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.

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

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

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

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

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

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

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

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

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

Hint: $\psi_2 = \dfrac{\psi_1 + \psi_1^*}{2}$ 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.

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:

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

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.

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

near $x=0$ constructive

$\phi(k)$ → amplitude of wave packet

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

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

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

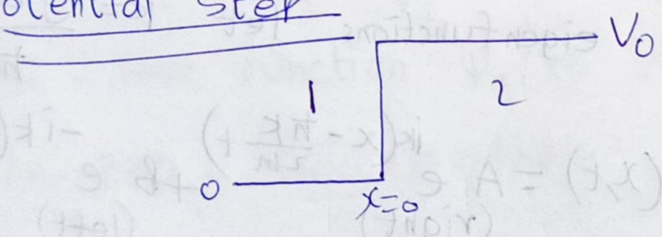
~~For~~ In general

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

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

V_g → classical analogue

2) Potential step



a) Case $E > V_0$

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

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

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

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

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

Bound states ($0 < E < V_0$)

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

odd or antisym

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

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

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

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

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 $\to \infty$. Approximately Infinite square well.

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

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

$$k = \sqrt{\frac{2mE}{\hbar}} \qquad \psi(x) = A e^{ikx} + B e^{-ikx} \quad x < -a$$

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

$$l = \sqrt{\frac{2m(E+V_0)}{\hbar^2}} \qquad F e^{ikx} \quad x > a$$

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

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

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5) **Barrier**

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

$E > V_0$

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

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

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

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

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

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

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

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

6) **Harmonic oscillator**

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

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

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

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

Algebraic

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

$$\boxed{[\hat{a}_-, \hat{a}_+] = 1} \qquad \hat{a}_+\hat{a}_- = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2}$$

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

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

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

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

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

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

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

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

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

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

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

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

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>

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

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

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

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

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

$\boxed{\text{Boundstate}}$

$\boxed{E<0}$

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

$$\psi(x) = \cancel{Ae}\ B e^{kx} \quad x<0$$

$$F e^{-kx} \quad x>0$$

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

10 $\boxed{E>0}$

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

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

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

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

8) Double delta potential

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

Bound state $(E<0)$

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

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

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

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

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

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

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

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

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

→ is Complete

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

Dirac Notation

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

Bra ← $\langle \phi |$; $| \psi \rangle$ → $\boxed{\text{Ket}}$

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

$\langle \phi |$ → Dualvector → Covariant → Row 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

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

Linear operators

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

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

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

1) State is a point in $x-p$ plane.

2) Every dynamic variable $w = w(x,p)$

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

4) $\dot{x} = \dfrac{\partial \mathcal{H}}{\partial p}$

$\dot{p} = \dfrac{-\partial \mathcal{H}}{\partial x}$

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

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

3) Measuring $\hat{\Omega}$

$\Rightarrow$ one of the eigenvalues will come

$\Rightarrow$ $p(w) \propto |\langle w|\psi\rangle|^2$

alters state

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

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

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

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

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

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

$$\Rightarrow \langle\psi| = (a_1^* \; a_2^* \; \text{---}, a_n^* \; \text{---})$$

Operator:

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

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

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

Trace:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Stationary states

time independent probability density.

Conservation of Probability

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

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

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

$\downarrow$ Probability current density

$\downarrow$ 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

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

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

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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 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 $\nexists$ eigenstate.

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Schrodinger picture

state vectors evolve but operators do not.

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

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

$$\boxed{\frac{d}{dt}\langle\hat{A}\rangle = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle} \quad \hat{U}(t,t_0) = e^{-\frac{i(t-t_0)}{\hbar}\hat{H}}$$

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

Heisenberg picture

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

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

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

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

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

Heisenberg equation of motion

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

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

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

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

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

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

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

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

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

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

$$\boxed{\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned}}$$

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

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

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

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

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

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

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

$[p_i, p_j] = 0$

$[x_i, x_j] = 0$

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

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

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

$\vec{V} = (V_1, V_2, V_3)^T$ 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 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 $u(r) = r R(r)$

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

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

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

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

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

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

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

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

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.

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

$$\boxed{\begin{aligned} R_n^l(r) &= D\,e^{-\frac{1}{2}\rho_r}\,\rho_r^l\,L_{n+l}^{2l+1}(\rho_r) \\ \rho_r &= \frac{2}{n a_0}\,r \qquad a_0 = \frac{\hbar^2}{m e^2}\,4\pi\epsilon_0 \\ D &= -\left[\left(\frac{2}{n a_0}\right)^3 \frac{(n-l-1)!}{2n\,[(n+l)!]}\right]^{\frac{1}{2}} \\ L_{n+l}^{2l+1}(\rho) &= \sum_{k=0}^{n-l-1} (-1)^{k+2l+1}\,\frac{((n+l)!)^2\,\rho^k}{(n-l-1-k)!\,(2l+1+k)!\,k!} \end{aligned}}$$

Assosiated Laguerre functions

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Spin:

spin magnetic moment

$$\mu_z = -g_s \mu_b m_s$$

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

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

For Harmonic oscillator

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

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

$\Longrightarrow$ Not hermitian

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

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

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

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

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

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

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

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

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

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

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

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

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

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

These equations becomes uncoupled

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

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

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

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

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

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

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

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

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

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

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

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

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

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

33 $\hat{\vec{J}}^2 |j,m\rangle = \hbar^2 j(j+1) |j,m\rangle$

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

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

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

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

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

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

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

<u>Similarily</u> spin

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

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

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

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

<u>Pauli matrices</u>

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

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

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

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

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

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

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

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

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

$$Tr(\sigma_j) = 0$$

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

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

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

$$(u_z \neq -1)$$

$$\downarrow$$

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

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

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

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

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

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

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

$$\boxed{[\pi_x, \pi_y]} = i\hbar eB$$

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

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

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

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

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

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

Many particle system

Permutation operator:

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

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

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

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

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

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

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

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.

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

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

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

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

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

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

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

$$\Downarrow$$

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

Limiting Cases

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

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

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

$$\Downarrow$$

☆

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

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

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

☆

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

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

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

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

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

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

	$\uparrow\uparrow$	$\uparrow\downarrow$	$\downarrow\uparrow$	$\downarrow\downarrow$
$J=1, m=1$	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

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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

$$A_0^{(1)} = A_z \qquad Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}$$

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

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

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

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

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

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

Tensors

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

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

Cartesian tensors

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

Antisymetric

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

symmetric

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

$$\left[\hat{J}_z, \hat{T}_q^{(k)}\right] = \hbar q \, \hat{T}_q^{(k)} \qquad q = -k, -k+1, \ldots, k$$

$$\left[\hat{J}_\pm, \hat{T}_q^{(k)}\right] = \hbar \sqrt{k(k+1) - q(q\pm1)} \; \hat{T}_{q\pm1}^{(k)}$$

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

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

$$\boxed{\left(A^{(1)} \otimes B^{(1)}\right)^{(2)}_{\pm2} = A^{(1)}_{\pm1} B^{(1)}_{\pm1}} \quad \left(A^{(1)} \otimes B^{(1)}\right)^{(2)}_{\pm1} = \frac{1}{\sqrt{2}}\left(A^{(1)}_{\pm1} B^{(1)}_{0} + A^{(1)}_{0} B^{(1)}_{\pm1}\right)$$

$$\boxed{\left(A^{(1)} \times B^{(1)}\right)^{(2)}_{0} = \frac{1}{\sqrt{6}}\left(A_{+1} B_{-1} + 2A_0 B_0 + A_{-1} B_{+1}\right)}$$

Wigner-Eckart Theorem

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

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

Geometrical factor

Reduced Matrix element
dynamical factor
(No dependence on orientation)

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

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

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

$\Downarrow$

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

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

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

Quadropole moment

$$Q_{jj} = \sum_{l} a_l \, r_{il} \, r_{jl}$$