13.5 Central Potential:

$$i\hbar \frac{\partial}{\partial t}\Psi = \hat{H}\Psi, \quad \hat{H} = c\vec{\alpha}\cdot\hat{\vec{p}} + mc^2\beta + q\varphi(\underbrace{r}_{=|\vec{x}|})$$

$$[\hat{H}, \hat{\vec{J}}]_- = 0, \quad \hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}, \quad \hat{\vec{L}} = \vec{x}\times\hat{\vec{p}}, \quad \hat{\vec{p}} = \frac{\hbar}{i}\vec{\nabla}, \quad \hat{\vec{S}} = \frac{\hbar}{2}\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}$$

$\Rightarrow$ we can find states, which are eigenstates of $\hat{H}, \hat{\vec{J}}^2, \hat{J}_z$

spinorial spherical harmonics are Weyl spinors, which are eigenfunctions of $\hat{\vec{J}}^2$, $\hat{J}_z = \frac{\hbar}{2}\vec{\sigma}$:

$$\boxed{\mathcal{Y}^{j=l\pm\frac{1}{2}, m}_{l, \frac{1}{2}=s}(\vartheta,\varphi)} = \begin{pmatrix} \pm\sqrt{\dfrac{l\pm m+\frac{1}{2}}{2l+1}}\; Y_l^{m-1/2}(\vartheta,\varphi) \\ \sqrt{\dfrac{l\mp m+\frac{1}{2}}{2l+1}}\; Y_l^{m+1/2}(\vartheta,\varphi)\end{pmatrix},$$

$$\hat{\vec{J}}^2\, \mathcal{Y}^{j=l\pm\frac{1}{2}, m}_{l,\frac{1}{2}}(\vartheta,\varphi) = \hbar^2 j(j+1)\, \mathcal{Y}^{j=l\pm\frac{1}{2}, m}_{l,\frac{1}{2}}(\vartheta,\varphi)$$

$$\hat{J}_z \quad \text{"} \quad = \hbar m \quad \text{"}$$

How to combine these spinorial spherical harmonics?

$$\Psi(\vec{x},t) = \Psi\, e^{-\frac{i}{\hbar}Et}, \quad \Psi = \begin{pmatrix} u \\ v\end{pmatrix}$$

$$[E - mc^2 - V(r)]\, u(\vec{x}) = c\,\boxed{\vec{\sigma}\cdot\hat{\vec{p}}}\, v(\vec{x}) \quad \longleftarrow$$

$$[E + mc^2 - V(r)]\, v(\vec{x}) = c\,\boxed{\vec{\sigma}\cdot\hat{\vec{p}}}\, u(\vec{x})$$

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

$$\vec A = \vec B = \vec x: \qquad (\vec\sigma\cdot\vec x)(\vec\sigma\cdot\vec x) = \vec x^2 = r^2$$

$$\boxed{\vec\sigma\cdot\hat{\vec p}} = \Big(\underbrace{\frac{\vec\sigma\cdot\vec x}{r}\cdot\frac{\vec\sigma\cdot\vec x}{r}}_{=1}\Big)(\vec\sigma\cdot\hat{\vec p}) = \frac{\vec\sigma\cdot\vec x}{r}\cdot\Big(\underbrace{\frac{\vec\sigma\cdot\vec x}{r}\cdot\vec\sigma\cdot\hat{\vec p}}\Big)$$

$$(*) = \underbrace{\frac{\vec x\cdot\hat{\vec p}}{r}}_{=\vec e_r\cdot\hat{\vec p} = \frac{\hbar}{i}\frac{\partial}{\partial r}} + i\underbrace{\vec\sigma\frac{\hbar}{2}}_{\hat{\vec S}}\underbrace{\frac{\vec x\times\hat{\vec p}}{r}}_{=\frac{\hat{\vec L}}{r}}\frac{2}{\hbar}$$

$$= \frac{\vec\sigma\cdot\vec x}{r}\Big\{-i\hbar\frac{\partial}{\partial r} + i\frac{1}{\hbar r}\,\underbrace{2\,\hat{\vec S}\cdot\hat{\vec L}}_{=\hat{\vec J}^2 - \hat{\vec L}^2 - \hat{\vec S}^2}\Big\}\,\mathcal{Y}$$

assume: $u, v \sim \mathcal{Y}_{\ell,\frac12}^{j=\ell\pm\frac12, m}$

$$\underbrace{= \hbar^2\{j(j+1) - \ell(\ell+1) - s(s+1)\}}_{= \varkappa = \pm(\lambda\mp1), \quad \underline{\lambda = j+\frac12}}$$

$j = \ell \pm \frac12 \;\hat=\; \ell = j \mp \frac12$:

Question: How is $\frac{\vec\sigma\cdot\vec x}{r}$ acting on $\mathcal{Y}$?

$$\underbrace{\frac{\vec x}{r}\cdot\vec\sigma}_{\text{polar axial}} = \sin\vartheta\cos\varphi\underbrace{\begin{pmatrix}0&1\\1&0\end{pmatrix}}_{=\sigma_x} + \sin\vartheta\sin\varphi\underbrace{\begin{pmatrix}0&-i\\i&0\end{pmatrix}}_{=\sigma_y} + \cos\vartheta\underbrace{\begin{pmatrix}1&0\\0&-1\end{pmatrix}}_{=\sigma_z}$$

pseudo-scalar

$$= \begin{pmatrix}\cos\vartheta & \sin\vartheta\, e^{-i\varphi}\\ \sin\vartheta\, e^{i\varphi} & -\cos\vartheta\end{pmatrix}$$

Smart approach: let us choose a special vector, e.g. $\frac{\vec x}{r} = \vec e_z \;\hat=\; \vartheta = 0$

$$\frac{\vec{x}}{r}\cdot\vec{\sigma} = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \sigma_z$$

$$Y_{lm}(\vartheta=0,\varphi) = \sqrt{\frac{2l+1}{4\pi}}\;\delta_{m,0}\;\underbrace{1}_{=P_l(\underbrace{1}_{=\cos 0})=1}$$ (has to be proven)

$$\mathcal{Y}^{j=l\pm\frac{1}{2},m}_{l,\frac{1}{2}}(0,\varphi) = \sqrt{\frac{j+\frac{1}{2}}{4\pi}}\begin{pmatrix}\pm\delta_{m,1/2}\\ \delta_{m,-1/2}\end{pmatrix}$$

$$\underbrace{\sigma_z}_{=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}\mathcal{Y}^{j,m}_{l=j\mp\frac{1}{2},\frac{1}{2}}(0,\varphi) = -\sqrt{\frac{j+\frac{1}{2}}{4\pi}}\begin{pmatrix}\cancel{\mp}\pm\,\delta_{m,1/2}\\ +\;\delta_{m,-1/2}\end{pmatrix} = -\,\mathcal{Y}^{j,m}_{l=j\pm\frac{1}{2},\frac{1}{2}}(0,\varphi)$$

due to the independence on ϑ:

$$\frac{\vec{\sigma}\cdot\vec{x}}{r}\,\mathcal{Y}^{j,m}_{l=j\mp\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi) = -\,\mathcal{Y}^{j,m}_{l=j\pm\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi) \qquad (*)$$

sign change

Option A:

$$\psi_A(\vec{x}) = \begin{pmatrix}u_A(\vec{x})\\ v_A(\vec{x})\end{pmatrix} = \begin{pmatrix}u_A(r)\;\mathcal{Y}^{j,m}_{j-\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi)\\ \underbrace{(-i)}_{\text{convention}}\,v_A(r)\;\mathcal{Y}^{j,m}_{j+\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi)\end{pmatrix}$$

1) $[E - Mc^2 - V(r)]\,u_A(r)\;\cancel{\mathcal{Y}^{j,m}_{j-\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi)} = c(\vec{\sigma}\cdot\vec{p})\,v_A(\vec{x})$

$$= \cancel{-}c\,\frac{\vec{\sigma}\cdot\vec{x}}{r}\,\mathcal{Y}^{jm}_{j\mp\frac{1}{2},\frac{1}{2}}(\vartheta,\varphi)\left\{-i\hbar\frac{\partial}{\partial r} + i\frac{\hbar}{r}(-\lambda-1)\right\}(-i)\,v_A(r)$$

$$= \hbar c\left(\frac{\partial}{\partial r} + \frac{\lambda+1}{r}\right) v_A(r)$$

2) other equation: $\left[E + mc^2 - V(r)\right] v_A(r) = -\hbar c\left(\frac{\partial}{\partial r} - \frac{\lambda-1}{r}\right) u_A(r)$

Option B: swap $+ \to -$ and $- \to +$ $\Rightarrow$ same equations!

Current state: angles eliminated, two radial differential equations

$$\left[E - Mc^2 - V(r)\right] u(r) - \hbar c\left(\frac{\partial}{\partial r} + \frac{\lambda\cancel{+1}}{r}\right) v(r) = 0$$

$$\left[E + mc^2 - V(r)\right] v(r) + \hbar c\left(\frac{\partial}{\partial r} - \frac{\lambda\cancel{-1}}{r}\right) u(r) = 0$$

substitution: $u(r) = \frac{F(r)}{r}$, $v(r) = \frac{G(r)}{r}$

$F(r)^2$ and $G(r)^2$ represent radial densities

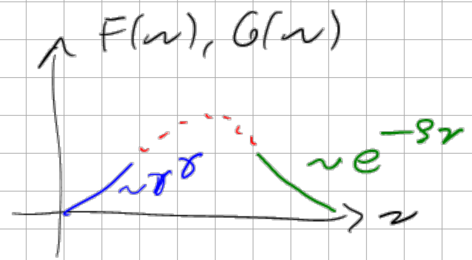
Bound states are normalizable

$$\int_0^\infty dr\, r^2\left\{|u(r)|^2 + |v(r)|^2\right\} = \int_0^\infty dr\left\{|F(r)|^2 + |G(r)|^2\right\} = 1$$

$$\begin{cases} G'(r) + \frac{\lambda}{r}G(r) = \left(\frac{E - Mc^2}{\hbar c} + \frac{\alpha}{r}\right) F(r) & (\mathrm{I}) \\ -F'(r) + \frac{\lambda}{r}F(r) = \left(\frac{E + Mc^2}{\hbar c} + \frac{\alpha}{r}\right) G(r) \end{cases}$$

$$V(r) = -\frac{\alpha\hbar c}{r}$$

13.6 Hydrogen Atom: $\quad 0 < E < mc^2, \quad mc^2 - E > 0$



asymptotic behaviour $r \to \infty$:

$$G'(r) = -\frac{mc^2 - E}{\hbar c} F(r), \qquad F'(r) = -\frac{mc^2+E}{\hbar c} G(r)$$

$$F''(r) = -\frac{mc^2+E}{\hbar c} G'(r) = \underbrace{\frac{(mc^2-E)(mc^2+E)}{\hbar^2 c^2}}_{=\rho^2} F(r),$$

$$F(r) \sim e^{\overset{(+)}{-}\rho r}, \quad G(r) \sim e^{-\rho r}, \qquad \rho = \overset{+}{(-)} \frac{\sqrt{m^2c^4 - E^2}}{\hbar c}$$

asymptotic behaviour $r \to 0$:

$$G'(r) + \frac{\lambda}{r} G(r) = \frac{\alpha}{r} F(r), \qquad F'(r) + \frac{\lambda}{r} F(r) = \frac{\alpha}{r} G(r)$$

ansatz: $\quad F(r) = \underline{a_0}\, r^\gamma, \quad G(r) = \underline{b_0}\, r^\gamma$

$$\begin{pmatrix} \alpha & -(\gamma+\lambda) \\ -(\gamma-\lambda) & -\alpha \end{pmatrix} \underbrace{\begin{pmatrix} a_0 \\ b_0 \end{pmatrix}}_{\neq \binom{0}{0}} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \begin{matrix} \Leftarrow (\mathrm{I}') \\ \Leftarrow (\mathrm{II}') \end{matrix} \qquad \lambda = j + \frac{1}{2}$$

$$\begin{vmatrix} \alpha & -(\gamma+\lambda) \\ -(\gamma-\lambda) & \alpha \end{vmatrix} = 0 \quad \Rightarrow \quad \gamma = \overset{+}{(-)} \sqrt{\lambda^2 - \alpha^2} = \sqrt{(j+\tfrac{1}{2})^2 - \alpha^2}$$

excluded due to normalizability

Interpolation between both asymptotic limits:

$$F(r) = r^\gamma e^{-\rho r} \underbrace{f(r)}_{= \sum_{n=0}^{\infty} a_n r^n}, \qquad G(r) = r^\gamma e^{-\rho r} \underbrace{g(r)}_{= \sum_{n=0}^{\infty} b_n r^n}$$

insert into (I)

$$(\gamma+\lambda)\sum_{n=\cancel{0}\,1}^{\infty} b_n r^{n\cancel{-1}} + \sum_{n=1}^{\infty} n b_n r^{n\cancel{-1}} - g\sum_{\substack{\cancel{n=0}\\ n'=1\\ n'=n+1}}^{\infty} \underbrace{b_n}_{n'-1} r^{\underbrace{n}_{n'\cancel{-1}}}$$

$$= \frac{E-mc^2}{\hbar c}\sum_{\substack{\cancel{n=0}\\ n'=1\\ n'=n+1}}^{\infty} \underbrace{a_n}_{n'-1} r^{\underbrace{n}_{n'\cancel{-1}}} + \alpha \sum_{n=\cancel{0}\,1}^{\infty} a_n r^{n\cancel{-1}}$$

$n=0$: $(\gamma+\lambda) b_0 = \alpha\, a_0$ (I')

$$\begin{matrix} \text{(II)} \\ \text{(I)} \end{matrix} \begin{pmatrix} \alpha & -(n+\gamma+\lambda) \\ -n-\gamma+\lambda & -\alpha \end{pmatrix} \boxed{\begin{pmatrix} a_n \\ b_n \end{pmatrix}} = \underbrace{\begin{pmatrix} \frac{mc^2-E}{\hbar c} & -g \\ -g & \frac{mc^2+E}{\hbar^2 c^2} \end{pmatrix}}_{\text{matrix}} \begin{pmatrix} a_{n-1} \\ b_{n-1} \end{pmatrix}$$

singular, determinant vanishes due to $r\to\infty$

left-hand eigenvector to eigenvalue 0:

$$\underline{\left(\frac{mc^2+E}{\hbar c},\ g\right)} \begin{pmatrix} \frac{mc^2-E}{\hbar c} & -g \\ -g & \frac{mc^2+E}{\hbar^2 c^2} \end{pmatrix} = 0\cdot \begin{pmatrix} \times & \times \\ \times & \times \end{pmatrix}$$

generic relation between a_n and b_n due to left-hand eigenvector:

$$\left[\frac{mc^2+E}{\hbar c}\alpha + g(-n_r-\gamma+\lambda)\right]\cdot a_{n_r} - \left[\frac{mc^2+E}{\hbar c}(n_r+\gamma+\lambda) + \alpha g\right] b_{n_r} = 0 \quad (*)$$

One can show that generically $f(r)$ and $g(r)$ go like e^{+2gr}

$\Rightarrow$ This we have to exclude. There must be a truncation of Taylor series.

$a_{n_r+1}=0$, provided that $\frac{mc^2-E}{\hbar c}\underbrace{a_{n_r}}_{\text{radial quantum number}} - \rho\, b_{n_r} = 0$ $\quad (**)$

$$\begin{pmatrix} \frac{mc^2-E}{\hbar c} & -\rho \\ \frac{mc^2+E}{\hbar c}\alpha + \rho(-n_r-\gamma+\lambda) & -\left[\frac{mc^2+E}{\hbar c}(n_r+\gamma+\lambda)+\alpha\rho\right]\end{pmatrix}\underbrace{\begin{pmatrix}a_{n_r}\\ b_{n_r}\end{pmatrix}}_{\neq\begin{pmatrix}0\\0\end{pmatrix}} = \begin{pmatrix}0\\0\end{pmatrix}$$

$$\begin{vmatrix} \cdots \end{vmatrix} = 0$$

$$-\rho^{\cancel{2}}(n_r+\gamma+\cancel{\lambda}) - \frac{mc^2\cancel{-E}}{\hbar c}\alpha\cancel{\rho} + \cancel{\rho}\frac{mc^2\cancel{+E}}{\hbar c}\alpha + \rho^{\cancel{2}}(-n_r-\gamma+\cancel{\lambda}) = 0$$

square this and solve for E: $\qquad \rho^2 = \frac{m^2c^4-E^2}{\hbar^2c^2}$

$$\underbrace{\rho^2}_{=\frac{m^2c^4-E^2}{\hbar^2c^2}}(n_r+\gamma)^2 = E^2\alpha^2 \quad\Longrightarrow\quad E = \frac{mc^2}{\sqrt{1+\frac{\alpha^2}{(n_r+\underbrace{\gamma}_{=\sqrt{l+\frac{1}{2}-\alpha}})^2}}}$$

$$E = \frac{mc^2}{\sqrt{1+\frac{\alpha^2}{\left[n_r+\sqrt{(j+\frac{1}{2})^2-\alpha^2}\right]^2}}}$$

principal quantum number: $n = n_r + j + 1/2 \to n_r = n - j - 1/2$

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

$\alpha \ll 1$

$$\approx \underset{\substack{\uparrow \\ \text{rest energy}}}{mc^2} + \underbrace{\underbrace{\underbrace{\left(-\frac{1}{2} mc^2 \alpha^2\right)}_{= Ry} \frac{1}{n^2}}_{= E_n^{(0)}}}_{\text{Schrödinger}} + \underbrace{\underbrace{\left(-\frac{1}{2} mc^2 \frac{\alpha^2}{n^2}\right)}_{= E_n^{(0)}} \frac{\alpha^2}{n}\left[\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right]}_{\text{fine structure}} + \dots$$