17.02.2012

$$H = \vec{\alpha}\cdot\vec{p} + \beta m + V(r)$$

$$H\Psi = E\Psi \quad \text{(eigenvalue equation)}$$

$$\vec{J} = \vec{L} + \vec{S} \rightarrow \frac{\hbar}{2}\begin{pmatrix}\sigma & 0\\ 0 & \sigma\end{pmatrix}$$

$$P\Psi(\vec{r}) = \beta\Psi(-\vec{r}) \qquad [H, J_i] = 0$$

$$[H, P] = 0$$

$$[J_i, J_j] = i\epsilon^{ijk}J_k$$

$\Rightarrow$ We have simultaneous eigenstates of

$$H,\ J^2,\ J_z,\ P.$$

Eigenstates of L^2, S^2, L_z, S_z

$$Y_{lm_l}(\theta,\phi)\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \text{ or } Y_{lm_l}(\theta,\phi)\begin{pmatrix}0\\0\\1\\0\end{pmatrix} \Big/ Y_{lm_l}(\theta,\phi)\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

$L^2 = l(l+1)$ $\quad S_z = \pm\frac{1}{2}$ $\quad$ & $\quad Y_{lm_l}(\theta,\phi)\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$

$L_z = m_l$

$$P \rightarrow (-1)^l \quad 1 \quad 1 \quad -1 \quad -1$$

$$(\theta,\phi) \rightarrow (\pi-\theta, \phi+\pi) \quad \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \begin{pmatrix}0\\1\\0\\0\end{pmatrix} \begin{pmatrix}0\\0\\1\\0\end{pmatrix} \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

$Y^l_{m_l}$'s transform as

$$(-1)^l Y^l_m.$$

First fix

$$J^2 = j(j+1), \quad J_z = m$$

$$\sum C^{j\ l\ s=\frac{1}{2}}_{m\ m_l\ m_s} |l, s, m_l, m_s\rangle$$

$m_l \rightarrow m - m_s$, $\quad m_s \rightarrow \pm\frac{1}{2}$

$l = j \pm \frac{1}{2}$. $\qquad$ Exercise $\rightarrow$ Check that

$$l = j - \frac{1}{2} \Rightarrow |l, s, j, m\rangle$$

$$= C^{j\ \ell\ \frac{1}{2}}_{m\ \ m-\frac{1}{2}\ \ \frac{1}{2}} \begin{pmatrix} Y_{\ell,\, m-\frac{1}{2}}(\theta,\phi) \\ 0 \\ \vdots \end{pmatrix} + C^{j\ \ell\ \frac{1}{2}}_{m\ \ m+\frac{1}{2}\ \ -\frac{1}{2}} \begin{pmatrix} 0 \\ Y_{\ell,\, m+\frac{1}{2}} \\ \vdots \end{pmatrix}$$

$$= \begin{pmatrix} \varphi^{(+)}_{jm} \\ 0 \\ \vdots \end{pmatrix} \qquad \varphi^{(+)}_{jm} = \begin{pmatrix} \sqrt{\dfrac{\ell+\frac{1}{2}+m}{2\ell+1}}\ Y_{\ell,\, m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\dfrac{\ell+\frac{1}{2}-m}{2\ell+1}}\ Y_{\ell,\, m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

$$\ell = j+\frac{1}{2} \implies \begin{pmatrix} \varphi^{(-)}_{jm} \\ 0 \\ 0 \end{pmatrix} \qquad \varphi^{(-)}_{jm} = \begin{pmatrix} \sqrt{\dfrac{\ell+\frac{1}{2}-m}{2\ell+1}}\ Y_{\ell,\, m-\frac{1}{2}}(\theta \\ -\sqrt{\dfrac{\ell+\frac{1}{2}+m}{2\ell+1}}\ Y_{\ell,\, m+\frac{1}{2}}(\theta \end{pmatrix}$$

A general state with $J^2 = j(j+1)$ & $J_z = m$ is

$$\begin{pmatrix} g^{(+)}(r)\ \varphi^{(+)}_{jm} + g^{(-)}(r)\ \varphi^{(-)}_{jm} \\ f^{(+)}(r)\ \varphi^{(+)}_{jm} + f^{(-)}(r)\ \varphi^{(-)}_{jm} \end{pmatrix}$$

generally depend on j's

[Now, we require these to be eigenstates of H & P

<u>Parity</u>

$\varphi^{(+)} \longrightarrow \ell = j-\frac{1}{2}, \quad \varphi^{(-)} \longrightarrow \ell = j+\frac{1}{2}$

$$P\psi = \begin{pmatrix} (-1)^{j-\frac{1}{2}}\ g^{(+)}\ \varphi^{(+)}_{jm} + (-1)^{j+\frac{1}{2}}\ g^{(-)}\ \varphi^{(-)}_{jm} \\ -(-1)^{j-\frac{1}{2}}\ f^{(+)}\ \varphi^{(+)}_{jm} - (-1)^{j+\frac{1}{2}}\ f^{(-)}\ \varphi^{(-)}_{jm} \end{pmatrix}$$

$$= (-1)^{j-\frac{1}{2}} \begin{pmatrix} g^{(+)}\ \varphi^{(+)} - g^{(-)}\ \varphi^{(-)} \\ -f^{(+)}\ \varphi^{(+)} + f^{(-)}\ \varphi^{(-)} \end{pmatrix}.$$

$\therefore$ Parity eigenstates are —

$$\begin{pmatrix} g^{(+)} \varphi^{(+)} \\ f^{(-)} \varphi^{(-)} \end{pmatrix} \quad \underline{\text{OR}} \quad \begin{pmatrix} g^{(-)} \varphi^{(-)} \\ f^{(+)} \varphi^{(+)} \end{pmatrix}$$

$(-1)^{j-\frac{1}{2}}$ $\qquad$ $(-1)^{j+\frac{1}{2}}$

eigenvalues

$\varphi^{(+)} \rightarrow l = j - \frac{1}{2}$

$\varphi^{(-)} \rightarrow l = j + \frac{1}{2}$

For $\varphi^{(+)} \longrightarrow (x \;\; y \;\; z)\, \varphi^{(+)}$

$J^2 = j(j+1) \longrightarrow j - \frac{3}{2},\; j + \frac{1}{2}$

$\Downarrow$

out

If we multiply $\varphi^{(+)}$ by an operator which commutes with J^2, it doesn't change j. So we get only $(j + \frac{1}{2})$

$$\left[\vec{J}, \frac{\vec{r} \cdot \vec{\sigma}}{|\vec{r}|} \right] = 0.$$

depends only on the angles

scalar operator

$$\varphi^{(-)}_{jm} = \frac{\vec{r} \cdot \vec{\sigma}}{r} \varphi^{(+)}_{jm}$$

upto a phase

<u>Exercise</u> $\rightarrow$ Check that phase $= 1$.

$$\varphi^{(+)}_{jm} = \frac{\vec{r} \cdot \vec{\sigma}}{r} \varphi^{(-)}_{jm}$$

$(\vec{r} \cdot \vec{\sigma})^2 = r^2$

Define : $\chi^{(j\,l)}_{jm} = \varphi^{(+)}_{jm}$ if $l = j - \frac{1}{2}$

2-component $= \varphi^{(-)}_{jm}$ if $l = j + \frac{1}{2}$

So, general form of $\psi = \begin{pmatrix} g\, \chi^{(j,l)}_{jm} \\ f\, \frac{\vec{\sigma} \cdot \vec{r}}{r} \chi^{(j,l)}_{jm} \end{pmatrix}$ Parity $(-1)^l$

Now comes H.

J^2, J_z, P eigenstates.

$$H\psi = \left(\vec{\alpha}\cdot\vec{p} + \beta m + V\right)\psi$$

$$= \begin{pmatrix} (m+V(r))\,\mathbb{1}_{2\times2} & \vec{\sigma}\cdot(-i\vec{\nabla}) \\ \vec{\sigma}\cdot(-i\vec{\nabla}) & (-m+V(r))\,\mathbb{1}_{2\times2} \end{pmatrix}\psi$$

$$\psi = \begin{pmatrix} g(r)\,\mathcal{X}^{(j\,l)}_{jm} \\ f(r)\,\dfrac{\vec{\sigma}\cdot\vec{r}}{r}\,\mathcal{X}^{(j\,l)}_{jm} \end{pmatrix}.$$

$H\psi = E\psi$
(To solve!)

$$E\,g(r)\,\mathcal{X}^{(j\,l)}_{jm} = \left(m+V(r)\right)\mathcal{X}^{(j\,l)}_{jm}\,g(r) + \vec{\sigma}\cdot\left(-i\vec{\nabla}\right)\left(f(r)\,\frac{\vec{\sigma}\cdot\vec{r}}{r}\mathcal{X}\right)$$

$$E\,f(r)\,\frac{\vec{\sigma}\cdot\vec{r}}{r}\,\mathcal{X}^{(j\,l)}_{jm} = \left(-m+V(r)\right)\frac{\vec{\sigma}\cdot\vec{r}}{r}\,\mathcal{X}^{(j\,l)}_{jm}\,f(r) + \vec{\sigma}\cdot(-i\vec{\nabla})\left\{g(r)\,\mathcal{X}^{(j\,l)}_{jm}\right\}$$

$$\vec{\nabla} f(r) = \frac{\partial f}{\partial r}\frac{\vec{r}}{r}$$

$$\vec{\sigma}\cdot\vec{\nabla}\left(f(r)\,\frac{\vec{\sigma}\cdot\vec{r}}{r}\mathcal{X}\right) = \frac{\partial(f/r)}{\partial r}\frac{\vec{\sigma}\cdot\vec{r}}{r}\,\vec{\sigma}\cdot\vec{r}\,\mathcal{X} + \frac{f(r)}{r}\,\vec{\sigma}\cdot\vec{\nabla}\,\vec{\sigma}\cdot\vec{r}\,\mathcal{X}$$

$$= r\frac{\partial}{\partial r}\left(f/r\right)\mathcal{X} + \frac{1}{r}f\,\sigma^i\sigma^j\,\nabla_i\left(r_j\,\mathcal{X}\right)$$

$$\cancel{\sigma_i\sigma_j}\quad \sigma^i\sigma^j\underbrace{\left(\vec{\nabla}_i\,r_j\right)}_{\delta_{ij}}\mathcal{X} + \sigma^i\sigma^j r_j\,\nabla_i\,\mathcal{X}$$

$$\downarrow$$

$$3\mathcal{X} + \left(\delta_{ij} + i\epsilon^{ijk}\sigma_k\right)r_j\,\nabla_i\,\mathcal{X}$$

$$= 3\mathcal{X} + \underbrace{\left(\vec{r}\cdot\vec{\nabla}\right)}_{r\frac{\partial}{\partial r}}\mathcal{X} + \vec{\sigma}\cdot\vec{L}\,\mathcal{X}.$$

(!!) $$= 3\mathcal{X} + \vec{\sigma}\cdot\vec{L}\,\mathcal{X}$$

$$= 3\mathcal{X} + 2\vec{S}\cdot\vec{L}\,\mathcal{X}$$

$$\Downarrow$$

$$\left(J^2 - L^2 - S^2\right)\mathcal{X}$$

$$= \left\{j(j+1) - l(l+1) - \frac{3}{4}\right\}\mathcal{X}$$

$\mathcal{X}$ has completely been factored out.

Result

An equation involving $g, f, \frac{dg}{dr}, f$. (1st one)

$$(\vec{\sigma}\cdot\vec{\nabla})(g(r)\,\chi)$$

$$= \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\,\vec{\sigma}\cdot\vec{r}\,\vec{\sigma}\cdot\vec{\nabla}\,(g(r)\,\chi)$$

$$\sigma^i\sigma^j r_i \nabla_j (\quad)$$

$$(\vec{\sigma}\cdot\vec{\nabla})\,g(r)\,\chi \longrightarrow \frac{\vec{\sigma}\cdot\vec{r}}{r}\frac{\partial g}{\partial r}\chi + g(r)\,\vec{\sigma}\cdot\vec{\nabla}\chi$$

$$\vec{\nabla} g(r) = \frac{\vec{r}}{r}\frac{\partial g}{\partial r}$$

$$\frac{\vec{\sigma}\cdot\vec{r}}{r}\,\frac{\vec{\sigma}\cdot\vec{r}}{r^2}\,\vec{\sigma}\cdot\vec{\nabla}\chi$$

$$\frac{\vec{\sigma}\cdot\vec{r}}{r}\frac{\partial g}{\partial r}\chi - \frac{\vec{\sigma}\cdot\vec{r}}{r^2}\,g\;\vec{\sigma}\cdot\vec{L}\chi = \underbrace{\sigma^i\sigma^j}_{(\delta^{ij} + i\epsilon^{ijk}\sigma^k)} r_i \nabla_j \chi$$

Second eq$^{\underline{n}}$ involves g, f & $\frac{dg}{dr}$.

22.02.2012

We were dealing with Hydrogen Atom.

· From symmetry considerations, we found that

$$\psi = \begin{pmatrix} g(r)\,\varphi^{l}_{jm} \\ f(r)\,\frac{\vec{\sigma}\cdot\vec{r}}{r}\,\varphi^{l}_{jm} \end{pmatrix}$$

$$\varphi^{l}_{jm} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\; Y_{l\,m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\; Y_{l\,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}$$

for $j = l + \frac{1}{2}$

$$\varphi^{l}_{jm} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\; Y_{l\,m-\frac{1}{2}}(\theta,\phi) \\ -\sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\; Y_{l\,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix} \quad \text{for } l = j + \frac{1}{2}$$

• Observe that ψ is not an $\hat{L}^2$ eigenstate.

$$\left(E - m - V(r)\right) g\, \varphi^{l}_{jm} = -i\, \vec{\sigma}\cdot\vec{\nabla}\left(f\, \frac{\vec{\sigma}\cdot\vec{r}}{r}\, \varphi^{l}_{jm}\right). \quad (1)$$

$$\left(E + m - V(r)\right) \frac{\vec{\sigma}\cdot\vec{r}}{r} f\, \varphi^{l}_{jm} = -i\, \vec{\sigma}\cdot\vec{\nabla}\left(g\, \varphi^{l}_{jm}\right). \quad (2)$$

$\hat{H}\psi = E$

We had manipulated the first equation to get -

$$\left(E - m - V(r)\right) g = -ir\frac{\partial}{\partial r}\left(\frac{f}{r}\right) - 3i\frac{f}{r} + i\frac{(K+1)}{r} f.$$

$$\left\{\begin{array}{l} (K+1) \longrightarrow l(l+1) + \frac{3}{4} - j(j+1) \\ \text{This is } -2\vec{S}\cdot\vec{L} \text{ eigenvalue} \end{array}\right\} \begin{array}{l} -l \text{ for } j = l \\ (l+1) \text{ for } j = \end{array}$$

$$\left(\frac{\vec{\sigma}\cdot\vec{r}}{r}\right)^2 = 1. \qquad \left(E + m - V(r)\right) f\, \varphi^{l}_{jm} = -i\, \vec{\sigma}\cdot\frac{\vec{r}}{r}\, \vec{\sigma}\cdot\vec{\nabla}\left(g\, \varphi\right.$$

[Multiplying (2) on both sides by $\frac{\vec{\sigma}\cdot\vec{r}}{r}$.]

So, $$\left(E + m - V(r)\right) f\, \varphi^{l}_{jm} = -i\, \frac{\vec{\sigma}\cdot\vec{r}}{r}\left(\vec{\sigma}\cdot\vec{\nabla} g\right) \varphi^{l}_{jm} - i\frac{g}{r}\, \vec{\sigma}\cdot\vec{r}\, \vec{\sigma}\cdot\vec{\nabla}\, \varphi^{l}_{jm}$$

• <u>Second term of RHS</u>

$$\vec{\sigma}\cdot\vec{r}\, \vec{\sigma}\cdot\vec{\nabla}\, \varphi^{l}_{jm} = \sigma^i \sigma^j r^i \nabla^j\, \varphi^{l}_{jm}$$

$$= \left(\underbrace{\delta_{ij}\, r^i \nabla^j}_{\vec{r}\cdot\vec{\nabla}} + \underbrace{i\, \epsilon^{ijk} \nabla^j \sigma^k}_{-\vec{L}\cdot\vec{\sigma}}\right)\varphi^{l}$$

$$r\frac{\partial}{\partial r}\varphi^{l}_{jm} = 0 \qquad \underbrace{-\vec{L}\cdot\vec{\sigma}}_{(K+1)\,\varphi^{l}_{jm}}$$

We get, $$\left(E + m - V(r)\right) f\, \varphi^{l}_{jm}$$

$$= \left\{-i\frac{dg}{dr} - i(K+1)\frac{g}{r}\right\} \varphi^{l}_{jm}.$$

$$\left(E + m - V(r)\right) f = \left\{ -i \frac{dg}{dr} - i(K+1)\frac{g}{r} \right\}$$

· To recover usual Schrödinger equation, we eliminate f. (anti-particle part)

Introduce new functions F & G defined as –

$$\left.\begin{aligned} g &= i\, G/r \\ f &= F/r \end{aligned}\right\} \qquad V(r) = -\frac{Ze^2}{r} \text{ (Coulomb potential)}$$

$Z \rightarrow$ atomic number

$$\left(E - m + \frac{Ze^2}{r}\right) \cancel{i}\frac{G}{r} = -\cancel{i}\, r \frac{d}{dr}\left(\frac{F}{r^2}\right) - 3\cancel{i}\frac{F}{r^2} + \cancel{i}(K+1)\frac{F}{r^2}.$$

(first equation)

$$\left(E + m + \frac{Ze^2}{r}\right)\frac{F}{r} = \frac{d}{dr}\left(\frac{G}{r}\right) + (K+1)\frac{G}{r^2}.$$

(second equation)

$$\left(E - m + \frac{Ze^2}{r}\right) G = -r^2\left(\frac{1}{r^2}\frac{dF}{dr} - \frac{2}{r^3}F\right) - 3\frac{F}{r} + (K+1)\frac{F}{r}.$$

$$= -\frac{dF}{dr} + \frac{K}{r}F. \quad \text{(simplifies !)}$$

Second equation similarly reduces to

$$\left(E + m + \frac{Ze^2}{r}\right) F = \frac{dG}{dr} + \frac{K}{r}G.$$

Bound states $\longrightarrow$ $E < m$. (analogous to $E < 0$ in non-rel. case)

$\underline{\underline{r \rightarrow \infty}}$ limit (asymptotic)

$$\left\{\begin{aligned} (E + m) f &= \frac{dG}{dr} \\ (E - m) G &= -\frac{dF}{dr} \end{aligned}\right\} \quad \left(\text{Dropping } o\left(\frac{1}{r}\right).\right)$$

$$\frac{d^2G}{dr^2} = (E+m)\frac{dF}{dr} = (m^2 - E^2)\, G$$

$$\Rightarrow \quad G \approx C\, e^{-\sqrt{m^2+E^2}\, r}.$$

(Ignoring + sign. . .)

$$F \cong \left(\frac{C}{E+m}\right)(-1)\sqrt{m^2-E^2}\; e^{-\sqrt{m^2-E^2}\, r} = -C\sqrt{\frac{m-E}{m+E}}\; e^{-\sqrt{m}}$$

$\underline{\underline{r \to 0}} \longrightarrow$ we expect $O\left(\frac{1}{r}\right)$ and $\frac{dG}{dr}$ or

are of the same order.

$$\left.\begin{aligned} \frac{Ze^2}{r} F &\approx \frac{dG}{dr} + \frac{K}{r} G. \\ \frac{Ze^2}{r} G &\approx -\frac{dF}{dr} + \frac{K}{r} F. \end{aligned}\right\} \qquad F/G \propto r^{n}$$

(we expect)

We should look for solutions like $F \simeq A r^{\gamma}$, $G \simeq B r^{\gamma}$.

$$Ze^2 A r^{\gamma-1} = \gamma B\, r^{\gamma-1} + K B\, r^{\gamma-1}$$

$$Ze^2 B\, r^{\gamma-1} = -\gamma A\, r^{\gamma-1} + K A\, r^{\gamma-1}$$

$$\Rightarrow \quad \begin{aligned} Ze^2 A &= (\gamma + K)\, B \\ Ze^2 B &= (K - \gamma)\, A \end{aligned}$$

$$-(\gamma^2 - K^2) = (Ze^2)^2$$

$$\Rightarrow \quad \gamma^2 = K^2 - (Ze^2)^2$$

$$\Rightarrow \quad \gamma = \sqrt{K^2 - (Ze^2)^2}$$

$$\left\{\begin{aligned} K &= -l-1 \quad \text{for } j = l + \tfrac{1}{2} \\ K &= l \quad \text{for } j = l - \tfrac{1}{2} \\ K &\neq 0 \end{aligned}\right\}$$

(Choice of positive root - $r \to 0$ behaviour)

- The analysis holds for $Ze^2 < 1$.

<u>Trial solution</u>

$$\left\{\begin{aligned} F &= e^{-\sqrt{m^2-E^2}\, r}\; r^{\gamma} \sum_{n=0}^{\infty} a_n r^n \\ G &= e^{-\sqrt{m^2-E^2}\, r}\; r^{\gamma} \sum_{n=0}^{\infty} b_n r^n \end{aligned}\right\}$$

Substitute in the original equation. Get recursion relations for a_n & b_n.

- One can take $a_0 = 1$. Get all a_n's & b_n's.
- Demand → series terminates.

What do we get ?? Define $\alpha = e^2$

$$E_{n,l,j,m} = m\left[1 + \left(\frac{Z\alpha}{n + l - (j+\frac{1}{2}) + \sqrt{(j+\frac{1}{2})^2 - Z^2\alpha^2}}\right)^2\right]^{-1/2}$$

m → mass

ψ : not L^2 eigenstate

$n \to 1, 2, 3, \ldots$ Quantum number

$l \to$ not angular momentum

↳ takes care of parity symmetry

$j \pm \frac{1}{2} \to$ allowed values

What about non-relativistic limit ?

- Restore c.

$$m \longrightarrow mc^2 \quad (\checkmark)$$

$$\alpha \to e^2 \qquad e^2/r^2 = \text{force} = [MLT^{-2}]$$

$$[e^2] = [ML^3T^{-2}]$$

$$[\hbar] = [ML^2T^{-1}]$$

$$[c] = [LT^{-1}] \qquad \hbar c \checkmark$$

$$\alpha \to e^2/\hbar c$$

dimensionless

⇝ $\alpha \to 0$ limit & keep leading terms

$$E = mc^2\left[1 + \frac{Z^2\alpha^2}{(n+l)^2}\right]^{-1/2}$$

$$= mc^2\left(1 - \frac{Z^2\alpha^2}{2(n+l)^2}\right)$$

$$= mc^2 - \frac{Z^2 e^4/\hbar^2c^2 \; mc^2}{2(n+l)^2}$$

$$= mc^2 - \frac{Z^2 e^4 m}{2\hbar^2(n+l)^2}$$

Rydberg formula

$l \longrightarrow$ angular mom. eigenvalue (status regained!)

Next order $\longrightarrow$? (upto $O(\alpha^4)$.)

<u>Exercise</u> Check that $E = mc^2 - \frac{1}{2}\frac{Z^2\alpha^2 mc^2}{(n+l)^2}$

$$- \frac{Z^4\alpha^4 mc^2}{2(n+l)^2}\left(\frac{1}{(n+l)(j+\frac{1}{2})} - \frac{3}{4(n+l)}\right) + O(\alpha^6).$$

$\rightsquigarrow$ Now, E depends on j

$\underbrace{n+l}_{1}$ (degenerate)

$^2S_{1/2} \longleftrightarrow {}^2P_{1/2}$ $\updownarrow$ splits for Rel. H-atom.

$l=0$, $j = 1/2$

$^2P_{3/2}$

all degenerate for N-R Schrödinger eq^n.

- This is called fine-structure splitting.

There are other interactions $\rightsquigarrow$ $\vec{S}_N \cdot \vec{S}_{electron}$

$\underbrace{J_{tot.} = 0 \text{ or } 1}_{(1/2 \oplus 1/2)}$. nuclear spin

- <u>Finer splitting</u> [hyperfine splitting]

- Finally. $^2S_{1/2}$ & $^2P_{1/2}$ levels also split $\longrightarrow$ Lamb shift (QFT)

<u>23.02.2012</u>

Electron in a uniform magnetic field :-

$\rightarrow$ 1) NR, no spin
2) add spin
3) Relativistic

$$H = \frac{1}{2m}\left(\vec{p} - e\vec{A}/c\right)^2$$

Put back factors of $\hbar$ & c.

$$H = \frac{\vec{p}^2}{2m} - \frac{e}{2mc}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{2mc^2}\vec{A}^2$$

(Not 'weak' magnetic field)

• Choose a specific gauge. We take $\vec{B} = B\hat{z}$ → constant

One possible choice →

$$A_y = \frac{Bx}{2}$$

$$A_x = -\frac{By}{2}$$

$$\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} = \frac{B}{2} - \left(-\frac{B}{2}\right) \quad \text{(symmetric gauge)}$$

$$= B.$$

$$H = \frac{p^2}{2m} - \frac{e}{2mc}\left(-\frac{B}{2}p_x y + \frac{B}{2}p_y x - \frac{B}{2}y p_x + \frac{B}{2}x p_y\right)$$

$$+ \frac{e^2}{2mc^2}\frac{B^2}{4}(x^2+y^2)$$

$$= \frac{p^2}{2m} - \frac{eB}{2mc}L_z + \frac{e^2B^2}{8mc^2}(x^2+y^2)$$

$$\therefore H = \underbrace{\frac{(p_x^2+p_y^2)}{2m} + \frac{e^2B^2}{8mc^2}(x^2+y^2)}_{H_1} - \underbrace{\frac{eB}{2mc}L_z}_{H_2} + \underbrace{\frac{p_z^2}{2m}}_{H_3}.$$

$L_z = x p_y - y p_x$. Mutually commuting parts

H.O. part : $(a_x^\dagger)^{n_x}(a_y^\dagger)^{n_y}|0\rangle$

• Choose eigenstates of L_z.

Define
$$a_+^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger + i a_y^\dagger)$$
$$a_-^\dagger = \frac{1}{\sqrt{2}}(a_x^\dagger - i a_y^\dagger)$$

$$\underbrace{[L_z, a_+^\dagger] = \hbar a_+^\dagger \qquad [L_z, a_-^\dagger] = -\hbar a_-^\dagger}_{\text{(Check !)}}$$

$|n_+, n_-\rangle = (a_+^\dagger)^{n_+}(a_-^\dagger)^{n_-}|0\rangle$ (Basis transformation)

$$|n_+, n_-, k\rangle = |n_+, n_-\rangle \otimes e^{ikz}.$$

(Total state)

Define $\omega = \frac{eB}{2mc}$

$$H_1|n_+, n_-, k\rangle = \frac{eB\hbar}{2mc}(n_+ + n_- + 1)|n_+, n_-, k\rangle$$

$$H_2|n_+, n_-, k\rangle = -\frac{eB}{2mc}(n_+ - n_-)\hbar|n_+, n_-, k\rangle$$

$$H_3 \,|n_+, n_-, k\rangle = \frac{\hbar^2 k^2}{2m} |n_+, n_-, k\rangle$$

$$E = \frac{\hbar^2 k^2}{2m} + \frac{eB\hbar}{2mc}(2n_- + 1)$$

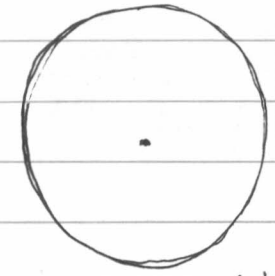
$$= \frac{\hbar^2 k^2}{2m} + \boxed{\frac{eB\hbar}{mc}\left(n_- + \frac{1}{2}\right)} \longrightarrow \hbar\omega_c\left(n_- + \frac{1}{2}\right)$$

(ignorable) $\omega_c \rightarrow$ cyclotron frequency

- Energy doesn't depend on $n_+ \longrightarrow$ infinite degeneracy of levels. . . $\rightsquigarrow$ arbitrary angular momentum

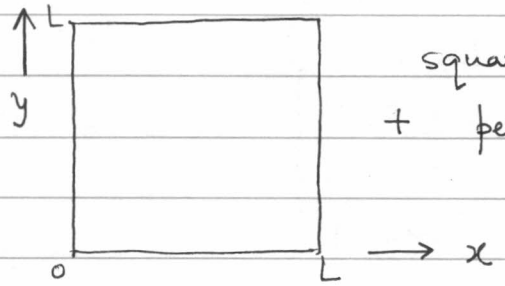
$\longrightarrow$ Assumption $\rightarrow$ INFINITE PLANE

What if confined? $\longrightarrow$ finite degeneracy



$\left\{\begin{matrix}\text{circular}\\ \text{box}\end{matrix}\right\} \rightsquigarrow$ [Rigorous way]

Degeneracy $\longrightarrow$ small B limit



square box + periodic boundary condition

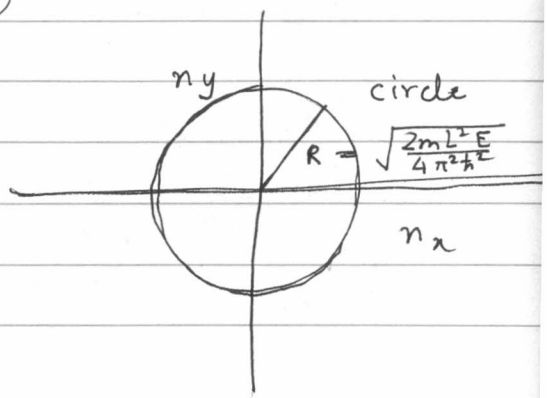
$$\psi = e^{i(k_x x + k_y y)}$$

$$\left[k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}\right]$$

$n_x, n_y \rightarrow$ integers

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

$$= \frac{\hbar^2 \cdot 4\pi^2}{2mL^2}\left(n_x^2 + n_y^2\right)$$



$$\# \text{ of states below } E = \pi \frac{2mL^2E}{h^2}$$

$$= \left(\frac{mL^2}{2\pi\hbar^2}\right)E$$

# of states with energy between E & $E+\delta E$

$$= \frac{mL^2}{2\pi\hbar^2}\,\cancel{\Delta E}\;\delta E$$

Now, the weak field problem. $\Rightarrow$

If D is the degeneracy per level then # of states with energy between $(E,\ E+\delta E)$

$$= D(E) \times \frac{\delta E}{\hbar\omega_c}$$

$\odot$ Match with previous result

$$D(E)\frac{\delta E}{\hbar\omega_c} = \frac{mL^2}{2\pi\hbar^2}\,\delta E$$

$$\Rightarrow D(E) = \frac{mL^2}{2\pi\hbar^2}\hbar\omega_c = \frac{\cancel{m}L^2}{2\pi\hbar}\frac{eB}{\cancel{m}c}$$

$$= \underbrace{(L^2B)}_{\text{flux}} \times \underbrace{\left(\frac{e}{2\pi\hbar c}\right)}_{(\phi_0)} \rightarrow \text{flux quantum}$$

$$D(E) = \text{flux} \times \frac{1}{\phi_0}$$

$\rightarrow$ $\boxed{\text{Flux quantization}}$ The levels in weak mag. field $\longrightarrow$ LANDAU LEVELS

<u>Adding spin</u>

Add new term $H_4 = -\frac{eB}{2mc}\cdot 2S_z$ to the Hamiltonian.

$$= -\frac{eB}{mc}S_z.$$

$$S_z|\ \rangle = m_s\hbar|\ \rangle$$

$$\begin{pmatrix}1\\0\end{pmatrix},\ \begin{pmatrix}0\\1\end{pmatrix}.$$

$$\Rightarrow \frac{\hbar^2k^2}{2m} + \underbrace{\frac{eB\hbar}{mc}}_{\omega_c}\left(n_- + \frac{1}{2} - m_s\right)$$

$n_- = 0, 1, 2, \ldots$ $\boxed{m_s = \pm\frac{1}{2}}$

(2D) $2\hbar\omega_c$ —— $n_- = 2,\ m_s = \frac{1}{2},\quad n_- = 1,\ m_s = -\frac{1}{2}$

(2D) $\hbar\omega_c$ —— $n_- = 1,\ m_s = \frac{1}{2},\quad n_- = 0,\ m_s = -\frac{1}{2}$

(D) 0 —— lowest level $\rightarrow$ zero

$n = 0,\ m_s = \frac{1}{2}$

- Every level excepting 0 will be "extra" <u>2-fold degenerat</u>

<u>Full relativistic problem</u>

$$\hat{H} = c\vec{\alpha}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right) + \beta mc^2$$

$$= \begin{pmatrix} mc^2 & c\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right) \\ c\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right) & -mc^2 \end{pmatrix}$$

$$H\Psi = E\Psi \quad . \qquad \Psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} .$$

Equation(s) $\rightarrow$

$$\begin{cases} (mc^2 - E)\varphi + c\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right)\chi = 0 \\ (mc^2 + E)\chi + c\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right)\varphi = 0 \end{cases}$$

Substitute $\chi = \frac{1}{mc^2 + E}\, c\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right)\varphi$ in first equation.

$$(mc^2 - E)\varphi + \frac{c^2}{mc^2 + E}\left(\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2\right)\phi = 0$$

$$(m^2c^4 - E^2)\varphi + \underbrace{c^2\cdot 2m\left\{\frac{1}{2m}\,\vec{\sigma}\cdot\left(\vec{p} - \frac{e\vec{A}}{c}\right)\right\}^2}_{\text{non-relativistic } H \text{ with spin (!)}}\varphi = 0$$

$$\sigma^i\sigma^j\left(p^i - \frac{eA_i}{c}\right)\left(p^j - \frac{eA_j}{c}\right)$$

$$\longleftrightarrow \left(\delta_{ij} + i\epsilon^{ijk}\sigma_k\right)$$

$$(m^2c^4 - E^2)\varphi + 2mc^2 \underset{\substack{\parallel \\ \text{non rel. Ham.}}}{H_{NR}}\varphi = 0 .$$

$$m^2c^4 - E^2 + 2mc^2 E_{NR} = 0 \quad (\text{with spin})$$

$\downarrow$

<u>eigenvalues of H_{NR}</u>

$$E = \sqrt{m^2c^4 + 2mc^2 E_{NR}} .$$