

# Quantum mechanics I notes

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# Quantum Mechanics I

## Recap of basic wave mechanics

- The wave function contains all information we can know about a system.
- Born's interpretation:  $|\Psi(x,t)|^2$  is the probability density
- $\Psi(x,t)$  are continuous and square integrable
- Discontinuous potentials

$$-\frac{\hbar^2}{2m} \left[ \frac{d\Psi(x)}{dx} \Big|_{x=e} - \frac{d\Psi(x)}{dx} \Big|_{x=-e} \right] + \int_{-e}^e (V(x) - E)\Psi(x) dx$$

For finite discontinuity  $\frac{d\Psi}{dx}$  is continuous.

$$\rightarrow \text{T.I.S.E} \left[ i\hbar \frac{d}{dt} \Psi(x,t) = \hat{H} \Psi(x,t) \right]$$

- Stationary states: If  $\frac{\partial}{\partial t} |\Psi(x,t)|^2 = 0$
- Boundary values cause quantization.

- It is only possible for a state to be eigenfunction of both A and B if  $[A, B]\Psi = 0$

## 1-D problems

→ Bound states are discrete and non degenerate.

Proof: Let  $\Psi_1$  and  $\Psi_2$  are degenerate.

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2\Psi_1}{dx^2} + V\Psi_1 &= E\Psi_1 \\ -\frac{\hbar^2}{2m} \frac{d^2\Psi_2}{dx^2} + V\Psi_2 &= E\Psi_2 \end{aligned}$$

$\Psi_1 \frac{d\Psi_2}{dx} - \Psi_2 \frac{d\Psi_1}{dx} = 0$

$$\Psi_1 \frac{d\Psi_2}{dx} - \Psi_2 \frac{d\Psi_1}{dx} = C \quad \leftarrow \frac{d}{dx} \left( \Psi_1 \frac{d\Psi_1}{dx} - \Psi_2 \frac{d\Psi_2}{dx} \right) = 0$$

$$\Rightarrow \Psi_1 = e^{\frac{d}{dx}x} \Psi_2 \quad (\text{disintegration constant})$$

$\boxed{\text{Same system}}$

→ Eigen functions of  $\hat{H}$  can always be chosen pure real.

Hint:  $\Psi_2 = \frac{\Psi_1 + \Psi_1^*}{2}$  is also an eigenfunction.  
 (true for higher dimensions also)

→ The wave function  $\Psi_n(x)$  in  $\boxed{1d}$  has  $n$  nodes

if  $n=0$  is considered as ground state.

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Bound state

If

 $V_{\min}$ 

$$E < \min(V(+\infty), V(-\infty))$$

Unbound states cannot be normalised and they have continuous states.

→ For symmetric potentials, the wave  $\psi(x)$  is either even or odd

Proof:  $\hat{P} \psi(\vec{r}, t) = \psi(-\vec{r}, t)$  (parity operator)

Operation is even if

$$\hat{P} \hat{A} \hat{P} = \hat{A}$$

odd if  $\hat{P} \hat{B} \hat{P} = -\hat{B}$

$$\Rightarrow \hat{A} \hat{P} = (\hat{P} \hat{A} \hat{P}) \hat{P} = \hat{P} \hat{A} \hat{P}^2 = \hat{P} \hat{A}$$

Similarly

$$\hat{B} \hat{P} = -\hat{P} \hat{B}$$

⇒ Even operator commute with P. So, both have same eigen functions.

Some Problems

1) Free particle.

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

For hamiltonian eigenfunctions let  $k = \sqrt{\frac{2mE}{\hbar}}$

$$\Rightarrow \psi(x, t) = A e^{ik(x - \frac{\hbar k}{2m} t)} + B e^{-ik(x + \frac{\hbar k}{2m} t)}$$

→ It is not normalizable. H eigen states may not be bound states.

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Wave packet: A localized wave function.

$$\boxed{\text{I.F.T}} \leftarrow \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega t)} dk$$

near  $x=0$  constructive  
amplitude of wave packet

$$\boxed{\text{F.T}} \leftarrow \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x_0) e^{-ikx} dx$$

near  $x=0$ , constructive interference.

$$\int_{-\infty}^{\infty} |\psi_0(x)|^2 dx = \int_{-\infty}^{\infty} |\phi(k)|^2 dk$$

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$\int_{-\infty}^{\infty} \frac{e^{-\frac{1}{2}(\frac{x-\mu}{\sigma})^2}}{\sigma \sqrt{2\pi}} = 1$$

For gaussian wave packets

$$\Delta x \Delta k = \frac{1}{2} \quad \text{or} \quad \Delta x \Delta p = \frac{\hbar}{2}$$

\* In general

$$\Delta x \Delta k \geq \frac{1}{2} \quad \Delta x \Delta p \geq \frac{\hbar}{2}$$

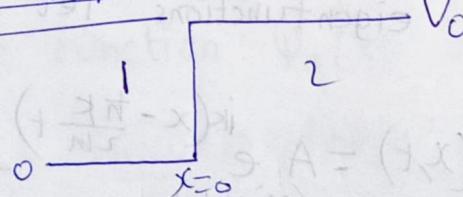
$$V_{ph} = \frac{\omega(k)}{k}$$

$$V_g = \frac{dw(k)}{dk}$$

$$\dot{V}_g = V_{ph} - 2 \frac{dV_{ph}}{dx}$$

classical analogue

## 2) Potential Step



a) Case  $E > V_0$

$$\psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$$

$$\psi_2(x) = Ce^{ik_2 x} + De^{-ik_2 x}$$

$$D=0, \quad B = \frac{K_1 - K_2}{K_1 + K_2} A, \quad C = \frac{2K_1}{K_1 + K_2} A$$

$$R = \frac{|B|^2}{|A|^2}$$

$$T = \frac{K_2}{K_1} \frac{|C|^2}{|A|^2}$$

$$b) E < V_0$$

$$\Psi(x,t) = \begin{cases} A e^{i(K_1 x - \omega t)} + B e^{-i(K_1 x + \omega t)} & x < 0 \\ C e^{-K_1' x} e^{-i\omega t} & x \geq 0 \end{cases}$$

$$B = \left( \frac{K_1 - iK_1'}{K_1 + iK_1'} \right) A \quad C = \left( \frac{2K_1}{K_1 + iK_1'} \right) A$$

$$R = 1$$

$$T = \text{undefined}$$

### 3) Infinite square well

$$V(x) = 0 \text{ if } 0 \leq x \leq a, \quad \infty \text{ otherwise}$$

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$$

$$\Psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

Zero point energy  $\Rightarrow E_1 > 0$

### 4) Finite square well

$$V(x) = \begin{cases} -V_0 & -a \leq x \leq a \\ 0 & |x| > a \end{cases}$$

Bound states ( $E < 0$ )

$$\text{even} \rightarrow \Psi(x) = \begin{cases} F e^{-Kx} & x > a \\ D \cos(kx) & 0 < x < a \\ \Psi(-x) & x < 0 \end{cases}$$

## 6) Finite square well

$$V(x) = \begin{cases} V_0 & x < -\frac{a}{2} \\ 0 & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ V_0 & x > \frac{a}{2} \end{cases}$$

$$k_1 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

Bound states ( $0 < E < V_0$ )

odd or antisym

$$\Psi_a(x) = \begin{cases} Ae^{k_1 x} & x < -\frac{a}{2} \\ C \sin(k_2 x) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ Pe^{-k_1 x} & x > \frac{a}{2} \end{cases}$$

$$\Psi_s(x) = \begin{cases} Ae^{k_1 x} & x < -\frac{a}{2} \\ B \cos(k_2 x) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\ De^{-k_1 x} & x > \frac{a}{2} \end{cases}$$

For  $\Psi_a$ , bound energies are given by

$$k_2 \cot\left(\frac{k_2 a}{2}\right) = -k_1$$

For  $\Psi_s$

$$k_2 \tan\left(\frac{k_2 a}{2}\right) = k_1$$

then number of bound states  $\rightarrow \infty$ .  
Infinite square well.

$\rightarrow$  If  $V_0 \rightarrow \infty$  approximately

always atleast one bound

$\rightarrow$  Even if  $V_0 \rightarrow 0$ , state exists.

Scattering

$$(E > V_0) \quad V(x) = -V_0$$

$$-a \leq x \leq a$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi(x) = Ae^{ikx} + Be^{-ikx} \quad x < -a$$

$$= C \sin(kx) + D \cos(kx) \quad -a < x < a$$

$$F e^{ikx} \quad x > a$$

$$F = \frac{e^{-2ika} A}{\cos(2ka) - i \frac{(E+V_0)}{2\hbar^2} \sin(2ka)}$$

$$T = \frac{|F|^2}{|A|^2}$$

$$= \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar} \sqrt{2m(E+V_0)}\right)}$$

Perfect transmission  $\rightarrow$

$$E_n + V_0 = \frac{\hbar^2 \pi^2 \hbar^2}{2m(2a)^2}$$

### 5) Barrier

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq a \\ 0 & x > a \end{cases}$$

$$E > V_0 \quad \Psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x \leq 0 \\ Ce^{ik_2 x} + De^{-ik_2 x} & 0 < x < a \\ Ee^{ik_1 x} & x \geq a \end{cases}$$

$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$   
 $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$$T = \frac{k_1 |E|^2}{k_1 |A|^2} = \left[ 1 + \frac{V_0^2}{4E(E-V_0)} \sin^2(a \sqrt{\frac{2mV_0}{\hbar^2}} \sqrt{\frac{E}{V_0} - 1}) \right]$$

$$T = \left[ 1 + \frac{1}{4E(E-1)} \sin^2(2\sqrt{E-1}) \right]^{-1} \Leftrightarrow \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sin^2(a \sqrt{\frac{2mV_0}{\hbar^2}} \sqrt{\frac{E}{V_0} - 1})}$$

$$R = \left[ 1 + \frac{4E(E-1)}{\sin^2(2\sqrt{E-1})} \right]^{-1} \quad x = a \sqrt{\frac{2mV_0}{\hbar^2}} \quad E = \frac{E}{V_0}$$

### 6) Harmonic oscillator

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \Psi = E\Psi$$

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

$$\Psi_n(x) = \frac{1}{\sqrt{\sqrt{\pi} 2^n n! x_0}} e^{-\frac{x^2}{2x_0^2}} H_n\left(\frac{x}{x_0}\right)$$

Algebraic

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}} (\mp i\hat{p} + m\omega x)$$

$$[\hat{a}_-, \hat{a}_+] = 1$$

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} e^{-y^2}$$

$$\hat{a}_+ \hat{a}_- = \frac{1}{\hbar\omega} \hat{H} - \frac{1}{2}$$

$$\hbar\omega (\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2}) \Psi = E\Psi$$

$$\hat{H}\psi = E\psi \Rightarrow \hat{H}(\hat{a}_{\pm}\psi) = (E \pm \hbar\omega)(\hat{a}_{\pm}\psi)$$

$$\Psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}$$

$$\Psi_n(x) = A_n (\hat{a}_+)^n \Psi_0(x), E_n = \hbar + \frac{1}{2} \hbar\omega$$

$$A_n = \frac{1}{\sqrt{n!}}$$

Analytic

$$k = \frac{2E}{\hbar\omega}$$

$$\xi \equiv \sqrt{\frac{m\omega}{\hbar}} x \Rightarrow \frac{d^2\psi}{d\xi^2} = (\xi^2 - k) \psi$$

$$\xi \gg k \Rightarrow \frac{d^2\psi}{d\xi^2} = \xi^2 \psi$$

$$\Rightarrow \psi(\xi) = A e^{-\frac{\xi^2}{2}}$$

$$\text{Let } \psi(\xi) = h(\xi) e^{-\frac{\xi^2}{2}}$$

$$\Rightarrow \frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (k-1)h = 0$$

$$\Psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}$$

$\Rightarrow$  Delta function potential

Dirac delta distribution or function

$$\int_{-\infty}^{\infty} f(x) \delta(x-a) dx = f(a)$$

$$\delta(-x) = \delta(x)$$

$$\delta(ax) = \frac{\delta(x)}{|a|}$$

$$\begin{cases} g(x_i) = 0 \\ g'(x_i) \neq 0 \end{cases}$$

$$\delta[g(x)] = \sum_i \frac{1}{|g'(x_i)|} \delta(x-x_i)$$

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$$\hat{\delta}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \delta(x) e^{-ikx} dx$$

$$\hat{\delta}(\xi) = \frac{1}{\sqrt{2\pi}} \Rightarrow \delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk$$

Heaviside fctn

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

$$\frac{d}{dx} \Theta(x) = \delta(x)$$

$$\frac{d\delta(x)}{dx} = \delta'(x) = \frac{i}{2\pi} \int_{-\infty}^{\infty} k e^{ikx} dk$$

Integration by parts  $\Rightarrow$ 

$$\int_{-\infty}^{\infty} f(x) \delta'(x-a) dx = -f'(a)$$

$$\int_{-\infty}^{\infty} f(x) \delta^{(n)}(x-a) dx = (-1)^n f^{(n)}(a)$$

In 3d

$$\begin{aligned} \delta(\vec{r} - \vec{r}') &= \delta(x-x') \delta(y-y') \delta(z-z') \\ &= \frac{1}{\vec{r}^2} \delta(\vec{r}-\vec{r}') \delta(\cos\theta - \cos\theta') \delta(\varphi - \varphi') \\ &= \frac{1}{\vec{r}^2 \sin\theta} \delta(\vec{r}-\vec{r}') \delta(\theta-\theta') \delta(\varphi-\varphi') \end{aligned}$$

$$\delta(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int d^3 k e^{i\vec{k} \cdot (\vec{r} - \vec{r}')}}$$

Boundstate

$$\Rightarrow \left( \frac{\vec{p}}{\vec{r}^2} \right) = 4\pi \delta(\vec{r}) \quad \nabla^2 \left( \frac{1}{\vec{r}} \right) = -4\pi \delta(\vec{r})$$

 $E < 0$ 

$$V(x) = -\alpha \delta(x)$$

$$k = \frac{\sqrt{-2mE}}{\hbar}$$

$$\Psi(x) = \begin{cases} Be^{kx} & x < 0 \\ Fe^{-kx} & x > 0 \end{cases}$$

$$\Psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha|x|}{\hbar^2}}$$

$$k = \frac{m\alpha}{\hbar^2} \rightarrow \text{only bound state.}$$

E &gt; 0

$$k = \frac{\sqrt{2mE}}{\hbar}$$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad \begin{cases} x < 0 \\ x > 0 \end{cases}$$

$$\beta = \frac{m\alpha}{\hbar^2 k}$$

$$\beta = \frac{iBA}{1-iF} A$$

$$F = \frac{1}{1-i\beta} A$$

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2}$$

$$T = \frac{|A|^2}{|A|^2} = \frac{1}{1+\beta^2}$$

### 8) Double delta potential

$$V(x) = -g\delta(x-a) - g\delta(x+a)$$

Bound state ( $E < 0$ )

$$\psi_{\text{even}} = A \cosh(\alpha x) \quad |x| < a$$

$$\alpha = \frac{\sqrt{-2mE}}{\hbar} \quad B e^{-\alpha x} \quad |x| > a$$

$$\Rightarrow \tanh \alpha a = \frac{2mg}{\hbar^2 \alpha} - 1$$

$$\psi_{\text{odd}} = A \sinh \alpha x \quad |x| < a$$

$$B e^{-\alpha x} \quad x > a$$

$$\Rightarrow \frac{2mg}{\hbar^2 \alpha} = 1 + \coth \alpha a$$

3D Box

$$\psi(\vec{r}) = \sqrt{\frac{8}{L_x L_y L_z}} \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right)$$

Harmonic

$$E = \left(n_x + \frac{1}{2}\right) \hbar \omega_x + \left(n_y + \frac{1}{2}\right) \hbar \omega_y + \left(n_z + \frac{1}{2}\right) \hbar \omega_z$$

$$V(x) = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_y^2 y^2 + \frac{1}{2} m \omega_z^2 z^2$$

## 2) Formulation of Quantum Mechanics

Linear Vector Space: a) Addition is commutative,  
Associative, Neutral Vector ( $\vec{0}$ ). Unique Inverse

$$\vec{a} + \vec{b} \in V$$

$$b) \alpha_1 \vec{a} + \alpha_2 \vec{b} \in V$$

→ Unique Identity scalar

→ Associativity + Distributivity  
w.r.t multiplication of  
scalars and addition.

### Hilbert space

→ Linear Vector Space

$$\langle \psi, \phi \rangle = (\phi, \psi)^* \quad \text{and} \quad \langle \psi, \psi \rangle \geq 0$$

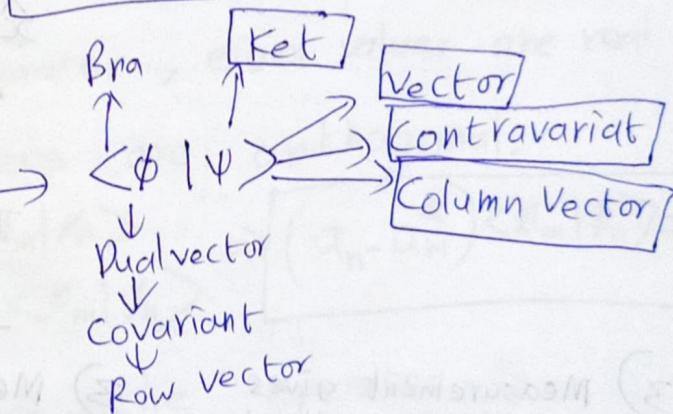
$$\langle \psi, \psi \rangle = 0 \Rightarrow \psi = 0$$

→ is Separable

→ is Complete

### Dirac Notation

$$(\phi, \psi) \rightarrow$$



Every Ket has  
unique bra

$$|\psi\rangle \leftrightarrow \langle\psi|$$

$$a|\psi\rangle + b|\phi\rangle \leftrightarrow a^* \langle\psi| + b^* \langle\phi|$$

$$|a\psi\rangle = a|\psi\rangle \quad \langle a\psi| = a^* \langle\psi|$$

$$\langle\psi|a_1\psi_1 + a_2\psi_2\rangle = a_1 \langle\psi|\psi_1\rangle + a_2 \langle\psi|\psi_2\rangle$$

$$\langle a_1\phi_1 + a_2\phi_2|\psi\rangle =$$

$$a_1^* \langle\phi_1|\psi\rangle + a_2^* \langle\phi_2|\psi\rangle$$

$$\langle a_1\phi_1 + a_2\phi_2 | b_1\psi_1 + b_2\psi_2 \rangle = a_1^* b_1 \langle\phi_1|\psi_1\rangle + a_1^* b_2 \langle\phi_1|\psi_2\rangle$$

$$\| |\psi + \phi\rangle \| \leq \| |\psi\rangle \| + \| |\phi\rangle \|$$

## Operator

$$\hat{A} |\psi\rangle = |\psi'\rangle \quad \langle \phi | \hat{A} = \langle \phi' |$$

**Linear  
operators**

$$\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1 \hat{A}|\psi_1\rangle + a_2 \hat{A}|\psi_2\rangle$$

$$(\langle \psi_1 | a_1 + \langle \psi_2 | a_2) \hat{A} = a_1 \langle \psi_1 | \hat{A} + a_2 \langle \psi_2 | \hat{A}$$

**Antilinear  
operator**

$$\hat{A}(a_1|\psi_1\rangle + a_2|\psi_2\rangle) = a_1^* \hat{A}|\psi_1\rangle + a_2^* \hat{A}|\psi_2\rangle$$

## Postulates

C - M

- 1) State is a point in  $x-p$  plane.
- 2) Every dynamic variable  $w = w(x, p)$

- Q - M
- 1) State is a vector  $|\psi(t)\rangle$  in a Hilbert space.
- 2) The independent  $x$  and  $p$  are represented by linear Hermitian operations

$\hat{x}$  and  $\hat{p}$ .

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

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

If  $w = w(x, p)$

$$\hat{w}(\hat{x}, \hat{p}) = w(x \rightarrow \hat{x}, p \rightarrow \hat{p})$$

- 3) Measurement gives  $w(x, p)$  without altering state

- 3) Measuring  $\hat{A}$   
 $\Rightarrow$  one of the eigenvalues will come  
 $\Rightarrow p(w) \propto | \langle w | \psi \rangle |^2$   
 alters state

$$(4) \quad \hat{x} = \frac{\partial \mathcal{S}}{\partial p}$$

$$(4) \quad i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle$$

$$\hat{p} = -\frac{\partial \mathcal{S}}{\partial x}$$

$$H(\hat{x}, \hat{p}) = \mathcal{S}(\hat{x} \rightarrow x, \hat{p} \rightarrow p)$$

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Hermitian Adjoint: is defined as  
 $\langle \psi | \hat{A}^\dagger | \phi \rangle = \langle \phi | \hat{A} | \psi \rangle$

Hermitian operator: If  $\hat{A}^\dagger = \hat{A}$

$\Rightarrow$  Eigen values are ~~not~~ real.  
 $\langle \psi | \hat{A} | \psi \rangle = \langle \psi | \hat{A}^\dagger | \psi \rangle$

Projection Operator: If  $\hat{P}^\dagger = \hat{P}$  and  $\hat{P}^2 = \hat{P}$

Unitary Operator: If  $\hat{U}^\dagger = \hat{U}^{-1}$   
Product of Unitary is also unitary.

Eigenvalues and Eigenvectors:

Eigenvector is non zero.

$$\hat{A}|\psi\rangle = a|\psi\rangle \Rightarrow \hat{A}^\dagger \hat{A}^{-1} |\psi\rangle = \frac{1}{a} |\psi\rangle$$

For a Hermitian operator, eigen values are real  
and the eigenvectors are orthogonal.

Proof:  $\langle \phi_m | \hat{A} | \phi_n \rangle = a_n \langle \phi_m | \phi_n \rangle$   
 $\langle \phi_m | \hat{A}^\dagger | \phi_n \rangle = a_m^* \langle \phi_m | \phi_n \rangle$   $\Rightarrow (a_n - a_m^*) \langle \phi_m | \phi_n \rangle = 0$

In the eigenbasis the operator is diagonal.

Q-3] If  $\hat{A}$  and  $\hat{B}$  commute and If  $\hat{A}$  has no degenerate eigenvalue,  $\Rightarrow$  eigenvector of  $\hat{A}$  is also an eigenvector of  $\hat{B}$ .

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## Matrix Representation in Discrete Bases

Let  $\{\phi_n\}$  be bases such that

$$\text{Orthonormal: } \langle \phi_n | \phi_m \rangle = \delta_{nm}$$

$$\boxed{\sum_{n=1}^{\infty} |\phi_n\rangle \langle \phi_n| = \hat{I}}$$

$$\begin{aligned} \text{State} \Rightarrow |\psi\rangle &= \left( \sum_{n=1}^{\infty} |\phi_n\rangle \langle \phi_n| \right) |\psi\rangle \\ &= \sum_{n=1}^{\infty} a_n |\phi_n\rangle \quad \left( \begin{array}{c} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \end{array} \right) \end{aligned}$$

$$\Rightarrow |\psi\rangle = (a_1^*, a_2^*, \dots, a_n^*)^\top$$

### Operator:

$$A_{nm} = \langle \phi_n | \hat{A} | \phi_m \rangle$$

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots \\ A_{21} & \cdots & \cdots \end{pmatrix}$$

$$A^+ = (A^T)^*$$

$$\text{Trace: } \text{Tr}(\hat{A}^+) = (\text{Tr}(\hat{A}))^*$$

$$\text{Tr}(\alpha \hat{A} + \beta \hat{B} + \gamma \hat{C} + \dots) = \alpha \text{Tr}(\hat{A}) + \beta \text{Tr}(\hat{B}) + \dots$$

$$\text{Tr}(\hat{A} \hat{B} \hat{C} \hat{D} \hat{E}) = \text{Tr}(\hat{B} \hat{C} \hat{D} \hat{E} \hat{A}) = \dots$$

If matrix multiplication is not possible then so is ket multiplication.

$$\text{Ex: } |\psi\rangle |\phi\rangle$$

15 Basis transformation

$$|\phi_n\rangle = \left( \sum_m |\phi'_m\rangle \langle \phi'_m| \right) |\phi_n\rangle = \sum_m v_{mn} |\phi'_m\rangle$$

$$v_{mn} = \langle \phi'_m | \phi_n \rangle$$

Basis transformation is a Unitary matrix.

### Eigenvalues

$$\det(A^+) = (\det(A))^*$$

$$\det(A^T) = \det(A) \Rightarrow \text{Tr}(A) = \sum_n a_n$$

$$\det(A) = e^{\text{Tr}(\ln A)}$$

$$\det(A) = \prod_n a_n$$

### Continuous Basis

$$\langle x_k | x_{k'} \rangle = \delta(k - k')$$

state:  $|\psi\rangle = \int_{-\infty}^{\infty} dk c(k) |x_k\rangle \langle x_k| |\psi\rangle$

$$= \int_{-\infty}^{\infty} dk b(k) |x_k\rangle, b(k) = \langle x_k | \psi \rangle$$

### Continuous matrix

Position:  $\hat{R} |\vec{r}\rangle = \vec{r} |\vec{r}\rangle$

$$\langle \vec{r} | \vec{r}' \rangle = \delta(\vec{r} - \vec{r}')$$

$$\langle \vec{r} | \psi \rangle = \Psi(\vec{r})$$

$$\langle \phi | \psi \rangle = \langle \phi | \int d^3r |\vec{r}\rangle \langle \vec{r}| \psi \rangle$$

$$= \int d^3r \phi^*(\vec{r}) \Psi(\vec{r})$$

Connecting  $x$  and  $p$  representations

$$\langle \vec{q} | \psi \rangle = \langle \vec{q} | (\int d^3 p |\vec{p}\rangle \langle \vec{p}|) |\psi \rangle$$

$$= \int d^3 p \langle \vec{q} | \vec{p} \rangle \Psi(\vec{p})$$

$$\langle \vec{p} | \psi \rangle = \int d^3 q \langle \vec{p} | \vec{q} \rangle \Psi(\vec{q})$$

$$\langle \vec{q} | \vec{p} \rangle = -\langle \vec{p} | \vec{q} \rangle = \frac{1}{(2\pi\hbar)^3} e^{i\frac{\vec{p} \cdot \vec{q}}{\hbar}}$$

Parseval's theorem

$$\int d^3 p \Psi^*(\vec{p}) \Psi(\vec{p}) = \int d^3 q \Psi^*(\vec{q}) \Psi(\vec{q})$$

Momentum Operator in  $x$  representation

$$\langle \vec{q} | \hat{p} | \psi \rangle = -i\hbar \vec{\nabla} \langle \vec{q} | \psi \rangle$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

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

$\hat{x}$  in  $p$  representation

$$\langle \vec{p} | \hat{x} | \psi \rangle = i\hbar \left( i \frac{\partial}{\partial p_x} + i \frac{\partial}{\partial p_y} + \hat{r} \frac{\partial}{\partial p_z} \right) \Psi(\vec{p})$$

$$\Rightarrow \hat{x} = i\hbar \frac{\partial}{\partial p_x}$$

Connection between QM and CM

$$\{A, B\} = \sum_j \left( \frac{\partial A}{\partial q_j} \frac{\partial B}{\partial p_j} - \frac{\partial A}{\partial p_j} \frac{\partial B}{\partial q_j} \right)$$

$$\{q_j, q_k\} = \{p_j, p_k\} = 0 \quad \{q_j, p_k\} = \delta_{jk}$$

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$$\frac{dA}{dt} = \{A, H\}^p + \frac{\partial A}{\partial t}$$

$$= \sum_j \left( \frac{\partial A}{\partial q_j} \frac{\partial p_j}{\partial t} + \frac{\partial A}{\partial p_j} \frac{\partial q_j}{\partial t} \right) + \frac{\partial A}{\partial t}$$

Proof:

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j} \quad , \quad \frac{dp_j}{dt} = -\frac{\partial H}{\partial q_j}$$

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, A] \rangle + \langle \frac{\partial \hat{A}}{\partial t} \rangle$$

$$\frac{1}{i\hbar} [\hat{A}, \hat{A}] \rightarrow \{A, A\}_{\text{classical}}$$

Ehrenfest theorem

$$\frac{d}{dt} \langle \hat{R} \rangle = \frac{1}{i\hbar} \langle [\hat{R}, \frac{\hat{p}^2}{2m} + V(\vec{r}, t)] \rangle + 0$$

$$= \frac{1}{2im\hbar} \langle [\hat{R}, \hat{p}^2] \rangle = \frac{\langle \hat{p} \rangle}{m}$$

$$\frac{d}{dt} \langle \hat{p} \rangle = \frac{1}{i\hbar} \langle [\hat{p}, \nabla(\vec{r}, t)] \rangle + 0$$

$$= - \langle \vec{\nabla} \cdot \vec{v}(\vec{r}, t) \rangle$$

$$\lim_{h \rightarrow 0} Q \cdot M = C \cdot M$$

$$\langle \psi(t) | \psi(t) \rangle = \langle \psi(t_0) | \psi(t) \rangle$$

Time Evolution operator

$$\frac{\partial \hat{U}(t, t_0)}{\partial t} = -\frac{i}{\hbar} \hat{H} \hat{U}(t, t_0)$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

$$|\psi(t)\rangle = e^{-\frac{i\hat{H}}{\hbar}(t-t_0)} |\psi(t_0)\rangle$$

$$\hat{U}(t, t_0) = e^{-\frac{i(t-t_0)\hat{H}}{\hbar}}$$

$$U^\dagger = U^{-1}$$

## Time Independent Potentials

$$\hat{V}(\vec{r}, t) = V(\vec{r})$$

$\Rightarrow$  Some solutions are separable

$$\Psi(\vec{r}, t) = \psi(\vec{r})f(t)$$

$$E = \frac{i\hbar}{f(t)} \frac{df(t)}{dt} = \frac{1}{\psi(\vec{r})} \left[ \frac{-\hbar^2}{2m} \nabla^2 \psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) \right]$$

## Stationary States

time independent

probability density.

## Conservation of Probability

$$\frac{\partial e(\vec{r}, t)}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0$$

$$e(\vec{r}, t) = \psi^*(\vec{r}, t)\psi(\vec{r}, t) \quad \vec{j}(\vec{r}, t) = \frac{i\hbar}{2m} (\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi)$$

$$\downarrow \text{probability density}$$

$$\begin{aligned} \hat{e}(t) &= |\psi(t)\rangle \langle \psi(t)| \\ &= \hat{U}(t, t_0) |\psi(0)\rangle \langle \psi(0)| \hat{U}^\dagger(t, t_0) \\ &= \boxed{\hat{U}(t, t_0) \hat{P}(t_0) \hat{U}^\dagger(t, t_0)} \end{aligned}$$

## Gram-Schmidt process

$$|\phi_n\rangle = |\psi_n\rangle - \sum_{i,j=1}^{n-1} (\omega^{-1})_{ji} |\psi_j\rangle \langle \psi_i, \psi_n \rangle$$

$$\boxed{\hat{U} = \hat{U}}$$

$$\boxed{w_{ij} = \langle \psi_i | \psi_j \rangle}$$

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UncertaintyRelations

$$\Delta A = \sqrt{\langle (\Delta \hat{A})^2 \rangle} = \sqrt{\langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle}$$

$$= \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

$$= \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}$$

$$\Rightarrow \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq |\langle \Delta \hat{A} \Delta \hat{B} \rangle|^2$$

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

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

$$|\langle \Delta \hat{A} \Delta \hat{B} \rangle|^2 = \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2 + \frac{1}{4} |\langle \{ \hat{A}, \hat{B} \} \rangle|^2$$

$$\Rightarrow \langle (\Delta \hat{A})^2 \rangle \langle (\Delta \hat{B})^2 \rangle \geq \frac{1}{4} |\langle [\hat{A}, \hat{B}] \rangle|^2$$

$$\Rightarrow \boxed{\Delta A \Delta B \geq \frac{1}{2} | \langle [\hat{A}, \hat{B}] \rangle |}$$

Functions of operators

$$F(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n$$

$$\text{Adjoint of } F(\hat{A}) = [F(\hat{A})]^+ = F^*(\hat{A}^+)$$

$$= \sum_{n=0}^{\infty} a_n^* (\hat{A}^+)^n$$

## Compatible Observable

$$\rightarrow [A, B] = 0$$

~~→ Not necessary that~~

→ If 2 operators are compatible, they possess a set of common (or simultaneous) eigenstates. (irrespective of degeneracy)

→ In FDHS we can simultaneously diagonalise them.

## Non compatible observable

→ still it is possible that a state is eigenstate of A and not for B if A is degenerate.

## Non-compatible observables

$$\rightarrow [A, B] \neq 0$$

→ But it is possible that

$$[A, B] \psi = 0 \quad \text{for some } \psi$$

→ Here eigenstate.

→ If  $[A, B] \psi \neq 0 \quad \forall \psi \in \mathcal{H}$   
then no simultaneous eigenstate.

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## Schrödinger picture

state vectors evolve but operators do not.

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

$$|\Psi(t)\rangle = U(t, t_0) |\Psi(t_0)\rangle$$

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} [\langle \hat{A}, \hat{H} \rangle] + \left( \frac{\partial \hat{A}}{\partial t} \right)$$

$$U(t, t_0) = e^{-i\frac{(t-t_0)}{\hbar} \hat{H}}$$

$$U^+(t, t_0) = U^{-1}(t, t_0) = U(t_0, t)$$

## Heisenberg picture

$$|\Psi(t)\rangle_H = U^+(t) |\Psi(t)\rangle = |\Psi(0)\rangle$$

Operators do not evolve state vectors do not.

$$|\Psi(t)\rangle_H = e^{i\frac{t\hat{H}}{\hbar}} |\Psi(0)\rangle \quad (t_0=0)$$

$$\langle \Psi(t) | \hat{A} | \Psi(t) \rangle = \langle \Psi(0) | e^{i\frac{t\hat{H}}{\hbar}} \hat{A} e^{-i\frac{t\hat{H}}{\hbar}} | \Psi(0) \rangle$$

$$\Rightarrow \hat{A}_H(t) = U^+(t) \hat{A} U(t) = e^{i\frac{t\hat{H}}{\hbar}} \hat{A} e^{-i\frac{t\hat{H}}{\hbar}}$$

## Heisenberg equation of motion

$$\frac{d \hat{A}_H(t)}{dt} = \frac{1}{i\hbar} [\hat{A}_H, U^+ \hat{A} U]$$

since  $\hat{H}$  and  $U(t)$  commute

$$\frac{d \hat{A}_H(t)}{dt} = \frac{1}{i\hbar} [\hat{A}_H, \hat{A}]$$

$$\frac{d}{dt} A_H(t) = \frac{i}{\hbar} [H_H, A_H(t)] + \left( \frac{\partial A_S}{\partial t} \right)_H$$

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Some potential energies

Ex:  $V(x,y) = (2xy)^2 \Rightarrow U(x,y) = 2x^2$

$$x = \frac{x+y}{\sqrt{2}} \quad \boxed{\psi(x,y) = \psi(x)\psi(y)}$$

$$y = \frac{x-y}{\sqrt{2}}$$

Ex:  $V(x) = \frac{1}{2}kx^2 + qEx = \frac{1}{2}k\left(x + \frac{qE}{2k}\right)^2 - \frac{q^2E^2}{4k}$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{q^2E^2}{4k}$$

Electromagnetic minimal coupling

$$\hat{H} = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + q\phi$$

$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} \quad \vec{B} = \vec{\nabla} \times \vec{A}$$

$$\hat{H} = \frac{1}{2m}(-i\hbar\vec{\nabla} - q\vec{A})^2 + q\phi$$

$$i\hbar \frac{\partial \psi}{\partial t} = \left[ \frac{1}{2m}(-i\hbar\vec{\nabla} - q\vec{A})^2 + q\phi \right] \psi$$

Gauge invariance

$$\psi' = \psi - \frac{\partial \Lambda}{\partial t} \quad \vec{A}' = \vec{A} + \vec{\nabla}\Lambda$$

$$\Rightarrow \psi' = e^{\frac{iq\Lambda}{\hbar}} \psi$$

$\Rightarrow$  Quantum mechanics is gauge invariant.

$$\boxed{[\vec{A}, \vec{A}'] \frac{1}{\hbar} = (\vec{J})_{\vec{A}} \vec{A}'}$$

$$\boxed{\left(\frac{\partial A_i}{\partial x_j}\right) + [(\vec{J})_{\vec{A}}, \vec{A}] \frac{1}{\hbar} = (\vec{J})_{\vec{A}} \frac{\partial \vec{A}}{\partial x_j}}$$

## Angular momentum operator

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

$$\Rightarrow \hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = -i\hbar \hat{\vec{r}} \times \hat{\vec{p}}$$

$$\Rightarrow L_i = -i\hbar \sum_{jk} \epsilon_{ijk} x_j \frac{\partial}{\partial x_k}$$

$$x = r \sin \theta \cos \phi$$

$$y = r \sin \theta \sin \phi$$

$$z = r \cos \theta$$

$$L_x = L_1 = i\hbar \left( \sin \theta \frac{\partial}{\partial \phi} + \cot \theta \cos \phi \frac{\partial}{\partial \theta} \right)$$

$$L_y = i\hbar \left( -\cos \phi \frac{\partial}{\partial \theta} + \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right)$$

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2 \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

## Commutator Algebra

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

$$\{ \hat{A}, \hat{B} \} = \hat{A}\hat{B} + \hat{B}\hat{A}$$

$$[\hat{A}, \hat{B} + \hat{C} + \dots] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] + \dots$$

$$[\hat{A}, \hat{B}]^+ = [\hat{B}^+, \hat{A}^+]$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$$

$$[\hat{A}, \hat{B}^n] = \sum_{j=0}^{n-1} \hat{B}^j [\hat{A}, \hat{B}] \hat{B}^{n-j-1}$$

$$[\hat{A}^n, \hat{B}] = \sum_{j=0}^{n-1} \hat{A}^{n-j-1} [\hat{A}, \hat{B}] \hat{A}^j$$

Jacobi Identity:  $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$

## 24 Commutators in Q.M

$$\left[ \frac{\partial}{\partial x_k}, x_j \right] = \delta_{kj}$$

$$[P_i, P_j] = 0$$

$$[x_j, P_k] = i\hbar \delta_{jk}$$

$$[x_i, x_j] = 0$$

$$[L_i, x_j] = i\hbar \sum_k \epsilon_{ijk} x_k$$

$$[L_i, v_j] = i\hbar \sum_k \epsilon_{ijk} v_k$$

$\vec{v} = (v_1, v_2, v_3)^T$  is any vector constructed

from  $x_i$  and  $\frac{\partial}{\partial x_i}$ .

$$\vec{v} = \vec{x} \text{ or } \vec{P} \text{ etc. or } \vec{L}$$

$$[L_i, \vec{v}] = i\hbar \sum_{jk} \epsilon_{ijk} (v_k v_j + v_j v_k)$$

$= 0$  (since by reversing  
j and k  
we get)

$$[L_i, \vec{v}^2] = -[L_i, \vec{v}]$$

## Hydrogen Atom

### Central Potential

$$\vec{\nabla} f(\rho, \theta, \phi) = \frac{\partial f}{\partial \rho} \hat{e}_\rho + \frac{1}{\rho} \frac{\partial f}{\partial \theta} \hat{e}_\theta + \frac{1}{\rho \sin \theta} \frac{\partial f}{\partial \phi} \hat{e}_\phi$$

$$\vec{\nabla}^2 f = \Delta f = \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left( \rho^2 \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \theta^2} + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}$$

$$+ \frac{1}{\rho^2 \sin \theta} \frac{\partial^2 f}{\partial \phi^2}$$

$$\hat{P}_\theta = \frac{1}{2} \left[ \left( \frac{\partial}{\partial \theta} \right) \cdot \hat{P} + \hat{P} \cdot \left( \frac{\partial}{\partial \theta} \right) \right]$$

$$\boxed{\hat{P}_\theta = -i\hbar \frac{1}{2} \frac{\partial^2}{\partial \theta^2}}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = E\psi$$

$$\text{Let } \psi(\theta, \phi) = R(\theta) Y(\theta, \phi)$$

$$\Rightarrow -\frac{\hbar^2}{2m} \left[ Y \frac{d}{d\theta} \left( \theta^2 \frac{dR}{d\theta} \right) + \frac{R}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{R}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right]$$

$$+ V R Y = E R Y$$

divide by  $Y R$  and multiply by  $-\frac{2m\theta^2}{\hbar^2}$

$$\left\{ \frac{1}{R} \frac{d}{d\theta} \left( \theta^2 \frac{dR}{d\theta} \right) - \frac{2m\theta^2}{\hbar^2} [V(\theta) - E] \right\} + \frac{1}{Y} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right] = 0$$

↓                            ↓

$l(l+1)$                      $-l(l+1)$

Angular equation by multiplying  $Y \sin^2 \theta$

$$\sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{\partial^2 Y}{\partial \phi^2} = -l(l+1) \sin^2 \theta Y$$

$$Y(\theta, \phi) = \Theta(\theta) \Phi(\phi) = \Theta(\theta) \Psi(\phi)$$

plugging and dividing by  $\Theta \Psi$

$$\left\{ \frac{1}{\Theta} \left[ \sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) \right] + l(l+1) \sin^2 \theta \right\} + \frac{1}{\Psi} \frac{d^2 \Psi}{d\phi^2} = 0$$

↓                            ↓

$m^2$                              $-m^2$

$$\Psi(\phi) = e^{im\phi}$$

$$\Psi(\phi + 2\pi) = \Psi(\phi)$$

$$\Rightarrow m=0, \pm 1, \pm 2, \dots$$

$$\sin \theta \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + [l(l+1) \sin^2 \theta - m^2] \Theta = 0$$

$$\Theta(\theta) = A P_l^m(\cos \theta)$$

↑ Not polynomial

$P_l^m$  are associated Legendre functions

$$P_l^m(x) = (-1)^m (1-x^2)^{\frac{m}{2}} \left( \frac{d}{dx} \right)^m P_l(x)$$

$P_l(x)$  is a legendre polynomial.

Rodrigues formula:  $P_l(x) = \frac{1}{2^l l!} \left( \frac{d}{dx} \right)^l (x^2 - 1)^l$

$$d^3r = r^2 \sin \theta dr d\theta d\phi = r^2 dr d\theta d\phi$$

Normalize  $\Rightarrow \int_{-1}^1 |P_l(x)|^2 dx = \int_0^\pi \int_0^{2\pi} |Y|^2 \sin \theta d\theta d\phi = 1$

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

Radial part

$V(r)$  only affect radial part

$$\frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{h^2} [V(r) - E] R = l(l+1) R$$

Let  $V(r) = rR(r)$

$$\frac{-\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[ V + \frac{\hbar^2 \lambda(\ell+l)}{2m r^2} \right] u = Eu$$

$V_{eff}$

$$\int_0^\infty |u|^2 dr = 1$$

Hydrogen

Atom

$$V = -\frac{e^2}{4\pi\epsilon_0} \frac{1}{r}$$

$$E < 0 \Rightarrow \text{Let } K = \frac{\sqrt{-2m_e E}}{\hbar}$$

$$P \neq K r, \text{ and } P_0 = \frac{m_e e^2}{2\pi\epsilon_0\hbar^2 K^2}$$

$$\Rightarrow \frac{d^2u}{dr^2} = \left[ 1 - \frac{P_0}{P} + \frac{\lambda(\ell+l)}{e^2} \right] u$$

$$r \rightarrow \infty \quad \frac{d^2u}{dr^2} = u$$

$$V(r) \sim A e^{-er} + B e^{+er}$$

$$r \rightarrow 0 \quad \frac{d^2u}{dr^2} = \frac{\lambda(\ell+l)}{r^2} u$$

$$u(r) = C r^{\ell+l} + D r^{-\ell-l}$$

$$\text{Let } u(P) = P^{\ell+l} e^{-Pr} V(P)$$

$$\Rightarrow P \frac{d^2V}{dr^2} + 2(\ell+l-r) \frac{dV}{dr} + [P_0 - 2(\ell+l)] V = 0$$

$$\Psi_{nlm}(\eta, \theta, \phi) = R_n^l(\eta) \Theta_{lm}(\theta) \Phi_m(\phi)$$

or

$$\Rightarrow \Psi_{nlm}(\eta, \theta, \phi) = R_{nl}(\eta) Y_l^m(\theta, \phi)$$

$$R_{nl}(\eta) = \frac{1}{\eta} e^{i\ell+1} V(P) e^{-P}$$

$V(P)$  is a polynomial of degree  $n-l-1$  in  $P$

$$C_{j+l} = \frac{2(j+l+1-n)}{(j+l)(j+l+2)} C_j V$$

$$R_n^l(\eta) = D e^{-\frac{1}{2}\eta} e^{\ell} e^{\eta} L_{n+l}^{2\ell+1}(\eta)$$

$$\eta = \frac{2}{na_0} \eta = q_0 = \frac{\hbar^2}{me^2} 4\pi E_0$$

$$D = - \left[ \left( \frac{2}{na_0} \right)^3 \frac{(n-\ell-1)!}{2n [(n+\ell)!]} \right]^{\frac{1}{2}}$$

$$L_{n+l}^{2\ell+1}(P) = \sum_{k=0}^{n-\ell} (-1)^{k+2\ell+1} \frac{(2\ell+1)!}{(n-\ell-1-k)!} \frac{P^k}{(2\ell+1+k)!}$$

↓ Assosiated Laguerre functions

$$\Psi_{1,0,0}(\eta, \theta, \phi) = \left( \frac{1}{\pi a_0} \right)^{\frac{3}{2}} e^{-\frac{\eta}{a_0}}$$

$$\Psi_{2,0,0}(\eta, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{\frac{3}{2}} \left( 2 - \frac{\eta}{a_0} \right) e^{-\frac{\eta}{2a_0}}$$

$$\Psi_{2,1,0}(\eta, \theta, \phi) = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{\frac{3}{2}} \frac{\eta}{a_0} e^{-\frac{\eta}{2a_0}} \cos \theta$$

$$\Psi_{2,1,\pm}(\eta, \theta, \phi) = \frac{1}{8\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{\frac{3}{2}} \frac{\eta}{a_0} e^{-\frac{\eta}{2a_0}} \sin \theta e^{\pm i\phi}$$

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} r^2 \sin \theta dr d\theta d\phi |\Psi(r, \theta, \phi)|^2 = 1$$

$$\boxed{\int_0^\infty dr r^{n-1} e^{-r} = \Gamma(n) = (n-1)!}$$

$$\int_0^\infty r^2 |R(r)|^2 dr \int_0^\pi \sin \theta |\Theta(\theta)|^2 d\theta \int_0^{2\pi} |\Phi(\phi)|^2 d\phi = 1$$

$$E_n = -\frac{13.6}{n^2} \text{ eV}$$

$$\sum_{l=0}^{n-1} \sum_{m_l=-l}^l = n^2$$

Selection rules:  $\Delta l = \pm 1, \Delta m_l = \pm 1, 0$

$$\Psi = a \Psi_m e^{\frac{i(E_m t)}{\hbar}} + b \Psi_n e^{\frac{-i(E_n t)}{\hbar}}$$

$$\langle x \rangle \propto \cos\left(\frac{(E_m - E_n)t}{\hbar}\right) \text{ iff } \uparrow$$

## Angular momentum continued

$$\hat{\sum}_z \Psi_{n,l,m_l}(r, \theta, \phi) = m_l \hbar \Psi_{n,l,m_l}(r, \theta, \phi)$$

$$\hat{\sum}_z^2 \Psi_{n,l,m_l}(r, \theta, \phi) = l(l+1) \hbar^2 \Psi_{n,l,m_l}(r, \theta, \phi)$$

Orbital magnetic dipole moment

$$\vec{\mu} = -\frac{\mu_B}{\hbar} \vec{l} \quad \mu_B = \frac{e \hbar}{2m} = \text{bohr magneton.}$$

$$\hat{\mu}_z \Psi_{n,l,m_l}(r, \theta, \phi) = -m_l \mu_B \Psi_{n,l,m_l}(r, \theta, \phi)$$

$$|\hat{\mu}_z| \Psi_{n,l,m_l}(r, \theta, \phi) = \mu_B \sqrt{l(l+1)} \Psi_{n,l,m_l}(r, \theta, \phi)$$

$$U = -\vec{M} \cdot \vec{B}$$

$$\hat{H} \Psi_{n,l,m_l}(r, \theta, \phi) = E_n - m_l M_b B$$

$(2l+1)$  states  $\rightarrow$  but experimentally  
 $2(2l+1)$  states.

### Spin:

spin magnetic moment

$$M_z = -g_s \mu_b m_s$$

$$s = \frac{1}{2}$$

$$m_s = \pm \frac{1}{2}$$

$$m_s = -s, -s+1, -s+2, s$$

For Harmonic oscillator

$$\hat{a} = \frac{m\omega \hat{x} + i\hat{p}}{\sqrt{2\hbar m\omega}}$$

Not hermitian

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

$$\hat{x} = \frac{1}{2}(\hat{a} + \hat{a}^\dagger) \sqrt{\frac{2\hbar}{m\omega}}$$

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

$$[\hat{a}, \hat{a}^\dagger] = I$$

$$\hat{H} = \hbar\omega (\hat{a}^\dagger \hat{a} + \frac{1}{2})$$

$$\hat{N} = \hat{a}^\dagger \hat{a}$$

$$\hat{N} |n\rangle = n |n\rangle$$

$$a |n\rangle = \sqrt{n} |n-1\rangle$$

$$a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle$$

annihilation

creation

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$$\langle m | \hat{x} | n \rangle = \sqrt{\frac{\hbar}{2mw}} (\sqrt{n} s_{m,n-1} + \sqrt{n+1} s_{m,n+1})$$

$$\langle m | \hat{p} | n \rangle = i \sqrt{\frac{\hbar mw}{2}} (\sqrt{n+1} s_{m,n+1} - \sqrt{n} s_{m,n-1})$$

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

$$\langle n | \hat{x}^2 | n \rangle = (n + \frac{1}{2}) \frac{\pi}{mw} \quad \langle n | \hat{p}^2 | n \rangle = (n + \frac{1}{2}) \pi mw$$

$$\frac{\partial \hat{A}}{\partial t} = 0 \Rightarrow \frac{d \hat{A}}{dt} = \frac{1}{i\hbar} [\hat{A}, \hat{A}]$$

$$\frac{dp}{dt} = -m\omega \hat{x}; \quad \frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}$$

These equations becomes uncoupled

$$i\hbar \frac{d\hat{a}}{dt} = \hbar\omega \hat{a}; \quad i\hbar \frac{d\hat{a}^\dagger}{dt} = -\hbar\omega \hat{a}^\dagger$$

$$\Rightarrow \hat{a}(t) = \hat{a}(0) e^{-i\omega t}; \quad \hat{a}^\dagger(t) = \hat{a}^\dagger(0) e^{i\omega t}$$

$$\hat{x} = \sqrt{\frac{\hbar}{2mw}} (\hat{a}^\dagger + \hat{a}) \pm \sqrt{\frac{\hbar}{2mw}} ((\hat{a}^\dagger(0) + \hat{a}(0)) \cos(\omega t) + i(\hat{a}^\dagger(0) - \hat{a}(0)) \sin(\omega t))$$

$$\Rightarrow \hat{x} = \hat{x}(0) \cos(\omega t) + \frac{1}{mw} \hat{p}(0) \sin(\omega t)$$

$$\hat{p} = \hat{p}(0) \cos(\omega t) - mw \hat{x}(0) \sin(\omega t)$$

Baker-Hausdorff Lemma

$$e^{i\hat{a}^\dagger \hat{A}} e^{-i\hat{a}^\dagger} = A + it [\hat{a}^\dagger, \hat{A}] + \frac{(it)^2}{2!} [\hat{a}^\dagger, [\hat{a}^\dagger, \hat{A}]] + \frac{(it)^3}{3!} [0, [0, [0, \hat{A}]]] + \dots$$

For  $\hat{a}^\dagger \xi(x) = \xi(x)$   $\rightarrow$  no non trivial solution.

Coherent states

$$\hat{a} \xi(x) = \alpha(\xi(x))$$

$$\alpha(\xi) = e^{-\frac{\alpha^2}{2} + \alpha x}$$

$$|\xi\rangle = \sum_n \frac{\alpha^n}{n!} e^{-\frac{|\alpha|^2}{2}} (a^\dagger)^n |0\rangle$$

$$|\alpha\rangle = \sum_n \frac{\alpha^n e^{-\frac{|\alpha|^2}{2}}}{\sqrt{n!}} |n\rangle$$

$$= e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} |\alpha\rangle$$

$$= e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} \hat{e}^{\alpha \hat{a}^\dagger} |\alpha\rangle$$

If  $[\hat{A}, \hat{B}] = \text{constant}$   $\Rightarrow e^{\hat{A}} e^{\hat{B}} e^{-\frac{[\hat{A}, \hat{B}]}{2}} = e^{\hat{A} + \hat{B}} = e^{\hat{B}} e^{\hat{A}}$

 $|\alpha\rangle = e^{(\alpha \hat{a}^\dagger - \frac{1}{2}\alpha^2)} |\alpha\rangle = D(\alpha) |\alpha\rangle$ 
 $D(\alpha) = e^{\alpha \hat{a}^\dagger - \frac{1}{2}\alpha^2} \quad [D(\alpha) \hat{a} D(\alpha)^\dagger = \hat{a} + \alpha]$

$$D(\alpha)^\dagger D(\alpha) = I$$

$$\bar{n} = \text{average number} = \langle n | \hat{n} | n \rangle$$

$$p(n) = |\langle n | \alpha \rangle|^2 = \frac{(1|\alpha|^2)^n}{n!} e^{-|\alpha|^2} e^{-\alpha \hat{a}^\dagger} |\alpha\rangle = |\alpha\rangle$$

### General      Angular      Momentum      Theory

$$[J_i, J_j] = i\hbar \sum_k \epsilon_{ijk} J_k$$

$$\text{or} \quad [\vec{J} \times \vec{J}] = i\hbar \vec{J}$$

$$[\vec{J}^2, J_i] = 0$$

$$\hat{J}_z = \hat{J}_x \pm i \hat{J}_y$$

$$[\hat{J}_z^2, \hat{J}_\pm] = 0$$

$$[\hat{J}_+, \hat{J}_\pm] = \pm \hbar \hat{J}_2$$

$$[\hat{J}_-, \hat{J}_\pm] = \pm \hbar \hat{J}_1$$

$$\hat{J}_z^2 = \hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ + \hbar^2 \hat{J}_z^2$$

$$\hat{J}_z^2 = \frac{1}{2} (\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+) + \hat{J}_z^2$$

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$$\hat{J}_z^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$$

$$\hat{J}_z |j, m\rangle = \hbar m |j, m\rangle$$

$$m = -j, -(j-1), \dots, j$$

$$\langle j', m' | j, m \rangle = \delta_{j', j} \delta_{m', m}$$

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

$$\hat{J}_z^{\pm} |j, m\rangle = \hbar \sqrt{(j\mp m)(j\pm m+1)} |j, m\pm 1\rangle$$

$$\langle \hat{J}_x^2 \rangle = \langle J_x^2 \rangle = \frac{\hbar^2}{2} (j(j+1) - m^2)$$

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

Similarly

Spin

$$[\hat{s}_i, \hat{s}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{s}_k$$

$$[L_i, S_i] = 0$$

$$\hat{s}_z^2 |s, m_s\rangle = \hbar^2 s(s+1) |s, m_s\rangle$$

$$\hat{s}_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$$

$$\hat{s}_z^{\pm} |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s\pm 1)} |s, m_s\pm 1\rangle$$

Pauli Matrices

$$\hat{s} = \frac{\hbar}{2} \vec{\sigma} \Rightarrow$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_z^2 = 1$$

$$\sigma_3^2 = I$$

$$\left[ \sigma_j, \sigma_k \right] = 2i \hat{J}_z \delta_{j,k} \quad \rightarrow \quad \sum_j \sigma_j^2 + \sum_k \sigma_k^2 = 0 \quad (j \neq k)$$

$$[\sigma_j, \sigma_k] = 2i \epsilon_{jkl} \sigma_l$$

$$\boxed{\sigma_j \sigma_k = \delta_{jk} + i \sum_l \epsilon_{jkl} \sigma_l}$$

$$(\vec{e} \cdot \vec{A})(\vec{e} \cdot \vec{B}) = (\vec{A} \cdot \vec{B}) \hat{I} + i \vec{e} \cdot (\vec{A} \times \vec{B})$$

$$\sigma_j^T = \sigma_j$$

$$\sigma_x \sigma_y \sigma_z = i \hat{I}$$

$$\text{Tr}(\sigma_j) = 0$$

$$\det(\sigma_j) = -1$$

$$e^{i\alpha \sigma_j} = \hat{I} \cos \alpha + i \sigma_j \sin \alpha$$

$$S_u = \frac{i}{2} (u_x \sigma_x + u_y \sigma_y + u_z \sigma_z)$$

$$|S, S_u = \frac{1}{2}\rangle = \frac{1}{\sqrt{2+u_z}} \begin{pmatrix} 1+u_z \\ u_x + i u_y \end{pmatrix}$$

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\hat{S}^2 = \frac{3}{4} \hbar^2 \hat{I}$$

$$e^{-i\alpha(\vec{\sigma} \cdot \hat{n})} = \begin{pmatrix} 0 \\ -1 \end{pmatrix} = \hat{I} \cos(\alpha) - i(\vec{\sigma} \cdot \hat{n}) \sin(\alpha)$$

Schwinger oscillator method

$$\text{Let } [a, a^\dagger] = [b, b^\dagger] = I \quad \& \quad [a, b] = [a, b^\dagger] = 0$$

$$J_+ = \hbar a^\dagger b$$

$$J_- = \hbar a b^\dagger$$

$$J_3 = \frac{\hbar}{2} (N_a - N_b)$$

$$J^2 = \frac{\hbar^2}{2} \left( \frac{(N_a + N_b)}{2} \right) \left( \frac{(N_a + N_b)}{2} + 1 \right)$$

$$Q = Q_T + P_T K$$

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# charged particle in $B_2$

$$\hat{H} = \frac{\pi_x^2}{2m} + \frac{\pi_y^2}{2m} + \frac{p_z^2}{2m} \quad \pi_i = p_i - eA_i$$

$$\hat{N}|n\rangle = n|n\rangle$$

$$\hat{A}|n\rangle = (h\omega_c) \hat{n}w|n\rangle$$

Trial

$$E_{n, k_2} = (n + \frac{1}{2}) \hbar \omega_c + \frac{\hbar^2 k_2^2}{2}$$

$$\boxed{\omega_c = \frac{eB}{m}}$$

$$[\pi_x, \pi_y] = i\hbar eB$$

$$\text{Let } \hat{b} = \frac{\pi_{2c} + i\pi_y}{\sqrt{2eB\hbar}}$$

$$\hat{b}^\dagger = \frac{\pi_x - i\pi_y}{\sqrt{2eB\hbar}}$$

$$I+ = (\hat{b}^\dagger b + \frac{1}{2}) \frac{\hbar eB}{m} + \frac{p_z^2}{2m}$$

$$\frac{d\vec{x}_i}{dt} = \frac{1}{i\hbar} [\vec{x}_i, \hat{A}] = \frac{p_i - eA_i}{m}$$

$$m \frac{d\vec{x}_i^2}{dt^2} = m \frac{1}{i\hbar} \left[ \frac{d\vec{x}_i}{dt}, \hat{A} \right] = F_i$$

$$\vec{F} = e\hat{E} + \frac{1}{c} \left( \frac{d\vec{p}}{dt} \times \vec{B} - \vec{B} \times \frac{d\vec{p}}{dt} \right)$$

# Many particle system

Permutation operator:

$$\hat{P}_{jk} \Psi(\varepsilon_1, \dots, \varepsilon_j, \dots, \varepsilon_k, \dots, \varepsilon_N)$$

$$= \Psi(\varepsilon_1, \dots, \varepsilon_{\bar{k}}, \dots, \varepsilon_j, \dots, \varepsilon_N)$$

$\Rightarrow$

$$\hat{P}_{jk} = \hat{P}_{kj}$$

eigen values  $\hat{P}_{ij}^2 = \pm 1$

eigen values  $\hat{P}_{ij} = \pm 1$  (+1 for Bosons)  
(-1 for Fermions)

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} \Psi(x_1, x_2) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} \Psi(x_1, x_2) = E \Psi(x_1, x_2)$$

$$\Psi(x_1, x_2) = \phi(x_1) \phi(x_2)$$

$$\Psi_{n_1, n_2}^{\pm}(x_1, x_2) = \frac{1}{\sqrt{2}} (\phi_{n_1}(x_1) \phi_{n_2}(x_2) \pm \phi_{n_2}(x_1) \phi_{n_1}(x_2))$$

Let  $\alpha \equiv (n_\alpha, l_\alpha, m_\alpha, m_S)$

Fermions  $\Psi_{\alpha, \beta}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\Psi_\alpha(\vec{r}_1) \Psi_\beta(\vec{r}_2) - \Psi_\beta(\vec{r}_1) \Psi_\alpha(\vec{r}_2))$

Bosons  $\Psi_{\alpha, \beta}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\Psi_\alpha(\vec{r}_1) \Psi_\beta(\vec{r}_2) + \Psi_\beta(\vec{r}_1) \Psi_\alpha(\vec{r}_2))$

Classical Mechanics

$$\vec{x}' = R \vec{x} \quad R = \text{orthogonal}$$

$$|\vec{x}'| = |\vec{x}| \quad R R^T = I$$

$$R_x(\theta) R_y(\theta) - R_y(\theta) R_x(\theta) = R_z(\theta^2) - 1 \quad |R| = 1$$

2D-matrix representation

$$2D \text{ matrix} \leftarrow X = \vec{x} \cdot \vec{\sigma}$$

$$X' = R \times R^T$$

$$R = \exp\left(-\frac{i\theta}{2}(\vec{\sigma} \cdot \hat{n})\right) = \cos\left(\frac{\theta}{2}\right) - i \frac{(\vec{\sigma} \cdot \hat{n})}{\sin\left(\frac{\theta}{2}\right)}$$

(since  $(\vec{\sigma} \cdot \hat{n})^2 = 1$ )

Quantum Mechanics

$$|\psi'\rangle = \hat{R}|\psi\rangle \quad \hat{A}' = \hat{R} \hat{A} \hat{R}^T$$

$$\text{Ex: } \hat{R}_z(\theta) \psi(g, \theta, \phi) = \psi(g, \theta, \phi - \delta\theta)$$

$$U_R(\hat{n}, \phi) = \hat{R}_n(\phi) = \exp\left(-i \frac{\vec{\sigma} \cdot \hat{n}}{\hbar} \phi\right)$$

It generates rotations

$$\hat{R}_x(\theta) \hat{R}_y(\theta) - \hat{R}_y(\theta) \hat{R}_x(\theta) = -\frac{s^2}{\hbar^2} [\hat{J}_x, \hat{J}_y]$$

$$\hat{R}_z(\theta^2) - 1 = -\frac{i s^2}{\hbar} \hat{J}_z$$

$$[\hat{J}_i, \hat{J}_j] = i \hbar \sum_k \epsilon_{ijk} \hat{J}_k$$

Rotations don't commute  $\Leftrightarrow [J_i, J_k] \neq 0$

Unlike traslations & ~~rot~~ momentum.

Space-time transformation

$$\vec{x} \rightarrow R(\theta) \vec{x}$$

$$\vec{x} \rightarrow \vec{x} + \vec{a}$$

$$\vec{x} \rightarrow \vec{x} + \vec{v}t$$

Unitary operator:

$$e^{-i \frac{\vec{J} \cdot \vec{n}}{\hbar} \theta}$$

$$e^{-i \frac{\vec{p} \cdot \vec{a}}{\hbar}}$$

$$e^{i \frac{\vec{v} \cdot \vec{G}}{\hbar} t}$$

$$\vec{G} = \vec{t} \vec{p} - m \vec{r}$$

$$e^{i \frac{\vec{A} \cdot \vec{t}_0}{\hbar}}$$

All classical rotation matrices with  $\det(R)=+1$

~~are~~ form a group called  $SO(3)$

If  $\det(R)=\pm 1$

then it is  $O(3)$ .

In QM the set of  $\{U_R(\vec{n}, \theta)\}$  forms

the group  $\xrightarrow{\text{Unitary}} SU(2)$

In H atom apart from  $\vec{E}$ , the

Runge-Lenz vector ( $\vec{A}$ ) is conserved.

$$\vec{A} = \vec{p} \times \vec{r} - m k \vec{r} \quad (\vec{F}_{(g)} = -\frac{k}{r^2} \vec{a})$$

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

### 39 Euler rotations

zyz

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_z(\gamma) \hat{R}_y(\beta) \hat{R}_z(\alpha)$$

$$\hat{R}^{-1}(\alpha, \beta, \gamma) = \hat{R}_z(-\gamma) \hat{R}_y(-\beta) \hat{R}_z(-\alpha)$$

$$\hat{R}(\alpha, \beta, \gamma) = \hat{R}_z(\alpha) \hat{R}_y(\beta) \hat{R}_z(\gamma)$$

$$\hat{R}^{-1}(\alpha, \beta, \gamma) = \hat{R}_z(-\gamma) \hat{R}_y(-\beta) \hat{R}_z(-\alpha)$$

$$\hat{R}(\alpha, \beta, \gamma) |j, m\rangle = \sum_{m'=-j}^j D_{m'm}^{(j)}(\alpha, \beta, \gamma) |j, m'\rangle$$

$$D_{m'm}^{(j)}(\alpha, \beta, \gamma) = \langle j, m' | \hat{R}(\alpha, \beta, \gamma) | j, m \rangle$$

$$D_{m'm}^{(j)}(\alpha, \beta, \gamma) = e^{-i(m'\alpha + m\gamma)} d_{m'm}^{(j)}(\beta)$$

$$d_{m'm}^{(j)}(\beta) = \langle j, m' | e^{-i\beta \frac{\partial}{\partial z}} | j \rangle$$

Wigner formula

$$d_{m'm}^{(j)}(\beta) = \sum_k (-1)^{k+m-m'} \frac{\sqrt{(j+m)! (j-m)! (j+m)! (j-m)!}}{(j-m-k)! (j+m-k)! (k+m'-m)! k!}$$

$$(cos \frac{\beta}{2})^{2j+m-m'-2k} (sin \frac{\beta}{2})^{m'-m+2k}$$

$$\sin \beta = i = \beta - \bar{\beta} \quad \beta = m + im$$

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## Addition of Angular Momenta

$$[J_{1i}, J_{1j}] = i\hbar \sum_k \epsilon_{ijk} J_{1k}$$

$$[J_{1i}, J_{2j}] = 0$$

$$\vec{J} = \vec{J}_1 + \vec{J}_2$$

$$\hat{\vec{J}}_1^2, \hat{\vec{J}}_2^2, \hat{J}_{1z}, \hat{J}_{2z}$$

$$\vec{J} = \vec{J}_1 \otimes \mathbf{1} + \mathbf{1} \otimes \vec{J}_2 = \vec{J}_1 + \vec{J}_2$$

$$\hat{\vec{J}}_1^2, \hat{\vec{J}}_2^2, \hat{J}_1, \hat{J}_2$$

$$|j_1, j_2; m_1, m_2\rangle$$

or

$$|j_1, j_2; j, m\rangle$$

or

$$|j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

Uncoupled basis

$$(j, m)$$

coupled basis

## Clebsch-Gordan Coefficients

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

Convention: Take them as real

$$\langle j_1, j_2; m_1, m_2 | j, m \rangle = \langle j, m | j_1, j_2; m_1, m_2 \rangle$$

$$\langle j_1, j_2; j_1, (j-j_1) | j, j \rangle = +ve \text{ real.}$$

$$\Rightarrow \langle j_1, j_2; m_1, m_2 | j, m \rangle = (-1)^{j-j_1-j_2} \langle j_2, j_1; m_2, m_1 | j, m \rangle$$

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j+1) = (2j_1+1)(2j_2+1) = \text{dimensionality.}$$

## Selection Rules for CG coefficients

$$m_1 + m_2 = m \quad \& \quad |j_1 - j_2| \leq j \leq j_1 + j_2$$

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$$\langle j_1^{\pm}, j_2^{\pm}; m_1^{\pm}, m_2^{\pm} | j_1, j_2; m_1, m_2 \rangle = \delta_{j_1^{\pm}, j_1} \delta_{j_2^{\pm}, j_2} \\ \delta_{m_1^{\pm}, m_1} \delta_{m_2^{\pm}, m_2}$$

$$\boxed{\begin{aligned}\hat{j}_{1\pm} &= \hat{j}_{1x} \pm i \hat{j}_{1y} \\ \hat{j}_{2\pm} &= \hat{j}_{2x} \pm i \hat{j}_{2y}\end{aligned}}$$

$$\hat{j}_{\pm} = \hat{j}_{1\pm} + \hat{j}_{2\pm}$$

$$\sum_j \sum_{m=j}^j \langle j_1, j_2; m_1, m_2 | j, m \rangle \langle j_1, j_2; m_1, m_2 | j, m \rangle \\ = \delta_{m_1^{\pm}, m_1} \delta_{m_2^{\pm}, m_2}$$

↓

$$\sum_j \sum_m \langle j_1, j_2; m_1, m_2 | j, m \rangle^2 = 1$$

Limiting Cases

$$\langle j_1, j_2; j_1, j_2 | (j_1 + j_2), (j_1 + j_2) \rangle = 1$$

$$\langle j_1, j_2; -j_1, -j_2 | (j_1 + j_2), -(j_1 + j_2) \rangle = 1$$

$$\hat{j}_{\pm} = \hat{j}_{1\pm} + \hat{j}_{2\pm}$$

★

$$\sqrt{(j \mp m)(j \pm m+1)} \langle j_1, j_2; m_1, m_2 | j, m \pm 1 \rangle$$

$$= \sqrt{(j_1 \pm m_1)(j_1 \mp m_1 + 1)} \langle j_1, j_2; m_1 \mp 1, m_2 | j, m \rangle$$

$$+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)} \langle j_1, j_2; m_1, m_2 \mp 1 | j, m \rangle$$

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$$\sqrt{(j \mp m+1)(j \pm m)} \langle j_1, j_2; m_1, m_2 | j, m \rangle$$

$$= \sqrt{(j_1 \mp m_1)(j_1 \mp m_1 + 1)} \langle j_1, j_2; m_1 \neq 1, m_2 | j, m \mp 1 \rangle$$

$$+ \sqrt{(j_2 \pm m_2)(j_2 \mp m_2 + 1)} \langle j_1, j_2; m_1, m_2 \mp 1 | j, m \mp 1 \rangle$$

$$\boxed{\langle j_1, j_2; j_1, (j_2 - 1) | (j_1 + j_2), (j_1 + j_2 - 1) \rangle = \sqrt{\frac{j_2}{j_1 + j_2}}}$$

$$\langle j_1, j_2; (j_1 - 1), j_2 | (j_1 + j_2), (j_1 + j_2 - 1) \rangle = \sqrt{\frac{j_1}{j_1 + j_2}}$$

$$\langle j_1, 1; m_1, 0 | j_1, m \rangle = \frac{m}{\sqrt{j(j+1)}} \langle j_1, 0; m_1, 0 | j_1, m \rangle = 1$$

	$\uparrow\uparrow$	$\uparrow\downarrow$	$\downarrow\uparrow$	$\downarrow\downarrow$
$j=1, m=1$	1	0	0	0
$j=1, m=0$	0	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$	0
$j=0, m=0$	0	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$	0
$j=1, m=-1$	0	0	0	1

$$\langle j_1, j_2; j_1, j_2 | (j_1 + j_2, j_1 + j_2 - 1) \rangle (1 + m_1 \pm i)(m_2 \mp i)$$

$$\langle m_1, i | (m_1 + 1, m_1); m_2, i \rangle (1 + m_2 \mp i)(m_2 \pm i) =$$

$$\langle m_1, i | (1 + m_1, m_1); m_2, i \rangle (1 + m_2 \mp i)(m_2 \pm i) +$$

# 43) Tensor Operators

Scalar

$$[\hat{A}, \hat{J}_k] = 0$$

Vector

Cartesian

$$[\vec{A}, \hat{n} \cdot \vec{J}] = i\hbar \hat{n} \times \vec{A}$$

$$[\partial J_i, A_j] = i\hbar \sum_k \epsilon_{ijk} A_k$$

## Spherical Tensors in spherical basis

$$A_0^{(1)} = A_z$$

$$A_{+1}^{(1)} = -\frac{1}{\sqrt{2}}(A_x + iA_y)$$

$$A_{-1}^{(1)} = \frac{1}{\sqrt{2}}(A_x - iA_y)$$

$$A_{\pm 1}^{(1)} = \mp \frac{1}{\sqrt{2}}(A_x \pm iA_y)$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \frac{z}{\sqrt{2}r_1}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} e^{i\phi} \sin \theta = -\sqrt{\frac{3}{8\pi}} \frac{(x+iy)}{\sqrt{2}r_1}$$

$$Y_{1,-1} = \sqrt{\frac{3}{8\pi}} e^{-i\phi} \sin \theta = \sqrt{\frac{3}{8\pi}} \frac{(x-iy)}{\sqrt{2}r_1}$$

$$\hat{J}_z, \hat{A}_q^{(1)} = \hbar q \hat{A}_q$$

$$\hat{J}_{\pm}, \hat{A}_q^{(1)} = \hbar \sqrt{2-q(q\pm 1)} \hat{A}_{q\pm 1}$$

$$q = -1, 0, 1$$

## Tensors

Cartesian  
Tensors

$$\hat{T}_{ij}^F = \hat{T}_{ij}^{(0)} + \hat{T}_{ij}^{(1)} + \hat{T}_{ij}^{(2)}$$

$$\hat{T}_{ij}^{(0)} = \frac{1}{3} \delta_{ij} \sum_{l=1}^3 \hat{T}_{ll}$$

$$\text{Antisymmetric } \hat{T}_{ij}^{(1)} = \frac{1}{2} (\hat{T}_{ij} - \hat{T}_{ji}) \quad i \neq j$$

$$\text{symmetric } \hat{T}_{ij}^{(2)} = \frac{1}{2} (\hat{T}_{ij} + \hat{T}_{ji}) - \hat{T}_{ij}^{(0)}$$

$$[\hat{J}_z, \hat{T}_a^{(k)}] = \hbar q \hat{T}_a^{(k)} \quad q = -k, -k+1, \dots, k$$

$$[\hat{J}_\pm, \hat{T}_a^{(k)}] = \hbar \sqrt{k(k+1) - q(q\pm 1)} \hat{T}_{a\pm 1}^{(k)}$$

$$[\hat{J}, \hat{T}_a^{(k)}] = \sum_{a'=-k}^k \hat{T}_{a'}^{(k)} \langle k, a' | \hat{J} | k, a \rangle$$

$$[\vec{n} \cdot \hat{J}, \hat{T}_a^{(k)}] = \sum_{a'=-k}^k \hat{T}_{a'}^{(k)} \langle k, a' | \vec{n} \cdot \hat{J} | k, a \rangle$$

$$(A^{(1)} \otimes B^{(1)})_{\pm 2}^{(2)} = A_{\pm 1}^{(1)} B_{\pm 1}^{(1)} \quad (A^{(1)} \otimes B^{(1)})_{\pm 1}^{(2)} = \frac{1}{\sqrt{2}} (A_{\pm 1}^{(1)} B_0^{(1)} + A_0^{(1)} B_{\pm 1}^{(1)})$$

$$(A^{(1)} \times B^{(1)})_0^{(2)} = \frac{1}{\sqrt{6}} (A_{+1} B_{-1} + 2A_0 B_0 + A_{-1} B_{+1})$$

Wigner-Eckart Theorem

$$\hat{T}_a^{(k)} = T(k, a)$$

$$\langle j', m' | \hat{T}_a^{(k)} | j, m \rangle = \langle j, k; m, a | j', m' \rangle \langle j' | \hat{T}^{(k)} | j \rangle$$

Selection rule:  $m+a = m'$

↓ Geometrical factor      ↓ Reduced Matrix element

dynamical factor  
(No dependence on orientation)

Scalar operator

$$\langle j, 0; m, 0 | j', m' \rangle = \delta_{j,j'} \delta_{m,m'}$$

$$\langle j', m' | \hat{B} | j, m \rangle = \langle j' | \hat{B} | j \rangle \delta_{j,j'} \delta_{m,m'}$$

Vector operator

$$\langle j', m' | \hat{J}_a | j, m \rangle = \langle j, m, a | j', m' \rangle$$

$$\downarrow \qquad \qquad \qquad \langle j' | \hat{J} | j \rangle$$

spin zero particle cannot have a dipole moment  
since  $\langle 0, 0, 0 | q_0 \rangle = 0$

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$$\vec{M}_L = \frac{e}{2mc} \vec{P}$$

Similarly, a spin half particle cannot have a quadratic moment since  $\langle \frac{1}{2}, 2; m, a | \frac{1}{2}, m \rangle = 0$

↓  
2nd rank tensor.

$\Rightarrow J$  cannot have a non-vanishing expectation value for  $2^{\lambda}$  electric or magnetic multipole moment tensor unless  $\lambda \leq 2j$ . (i.e zero if  $\lambda > 2j$ )  
 $\langle j_m | T_{kl}^a | j_m \rangle = 0$  if  $\lambda > 2j$

Scalar product

$$\hat{J} \cdot \hat{A} = \hat{J}_0 \hat{A}_0 - \hat{J}_{+1} \hat{A}_{-1} - \hat{J}_{-1} \hat{A}_{+1}$$

$$\boxed{\langle j_1, m' | \hat{A}_a | j_1, m \rangle = \frac{\langle j_1, m | \hat{J} \cdot \hat{A} | j_1, m \rangle}{\pi^2 j_1 (j_1 + 1)} \langle j_1, m' | \hat{J}_a | j_1, m \rangle}$$

Quadropole moment

$$Q_{jj} = \sum_l a_l g_{1il} g_{1jl}$$