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 continous and squre integrable

→ Discontinous potentials

$$-\frac{\hbar^2}{2m}\left[\left.\frac{d\psi(x)}{dx}\right|_{x=\epsilon} - \left.\frac{d\psi(x)}{dx}\right|_{x=-\epsilon}\right] + \int_{-\epsilon}^{\epsilon}(V(x)-E)\psi(x)\,dx = 0$$

For finite discontinuity $\frac{d\psi}{dx}$ is continous.

→ T.I.S.E $\boxed{i\hbar \frac{d}{dt}\psi(x,t) = \hat{H}\psi(x,t).}$

→ 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 $\boxed{[A,B]\psi=0}$

1-D problems

→ Bound states are discrete and non degenerate.

Proof: Let ψ_1 and ψ_2 are degenerate.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + V\psi_1 = E\psi_1$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2$$

$$\longrightarrow \psi_1\frac{d^2\psi_2}{dx^2} - \psi_2\frac{d^2\psi_2}{dx^2} = 0$$

$$\downarrow$$

$$\frac{d}{dx}\left(\psi_1\frac{d\psi_1}{dx} - \psi_2\frac{d\psi_2}{dx}\right) = 0$$

$$\longleftarrow$$

$$\psi_1\frac{d\psi_2}{dx} - \psi_2\frac{d\psi_1}{dx} = c$$

$$\downarrow \; |x| \to \infty \Rightarrow \boxed{c=0}$$

$$\Rightarrow \psi_1 = e^{d}\psi_2 \quad \text{(dis integration contand)}$$

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

→ 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 $\boxed{\text{1d}}$ 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 continous 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)

Operator is even if $\boxed{\hat{P}\hat{A}\hat{P} = \hat{A}}$ odd if $\boxed{\hat{P}\hat{B}\hat{P} = -\hat{B}}$

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

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

⇒ Even operator commute wit 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 $k = \frac{\sqrt{2mE}}{\hbar}$

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

→ It is not normalizable. $\hat{H}$ eigen states may not be bound states.

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

$\phi(k)$ → amplitude of wave packet

$$\boxed{\text{F.T}} \leftarrow \boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0)\, e^{-ikx}\, dx}$$

near $x=0$ constructive interference.

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

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

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

For gaussian wave packets

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

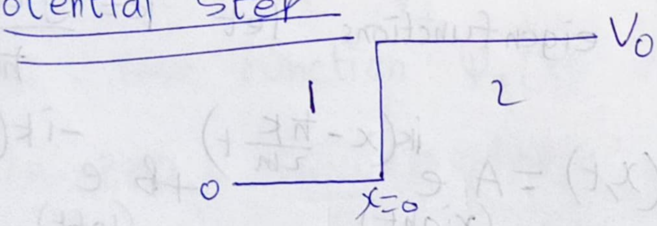
~~For~~ In general

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

$$\boxed{V_{ph} = \frac{\omega(k)}{k}} \qquad \boxed{V_g = \frac{d\omega(k)}{dk}} \Rightarrow \boxed{V_g = V_{ph} - \lambda \frac{dV_{ph}}{d\lambda}}$$

V_g → classical analogue

2) Potential step



a) Case $E > V_0$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$D=0$, $B=\frac{k_1-k_2}{k_1+k_2}A$, $C=\frac{2k_1}{k_1+k_2}A$

$\boxed{R+T=1}$ $R=\frac{|B|^2}{|A|^2}$ $\boxed{T=\frac{k_2}{k_1}\frac{|C|^2}{|A|^2}}$

b) $E<V_0$

$$\psi(x,t)=\begin{cases} Ae^{i(k_1x-\omega t)}+Be^{-i(k_1x+\omega t)} & x<0 \\ Ce^{-k_2'x}e^{-i\omega t} & x\geq 0 \end{cases}$$

$$B=\left(\frac{k_1-ik_2'}{k_1+ik_2'}\right)A \qquad C=\left(\frac{2k_1}{k_1+ik_2'}\right)A$$

$\boxed{R=1}$ $\boxed{T = \text{Undefined}}$

3) Infinite square well

$V(x)=0$ if $0\leq x\leq a$, ∞ otherwise

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

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

Zero point energy $\Rightarrow$ $\boxed{E_1>0}$

4) Finite square well

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

Bound states ($E<0$)

even $\rightarrow$ $\psi(x)=\begin{cases} Fe^{-kx} & x>a \\ D\cos(lx) & 0<x<a \\ \psi(-x) & x<0\end{cases}$

4) Finite square well

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

$$k_1 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \quad \boxed{k_1^2 + k_2^2 = \frac{2mV_0}{\hbar^2}}$$

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

Bound states ($0 < E < V_0$)

odd or antisym

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

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

For ψ_a, bound energies are given by

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

For ψ_s

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

→ If $V_0 \to \infty$ then number of bound states → ∞. Approximately Infinite square well.

→ Even if $V_0 \to 0$, always atleast one bound state exists.

Scattering ($E > 0$) $V(x) = -V_0 \quad -a \le x \le a$

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

$$\lambda = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ C\sin(\lambda x) + D\cos(\lambda x) & -a < x < a \\ Fe^{ikx} & x > a \end{cases}$$

$$F = \frac{e^{-2ika} A}{\cos(2\lambda a) - i\frac{(k^2+\lambda^2)}{2k\lambda}\sin(2\lambda a)} \qquad T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)}$$

Perfect transmission ⇒ $\boxed{E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}}$

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5) Barrier

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

$E>V_0$

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x} & x\le 0 \\ Ce^{ik_2x} + De^{-ik_2x} & 0<x<a \\ Ee^{ik_1x} & x\ge a \end{cases}$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

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

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

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

$$\boxed{T = \left[1+\frac{1}{4\epsilon(\epsilon-1)}\sin^2(a\sqrt{\epsilon-1})\right]^{-1}} \Leftarrow$$

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

$$\epsilon = \frac{E}{V_0}$$

6) Harmonic oscillator

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

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

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

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

Algebraic

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

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

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

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

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

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}}$$

$$\boxed{\psi_n(x) = A_n(\hat{a}_+)^n\psi_0(x) \quad , E_n = n+\tfrac{1}{2}\hbar\omega}$$

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

Analytic

$$\boxed{K = \frac{2E}{\hbar\omega}}$$

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

$$\xi >> K \Rightarrow \frac{d^2\psi}{d\xi^2} = \xi^2\psi$$

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

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

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

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

→ Delta function potential

Dirac delta distribution or function

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

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

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

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

$$\boxed{g(x_i) = 0 \;\&\; g'(x_i) \neq 0}$$

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

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

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

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

Integration by parts $\Rightarrow$ $\boxed{\int_{-\infty}^{\infty} f(x)\, \delta'(x-a)\, dx = -f'(a)}$

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

<u>In 3d</u>

$$\delta(\vec{r}-\vec{r}') = \delta(x-x')\,\delta(y-y')\,\delta(z-z')$$

$$= \frac{1}{r^2}\,\delta(r-r')\,\delta(\cos\theta-\cos\theta')\,\delta(\varphi-\varphi')$$

$$\boxed{\int d^3r\, f(\vec{r})\,\delta(\vec{r}) = f(0)} \quad = \boxed{\frac{1}{r^2\sin\theta}\,\delta(r-r')\,\delta(\theta-\theta')\,\delta(\varphi-\varphi')}$$

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

$$\vec{\nabla}\cdot\left(\frac{\hat{r}}{r^2}\right) = 4\pi\,\delta(\vec{r}) \qquad \nabla^2\left(\frac{1}{r}\right) = -4\pi\,\delta(\vec{r})$$

$\boxed{\text{Boundstate}}$

$\boxed{E<0}$

$$V(x) = -\alpha\,\delta(x) \qquad k = \frac{\sqrt{-2mE}}{\hbar}$$

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

$$\boxed{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\, e^{-\frac{m\alpha|x|}{\hbar^2}}} \Rightarrow \boxed{k = \frac{m\alpha}{\hbar^2}} \rightarrow \text{only bound state.}$$

10 $\boxed{E>0}$

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

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

$$\boxed{\beta = \frac{m\alpha}{\hbar^2 k}} \qquad B = \frac{i\beta A}{1-i\beta} A \qquad F = \frac{1}{1-i\beta} A$$

$$\boxed{R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2}} \qquad \boxed{T = \frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2}}$$

8) Double delta potential

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

Bound state $(E<0)$

$$\psi_{even} = \begin{cases} A\cosh(\alpha x) & |x|<a \\ Be^{-\alpha x} & |x|>a \end{cases}$$

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

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

$$\psi_{odd} = \begin{cases} A\sinh \alpha(x) & |x|<a \\ Be^{-\alpha x} & x>a \end{cases}$$

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

$\boxed{\text{3D Box}}$ $$\psi(\vec{r}) = \sqrt{\frac{8}{L_x L_y L_z}} \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

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

$\boxed{\text{Harmonic}}$

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

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

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2) Formulation of Quantm Mechanics

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

$\boxed{\bar{a}+\bar{b} \in V}$

b) $\lambda_1 \bar{a} + \lambda_2 \bar{b} \in V$

→ $\boxed{\text{Uniqe Identity scalar}}$ → $\boxed{\text{Associativity + Distributivity w.r.t multiplication of scalars and addition.}}$

Hibert space

→ Linear Vector Space

→ Salar product. $(\psi, \phi) = (\phi, \psi)^*$ & $\boxed{(\psi, \psi) \geq 0}$

$(\psi, \psi) = 0 \Rightarrow \psi = 0$

→ is Seperable $\boxed{(\psi, \phi) = \int \psi^* \phi \, dx}$

→ is Complete

Dirac Notation

$(\phi, \psi) \longrightarrow \langle \phi | \psi \rangle$

$\langle \phi |$: Bra ↓ Dualvector ↓ Covariant ↓ Row vector

$| \psi \rangle$: $\boxed{\text{Ket}}$, $\boxed{\text{Vector}}$, $\boxed{\text{Contravariat}}$, $\boxed{\text{Column Vector}}$

Every ket has uniaue bra

$| \psi \rangle \Longleftrightarrow \langle \psi |$

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

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

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

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

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

$\boxed{\| |\psi + \phi\rangle \| \leq \| |\psi\rangle \| + \| |\phi\rangle \|}$

Operator

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

$\boxed{\text{Linear operators}}$

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

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

$\boxed{\text{Antilinear Operator}}$

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

Postulates

C.M	Q.M
1) State is a point in x-p plane.	1) State is a vector $\lvert\psi(t)\rangle$ in a Hilbert space.
2) Every dynamic variable $w = w(x,p)$	2) The independent x and p are represented by linear Hermitian operators $\hat{x}$ and $\hat{p}$. $\langle x\lvert\hat{x}\rvert x'\rangle = x\,\delta(x-x')$; $\langle x\lvert\hat{p}\rvert x'\rangle = -i\hbar\,\delta'(x-x')$; If $w = w(x,p)$: $\hat{\Omega}(\hat{x},\hat{p}) = w(x\to\hat{x}, p\to\hat{p})$
3) Measurement gives $w(x,p)$ without altering state	3) Measuring $\hat{\Omega}$ $\Rightarrow$ one of the eigenvalues will come $\Rightarrow$ $p(w) \propto \lvert\langle w\lvert\psi\rangle\rvert^2$ alters state
4) $\dot{x} = \dfrac{\partial \mathcal{H}}{\partial p}$, $\dot{p} = \dfrac{-\partial \mathcal{H}}{\partial x}$	4) $i\hbar\dfrac{d}{dt}\lvert\psi(t)\rangle = H\lvert\psi(t)\rangle$; $H(\hat{x},\hat{p}) = \mathcal{H}(x\to\hat{x}, p\to\hat{p})$

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Hermition Adjoint: is defined as

$$\langle \psi | \hat{A}^{\dagger} | \phi \rangle = \langle \phi | \hat{A} | \psi \rangle^{*}$$

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

$\Rightarrow$ Eigen values are ~~not~~ real.

$$\langle \psi | \hat{A} | x \rangle = \langle x | \hat{A} | \psi \rangle^{*}$$

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

Unitary Operator: If $\boxed{\hat{U}^{\dagger} = \hat{U}^{-1}}$

Product of Unitary is also unitary.

Eigenvalues and Eigenvectors:

Eigenvetor is non zero.

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

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

Proof: $\langle \phi_m | \hat{A} | \phi_n \rangle = a_n \langle \phi_m | \phi_n \rangle$

$\langle \phi_m | \hat{A}^{\dagger} | \phi_n \rangle = a_m^{*} \langle \phi_m | \phi_n \rangle$

$\Rightarrow \boxed{(a_n - a_m^{*}) \langle \phi_m | \phi_n \rangle = 0}$

In the eigenbasis the operator is diagnol.

2.3 $\Rightarrow$ 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 $\hat{B}$.

Matrix Representation in Discrete Bases

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

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

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

State $\Rightarrow$ $|\psi\rangle = \left(\sum_{n=1}^{\infty} |\phi_n\rangle\langle\phi_n|\right)|\psi\rangle$

$$= \sum_{n=1}^{\infty} a_n |\phi_n\rangle \doteq \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}$$

$$\Rightarrow \langle\psi| = (a_1^* \; a_2^* \; \cdots, a_n^* \; \cdots)$$

Operator:

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

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

$$A^{\dagger} = (A^T)^*$$

Trace: $\mathrm{Tr}(\hat{A}^{\dagger}) = (\mathrm{Tr}(\hat{A}))^*$

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

$$\mathrm{Tr}(\hat{A}\hat{B}\hat{C}\hat{D}\hat{E}) = \mathrm{Tr}(\hat{B}\hat{C}\hat{D}\hat{E}\hat{A}) = \cdots$$

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

Ex: $|\psi\rangle|\phi\rangle$

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

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

Basis transformation is a Unitary matrix.

Eigenvalues

$$\det(A_{mn} - a\delta_{mn}) = 0$$

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

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

$\boxed{\det(A) = e^{\mathrm{Tr}(\ln A)}}$ $\quad \det(A) = \prod_n a_n$

Continous Basis

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

state: $|\psi\rangle = \left(\int_{-\infty}^{\infty} dk\,|x_k\rangle\langle x_k|\right)|\psi\rangle$

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

Continous matrix

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

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

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

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

$$= \boxed{\int d^3r\,\phi^*(\vec{r})\,\psi(\vec{r})}$$

Connecting x and p representations

$$\langle \vec{r}|\psi\rangle = \langle \vec{r}|\left(\int d^3p\, |\vec{p}\rangle\langle\vec{p}|\right)|\psi\rangle$$

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

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

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

Parseval's theorem

$$\int d^3p\, \psi^*(\vec{p})\psi(\vec{p}) = \int d^3r\, \psi^*(\vec{r})\, \psi(\vec{r})$$

Momentum Operator in x representation

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

$$\boxed{\hat{p}_x = -i\hbar\frac{\partial}{\partial x}} \qquad \boxed{\hat{\vec{p}} = -i\hbar\vec{\nabla}}$$

$\hat{x}$ in p representation

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

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

Connection between QM and CM

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

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

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$$\boxed{\frac{dA}{dt} = \{A, H\}_P + \frac{\partial A}{\partial t}}$$

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

Proof:

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

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

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

Ehrenfest theorem

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

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

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

$$= -\langle \vec{\nabla} \hat{V}(\vec{R}, t) \rangle$$

$$\boxed{\lim_{\hbar \to 0} Q.M = C.M}$$

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

Time Evolution operator

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

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

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

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

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

Time Independent Potentials

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

$\Rightarrow$ Some solutions are seperable

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

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

Stationary states

time independent probability density.

Conservation of Probability

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

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

$\downarrow$

Probability current density

$$\rho(\vec{r}, t) = \psi^*(\vec{r}, t) \psi(\vec{r}, t)$$

$\downarrow$

probability density

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

Gram-Schmidt process

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

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

Uncertainity Relations

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

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

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

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

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

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

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

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

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

Functions ~~of~~ of operators

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

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

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

Compatible Observable

→ $[A, B] = 0$

→ ~~Not necessary that~~

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

→ In FDHS we can simultaneosly diagnolise 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

→ $[A, B] \neq 0$

→ But it is possible that $[A, B]\,\psi = 0$ for some ψ

→ Here we can write simultaneous eigenstate.

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

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Schrodinger picture

state vectors evolve but operators do not.

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

$$|\psi(t)\rangle = \hat{U}(t,t_0)\,|\psi(t_0)\rangle$$

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

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

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

Heisenberg picture

$$|\psi(t)\rangle_H = \hat{U}^{+}(t)\,|\psi(t)\rangle = |\psi(0)\rangle$$

Operators ~~an~~ evolve state vectors do not.

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

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

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

Heisenberg equation of motion

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

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

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

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

Some potential energies

Ex: $V(x,y) = (x+y)^2 \Rightarrow U(X,Y) = 2X^2$

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

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

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

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

Electromagnetic minimal coupling

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

$$\vec{E} = -\vec{\nabla}\varphi - \frac{\partial \vec{A}}{\partial t} \qquad \vec{B} = \vec{\nabla} \times A$$

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

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

Gauge invariance

$$\varphi' = \varphi - \frac{\partial\Lambda}{\partial t} \qquad \vec{A}' = \vec{A} + \vec{\nabla}\Lambda$$

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

$\Rightarrow$ Quantum mechanics is guage invariant.

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Angular momentum operator

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

$$\Rightarrow \hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = -i\hbar\, \vec{R} \times \vec{\nabla}$$

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

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

$$\frac{\partial}{\partial\phi} = \sum_i \frac{\partial x_i}{\partial\phi} \frac{\partial}{\partial x_i}$$

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

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

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

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

Commutator Algebra

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

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

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

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

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

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

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

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

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

Commutators in Q.M

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

$[P_i, P_j] = 0$

$[x_i, x_j] = 0$

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

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

$$\boxed{[L_i, V_j]} = i\hbar \sum_k \epsilon_{ijk} V_k$$

$\vec{V} = (V_1, V_2, V_3)^T$ is any vector constructed from x_i and $\frac{\partial}{\partial x_i}$.

$$\boxed{\vec{V} = \vec{x} \text{ or } \vec{P} \text{ etc} \boxed{\text{or } \vec{L}}}$$

$$[L_i, \vec{V}^2] = i\hbar \sum_{jk} \epsilon_{ijk} (V_k V_j + V_j V_k)$$

$= 0$ (since by reversing j and k we get $\boxed{[L_i, \vec{V}^2] = -[L_i, \vec{V}^2]}$

~~Hydrogen Atom~~

Central Potential

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

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

$$\hat{p}_r = \frac{1}{2}\left[\left(\frac{\vec{r}}{r}\right)\cdot\vec{p} + \vec{p}\cdot\left(\frac{\vec{r}}{r}\right)\right]$$

$$\boxed{\hat{p}_r = -i\hbar\frac{1}{r}\frac{\partial}{\partial r}r}$$

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

Let $\psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$

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

$$+ VRY = ERY$$

divide by YR and multiply by $-\frac{2mr^2}{\hbar^2}$

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

Angular equation

By multiplying $Y\sin^2\theta$

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

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

plugging and dividing by $\Theta\Phi$

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

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

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

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

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

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

Not polynomial

P_l^m are associated Legendre ~~f~~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: $P_l(x) = \frac{1}{2^l l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l$

$$d^3\vec{r} = r^2 \sin\theta \, dr \, d\theta \, d\phi = r^2 \, dr \, d\Omega$$

Normalize $\Rightarrow \int_0^\infty |R|^2 r^2 dr = 1 \quad \int_0^\pi \int_0^{2\pi} |Y|^2 \sin\theta \, d\theta \, d\phi = 1$

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

Radial part

$V(r)$ only affect radial part

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

Let $\quad u(r) = r R(r)$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left[V + \frac{\hbar^2 l(l+1)}{2m r^2}\right]}_{V_{eff}} u = Eu$$

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

Hydrogen Atom

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

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

$\rho = Kr$ and $\rho_0 = \frac{m_e e^2}{2\pi\epsilon_0 \hbar^2 K}$

$$\Rightarrow \frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u$$

$\rho \to \infty$ $\frac{d^2u}{d\rho^2} = u$

$$u(\rho) \sim Ae^{-\rho} + \cancel{Be^{+\rho}}$$

$\rho \to 0$ $\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2} u$

$$u(\rho) = C\rho^{l+1} + \cancel{D\rho^{-l}}$$

Let $u(\rho) = \rho^{l+1} e^{-\rho} v(\rho)$

$$\Rightarrow \rho\frac{d^2v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0$$

$$\psi_{n l m_l}(r,\theta,\phi) = R_n^l(r)\,\Theta_{l m_l}(\theta)\,\Phi_{m_l}(\phi)$$

or

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

$$R_{nl}(r) = \frac{1}{r}\,\rho^{l+1}\,v(\rho)\,e^{-\rho}$$

$v(\rho)$ is a polynomial of degree $n-l-1$ in ρ.

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}\,c_j$$

$$R_n^l(r) = D\,e^{-\frac{1}{2}\rho_r}\,\rho_r^{\,l}\,L_{n+l}^{2l+1}(\rho_r)$$

$$\rho_r = \frac{2}{na_0}\,r \qquad a_0 = \frac{\hbar^2}{me^2}\,4\pi\epsilon_0$$

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

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

Assosiated Laguerre functions

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

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

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

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

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

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

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

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

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

Selection rules: $\boxed{\Delta l = \pm 1 \,, \; \Delta m_l = \pm 1, 0}$

$$\Psi = a\Psi_m e^{-\frac{iE_m t}{\hbar}} + b\Psi_n e^{-\frac{E_n t}{\hbar}}$$

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

Angular momentum continued

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

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

Orbital magnetic dipole moment

$$\vec{\mu} = \frac{-\mu_b}{\hbar}\vec{L} \qquad \mu_b = \frac{e\hbar}{2m} = \text{bohr magneton.}$$

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

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

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

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

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

Spin:

spin magnetic moment

$$\mu_z = -g_s\,\mu_b\,m_s \qquad s=\frac{1}{2} \downarrow m_s = \pm\frac{1}{2}$$

$$m_s = -s, -s+1, \ldots, s$$

For Harmonic oscillator

$$\hat{a} = \frac{m\omega\hat{x} + i\hat{p}}{\sqrt{2\hbar m\omega}} \Longrightarrow \text{Not hermitian}$$

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

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

$$\hat{p} = \frac{1}{2i}(\hat{a}-\hat{a}^{+})\sqrt{2\hbar m\omega}$$

$$\boxed{[\hat{a}\ \hat{a}^{+}] = I}$$

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

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

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

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

creation $\quad a^{+}|n\rangle = \sqrt{n+1}\,|n+1\rangle$

$$\langle m|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{m,n-1} + \sqrt{n+1}\,\delta_{m,n+1}\right)$$

$$\langle m|\hat{p}|n\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\left(\sqrt{n+1}\,\delta_{m,n+1} - \sqrt{n}\,\delta_{m,n-1}\right)$$

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

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

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

$$\frac{dp}{dt} = -m\omega^2\hat{x} \; ; \; \frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}$$

These equations becomes uncoupled

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

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

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

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

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

Baker-Hausdorff lemma

$$e^{i\hat{O}t}\hat{A}\,e^{-i\hat{O}t} = A + it[\hat{O},\hat{A}] + \frac{(it)^2}{2!}[\hat{O},[\hat{O},\hat{A}]] + \frac{(it)^3}{3!}[O,[O,[O,A]]] + \cdots$$

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

Coherent states

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

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

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

$$\boxed{|\alpha\rangle = \sum_n \frac{\alpha^n e^{-\frac{|\alpha|^2}{2}}}{\sqrt{n!}} |n\rangle} = e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} |0\rangle$$

$$= e^{-\frac{|\alpha|^2}{2}} e^{\alpha \hat{a}^\dagger} e^{-\alpha^* \hat{a}} |0\rangle$$

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

$$|\alpha\rangle = e^{(\alpha \hat{a}^\dagger - \alpha^* \hat{a})} |0\rangle = D(\alpha)|0\rangle$$

$$D(\alpha) = e^{\alpha \hat{a}^\dagger - \alpha^* \hat{a}} \qquad \boxed{D^\dagger(\alpha)\, \hat{a}\, D(\alpha) = \hat{a} + \alpha}$$

$$\boxed{D^\dagger(\alpha) D(\alpha) = I}$$

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

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

$$e^{-\alpha^* \hat{a}} |0\rangle = |0\rangle$$

General Angular Momentum Theory

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

or

$$\boxed{\vec{J} \times \vec{J} = i\hbar \vec{J}}$$

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

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

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

$$[\hat{J}_+, \hat{J}_-] = 2\hbar \hat{J}_z$$

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

$$\hat{\vec{J}}^2 = \hat{J}_\pm \hat{J}_\mp + \hat{J}_z^2 \mp \hbar \hat{J}_z$$

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

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

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

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

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

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

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

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

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

Similarily spin

$$[\hat{S}_i, \hat{S}_j] = i\hbar \sum_k \epsilon_{ijk} \hat{S}_k \qquad \boxed{[L_i, S_i] = 0}$$

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

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

$$\hat{S}_\pm |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s\pm1)} \, |s, m_s\pm1\rangle$$

Pauli matrices

$$\hat{\vec{S}} = \frac{\hbar}{2} \vec{\sigma}$$

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

$$\sigma_j^2 = \hat{I}$$

$$\boxed{\{\sigma_j, \sigma_k\} = 2\hat{I}\,\delta_{j,k}} \rightarrow \sigma_j^2 = I$$

$$\rightarrow \sigma_j\sigma_k + \sigma_k\sigma_j = 0 \quad (j \neq k)$$

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

$$\boxed{\sigma_j \sigma_k = \delta_{j,k} + i \sum_l \epsilon_{jkl} \sigma_l}$$

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

$$\sigma_j^\dagger = \sigma_j \qquad \sigma_x \sigma_y \sigma_z = i\hat{I}$$

$$Tr(\sigma_j) = 0$$

$$det(\sigma_j) = -1 \qquad \boxed{e^{i\alpha\sigma_j} = \hat{I}\cos\alpha + i\sigma_j \sin\alpha}$$

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

$$|s, s_u = \tfrac{1}{2}\rangle = \frac{1}{\sqrt{2+2u_z}}\begin{pmatrix} 1+u_z \\ u_x + iu_y \end{pmatrix}$$

$$(u_z \neq -1)$$

$$\begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

$$\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

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

$$\boxed{e^{-i\alpha(\vec{\sigma}\cdot\hat{n})} = \hat{I}\cos(\alpha) - i(\vec{\sigma}\cdot\hat{n})\sin(\alpha)}$$

Schwinger oscillator method

Let $[a, a^\dagger] = [b, b^\dagger] = I$ & $[a, b] = [a, b^\dagger] = 0$

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

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

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

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

Charged particle in B_z

$$\hat{H} = \frac{\Pi_x^2}{2m} + \frac{\Pi_y^2}{2m} + \frac{P_z^2}{2m} \qquad \Pi_i = P_i - eA_i$$

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

$$\hat{H}\,|n\rangle = (n+\tfrac{1}{2})\,\hbar\omega\,|n\rangle$$

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

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

$$\boxed{[\Pi_x, \Pi_y]} = i\hbar eB$$

Let $\quad \hat{b} = \frac{\Pi_x + i\Pi_y}{\sqrt{2eB\hbar}}$

$$\hat{b}^{+} = \frac{\Pi_x - i\Pi_y}{\sqrt{2B\hbar}}$$

$$H = (b^{+}b + \tfrac{1}{2})\frac{\hbar eB}{m} + \frac{P_z^2}{2m}$$

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

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

$$\vec{F} = e\hat{E} + \frac{1}{2}\left(\frac{d\vec{r}}{dt}\times\vec{B} - \vec{B}\times\frac{d\vec{r}}{dt}\right)$$

Many particle system

Permutation operator:

$$\hat{P}_{jk}\Psi(\xi_1,\dots\xi_j,\dots\xi_k,\dots\xi_N)$$

$$:= \Psi(\xi_1,\dots\xi_k,\dots\xi_j,\dots\xi_N)$$

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

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

eigen values $\hat{P}_{ij} = \pm 1$ $\begin{pmatrix} +1 \text{ for Bosons} \\ -1 \text{ for fermions} \end{pmatrix}$

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

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

$$\Psi^{\pm}_{n_1,n_2}(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\phi_{n_1}(x_1)\phi_{n_2}(x_2) \pm \phi_{n_2}(x_1)\,\phi_{n_1}(x_2)\right)$$

Let $\alpha \equiv (n_\alpha, l_\alpha, m_{l\alpha}, m_{s\alpha}$

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

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

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Classical Mechanics

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

$$|\vec{x}'| = |\vec{x}| \qquad RR^T = I$$

$$\boxed{|R| = 1}$$

$$\boxed{R_x(\delta)\, R_y(\delta) - R_y(\delta)\, R_x(\delta) = R_z(\delta^2) - 1}$$

2D-matrix representation

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

$$X' = R X R^{\dagger}$$

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

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

Quantum Mechanics

$$|\psi'\rangle = \hat{R}|\psi\rangle \qquad \hat{A}' = \hat{R}\hat{A}\hat{R}^{\dagger}$$

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

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

$\vec{J}$ $\downarrow$ It generates rotations

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

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

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

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

Unlike traslations & ~~pom~~ momentum.

Space-time transformation	Unitary operator
$\vec{x} \to R_n(\theta)\vec{x}$	$e^{-i\frac{\hat{\vec{J}}\cdot\hat{n}}{\hbar}\theta}$
$\vec{x} \to \vec{x} + \vec{a}$	$e^{-i\frac{\vec{p}\cdot\vec{a}}{\hbar}}$
$\vec{x} \to \vec{x} + \vec{v}t$	$e^{i\frac{\vec{v}\cdot\vec{G}}{\hbar}}$, $\vec{G} = t\vec{p} - m\vec{r}$
$t \to t + t_0$	$e^{\frac{i}{\hbar}\hat{H}t_0}$

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 $\{U_R(\hat{n}, \theta)\}$ forms

the group $SU(2)$ $\to$ Unitary

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

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

$$\vec{A} = \vec{p} \times \vec{L} - mk\vec{r} \quad \left(\vec{F}(r) = \frac{-k}{r^2}\hat{r}\right)$$

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Euler rotations zyz

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

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

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

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

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

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

$$\boxed{D^{(j)}_{m'm}(\alpha,\beta,\gamma) = e^{-i(m'\alpha+m\gamma)}\,d^{(j)}_{m'm}(\beta)}$$

$$d^{(j)}_{m'm}(\beta) = \langle j,m'|e^{\frac{-i\beta\hat{J}_y}{\hbar}}|j,m\rangle$$

Wignerformula

$$d^{(j)}_{m'm}(\beta) = \sum_k (-1)^{k+m'-m}\frac{\sqrt{(j+m)!\,(j-m)!\,(j+m')!\,(j-m')!}}{(j-m'-k)!\,(j+m-k)!\,(k+m'-m)!\,k!}\left(\cos\frac{\beta}{2}\right)^{2j+m-m'-2k}\left(\sin\frac{\beta}{2}\right)^{m'-m+2k}$$

Addition of Angular Momenta

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

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

$$\boxed{\vec{J} = \vec{J}_1 + \vec{J}_2} \qquad \boxed{\vec{J} = \vec{J}_1 \otimes 1 + 1 \otimes \vec{J}_2 \equiv \vec{J}_1 + \vec{J}_2}$$

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

$|j_1, j_2; m_1, m_2\rangle$ or $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ — Uncoupled basis

$|j_1, j_2; j, m\rangle$ or $|j, m\rangle$ — Coupled basis

Clebsh-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

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

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

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

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

Selection Rules for CG coefficients

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

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

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

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

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

$$\Downarrow$$

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

Limiting Cases

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

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

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

$$\Downarrow$$

☆

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

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

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

★

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

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

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

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

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

↓

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

	↑↑	↑↓	↓↑	↓↓
$J=1, m=1$	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

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Tensor Operators

Scalar

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

Vector

Cartesian

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

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

spherical Tensors in spherical basis

$$A^{(1)}_0 = A_z \qquad Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}$$

$$A^{(1)}_{+1} = -\frac{1}{\sqrt{2}}(A_x + iA_y) \qquad Y_{1,1} = -\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin\theta = -\sqrt{\frac{3}{4\pi}}\left(\frac{x+iy}{\sqrt{2}r}\right)$$

$$A^{(1)}_{-1} = \frac{1}{\sqrt{2}}(A_x - iA_y) \qquad Y_{1,-1} = \sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin\theta = \sqrt{\frac{3}{4\pi}}\left(\frac{x-iy}{\sqrt{2}r}\right)$$

$$\boxed{A^{(1)}_{\pm1} = \mp\frac{1}{\sqrt{2}}(A_x \pm A_y)}$$

$$\boxed{q = -1, 0, 1}$$

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

$$\hat{J}_\pm, \hat{A}^{(1)}_q = \hbar\sqrt{2 - q(q\pm1)}\,\hat{A}_{q\pm1}$$

Tensors

$$3^K \qquad 2K+1$$

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

Cartesian tensors

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

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

Antisymetric

symmetric

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

$$\boxed{\begin{aligned}&\left[\hat{J}_z, \hat{T}^{(k)}_q\right] = \hbar q \hat{T}^{(k)}_q \qquad q=-k,-k+1,\dots,k\\ &\left[\hat{J}_\pm, \hat{T}^{(k)}_q\right] = \hbar\sqrt{k(k+1)-q(q\pm1)}\,\hat{T}^{(k)}_{q\pm1}\end{aligned}}$$

$$\left[\vec{\hat{J}}, \hat{T}^{(k)}_q\right] = \sum_{q'=-k}^{k} \hat{T}^{(k)}_{q'} \langle k,q' | \vec{\hat{J}} | k,q\rangle$$

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

$$\boxed{\left(A^{(1)}\otimes B^{(1)}\right)^{(2)}_{\pm2} = A^{(1)}_{\pm1} B^{(1)}_{\pm1}} \quad \left(A^{(1)}\otimes B^{(1)}\right)^{(2)}_{\pm1} = \frac{1}{\sqrt{2}}\left(A^{(1)}_{\pm1} B^{(1)}_0 + A^{(1)}_0 B^{(1)}_{\pm1}\right)$$

$$\boxed{\left(A^{(1)}\times B^{(1)}\right)^{(2)}_0 = \frac{1}{\sqrt{6}}\left(A_{+1}B_{-1} + 2A_0B_0 + A_{-1}B_{+1}\right)}$$

Wigner-Eckart Theorem

$$\hat{T}^{(k)}_q = T(k,q)$$

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

Selection rule: $\boxed{m+q=m'}$

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

$$\langle j',m' | \hat{J}_q | j,m\rangle = \langle j,1; m,q | j',m'\rangle \langle j' \| \hat{\vec{J}} \| j\rangle$$

Spin zero particle cannot have a dipole moment since $\langle 0,1; 0,q | 0,0\rangle = 0$.

$$\vec{\mu}_L = \frac{a}{2mc}\vec{L}$$

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

$\underbrace{\text{a quadratic moment}}_{\text{2nd rank tensor.}}$

$\Rightarrow$ J cannot have a non-vanishing expectation value for 2^λ electric or magnetic multipole moment tensor unless $\lambda \leq 2j$. (i.e zero if $\lambda > 2j$)

$\langle j\, m | T^a_k | j\, m \rangle = 0$ if $\boxed{\lambda > 2j}$

Scalar product

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

$$\boxed{\langle j, m' | \hat{A}_q | j, m \rangle = \frac{\langle j, m | \hat{\vec{J}} \cdot \hat{\vec{A}} | j, m \rangle}{\hbar^2 j(j+1)} \langle j, m' | \hat{J}_q | j, m \rangle}$$

Quadropole moment

$$Q_{ij} = \sum_l a_l\, x_{il}\, x_{jl}$$