

Schrodinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi \quad \hat{H} = \frac{\hat{p}^2}{2m} + V \quad \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

(Hamiltonian operator) (momentum operator)

Some probability (age group)

Median: age value T s.t. half $< T$ and half population $> T$.

Deviation: $\Delta j = j - \langle j \rangle$; variance: $\sigma^2 = \langle \Delta j^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2$; stand. dev. σ

Operators

$$\langle x \rangle = \int \psi^* x \psi dx = \langle \psi | x | \psi \rangle$$

$$\langle p \rangle = \langle \psi | \frac{\hbar}{i} \frac{\partial}{\partial x} | \psi \rangle$$

$$\langle Q(x, p) \rangle = \langle \psi | Q(x, \frac{\hbar}{i} \frac{\partial}{\partial x}) | \psi \rangle \quad \text{ex } T = \frac{p^2}{2m} \rightarrow \langle T \rangle = \langle \psi | \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} | \psi \rangle$$

Formalism: $\langle f | g \rangle = \int f^* g \Rightarrow \langle a_n f_n | b_m g_m \rangle = a_n^* b_m \langle f_n | g_m \rangle$

$$\langle f | g \rangle \leq \|f\| \|g\| \text{ Schwartz ineq.}$$

complex inner product

$$\langle u | v \rangle = \langle v | u \rangle^*$$

$$\langle k | u | v \rangle = k \langle u | v \rangle \quad \langle u | k | v \rangle = k^* \langle u | v \rangle$$

Hermitian:

$$\langle Q \rangle = \langle \psi | \hat{Q} \psi \rangle = \langle \hat{Q} \psi | \psi \rangle \Rightarrow \hat{Q}^\dagger = \hat{Q}$$

observable operator

$$\begin{aligned} \int (\hat{Q} \psi)^\dagger \psi &= \int \psi^\dagger \hat{Q}^\dagger \psi \\ &= \int \psi^\dagger \hat{Q} \psi \end{aligned}$$

Determinate state are eigfunc of \hat{Q} . ex stationary state $\langle Q \rangle = q$ time indept

Collection of eig.vals of \hat{Q} is its spectrum.

Hermitian Spectrum

- discrete: in Hilbert space, physical ex Harmonic oscillator
- continuum: not in Hilbert space, not normalizable ex free particles
- ex finite well (Both)

Axiom: Eigenfunc. of observable are complete.

Continuous Spectrum de Broglie $\left| \lambda = \frac{2\pi\hbar}{p} = \frac{h}{p} \right|$ from momentum operator (solve)

Here Eig.func. of Hermitian are Dirac Orthonormal

$$\langle f_p | f_p \rangle = \delta(p - \bar{p})$$

and complete

$$f(x) = \int_{-\infty}^{\infty} c(p) f_p(x) dp \quad \text{w/} \quad c(p) = \langle f_p | f \rangle$$

ex position operator: $x g_y = y g_y \Rightarrow g_y = \delta(x - y)$

Generalized Stat. Interpretation

Discrete: $\psi(x,t) = \sum_n C_n f_n(x)$; $|C_n|^2$ - Probability getting eigval q_n of \hat{Q}

Continuous: Probability $|C(z)|^2 dz$ and $C(z) = \langle f_z | \psi \rangle$ ex $C(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{\frac{ipx}{\hbar}} \psi(x,t) dx$

Generalized uncertainty principle

$$\sigma_A \sigma_B \geq \left| \frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right|$$

ex $[\hat{x}, \hat{p}] = i\hbar$, $\Delta x \Delta p \geq \frac{\hbar}{2}$ Heisenberg's

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

$$\Delta t \Delta E \geq \frac{\hbar}{2}$$

Δt - time taken to change $\langle Q \rangle$ by a standard deviation

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

momentum space $\Phi(p,t)$

Q observable not explicitly time dependent, then

$$\frac{d\langle Q \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{Q}] \rangle$$

if \hat{H} & \hat{Q} commute

Q is a constant of motion

(ii) $[\hat{Q}, \hat{H}] = 0$ same idea

Commutator. $[A, B] = 0$ iff simultaneous diagonalizable (i.e. A, B have common eig. func.)

$$[AB, C] = A[B, C] + [A, C]B$$

$$[A, BC] = [A, C]B + C[A, B] \quad (A, B)C + B[A, C]$$

measurement of A won't disturb B .

Dirac Notation

$|S\rangle$ vector

$$|S\rangle = \sum_i C_i |x_i\rangle \quad \text{basis}$$

$$C_i = \langle x_i | S \rangle = \psi(x_i, t)$$

ex $\psi(x,t) = \langle x | S \rangle$

$$\Phi(p,t) = \langle p | S \rangle$$

$$C_n(t) = \langle n | S \rangle$$

n - n^{th} eig. state of \hat{H}

Wave func. is coeff in expansion of $|S\rangle$ there is in basis of position eig. func.

$$\psi(x,t) = \int \psi(y,t) \delta(x-y) dy = \int \Phi(p,t) \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}} dp = \sum_n C_n e^{-\frac{iE_n t}{\hbar}} \psi_n(x)$$

(seeing thing in different coordinates!)

bra, ket, transformation

$$Q_{mn} = \langle e_m | \hat{Q} | e_n \rangle$$

from $|S\rangle = \hat{Q} |\alpha\rangle$ i.e. write $|\alpha\rangle = \sum a_n |e_n\rangle$

bra $\langle \alpha |$ func. space

$$\langle f | = \int f^*(x) dx$$

shouldn't it more appropriate to define $\langle f | = f^*(x)$ if $|S\rangle = f(x)$

finite space

$$\langle \alpha | = (a_1^*, a_2^*, \dots, a_n^*)$$

dual space of ket

$$\text{ket } |\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

Projection Operator (outer product)

$$\hat{P} \equiv |\alpha\rangle \langle \alpha| \Rightarrow \hat{P} |\beta\rangle = \langle \alpha | \beta \rangle |\alpha\rangle$$

$$\sum_n |e_n\rangle \langle e_n| = I, \quad \langle e_n | e_m \rangle = \delta_{nm}$$

Continuous space

$$\langle e_z | e_{\tilde{z}} \rangle = \delta(z - \tilde{z}) \quad \& \quad \int |e_z\rangle \langle e_z| dz = I$$

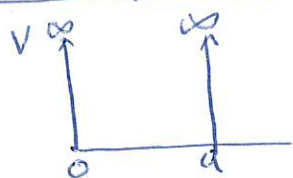
Sol Schrödinger Eq for Special V(x) by sep. var. $\Psi(x,t) = \psi(x)\phi(t) \Rightarrow$ stationary state Δ delta

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

$$\psi_n(t) = e^{-iE_n t/\hbar}$$

$$(\hat{p} + V(x))\psi = E\psi \Rightarrow E_n$$

1 Infinite Square Well



like standing wave

$$E = \frac{p^2}{2m} \quad p = \frac{2\pi\hbar}{\lambda} \quad \lambda = \frac{2a}{n}$$

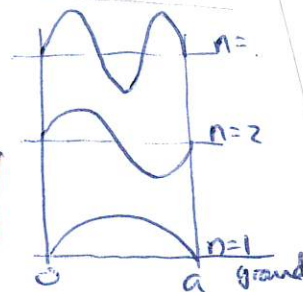
$$E_n = \frac{\hbar^2 k_n^2}{2m} \quad k_n = \frac{n\pi}{a}$$

Solve,

$$\psi'' = -k^2\psi \quad k = \frac{\sqrt{2mE}}{\hbar}$$

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

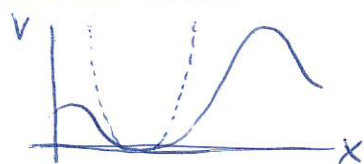
$n=1, 2, 3, \dots$



Lead to Fourier Series

$$\psi(x,t) = \sum_{n=1}^{\infty} C_n \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad w/ \quad \int_0^a \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{m\pi x}{a}\right) dx = \delta_{mn}$$

2 Harmonic Oscillator



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

rewrite H

$$\frac{1}{2m} [p^2 + (m\omega x)^2] \psi = E\psi$$

raising/lowering operator

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

$$a_+ \psi_n = \sqrt{n+1} \psi_{n+1}$$

$$a_- \psi_n = \sqrt{n} \psi_{n-1}$$

$$H(a_{\pm} \psi) = (E \pm \hbar\omega)(a_{\pm} \psi)$$

$$[x, p] = i\hbar$$

$$[a_-, a_+] = 1$$

$$H = \hbar\omega (a_+ a_- + \frac{1}{2})$$

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

$$E_0 = \frac{\hbar\omega}{2}$$

$$a_- \psi_0 = 0$$

also

$$a_+ |n\rangle = \sqrt{n+1} |n+1\rangle$$

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

$$x = \frac{\hbar}{\sqrt{2m\omega}} (a_+ + a_-)$$

$$p = i\sqrt{\frac{\hbar m\omega}{2}} (a_+ - a_-)$$

useful!!

$$\psi_n \sim H_n(x) e^{-\frac{V(x)}{\hbar\omega}} = H_n(x) e^{-\frac{m\omega x^2}{2\hbar}}$$

Hermite Poly. $\frac{1}{2} \hbar\omega$

3 Free Particle ($V=0$) Solve $\psi'' = -k^2\psi$

Wave packet (represent true particle)

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \frac{\hbar k^2}{2m} t)} dk$$

$$i.e. \quad \psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk$$

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

$k > 0$ wave move right
 $k < 0$ wave move left

$$V_g = V_{class} = 2V_p = \frac{2E}{m}$$

$$v_p = \frac{\omega}{k}$$

$$v_g = \frac{d\omega}{dk}$$

$$\frac{1}{2} m v^2 = E$$

$$\text{Quick solve.} \quad -\frac{i\hbar \partial}{\partial t} \psi = E \psi \quad V_p = \frac{E_n}{\hbar k} = \frac{E}{2m}$$

Fourier Transform

$$\text{IFT: } f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{ikx} dk$$

$$\text{FT: } f(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

why e^{ikx} ?

$$\psi'' = -k^2\psi \Rightarrow \psi(x) = e^{ikx}$$

Dirac notation

$$f(k) = \langle p | f \rangle \quad \text{given}$$

$$\langle p | \sim e^{-ikx}$$

$$f(x) = \langle x | f \rangle$$

$$\langle x | \sim e^{ikx}$$

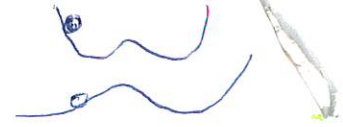
$$p = \hbar k$$

$$E = \hbar\omega$$

$$\Rightarrow \omega(k) = \frac{\hbar k^2}{2m}$$

dispersion relation

atunc. Potential: Def Bound State $E < V(\infty)$ and $V(\infty)$
 Scattering State $E > V(\infty)$ or $V(\infty)$



$V(x) = -\alpha \delta(x)$ $\alpha > 0$

$\therefore E < 0$

Bound ($E < 0$)

Solve $\psi'' = k^2 \psi$

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

$E = -\frac{\hbar^2 k^2}{2m}$ (unknown)

dimensional analysis

$E \propto \frac{m}{2} \hbar^2 \alpha^2 \Rightarrow E = -\frac{m\alpha^2}{2\hbar^2}$ solve k

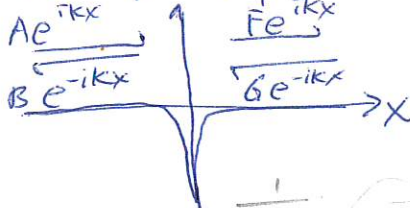
factor $\frac{1}{2}$

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

delta func only has 1 bound state !!

Scattering ($E > 0$)

Solve $\psi'' = -k^2 \psi$ $k = \frac{\sqrt{2mE}}{\hbar}$



Assume incident from left

A incident

B reflection

F transmission

$G = 0$

Probability

$R = \frac{|B|^2}{|A|^2} = \frac{1}{1 + \left(\frac{2\hbar^2 E}{m\alpha^2}\right)}$

$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \left(\frac{m\alpha^2}{2\hbar^2 E}\right)}$

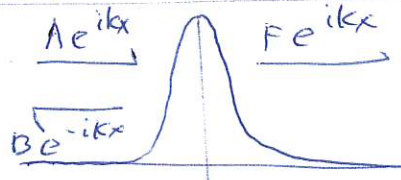
$T + R = 1$

def. $|E_0| = \frac{m\alpha^2}{2\hbar^2}$

Delta Barrier $\alpha < 0$

No bound state

Scattering $0 < E < V_{max}$



everything the same except now with tunneling effect

$T = \frac{1}{1 + \left(\frac{m\alpha^2}{2\hbar^2 E}\right)}$

⑤ Finite square well Gives continuity of $\frac{d\psi}{dx}$ except at jump.

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

Bound ($E < 0$)

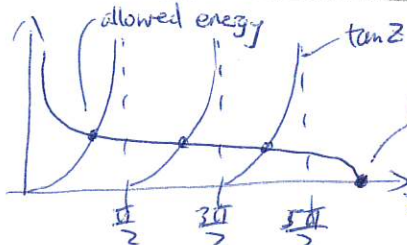
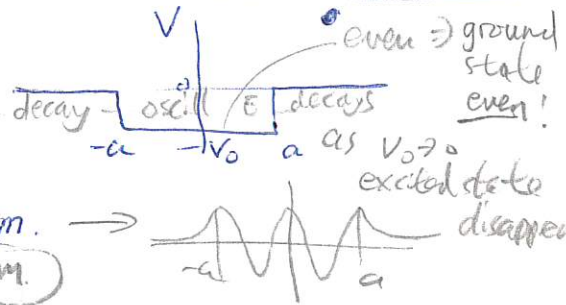
no oscillation

$\psi'' = k^2 \psi$

$-\frac{\hbar^2}{2m} \psi'' = (E + V_0) \psi$

Solve by transcendental eqn.

$a \frac{\sqrt{2mV_0}}{\hbar}$ like k



$z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$

size of well determine # of bound state

$z_0 \ll 1$ will always has 1 ground/bound state

$z_0 \rightarrow \infty$ becomes infinite well bound

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

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

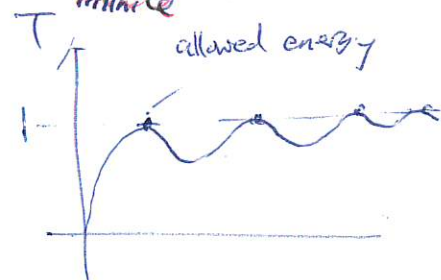
Scattering $E > 0$

$T^{-1} \propto 1 + \sin^2(x)$

Energy of Perfect transmission $T=1$, $x = n\pi$

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

$V_0 = 0$ infinite well



3D Schrödinger

Ang

$$\vec{p} = \frac{\hbar}{i} \nabla \quad p^2 = p_x^2 + p_y^2 + p_z^2 \quad [x_j, p_k] = i\hbar \delta_{jk} \quad \Delta x_i \Delta p_i \geq \frac{\hbar}{2}$$

Sep. var. $\psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$ Normalization: $\int_0^\infty |R|^2 r^2 dr = 1 \quad \int |Y|^2 d\Omega = 1$

Angular eqn: Spherical harmonic soln. (part due to spherical symmetric potential $V(r) = V(r)$)

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

orthonormality: $\int_0^{2\pi} \int_0^\pi Y_l^m(\theta, \phi) Y_l^m(\theta, \phi) d\Omega = \delta_{ll} \delta_{mm}$

reflection sym. l - azimuthal quantum # $l = 0, 1, 2, \dots$
 m - magnetic quantum # $m = -l, -l+1, \dots, 0, \dots, l-1, l$

Legendre Polynomials: $P_l(x) = \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2-1)^l$
 $P_0(x) = 1$
 $P_1(x) = x$
 $P_2(x) = \frac{1}{2}(3x^2-1)$
 $P_3(x) = \frac{1}{4}(5x^3-3x)$
 $P_4(x) = \frac{1}{8}(35x^4-30x^2+3)$
 $P_5(x) = \frac{1}{8}(63x^5-70x^3+15x)$
 $P_6(x) = \frac{1}{16}(231x^6-315x^4+105x^2-5)$
 $P_7(x) = \frac{1}{16}(429x^7-693x^5+315x^3-63x)$
 $P_8(x) = \frac{1}{128}(6435x^8-14620x^6+9009x^4-2728x^2+253)$
 $P_9(x) = \frac{1}{128}(12870x^9-35277x^7+31528x^5-12012x^3+143x)$
 $P_{10}(x) = \frac{1}{2048}(17325x^{10}-55460x^8+54286x^6-26520x^4+5412x^2-231)$
 $P_{11}(x) = \frac{1}{2048}(35277x^{11}-14620x^9+14620x^7-6930x^5+1287x^3-66x)$
 $P_{12}(x) = \frac{1}{16384}(48525x^{12}-17325x^{10}+17325x^8-6930x^6+1287x^4-66x^2+11)$
 $P_{13}(x) = \frac{1}{16384}(104253x^{13}-48525x^{11}+48525x^9-17325x^7+35277x^5-14620x^3+143x)$
 $P_{14}(x) = \frac{1}{16384}(208395x^{14}-104253x^{12}+104253x^{10}-48525x^8+9009x^6-12012x^4+5412x^2-231)$
 $P_{15}(x) = \frac{1}{16384}(401775x^{15}-208395x^{13}+208395x^{11}-104253x^9+17325x^7-35277x^5+14620x^3-143x)$
 $P_{16}(x) = \frac{1}{131072}(643500x^{16}-401775x^{14}+401775x^{12}-208395x^{10}+48525x^8-9009x^6+12012x^4-5412x^2+231)$
 $P_{17}(x) = \frac{1}{131072}(1287000x^{17}-643500x^{15}+643500x^{13}-35277x^{11}+9009x^9-12012x^7+5412x^5-1287x^3+66x)$
 $P_{18}(x) = \frac{1}{131072}(2431005x^{18}-1287000x^{16}+1287000x^{14}-643500x^{12}+12012x^{10}-35277x^8+14620x^6-143x^4+11x^2-1)$
 $P_{19}(x) = \frac{1}{131072}(4852500x^{19}-2431005x^{17}+2431005x^{15}-1287000x^{13}+208395x^{11}-48525x^9+9009x^7-12012x^5+5412x^3-1287x)$
 $P_{20}(x) = \frac{1}{131072}(9009000x^{20}-4852500x^{18}+4852500x^{16}-2431005x^{14}+401775x^{12}-9009x^{10}+12012x^8-5412x^6+1287x^4-66x^2+1)$
 $P_{21}(x) = \frac{1}{131072}(17325000x^{21}-9009000x^{19}+9009000x^{17}-4852500x^{15}+900900x^{13}-12012x^{11}+35277x^9-14620x^7+143x^5-11x^3+1)$
 $P_{22}(x) = \frac{1}{131072}(33264000x^{22}-17325000x^{20}+17325000x^{18}-9009000x^{16}+1201200x^{14}-352770x^{12}+90090x^{10}-12012x^8+5412x^6-1287x^4+66x^2-1)$
 $P_{23}(x) = \frac{1}{131072}(63523200x^{23}-33264000x^{21}+33264000x^{19}-17325000x^{17}+2083950x^{15}-485250x^{13}+120120x^{11}-352770x^9+146200x^7-14300x^5+1100x^3-1)$
 $P_{24}(x) = \frac{1}{131072}(120120000x^{24}-63523200x^{22}+63523200x^{20}-33264000x^{18}+4017750x^{16}-900900x^{14}+120120x^{12}-352770x^{10}+90090x^8-12012x^6+5412x^4-1287x^2+1)$
 $P_{25}(x) = \frac{1}{131072}(231000000x^{25}-120120000x^{23}+120120000x^{21}-63523200x^{19}+7590000x^{17}-1201200x^{15}+352770x^{13}-90090x^{11}+12012x^9-5412x^7+1287x^5-66x^3+1)$
 $P_{26}(x) = \frac{1}{131072}(435456000x^{26}-231000000x^{24}+231000000x^{22}-120120000x^{20}+14620000x^{18}-2083950x^{16}+485250x^{14}-120120x^{12}+352770x^{10}-90090x^8+12012x^6-5412x^4+1287x^2-1)$
 $P_{27}(x) = \frac{1}{131072}(835200000x^{27}-435456000x^{25}+435456000x^{23}-231000000x^{21}+27900000x^{19}-4017750x^{17}+900900x^{15}-120120x^{13}+352770x^{11}-90090x^9+12012x^7-5412x^5+1287x^3-66x)$
 $P_{28}(x) = \frac{1}{131072}(1581312000x^{28}-835200000x^{26}+835200000x^{24}-435456000x^{22}+52700000x^{20}-7590000x^{18}+1201200x^{16}-2083950x^{14}+485250x^{12}-120120x^{10}+352770x^8-90090x^6+12012x^4-5412x^2+1)$
 $P_{29}(x) = \frac{1}{131072}(3003000000x^{29}-1581312000x^{27}+1581312000x^{25}-835200000x^{23}+100000000x^{21}-14620000x^{19}+2083950x^{17}-485250x^{15}+120120x^{13}-352770x^{11}+90090x^9-12012x^7+5412x^5-1287x^3+66x)$
 $P_{30}(x) = \frac{1}{131072}(5643000000x^{30}-3003000000x^{28}+3003000000x^{26}-1581312000x^{24}+187000000x^{22}-27900000x^{20}+4017750x^{18}-900900x^{16}+120120x^{14}-352770x^{12}+90090x^{10}-12012x^8+5412x^6-1287x^4+66x^2-1)$
 $P_{31}(x) = \frac{1}{131072}(10665600000x^{31}-5643000000x^{29}+5643000000x^{27}-3003000000x^{25}+369000000x^{23}-52700000x^{21}+7590000x^{19}-1201200x^{17}+2083950x^{15}-485250x^{13}+120120x^{11}-352770x^9+90090x^7-12012x^5+5412x^3-1287x)$
 $P_{32}(x) = \frac{1}{131072}(20160000000x^{32}-10665600000x^{30}+10665600000x^{28}-5643000000x^{26}+690000000x^{24}-100000000x^{22}+14620000x^{20}-2083950x^{18}+485250x^{16}-120120x^{14}+352770x^{12}-90090x^{10}+12012x^8-5412x^6+1287x^4-66x^2+1)$
 $P_{33}(x) = \frac{1}{131072}(38016000000x^{33}-20160000000x^{31}+20160000000x^{29}-10665600000x^{27}+1290000000x^{25}-187000000x^{23}+27900000x^{21}-4017750x^{19}+900900x^{17}-120120x^{15}+352770x^{13}-90090x^{11}+12012x^9-5412x^7+1287x^5-66x^3+66x)$
 $P_{34}(x) = \frac{1}{131072}(70560000000x^{34}-38016000000x^{32}+38016000000x^{30}-20160000000x^{28}+2430000000x^{26}-369000000x^{24}+52700000x^{22}-7590000x^{20}+1201200x^{18}-2083950x^{16}+485250x^{14}-120120x^{12}+352770x^{10}-90090x^8+12012x^6-5412x^4+1287x^2-1)$
 $P_{35}(x) = \frac{1}{131072}(132096000000x^{35}-70560000000x^{33}+70560000000x^{31}-38016000000x^{29}+4590000000x^{27}-690000000x^{25}+100000000x^{23}-14620000x^{21}+2083950x^{19}-485250x^{17}+120120x^{15}-352770x^{13}+90090x^{11}-12012x^9+5412x^7-1287x^5+66x^3-66x)$
 $P_{36}(x) = \frac{1}{131072}(246960000000x^{36}-132096000000x^{34}+132096000000x^{32}-70560000000x^{30}+5670000000x^{28}-835200000x^{26}+120120000x^{24}-18700000x^{22}+2790000x^{20}-4017750x^{18}+900900x^{16}-120120x^{14}+352770x^{12}-90090x^{10}+12012x^8-5412x^6+1287x^4-66x^2+66x)$
 $P_{37}(x) = \frac{1}{131072}(462000000000x^{37}-246960000000x^{35}+246960000000x^{33}-132096000000x^{31}+16380000000x^{29}-2430000000x^{27}+369000000x^{25}-52700000x^{23}+7590000x^{21}-1201200x^{19}+2083950x^{17}-485250x^{15}+120120x^{13}-352770x^{11}+90090x^9-12012x^7+5412x^5-1287x^3+66x)$
 $P_{38}(x) = \frac{1}{131072}(864000000000x^{38}-462000000000x^{36}+462000000000x^{34}-246960000000x^{32}+29160000000x^{30}-4354560000x^{28}+643500000x^{26}-900900x^{24}+120120x^{22}-1870000x^{20}+2790000x^{18}-4017750x^{16}+900900x^{14}-120120x^{12}+352770x^{10}-90090x^8+12012x^6-5412x^4+1287x^2-1287x)$
 $P_{39}(x) = \frac{1}{131072}(1612800000000x^{39}-864000000000x^{37}+864000000000x^{35}-462000000000x^{33}+56160000000x^{31}-8352000000x^{29}+120120000x^{27}-1870000x^{25}+2790000x^{23}-4017750x^{21}+900900x^{19}-120120x^{17}+352770x^{15}-90090x^{13}+12012x^{11}-5412x^9+1287x^7-1287x^5+66x^3-66x)$
 $P_{40}(x) = \frac{1}{131072}(3024000000000x^{40}-1612800000000x^{38}+1612800000000x^{36}-864000000000x^{34}+103680000000x^{32}-15813120000x^{30}+2310000000x^{28}-332640000x^{26}+485250x^{24}-643500x^{22}+900900x^{20}-120120x^{18}+1870000x^{16}-2790000x^{14}+4017750x^{12}-900900x^{10}+120120x^8-5412x^6+1287x^4-1287x^2+1287x)$
 $P_{41}(x) = \frac{1}{131072}(5644800000000x^{41}-3024000000000x^{39}+3024000000000x^{37}-1612800000000x^{35}+196560000000x^{33}-29160000000x^{31}+4354560000x^{29}-643500000x^{27}+900900x^{25}-120120x^{23}+1870000x^{21}-2790000x^{19}+4017750x^{17}-900900x^{15}+120120x^{13}-352770x^{11}+90090x^9-12012x^7+5412x^5-1287x^3+1287x)$
 $P_{42}(x) = \frac{1}{131072}(10560000000000x^{42}-5644800000000x^{40}+5644800000000x^{38}-3024000000000x^{36}+362880000000x^{34}-54288000000x^{32}+8073600000x^{30}-1197000000x^{28}+1732500x^{26}-2310000x^{24}+3326400x^{22}-485250x^{20}+643500x^{18}-900900x^{16}+120120x^{14}-1870000x^{12}+2790000x^{10}-4017750x^8+900900x^6-120120x^4+1287x^2-1287x)$
 $P_{43}(x) = \frac{1}{131072}(19968000000000x^{43}-10560000000000x^{41}+10560000000000x^{39}-5644800000000x^{37}+684000000000x^{35}-100800000000x^{33}+15120000000x^{31}-2277000000x^{29}+3326400x^{27}-4354560x^{25}+643500x^{23}-900900x^{21}+120120x^{19}-1870000x^{17}+2790000x^{15}-4017750x^{13}+900900x^{11}-120120x^9+5412x^7-1287x^5+1287x^3-1287x)$
 $P_{44}(x) = \frac{1}{131072}(37824000000000x^{44}-19968000000000x^{42}+19968000000000x^{40}-10560000000000x^{38}+1296000000000x^{36}-196560000000x^{34}-29160000000x^{32}+4354560000x^{30}-643500000x^{28}+900900x^{26}-120120x^{24}+1870000x^{22}-2790000x^{20}+4017750x^{18}-900900x^{16}+120120x^{14}-1870000x^{12}+2790000x^{10}-4017750x^8+900900x^6-120120x^4+1287x^2-1287x)$
 $P_{45}(x) = \frac{1}{131072}(71424000000000x^{45}-37824000000000x^{43}+37824000000000x^{41}-19968000000000x^{39}+2430000000000x^{37}-369000000000x^{35}-54288000000x^{33}+8073600000x^{31}-1197000000x^{29}+1732500x^{27}-2310000x^{25}+3326400x^{23}-485250x^{21}+643500x^{19}-900900x^{17}+120120x^{15}-1870000x^{13}+2790000x^{11}-4017750x^9+900900x^7-120120x^5+5412x^3-1287x)$
 $P_{46}(x) = \frac{1}{131072}(134400000000000x^{46}-71424000000000x^{44}+71424000000000x^{42}-37824000000000x^{40}+4536000000000x^{38}-684000000000x^{36}-100800000000x^{34}+15120000000x^{32}-2277000000x^{30}+3326400x^{28}-4354560x^{26}+643500x^{24}-900900x^{22}+120120x^{20}-1870000x^{18}+2790000x^{16}-4017750x^{14}+900900x^{12}-120120x^{10}+5412x^8-1287x^6+1287x^4-1287x^2+1287x)$
 $P_{47}(x) = \frac{1}{131072}(255360000000000x^{47}-134400000000000x^{45}+134400000000000x^{43}-71424000000000x^{41}+8712000000000x^{39}-1312200000000x^{37}-196560000000x^{35}+29160000000x^{33}-4354560000x^{31}+643500x^{29}-900900x^{27}+120120x^{25}-1870000x^{23}+2790000x^{21}-4017750x^{19}+900900x^{17}-120120x^{15}+1870000x^{13}-2790000x^{11}+4017750x^9-900900x^7+120120x^5-5412x^3+1287x^2-1287x)$
 $P_{48}(x) = \frac{1}{131072}(483840000000000x^{48}-255360000000000x^{46}+255360000000000x^{44}-134400000000000x^{42}+17280000000000x^{40}-2613600000000x^{38}-398160000000x^{36}-58752000000x^{34}+8640000000x^{32}-1296000000x^{30}+1732500x^{28}-2310000x^{26}+3326400x^{24}-485250x^{22}+643500x^{20}-900900x^{18}+120120x^{16}-1870000x^{14}+2790000x^{12}-4017750x^{10}+900900x^8-120120x^6+5412x^4-1287x^2+1287x)$
 $P_{49}(x) = \frac{1}{131072}(912960000000000x^{49}-483840000000000x^{47}+483840000000000x^{45}-255360000000000x^{43}+30240000000000x^{41}-4536000000000x^{39}-684000000000x^{37}-100800000000x^{35}+15120000000x^{33}-2277000000x^{31}+3326400x^{29}-4354560x^{27}+643500x^{25}-900900x^{23}+120120x^{21}-1870000x^{19}+2790000x^{17}-4017750x^{15}+900900x^{13}-120120x^{11}+5412x^9-1287x^7+1287x^5-1287x^3+1287x^2-1287x)$
 $P_{50}(x) = \frac{1}{131072}(1728000000000000x^{50}-912960000000000x^{48}+912960000000000x^{46}-483840000000000x^{44}+58320000000000x^{42}-8712000000000x^{40}-1312200000000x^{38}-196560000000x^{36}-29160000000x^{34}+4354560000x^{32}-643500x^{30}+900900x^{28}-120120x^{26}+1870000x^{24}-2790000x^{22}+4017750x^{20}-900900x^{18}+120120x^{16}-1870000x^{14}+2790000x^{12}-4017750x^{10}+900900x^8-120120x^6+5412x^4-1287x^2+1287x)$
 $P_{51}(x) = \frac{1}{131072}(3264000000000000x^{51}-1728000000000000x^{49}+1728000000000000x^{47}-912960000000000x^{45}+70560000000000x^{43}-10665600000000x^{41}-1581312000000x^{39}-231000000000x^{37}-3326400x^{35}+485250x^{33}-643500x^{31}+900900x^{29}-120120x^{27}+1870000x^{25}-2790000x^{23}+4017750x^{21}-900900x^{19}+120120x^{17}-1870000x^{15}+2790000x^{13}-4017750x^{11}+900900x^9-120120x^7+5412x^5-1287x^3+1287x^2-1287x)$
 $P_{52}(x) = \frac{1}{131072}(6182400000000000x^{52}-3264000000000000x^{50}+3264000000000000x^{48}-1728000000000000x^{46}+212400000000000x^{44}-32640000000000x^{42}-485250x^{40}-714240000000x^{38}-106656000000x^{36}-158131200000x^{34}+2310000x^{32}-3326400x^{30}+485250x^{28}-643500x^{26}+900900x^{24}-120120x^{22}+1870000x^{20}-2790000x^{18}+4017750x^{16}-900900x^{14}+120120x^{12}-1870000x^{10}+2790000x^8-4017750x^6+900900x^4-120120x^2+1287x)$
 $P_{53}(x) = \frac{1}{131072}(11776000000000000x^{53}-6182400000000000x^{51}+6182400000000000x^{49}-3264000000000000x^{47}+378240000000000x^{45}-56448000000000x^{43}-8352000000000x^{41}-120120x^{39}-1870000x^{37}-2790000x^{35}+4017750x^{33}-900900x^{31}+120120x^{29}-1870000x^{27}+2790000x^{25}-4017750x^{23}+900900x^{21}-120120x^{19}+1870000x^{17}-2790000x^{15}+4017750x^{13}-900900x^{11}+120120x^9-5412x^7+1287x^5-1287x^3+1287x^2-1287x)$
 $P_{54}(x) = \frac{1}{131072}(22464000000000000x^{54}-11776000000000000x^{52}+11776000000000000x^{50}-6182400000000000x^{48}+453600000000000x^{46}-68400000000000x^{44}-10080000000000x^{42}-1512000000000x^{40}+2277000000x^{38}-3326400x^{36}+485250x^{34}-643500x^{32}+900900x^{30}-120120x^{28}+1870000x^{26}-2790000x^{24}+4017750x^{22}-900900x^{20}+120120x^{18}-1870000x^{16}+2790000x^{14}-4017750x^{12}+900900x^{10}-120120x^8+5412x^6-1287x^4+1287x^2-1287x)$
 $P_{55}(x) = \frac{1}{131072}(42816000000000000x^{55}-22464000000000000x^{53}+22464000000000000x^{51}-11776000000000000x^{49}+1396800000000000x^{47}-212400000000000x^{45}-32640000000000x^{43}-485250x^{41}-714240000000x^{39}-106656000000x^{37}-158131200000x^{35}+2310000x^{33}-3326400x^{31}+485250x^{29}-643500x^{27}+900900x^{25}-120120x^{23}+1870000x^{21}-2790000x^{19}+4017750x^{17}-900900x^{15}+120120x^{13}-1870000x^{11}+2790000x^9-4017750x^7+900900x^5-120120x^3+5412x-1287x)$
 $P_{56}(x) = \frac{1}{131072}(81216000000000000x^{56}-42816000000000000x^{54}+42816000000000000x^{52}-22464000000000000x^{50}+2721600000000000x^{48}-4017750x^{46}-5875200000000x^{44}-864000000000x^{42}-1296000000x^{40}+1732500x^{38}-2310000x^{36}+3326400x^{34}-485250x^{32}+643500x^{30}-900900x^{28}+120120x^{26}-1870000x^{24}+2790000x^{22}-4017750x^{20}+900900x^{18}-120120x^{16}+1870000x^{14}-2790000x^{12}+4017750x^{10}-900900x^8+120120x^6-5412x^4+1287x^2-1287x)$
 $P_{57}(x) = \frac{1}{131072}(154896000000000000x^{57}-8121600000000$

Orbital Angular Momentum

$$\vec{L} = \vec{r} \times \vec{p} \quad (\text{ie } L_x = y p_z - z p_y)$$

$$\text{uncertainty: } \Delta L_x \Delta L_y \geq \frac{\hbar}{2} |\langle L_z \rangle|$$

commutator (Right hand rule)

$$[L_x, L_y] = i\hbar L_z \quad ; \quad [L_y, L_z] = i\hbar L_x \quad ; \quad [L_z, L_x] = i\hbar L_y$$

Total angular momentum

$$L^2 = L_x^2 + L_y^2 + L_z^2 \quad , \quad [L^2, \vec{L}] = 0 \quad \text{commute}$$

Ladder operators

$$L_{\pm} = L_x \pm iL_y$$

$$[L_z, L_{\pm}] = \pm \hbar L_{\pm} \quad , \quad [L^2, L_{\pm}] = 0$$

$$L^2(L_{\pm}f) = \lambda(L_{\pm}f) \quad (\lambda \text{ eigenval of } L^2)$$

$$L_z(L_{\pm}f) = (\mu \pm \hbar)(L_{\pm}f) \quad (\mu \text{ eigenval of } L_z)$$

$\lambda \geq \mu^2$ bounded by total λ .

$$L^2 Y_{\ell}^m = \ell(\ell+1)\hbar^2 Y_{\ell}^m \quad L_z Y_{\ell}^m = m\hbar Y_{\ell}^m$$

(Spherical harmonics are eig.func of L^2, L_z)

$m = -\ell, -\ell+1, \dots, 0, \ell-1, \ell$ in N steps.

so $\ell = \frac{N}{2}$ either integer or half integer

Notice that $\sqrt{\ell(\ell+1)} > \ell = m_{\text{max}}$ except for $\ell=0$

Spherical coordinates

$$\vec{L} = \frac{\hbar}{i} (\vec{r} \times \nabla) \quad \nabla = \hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi}$$

$$L_z = \frac{\hbar}{i} \left[\phi \frac{\partial}{\partial \theta} - \theta \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \quad L^2 = -\hbar^2 \nabla^2$$

Spin

commutator (Right hand rule)

$$[S_x, S_y] = i\hbar S_z \quad ; \quad [S_y, S_z] = i\hbar S_x \quad ; \quad [S_z, S_x] = i\hbar S_y$$

$$S^2 |s, m\rangle = s(s+1)\hbar^2 |s, m\rangle$$

$$S_z |s, m\rangle = m\hbar |s, m\rangle$$

raising & lowering operator

$$S_{\pm} = S_x \pm iS_y \quad \begin{cases} S_x = \frac{S_+ + S_-}{2} \\ S_y = \frac{S_+ - S_-}{2i} \end{cases}$$

$$S_{\pm} |s, m\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)} |s, m \pm 1\rangle$$

where $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots$

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

Spin $\frac{1}{2}$: State $|s, m\rangle$

Vector

spin up $|\frac{1}{2}, \frac{1}{2}\rangle$

\uparrow

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

spin down $|\frac{1}{2}, -\frac{1}{2}\rangle$

\downarrow

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

Matrix Representation

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

$$\vec{S}_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \vec{S}_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\vec{S}^2 = \frac{3}{4} \hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

$$\sigma^2 = \sigma^x^2 + \sigma^y^2 + \sigma^z^2 = 3I$$

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Eigenval.

$$S^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$$

$$S_z |j, m\rangle = m\hbar |j, m\rangle$$

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

Here a single electron

$$s = \frac{1}{2} \Rightarrow m = \pm \frac{1}{2}$$

$$S_z |\frac{1}{2}, \frac{1}{2}\rangle = \frac{1}{2} \hbar |\frac{1}{2}, \frac{1}{2}\rangle$$

or \uparrow

$$S_+ |\frac{1}{2}, \frac{1}{2}\rangle = 0$$

$$S_+ |\frac{1}{2}, \frac{1}{2}\rangle = 0$$

$$S_+ |\frac{1}{2}, \frac{1}{2}\rangle = 0$$

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$$S_+ |\frac{1}{2}, \frac{1}{2}\rangle = 0$$

Spin Addition (Composite Spin)

Assume atom has two particles with spin $\frac{1}{2}$.

What is the total momentum of the atom? (i.e. m , the z-component)

$$(S_z^{(1)} \otimes S_z^{(2)})(\chi_1 \otimes \chi_2) = (S_z^{(1)}\chi_1) \otimes \chi_2 + \chi_1 \otimes (S_z^{(2)}\chi_2) = m_1\chi_1 \otimes \chi_2 + \chi_1 \otimes m_2\chi_2 = (m_1 + m_2)(\chi_1 \otimes \chi_2)$$

so m-component adds. And $S = S_1 + S_2$, $(S_1 + S_2 - 1), \dots, |S_1 - S_2|$

Possible combination of m :

m_1	m_2	arrow rep.	m
$\frac{1}{2}$	$\frac{1}{2}$	$\uparrow\uparrow$	1
$\frac{1}{2}$	$-\frac{1}{2}$	$\uparrow\downarrow$	0
$-\frac{1}{2}$	$\frac{1}{2}$	$\downarrow\uparrow$	0
$-\frac{1}{2}$	$-\frac{1}{2}$	$\downarrow\downarrow$	-1

notice that w/o $\uparrow\downarrow$
 $\uparrow\uparrow$ implies m_z component
 with $\uparrow\downarrow$ implies $|S, m\rangle$

we have extra $m=0$!

check.

$$S_-(\uparrow\uparrow) = (S_-^{(1)}\uparrow)\uparrow + \uparrow(S_-^{(2)}\uparrow) = \hbar(\downarrow\uparrow + \uparrow\downarrow)$$

make use of $S_{\pm}|S, m\rangle = \hbar\sqrt{S(S \pm 1) - m(m \pm 1)}|S, m \pm 1\rangle$ formula for computation.

and

$$S_-(\downarrow\uparrow + \uparrow\downarrow) = 2\hbar(\downarrow\downarrow)$$

thus for $S=1$ we have combination of the "triplet"

$$\begin{cases} |1, 1\rangle = \uparrow\uparrow \\ |1, 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ |1, -1\rangle = \downarrow\downarrow \end{cases}$$

For $S=0$ the combination of m_1, m_2 must be "0", so ~~ansatz~~

~~Ansatz~~

$$\text{Ansatz } |0, 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow) \quad \text{"singlet"}$$

Can check they are indeed eig. vector of S^2

Note that
$$S^2 = (S^{(1)} + S^{(2)}) \cdot (S^{(1)} + S^{(2)}) = (S^{(1)})^2 + (S^{(2)})^2 + 2S^{(1)} \cdot S^{(2)}$$

Ex Net angular momentum of hydrogen atom:

for Ψ_{nlm} , $\vec{J} = (\text{spin} + \text{orbital})$; $J = l + \frac{1}{2}$ or $l - \frac{1}{2}$

if throw in proton, total angular momentum ~~$J = J' + l$ or $J' - l$~~

$$J = J' + 1 \text{ or } J' - 1$$

Composite spin
of composite
particle

Mathematically, the combine state $|S m\rangle$

$$|S m\rangle = \sum_{m_1+m_2=m} \underbrace{C_{m_1 m_2 m}^{S_1 S_2 S}}_{\text{Clebsch-Gordan coefficients}} |S_1 m_1\rangle |S_2 m_2\rangle$$

can also reverse as

$$|S_1 m_1\rangle |S_2 m_2\rangle = \sum_S C_{m_1 m_2 m}^{S_1 S_2 S} |S m\rangle$$

Spin facts

S_x, S_y, S_z, S^2 Hermitian, S_{\pm} Not (nonobservable)

replace by App 1

Eigenspinor of S_z : $\chi_{\pm} \leftrightarrow \pm \frac{\hbar}{2}$; S_x 's equal $\pm \frac{\hbar}{2}$ (from matrix representation)

Adding Angular Momentum

Composite spin S_1, S_2 :
results from direct product

$$\begin{aligned} S &= (S_1 + S_2), \quad S_1 + S_2 - 1, \dots, |S_1 - S_2| \\ m &= m_1 + m_2, \quad m_1 = -S_1, -S_1 + 1, \dots, S_1 \end{aligned}$$

$m = -S + 1, \dots, S$

ex Net angular momentum: hydrogen atom (Spin + orbital) = $l + \frac{1}{2}$ or $l - \frac{1}{2}$
Add proton = $l + 1, l, l - 1$

arrows in z component

Two spin $\frac{1}{2}$ particles:

$$\begin{aligned} \uparrow\uparrow & (m_1 = \frac{1}{2}, m_2 = \frac{1}{2}) \\ \uparrow\downarrow & (m_1 = \frac{1}{2}, m_2 = -\frac{1}{2}) \\ \downarrow\uparrow & (m_1 = -\frac{1}{2}, m_2 = \frac{1}{2}) \\ \downarrow\downarrow & (m_1 = -\frac{1}{2}, m_2 = -\frac{1}{2}) \end{aligned}$$

$$\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)}$$

(i) acts on i^{th} particle only

ex $\uparrow\uparrow: m = 1 \Rightarrow \uparrow\uparrow = |1, 1\rangle$

$$S_1 S_2 = \frac{\hbar^2}{4}$$

$$|S_1 m_1\rangle |S_2 m_2\rangle$$

$$m_1 = \pm \frac{1}{2}, \quad m_2 = \pm \frac{1}{2}$$

possible $m = -1, 0, 1$

$$S_z(|\uparrow\uparrow\rangle) = \hbar(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle)$$

$$|S, m\rangle = |1, 1\rangle: m=1 \quad \frac{1}{2}\uparrow \frac{1}{2}\uparrow \Rightarrow \uparrow\uparrow$$

$$|1, 0\rangle: m=0 \quad \frac{1}{2}\uparrow \frac{1}{2}\downarrow \Rightarrow \uparrow\downarrow$$

$$|1, -1\rangle: m=-1 \quad \frac{1}{2}\downarrow \frac{1}{2}\downarrow \Rightarrow \downarrow\downarrow$$

$$S_{\pm} |S, m\rangle = \hbar \sqrt{S(S+1) - m(m\pm 1)} |S, m\pm 1\rangle$$

$$|1, 1\rangle: m=1 \quad \frac{1}{2}\uparrow \frac{1}{2}\downarrow \Rightarrow \uparrow\downarrow$$

$$|1, 0\rangle: m=0 \quad \frac{1}{2}\downarrow \frac{1}{2}\uparrow \Rightarrow \downarrow\uparrow$$

$$|1, -1\rangle: m=-1 \quad \frac{1}{2}\downarrow \frac{1}{2}\downarrow \Rightarrow \downarrow\downarrow$$

Given:

$$2S+1 = 3$$

Triplet

$$(S=1)$$

$$|1, 1\rangle = \uparrow\uparrow$$

$$|1, 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$$

$$|1, -1\rangle = \downarrow\downarrow$$

$$\text{Singlet } -2S+1 = 1$$

$$(S=0) \quad |0, 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$$

Application:

Electron in Magnetic field

Magnetic dipole $\vec{\mu}$, spinning charged particle $\vec{\mu} = \gamma \vec{S}$

Torque $\vec{\tau} = \vec{\mu} \times \vec{B}$, energy $H = -\vec{\mu} \cdot \vec{B} \Rightarrow$ Hamiltonian $H = -\gamma \vec{B} \cdot \vec{S}$

gyromagnetic ratio

$$\vec{B} = B_0 \hat{k} \quad \vec{H} = -\gamma B_0 \vec{S}_z = -\frac{\gamma B_0 \hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

electron spin $\frac{1}{2}$ at rest point in \vec{B} , the hamiltonian as above!

w/ energy $\frac{\partial E}{\partial B_0} = \frac{\gamma \hbar}{2} \leftrightarrow \lambda \pm \frac{\hbar}{2}$
time-independent
yield Larmor freq. γB_0

Stern-Gerlach Experiment: Electron deflected under inhomogeneous magnetic field shows existence of spin $\uparrow\downarrow$.

Details:

Under inhom B-field say

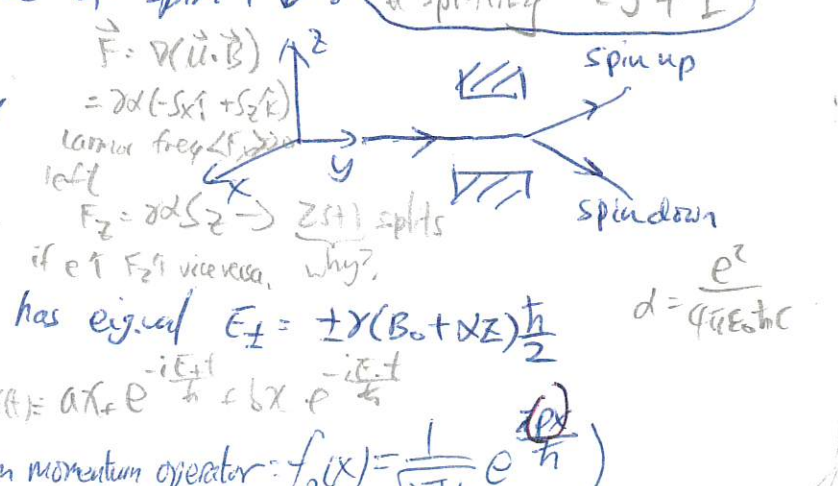
$$\vec{B}(x, y, z) = -\alpha x \hat{i} + (B_0 + \alpha z) \hat{k}$$

resulting Hamiltonian. $\langle H_x \rangle$ negligible due to Larmor freq.

$$H(t) = \begin{cases} 0 & t < 0 \text{ off} \\ -\gamma(B_0 + \alpha z) S_z & 0 < t < T \text{ on} \\ 0 & t > T \text{ off} \end{cases}$$

$$\text{acts on } \chi(t) = a \chi_+ + b \chi_- \quad (t \leq 0) \rightarrow (t > 0) \quad \chi(t) = a \chi_+ e^{-iE_+ t/\hbar} + b \chi_- e^{-iE_- t/\hbar}$$

$$\text{yields momentum } p_z = \pm \frac{\hbar}{2} \gamma \alpha T$$



$$\text{has eigval } E_{\pm} = \pm \gamma(B_0 + \alpha z) \frac{\hbar}{2}$$

$$\text{From momentum operator: } p_z(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\pm i p_z x/\hbar}$$

Two Particle system

State of 2 particles: $\psi(\vec{r}_1, \vec{r}_2, t)$

In Schrödinger eqn: $H = -\frac{\hbar^2}{2m_1} \nabla_1^2 - \frac{\hbar^2}{2m_2} \nabla_2^2 + V(\vec{r}_1, \vec{r}_2, t)$

using reduced mass, center of mass R, relative motion:

$$-\frac{\hbar^2}{2(m_1+m_2)} \nabla_R^2 \psi - \frac{\hbar^2}{2\mu} \nabla_r^2 \psi + V(\vec{r}) \psi = E \psi$$

- Center of mass as free particle
- Reduced mass as single particle subject to V in rel. motion.

this explains reduced mass in hydrogenic atom

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$E = E_R + E_r$$

Boson & Fermions

distinct particles: $\psi(\vec{r}_1, \vec{r}_2) = \psi_a(\vec{r}_1) \psi_b(\vec{r}_2)$

Indistinguishable identical particles: (allow position exchange)

Exchange Operator w/ equal \pm
 $P \psi(\vec{r}_1, \vec{r}_2) = \psi(\vec{r}_2, \vec{r}_1)$
 $[P, H] = 0$

state of P_1 particle in state $\psi_b(\vec{r})$

$$\psi(\vec{r}_1, \vec{r}_2) = \pm \psi(\vec{r}_2, \vec{r}_1)$$

+ sym
- anti sym

linear comb:
Boson

$$\psi_+(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) + \psi_a(\vec{r}_2) \psi_b(\vec{r}_1))$$

Fermion

$$\psi_-(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_a(\vec{r}_1) \psi_b(\vec{r}_2) - \psi_a(\vec{r}_2) \psi_b(\vec{r}_1))$$

$\frac{1}{\sqrt{2}}$ for orthonormal ψ_a, ψ_b
 (or more accurately symmetric \Rightarrow attraction)

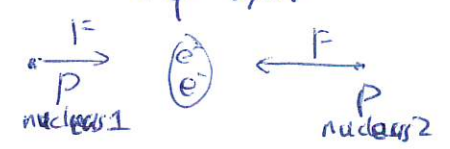
Distance separation shows: $\langle \Delta x^2 \rangle_{\pm} = \langle \Delta x^2 \rangle_{\text{distinct}} \mp 2|\langle x \rangle_{ab}|^2$

Boson attraction integer spin
Fermion repulsion half-spin

App. (Explain Covalent bond) Add spin!

Fermion \Rightarrow antisym $\psi = \psi(\vec{r}) \chi(\vec{s})$ @ ground state

ex $\psi(x_1, x_2, x_3) = \psi(x_1, x_3, x_2)$ sym under permutation
Boson



$\psi(x_1, x_2, x_3) = \sum_{ijk} \psi(x_i, x_j, x_k)$
Fermion

Fermion ψ show Pauli principle.

two identical fermion cannot occupy same state
else $\psi = 0$ has no wavefunction.

so $\psi = \psi(\vec{r}) \chi(\vec{s})$ ground state singlet $\rightarrow \psi(\vec{r})$ sym.

we have covalent bond!
 $\chi(\vec{s})$ tells us covalent bond requires electrons to occupy the singlet state w/ total spin $\hat{S}^2 = 0$.

ex CO_2
 $(1s)^2 (2s)^2 (2p)^2$ 8 electron state core 4-filled
 $(1s)^2 (2s)^2 (2p)^4$ 8 core 6 filled need 2 more

