QUANTUM MECHANICS - I

M1 - March 27
M2 - May 8

HYDROGEN ATOM

$i\hbar \frac{\partial \psi}{\partial t} = H\psi$, $H = \frac{1}{2m}(P_x^2 + P_y^2 + P_z^2) + V$

$P_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i}$, $i = 1,2,3.$ $\Rightarrow$ $\boxed{\vec{P} = \frac{\hbar}{i}\vec{\nabla}}$

- $i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$

  ↳ $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ → If you can find $\psi(x,y,z)$, you can find $|\psi(x,y,z)|^2$, $\int |\psi(x,y,z)|^2 d^3r = 1$. particle.

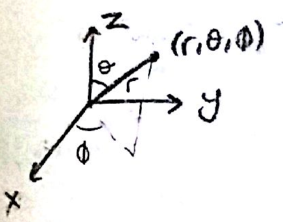
- Time dependent form of the stationary states: $\psi_n(\vec{r},t) = \psi_n(\vec{r})e^{-iE_nt/\hbar}$
- Superposition: $\psi(\vec{r},t) = \sum c_n \psi_n(\vec{r})e^{-iE_nt/\hbar}$ where $|c_n|^2$ is the probability of finding the particle in n^{th} state.

- Schrödinger Equation in spherical coordinates

hit stationary states to T.D.S.E.

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right] + V\psi = E\psi.$$

Here, $\psi = \psi(r,\theta,\phi) = R(r)\cdot Y(\theta,\phi)$ ↗ plug it in.



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

↳ divide to YR, multiply w/ $-\frac{2mr^2}{\hbar^2}$

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

$\ell(\ell+1)$ → coming from series soln. ← $-\ell(\ell+1)$
(assume $R = \sum a_\ell r^\ell$)

↳ multiply everything w/ $\sin^2\theta$:

$$\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)\sin^2\theta\, Y . \longrightarrow \text{angular part.}$$

↳ one more separation of variables: $Y(\theta,\phi) = \Theta(\theta)\cdot\Phi(\phi)$ → plug it in, divide to $\Theta\Phi$

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

- $\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 \Rightarrow \frac{d^2\Phi}{d\phi^2} + m^2\Phi = 0$ → it is clear why we said $-m^2$.

  $\Phi(\phi) = e^{im\phi}$, $\Phi(\phi+2\pi) = \Phi(\phi)$ should be true.

  $\boxed{m = 0, \pm1, \pm2, \dots} \Longleftarrow e^{im(\phi+2\pi)} = e^{im\phi} \Rightarrow e^{im2\pi} = 1$

  Magnetic Quantum Number is quantized...

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

  ↳ This has the solution: $\Phi(\phi) = A\, P_\ell^m(\theta)$ → Associated Legendre F. (θ ← $\cos\theta$)

  (for the solution, check Grad. book: Jackson)

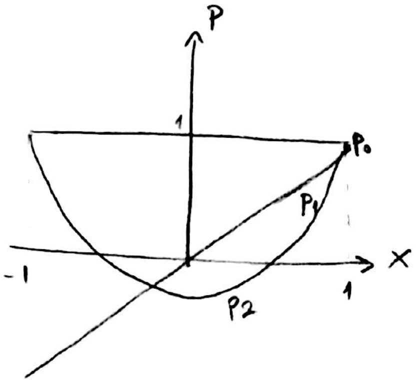
↳ $P_\ell^m(x) = (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|} \underbrace{P_\ell(x)}_{\ell^{th}\text{ Legendre Polynomial}}$ → notice $P_\ell^m = P_\ell^{-m}$

here, $-1 \le x = \cos\theta \le 1$.

$P_\ell(x) = \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell \Rightarrow P_0 = 1$ → constant

$P_1 = x$ → linear

$P_2 = \frac{1}{2}(3x^2-1)$ → quadratic

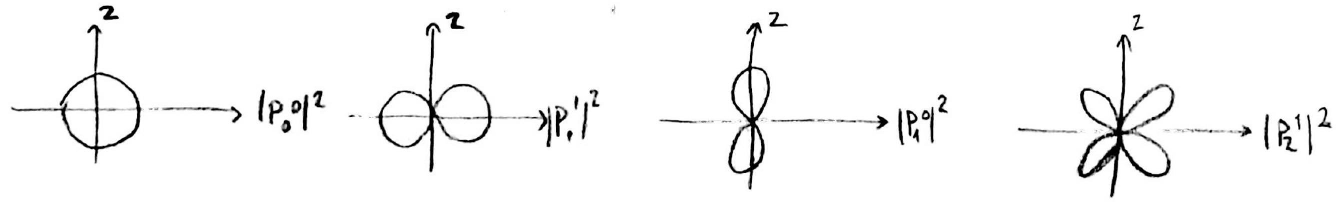


all Legendre Polynomials are mutually orthogonal in $[-1,1]$.

If $\underline{|m|>\ell}$, it is now obvious that $P_\ell^m(\theta) = 0$.

$P_0^0 = 1$ $\quad P_1^1 = \sin\theta$ $\quad P_2^1 = 3\sin\theta\cos\theta$

$P_1^0 = \cos\theta$ $\quad P_2^2 = 3\sin^2\theta$



(check Griffiths)

$\boxed{l = 0, 1, 2, 3, \ldots}$ and $\boxed{m = -l, \ldots, 0, \ldots, l}$

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

$\int |\psi(r,\theta,\phi)|^2 r^2 \sin\theta \, dr \, d\theta \, d\phi = 1$ is known. Use separation of variables,

$$\underbrace{\int |R(r)|^2 r^2 dr}_{1} \underbrace{\int |Y(\theta,\phi)|^2 \sin\theta \, d\theta \, d\phi}_{1} = 1 .$$

Then, $\boxed{\int_0^\infty |R(r)|^2 r^2 dr = 1}$, $\boxed{\int_0^{2\pi}\int_0^{\pi} |Y(\theta,\phi)|^2 \sin\theta \, d\theta \, d\phi = 1}$.

Spherical harmonics: $Y_l^m(\theta,\phi) = (-1)^m \sqrt{\dfrac{(2l+1)}{4\pi} \dfrac{(l-|m|)!}{(l+|m|)!}} \, e^{im\phi} \cdot P_l^m(\cos\theta)$.

This function is such that all Y_l^m are orthogonal to eachother.

$$\int_0^{2\pi}\int_0^{\pi} \left(Y_l^m(\theta,\phi)\right)^* \left(Y_{l'}^{m'}(\theta,\phi)\right) \sin\theta \, d\theta \, d\phi = \delta_{ll'} \delta_{mm'} .$$

l = azimuthal quantum number

m = magnetic quantum number → effect of it can be seen in a magnetic field.

$\boxed{Y_l^{-m} = (-1)^m (Y_l^m)^*}$

$$\int_{-1}^{1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{ll'} \quad (\text{when we choose } x = \cos\theta)$$

$\boxed{\text{HW}}$ 4.1.

The radial equation

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

→ let $u(r) = rR(r)$ OR $R = u/r$

Then, $\dfrac{dR}{dr} = \dfrac{1}{r}\dfrac{du}{dr} - \dfrac{1}{r^2}u = \dfrac{1}{r^2}\left(r\dfrac{du}{dr} - u\right)$ → multiply with r^2, insert

$$\rightarrow \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = \frac{d}{dr}\left(r\frac{du}{dr} - u\right) = \frac{du}{dr} + r\frac{d^2u}{dr^2} - \frac{du}{dr} = r\frac{d^2u}{dr^2}$$

$$\rightarrow r\frac{d^2u}{dr^2} - \frac{2mr^2}{\hbar^2}(V(r) - E)\frac{u}{r} = l(l+1)\frac{u}{r}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \underbrace{\left[V + \overbrace{\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}^{\text{centrifugal term}}\right]}_{\text{effective potential}} u = Eu$$

$\oint \int_0^\infty |u(r)|^2 dr = 1$ → due to centrifugal term, normalization changed.

ex Infinite spherical well → $V(r) = 0, \; r \leq a$
$V(r) \to \infty, \; r > a$

→ Outside the well, wave function is zero.

→ define $K = \frac{\sqrt{2mE}}{\hbar}$. Then, the radial equation becomes

$$\frac{d^2u}{dr^2} = \left[\frac{\ell(\ell+1)}{r^2} - k^2\right]u$$

Simplicity : $\ell = 0 \to m = 0$
boundary cond : $R(a) = 0$

given → $Y_{00} = \left(\frac{1}{4\pi}\right)^{1/2}$, $Y_{10} = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$, $Y_1^{\pm 1} = \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \, e^{\pm i\phi}$

Solution: $u(r) = A\sin(Kr) + B\cos(Kr)$

$$R(r) = A\frac{\sin(kr)}{r} + B\frac{\cos(kr)}{r}$$

blows when $r \to 0$. Then, $B = 0$.

$R(r) = A\frac{\sin(kr)}{r}$, $R(a) = 0 \Rightarrow 0 = \frac{A}{a}\sin(ka)$

$Ka = n\pi \Rightarrow \boxed{E_{n0} = \frac{n^2\pi^2\hbar^2}{2ma^2}}$

$\ell = 0$ $\quad n = 1, 2, \ldots$

→ Normalize : $\int_0^a |u(r)|^2 dr = 1$

$\int_0^a A^2 \sin^2(Kr) dr = 1 \Rightarrow A = \sqrt{2/a}$

$R(r) = \frac{\sqrt{2}}{a}\frac{\sin(kr)}{r}$

$$\boxed{\psi_{n00} = \sqrt{\frac{2}{a}}\frac{\sin(kr)}{r}\left(\frac{1}{4\pi}\right)^{1/2}}$$

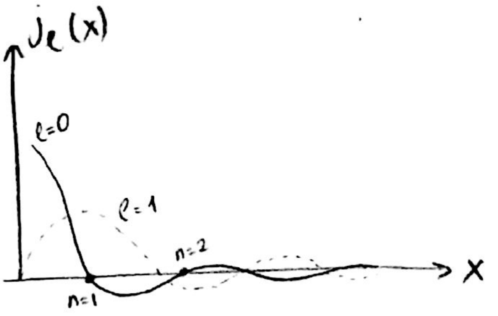
→ stationary state,
you now the time dependence

→ when $\ell \neq 0$, $u(r) = A\, r\, j_\ell(Kr) + B\, r\, n_\ell(Kr)$

j_ℓ: Spherical Bessel function of order ℓ
n_ℓ: Spherical Neuman function of order ℓ

$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}, \quad n_\ell(x) = -(-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}$$

↳ blows at the origin!
$B = 0$ should be chosen.



→ Since at the surface, ψ should vanish, "a" is basically one of the zeros.

$$\rightarrow R(r) = \frac{u(r)}{r} = A\, j_\ell(kr) \quad , \quad R(a) = A\, j_\ell(ka) = 0 .$$

→ Terminology : $ka = \beta_{n\ell}$ → representation of the zeros of the Bessel function.

Then, $\boxed{E_{n\ell} = \frac{\hbar^2}{2ma^2}\beta_{n\ell}^2}$ and $\boxed{\psi_{n\ell m}(r,\theta,\phi) = A_{n\ell}\, j_\ell(\beta_{n\ell} r/a)\, Y_\ell^m(\theta,\phi)}$

$\boxed{\text{HW}}$ 4.9 , $V(r) = \begin{cases} -V_0 , & r \le a \\ 0 , & r > a \end{cases}$

Hydrogen Atom

All you need to do is write $\frac{-e^2}{4\pi\varepsilon_0 r}$ instead of $V(r)$.

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r} + \underbrace{\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}}_{\text{decreases the effect of Coulomb potential}}\right]u = Eu$$

→ In bound states, $E<0$ ⇒ define $k = \sqrt{\frac{-2mE}{\hbar^2}}$

$$\frac{1}{k^2}\frac{d^2u}{dr^2} = \left[1 - \frac{me^2}{2\pi\varepsilon_0\hbar^2 k}\frac{1}{kr} + \frac{\ell(\ell+1)}{(kr)^2}\right]u \quad (*)$$

→ Let $\rho = kr$, $\rho_0 = \frac{me^2}{2\pi\varepsilon_0\hbar^2 k}$. Then, $(*)$ becomes

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

- $\rho \to \infty \Rightarrow \frac{d^2u}{d\rho^2} = u \Rightarrow u(\rho) = \underline{Ae^{-\rho}} + \cancel{Be^{+\rho}}$ → not physical. blowing.
- $\rho \to 0 \Rightarrow \frac{d^2u}{d\rho^2} = \frac{\ell(\ell+1)}{\rho^2}u \Rightarrow u(\rho) = \underline{C\rho^{\ell+1}} + \cancel{D\rho^{-\ell}}$ → not physical. blowing.

$$u(\rho) = e^{-\rho}\cdot\rho^{\ell+1}\cdot \underbrace{v(\rho)}_{\text{intermediate regions}}$$ —→ plug it into the eqn.

$$\rightarrow \frac{du}{d\rho} = (\ell+1)\rho^{\ell} e^{-\rho} V(\rho) - \rho e^{-\rho} \rho^{\ell+1} V(\rho) + \rho^{\ell+1} e^{-\rho} \frac{dV}{d\rho}$$

$$= \rho^{\ell} e^{-\rho} \left[(\ell+1-\rho) V + \rho \frac{dV}{d\rho} \right]$$

* as an exercise, show that

$$\frac{d^2u}{d\rho^2} = \rho^{\ell} e^{-\rho} \left[\left(-2\ell-2+\rho+\frac{\ell(\ell+1)}{\rho}\right) V + 2(\ell+1-\rho)\frac{dV}{d\rho} + \rho \frac{d^2V}{d\rho^2} \right] \rightarrow \text{plug it in!}$$

$$\rightarrow \rho \frac{d^2V}{d\rho^2} + 2(\ell+1-\rho)\frac{dV}{d\rho} + (\rho_0 - 2(\ell+1))V = 0$$

Suggest a solution $V(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$

$$\frac{dV}{d\rho} = \sum_{j=0}^{\infty} j c_j \rho^{j-1}$$

$$= \sum_{j=-1}^{\infty} (j+1) c_{j+1} \rho^j$$

plug them in!

$$= \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j \Rightarrow \frac{d^2V}{d\rho^2} = \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^{j-1}$$

$$\rightarrow \sum_{j=0}^{\infty} j(j+1) c_{j+1} \rho^j + 2(\ell+1) \sum_{j=0}^{\infty} (j+1) c_{j+1} \rho^j - 2 \sum_{j=0}^{\infty} j c_j \rho^j + (\rho_0 - 2(\ell+1)) \sum_{j=0}^{\infty} c_j \rho^j = 0$$

equate like-powers,

$$j(j+1) c_{j+1} + 2(\ell+1)(j+1) c_{j+1} - 2 j c_j + (\rho_0 - 2(\ell+1)) c_j = 0$$

$$c_{j+1} = \left[\frac{2(j+\ell+1) - \rho_0}{(j+1)(2\ell+2+j)} \right] c_j \quad //$$

* When $j \gg 1$, $c_{j+1} \simeq \frac{2j}{j(j+1)} c_j = \frac{2c_j}{j+1}$

with this assumption, we find $c_1 = \frac{2c_0}{1}$, $c_2 = \frac{2c_1}{2} = \frac{2}{2} \cdot \frac{2c_0}{1}$,

$c_3 = \frac{2c_2}{3} = \frac{2}{3} \cdot \frac{2}{2} \cdot \frac{2c_0}{1}$, ... $\Rightarrow c_j = \frac{2^j}{j!} c_0 \Rightarrow V(\rho) = \left(\sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j \right) c_0$

$$= e^{2\rho} c_0$$

Then, $u(\rho) = \rho^{l+1} e^{-\rho} e^{2\rho} c_0 = \rho^{l+1} e^{\rho} c_0$ → blows out when $\rho \to \infty$.

(this is not a nice way to show this, i believe.)

→ Conditions

- $C_{j_{max}+1} = 0$
- $2(\underbrace{j_{max} + l + 1}_{n}) - \rho_0 = 0$

n : principal quantum number

$\Big\}\ \rho_0 = 2n = \dfrac{me^2}{2\pi\varepsilon_0 \hbar^2 K}$, $K = \sqrt{\dfrac{-2mE}{\hbar^2}}$

These conditions will tell you that $E = \dfrac{-\hbar^2 K^2}{2m} = \dfrac{-me^4}{8\pi^2\varepsilon_0^2\hbar^2\rho_0^2}$

Bohr formula (1913)

$$\boxed{E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2}}$$

: energy is quantized for the bound states of H.

$n = 1, 2, \dots$

. Schrödinger (1924)

→ $\rho = Kr \Rightarrow K = \left(\dfrac{m_e \cdot e^2}{4\pi\varepsilon_0 \hbar^2}\right) \cdot \dfrac{1}{n} = \dfrac{1}{an}$ where a : Bohr radius

$$\boxed{a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \simeq 0.59 \cdot 10^{-10}\ m}$$

then, $\boxed{\rho = \dfrac{r}{an}}$: quantized

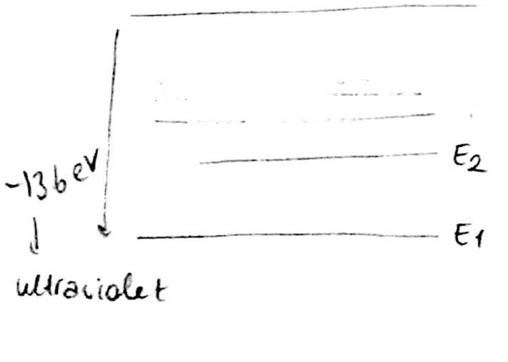
※ Spatial wave function for the Hydrogen atom labeled by three quantum numbers : (n, l, m).

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

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

→ $n = 1$ Solution (ground state)

$E_1 = -13.6$ eV



What is j_{max}?

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

* $n=0 \Rightarrow l=1 \Rightarrow$ for $C_{j_{max}+1}=0$, $j=0$

$C_{j_{max}+1} = C_1 = 0 \rightarrow$ the order is zero.

$\equiv V(\rho)$ is constant!

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

$\hookrightarrow R_{10} = \frac{1}{r}\rho e^{-\rho} C_0 = \frac{1}{r}\cdot\frac{r}{a}\cdot e^{-r/a} C_0 = \frac{C_0}{a} e^{-r/a}$ normalize and found

$$\int_0^\infty |R_{10}(r)|^2 r^2 dr = 1 \Rightarrow \frac{C_0^2}{a^2}\int_0^\infty e^{-2r/a} r^2 dr = 1$$

$$\Rightarrow \boxed{C_0 = \frac{2}{\sqrt{a}}}$$

Then, $\psi_{100} = \frac{2}{a^{3/2}} e^{-r/a}\left(\frac{1}{4\pi}\right)^{1/2} = \boxed{\frac{1}{\sqrt{\pi a^3}} e^{-r/a}}$

n	l	m	
1	$\rightarrow 0$	$\rightarrow 0$	
2	$\rightarrow 1$	$\rightarrow -1,0,1$	: 4-fold degenerate
	$\rightarrow 0$	$\rightarrow 0$	
3	$\rightarrow 2$	$\rightarrow -2,-1,0,1,2$	
	$\rightarrow 1$	$\rightarrow -1,0,1$	: 9-fold degenerate
	$\rightarrow 0$	$\rightarrow 0$	

ex $n=2$, $l=0$

$$C_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)} C_j \rightarrow C_{j_{max}+1} = \frac{2(j_{max}-1)}{(j_{max}+1)(j+2l+2)} C_{j_{max}} = 0 \Rightarrow j_{max}=1$$

and $\boxed{C_1 = -C_0}$

$(j=0)$

Then, $V(\rho) = c_0 + c_1\rho = c_0(1-\rho) = c_0\left(1 - \frac{r}{2a}\right)$

$$R_{20} = \frac{1}{r}\rho e^{-\rho} c_0\left(1 - \frac{r}{2a}\right) = \frac{1}{\cancel{r}}\frac{\cancel{r}}{2a} e^{-r/2a} \underbrace{c_0}_{\text{find from normalization.}}\left(1 - \frac{r}{2a}\right)$$

ex $\underline{n=2,\ l=1}$

$c_{j+1} = \frac{2j}{\sim} c_j \Rightarrow j_{max} = 0 \rightarrow V(\rho) = c_0$; find from normalization.

$\boxed{\text{HW}}$ 4.11 (do at least one normalization)

! $n = j_{max} + l + 1$

$\downarrow$

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

For each l, there are $(2l+1)$ m values.

$$\underbrace{d(n)}_{\text{degeneracy of energy } E_n} = \sum_{l=0}^{n-1} (2l+1) = n^2$$

e.g: $n=3 \rightarrow l = 2, 1, 0$

$5 + 3 + 1 = 9 = 3^2$

! $V(\rho) = L_{n-l-1}^{2l+1}(2\rho)$: not normalized

Associated Laguerre polynomials : $L_{q-p}^{p} = (-1)^p \left(\frac{d}{dx}\right)^p \underbrace{L_q(x)}_{\text{Laguerre polynomials}}$

Laguerre polynomials : $L_q(x) = e^x\left(\frac{d}{dx}\right)^q (e^{-x}x^q)$

$\hookrightarrow L_0 = 1$

$L_1 = -x + 1$

$L_2 = x^2 - 4x + 2 \quad \ldots$

$\hookrightarrow L_0^0 = 1$

$L_1^0 = -x + 1$

$L_1^2 = L_{3-2}^2 = \ldots$

* look at the curves to understand better.

$$\psi_{n\ell m} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \cdot e^{-r/na} \cdot \left(\frac{2r}{na}\right)^{\ell} \cdot \left[L^{2\ell+1}_{n-\ell-1}\left(\frac{2r}{na}\right)\right] \cdot Y^m_\ell(\theta,\phi)$$

for normalization   radial θ, ϕ

$$\hookrightarrow \int \psi^*_{n'\ell'm'} \psi_{n\ell m} \, r^2 dr \sin\theta d\theta d\phi = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'}.$$

Quantum Jumps!

$$E_\gamma = E_i - E_f = -13.6\,\text{eV}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

Planck's formula : $E_\gamma = h\nu$, $\lambda = \frac{c}{\nu}$ (in vacuum)

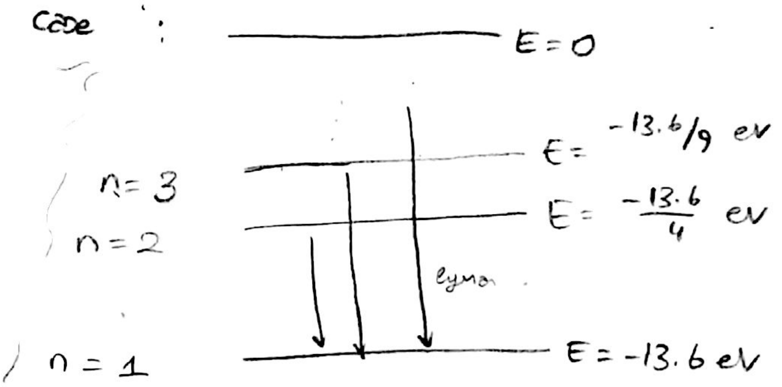
Then, $$\boxed{\frac{1}{\lambda_\gamma} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)}$$ where R: Rydberg constant

! $n \to \infty$: unbound case :

Lyman series : ultraviolet ($n_f = 1$)

Balmer series : visible ($n_f = 2$)

Paschen series : infrared ($n_f = 3$)



Angular Momentum

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

$$\vec{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix} \rightarrow \begin{aligned} L_x &= yP_z - zP_y \\ L_y &= zP_x - xP_z \\ L_z &= xP_y - yP_x \end{aligned}$$

where $P_x = i\hbar\frac{\partial}{\partial x}$, $P_y = i\hbar\frac{\partial}{\partial y}$, $P_z = i\hbar\frac{\partial}{\partial z}$

! $\vec{L} \times \vec{L}$ is not necessarily zero here since $\vec{p}$ is an operator.

- $[L_x, L_y] = [yP_z - zP_y, zP_x - xP_z]$

$$= [yP_z, zP_x] - [yP_z, xP_z) - [zP_y, zP_x] + [zP_y, xP_z]$$

$$\qquad\qquad\qquad\qquad 0 \qquad\qquad\qquad 0$$

$$\left(\text{Recall} \quad \begin{array}{l} [r_i, p_j] = -[p_j, r_i] = i\hbar\delta_{ij} \\ [r_i, r_j] = [p_i, p_j] = 0 \end{array} \right)$$

$$\rightsquigarrow [L_x, L_y] = [yP_z, zP_x] + [zP_y, xP_z]$$

$$= (yP_z zP_x - zP_x yP_z) + (zP_y xP_z - xP_z zP_y)$$

$$= (yP_x P_z z - yP_x zP_z) + (P_y x z P_z - xP_y P_z z)$$

$$= yP_x \underbrace{[P_z, z]}_{-i\hbar} + xP_y \underbrace{[z, P_z]}_{i\hbar} = i\hbar(xP_y - yP_x) = \boxed{i\hbar L_z}$$

- $$\boxed{\begin{array}{l} [L_x, L_y] = i\hbar L_z \\ [L_y, L_z] = i\hbar L_x \\ [L_z, L_x] = i\hbar L_y \end{array}}$$

$\longrightarrow$ then, you will have a bunch of things in $\vec{L} \times \vec{L}$

$$\vec{L} \times \vec{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{vmatrix} = \hat{i}(i\hbar L_x) - \hat{j}(-i\hbar L_x) + \hat{k}(i\hbar L_z)$$

$$= i\hbar [L_x \hat{i} + L_y \hat{j} + L_z \hat{k}] = \boxed{i\hbar \vec{L}}$$

! Uncertainty principle in general : $\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2$

$$\longrightarrow \sigma_{L_x}^2 \sigma_{L_y}^2 \geq \left(\frac{1}{2i} \langle i\hbar L_z \rangle \right)^2 = \frac{\hbar^2}{4} L_z^2 \Rightarrow \boxed{\sigma_{L_x} \sigma_{L_y} \geq \frac{\hbar L_z}{2}}$$

! Derivation of uncertainty principle

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

$$\sigma_B^2 = \langle g | g \rangle \quad \text{where} \quad g = (\hat{B} - \langle \hat{B} \rangle)\psi$$

$$* \ \langle f | g \rangle = \int_a^b f^*(x)\, g(x)\, dx$$

Schwartz inequality : $\left| \int_a^b f^*(x) g(x) dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$

⇝ We know $\langle f|g \rangle^* = \langle g|f \rangle$

⇝ $\sigma_A^2 \sigma_B^2 = \langle f|f \rangle \langle g|g \rangle$: like Schwartz

$\sigma_A^2 \sigma_B^2 \geq \langle f|g \rangle^2$

! If you have any complex number z,

$$|z|^2 = (Re\{z\})^2 + (Im\{z\})^2 \geq (Im\{z\})^2 = \left(\frac{z - z^*}{2i}\right)^2$$

If you say $z = \langle f|g \rangle$,

! $\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\left[\langle f|g \rangle - \langle g|f \rangle\right]\right)^2$

! $\langle f|g \rangle = \langle (\hat{A} - \langle \hat{A} \rangle)\psi | (\hat{B} - \langle \hat{B} \rangle)\psi \rangle$

$= \langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle)\psi \rangle$ (assuming Hermitian)

$= \langle \psi | (\hat{A}\hat{B} - \hat{A}\langle \hat{B} \rangle - \langle \hat{A} \rangle \hat{B} + \langle \hat{A} \rangle \langle \hat{B} \rangle)\psi \rangle$

$= \langle \hat{A}\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle - \cancel{\langle \hat{A} \rangle \langle \hat{B} \rangle} + \cancel{\langle \hat{A} \rangle \langle \hat{B} \rangle}$

$= \langle \hat{A}\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$

$\langle g|f \rangle = \langle \hat{B}\hat{A} \rangle - \langle \hat{B} \rangle \langle \hat{A} \rangle$

$\Rightarrow \langle f|g \rangle - \langle g|f \rangle = \langle \hat{A}\hat{B} \rangle - \langle \hat{B}\hat{A} \rangle = \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle$

Hence, $\boxed{\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle\right)^2}$ perfect...

! $L^2 = L_x^2 + L_y^2 + L_z^2$

$[L^2, L_x] = \underbrace{[L_x^2, L_x]}_{0} + [L_y^2, L_x] + [L_z^2, L_x]$

Recall: $[\hat{A}^2, \hat{B}] = \hat{A}[\hat{A},\hat{B}] + [\hat{A},\hat{B}]\hat{A}$

$\rightsquigarrow [L^2, L_x] = L_y[L_y, L_x] + [L_y, L_x]L_y + L_z[L_z, L_x] + [L_z, L_x]L_z$

$= -i\hbar L_y L_z - i\hbar L_z L_y + i\hbar L_z L_y + i\hbar L_y L_z = 0.$

! L^2 commutes with L_x, L_y and L_z.

OR, $\boxed{[L^2, L_x] = [L^2, L_y] = [L^2, L_z] = [L^2, \vec{L}] = 0.}$

! $L^2 f = \lambda f$) what are these eigenvalues?

$L_z f = \mu f$ → L_z is chosen since it is related to $\frac{\partial^2}{\partial\phi^2}$ in Schrödinger eqn.

Define dagger operators: $\boxed{\begin{aligned} L_+ &= L_x + iL_y \\ L_- &= L_x - iL_y \end{aligned}}$

→ $[L_z, L_\pm] = [L_z, L_x] \pm i[L_z, L_y]$

$= i\hbar L_y \pm i \cdot (-i\hbar L_x)$

$= i\hbar L_y \pm \hbar L_x$

$[L_z, L_\pm] = \pm\hbar\underbrace{(L_x \pm L_y)}_{L_\pm}$

$\boxed{[L_z, L_\pm] = \pm\hbar L_\pm}$

→ $[L^2, L_\pm] = 0$ since $L_\pm = L_x \pm iL_y$.

→ $L^2(L_\pm f) = \underbrace{L_\pm(L^2 f)}_{\text{since commutes}} = L_\pm(\lambda f) = \lambda L_\pm f$

$\boxed{L^2(L_\pm f) = \lambda(L_\pm f)}$

→ $L_z(L_\pm f) = (L_z L_\pm - L_\pm L_z)f + L_\pm L_z f$

$= \pm\hbar L_\pm f + L_\pm(\mu f)$

$\boxed{L_z(L_\pm f) = (\mu \pm \hbar)(L_\pm f)}$

→ Go to the top state.

$$\boxed{L_+ f_t = 0} \quad \longleftarrow \text{constraint equation}$$

$$\boxed{L_z f_t = \underbrace{\hbar l}_{\text{maximum value}} f_t}$$

$$\boxed{L^2 f_t = \lambda f_t} \quad (*)$$

$$L_\pm L_\mp = (L_x \pm iL_y)(L_x \mp iL_y)$$

$$= L_x^2 + L_y^2 \mp i\underbrace{(L_xL_y - L_yL_x)}_{i\hbar L_z} + L_z^2 - L_z^2$$

$$\Rightarrow L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z \quad \text{insert into } (*)$$

Choose one: $L^2 = L_-L_+ + L_z^2 + \hbar L_z$

then, $L^2 f_t = (L_-L_+ + L_z^2 + \hbar L_z) f_t = \lambda f_t$

$$= 0 + \hbar^2 l^2 f_t + \hbar^2 l f_t = \lambda f_t$$

$$\hbar^2 l(l+1) f_t = \lambda f_t \Rightarrow \boxed{\lambda = \hbar^2 l(l+1)}$$

Therefore, in general, $\boxed{L^2 f_t = \hbar^2 l(l+1) f_t}$

→ Go to the bottom state,

$$\boxed{L_- f_b = 0} \quad \leftarrow \text{constraint eqn.}$$

$$\boxed{L_z f_b = \hbar \bar{l} f_b}$$

$$\boxed{L^2 f_b = \lambda f_b} \quad \text{use } L^2 \text{ again.}$$

Choose the other: $L^2 = L_+L_- + L_z^2 - \hbar L_z$

then, $L^2 f_b = (L_+L_- + L_z^2 - \hbar L_z) f_b = \lambda f_b$

$$= 0 + \hbar^2 \bar{l}^2 f_b - \hbar^2 \bar{l} f_b = \hbar^2 \bar{l}(\bar{l}-1) f_b = \lambda f_b$$

$$\Rightarrow \boxed{\lambda = \hbar^2 \bar{l}(\bar{l}-1)} \Rightarrow \text{in general, } \boxed{L^2 f_b = \hbar^2 \bar{l}(\bar{l}-1) f_b}$$

equate those λ's : $\underbrace{\hbar^2 \ell(\ell+1) = \hbar^2 \bar{\ell}(\bar{\ell}-1)}$

$\boxed{\bar{\ell} = -\ell}$: but what are the steps?

$\rightarrow -\ell \cdots\cdots \ell$ integer steps $N \Rightarrow \ell = -\ell + N \Rightarrow \boxed{\ell = N/2}$: integer or half integer!

we didn't see this in sep. of var.

Then, $\boxed{\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots}$ and $\boxed{m = -\ell, -\ell+1, \ldots, \ell-1, \ell}$

this half integers are related to spin angular momentum.

HW 4.13 & 4.15

! We know $L^2 f_\ell^m = \hbar \ell(\ell+1) f_\ell^m$ and $L_z f_\ell^m = m\hbar f_\ell^m$

$L_\pm = L_x \pm i\hbar$, $\boxed{L_\pm f_\ell^m = A_\ell^m f_\ell^{m\pm 1}}$ $\rightarrow A_\ell^m = ?$

$\rightarrow \langle f | L_\pm g \rangle = \langle f | L_x g \rangle \pm i \langle f | L_y g \rangle$

HW Show that L_x and L_y are Hermitian. (use $\vec{r} \times \vec{p}$) hermitian hermitian

$$\rightarrow \langle f | L_\pm g \rangle = \langle L_x f | g \rangle \pm i \langle L_y f | g \rangle$$
$$= \langle (L_x \mp L_y) f | g \rangle$$
$$= \langle L_\mp f | g \rangle \Rightarrow \boxed{(L_\pm)^\dagger = L_\mp}$$

$$\rightarrow \langle L_\pm f_\ell^m | L_\pm f_\ell^m \rangle = \langle f_\ell^m | L_\mp L_\pm f_\ell^m \rangle$$
$$= \langle f_\ell^m | (L^2 - L_z^2 \mp \hbar L_z) f_\ell^m \rangle$$
$$= \hbar^2 \ell(\ell+1) - \hbar^2 m^2 \mp \hbar^2 m$$

$$\Rightarrow |A_\ell^m|^2 = \hbar^2 \ell(\ell+1) - \hbar^2 m^2 \mp m\hbar^2$$

$$\boxed{A_\ell^m = \hbar \sqrt{\ell(\ell+1) - m(m \pm 1)}}$$

$$\left(\begin{aligned} L_\mp L_\pm &= (L_x \mp i L_y)(L_x \pm i L_y) = L_x^2 \pm i L_x L_y \mp i L_y L_x + L_y^2 + L_z^2 - L_z^2 \\ &= L^2 - L_z^2 \mp \hbar L_z \ // \end{aligned} \right)$$

Eigenfunctions of L

$$\vec{L} = \frac{\hbar}{i}\, \vec{r} \times \vec{\nabla} \quad \text{where} \quad \vec{\nabla} = \left[\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\hat{\phi}\right]$$

then, $\vec{L} = \frac{\hbar}{i}\, r\hat{r} \times \left[\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}\hat{\phi}\right]$

$$= \frac{\hbar}{i}\left(\frac{\partial}{\partial\theta}\hat{\phi} - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\hat{\theta}\right)$$

We know that $\hat{\theta} = \cos\theta\cos\phi\,\hat{i} + \cos\theta\sin\phi\,\hat{j} - \sin\theta\,\hat{k}$
$\hat{\phi} = -\sin\phi\,\hat{i} + \cos\phi\,\hat{j}$ } insert.

$$\boxed{\begin{aligned} L_x &= \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_y &= \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right) \\ L_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi} \end{aligned}}$$

→ $L_\pm = L_x \pm L_y$

$$\boxed{L_\pm = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)}$$

HW 4.21: a,b.
not necessarily L_+L_- L^2

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

→ $Y_\ell^m(\theta,\phi)$ are the eigenfunctions of L^2 and L_z (not the half integers)

→ $H\psi = E\psi$
$L^2\psi = \hbar^2\ell(\ell+1)\psi$
$L_z\psi = \hbar m\psi$
} $\boxed{\psi = R\,Y_\ell^m}$

! $$\frac{1}{2mr^2}\left[-\hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + L^2\right]\psi + V\psi = E\psi$$: Schrödinger equation in spherical coordinates

- $$[L_z, x] = [xp_y - yp_x, x]$$
$$= [xp_y, x] - [yp_x, x]$$
$$= x\underbrace{[p_y, x]}_{0} + \underbrace{[x, x]}_{0}p_y - y[p_x, x] - \underbrace{[y, x]}_{0}p_x$$

$$\boxed{\begin{aligned} [L_z, x] &= i\hbar y \\ [L_z, y] &= -i\hbar x \\ [L_z, z] &= 0 \end{aligned}}$$

- $$[L_z, p_x] = [xp_y - yp_x, p_x]$$
$$= x\underbrace{[p_y, p_x]}_{0} + [x, p_x]p_y - y\underbrace{[p_x, p_x]}_{0} - \underbrace{[y, p_x]}_{0}p_x$$

$$\boxed{\begin{aligned} [L_z, p_x] &= i\hbar p_y \\ [L_z, p_y] &= -i\hbar p_x \\ [L_z, p_z] &= 0 \end{aligned}}$$

- $$[L_z, r^2] = [L_z, x^2] + [L_z, y^2] + [L_z, z^2]$$
$$= x[L_z, x] + [L_z, x]x + y[L_z, y] + [L_z, y]y + \cancelto{0}{z[L_z, z]} + \cancelto{0}{[L_z, z]z}$$
$$= i\hbar xy + i\hbar yx - i\hbar yx - i\hbar xy = 0.$$

- $$[L_z, p^2] = [L_z, p_x^2] + [L_z, p_y^2] + [L_z, p_z^2]$$
$$= p_x[L_z, p_x] + [L_z, p_x]p_x + p_y[L_z, p_y] + [L_z, p_y]p_y + \cancelto{0}{p_z[L_z, p_z]} + \cancelto{0}{[L_z, p_z]p_z}$$
$$= i\hbar \cancel{p_x p_y} + i\hbar \cancel{p_y p_x} - i\hbar \cancel{p_y p_x} - i\hbar \cancel{p_x p_y} = 0.$$

- Notice that $[L_x, r^2] = [L_y, r^2] = [L_x, p^2] = [L_y, p^2] = 0$.

Then, $$\boxed{\begin{aligned} [\vec{L}, r^2] &= 0 \\ [\vec{L}, p^2] &= 0 \end{aligned}}$$

$\hat{H} = \frac{\hat{p}^2}{2m} + V$ → Consider harmonic oscillator, $V \propto x^2+y^2+z^2$

Then, $[H, L^2] = 0$

$[H, L_z] = 0$

If there is a potential, $\frac{d}{dt}\langle L\rangle = \langle N\rangle$ torque

This comes from $\frac{d}{dt}\langle\hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle$

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

$* \ [H, L_x] = \frac{1}{2m}\underbrace{[p^2, L_x]}_{0} + [V, L_x]$

$= [V, yp_z - zp_y]$

$= y[V, p_z] + \cancel{[V, y]p_z}^{\,0} - z[V, p_y] - \cancel{[V, z]}^{\,0}p_y$

$= yi\hbar\frac{\partial V}{\partial z} - zi\hbar\frac{\partial V}{\partial y}$

$\boxed{[H, L_x] = i\hbar(\vec{r}\times\vec{\nabla}V)_x}$ → if you do this for y & z, you will see that

$\Downarrow$

$\frac{d}{dt}\langle L_x\rangle = -\langle(\vec{r}\times\vec{\nabla}V)_x\rangle$

$$\boxed{\frac{\partial}{\partial t}\langle\vec{L}\rangle = -\langle\vec{r}\times\vec{\nabla}V\rangle}$$

force

torque!

Notice that when $V = V(r)$, ∇V gives a function $\hat{r}$, then angular momentum is conserved.

HW 4.23, Read "What is spin", American Journal of Physics, V. 54, p. 500, 1986, Hans Ohanian

HW | 4.38 & 4.39 → important!

Spin

$\vec{L} = \vec{r} \times \vec{p}$, $l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$

$\vec{S} = I\vec{w}$

spin

! Assume $l = 2$ $\Rightarrow \langle L^2 \rangle = \hbar^2 l(l+1) = 6\hbar^2 \Rightarrow \sqrt{\langle L^2 \rangle} = \hbar\sqrt{3}$? $\langle L_z \rangle < \sqrt{\langle L^2 \rangle}$

$m = -2, -1, 0, 1, 2$ $\quad \langle L_z \rangle = 2\hbar$ (assume max)

since L_x, L_y, L_z do not commute and it is not possible $L_x = L_y = 0$.

! $\boxed{\begin{aligned} [S_x, S_y] &= i\hbar S_z \\ [S_y, S_z] &= i\hbar S_x \\ [S_z, S_x] &= i\hbar S_y \end{aligned}}$: same with $\vec{L}$.

! $\boxed{\begin{aligned} S^2 |sm\rangle &= \hbar s(s+1) |sm\rangle \\ S_z |sm\rangle &= \hbar m |sm\rangle \\ S_\pm |sm\rangle &= \hbar \sqrt{s(s+1) - m(m\pm1)}\, |s\, m\pm1\rangle \end{aligned}}$

where $\boxed{S_\pm = S_x \pm i S_y}$

! $S = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$

pi meson, electron, photon, graviton

→ We will be working with the electron : $s = 1/2$

$|\frac{1}{2}\ \frac{1}{2}\rangle$: spin up ↑

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

! spin $\frac{1}{2}$ particle column matrix (spinor) : $\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$

where $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$: spin up

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

$\rightarrow$ $S^2 \chi_+ = \frac{3}{4}\hbar^2 \chi_+$
$S^2 \chi_- = \frac{3}{4}\hbar^2 \chi_-$ $\Big\}$ $S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$

$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} c \\ e \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} d \\ f \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Then, $c = \frac{3}{4}\hbar^2 = f$, $d = e = 0$: $\Rightarrow$ $\boxed{S^2 = \frac{3}{4}\hbar^2 I}$

$\rightarrow$ $S_z \chi_+ = \frac{\hbar}{2}\chi_+$
$S_z \chi_- = -\frac{\hbar}{2}\chi_-$ $\Big\}$ $\boxed{S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$

$\rightarrow$ To find S_x & S_y, we use the ladder operators.

$S_+ \chi_- = \hbar\sqrt{\frac{1}{2}\cdot\frac{3}{2} + \frac{1}{2}\frac{1}{2}}\,\chi_+ = \hbar\chi_+$
$S_+ \chi_+ = 0$ $\Big\}$ $\boxed{S_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}$

$S_- \chi_+ = \hbar\sqrt{\frac{1}{2}\cdot\frac{3}{2} - \frac{1}{2}\cdot\left(\frac{-1}{2}\right)}\,\chi_- = \hbar\chi_-$
$S_- \chi_- = 0$ $\Big\}$ $\boxed{S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}$

$\rightarrow$ Then,
$$\boxed{\begin{aligned} S_x &= \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ S_y &= \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \end{aligned}}$$

Then, $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$ where

$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\Big\}$ Pauli spin matrices
$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- $\underbrace{S_x, S_y, S_z, S^2}_{\text{observable}}$ are all Hermitians, $\underbrace{S_+ \& S_-}_{\text{not observable}}$ are not.

- $S_z \chi_\pm = \underbrace{\pm \frac{\hbar}{2}}_{\text{eigenvalues}} \chi_\pm$

- Any χ can be expressed as $\chi = a\chi_+^z + b\chi_-^z$

  then, spin is $+\frac{\hbar}{2}$ with probability a^2,

  $-\frac{\hbar^2}{2}$ with probability b^2. } where $a^2 + b^2 = 1$.

- $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ → what are the spinors?

$$\begin{vmatrix} -\lambda & \hbar/2 \\ \hbar/2 & -\lambda \end{vmatrix} = \lambda^2 - \frac{\hbar^2}{4} = 0 \Rightarrow \boxed{\lambda = \pm\frac{\hbar}{2}} \text{ : eigenvalue of } S_x.$$

$$\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\frac{\hbar}{2}\begin{pmatrix} \beta \\ \alpha \end{pmatrix} = +\frac{\hbar}{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \rightsquigarrow \beta = \alpha \quad : \lambda = \frac{\hbar}{2} \Rightarrow \chi_+^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\frac{\hbar}{2}\begin{pmatrix} \beta \\ \alpha \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \rightsquigarrow \beta = -\alpha \quad : \lambda = -\frac{\hbar}{2} \Rightarrow \chi_-^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

- S_y → derive.

- $$\chi = \left(\frac{a+b}{\sqrt{2}}\right)\underbrace{\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}}_{\chi_+^x} + \left(\frac{a-b}{\sqrt{2}}\right)\underbrace{\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}}_{\chi_-^x} = a\underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix}}_{\chi_+} + b\underbrace{\begin{pmatrix} 0 \\ 1 \end{pmatrix}}_{\chi_-}$$

ex spin $\frac{1}{2}$ with $\chi = \frac{1}{\sqrt{6}}\begin{pmatrix}1+i\\ 2\end{pmatrix}$. What are the probabilities of getting $\frac{\hbar}{2}$ when measuring S_x & S_z?

for S_z: $\frac{1+i}{\sqrt{6}}\begin{pmatrix}1\\0\end{pmatrix} + \frac{2}{\sqrt{6}}\begin{pmatrix}0\\1\end{pmatrix} \Rightarrow P = |a|^2 = \frac{(1+i)(1-i)}{6} = \boxed{1/3}$

S_x: $\frac{3+i}{2\sqrt{3}}\begin{pmatrix}1/\sqrt{2}\\ 1/\sqrt{2}\end{pmatrix} + \frac{-1+i}{2\sqrt{3}}\begin{pmatrix}1/\sqrt{2}\\ -1/\sqrt{2}\end{pmatrix} \Rightarrow P = \left|\frac{a+b}{\sqrt{2}}\right|^2 = \frac{(3+i)(3-i)}{12} = \boxed{\frac{5}{6}}$

expectation value: $\langle S_z\rangle = \chi^\dagger S_z \chi$

$$= \frac{1}{\sqrt{6}}\begin{pmatrix}1-i & 2\end{pmatrix}\begin{pmatrix}\hbar/2 & 0\\ 0 & -\hbar/2\end{pmatrix}\frac{1}{\sqrt{6}}\begin{pmatrix}1+i\\ 2\end{pmatrix}$$

$$= \frac{1}{6}\frac{\hbar}{2}\begin{pmatrix}1-i & -2\end{pmatrix}\begin{pmatrix}1+i\\ 2\end{pmatrix}$$

$$= \frac{1}{6}\frac{\hbar}{2}(2-4) = \boxed{\frac{-\hbar}{6}}$$

expectation value: $\langle S_x\rangle = \chi^\dagger S_x \chi$

or use the probabilities,

$$\langle S_x\rangle = \frac{\hbar}{2}\cdot\frac{5}{6} - \frac{\hbar}{2}\cdot\frac{1}{6} = \boxed{\frac{\hbar}{3}}$$

$\boxed{\text{HW}}$ 4.27

Spin in a Magnetic Field

$\vec{B}$

$\vec{\tau} = \vec{\mu}\times\vec{B}$

$\vec{\mu} = \gamma\vec{S}$

↳ spin angular momentum

magnetic dipole moment

gyromagnetic ratio

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

$\hookrightarrow H = -\vec{\mu}\cdot\vec{B} = -\gamma\vec{S}\cdot\vec{B}$

Assume electron is in a uniform magnetic field : $\vec{B} = B_0 \hat{k}$.

Then, $H = -\gamma S_z B_0 = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ → eigenstates of the Hamiltonian are eigenstates of S_z.

do for $\vec{B} = B_0 \hat{i}$ or $\vec{B} = B_0 \hat{j}$

eigenstates : $\boxed{\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}}$, eigenvalues are the energy.

$$H\chi_+ = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \left(-\gamma B_0 \frac{\hbar}{2}\right) \chi_+ \Rightarrow \boxed{E_+ = -\gamma B_0 \frac{\hbar}{2}}$$

$$H\chi_- = -\gamma B_0 \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \left(\gamma B_0 \frac{\hbar}{2}\right) \chi_- \Rightarrow \boxed{E_- = \gamma B_0 \frac{\hbar}{2}}$$

→ Time evolution :

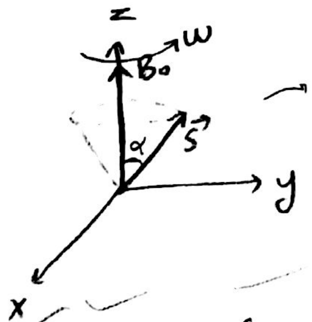
$$i\hbar \frac{\partial \chi}{\partial t} = H\chi \Rightarrow \chi(t) = a \underbrace{\chi_+}_{\begin{pmatrix} 1 \\ 0 \end{pmatrix}} e^{-iE_+t/\hbar} + b \underbrace{\chi_-}_{\begin{pmatrix} 0 \\ 1 \end{pmatrix}} e^{-iE_-t/\hbar}.$$

$$\Rightarrow \boxed{\chi(t) = \begin{pmatrix} a \exp(i\gamma B_0 t/2) \\ b \exp(-i\gamma B_0 t/2) \end{pmatrix}} , \quad \boxed{\chi(0) = \begin{pmatrix} a \\ b \end{pmatrix}}$$

not normalized !

! Check Schrödinger & Heisenberg pictures !

$$\chi^\dagger(0)\chi = (a \;\; b) \begin{pmatrix} a \\ b \end{pmatrix} = \boxed{a^2 + b^2 = 1}$$ → normalization holds both for $\chi(0)$ and $\chi(t)$, obviously.



→ not completely true due to uncertainty. though, it helps us to understand.

$\boxed{a = \cos\left(\frac{\alpha}{2}\right), \quad b = \sin\left(\frac{\alpha}{2}\right)}$

you can choose a & b like this.

$$\chi(t) = \begin{pmatrix} \cos\left(\frac{\alpha}{2}\right) \exp(i\gamma B_0 t/2) \\ \sin\left(\frac{\alpha}{2}\right) \exp(-i\gamma B_0 t/2) \end{pmatrix}$$

$\rightarrow \quad \langle S_x \rangle = \langle \chi | S_x | \chi \rangle$

$= \chi^{+} S_x \chi$ — you will find a number.

$$= \left(\cos(\tfrac{\alpha}{2})\exp(-i\gamma B_0 t/2) \quad \sin(\tfrac{\alpha}{2})\exp(i\gamma B_0 t/2)\right)\frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\cos(\frac{\alpha}{2})\exp(i \ldots)\\ \sin(\frac{\alpha}{2})\exp(-i\ldots)\end{pmatrix}$$

$$= \frac{\hbar}{2}\left(\cos\cdot\exp(-) \quad \sin\cdot\exp(+)\right)\begin{pmatrix}\sin\cdot\exp(-)\\ \cos\cdot\exp(+)\end{pmatrix}$$

$$= \frac{\hbar}{2}\left(\cos\frac{\alpha}{2}\sin\frac{\alpha}{2}\exp(-i\gamma B_0 t) + \sin\frac{\alpha}{2}\cos\frac{\alpha}{2}\exp(i\gamma B_0 t)\right)$$

$\boxed{\langle S_x \rangle = \frac{\hbar}{2}\sin\alpha\cos(\gamma B_0 t)}$ → if you integrate over $\alpha: 0 \to 2\pi$ or $\omega = \gamma B_0 : 0 \to 2\pi$ you get zero!

↳ Larmor frequency

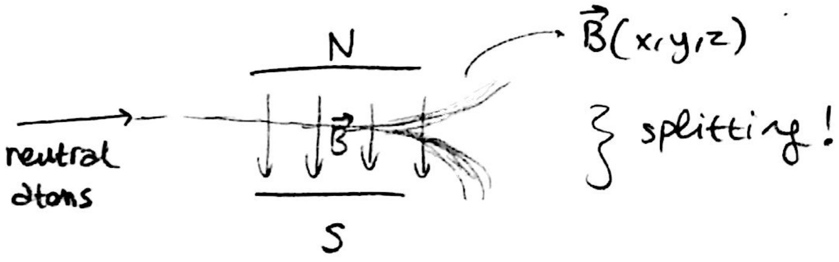
→ $\boxed{\langle S_y \rangle = \frac{-\hbar}{2}\sin\alpha\sin(\gamma B_0 t)}$ → do it.

→ $\boxed{\langle S_z \rangle = \frac{\hbar}{2}\cos\alpha}$: not time dependent! (do it, though)

Notice that $\alpha = 0$ is not real!

↳ time evolution is finite!

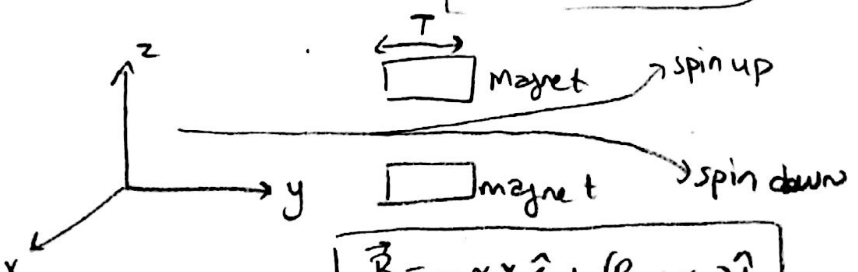
! The Stern-Gerlach Experiment



* Lorentz force is not possible since the particles are neutral.

So, what is happening?

* $U = -\vec{\mu}\cdot\vec{B} \Rightarrow \boxed{\vec{F} = \vec{\nabla}(\vec{\mu}\cdot\vec{B})}$ wooaaah.



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

notice We know that $\nabla \cdot \vec{B} = 0$. This field is arranged in that way.
that

$\vec{B} = (B_0 + \alpha z)\hat{k}$ does not work.

you can choose $\vec{B} = -\alpha y \hat{j} + (B_0 + \alpha z)\hat{k}$ though.

but in the figure, it is not logical. ≡ change the arrangement

$$\vec{F} = \nabla(\vec{\mu} \cdot \vec{B}) = \nabla\{\gamma \vec{S} \cdot [-\alpha x \hat{i} + (B_0 + \alpha z)\hat{k}]\}$$

$$= \nabla(-\alpha\gamma S_x x + \gamma B_0 S_z + \alpha\gamma S_z z)$$

$$\boxed{\vec{F} = -\alpha\gamma S_x \hat{i} + \alpha\gamma S_z \hat{k}}$$ → Constant $\vec{B}$ does not work.

→ the constant field is only in $\hat{k}$ direction → only $\hat{k}$ contributes to the splitting since in other directions, $\langle S_x \rangle, \langle S_y \rangle, \langle S_z \rangle$ would be time dependent: no net splitting

$$\boxed{\vec{F} = \alpha\gamma S_z \hat{k}}$$

(α depends on the matter, magnetic field etc.)

→ Basically, the beam splits in $2s+1$ states.

for electron: 2

for photon → no magnetic moment, no mass; what do you expect?
however, it has a polarization

different experiment, 3 states

$+1, -1$ → RH-LH

→ Classically, $\vec{F} = \alpha\gamma S_z \hat{k}$ means not splitting but deflecting. Splitting comes from QM: $S_z \in \mathbb{R}^{2\times 2}$

→ $H(t)$ in the magnet:

$$H = \begin{cases} -\gamma \vec{B} \cdot \vec{S} = -\gamma(B_0 + \alpha z)S_z, & 0 \le t \le T \\ 0, & \text{otherwise } [t \le 0 \;\&\; t \ge T] \end{cases}$$

we know that $\chi(t) = a\chi_+(t) + b\chi_-(t)$, $a^2 + b^2 = 1$.

$$\chi(t) = a\chi_+ e^{-iE_+ t/\hbar} + b\chi_- e^{-iE_- t/\hbar}, \quad 0 \le t \le T$$

* What will be the eigenvalues?

$$\boxed{E_\pm = \mp \gamma(B_0 + \alpha z)\frac{\hbar}{2}}$$

$$\chi(t>T) = \left[a \exp\left(\frac{i\gamma T B_0}{2}\right)\chi_+\right] e^{i\alpha\gamma\frac{T}{2}z}$$ additional term

$$+ \left[b \exp\left(-\frac{i\gamma T B_0}{2}\right)\chi_-\right] e^{-i\alpha\gamma\frac{T}{2}z}$$

$\Rightarrow$ You have some z dependence when you leave the apparatus!

Notice that the eigenfunctions of momentum ~ z dependence

$$\frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar} \quad \sim e^{i\left(\frac{\alpha\gamma T}{2}\right)z}$$

$$\sim e^{-i\left(\alpha\frac{\gamma T}{2}\right)z}$$

$\Rightarrow$ one momentum in +z,
one momentum in −z, $\Bigg\}$ $\boxed{P_z = \pm\frac{\alpha\gamma T\hbar}{2}}$

Actual force: $F = \alpha\gamma S_z$

measure $S_z \rightarrow$ you get $\frac{\hbar}{2}$

measure $F \longrightarrow$ you get $\frac{\alpha\gamma\hbar}{2}$

Then, $\langle F\rangle T = \frac{\alpha\gamma\hbar T}{2} = P_z$

for spin up case, of course

ex $B = -B_0\cos\omega t\,\hat{k}$ $\rightarrow$ time averages will be zero.
solve.

$\boxed{\text{HW}}$ 4.32, 4.33 (simple)
4.49 (meh)

(check the notation differences between Griffiths, Liboff & Gasiorowicz)
especially

Addition of Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

$\vec{J}$: total angular momentum; $\vec{L}$: angular; $\vec{S}$: spin

Suppose two spin half particle in the ground state of H.

possibilities: $\uparrow\uparrow \quad \uparrow\downarrow \quad \downarrow\uparrow \quad \downarrow\downarrow$

$\vec{S} = \vec{S}^1 + \vec{S}^2$ → we want to do this.

↳ $S_z = S_z^1 + S_z^2$ → you need an addition,

$$S_z \chi_1 \chi_2 = (S_z^1 + S_z^2)\chi_1\chi_2$$
$$= (S_z^1\chi_1)\chi_2 + \chi_1(S_z^2\chi_2)$$
$$= (\hbar m_1 \chi_1)\chi_2 + \chi_1(\hbar m_2 \chi_2)$$
$$= \hbar(\underbrace{m_1}_{\pm\frac{1}{2}} + \underbrace{m_2}_{\pm\frac{1}{2}})\chi_1\chi_2$$

⇒ the eigenvalue of S_z : $\underline{\hbar(m_1+m_2)}$

Then,
$\uparrow\uparrow$: $m = 1$
$\uparrow\downarrow$: $m = 0$
$\downarrow\uparrow$: $m = 0$
$\downarrow\downarrow$: $m = -1$

\# of total states should be 3, not 4.

↳ $S_- = S_-^1 + S_-^2$, take $\uparrow\uparrow$ state.

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

: three states with $s = 1$.

(recall $S_+\chi_- = \hbar\chi_+$
$S_-\chi_+ = \hbar\chi_-$)

hit again, you get $\downarrow\downarrow$.

$\lvert s\ m\rangle$
$\lvert 1\ 1\rangle = \uparrow\uparrow$
$\lvert 1\ 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$
$\lvert 1\ {-1}\rangle = \downarrow\downarrow$

all this is for $s = 1$. ≡ triplet states

all these states are orthogonal

another possibility: $\boxed{\lvert 0\ 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)}$ → for $s = 0$. singlet state

! for s, you get states from $(s_1 + s_2)$ to $|s_1 - s_2|$

$\overset{?}{\vec{S}} = \vec{S}^1 + \vec{S}^2$

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

$\longrightarrow$ Let us pick $|1\ 0\rangle$. We know that S^2 has eigenvalues $\hbar s(s+1)$.

eigenvectors of S_z

$\longrightarrow$ $S^{(1)} \cdot S^{(2)} (\uparrow\downarrow) = (S_x^{(1)} \uparrow)(S_x^{(2)} \downarrow) + (S_y^{(1)} \uparrow)(S_y^{(2)} \downarrow) + (S_z^{(1)} \uparrow)(S_z^{(2)} \downarrow)$

$\qquad\qquad \binom{1}{0} \quad \binom{0}{1} \quad \binom{1}{0} \quad \binom{0}{1} \quad \binom{1}{0} \quad \binom{0}{1}$

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\Rightarrow S^{(1)} \cdot S^{(2)} (\uparrow\downarrow) = \left(\frac{\hbar}{2}\downarrow\right)\left(\frac{\hbar}{2}\uparrow\right) + \left(\frac{i\hbar}{2}\downarrow\right)\left(\frac{-i\hbar}{2}\uparrow\right) + \left(\frac{\hbar}{2}\uparrow\right)\left(\frac{-\hbar}{2}\downarrow\right)$$

$$= \frac{\hbar^2}{4}(2\downarrow\uparrow - \uparrow\downarrow) \,//$$

Then, $S^{(1)} \cdot S^{(2)} (\downarrow\uparrow) = \frac{\hbar^2}{4}(2\uparrow\downarrow - \downarrow\uparrow) \,//$

keep this $\longrightarrow$ $\vec{S}^{(1)} \cdot \vec{S}^{(2)} |1\ 0\rangle = \vec{S}^{(1)} \cdot \vec{S}^{(2)} \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$

$$= \frac{\hbar^2}{4} \cdot \frac{1}{\sqrt{2}} \left[2\downarrow\uparrow - \uparrow\downarrow + 2\uparrow\downarrow - \downarrow\uparrow\right]$$

$$= \frac{\hbar^2}{4} \frac{1}{\sqrt{2}} (\uparrow\downarrow + \downarrow\uparrow) = \boxed{\frac{\hbar^2}{4} |1\ 0\rangle}$$

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

$$= \frac{3\hbar^2}{4} |1\ 0\rangle \quad \left(\text{recall } S^2 = \frac{3\hbar}{4} \mathbb{I}\right)$$

The same is true for $(S^{(2)})^2$.

$\longrightarrow$ Altogether, $S^2 |1\ 0\rangle = \left(\frac{3\hbar^2}{4} + \frac{3\hbar^2}{4} + \frac{2\hbar^2}{4}\right) |1\ 0\rangle$

$$= 2\hbar\, |1\ 0\rangle = \hbar s(s+1)\, |1\ 0\rangle$$

where $s = 1$.

YES!

$\boxed{S^2 |s\ m\rangle = \hbar^2 s(s+1)\, |s\ m\rangle}$ is shown to be true.

$\hookrightarrow S^2 |0\ 0\rangle = 0 \cdot |0\ 0\rangle$

$\rightarrow \boxed{S = (s_1 + s_2), (s_1 + s_2 - 1), \dots, |s_1 - s_2|}$ (the spins you get.)

ex

$$\left.\begin{array}{l} s_1 = \frac{3}{2} \\ \\ s_2 = 2 \end{array}\right\} \begin{array}{lcl} \underline{s} & & \underline{m} \\ \frac{7}{2} & \rightarrow & \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, \frac{-1}{2}, \frac{-3}{2}, \frac{-5}{2}, \frac{-7}{2} \\ \vdots & & \\ \frac{1}{2} & \rightarrow & \frac{1}{2}, \frac{-1}{2} \end{array}$$

$$\left.\begin{array}{l} l = 2 \\ \\ s = \frac{1}{2} \end{array}\right\} \begin{array}{lcl} \underline{J} & & \underline{m} \\ \frac{5}{2} & \rightarrow & \frac{-5}{2}, \frac{-3}{2}, \frac{-1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{5}{2} \\ \vdots & & \\ \frac{3}{2} & \rightarrow & \frac{-3}{2}, \frac{-1}{2}, \frac{1}{2}, \frac{3}{2} \end{array}$$

$$|s\ m\rangle = \sum_{m_1 + m_2 = m} C^{s_1 s_2 s}_{m_1 m_2 m} |s_1\ m_1\rangle |s_2\ m_2\rangle$$

$\hookrightarrow$ Clebsh Gordon Coefficients $\rightarrow$ hard!

ex $\underline{\overset{s_1}{2} \times \overset{s_2}{1}}$

$$\begin{pmatrix} 2 \\ 1 \\ 0 \\ -1 \\ -2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\begin{array}{lcl} \underline{s} & & \underline{m} \\ 3 & \longrightarrow & +3, 2, 1, 0, -1, -2, -3 \\ 2 & \longrightarrow & +2, 1, 0, -1, -2 \\ 1 & \longrightarrow & +1, 0, -1 \end{array}$$

Check the book! There is a table!

you pick a value: $|3\ 0\rangle$

$$|3\ 0\rangle = \frac{1}{\sqrt{5}} |\overset{3}{2\ 1}\rangle |1\ -1\rangle + \sqrt{\frac{3}{5}} |\overset{3}{2\ 0}\rangle |1\ 0\rangle \frac{1}{\sqrt{5}} + |\overset{3}{2\ -1}\rangle |1\ 1\rangle$$

(s_1 m_1, s_2 m_2; 0, 0, 0)

$\uparrow$ from the book

S'_z getting eigenvalue $\hbar$ $\rightarrow$ probability?

$\hbar \rightarrow \frac{1}{5}$ since $|2\ 1\rangle |1\ -1\rangle$ would get $\hbar$

$0 \rightarrow \frac{3}{5}$ since $|2\ 0\rangle |1\ 0\rangle$ " " 0

$-\hbar \rightarrow \frac{1}{5}$ since $|2\ -1\rangle |1\ 1\rangle$ " " $-\hbar$

! We can also write $|s_1\, m_1\rangle|s_2\, m_2\rangle = \sum \quad |s\, m\rangle$

let us choose $|2\ 1\rangle|1\ -1\rangle = \frac{1}{\sqrt{5}}|3\ 0\rangle + \frac{1}{\sqrt{2}}|2\ 0\rangle + \sqrt{\frac{3}{10}}|1\ 0\rangle$

from the book

$\Rightarrow$ CHECK THE BOOK!

$\boxed{\text{HW}}$ 4.51 ($\frac{1}{2}\times 5$): very important!, Gasiorowicz: prob # 14.
3rd edt

Check Liboff.

(If you need $L\cdot S$ anytime, use $J = L + S \Rightarrow J^2 = L^2 + S^2 + 2L\cdot S$)

In some cases they do not commute.

Midterm 1 is up to here.

$\boxed{\text{HW}}$ 4.40 - 4.41 - 4.55

Basics

$\rightarrow \int_{-\infty}^{\infty} dx\, u_m(x) u_n(x) = \delta_{nm}$

$\rightarrow \langle\phi|\psi\rangle = \int_{-\infty}^{\infty}\phi^*(x)\psi(x)\,dx$ } scalar product of two wave function

bra, ket

$\rightarrow \langle\phi|\psi\rangle^* = \langle\psi|\phi\rangle$

$\rightarrow A|\psi\rangle = |A\psi\rangle$

$\hookrightarrow \langle\phi|A\psi\rangle = \langle\phi|A|\psi\rangle = \int_{-\infty}^{\infty}\phi^*(x)A\psi(x)\,dx$

$\rightarrow \int_{-\infty}^{\infty}(A\phi(x))^*\psi(x) = \int_{-\infty}^{\infty} dx\,\phi^*(x)A^\dagger\psi(x)$

$\hookrightarrow \langle A\phi|\psi\rangle = \langle\phi|A^\dagger\psi\rangle$

$\rightarrow \langle\phi|A^\dagger|\psi\rangle^* = \langle A\phi|\psi\rangle^* = \langle\psi|A\phi\rangle = \langle\psi|A|\phi\rangle$

$\rightarrow |\psi\rangle = \sum_n c_n \underbrace{|n\rangle}_{\text{orthonormal eigenstates}}$

discrete distribution

$\downarrow$

$\langle m|\psi\rangle = \sum_n c_n \langle m|n\rangle = c_m$, $|c_n|^2$ gives the probabilities.

$\searrow |\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$

$\rightarrow$ Completeness relation: $\sum_n |n\rangle\langle n| = 1 \rightarrow$ unit operation $\rightarrow$ For any orthonormal series, you'll get some comp. rel

$X|x\rangle = x\,|x\rangle$ $\rightarrow |\psi\rangle = \int dx\, c(x)\,|x\rangle$ $\rightarrow$ continuous distribution

eigenkets

$\rightarrow \langle x'|\psi\rangle = \int dx\, c(x)\,\underbrace{\langle x'|x\rangle}_{\delta_{x'x}} = c(x') \Rightarrow c(x) = \langle x|\psi\rangle$

$\rightarrow \langle x|\psi\rangle$: projection of ψ on x $\Rightarrow \psi(x) = \langle x|\psi\rangle$ } a change of notation

$\langle p|\phi\rangle$: projection of ϕ on p $\rightarrow \phi(p) = \langle p|\phi\rangle$

$\downarrow$ momentum space wave function

$\rightarrow$ Completeness relation: $\int_{-\infty}^{\infty} dx\, |x\rangle\langle x| = 1$ $\rightarrow$ continuous one. Insert anytime!

$\rightarrow \langle\psi_1|\psi_2\rangle = \langle\psi_1|1|\psi_2\rangle$

$= \int_{-\infty}^{\infty} dx\, \langle\psi_1|x\rangle\langle x|\psi_2\rangle = \int_{-\infty}^{\infty} dx\, \psi_1^*(x)\,\psi_2(x)$ well. notation works well.

ex $\langle x|\psi\rangle = \langle x|1|\psi\rangle$ you can call anything!

$\psi(x) = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\langle p|\psi\rangle$ d'you reckon fourier?

$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(p)\, e^{ipx/\hbar}\, dp = \int_{-\infty}^{\infty} dp\, \langle x|p\rangle\,\psi(p)$

Then, $\boxed{\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}}$

→ $|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle$ is obvious.

projection operator : $\boxed{P_n = |n\rangle\langle n|}$ (if you sum, that's unity)

↳ $P_m P_n = |m\rangle\langle m|n\rangle\langle n| = |m\rangle \delta_{nm} \langle n| = \delta_{nm} P_n$

↳ Then, $P_n^2 = P_n$.

→ $\langle \psi | H | \psi \rangle = \sum_n \langle n|\psi\rangle^2 E_n$

$= \sum_n \langle \psi | n \rangle\langle n|\psi\rangle E_n$ } $H = \sum_n E_n P_n$

→ $H|\psi_1 + \psi_2 + \dots\rangle = |E_1\psi_1 + \dots\rangle$

$\langle \psi_1 + \psi_2 + \dots | E_1 \psi_1 + \dots \rangle = E_1 + E_2 + \dots$

→ Harmonic Oscillator

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

$$H = \omega \underbrace{\left[\sqrt{\frac{m\omega}{2}}\, x - i\frac{p}{\sqrt{2m\omega}}\right]}_{A/\sqrt{\hbar} = A} \underbrace{\left[\sqrt{\frac{m\omega}{2}}\, x + i\frac{p}{\sqrt{2m\omega}}\right]}_{A^+/\sqrt{\hbar} = A^+}$$

$= \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2 - \frac{i\omega}{2}(px - xp)$

$\boxed{[A, A^+] = 1}$

$\boxed{H = H - \frac{1}{2}\hbar\omega}$

$H = \hbar\omega\,(A^+A + \frac{1}{2})$

→ $[H, A] = \hbar\omega\,[A^+A, A] = -\hbar\omega A$

$[H, A^+] = \hbar\omega\,[A^+A, A^+] = \hbar\omega A^+$

→ $H|E\rangle = E|E\rangle$

$HA|E\rangle = AH|E\rangle - \hbar\omega A|E\rangle$

$= (E - \hbar\omega)A|E\rangle$

A lowering the degree by one

$HA^+|E\rangle = (E + \hbar\omega)A^+|E\rangle$

A^+ increasing the degree by one

$\rightarrow H|0\rangle = \hbar w\,(A^{\dagger}A + \tfrac{1}{2})\,|0\rangle$

zero

$= \tfrac{1}{2}\hbar w|0\rangle$, energy of the zero state! ≡ zero point energy

$\rightarrow \langle H\rangle = \dfrac{(\Delta p)^2}{2m} + \dfrac{1}{2} m w^2 \langle \Delta x\rangle^2$

take zero for simplicity

$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2$

$(\Delta x)^2 = \langle x^2\rangle - \cancel{\langle x\rangle}^2$

consists

$\langle H\rangle = \dfrac{\langle p^2\rangle}{2m} + \dfrac{1}{2} m w^2 \langle x^2\rangle$

can never be zero since $\langle p^2\rangle, \langle x^2\rangle > 0$.

$\rightarrow H A^{\dagger}|0\rangle = (A^{\dagger}H + \hbar w A^{\dagger})|0\rangle$

$= A^{\dagger}H|0\rangle + \hbar w A^{\dagger}|0\rangle$

$= A^{\dagger}\tfrac{1}{2}\hbar w|0\rangle + \hbar w A^{\dagger}|0\rangle = \hbar w(\tfrac{1}{2}+1)A^{\dagger}|0\rangle$

Then, $\boxed{E_n = (n+\tfrac{1}{2})\hbar w}$, $n = 0, 1 \ldots$

$\rightarrow |n\rangle = \dfrac{1}{\sqrt{n!}}(A^{\dagger})^n|0\rangle$

$\hookrightarrow A(A^{\dagger})^n|0\rangle = (A^{\dagger}A + \underbrace{[A, A^{\dagger}]}_{1})(A^{\dagger})^{n-1}|0\rangle$

$= (A^{\dagger})^{n-1}|0\rangle + (A^{\dagger}A)(A^{\dagger})^{n-1}|0\rangle$

: etc you know it.

$A(A^{\dagger})^n|0\rangle = n(A^{\dagger})^{n-1}|0\rangle$

→ derivatives, numbers, etc.

$= n(A^{\dagger})^{n-1}|0\rangle + (A^{\dagger})^n \underbrace{A|0\rangle}_{0}$

$\langle 0|\left(\dfrac{d}{dA^{\dagger}}\right)^n (A^{\dagger})^n|0\rangle = n(n-1)\ldots 1 = n!$

A^n

$\downarrow$

$\langle (A^{\dagger})^n 0|(A^{\dagger})^n 0\rangle = n!$ → explains $\dfrac{1}{\sqrt{n!}}$

→ Time dependence of operators

$$i\hbar \frac{d}{dt}|\psi\rangle = H|\psi\rangle \quad \Rightarrow \left| |\psi(t)\rangle = e^{-iHt/\hbar}\,|\psi(0)\rangle \right| \rightarrow \textbf{SCHROEDINGER PICTURE}$$

$$\boxed{e^{-iHt/\hbar} = \sum_{n=0}^{\infty} \frac{1}{n!}\left(-\frac{iHt}{\hbar}\right)^n}$$ ← if you need commutation relations or something.

$$\rightarrow \langle B\rangle_t = \langle \psi(t)|B|\psi(t)\rangle$$
$$= \langle e^{-iHt/\hbar}\psi(0)|\,B\,|e^{-iHt/\hbar}\psi(0)\rangle$$
$$= \langle \psi(0)|\underbrace{e^{iHt/\hbar}\,B\,e^{-iHt/\hbar}}_{B(t)}|\psi(0)\rangle$$ ← (assuming $H^\dagger = H$)

$B(t)$ → **HEISENBERG PICTURE**

where $\boxed{\frac{dB}{dt} = \frac{i}{\hbar}[H, B(t)]}$

Matrices in Quantum Mechanics

→ $L^2|\ell m\rangle = \hbar^2 \ell(\ell+1)|\ell m\rangle$

→ $L_z|\ell m\rangle = \hbar m|\ell m\rangle$

} Recall that S^2 & S_z were very similar.

→ $H|n\rangle = \hbar\omega(n+\frac{1}{2})|n\rangle$ where $|n\rangle = \frac{1}{\sqrt{n!}}(A^\dagger)^n|0\rangle$

→ $A^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$ → creation operator

$A|n\rangle = \sqrt{n}\,|n-1\rangle$ → annihilation operator

} Quantum Harmonic Oscillator

! $\langle m|H|n\rangle = \hbar\omega(n+\frac{1}{2})\langle m|n\rangle = \hbar\omega(n+\frac{1}{2})\delta_{mn}$ → Matrix!

$$\boxed{H = \hbar\omega\begin{pmatrix} \frac{1}{2} & 0 & 0 & \cdots & 0 \\ 0 & \frac{3}{2} & 0 & & \\ \vdots & \vdots & \frac{5}{2} & & \\ 0 & 0 & 0 & & \end{pmatrix}}$$

→ Diagonal matrix with eigenvalues as diagonal entries.

$\forall \quad \langle m|A^{+}|n\rangle = \sqrt{n+1}\,\langle m|n+1\rangle = \sqrt{n+1}\,\delta_{m\,n+1}$

$$A^{+} = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \cdots \\ \vdots & & \sqrt{3} & \ddots \\ & & & 0 \end{pmatrix}$$

diagonal

$\forall \quad \langle m|A|n\rangle = \sqrt{n}\,\langle m|n-1\rangle = \sqrt{n}\,\delta_{m\,n-1}$

$$A = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots \\ & 0 & \sqrt{2} & 0 & \cdots \\ & & 0 & \sqrt{3} & \cdots \\ & & & \ddots & \\ & & & & 0 \end{pmatrix}$$

diagonal

$\rightarrow \quad (FG)_{ij} = \sum_k F_{ik} G_{kj} = (F_{ik})(G_{kj})$

$\rightarrow \quad \boxed{G|j\rangle = \sum_n c_n |n\rangle}$

$\langle m|G|j\rangle = \sum_n c_n \underbrace{\langle m|n\rangle}_{\delta_{mn}} = c_m \quad \Rightarrow \quad \boxed{c_n = \langle n|G|j\rangle}$

$$\boxed{G|j\rangle = \sum_n |n\rangle\langle n|G|j\rangle}$$

$\boxed{\langle i|G|j\rangle = \sum_n \langle i|n\rangle\langle n|G|j\rangle}$ etc.

$$\downarrow$$

$\rightarrow \quad \boxed{\langle i|FG|j\rangle = \sum_n \underbrace{\langle i|F|n\rangle}_{F_{in}}\underbrace{\langle n|G|j\rangle}_{G_{nj}}}$

$\rightarrow \quad \langle m|F|n\rangle^{*} = \langle m|Fn\rangle^{*} = \langle Fn|m\rangle$
$\quad = \langle n|F^{+}|m\rangle$

$$\boxed{F^{*}_{mn} = F^{+}_{nm}}$$

where the definition is coming

$\rightarrow \langle u_n | A | u_m \rangle = \langle u_n | a_m u_m \rangle = a_m \langle u_n | u_m \rangle = a_m \delta_{nm} = a_n$ (basis)

↳ then, A is diagonal and a_n are the eigenvalues.

$\rightarrow A_{mn} = \langle u_m | A | u_n \rangle$

$$|a_m\rangle = \sum_k |u_k\rangle \langle u_k | a_m \rangle$$

new basis

$$\langle a_n | = \sum_\ell \langle a_n | u_\ell \rangle \langle u_\ell |$$

$$\langle a_n | a_m \rangle = \sum_{\ell,k} \langle a_n | u_\ell \rangle \langle u_\ell | u_k \rangle \langle u_k | a_m \rangle$$

$$= \sum_{\ell,k} \langle a_n | u_\ell \rangle \delta_{\ell k} \langle u_k | a_m \rangle$$

$$= \sum_k \langle a_n | u_k \rangle \langle u_k | a_m \rangle = \sum_k u^+_{nk} u_{km} = \delta_{nm}$$

$$\Downarrow$$

$$\boxed{u^+ u = 1}$$

↓ unitary matrix (definition)

$$\langle a_n | A | a_m \rangle = \sum_{\ell,k} \langle a_n | u_\ell \rangle \langle u_\ell | A | u_k \rangle \langle u_k | a_m \rangle$$

$\langle a_n | A | a_m \rangle = A_{nm}$ ↓ we want this to be diagonal

$\langle a_n | u_\ell \rangle = \langle u_\ell | a_n \rangle^* = u^*_{\ell n} \equiv u^+_{n\ell}$

$\langle u_\ell | A | u_k \rangle = A_{\ell k}$

$\langle u_k | a_m \rangle = u_{km}$

$$A_{nm} = \sum_{\ell,k} u^+_{n\ell} A_{\ell k} u_{km}$$

since diagonal ↓

$$a_m \delta_{mn} = \sum_{\ell,k} u^+_{n\ell} A_{\ell k} u_{km}$$

Similarity transformations

! Then, if you find some u to diagonalize A, $\boxed{A' = u^+ A u}$ equal $\boxed{u A' u^+ = A}$

(remember: to find u, write orthonormal eigenvectors side by side)

Matrix Mechanics

$\forall\ |\psi\rangle = A|\phi\rangle$

$$\boxed{\langle i|\psi\rangle = \langle i|A|\phi\rangle}$$

column vector

$$= \sum_n \langle i|A|n\rangle\langle n|\phi\rangle$$

column vector : $\langle 1|\phi\rangle \to \alpha_1$
$\langle 2|\phi\rangle \to \alpha_2$
$\vdots$
$\langle k|\phi\rangle \to \alpha_k$
$\vdots$

$\beta_1 \leftarrow \langle 1|\psi\rangle$
$\beta_2 \leftarrow \langle 2|\psi\rangle$
$\vdots$
$\beta_k \leftarrow \langle k|\psi\rangle$
$\vdots$

Then, $\boxed{\beta_i = \sum_n A_{in}\alpha_n}$

! $\langle n|\phi\rangle^* = \langle\phi|n\rangle \longrightarrow (\alpha_1^*, \alpha_2^*, \ldots, \alpha_k^*, \ldots)$

$\hookrightarrow \langle\phi|\psi\rangle = \sum_n \langle\phi|n\rangle\langle n|\psi\rangle = \sum_n \alpha_n^*\beta_n = (\alpha_1^*\ \alpha_2^* \cdots)\begin{pmatrix}\beta_1\\ \beta_2\\ \vdots\end{pmatrix}$

! $\langle\psi|Q|\psi\rangle = \sum_{n,m} \underbrace{\langle\psi|n\rangle}_{\beta_n^*}\underbrace{\langle n|Q|m\rangle}_{Q_{nm}}\underbrace{\langle m|\psi\rangle}_{\beta_m} = \langle Q\rangle$

matrix öğrenip QM unuttuğumuzun kanıtı.

! $A|\phi\rangle = a|\phi\rangle$

eigenvalue eqn!

$$\boxed{\sum_n A_{in}\alpha_n = a\alpha_i} \to = \sum_n a\,\delta_{in}\alpha_n$$

$$\begin{pmatrix} A_{11}-a & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22}-a & A_{23} & \cdots \\ & & \ddots & \\ & & & \ddots \end{pmatrix}\begin{pmatrix}\alpha_1\\ \alpha_2\\ \vdots\end{pmatrix} = 0 \Rightarrow \boxed{\det(A_{in} - a\,\delta_{in}) = 0}$$

! you have $(2l+1)$ or $(2s+1)$ as matrix dim.

$l=1 \rightarrow L_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$

$l=1 \rightarrow L_+ = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix}$, $L_- = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$

$\Rightarrow L_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$, $L_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$.

! $s = \frac{3}{2}$

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

$2s+1 = 4\times 4$ matrices! $S_x = ?$

$S_+ = \hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}$ $\quad S_- = \hbar \begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$

we'll have

eigenstates of S_z

$|\frac{3}{2} \; \frac{3}{2}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

$|\frac{3}{2} \; \frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$|\frac{3}{2} \; \frac{-1}{2}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$

$|\frac{3}{2} \; \frac{-3}{2}\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$

$S_+ |\frac{3}{2} \; \frac{3}{2}\rangle = 0$

$S_+ |\frac{3}{2} \; \frac{1}{2}\rangle = \sqrt{3}\hbar \, |\frac{3}{2} \; \frac{3}{2}\rangle$

$S_+ |\frac{3}{2} \; \frac{-1}{2}\rangle = 2\hbar \, |\frac{3}{2} \; \frac{1}{2}\rangle$

$S_+ |\frac{3}{2} \; \frac{-3}{2}\rangle = \sqrt{3}\hbar \, |\frac{3}{2} \; \frac{-1}{2}\rangle$

$S_- |\frac{3}{2} \; \frac{3}{2}\rangle = \quad |\frac{3}{2} \; \frac{1}{2}\rangle$

etc

Then, $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$ → what are the eigenvalues?

$\det(S_x - \lambda I) = 0$

$$\begin{vmatrix} -\lambda & \sqrt{3} & 0 & 0 \\ \sqrt{3} & -\lambda & 2 & 0 \\ 0 & 2 & -\lambda & \sqrt{3} \\ 0 & 0 & \sqrt{3} & -\lambda \end{vmatrix} = -\lambda \cdot \begin{vmatrix} -\lambda & 2 & 0 \\ 2 & -\lambda & \sqrt{3} \\ 0 & \sqrt{3} & -\lambda \end{vmatrix} - \sqrt{3}\begin{vmatrix} \sqrt{3} & 0 & 0 \\ 2 & -\lambda & \sqrt{3} \\ 0 & \sqrt{3} & -\lambda \end{vmatrix}$$

$$= -\lambda\left[-\lambda^3 + 3\lambda + 4\lambda\right] - \sqrt{3}\left[\sqrt{3}\lambda^2 - 3\sqrt{3}\right] = \lambda^4 - 7\lambda^2 - 3\lambda^2 + 9$$

$$= \lambda^4 - 10\lambda^2 + 9 = 0$$

$$\left.\begin{matrix} \lambda^2 = 9 \\ \lambda^2 = 1 \end{matrix}\right\} \lambda = \pm 1, \pm 3$$

$\Rightarrow$ eigenvalues: $\boxed{\pm\frac{\hbar}{2}, \pm\frac{3\hbar}{2}}$ as expected.

$\boxed{\text{HW}}$ Find the eigenvectors of S_x.

The Interaction of the Charged Particles with the Electromagnetic Field

Maxwell's
- $\nabla \cdot \vec{B} = 0$ (there is no magnetic monopoles)
- $\nabla \cdot \vec{E} = \frac{\rho}{\varepsilon_0}$ (source of the electric field are the charges)

Faraday's
- $\nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0$

Ampere's
- $\nabla \times \vec{B} = \mu_0 \vec{J}$ (source of the magnetic field is the current density)

$\nabla \times \vec{B} = \mu_0 \vec{J} + \frac{1}{c^2}\frac{\partial \vec{E}}{\partial t}$ (Modified Ampere's law)

- $\boxed{\underbrace{\frac{\partial}{\partial t}\rho}_{\text{charge density}} + \nabla \cdot \underbrace{\vec{J}}_{\text{current density}} = 0} \rightsquigarrow \frac{d}{dt}\underbrace{\int_{\mathcal{V}} \rho\, d^3r}_{\text{charge}} = -\oint_S d\vec{a} \cdot \vec{J}$

- Lorentz Force : $\boxed{m_e \frac{d^2\vec{r}}{dt^2} = -e\left[\vec{E} + \vec{v}\times\vec{B}\right]}$

- $\boxed{\vec{B} = \nabla \times \vec{A}}$ since $\nabla\cdot\vec{B} = \nabla\cdot(\nabla\times\vec{A}) = 0,\ \forall\vec{A}$.

vector potential

- $\vec{E} + \frac{\partial\vec{A}}{\partial t} = -\nabla\phi$ since $\nabla\times\vec{E} + \frac{\partial\vec{B}}{\partial t} = \nabla\times\vec{E} + \frac{\partial}{\partial t}(\nabla\times\vec{A}) = \nabla\times\left(\vec{E} + \frac{\partial\vec{A}}{\partial t}\right)$

scalar potential

$$\boxed{\vec{E} = -\nabla\phi - \frac{\partial\vec{A}}{\partial t}}$$

! Let $\boxed{\vec{A}' = \vec{A} - \nabla g(\vec{r},t)}$.

$\vec{B}' = \underbrace{\nabla\times\vec{A}' = \nabla\times\vec{A} - \nabla\times\nabla g = \nabla\times\vec{A} = \vec{B}}_{\text{nothing changed for magnetic field}}$

Gauge transformation for magnetic field. → Gauge invariance

Let $\boxed{\phi' = \phi + \frac{\partial g}{\partial t}}$.

$$\vec{E}' = -\nabla\phi' - \frac{\partial\vec{A}'}{\partial t} = -\nabla\phi - \nabla\frac{\partial g}{\partial t} - \frac{\partial\vec{A}}{\partial t} + \frac{\partial}{\partial t}\nabla g$$

$$= -\nabla\phi - \frac{\partial\vec{A}}{\partial t} - \nabla\frac{\partial g}{\partial t} + \frac{\partial}{\partial t}\nabla g$$

they commute

$= \vec{E}$ → Gauge invariance

Gauge transformation for electric field

HW. Radial Schroedinger equation, $V=0$ & $V=-V_0$ — solve. Check Gasiorowicz, 2nd edt

! $\nabla\cdot\vec{E} = \nabla\cdot\left(-\nabla\phi - \frac{\partial\vec{A}}{\partial t}\right) = \frac{\rho}{\varepsilon_0}$ ← Maxwell

$$-\nabla^2\phi - \frac{\partial}{\partial t}\nabla\cdot\vec{A} = \frac{\rho}{\varepsilon_0}$$

Arrange the potential to let $\boxed{\nabla\cdot\vec{A} = 0}$ → $\boxed{\nabla^2\phi = \frac{-\rho}{\varepsilon_0}}$: Poisson equation

Coulomb Gauge

$$\phi = \frac{1}{4\pi\varepsilon_0}\int\frac{\rho\, d^3x'}{|x-x'|}$$

! $\nabla\times(\nabla\times\vec{A}) - \frac{1}{c^2}\frac{\partial}{\partial t}\left(-\nabla\phi - \frac{\partial\vec{A}}{\partial t}\right) = \mu_0\vec{J}$ ← Faraday

$$\nabla(\nabla\cdot\vec{A}) - \nabla^2\vec{A} - \frac{1}{c^2}\left[-\nabla\frac{\partial\phi}{\partial t} - \frac{\partial^2\vec{A}}{\partial t^2}\right] = \mu_0\vec{J}$$

$$\nabla\left(\underbrace{\nabla\cdot\vec{A} + \frac{1}{c^2}\frac{\partial\phi}{\partial t}}\right) - \nabla^2 A + \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = \mu_0\vec{J}$$

fix this to zero : Lorentz Gauge : $\nabla\cdot\vec{A} + \frac{1}{c^2}\frac{\partial\phi}{\partial t} = 0$

$$\rightarrow \boxed{-\nabla^2 A + \frac{1}{c^2}\frac{\partial^2\vec{A}}{\partial t^2} = \mu_0\vec{J}} \quad (1)$$

: nonhomogeneous wave equation for the vector potential

- Insert L.G. into C.G :

$$-\nabla^2\phi - \frac{\partial}{\partial t}\left(\frac{-1}{c^2}\frac{\partial\phi}{\partial t}\right) = \frac{\rho}{\varepsilon_0} \equiv \boxed{-\nabla^2\phi + \frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = \frac{\rho}{\varepsilon_0}} \quad (2)$$

: nonhomogeneous wave equation for the scalar potential.

→ Notice that under these conditions, (1) & (2) are independent!

- Hamiltonian equation (classical mechanics)

$$\rightarrow \frac{dx_i}{dt} = \frac{\partial H}{\partial p_i}, \quad \frac{dp_i}{dt} = \frac{-\partial H}{\partial x_i}$$

$$H = \frac{p^2}{2m} + V(x) \Rightarrow \frac{dp_i}{dt} = \frac{-\partial V}{\partial x}$$

$$\Rightarrow m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

Nonrelativistic charged particle interacting with EM field.

$\dot{x}_i$ here

$$\rightarrow H = p_i\dot{q}_i - L, \quad p_i = \frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial \dot{x}_i}$$

momentum, position, Lagrangian; here

$$\boxed{L = \frac{m\dot{x}_i\dot{x}_i}{2} + q\,A_i\dot{x}_i - q\phi_i}$$

kinetic energy; relativistic electrodynamics; potential energy

Then, $H = \underbrace{(m\dot{x}_i + q\cdot A_i)}_{p_i}\cdot\underbrace{\dot{x}_i}_{\dot{q}_i} - \frac{m\dot{x}_i\dot{x}_i}{2} - q\cdot A_i\dot{x}_i + q\phi_i$

$$\boxed{H = \frac{m\dot{x}_i\dot{x}_i}{2} + q\phi_i}, \quad \boxed{p_i = m\dot{x}_i + q\cdot A_i}$$

canonical momentum

Then, $H = \frac{m}{2}\left(\frac{p_i - q\cdot A_i}{m}\right)^2 + q\phi_i = \boxed{\frac{1}{2m}(p_i - qA_i)^2 + q\phi_i = H}$

General Hamiltonian for a charged particle interacting with EM field.

$\rightarrow$ $i\hbar \frac{\partial \Psi}{\partial t} = H \Psi$

$$\boxed{i\hbar \frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m_e}(-i\hbar\nabla + e\vec{A})^2 - e\phi\right] \Psi(\vec{r},t)}$$

Schrödinger equation for a charged particle interacting with em.

$\rightarrow$ Gauge transformation: let $\vec{A}' = \vec{A} - \nabla g$, $\phi' = \phi + \frac{\partial g}{\partial t}$.

Recall that $\Psi'(\vec{r},t) = e^{i\Omega(\vec{r},t)} \cdot \Psi(\vec{r},t)$ (phase is unknown)

↑ If you insert a solenoid in front of the double slit, a phase shift occurs. This is due to that.

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[\frac{1}{2m_e}(-i\hbar\nabla + e\vec{A}' + e\nabla g)^2 - e\phi' + e\frac{\partial g}{\partial t}\right] \Psi$$

$$\left(\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left(e^{-i\Omega}\Psi'\right) = -i\frac{\partial \Omega}{\partial t}\underbrace{(e^{-i\Omega}\Psi')}_{\Psi} + e^{-i\Omega}\frac{\partial \Psi'}{\partial t} \right)$$

$$i\hbar \cancel{e^{-i\Omega}}\left[-i\underbrace{\frac{\partial \Omega}{\partial t}} + \frac{\partial}{\partial t}\right]\Psi' = \left[\frac{1}{2m_e}\left(e^{-i\Omega}(-\hbar\nabla\Omega - i\hbar\nabla + e\vec{A}' + e\nabla g)\right)^2 - e\phi' + e\underbrace{\frac{\partial g}{\partial t}}\right]\Psi' \cancel{e^{-i\Omega}}$$

If the Schroedinger eqn is Gauge invariant, 2 conditions must hold:

$$1 \rightarrow \boxed{\hbar \frac{\partial \Omega}{\partial t} = e\frac{\partial g}{\partial t}}$$

$$\left(-i\hbar\nabla\Psi = e^{-i\Omega}\left[-\hbar\nabla\Omega - i\hbar\nabla\right]\Psi'\right)$$

$$2 \rightarrow \boxed{\hbar\nabla\Omega = e\nabla g}$$

Under these condition, we'll have

$$i\hbar\frac{\partial \Psi'}{\partial t} = \left[\frac{1}{2m_e}(-i\hbar\nabla + eA')^2 - e\phi'\right]\Psi' \rightarrow$$ Schroedinger equation invariant under Gauge transformations.

$$(1) \,\&\, (2): \boxed{\Omega = \frac{e}{\hbar} g}$$

→ Let us open the paranthesis :

$$(-i\hbar\nabla+e\vec{A})\cdot(-i\hbar\nabla+e\vec{A})\psi=-\hbar^2\nabla^2\psi-i\hbar e\nabla\cdot(\vec{A}\psi)-i\hbar e\vec{A}\cdot\nabla\psi+e^2A^2\psi$$

$$=-\hbar^2\nabla^2\psi-i\hbar e\left[\underbrace{\cancel{(\nabla\cdot\vec{A})}^{0}}_{\text{coulomb gauge}}\psi+\vec{A}\cdot\nabla\psi\right]-i\hbar e\vec{A}\cdot\nabla\psi+e^2A^2\psi$$

$$=-\hbar^2\nabla^2\psi-2i\hbar e\vec{A}\cdot\nabla\psi+e^2A^2\psi$$

Then, since $\Psi(\vec{r},t)=e^{iEt/\hbar}\cdot\psi(\vec{r})$,

$$\boxed{\frac{-\hbar^2}{2m_e}\nabla^2\psi-\frac{i\hbar e}{m_e}\vec{A}\cdot\nabla\psi+\frac{e^2}{2m_e}|\vec{A}|^2\psi-e\phi\psi=E\psi}$$

T.I. Schroedinger equation for the charged particle interacting with the emf with **Coulomb** gauge.

Coulomb potential → $\phi=\frac{-Ze}{4\pi\varepsilon_0 r}$

For constant magnetic field, $\boxed{\vec{A}=-\frac{1}{2}(\vec{r}\times\vec{B})}$

↳ $\vec{B}=\nabla\times\vec{A}$, $\vec{A}=\frac{-1}{2}\begin{vmatrix}\hat{i}&\hat{j}&\hat{k}\\x&y&z\\B_x&B_y&B_z\end{vmatrix}=\frac{-1}{2}\left[(yB_z-zB_y)\hat{i}+(zB_x-xB_z)\hat{j}+(xB_y-yB_x)\hat{k}\right]$

Then, $\vec{B}=\frac{-1}{2}\begin{vmatrix}\hat{i}&\hat{j}&\hat{k}\\\partial_x&\partial_y&\partial_z\\A_x&A_y&A_z\end{vmatrix}=\frac{-1}{2}\left(-2B_x\hat{i}-2B_y\hat{j}-2B_z\hat{k}\right)$

$\vec{B}=B_x\hat{i}+B_y\hat{j}+B_z\hat{k}=\vec{B}$ (a very meaningful equality)

For Coulomb gauge ($\nabla\cdot\vec{A}=0$), constant magnetic field & $\vec{A}=\frac{-1}{2}(\vec{r}\times\vec{B})$,

$$\frac{-\hbar^2}{2m_e}\nabla^2\psi-\frac{i\hbar e}{m_e}\vec{A}\cdot\nabla\psi+\frac{e^2}{2m_e}|\vec{A}|^2\psi-e\phi\psi=E\psi$$

→ $-\frac{i\hbar e}{m_e}\left(\frac{-1}{2}\vec{r}\times\vec{B}\right)\nabla\psi=\frac{-i\hbar e}{2m_e}\vec{B}\cdot(\vec{r}\times\nabla\psi)=\frac{e}{2m_e}\vec{B}(\vec{r}\times\underbrace{(-i\hbar\nabla\psi)}_{\vec{P}})$

$\sum_i\sum_{jk}\varepsilon_{ijk}r_jB_k\partial_i\psi$

$=\varepsilon_{kij}r_jB_k\partial_i\psi=-\varepsilon_{kji}r_jB_k\partial_i\psi=-\varepsilon_{kji}r_j\partial_i\psi B_k$

$=-(\vec{r}\times\nabla\psi)\cdot\vec{B}$

Here, $\frac{-i\hbar e}{m_e}\left(\frac{-1}{2}\vec{r}\times\vec{B}\right)\nabla\psi = \frac{e}{2m_e}(\vec{B}\cdot\vec{L})\psi$

$$\longrightarrow \frac{e^2}{2m_e}\left|\frac{-1}{2}(\vec{r}\times\vec{B})\right|^2\psi = \frac{e^2}{8m_e}r^2B^2\sin^2\theta\,\psi = \frac{e^2}{8m_e}\underbrace{r^2B^2(1-\cos^2\theta)}_{r^2B^2-(\vec{r}\cdot\vec{B})^2}\psi$$

Let $\vec{B}=B\hat{k}$ $\longrightarrow$ $r^2B^2-(\vec{r}\cdot\vec{B})^2 = (x^2+y^2+z^2)B^2 - z^2B^2$

$$= (x^2+y^2)B^2$$

$$\Rightarrow \frac{e^2}{2m_e}\left|\frac{-1}{2}(\vec{r}\times\vec{B})\right|^2\psi = \frac{e^2}{8m_e}(x^2+y^2)B^2\psi$$ — did you see the Harmonic osc?

$\longrightarrow$ Schroedinger equation becomes:

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi + \frac{e}{2m_e}\vec{B}\cdot\vec{L}\psi + \frac{e^2B^2}{8m_e}(x^2+y^2)\psi - \underbrace{e\phi\psi}_{\text{take this as zero.}} = E\psi$$

Coordinate change: $x=\rho\cos\phi$, $y=\rho\sin\phi$

propose a solution: $\psi(r)=U_m(\rho)e^{im\phi}e^{ikz}$

$$\nabla = \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\underbrace{\frac{\partial^2}{\partial\phi^2}}_{-m^2} + \underbrace{\frac{\partial^2}{\partial z^2}}_{-k^2} \quad \text{(cylindrical)}$$

make some arrangements (check!):

HW $\Rightarrow$
$$\frac{d^2U_m}{d\rho^2} + \frac{1}{\rho}\frac{dU_m}{d\rho} - \frac{m^2}{\rho}U_m - \frac{e^2B^2}{4\hbar^2}\rho^2U_m + \left(\frac{2m_eE}{\hbar^2} - \frac{eB\hbar m}{\hbar^2} + k^2\right)U_m = 0$$

$\longrightarrow$ Let $\boxed{X=\sqrt{\frac{eB}{2\hbar}}\,\rho}$ $\Rightarrow dX = \sqrt{\frac{eB}{2\hbar}}\,d\rho$ $\longrightarrow$ plug it in:

$$\frac{d^2U_m}{dx^2} + \frac{1}{x}\frac{dU_m}{dx} - \frac{m^2}{x^2}U_m - x^2U_m + \lambda U_m = 0$$

$$\boxed{\lambda = \frac{4m_e}{eB\hbar}\left(E - \frac{\hbar^2k^2}{2m_e}\right) - 2m}$$

* $U_m(x\to\infty)$: $\frac{dU_m^2}{dx^2} - x^2U_m = 0 \Rightarrow U_m(x)\sim e^{-x^2/2}$
* $U_m(x\to 0)$: $\frac{d^2U_m}{dx^2} + \frac{1}{x}\frac{dU_m}{dx} - \frac{m^2}{x^2}U_m = 0 \Rightarrow U_m(x)\sim x^{|m|}$

Then, $U_m(x) = x^{|m|} e^{-x^2/2} G(x)$ $\longrightarrow$ plug it into the D.E.:

$$\frac{d^2G}{dx^2} + \left(\frac{2|m|+1}{x} - 2x\right)\frac{dG}{dx} + (\lambda - 2 - 2|m|)G = 0$$

$\rightarrow$ Let $y = x^2 \rightarrow dy = 2x\,dx$ $\rightarrow$ plug it in:

$$\underbrace{\frac{d^2G}{dy^2} + \left(\frac{|m|+1}{y} - 1\right)\frac{dG}{dy} + \frac{\lambda - 2 - 2|m|}{4y}\,G = 0}$$

exactly like Hydrogen atom! plug the solution:

$$\frac{\lambda}{4} - \frac{1+|m|}{2} = n_r \;, \quad n_r = 0, 1, \ldots$$

$$\boxed{E - \frac{\hbar^2 k^2}{2m_e} = \frac{eB\hbar}{2m_e}(2n_r + 1 + |m| + m)}$$: quantized!

and $G(r)$ are the Laguerre polynomials,

$$G(r) = L_n^{m}(y)$$

Landau Levels

$\rightarrow$ Let $\vec{B} = B_z\hat{k}$, $\vec{A} = \frac{-1}{2}(\vec{r}\times\vec{B}) = \frac{-1}{2}\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ 0 & 0 & B_z \end{vmatrix} = \frac{-1}{2}(yB_z\hat{i} - xB_z\hat{j})$

$$= \frac{-1}{2}yB_z\hat{i} + \frac{1}{2}xB_z\hat{j}$$

$$\boxed{\vec{A} = \left(\frac{-yB}{2}, \frac{xB}{2}, 0\right)}$$

$\rightarrow$ Let $\vec{A}' = \vec{A} - \nabla g$

$$\left(\frac{-yB}{2}, \frac{xB}{2}, 0\right) = \underbrace{(0, xB, 0)}_{\text{easier!}} - \nabla\left(\frac{yxB}{2}\right)$$

$\rightarrow$ Hamiltonian: $H = \frac{1}{2m_e}\left(\vec{P} - (-e)\vec{A}\right)^2 = \frac{1}{2m_e}\left(P_x\hat{i} + (P_y + eBx)\hat{j} + P_z\hat{k}\right)^2$

$$= \frac{1}{2m_e}\left(P_x^2 + P_y^2 + P_z^2 + 2P_y eBx + e^2B^2x^2\right)$$

$\rightarrow$ TISE : $H\Psi = E\Psi$. assume only motion is in the xy plane

$P_z|n\rangle = 0|n\rangle$, $[H, P_z] = 0$

$P_y|n\rangle = \hbar k|n\rangle$, $[H, P_y] = 0$

$$\Psi(x,y) = e^{iky}V(x).$$

$$\frac{1}{2m_e}\left(-\hbar^2\frac{d^2}{dx^2}+e^2B^2\left(x+\frac{\hbar k}{eB}\right)^2\right)V(x)=E\,V(x)$$ — Harmonic oscillator!

Same shifted term, $x_0=\frac{\hbar k}{eB}$ shifted by equilibrium pos.

$$\Rightarrow \psi(x,y)=e^{iky}V(x)=e^{i\frac{eBx_0}{\hbar}y}\,u(x-x_0)$$

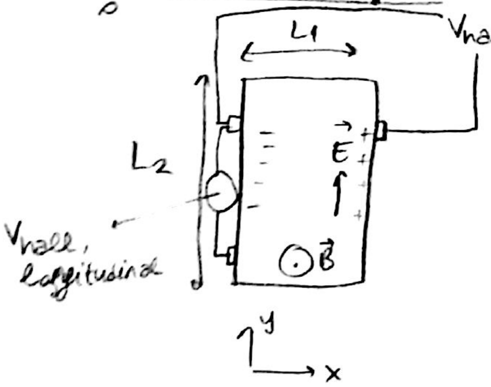
$u(x-x_0)$: solution of the H.O

$$\boxed{E=\hbar\omega\left(n+\frac{1}{2}\right),\quad \omega=\frac{eB}{m_e}}$$

same with the previous solution when $m=0$.

↓ Landau levels!

QM Hall effect



$$\psi(y)=\psi(y+L_2)\rightarrow e^{i\frac{eBx_0}{\hbar}y}$$

$$\rightarrow \frac{eBx_0L_2}{\hbar}=2\pi n^*,\quad n^*=0,1,2\dots$$

$$\rightarrow 0\le x_0\le L_1 \quad\Rightarrow\quad 0\le n^*\le\frac{eB}{2\pi\hbar}L_1L_2$$

L_1L_2: area; ℓ_B^2: magnetic length

degeneracy: $\boxed{n^*_{max}=\frac{L_1L_2}{2\pi\ell_B^2}}$

$$\boxed{\ell_B=\frac{25.6\cdot10^{-10}}{\sqrt{B(\text{tesla})}}\,m}$$

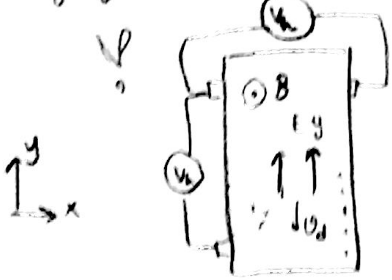
notice: $\hbar\omega=\hbar\left(\frac{eB}{m_e}\right)=\boxed{\frac{\hbar^2}{m_e\ell_B^2}=\hbar\omega}$ — energy spacing of Landau levels

$(n^*_{max}=n_BL_1L_2)$ $\Rightarrow n_B=2\pi\ell_B^2$

HW

Integral QMHE (google)

$$\vec{J}_{x,y}=\sigma_{x,y}\vec{E}_{x,y}\rightarrow \frac{\sigma_x}{\sigma_y}(n_B),\quad \sigma=\frac{n_ee^2\tau_0}{m_e^*}\rightarrow n_e=f\,n_B$$



$$J_y=\sigma_0E_y,\quad \sigma_0=\frac{n_ee^2\tau_0}{m_e^*}$$

n_e: density of free electrons; τ_0: mean collision time; m_e^*: effective mass

$$\vec{F}=\frac{\overbrace{-en_e\vec{v}}^{\vec{J}}\times\vec{B}}{n_e}=\frac{\vec{J}\times\vec{B}}{n_e}=-e\vec{E}'$$

$$\vec{J}=\sigma_0\left(\vec{E}-\frac{\vec{J}\times\vec{B}}{n_e\cdot e}\right)\Rightarrow J_x=-\sigma_0\frac{J_yB}{n_ee}=-\frac{e\tau_0}{m_e^*}J_yB$$

$$\Rightarrow J_y=\sigma_0\left(E_y+\frac{J_xB}{n_e\cdot e}\right)=\sigma_0E_y+\frac{e\tau_0}{m_e^*}J_xB$$

$$J_y = \sigma_0 E_y + \frac{e\tau_0}{m_e^*} B \cdot \left(\frac{-e\tau_0}{m_e} J_y B \right) = \sigma_0 E_y - \frac{e^2 \tau_0^2}{m_e^{*2}} B^2 J_y$$

$$\boxed{J_y = \frac{\sigma_0 E_y}{1 + \left(\frac{e\tau_0 B}{m_e^*} \right)^2}}$$

some kind of σ_0

Notice that $\frac{\vec{J} \times \vec{B}}{ne} = -e\vec{E} \equiv \frac{JB}{ne} = -eE \equiv J = \left(\frac{-ene}{B} \right) E$

$$J_y = \sigma_0 E_y + \sigma_0 J_x \frac{B}{n_e e} = \sigma_0 E_y - J_x \Rightarrow J_x = \sigma_0 E_y - J_y$$

$$\boxed{J_x = \left(\frac{-en_e}{B} \right) E_y \cdot \frac{\left(\frac{e\tau_0 B}{m_e^*} \right)^2}{1 + \left(\frac{e\tau_0 B}{m_e^*} \right)^2}}$$

Landau levels $\longrightarrow \Delta E = \hbar\omega = \hbar \underbrace{\frac{eB}{m_e}}_{\frac{\hbar^2}{m_e l_B^2}}$, $l_B^2 = \frac{\hbar^2}{eB}$

Look at the Google, find some simulation, σ_{xx}, σ_{yx}

$$n_B = \frac{eB}{2\pi\hbar} = \frac{1}{2\pi l_B^2}$$

full states of Landau levels

$n_e = \underset{1,2,\dots}{f} n_B \rightarrow \tau_0 \rightarrow \infty$

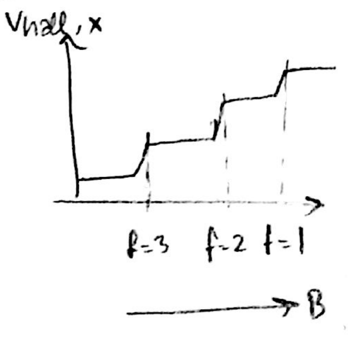
integer; density of the full states

$\Rightarrow J_x$ will be constant

$\Rightarrow V_{h,x}$ will be constant.

$\Rightarrow J_y$ will be zero

$\Rightarrow V_{h,y}$ will be zero.



! Additional comment on gauge invariance

$\vec{B} = B\hat{k}$, $0 \le \rho \le a$

Flux: $\int_0^a d\vec{s} \cdot \vec{B} = \int_0^a d\vec{s} \cdot \nabla \times \vec{A}$

$$\Phi = \pi a^2 B = \oint \vec{A} \cdot d\vec{l} = A_\phi \cdot 2\pi\rho \rightarrow A_\phi = \frac{\Phi}{2\pi\rho} = \frac{\pi a^2 B}{2\pi\rho}$$, true for also $\rho > a$.

no magnetic field yes scalar potential $\Rightarrow A_\phi = \nabla g = \frac{1}{\rho} \frac{dg}{d\phi}$, $\rho > a$

$\vec{B} = \nabla \times \nabla g = 0$.

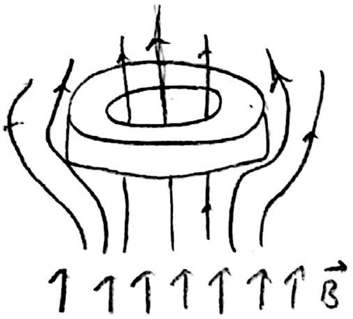
Equate both: $\frac{1}{\rho}\frac{dg}{d\phi} = \frac{\Phi}{2\pi\rho} \Rightarrow \boxed{g = \frac{\Phi}{2\pi}\cdot\phi}$

remember: $e^{i\Omega} = e^{i\frac{e}{\hbar}g}$

Then, $e^{i\Omega} = e^{i\frac{e}{\hbar}\frac{\Phi}{2\pi}\phi} \Rightarrow \boxed{\frac{e\Phi}{2\pi\hbar} = n} \Rightarrow$ Magnetic flux is quantized!

$\boxed{\Phi = \frac{2\pi n\hbar}{e}}$ $n = 1, 2, 3$

used in superconductivity



$T < T_c$: Meissner effect

$q=-e$

$$H = \frac{1}{2m}(\vec{P}-q\vec{A})\cdot(\vec{P}-q\vec{A}) + q\phi$$

$$= \frac{1}{2m}\left[P^2 - q(\vec{P}\cdot\vec{A}+\vec{A}\cdot\vec{P}) + q^2A^2\right] + q\phi$$

$$\rightarrow [H,x] = \frac{1}{2m}[P^2,x] - \frac{q}{2m}[(\vec{P}\cdot\vec{A})+(\vec{A}\cdot\vec{P}),x]$$

$$= \frac{1}{2m}[P_x^2,x] - \frac{q}{2m}[P_xA_x,x] - \frac{q}{2m}[A_xP_x,x]$$

$$= \frac{1}{2m}\Big(P_x\underbrace{[P_x,x]}_{-i\hbar} + \underbrace{[P_x,x]}_{-i\hbar}P_x\Big) - \frac{q}{2m}\Big(P_x\cancel{[A_x,x]}^{0} + \underbrace{[P_x,x]}_{-i\hbar}A_x\Big) - \frac{q}{2m} \sim \text{similar}$$

$$= -\frac{i\hbar}{m}P_x - \frac{qi\hbar}{m}A_x = \boxed{-\frac{i\hbar}{m}(P_x - qA_x)}$$

Then, $\langle[H,\vec{r}]\rangle\frac{i}{\hbar} = \boxed{\frac{\partial}{\partial t}\langle\vec{r}\rangle = \frac{1}{m}\langle(\underbrace{\vec{P}-q\vec{A}}_{\text{canonical momentum}})\rangle}$

$$\rightarrow \frac{d}{dt}\langle\vec{v}\rangle = \frac{i}{\hbar}\langle[H,\vec{v}]\rangle + \underbrace{\left\langle\frac{\partial\vec{v}}{\partial t}\right\rangle}_{\left\langle-\frac{q}{m}\frac{\partial\vec{A}}{\partial t}\right\rangle}$$

$$H = \frac{1}{2}m\overbrace{v}^{p-qA}{}^2 + q\phi \Rightarrow [H,v] = \frac{m}{2}[v^2,v] + q\underbrace{[\phi,v]}_{\frac{1}{m}[\phi,p]}$$

- $\frac{1}{m}[\phi, P_x] = \frac{-1}{m}\frac{\hbar}{i}\frac{\partial \phi}{\partial x} \Rightarrow \frac{1}{m}[\phi, \vec{P}] = \frac{i\hbar}{m}\nabla\phi$

- $[H, \vartheta] = \frac{m}{2}[\vartheta^2, \vartheta] + \frac{q}{m} i\hbar \nabla\phi$

- $[\vartheta^2, \vartheta] \longrightarrow [(\vartheta_x^2 + \vartheta_y^2 + \vartheta_z^2), \vartheta_x] = [\vartheta_y^2, \vartheta_x] + [\vartheta_z^2, \vartheta_x]$

$$= \vartheta_y[\vartheta_y, \vartheta_x] + [\vartheta_y, \vartheta_x]\vartheta_y + \vartheta_z[\vartheta_z, \vartheta_x] + [\vartheta_z, \vartheta_x]\vartheta_z$$

commute

- $[\vartheta_y, \vartheta_x] = \frac{1}{m^2}[(P_y - qA_y), (P_x - qA_x)]$ commute like $[\phi, P_x]$

$$= \frac{-q}{m^2}\left([P_y, A_x] + [A_y, P_x]\right)$$

$$= \frac{-q}{m^2}\left(-i\hbar\frac{\partial A_x}{\partial y} + i\hbar\frac{\partial A_y}{\partial x}\right)$$

$$= -\frac{i\hbar q}{m^2}(\nabla \times \vec{A})_z = \frac{-i\hbar q}{m^2} B_z$$

$$\Rightarrow [\vartheta^2, \vartheta_x] = \frac{i\hbar q}{m^2}\left[-\vartheta_y B_z - B_z\vartheta_y + \vartheta_z B_y + B_y\vartheta_z\right]$$

$$= \frac{i\hbar q}{m^2}\left[-(\vec{\vartheta}\times\vec{B})_x + (\vec{B}\times\vec{\vartheta})_x\right]$$

$$\Rightarrow \frac{d}{dt}\langle\vec{\vartheta}\rangle = \frac{i}{\hbar}\left\langle\left(\frac{m}{2}\frac{iq\hbar}{m^2}\left(-(\vec{\vartheta}\times\vec{B}) + (\vec{B}\times\vec{\vartheta})\right)\right) + \frac{q\, i\hbar}{m}\nabla\phi\right\rangle + \left\langle\frac{-q}{m}\frac{\partial\vec{A}}{\partial t}\right\rangle$$

$$\boxed{m\frac{d}{dt}\langle\vec{\vartheta}\rangle = \frac{q}{2}\left(\langle\vec{\vartheta}\times\vec{B}\rangle - \langle\vec{B}\times\vec{\vartheta}\rangle\right) + q\langle\underbrace{-\nabla\phi - \frac{\partial\vec{A}}{\partial t}}_{\vec{E}}\rangle}$$ → almost Lorentz

actual **Ehrenfest Thm.**

If $\vec{B}$ is uniform, $\vec{\vartheta}\times\vec{B} = -\vec{B}\times\vec{\vartheta}$,

$$\boxed{m\frac{d}{dt}\langle\vec{\vartheta}\rangle = q\langle\vec{\vartheta}\times\vec{B}\rangle + q\langle\vec{E}\rangle}$$ ← **Lorentz force.**

IDENTICAL PARTICLES

Two Particle Systems

$\rightarrow \Psi = (\vec{r}_1, \vec{r}_2, t)$, $i\hbar \frac{\partial \Psi}{\partial t} = H\Psi$

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

$\longrightarrow \int |\Psi(\vec{r}_1, \vec{r}_2, t)|^2 \, d^3r_1 \, d^3r_2 = 1$

Time dependent form: $\Psi(\vec{r}_1, \vec{r}_2, t) = \Psi(\vec{r}_1, \vec{r}_2) e^{-iEt/\hbar}$

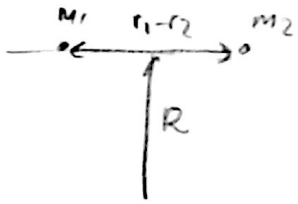
$\longrightarrow (m_1 - m_2)\vec{R} = m_1 \vec{r}_1 + m_2 \vec{r}_2$ } center of mass

let $\vec{r} = \vec{r}_1 - \vec{r}_2$, then,

$(m_1 + m_2)\vec{R} = m_1 \vec{r}_1 + (\vec{r}_1 - \vec{r}) m_2$

$(m_1 + m_2)\vec{R} = (m_1 + m_2)\vec{r}_1 - m_2 \vec{r}$

$\Rightarrow \boxed{\vec{r}_1 = \vec{R} + \frac{m_2}{m_1 + m_2} \vec{r}}$



Define $\mu = \frac{m_1 m_2}{m_1 + m_2}$: reduced mass,

$\boxed{\vec{r}_1 = \vec{R} + \frac{\mu}{m_1} \vec{r}}$ $\longrightarrow x_1 = X + \frac{\mu}{m_1} x$

and $\boxed{\vec{r}_2 = \vec{R} - \frac{\mu}{m_2} \vec{r}}$ $\longrightarrow x_2 = X - \frac{\mu}{m_2} x$

say $\vec{R} = \vec{R}(X, Y, Z)$ and $\vec{r} = \vec{r}(x, y, z)$.

$\longrightarrow (\nabla_1)_x = \frac{\partial}{\partial x_1} = \frac{\partial X}{\partial x_1} \frac{\partial}{\partial X} + \frac{\partial x}{\partial x_1} \frac{\partial}{\partial x}$

$X(m_1 + m_2) = m_1 x_1 + m_2 x_2 \Rightarrow \frac{\partial X}{\partial x_1} = \frac{m_1}{m_1 + m_2}$

$x = x_1 - x_2 \Rightarrow \frac{\partial x}{\partial x_1} = 1$

$\Rightarrow (\nabla_1)_x = \frac{m_1}{m_1 + m_2} \frac{\partial}{\partial X} + \frac{\partial}{\partial x} = \frac{\mu}{m_2} \frac{\partial}{\partial X} + \frac{\partial}{\partial x}$

Then, $\nabla_1 = \frac{\mu}{m_2}\nabla_R + \nabla_r$

similarly, $\nabla_2 = \frac{\mu}{m_1}\nabla_R - \nabla_r$

$$\nabla_1^2\psi = \nabla_1 \cdot (\nabla_1 \psi) = \left(\frac{\mu}{m_2}\nabla_R + \nabla_r\right)\cdot\left(\frac{\mu}{m_2}\nabla_R + \nabla_r\right)\psi$$

$$= \left(\frac{\mu^2}{m_2^2}\nabla_R^2 + \nabla_r^2 + \frac{2\mu}{m_2}(\nabla_R\cdot\nabla_r)\right)\psi$$

similarly, $\nabla_2^2\psi = \left(\frac{\mu^2}{m_1^2}\nabla_R^2 + \nabla_r^2 - \frac{2\mu}{m_1}(\nabla_R\cdot\nabla_r)\right)\psi$

insert into Schrödinger

$$\frac{-\hbar^2}{2m_1}\nabla_1^2\psi = \frac{-\hbar^2}{2m_1}\left(\frac{\mu^2}{m_2^2}\nabla_R^2\psi + \frac{2\mu}{m_2}(\nabla_R\cdot\nabla_r)\psi + \nabla_r^2\psi\right)$$

$$\frac{-\hbar^2}{2m_2}\nabla_2^2\psi = \frac{-\hbar^2}{2m_2}\left(\frac{\mu^2}{m_1^2}\nabla_R^2\psi - \frac{2\mu}{m_1}(\nabla_R\cdot\nabla_r)\psi + \nabla_r^2\psi\right)$$

make some arrangements

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

, let $\psi_r(r)\psi_R(r) = \psi$

substitute, divide etc.

$$\boxed{\frac{-\hbar^2}{2(m_1+m_2)}\nabla_R^2\psi_R = E_R\psi_R}$$

$$\boxed{\frac{-\hbar^2}{2\mu}\nabla_r^2\psi_r + V(r)\psi_r = E_r\psi_r}$$

Schrödinger eqn. for a free particle

$$\boxed{E = E_R + E_r}$$

$\boxed{\text{HW}}$ 5.2

Bosons and Fermions

$\psi(\vec{r_1}, \vec{r_2}) = \psi_a(r_1)\psi_b(r_2)$ — which one is which?

$\psi_\pm(\vec{r_1}, \vec{r_2}) = \frac{1}{\sqrt{2}}\left(\psi_a(r_1)\psi_b(r_2) \pm \psi_b(r_1)\psi_a(r_2)\right)$ — everything is possible.

- − is chosen for fermions (half integer spin)
- + is chosen for bosons (full integer spin)

+ refers to symmetric

− refers to antisymmetric

- Two identical Fermions cannot occupy the same state.

$$\psi_-(r_1,r_2) = \frac{1}{\sqrt{2}}\left[\psi_a(r_1)\psi_a(r_2) - \psi_a(r_1)\psi_a(r_2)\right] = 0.$$

≡ PAULI EXCLUSION PRINCIPLE

- Exchange operator

$$Pf(\vec{r}_1,\vec{r}_2) = f(\vec{r}_2,\vec{r}_1) \quad , \quad P^2 = 1 \Rightarrow \text{eigenvalues: } \pm 1$$

symmetric / antisymmetric

commuting with the Hamiltonian if the particles are identical.

$$P\psi_+ = +1\cdot\psi_+ \longrightarrow \text{boson}$$

$$P\psi_- = -1\cdot\psi_- \longrightarrow \text{fermion}$$

ex Particle in a box!

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} = n^2 K$$

$$\psi_{n_1n_2}(x_1,x_2) = \psi_{n_1}(x_1)\psi_{n_2}(x_2) \longrightarrow \text{not quite correct.}$$

$$E_{n_1n_2} = (n_1^2+n_2^2)K$$

ground state → $n_1 = n_2 = 1 \Rightarrow E_{11} = 2K$, $\underbrace{\psi_{11} = \sqrt{\frac{2}{a}}^{\,2}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)}_{\text{symmetric}}$

first excited state → $E_{12} = 5K$, $E_{21} = 5K$: 2-fold degeneracy

$$\psi_{12} = \sqrt{\frac{2}{a}}^{\,2}\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) \qquad \psi_{21} = \sqrt{\frac{2}{a}}^{\,2}\sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)$$

$$\psi \quad \frac{\sqrt{2}}{a}\left[\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{2\pi x_2}{a}\right) \underset{\text{fermion}}{\overset{\text{boson}}{\pm}} \sin\left(\frac{2\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right)\right]$$

Three Particle Systems ↳ 6 options

$$\Psi_{S,A} = A\left[\psi(1,2,3) \pm \psi(2,1,3) \pm \psi(3,2,1) + \psi(3,1,2) \pm \psi(1,3,2) + \psi(2,3,1)\right]$$

↳ exchange operator: replace any two..

N Fermions in a potential well

$$H = \sum_{i=1}^{N} H_i \quad , \quad H_i = \frac{p_i^2}{2m} + V(x_i)$$

$H_k u_{E_{\sigma_k}} = E_{k_{\sigma_k}} u_E$, each value of k, there are 2 possible values of the spin, labeled σ_k.

! Slater determinant }

$$u^A(1,2,\dots,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{E_1}(x_1) & \cdots & u_{E_N}(x_1) \\ u_{E_2}(x_1) & u_{E_2}(x_2) & \vdots \\ \vdots & \ddots & \vdots \\ u_{E_N}(x_N) & \cdots & u_{E_N}(x_N) \end{vmatrix}$$

- $\langle (x_1 - x_2)^2 \rangle = \langle x_1^2 \rangle + \langle x_2^2 \rangle - 2\langle x_1 x_2 \rangle$

$\langle x^2 \rangle = \int \psi_\pm^* x^2 \psi_\pm dx$ — you can do this. plug the wf's for bosons & fermions.

$$\ldots \langle (x_1 - x_2)^2 \rangle = \langle (\Delta x)^2 \rangle_\pm = \langle (\Delta x)^2 \rangle_d \mp 2 |\langle x \rangle_{ab}|^2$$

symmetric / antisymmetric

Exchange forces = useful in periodic table {

Symmetric → they tend to get together, the force between them is attractive, they use common orbits (like a covalent bond)

antisymmetric → separation increases

Atoms

$$H = \sum_{j=1}^{Z} \frac{-\hbar^2}{2m} \nabla_j^2 - \frac{1}{4\pi\varepsilon_0}\left(\frac{Ze^2}{r_j}\right) + \frac{1}{2} \cdot \frac{1}{4\pi\varepsilon_0} \sum_{j \neq k}^{Z} \frac{e^2}{|\vec{r}_j - \vec{r}_k|}$$

$H\Psi = E\Psi$, $\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z)\, \chi(\vec{s}_1, \vec{s}_2, \dots, \vec{s}_Z)$

↑ spatial (function) ↑ spin (vector)

Helium

$Z=2$ $\Rightarrow H = \left[\frac{-\hbar^2}{2m}\nabla_1^2 - \frac{1}{4\pi\varepsilon_0}\frac{2e^2}{r_1}\right] + \left[\frac{-\hbar^2}{2m}\nabla_2^2 - \frac{1}{4\pi\varepsilon_0}\frac{2e^2}{r_2}\right] + \underbrace{\frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\vec{r}_1-\vec{r}_2|}}$

ignore this & spins

$\Psi(\vec{r}_1,\vec{r}_2) = \psi_{nlm}(\vec{r}_1)\,\psi_{n'l'm'}(\vec{r}_2)$

It's like two hydrogen atoms.

$a = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \xrightarrow{\text{converts}} a(z) = \frac{a}{z} = \frac{4\pi\varepsilon_0\hbar^2}{z\,me^2}$ ↑ bohr radius is halved

$E_n = \left[-\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} \xrightarrow{\text{convert}} E_n(z) = z^2 E_n$ ↑ $E_n' = 4E_n$

Then, $E = 4(E_n + E_n')$

ground $\binom{n=1}{n'=1} \Rightarrow E_1 = 4\cdot 2\cdot(-13.6) = -109\ \text{eV}$ — binding energy for Helium which is not correct experimentally

$E_{1,exp} = -78.795\ \text{eV}$ ← coulombic repulsive force is ignored.

HW 5.11

$\psi_{ground} = \psi_{100}(\vec{r}_1)\,\psi_{100}(\vec{r}_2) = \psi_0(\vec{r}_1,\vec{r}_2)$ ← insert ψ's

symmetric

$\psi_0(\vec{r}_1,\vec{r}_2) = \frac{8}{\pi a^3}e^{-2(r_1+r_2)/a}$ ← for electrons, something must be antisymmetric → spin!

Then the full wf: $\psi_{antisym} = \psi_0\chi$

sym. antisym. → you should choose the singlet state!

calculate the contribution of the potential.

$\left\langle \frac{1}{4\pi\varepsilon_0}\frac{e^2}{|\vec{r}_1-\vec{r}_2|}\right\rangle$ with $\psi_0(\vec{r}_1,\vec{r}_2)$

Excited States

$\psi = \underbrace{\psi_{nlm}\,\psi_{100}}\,\chi$

$\psi_S \rightarrow$ singlet $\Longrightarrow$ parahelium ($S=0$)
$\psi_A \rightarrow$ triplet $\Longrightarrow$ orthohelium — highest spin ($S=1$)

] look at the energies from the book.

Periodic Table

n, ℓ, m

degeneracy for 2 electron: $2n^2$

2, 8, 18, 32 ? No!

True one: 2, 8, 8, 18, 18, ... → due to fermionic structure (← exchange forces)
→ due to screening effect (charge cloud screens the central source)

$\ell = 0 \rightarrow$ s orbital (sharp)
$\ell = 1 \rightarrow$ p orbital (principle)
$\ell = 2 \rightarrow$ d orbital (diffuse)
$\ell = 3 \rightarrow$ f orbital (fundamental)

Carbon

$Z = 6 \longrightarrow (1s)^2\,(2s)^2\,(2p)^2$

2 electrons in the 1st state	2 electrons in the 2nd state	2 electrons in the 2nd state
$n=1,\ \ell=0,\ m=0$, singlet	$n=2,\ \ell=0,\ m=0$,	$n=2,\ \ell=1,\ m=\pm1, 0$
Some combinations: $(1,0,0)$;	$(2,0,0)$;	$(2,1,0)$, $(2,1,1)$, $(2,1,-1)$

For two spins, we have → triplet, 1 ; angular momentums, we have ↳ singlet, 0

S	L	J
triplet, 1	2	3
singlet, 0	1	2
	0	1
		0

Check this rule from the book

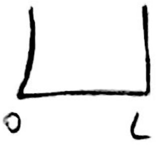
Hund's Rule → $\boxed{\text{HW } 5.13}$

${}^{2S+1}L_J \longrightarrow$ find the minimum value of the energy you can get.

$(2)(1)+(1)$: triplet, symmetric

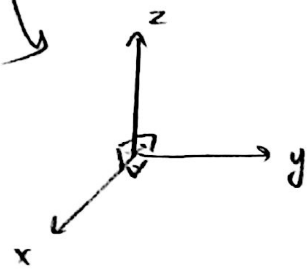
$\rightarrow L_J$, $L = 2 \ \&\ 0$ is symmetric $\Rightarrow L=1 \Longrightarrow {}^3P_0$ — description of the carbon atom

Exclusion Principle & Noninteracting Particles



$\rightarrow \psi = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$, $E_n = \frac{n^2 \pi^2 \hbar^2}{2m L^2}$ — for each n, there are 2 electrons.

In 3-D



$$u_E(x,y,z) = \underbrace{\left(\frac{2}{L}\right)^{3/2}}_{\text{size of the box}} \sin\left(\frac{n_1 \pi x}{L}\right) \sin\left(\frac{n_2 \pi y}{L}\right) \sin\left(\frac{n_3 \pi z}{L}\right)$$

$$\Rightarrow \boxed{E = \frac{\hbar^2 \pi^2}{2mL^2} \overbrace{(n_1^2 + n_2^2 + n_3^2)}^{R^2}}$$

$n_x^2 \quad n_y^2 \quad n_z^2$ — lots values

— Val.

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi = E_x \psi \Rightarrow k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$$ — wave number.

Then, $R^2 = \frac{2mEL^2}{\hbar^2 \pi^2} \Rightarrow R = \sqrt{\frac{2mEL^2}{\hbar^2 \pi^2}}$

in each lattice point you have $2\bar{e}$

$$2\left[\frac{4\pi}{8 \cdot 3} R^3\right] = \underbrace{\frac{\pi}{3} R^3}_{} = \frac{\pi}{3} \cdot \frac{(2mE)^{3/2} L^3}{\hbar^3 \pi^3}$$ — highest state!

one eight of the sphere is positive

L^3 — volume

# of lattice pts

E — Fermi energy

N = # of $\bar{e}$

N/L^3 : density of free electrons

$$\boxed{E_F = \frac{\hbar^2 \pi^2}{2m}\left(\frac{3n}{\pi}\right)^{2/3}} = \boxed{\frac{\hbar^2}{2m} k_F^2}$$ → Fermi energy

highest possible energy for the free electrons (all states are filled)

$$k_F = (3\pi^2 n)^{1/3} = \frac{2\pi}{\lambda_F}$$ — de broglie

$$\boxed{\lambda = 2.03 n^{-1/3}} \quad \boxed{\simeq 2d}$$

$n^{-1/3}$ → d (interparticle spacing)

$$\boxed{d \simeq \frac{\lambda_F}{2}}$$

Total energy : $E_{tot} = \frac{\hbar^2 \pi^2}{2mL^2} \int_0^{R} 2\, n^2 (4\pi n^2 dn) \cdot \frac{1}{8}$ ~ volume element of n-space ~ positive

$$\boxed{E_{total} = \frac{\hbar^2 \pi^3}{10 mL^2} R^5}$$

~ good for the condensed matter.

~ total energy of the condensed matter

$$\boxed{E_{total} = \frac{\hbar^2 \pi^3}{10 mL^2} \left(\frac{3N}{\pi}\right)^{5/3}}$$

$$\boxed{E_{total} = \frac{\hbar^2 \pi^3}{10 m} \left(\frac{3n}{\pi}\right)^{5/3} L^3}$$

→ $P_{(pressure)} = -\frac{\partial E_{total}}{\partial V_{\to L^3}} =$ ~~~ yeah

$B = V \frac{\partial P}{\partial V} =$ ~~~ yeah

bulk modulus

TIME INDEPENDENT PERTURBATION THEORY

Nondegenerate Perturbation Theory

unperturbed hamiltonian $H^0 \psi_n^0 = E \psi_n^0$

$$H = H^0 + \lambda H'$$

λ: $0 < \lambda < 1$, degree of perturbation

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm}$$

$$\psi_n = \psi_n^0 + \underbrace{\lambda \psi_n^1}_{\text{first order perturbation}} + \underbrace{\lambda^2 \psi_n^2}_{\text{second order perturbation}} + \lambda^3 \psi_n^3 + \dots \quad \text{---}$$

like Taylor series. (not Taylor series)

$$E_n = E_n^0 + \underbrace{\lambda E_n^1}_{\text{first order correction to energy}} + \underbrace{\lambda^2 E_n^2}_{\text{second order correction to energy}} + \dots$$

how to solve? take the wave function and plug into the eqn.

$$\rightarrow \underbrace{(H^0 + \lambda H')}_{H} \underbrace{(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots)}_{\psi_n} = \underbrace{(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)}_{E_n} \underbrace{(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \dots)}_{\psi_n}$$

collect like λ's

$$H^0 \psi_n^0 + \lambda [H^0 \psi_n^1 + H' \psi_n^0] + \lambda^2 [H^0 \psi_n^2 + H' \psi_n^1] = E_n^0 \psi_n^0 + \lambda [E_n^0 \psi_n^1 + E_n^1 \psi_n^0] + \dots$$

$$\dots \lambda^2 [E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0]$$

$\lambda^0 = 1 \rightarrow$ lowest order: unperturbed Schroedinger eqn: $\boxed{H^0 \psi_n^0 = E_n^0 \psi_n^0}$

$\lambda^1 \rightarrow$ first order: $H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$

$\lambda^2 \rightarrow$ second order: $H^0 \psi_n^2 + H' \psi_n^1 = E_n^0 \psi_n^2 + E_n^1 \psi_n^1 + E_n^2 \psi_n^0$

First Order Perturbation Theory

inner product with ψ_n^0: $\langle \psi_n^0 | H^0 \psi_n^1 \rangle + \langle \psi_n^0 | H' \psi_n^0 \rangle = E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle + E_n^1 \cancelto{1}{\langle \psi_n^0 | \psi_n^0 \rangle}$

$\langle H^0 \psi_n^0 | \psi_n^1 \rangle$

$E_n^0 \langle \psi_n^0 | \psi_n^1 \rangle$

Hence, $\boxed{\langle \psi_n^0 | H' \psi_n^0 \rangle = E_n^1} \rightarrow$ easy !

$$\boxed{E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle} \rightarrow \text{first order correction to the energy.}$$

ex Particle in a box, $V = 0$, $w = a$,

$\rightarrow V_0$: perturbation $\Rightarrow H' = V_0$

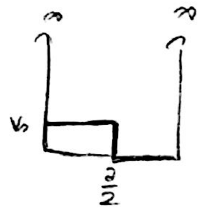
$$\left.\begin{matrix} \\ \\ \end{matrix}\right\} \psi_n^0 = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$\leftarrow a \rightarrow$.

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle, \quad H' = V_0 \Rightarrow \boxed{E_n^1 = V_0}$$

$$E_n = E_n^0 + \lambda V_0 = \boxed{\frac{n^2 \pi^2 \hbar^2}{2ma^2} + \lambda V_0}$$

ex



$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle = \frac{2}{a} V_0 \int_0^{a/2} \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \cdots = \boxed{\frac{V_0}{2}} \Rightarrow \boxed{E_n = E_n^0 + \lambda \frac{V_0}{2}}$$

you can do small examples like these, easy. you can do many things.

harmonic oscillator

etc. $\longrightarrow$ non degenerate in 1-D.

$\longrightarrow$ Eigenfunctions of 1^{st} order perturb.

$$H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$$

$$(H^0 - E_n^0) \psi_n^1 = -(H' - E_n^1) \psi_n^0 \quad (*)$$

can we do this? $\longrightarrow \psi_n^1 = \sum_{m \neq n} c_m^{(n)} \psi_m^0 \rightarrow$ if $m = n$, ψ_n^1 is already satisfies eqn. $(*)$ $[0=0]$

$$(H^0 - E_n^0) \sum_{m \neq n} c_m^{(n)} \psi_m^0 = -(H' - E_n^1) \psi_n^0$$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \psi_m^0 = -(H' - E_n^1) \psi_n^0$$

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^{(n)} \underbrace{\langle \psi_l^0 | \psi_m^0 \rangle}_{\delta_{lm}} = -\langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \overbrace{\langle \psi_l^0 | \psi_n^0 \rangle}^{0 \text{ since } l \neq n}$$

$$(E_l^0 - E_n^0) c_l^n = -\langle \psi_l^0 | H' | \psi_n^0 \rangle$$

Then $\boxed{c_m^n = \dfrac{-\langle \psi_m^0|H'|\psi_n^0\rangle}{E_m^0 - E_n^0} = \dfrac{\langle \psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}}$

Hence $\boxed{\psi_n^1 = \sum_{n\neq m} \dfrac{\langle \psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0}$ → $n=m$ blows

$\boxed{\text{HW}}$ harmonic oscillator, 6.2

$V=\frac{1}{2}kx^2$, $k\to(1+\varepsilon)k \Rightarrow V' = \frac{1}{2}\varepsilon k^2x^2$

Second Order Perturbation Theory → not <u>very</u> important in real life

$$H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0$$ — we want to find E_n^2 & ψ_n^2

$$\langle\psi_n^0|H^0\psi_n^2\rangle + \langle\psi_n^0|H'\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^2\rangle + E_n^1\langle\psi_n^0|\psi_n^1\rangle + E_n^2\underbrace{\langle\psi_n^0|\psi_n^0\rangle}_{1}$$

$=$

$\langle H^0\psi_n^0|\psi_n^2\rangle$

$=$

$E_n^0\langle\psi_n^0|\psi_n^2\rangle$ ← same

$$\longrightarrow E_n^2 = \langle\psi_n^0|H'|\psi_n^1\rangle - E_n^1\underbrace{\langle\psi_n^0|\psi_n^1\rangle}$$ orthogonal

$$\sum_{m\neq n} c_m^n\langle\psi_n^0|\psi_m^0\rangle = 0.$$

$$\rightarrow E_n^2 = \langle\psi_n^0|H'|\sum_{n\neq m} c_n^m\psi_m^0\rangle$$

$$= \sum_{n\neq m}\frac{\langle\psi_m^0|H'|\psi_n^0\rangle}{E_n^0 - E_m^0}\langle\psi_n^0|H'|\psi_m^0\rangle$$

$$\boxed{E_n^2 = \sum_{n\neq m}\frac{|\langle\psi_n^0|H'|\psi_m^0\rangle|^2}{E_n^0 - E_m^0}}$$

Correction to the wave function → $\psi_n^2 = \sum_{n\neq m} A_m^n\psi_m^1$ → complicated

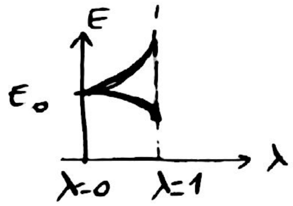
bi' try them annem. $\Big\{$ $\psi_n^2 = \sum K_m^n\psi_m^0$ → complicated

Degenerate Perturbation Theory

2-fold Degeneracy

$$H^0 \psi_a^0 = E^0 \psi_a^0$$
$$H^0 \psi_b^0 = E^0 \psi_b^0$$
where $\langle \psi_a^0 | \psi_b^0 \rangle = 0$ given that $a \neq b$ [orthogonality]

perturbation $\rightarrow$ H' will break / lift the degeneracy (for example magnetic field shifts the energies = Landau levels), when $\lambda: 0 \rightarrow 1$.



$$H = H^0 + \lambda H'$$
$$H\psi = E\psi$$

do the same things, with the deg. eig.-f.

*** FIRST ORDER:** $H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0$

notice $\psi^0 = \alpha \psi_a^0 + \beta \psi_b^0$ $\rightarrow$ insert stuff:

$$\cancel{\langle \psi_a^0 | H^0 | \psi^1 \rangle} + \langle \psi_a^0 | H' | \psi^0 \rangle = \cancel{E^0 \langle \psi_a^0 | \psi^1 \rangle} + E^1 \underbrace{\langle \psi_a^0 | \psi^0 \rangle}_{\alpha}$$

$$\boxed{\begin{gathered}\alpha \langle \psi_a^0 | H' | \psi_a^0 \rangle + \beta \langle \psi_a^0 | H' | \psi_b^0 \rangle = \alpha E^1 \\ \text{or, simply, } \langle \psi_a^0 | H' | \psi^0 \rangle = \alpha E^1\end{gathered}}$$

notation $\boxed{\langle \psi_i^0 | H' | \psi_j^0 \rangle = W_{ij}}$

here, $\boxed{\alpha W_{aa} + \beta W_{ab} = \alpha E^1}$ (1)

do with $\langle \psi_b^0 |$ $\rightarrow$ $\boxed{\alpha W_{ba} + \beta W_{bb} = \beta E^1}$ (2) (show this)

(2): multiply W_{ab} $\rightarrow$ $\alpha W_{ab} W_{ba} + \underbrace{\beta W_{ab}}_{\alpha E^1 - \alpha W_{aa}} W_{bb} = \underbrace{\beta W_{ab}}_{} E^1$

$$\boxed{\alpha W_{ab} W_{ba} + \alpha (E^1 - W_{aa})(W_{bb} - E^1) = 0}$$

$W_{ab}^* = W_{ba}$

$\alpha \neq 0 \Rightarrow (E^1)^2 - E^1 (W_{aa} + W_{bb}) + (W_{aa} W_{bb} - W_{ab} W_{ba}) = 0$

$$E^1_\pm = \frac{1}{2}(W_{aa} + W_{bb}) \pm \frac{1}{2}\sqrt{(W_{aa} + W_{bb})^2 - 4(W_{aa}W_{bb} - |W_{ab}|^2)}$$

$$\boxed{E^1_\pm = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right]}$$

Simple cases: $\alpha = 0, \beta = 1 \Rightarrow W_{ab} = 0 = W_{ba} \Rightarrow E^1 = W_{bb}$ (see (1)&(2))

$E^1 = \langle \psi_b^0 | H' | \psi_b^0 \rangle$ → non-degenerate 1st order perturbation

$\alpha = 1, \beta = 0 \Rightarrow W_{ba} = 0 = W_{ab} \Rightarrow E^1 = W_{aa}$ (see (1)&(2))

$E^1 = \langle \psi_a^0 | H' | \psi_a^0 \rangle$ → non degenerate 1st order perturbation

matrix representation :

$$\boxed{\underbrace{\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix}}_{\text{perturbed Hamiltonian matrix}} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}}$$

→ diagonalize & get α & β, ⇒ good states!

Theorem Let A be a Hermitian operator commutes with H^0 and H'. If ψ_a^0 and ψ_b^0 (the degenerate eigenfunctions of unperturbed Hamiltonian) are also eigenfunctions of A with distinct eigenvalues,

$$A\psi_a^0 = \mu\psi_a^0 \quad , \quad A\psi_b^0 = \nu\psi_b^0 , \quad \mu \neq \nu,$$

then, $W_{ab} = W_{ba} = 0$ ⇒ perturbed Hamiltonian matrix is diagonal already.
hence, ψ_a^0 and ψ_b^0 are the "good" states to use in perturbation theory.

proof | $[A, H'] = 0$

$$\langle \psi_a^0 | [A, H'] | \psi_b^0 \rangle = 0$$

$$\begin{aligned}
\langle \psi_a^0 | AH' - H'A | \psi_b^0 \rangle &= \langle \psi_a^0 | AH' | \psi_b^0 \rangle - \langle \psi_a^0 | H'A | \psi_b^0 \rangle \\
&= \langle A\psi_a^0 | H'\psi_b^0 \rangle - \langle \psi_a^0 | H' \nu \psi_b^0 \rangle \\
&= \mu \langle \psi_a^0 | H' | \psi_b^0 \rangle - \nu \langle \psi_a^0 | H' | \psi_b^0 \rangle = 0
\end{aligned}$$

If $\mu \neq \nu$, $\langle \psi_a^0 | H' | \psi_b^0 \rangle = W_{ab} = 0 \Rightarrow W_{ba} = 0$ ✓

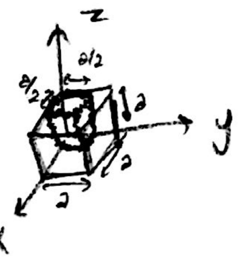
> For the real hydrogen atom, this will be useful.

n-fold degeneracy

$$W_{ij} = \langle \psi_i^0 | H' | \psi_j^0 \rangle$$

$$\begin{pmatrix} & \vdots & \\ \cdots & W_{ij} & \cdots \\ & \vdots & \end{pmatrix}_{n\times n} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \vdots \end{pmatrix}_{n\times 1} = E' \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \vdots \end{pmatrix}_{n\times 1}$$

ex Particle in a box: $V(x,y,z) = \begin{cases} 0, & 0<x<a,\ 0<y<a,\ 0<z<a \\ \infty, & \text{elsewhere} \end{cases}$



$\rightsquigarrow$ Recall: $\psi^0_{n_x n_y n_z} = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right)$

$\rightsquigarrow$ Perturbation: $x: 0 \to \frac{a}{2}$, $y: 0 \to \frac{a}{2}$, $z: 0 \to a$

$\hookrightarrow$ Recall: $E_n^0 = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)$

· Look at the ground state: $n_x = n_y = n_z = 1 \Rightarrow E_n^0 = \frac{3\pi^2\hbar^2}{2ma^2}$ → not degenerate, only possibility!!!

Perturbation: $H' = \begin{cases} V_0, & 0<x<\frac{a}{2},\ 0<y<\frac{a}{2},\ 0<z<a \\ 0, & \text{elsewhere} \end{cases}$

$$\hookrightarrow E_0' = \langle \psi_{111} | H' | \psi_{111} \rangle$$ → good state since non-degenerate

$$= \int_0^{a/2}\int_0^{a/2}\int_0^{a} \left(\frac{2}{a}\right)^3 V_0 \sin^2\left(\frac{\pi x}{a}\right) \sin^2\left(\frac{\pi y}{a}\right) \sin^2\left(\frac{\pi z}{a}\right) dz\,dy\,dx$$

$$= \frac{8}{a^3} V_0 \int_0^{a/2} \sin^2\left(\frac{\pi x}{a}\right) dx \int_0^{a/2} \sin^2\left(\frac{\pi y}{a}\right) dy \int_0^{a} \sin^2\left(\frac{\pi z}{a}\right) dz$$

$$= \cdots = \boxed{\frac{1}{4} V_0} \Rightarrow \boxed{E_n = \frac{3\hbar^2\pi^2}{2ma^2} + \lambda \frac{1}{4} V_0, \quad \lambda: 0 \to 1}$$

first excited state: 3-fold degeneracy!

$$\psi_a = \psi_{112},\ \psi_b = \psi_{121},\ \psi_c = \psi_{211},\ E_n^0 = \frac{6\pi^2\hbar^2}{2ma^2} = \boxed{\frac{3\pi^2\hbar^2}{ma^2}}$$

$\psi^0 = \alpha\psi_a + \beta\psi_b + \gamma\psi_c$ → good state. $\alpha = ?\ \beta = ?\ \gamma = ?$

$$\begin{pmatrix} W_{aa} & W_{ab} & W_{ac} \\ W_{ba} & W_{bb} & W_{bc} \\ W_{ca} & W_{cb} & W_{cc} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = E_n^1 \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \quad \text{where } W_{ij} = \langle \psi_i | H' | \psi_j \rangle$$

Doable: $W_{aa} = \langle \psi_{112} | H' | \psi_{112} \rangle = W_{bb} = W_{cc} = \frac{1}{4} V_0$
(sort of)

$W_{ab} = \langle \psi_{112} | H' | \psi_{121} \rangle = W_{ba} = 0$ (orthogonal z's)

$W_{ac} = W_{ca} = 0$ (orthogonal z's)

you'll see when you solve the integral

$$W_{bc} = \left(\frac{2}{a}\right)^3 \cdot V_0 \int_0^{a/2} \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx \int_0^{a/2} \sin\left(\frac{\pi y}{a}\right)\sin\left(\frac{2\pi y}{a}\right)dy \int_0^{a} \sin^2\left(\frac{\pi z}{a}\right)dz \neq 0$$

$W_{bc} = W_{cb} = \frac{16\pi^2}{9} V_0 = \frac{V_0}{4} \cdot K$ where $K = \left(\frac{8}{3\pi}\right)^2$

our perturbed Hamiltonian matrix $\Big\}$ $W = \frac{V_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix}$

$$\begin{vmatrix} 1-w & 0 & 0 \\ 0 & 1-w & K \\ 0 & K & 1-w \end{vmatrix} = (1-w)^3 - K^2(1-w) = 0 \begin{cases} \to w = 1 \\ \to w = 1-K \\ \to w = 1+K \end{cases}$$

$$E_1 = \frac{3\pi^2\hbar^2}{ma^2} + \lambda\frac{V_0}{4}$$

$$E_1 = \frac{3\pi^2\hbar^2}{ma^2} + \lambda(1+K)\frac{V_0}{4}$$

$$E_1 = \frac{3\pi^2\hbar^2}{ma^2} + \lambda(1-K)\frac{V_0}{4}$$

see? 3-fold.

What are the good states, then?

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & K \\ 0 & K & 1 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = w\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}$$

$w=1 \to \alpha = \alpha$; $\beta + K\gamma = \beta \to \gamma = 0$; $K\beta = 0 \to \beta = 0$ $\Big\}$ $\psi^0 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \psi_a$, $w=1$

$w = 1-K \to \alpha = (1-K)\alpha \to \alpha = 0$; $\beta + K\gamma = \beta - K\beta \to \gamma = -\beta$; $K\beta + \gamma = \dots$ $\Big\}$ $\psi^0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(\psi_b - \psi_c)$, $w = 1-K$

$w = 1+K \to \alpha = (1+K)\alpha \to \alpha = 0$; $\beta + K\gamma = \beta + K\beta \to \gamma = \beta$ $\Big\}$ $\psi^0 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(\psi_b + \psi_c)$, $w = 1+K$

So, good states: $\psi^0 = \begin{cases} \psi_a & , w = 1 \\ \frac{1}{\sqrt{2}}(\psi_b + \psi_c) & , w = 1+K \\ \frac{1}{\sqrt{2}}(\psi_b - \psi_c) & , w = 1-K \end{cases}$

so good states: $\psi^0 = \begin{cases} \psi_a & , w \cdot 1 \\ \frac{1}{\sqrt{2}}(\psi_a + \psi_b), & w \cdot 1+K \\ \frac{1}{\sqrt{2}}(\psi_a - \psi_b), & w \cdot 1-K \end{cases}$

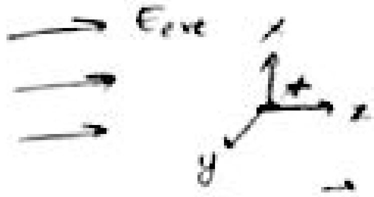
M1Q3] Show that $(\vec{\sigma}\cdot\vec{A})(\vec{\sigma}\cdot\vec{B}) = \vec{A}\cdot\vec{B} + i\vec{\sigma}\cdot(\vec{A}\times\vec{B})$

In a low energy neutron proton system, zero orbital momentum

$$V(r) = V_1(r) + V_2(r)\left[3\frac{(\vec{\sigma}_1\cdot r)(\vec{\sigma}_2\cdot r)}{r^2} - \vec{\sigma}_1\cdot\vec{\sigma}_2\right] + V_3(r)(\vec{\sigma}_1 + \vec{\sigma}_2)$$

r → vector connecting two particles V ? for spin singlet & triplet

ex Stark effect



well polarized : perturbation : $\vec{p} = \int \vec{x}\rho\, d^3x = -e\vec{r}$ ← separation

$U = -\vec{p}\cdot\vec{E}$
$= -pE\cos\theta$
$= -ezE\cos\theta$

stored potential energy, you can write this as a perturbation for the Hamiltonian

$H' = erE\cos\theta$ ← check the minus sign

n=1 → $|100\rangle = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$ non-degenerate
n=2

$$E_s^1 = \langle 100|H'|100\rangle = \frac{1}{\pi a^3}\int_0^\infty\int_0^\pi\int_0^{2\pi} e^{-2r/a}(erE\cos\theta)\,r^2\sin\theta\, d\phi\, d\theta\, dr = 0$$

1st order nondegenerate perturbation in ground state

⇒ ground state is not effected.

(a) $|1\rangle = |2\,0\,0\rangle$
(b) $|2\rangle = |2\,1\,1\rangle$
(c) $|3\rangle = |2\,1\,0\rangle$
(d) $|4\rangle = |2\,1\,-1\rangle$

4-fold degen

degenerate perturbation theory: $W_{ij} = \langle \psi_i^0|H'|\psi_j^0\rangle$

→ check the states from the book

16 possibilities)

do it: $W = -3a e E_{ext} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \rightarrow$ not diagonal

$$\begin{vmatrix} -\lambda & 0 & 1 & 0 \\ 0 & -\lambda & 0 & 0 \\ 1 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & -\lambda \end{vmatrix} = -\lambda \cdot \begin{vmatrix} -\lambda & 0 & 1 \\ 0 & -\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix}$$

$$= -\lambda\left(-\lambda^3 + \lambda\right) = \lambda^4 - \lambda^2 = 0 \quad \begin{matrix} \rightarrow \lambda = 0 \\ \rightarrow \lambda = 1 \\ \rightarrow \lambda = -1 \end{matrix}$$

Then, $E = \begin{cases} E_2 + 0 \\ E_2 + 0 \\ E_2 - 3a e E_{ext} \\ E_2 + 3a_0 E_{ext} \end{cases}$

$n=2\ l=0\ m=0$

$n=2\ l=1\ m=\pm 1, 0$

$3a e E_{ext}$

$-3a e E_{ext}$

$|2\,1\,1\rangle$ 8

$|2\,1\,-1\rangle$

eigenfunctions!

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \eta \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \eta \end{pmatrix}$$

$\lambda = 0 \rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \rightarrow |b\rangle = |2\rangle$

$\qquad\quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \rightarrow |d\rangle = |4\rangle$

unaffected states!

$\rightarrow m = \pm 1$

$\lambda = 1 \longrightarrow \begin{matrix} \gamma = \alpha \\ 0 = \beta \\ \alpha = \gamma \\ 0 = \eta \end{matrix} \rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(\psi_a + \psi_c\right) \rightarrow m=0$

$\lambda = -1 \rightarrow \begin{matrix} \gamma = -\alpha \\ 0 = \beta \\ \alpha = -\gamma \\ 0 = \eta \end{matrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(\psi_a - \psi_c\right) \rightarrow m=0$

HW 6.33 - 6.32 (exam p.), (6.36 (exam p.)), 6.37
not hw

QUANTUM MECHANICS - II

THE REAL HYDROGEN ATOM

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} \quad , \text{let } \alpha = \frac{e^2}{4\pi\hbar\varepsilon_0 c} = \frac{1}{137.036}$$

Then, Bohr energies = $\alpha^2 mc^2$

- Fine structure . relativistic & spin-orbit coupling correction [TINY!]
  $= \alpha^2[\alpha^2 mc^2] = \alpha^4 mc^2$
- Lamb shift : quantum field theory (quantization of $\vec{E}$) [TINIER!]
  $= \alpha^5 mc^2$
- Hyperfine splitting . interaction of the $\vec{B}$ with hydrogen atom [THE TINIEST]
  $= \frac{m_e}{m_p}\alpha^4 mc^2$

Fine Structure

→ Relativistic correction & spin-orbit coupling

∴ $T = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ where $\vec{p} = \frac{\hbar}{i}\nabla$

Then, $\boxed{T = \frac{-\hbar^2}{2m}\nabla^2}$

∴ Relativistic energy = γmc^2 , γ: Lorentz factor , $\gamma = \frac{1}{\sqrt{1-v^2/c^2}}$

$\Rightarrow T = \gamma mc^2 - mc^2$: (total energy - rest energy = kinetic energy)

∴ At low speeds , $\gamma mc^2 = \frac{mc^2}{\sqrt{1-v^2/c^2}} \simeq mc^2\left[1+\frac{1}{2}\frac{v^2}{c^2}\right] = mc^2 + \frac{1}{2}mv^2$

$\Rightarrow T = \gamma mc^2 - mc^2 \simeq \frac{1}{2}mv^2$; our good old T in CM.

∴ Relativistic momentum = $\gamma m\vec{v} = \frac{m\vec{v}}{\sqrt{1-v^2/c^2}} = \vec{p}$

∴ $p^2c^2 + m^2c^4 = \frac{m^2v^2c^2}{1-\frac{v^2}{c^2}} + m^2c^4 = m^2c^2\left(\frac{\cancel{v^2}+c^2-\cancel{v^2}}{1-v^2/c^2}\right) = \frac{m^2c^4}{1-v^2/c^2}$

$$\boxed{p^2c^2 + m^2c^4 = (T+mc^2)^2} \Rightarrow \boxed{\underbrace{T}_{\text{kinetic energy}} = \underbrace{\sqrt{p^2c^2+m^2c^4}}_{\text{total energy}} - \underbrace{mc^2}_{\text{rest energy}}}$$

$$T + mc^2 = \sqrt{p^2c^2 + m^2c^4} = E \Rightarrow \underset{\text{operator}}{E^2} = \underset{\text{operator}}{p^2}c^2 + m^2c^4$$ → does not explain the negative energy

If you put the operators, Klein-Gordon eqn

$$\boxed{E = \pm\sqrt{p^2c^2 + m^2c^4}}$$

↳ If $p \ll mc$, $T = mc^2\left[\sqrt{1 + \left(\frac{p}{mc}\right)^2} - 1\right]$

$$T = mc^2\left[\cancel{1} + \frac{1}{2}\left(\frac{p}{mc}\right)^2 - \frac{1}{8}\left(\frac{p}{mc}\right)^4 + \dots - \cancel{1}\right]$$

$$T = \frac{p^2}{2m} - \underbrace{\frac{p^4}{8m^3c^2}}_{\text{relativistic correction}} + \dots$$

relativistic correction to the Hamiltonian!

$$\Rightarrow \boxed{H_r' = \frac{-p^4}{8m^3c^2}}$$ ← the rest is perturbation.

Then, $\langle E_r' \rangle = \langle H_r' \rangle = \frac{-1}{8m^3c^2} \langle p^2\psi | p^2\psi \rangle$

→ Recall $p^2\psi = 2m(V - E)\psi$ (Schrödinger eqn)

Then, $\langle E_r' \rangle = \frac{-1}{8m^3c^2}(2m)^2 \langle (E - V)^2 \rangle$ → p^4 commutes with H, wf are the same

$$E_r' = \langle E_r' \rangle = \frac{-1}{2mc^2}\left(E_n^2 - 2E_n\langle V \rangle + \langle V^2 \rangle\right)$$

→ Recall $V = \frac{-1}{4\pi\varepsilon_0}\frac{e^2}{r} \Rightarrow V^2 = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{r^2}$

Then, $E_r' = \frac{-1}{2mc^2}\left(E_n^2 + \frac{2E_ne^2}{4\pi\varepsilon_0}\underbrace{\left\langle \frac{1}{r} \right\rangle}_{\text{do it}} + \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\underbrace{\left\langle \frac{1}{r^2} \right\rangle}_{\text{do it}}\right)$

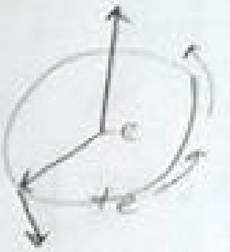
→ Recall $\left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2a}$, $\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{(l + \frac{1}{2})n^3a^2}$ → implicitly you are using A commutes with ... $\downarrow$ L^2, L_z

where a : Bohr radius $= \frac{4\pi\varepsilon_0\hbar^2}{me^2}$

HENCE, $\boxed{E_r' = \frac{-(E_n^2)}{2mc^2}\left[\frac{4n}{l + \frac{1}{2}} - 3\right]}$ ← do it! insert E_n,

↳ E_r' goes as α^4 something since $E_n \sim \alpha^2$

→ spin-orbit coupling



$H'_{so} = -\vec{\mu}\cdot\vec{B}$ → what is $\vec{\mu}$, what is $\vec{B}$?

∴ Biot-Savart law: $\vec{B} = \frac{\mu_0 I}{4\pi}\frac{d\vec{s}\times\hat{r}}{r^2} = \frac{\mu_0 I}{2r}$ (like a ring of current)

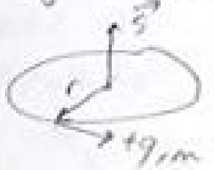
current due to single electron: $\frac{e}{T} \Rightarrow \vec{B}_{ele} = \frac{\mu_0 e}{2rT}\hat{L}$

for the electron: $L = rmv = rm\frac{2\pi r}{T} = \frac{2\pi m r^2}{T}$

then, $\boxed{\vec{B} = \frac{1}{4\pi\epsilon_0}\cdot\frac{e}{mc^2r^3}\vec{L}}$ → nice! we have $\vec{L}$.

$\left(\frac{1}{4\pi\epsilon_0}\cdot\frac{e\epsilon_0\mu_0}{mr^3}\cdot\frac{2\pi mr^2}{T} = \frac{e\mu_0}{2rT}\right)$

∴ Magnetic dipole moment of the electron:



very wrong approximation (electron is a ring spinning)

⇒ $S = I\omega = mr^2\omega = mr^2\frac{2\pi}{T'}$ a good point of care

Recall $\mu = I\pi r^2 = \frac{q}{T}\pi r^2 \Rightarrow \frac{\mu}{S} = \frac{q}{2m}$ gyromagnetic ratio

hence, $\boxed{\vec{\mu} = \left(\frac{q}{2m}\right)\vec{S}}$ → nice! we have $\vec{S}$.

Correction

coming from relativistic QM (Dirac theory): $\boxed{\vec{\mu} = \frac{q}{m}\vec{S}}$

introduce a 2 factor

∴ $H'_{so} = -\vec{\mu}\cdot\vec{B} = -\left(\frac{-e}{m}\vec{S}\right)\cdot\left(\frac{1}{4\pi\epsilon_0}\frac{e}{mc^2r^3}\vec{L}\right)$ → both operators

$H'_{so} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}$ (spin-orbit interaction)

Correction Thomas precession introduce a $\frac{1}{2}$ factor → $\boxed{H'_{so} = \frac{e^2}{8\pi\epsilon_0}\frac{1}{m^2c^2r^3}\vec{S}\cdot\vec{L}}$

$\vec{J} = \vec{S} + \vec{L} \rightarrow \underbrace{J^2 = S^2 + L^2 + 2\vec{S}\cdot\vec{L}}$ etc.

L^2 commutes, S^2 commutes,
eigenfunctions of L^2 & S^2 are the good states

also J^2, $\cancel{L_z}$ J_z commutes ⇒ we will use their eigenvalues

HW Question 16, Gasiorowicz

$\rightarrow \vec{L}\cdot\vec{S} = \frac{1}{2}(J^2 - L^2 - S^2)$

then eigenvalues of $\vec{L}\cdot\vec{S}$: $\frac{\hbar^2}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]$

$\longrightarrow$ notice that $Y_\ell^{m_\ell}$'s are the eigenfunction. Use it:

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{\ell(\ell+1)(\ell+\frac{1}{2})n^3 a^3}$$

insert

$$\langle jn\ell | H' | jn\ell \rangle = E_{so}^1 = \frac{e^2}{8\pi\varepsilon_0}\frac{1}{m^2c^2}\frac{1}{\ell(\ell+1)^2 n^3 a^3}\frac{\hbar^2}{2}\left[j(j+1) - \ell(\ell+1) - s(s+1)\right]$$

let $\underbrace{s=\frac{1}{2}}_{\text{electron}}$,

$$\boxed{E_{so}^1 = \frac{e^2\hbar^2}{16\pi\varepsilon_0 m^2c^2}\frac{\left[j(j+1) - \ell(\ell+1) - 3/4\right]}{\ell(\ell+1)(\ell+\frac{1}{2})n^3a^3}}$$

$\rightarrow$ Level of this is similar to relativistic correction

$$\boxed{E_{so}^1 = \frac{E_n^2}{mc^2}\left[\frac{n\left[j(j+1) - \ell(\ell+1) - 3/4\right]}{\ell(\ell+1)(\ell+\frac{1}{2})}\right]}$$

$\rightarrow$ do it

since $s = \frac{1}{2}$, $j = \ell + \frac{1}{2}, \dots, |\ell - \frac{1}{2}|$

$j = \ell + s \Rightarrow \ell = j - s = j - \frac{1}{2}$ $\rightarrow$ insert

$$E_{so}^1 = \frac{E_n^2}{mc^2}\left[\frac{n\left[j(j+1) - (j-\frac{1}{2})(j+\frac{1}{2}) - 3/4\right]}{(j-\frac{1}{2})(j+\frac{1}{2})j}\right]$$

$$E_{so}^1 = \frac{E_n^2}{mc^2}\left[\frac{n(\cancel{j^2} + j - \cancel{j^2} + \frac{1}{4} - \frac{3}{4})}{(j-\frac{1}{2})(j+\frac{1}{2})j}\right] = \boxed{\frac{E_n^2}{mc^2}\frac{n}{j(j+\frac{1}{2})}}$$

Spin orbit coupling correction

HENCE, first order correction to fine structure,

$$\boxed{E_{fs}^1 = E_r^1 + E_{so}^1 = \frac{E_n^2}{mc^2}\left[\frac{n}{j(j+\frac{1}{2})} - \frac{2n}{j} + 3\right]} \quad \boxed{= \frac{E_n^2}{2mc^2}\left(3 - \frac{4n}{j+\frac{1}{2}}\right.}$$

	$l=0$ (s)	$l=1$ (p)	$l=2$ (d)	$l=3$ (f)	
$n=3$	o	o	o	×	$j=5/2$, $j=3/2$, $j=\frac{1}{2}$
$n=2$	o	o	×	×	$j=3/2$, $j=\frac{1}{2}$
$n=1$	o	×	×	×	$j=\frac{1}{2}$

do it.

→ For a given n & j, $\boxed{E_{nj} = \frac{-13.6\,eV}{n^2}\left[1 + \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right]}$

do it.