Hydrogen atom

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton

(Date: April 30, 2017)

1. Central force problem: hydrogen atom

The Hamiltonian is given by

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 + eA_0$$

where

$$\boldsymbol{A} = (A_1, A_2, A_3) = (A_x, A_y, A_z),$$

$$\boldsymbol{p} = (p_1, p_2, p_3) = (p_x, p_y, p_z)$$

$$\boldsymbol{J} = (J_1, J_2, J_3) = (J_x, J_y, J_z)$$

$$\boldsymbol{\alpha} = (\alpha^1, \alpha^2, \alpha^3) = (\alpha_x, \alpha_y, \alpha_z)$$

with

$$\boldsymbol{A} = 0 \qquad eA_0 = eA^0 = V(r) \qquad \text{(spherical symmetry)}$$

(a) The commutation relation between J_3 and H

$$[H, J_3] = [H, J_z] = 0$$

((**Proof**))

$$\begin{aligned}
[H - eA_0, L_3] &= [c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2, L_3] \\
&= c[p_k, L_3]\alpha^k + mc^2[\beta, L_3] \\
&= c[p_k, x_1 p_2 - x_2 p_1]\alpha^k \\
&= c[p_1, x_1 p_2 - x_2 p_1]\alpha^1 + c[p_2, x_1 p_2 - x_2 p_1]\alpha^2 \\
&= \frac{\hbar}{i} c p_2 \alpha^1 - \frac{\hbar}{i} c p_1 \alpha^2 \\
&= \frac{\hbar}{i} c(p_2\alpha^1 - p_1\alpha^2) \\
&= \frac{c\hbar}{i}(\boldsymbol{\alpha}\times\boldsymbol{p})_3
\end{aligned}$$

or

$$[H, L_3] = -ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3 + [eA_0, L_3] = -ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3$$

since

$$\begin{aligned}[eA_0, L_3] &= [eA_0, xp_y - yp_x] \\ &= -x[p_y, eA_0] + y[p_x, eA_0] \\ &= -x\frac{\hbar}{i}\frac{\partial}{\partial y}eA_0 + y\frac{\hbar}{i}\frac{\partial}{\partial x}eA_0 \\ &= 0\end{aligned}$$

where

$$A_0 = A_0(r), \qquad r = \sqrt{x^2 + y^2 + z^2}$$

$$x\frac{\partial}{\partial y}A_0 - y\frac{\partial}{\partial x}A_0 = (x\frac{\partial r}{\partial y} - y\frac{\partial r}{\partial x})\frac{\partial A_0}{\partial r} = (\frac{xy}{r} - \frac{xy}{r})\frac{\partial A_0}{\partial r} = 0$$

Similarly

$$\begin{aligned}[H - eA_0, \Sigma^3] &= [c\alpha^k p_k + \beta mc^2, \Sigma^3] \\ &= [c\alpha^k p_k, \Sigma^3] + [\beta mc^2, \Sigma^3] \\ &= cp_k[\gamma^5\Sigma^k, \Sigma^3] + mc^2[\beta, \Sigma^3] \\ &= cp_k\gamma^5[\Sigma^k, \Sigma^3] \\ &= cp_1\gamma^5[\Sigma^1, \Sigma^3] + cp_2\gamma^5[\Sigma^2, \Sigma^3] \\ &= -cp_1\gamma^5[\Sigma^3, \Sigma^1] + cp_2\gamma^5[\Sigma^2, \Sigma^3] \\ &= -2icp_1\gamma^5\Sigma^2 + 2icp_2\gamma^5\Sigma^1 \\ &= 2ic(\alpha^1 p_2 - \alpha^2 p_1) \\ &= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3\end{aligned}$$

or

$$\begin{aligned}[H, \Sigma^3] &= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3 + [eA_0, \Sigma^3] \\ &= 2ic(\boldsymbol{\alpha} \times \boldsymbol{p})_3\end{aligned}$$

or

$$[H, \frac{\hbar}{2}\Sigma^3] = ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3$$

where

$$\boldsymbol{\Sigma} = (\Sigma^1, \Sigma^2, \Sigma^3), \qquad \boldsymbol{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$$

$$\alpha^k = \gamma^0\gamma^k = \Sigma^k\gamma^5 = \gamma^5\Sigma^k$$

$$[\gamma^5, \Sigma^k] = 0, \quad [\beta, \Sigma^k] = 0, \quad [\gamma^5, \alpha^k] = 0, \quad \{\beta, \gamma^5\} = 0$$

$$[\Sigma^i, \Sigma^j] = 2i\Sigma^k, \qquad \Sigma^i\Sigma^j = -\Sigma^j\Sigma^i = i\Sigma^k \qquad (i, j, \text{ and } k; \text{ cyclic})$$

$$[\gamma^5\Sigma^k, \Sigma^j] = \gamma^5\Sigma^k\Sigma^j - \Sigma^j\gamma^5\Sigma^k = \gamma^5[\Sigma^k, \Sigma^j]$$

$$\{\beta, \alpha^k\} = 0 \qquad (k = 1, 2, 3)$$

Thus we have

$$[H, J_3] = [H, L_3 + \frac{\hbar}{2}\Sigma^3] = -ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3 + ic\hbar(\boldsymbol{\alpha} \times \boldsymbol{p})_3 = 0$$

Note that

$$J_3 = L_3 + \frac{\hbar}{2}\Sigma^3$$

Similarly, we have

$$[H, J_1] = 0, \quad [H, J_2] = 0.$$

or

$$[H, \boldsymbol{J}] = 0.$$

where

$$\boldsymbol{J}=\boldsymbol{L}+\frac{\hbar}{2}\Sigma$$

(b) Definition of the operator K and the commutation relation $[K,H]=0$

$$K=\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}-\frac{\hbar}{2}\beta=\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar)$$

and

$$[H,K]=0, \qquad [H,K^2]=0$$

First we show that

$$[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}]=\frac{\hbar}{2}[H,\beta]$$

where

$$[H,\boldsymbol{J}]=0 \qquad \text{and} \qquad [\beta,\boldsymbol{\Sigma}]=0$$

((**Proof**))

$$\begin{aligned}[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}]&=H\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J})-\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J})H\\&=[H,\beta](\boldsymbol{\Sigma}\cdot\boldsymbol{J})+\beta[H,\boldsymbol{\Sigma}]\cdot\boldsymbol{J}\\&=-2c\beta(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})+2ic\beta(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}\end{aligned}$$

Here we note that

$$[H,\beta]=[c\boldsymbol{\alpha}\cdot\boldsymbol{p},\beta]=c\boldsymbol{\alpha}\cdot\boldsymbol{p}\beta-\beta c\boldsymbol{\alpha}\cdot\boldsymbol{p}=-2\beta c\boldsymbol{\alpha}\cdot\boldsymbol{p}$$

$$[H,\boldsymbol{\Sigma}]=2ic(\boldsymbol{\alpha}\times\boldsymbol{p})$$

$$\begin{aligned}(\boldsymbol{\alpha}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})&=\gamma^5(\boldsymbol{\Sigma}\cdot\boldsymbol{p})(\boldsymbol{\Sigma}\cdot\boldsymbol{J})\\&=\gamma^5[\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\Sigma}\cdot(\boldsymbol{p}\times\boldsymbol{J})]\\&=\gamma^5\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})\end{aligned}$$

Then we have

$$\begin{aligned}[H,\beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}] &= -2c\beta[\gamma^5\boldsymbol{p}\cdot\boldsymbol{J}+i\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})]+2ic\beta(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}\\ &= -2c\beta\gamma^5\boldsymbol{p}\cdot\boldsymbol{J}\\ &= -2c\beta\gamma^5\boldsymbol{p}\cdot(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma})\\ &= -c\hbar\beta\gamma^5\boldsymbol{p}\cdot\boldsymbol{\Sigma}\\ &= -c\hbar\beta\boldsymbol{\alpha}\cdot\boldsymbol{p}\\ &= \frac{\hbar}{2}[H,\beta]\end{aligned}$$

where

$$(\boldsymbol{\alpha}\times\boldsymbol{p})\cdot\boldsymbol{J}=\boldsymbol{\alpha}\cdot(\boldsymbol{p}\times\boldsymbol{J})$$

Then we define the operator K as

$$\begin{aligned}K &= \beta\boldsymbol{\Sigma}\cdot\boldsymbol{J}-\frac{\hbar}{2}\beta\\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{J}-\frac{\hbar}{2})\\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma}^2-\frac{\hbar}{2})\\ &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar)\end{aligned}$$

where

$$\boldsymbol{J}=\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma}$$

Then K commutes with H,

$$[K,H]=0.$$

This also implies that

$$[K^2,H]=0.$$

2. Commutation relations (continued)

We show that

$$[K,\boldsymbol{J}]=0$$

(i) $[\beta, \boldsymbol{J}] = 0$

$$[\beta, J_1] = [\beta, L_1 + \frac{\hbar}{2}\Sigma^1] = \frac{\hbar}{2}[\beta, \Sigma^1] = 0$$

(ii) $[\beta\boldsymbol{\Sigma} \cdot \boldsymbol{J}, \boldsymbol{J}] = 0$

$$\begin{aligned}
[\beta\boldsymbol{\Sigma} \cdot \boldsymbol{L}, J_1] &= [\beta\Sigma^1 L_1 + \beta\Sigma^2 L_2 + \beta\Sigma^3 L_3, L_1 + \frac{\hbar}{2}\Sigma^1] \\
&= [\beta\Sigma^1 L_1 + \beta\Sigma^2 L_2 + \beta\Sigma^3 L_3, L_1] \\
&\quad + [\beta\Sigma^1 L_1 + \beta\Sigma^2 L_2 + \beta\Sigma^3 L_3, \frac{\hbar}{2}\Sigma^1] \\
&= -\beta\Sigma^2[L_1, L_2] + \beta\Sigma^3[L_3, L_1] \\
&\quad + \frac{\hbar}{2}[\beta\Sigma^2 L_2, \Sigma^1] + \frac{\hbar}{2}[\beta\Sigma^3 L_3, \Sigma^1] \\
&= -i\hbar\beta\Sigma^2 L_3 + i\hbar\beta\Sigma^3 L_2 - \frac{\hbar}{2}L_2\beta[\Sigma^1, \Sigma^2] + \frac{\hbar}{2}L_3\beta[\Sigma^3, \Sigma^1] \\
&= -i\hbar\beta\Sigma^2 L_3 + i\hbar\beta\Sigma^3 L_2 - i\hbar L_2\beta\Sigma^3 + i\hbar L_3\beta\Sigma^2 \\
&= 0
\end{aligned}$$

since

$$[\beta, \Sigma^k] = 0$$

(iii) $[\beta\boldsymbol{\Sigma} \cdot \boldsymbol{J}, \boldsymbol{J}] = 0$

$$\begin{aligned}
[\beta\boldsymbol{\Sigma} \cdot \boldsymbol{J}, J_1] &= [\beta\boldsymbol{\Sigma} \cdot (\boldsymbol{L} + \frac{\hbar}{2}\Sigma), J_1] \\
&= [\beta\boldsymbol{\Sigma} \cdot \boldsymbol{L}, J_1] + \frac{\hbar}{2}[\beta\Sigma^2, J_1] \\
&= \frac{\hbar}{2}[3\beta, J_1] \\
&= 0
\end{aligned}$$

or

$$[\beta\boldsymbol{\Sigma} \cdot \boldsymbol{J}, \boldsymbol{J}] = 0$$

which leads to

$$[K, \boldsymbol{J}] = [\beta(\boldsymbol{\Sigma} \cdot \boldsymbol{L} + \hbar), \boldsymbol{J}] = 0$$

3. K^2 and J^2

$$\begin{aligned} K^2 &= \beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar)\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar) \\ &= (\boldsymbol{\Sigma}\cdot\boldsymbol{L})(\boldsymbol{\Sigma}\cdot\boldsymbol{L})+2\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2 \\ &= \boldsymbol{L}^2+i\Sigma\cdot(\boldsymbol{L}\times\boldsymbol{L})+2\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2 \\ &= \boldsymbol{L}^2+\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L}+\hbar^2 \end{aligned}$$

since

$$[\beta,\Sigma^k]=0.$$

We note that

$$\begin{aligned} \boldsymbol{J}^2 &= (\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma})\cdot(\boldsymbol{L}+\frac{\hbar}{2}\boldsymbol{\Sigma}) \\ &= \boldsymbol{L}^2+\frac{\hbar}{4}\boldsymbol{\Sigma}^2+\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L} \\ &= \boldsymbol{L}^2+\frac{3\hbar^2}{4}+\hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L} \end{aligned}$$

Thus we obtain

$$K^2=J^2+\frac{\hbar^2}{4}$$

Since $[K^2,H]=0$, we also have the commutation relation

$$[\boldsymbol{J}^2,H]=0$$

4. Parity operator *P*

The parity operator is defined by

$$P=\beta\pi$$

We show that $[P,H]$=0. Note that

$$P^2=\beta\pi\beta\pi=\beta^2\pi^2=1$$

((**Proof**))

$$
\begin{aligned}
[P,H] &= [\beta\pi, c\alpha^k p_k + \beta mc^2] \\
&= [\beta\pi, c\alpha^k p_k] \\
&= \beta\pi c\alpha^k p_k - c\alpha^k p_k \beta\pi \\
&= c\beta\alpha^k \pi p_k - c\alpha^k \beta p_k \pi \\
&= c(\beta\alpha^k + \alpha^k\beta)\pi p_k \\
&= c\{\beta,\alpha^k\}\pi p_k \\
&= 0
\end{aligned}
$$

5. Simultaneous eigenket

For an electron in a central potential, we can conduct a simultaneous eigenfunction of H, K, $\boldsymbol{J}^2$, and J_3,

$$H\psi = E\psi , \qquad K\psi = -\kappa\hbar\psi ,$$

$$\boldsymbol{J}^2\psi = \hbar^2 j(j+1)\psi , \qquad J_3\psi = j_3\hbar\psi$$

$$P\psi = \pm\psi$$

since

$$[H,K] = 0 , \quad [H,J_3] = 0 , \quad [H,J^2] = 0 , \quad [P,H] = 0$$

We also note that

$$K^2 = \boldsymbol{J}^2 + \frac{\hbar^2}{4}$$

This implies that

$$K^2\psi = \hbar^2\kappa^2\psi = [\hbar^2 j(j+1) + \frac{\hbar^2}{4}]\psi = \hbar^2(j+\frac{1}{2})^2\psi$$

or

$$\kappa^2\psi = [j(j+1) + \frac{1}{4}]\psi =^2 (j+\frac{1}{2})^2\psi$$

So we must have

$$\kappa = \pm(j+\frac{1}{2}),$$

Note that j is a half-integer and κ is an integer ($\kappa = \pm 1, \pm 2, ...$). So κ has integer eigenvalues which are not zero.

6. Operator K

We now consider the matrix of K.

$$\begin{aligned} K &= \beta(\boldsymbol{\Sigma} \cdot \boldsymbol{L} + \hbar) \\ &= \begin{pmatrix} \boldsymbol{1} & 0 \\ 0 & -\boldsymbol{1} \end{pmatrix} \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar & 0 \\ 0 & \boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar \end{pmatrix} \\ &= \begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar & 0 \\ 0 & -(\boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar) \end{pmatrix} \end{aligned}$$

The wave function ψ is a simultaneous function of K, $\boldsymbol{J}^2$, and J_3,

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Then we have

$$K\psi = -\hbar\kappa\psi$$

or

$$\begin{pmatrix} \boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar & 0 \\ 0 & -(\boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar) \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = -\hbar\kappa \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

or

$$(\boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar)\psi_A = -\hbar\kappa\psi_A, \qquad (\boldsymbol{\sigma} \cdot \boldsymbol{L} + \hbar)\psi_B = \hbar\kappa\psi_B$$

or

$$(\boldsymbol{\sigma} \cdot \boldsymbol{L})\psi_A = -\hbar(\kappa + 1)\psi_A, \qquad (\boldsymbol{\sigma} \cdot \boldsymbol{L})\psi_B = \hbar(\kappa - 1)\psi_B$$

7. Operators $\boldsymbol{J}^2$

$$\boldsymbol{J}^2\psi = \hbar^2 j(j+1)\psi$$

$$\boldsymbol{J} = \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}$$

$$\boldsymbol{J}^2 = \begin{pmatrix} \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix} \begin{pmatrix} \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma} \end{pmatrix}$$

$$= \begin{pmatrix} \left(\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 & 0 \\ 0 & \left(\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 \end{pmatrix}$$

Then we get

$$\boldsymbol{J}^2 \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \hbar^2 j(j+1) \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

or

$$\left(\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 \psi_A = \hbar^2 j(j+1)\psi_A, \qquad \left(\boldsymbol{L} + \frac{\hbar}{2}\boldsymbol{\sigma}\right)^2 \psi_B = \hbar^2 j(j+1)\psi_B$$

8. Operator J_3

$$J_3\psi = (L_3 + \frac{\hbar}{2}\Sigma_3)\psi = \begin{pmatrix} L_3 + \frac{\hbar}{2}\sigma_3 & 0 \\ 0 & L_3 + \frac{\hbar}{2}\sigma_3 \end{pmatrix} \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = j_3\hbar \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

or

$$(L_3 + \frac{\hbar}{2}\sigma_3)\psi_A = j_3\hbar\psi_A, \qquad (L_3 + \frac{\hbar}{2}\sigma_3)\psi_B = j_3\hbar\psi_B$$

9. The operator $\boldsymbol{L}^2$

Since $[H, \boldsymbol{L}^2] \neq 0$, ψ is not the eigenfunction of $\boldsymbol{L}^2$.

$$\boldsymbol{L}^2 = \boldsymbol{J}^2 - \hbar\boldsymbol{\Sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4}$$

we have

$$\boldsymbol{L}^2\psi = \begin{pmatrix} \boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4} & 0 \\ 0 & \boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4} \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

Then we get

$$\begin{aligned} \boldsymbol{L}^2\psi_A &= (\boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4})\psi_A \\ &= [\boldsymbol{J}^2 - \hbar(\boldsymbol{\sigma}\cdot\boldsymbol{L} + \hbar) + \frac{\hbar^2}{4}]\psi_A \\ &= [\hbar^2 j(j+1) + \hbar^2\kappa + \frac{\hbar^2}{4}]\psi_A \\ &= \hbar^2 l_A(l_A+1)\psi_A \end{aligned}$$

where

$$\boxed{j(j+1) + \kappa + \frac{1}{4} = l_A(l_A+1)}$$

Similarly,

$$\begin{aligned} \boldsymbol{L}^2\psi_B &= (\boldsymbol{J}^2 - \hbar\boldsymbol{\sigma}\cdot\boldsymbol{L} - \frac{3\hbar^2}{4})\psi_B \\ &= [\boldsymbol{J}^2 - \hbar(\boldsymbol{\sigma}\cdot\boldsymbol{L} + \hbar) + \frac{\hbar^2}{4}]\psi_B \\ &= [\hbar^2 j(j+1) - \hbar^2\kappa + \frac{\hbar^2}{4}]\psi_B \\ &= \hbar^2 l_B(l_B+1)\psi_B \end{aligned}$$

with

$$\boxed{j(j+1) - \kappa + \frac{1}{4} = l_B(l_B+1)}$$

Thus ψ_A and ψ_B are separately the eigenfunctions of $\boldsymbol{L}^2$. These eigenvalues are denoted by $l_A(l_A+1)\hbar^2$ and $\hbar^2 l_B(l_B+1)$, respectively.

Using these two equations, we can determine l_A and l_B for the given eigenvalue κ.

((**Non-relativistic case**))

Spin 1/2.

$n = 1$; $l = 0$

$$D_0 \times D_{1/2} = D_{1/2} \qquad (j = 1/2)$$

$n = 2$; $l = 0, 1$

$$D_0 \times D_{1/2} = D_{1/2} \qquad (j = 1/2)$$
$$D_1 \times D_{1/2} = D_{3/2} + D_{1/2} \qquad (j = 3/2, 1/2)$$

$n = 3$; $l = 0, 1, 2$

$$D_0 \times D_{1/2} = D_{1/2} \qquad (j = 1/2)$$
$$D_1 \times D_{1/2} = D_{3/2} + D_{1/2} \qquad (j = 3/2, 1/2)$$
$$D_2 \times D_{1/2} = D_{5/2} + D_{3/2} \qquad (j = 5/2, 3/2)$$

(a) For j = 1/2,

$$\kappa = \pm(j + \frac{1}{2}) = \pm 1.$$

(i) $\kappa = 1$, $l_A = 1$, and $l_B = 0$.
(ii) $\kappa = -1$, $l_A = 0$ and $l_B = 1$.

(b) For a half integer j,

$$\kappa = \pm(j + \frac{1}{2}).$$

(i) $\kappa = j + \frac{1}{2}$, $l_A = j + \frac{1}{2}$, $l_B = j - \frac{1}{2}$

(ii) $\kappa = -(j + \frac{1}{2})$, $l_A = j - \frac{1}{2}$, $l_B = j + \frac{1}{2}$

10. Normalized spin angular function

Spin orbit coupling

$$D_l \times D_{1/2} = D_{l+1/2} + D_{l-1/2}$$

For $j = l + 1/2$,

$$\begin{aligned}
y_l^{j=l+1/2, j_3} &= \sqrt{\frac{l + j_3 + 1/2}{2l+1}} Y_l^{j_3 - 1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l - j_3 + 1/2}{2l+1}} Y_l^{j_3 + 1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \frac{1}{\sqrt{2l+1}} \begin{pmatrix} \sqrt{l + j_3 + \frac{1}{2}} Y_l^{j_3 - 1/2} \\ \sqrt{l - j_3 + \frac{1}{2}} Y_l^{j_3 + 1/2} \end{pmatrix} \\
&= \frac{1}{\sqrt{2j}} \begin{pmatrix} \sqrt{j + j_3 + 1} Y_{l=j-1/2}^{j_3 - 1/2} \\ \sqrt{j - j_3 + 1} Y_{l=j-1/2}^{j_3 + 1/2} \end{pmatrix}
\end{aligned}$$

$$\rightarrow y_{l=j-1/2}^{j, j_3}$$

which has the parity of $(-1)^{j-1/2}$.

For $j = l - 1/2$,

$$\begin{aligned}
y_l^{j=l-1/2, j_3} &= -\sqrt{\frac{l - j_3 + 1/2}{2l+1}} Y_l^{j_3 - 1/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&\quad + \sqrt{\frac{l + j_3 + 1/2}{2l+1}} Y_l^{j_3 + 1/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \frac{1}{\sqrt{2l+1}} \begin{pmatrix} -\sqrt{l - j_3 + \frac{1}{2}} Y_l^{j_3 - 1/2} \\ \sqrt{l + j_3 + \frac{1}{2}} Y_l^{j_3 + 1/2} \end{pmatrix} \\
&= \frac{1}{\sqrt{2(j+1)}} \begin{pmatrix} -\sqrt{j - j_3 + 1}\, Y_{l=j+1/2}^{j_3 - 1/2} \\ \sqrt{j + j_3 + 1}\, Y_{l=j+1/2}^{j_3 + 1/2} \end{pmatrix}
\end{aligned}$$

$$\rightarrow y_{l=j+1/2}^{j, j_3}$$

which has the parity of $(-1)^{j+1/2}$.

((**Note**))
From the spin orbit interaction

$$|\,j=l+1/2,m\rangle=\sqrt{\frac{l+m+1/2}{2l+1}}|m_l=m-1/2,m_s=1/2\rangle$$
$$+\sqrt{\frac{l-m+1/2}{2l+1}}|m_l=m+1/2,m_s=-1/2\rangle$$

$$|\,j=l-1/2,m\rangle=-\sqrt{\frac{l-m+1/2}{2l+1}}|m_l=m-1/2,m_s=1/2\rangle$$
$$+\sqrt{\frac{l+m+1/2}{2l+1}}|m_l=m+1/2,m_s=-1/2\rangle$$

or

$$|\,j=l+1/2,m\rangle=\begin{pmatrix}\sqrt{\frac{l+m+1/2}{2l+1}}\\ \sqrt{\frac{l-m+1/2}{2l+1}}\end{pmatrix},$$

$$|\,j=l-1/2,m\rangle==\begin{pmatrix}-\sqrt{\frac{l-m+1/2}{2l+1}}\\ \sqrt{\frac{l+m+1/2}{2l+1}}\end{pmatrix}.$$

((Note))

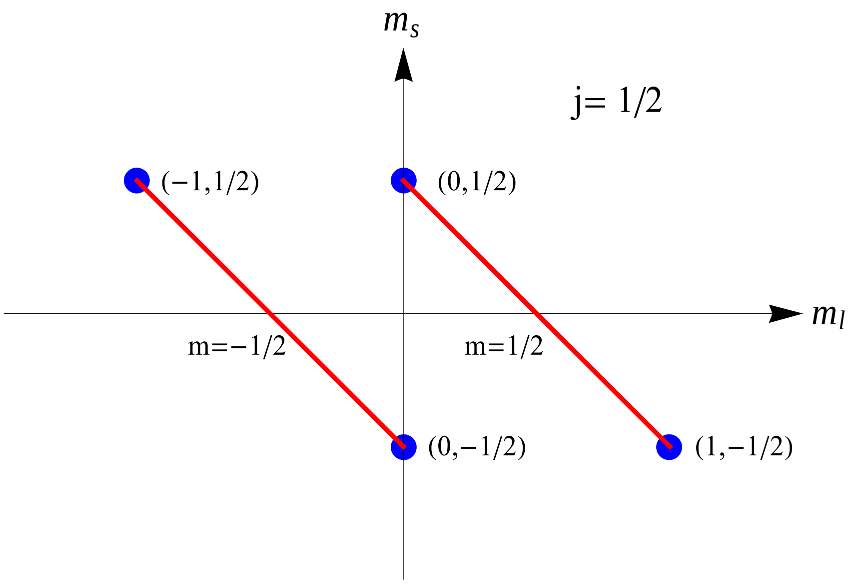

Fig. Clebsh-Gordan diagram for $\left| j,m \right\rangle$ with j = 1/2. m = 1/2 and -1/2.

---

11. Radial wave functions

(a) For $\kappa = j+\frac{1}{2}$, $l_A = j+\frac{1}{2}$, $l_B = j-\frac{1}{2}$

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} g(r) y^{j,j_3}_{l_A=j+\frac{1}{2}} \\ if(r) y^{j,j_3}_{l_B=j-\frac{1}{2}} \end{pmatrix}$$

(b) For $\kappa = -(j+\frac{1}{2})$, $l_A = j-\frac{1}{2}$, $l_B = j+\frac{1}{2}$

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} f(r) y^{j,j_3}_{l_A=j-\frac{1}{2}} \\ ig(r) y^{j,j_3}_{l_B=j+\frac{1}{2}} \end{pmatrix}$$

The parity of $y^{j,j_3}_{l_A=j-\frac{1}{2}}$ is given by $(-1)^{l_A}$, while the parity of $y^{j,j_3}_{l_B=j+\frac{1}{2}}$ is given by $(-1)^{l_B}$. Theses parities are different, since $l_B - l_A = \pm 1$. The radial functions f and g depend on κ. The factor i multiplying f and g is inserted to make f and g real for bound-state.

((**Note**))

$$\psi_A(-\boldsymbol{r},t) = (-1)^{l_A} \psi_A(\boldsymbol{r},t) = \pm\psi_A(\boldsymbol{r},t)$$

$$\psi_B(-\boldsymbol{r},t) = (-1)^{l_B} \psi_B(\boldsymbol{r},t) = \mp\psi_B(\boldsymbol{r},t)$$

Thus we have

$$(-1)^{l_A} = (-1)^{l_B+1}$$

or

$$l_A - l_B = \pm 1.$$

Table-1

κ	l_A	l_B
$\kappa = -(j + \frac{1}{2})$	$l_A = j - \frac{1}{2}$	$l_B = j + \frac{1}{2}$
$\kappa = (j + \frac{1}{2})$	$l_A = j + \frac{1}{2}$	$l_B = j - \frac{1}{2}$

Table-2

$j = \frac{1}{2}$

$\kappa = 1$, $l_A = 1$, $l_B = 0$

$\kappa = -1$, $l_A = 0$, $l_B = 1$

$j = \frac{3}{2}$

$\kappa = 2$, $l_A = 2$, $l_B = 1$

$\kappa = -2$, $l_A = 1$, $l_B = 2$

$j = \frac{5}{2}$

$\kappa = 3$, $l_A = 3$, $l_B = 2$

$\kappa = -3$, $l_A = 2$, $l_B = 3$

12. Expression of the two-component wave function

For a fixed κ [= *j*+1/2, or -(*j*+1/2)], we assume that the wave function is given by

$$\psi = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \begin{pmatrix} f(r) y_{l_A}^{j,j_3} \\ ig(r) y_{l_B}^{j,j_3} \end{pmatrix}$$

This function satisfies the Dirac equation given by

$$c(\boldsymbol{\sigma} \cdot \boldsymbol{p})\psi_B = (E - V(r) - mc^2)\psi_A ,$$

$$c(\boldsymbol{\sigma} \cdot \boldsymbol{p})\psi_A = (E - V(r) - mc^2)\psi_B$$

We note that

$$\begin{aligned}\boldsymbol{\sigma}\cdot\boldsymbol{p} &= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(\boldsymbol{\sigma}\cdot\boldsymbol{r})(\boldsymbol{\sigma}\cdot\boldsymbol{p}) \\ &= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})[\boldsymbol{r}\cdot\boldsymbol{p}+\boldsymbol{\sigma}\cdot(\boldsymbol{r}\times\boldsymbol{p})] \\ &= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(\boldsymbol{r}\cdot\boldsymbol{p}+i\boldsymbol{\sigma}\cdot\boldsymbol{L}) \\ &= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r}+i\boldsymbol{\sigma}\cdot\boldsymbol{L})\end{aligned}$$

where

$$(\boldsymbol{\sigma}\cdot\boldsymbol{r})(\boldsymbol{\sigma}\cdot\boldsymbol{r}) = r^2 + i\boldsymbol{\sigma}\cdot(\boldsymbol{r}\times\boldsymbol{r}) = r^2$$

$$\boldsymbol{r}\cdot\boldsymbol{p} = \frac{\hbar}{i}r\frac{\partial}{\partial r}$$

$$\boldsymbol{p} = \frac{\hbar}{i}\nabla = \frac{\hbar}{i}(\boldsymbol{e}_r\frac{\partial}{\partial r}+\boldsymbol{e}_\theta\frac{1}{r}\frac{\partial}{\partial\theta}+\boldsymbol{e}_\phi\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi})$$

For two arbitrary vectors ***A*** and ***B***,

$$(\boldsymbol{\sigma}\cdot\boldsymbol{A})(\boldsymbol{\sigma}\cdot\boldsymbol{B}) = (\boldsymbol{A}\cdot\boldsymbol{B})\hat{1} + i\boldsymbol{\sigma}\cdot(\boldsymbol{A}\times\boldsymbol{B})$$

Then we get

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B &= i(\boldsymbol{\sigma}\cdot\boldsymbol{p})f(r)y_{l_B}^{j,j_3} \\ &= \frac{i}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r}+i\boldsymbol{\sigma}\cdot\boldsymbol{L})f(r)y_{l_B}^{j,j_3} \\ &= (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})[-\hbar\frac{df}{dr}-\frac{(1-\kappa)\hbar}{r}f]y_{l_B}^{j,j_3} \\ &= -\hbar\frac{df}{dr}y_{l_A}^{j,j_3}-\frac{(1-\kappa)\hbar}{r}fy_{l_A}^{j,j_3}\end{aligned}$$

where

$$(\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_B = \hbar(\kappa-1)\psi_B, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3} = y_{l_A}^{j,j_3}.$$

Similarly, we get

$$
\begin{aligned}
(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A &= (\boldsymbol{\sigma}\cdot\boldsymbol{p})g y_{l_A}^{j,j_3} \\
&= \frac{1}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})(-i\hbar r\frac{\partial}{\partial r}+i\boldsymbol{\sigma}\cdot\boldsymbol{L})g y_{l_A}^{j,j_3} \\
&= \frac{\hbar}{r^2}(\boldsymbol{\sigma}\cdot\boldsymbol{r})[-ir\frac{dg}{dr}-i(\kappa+1)g]y_{l_A}^{j,j_3} \\
&= -[i\hbar\frac{dg}{dr}+i(\kappa+1)\hbar g]y_{l_B}^{j,j_3} \\
&= i\hbar\frac{dg}{dr}y_{l_B}^{j,j_3}+i\frac{(\kappa+1)\hbar}{r}g y_{l_B}^{j,j_3}
\end{aligned}
$$

where

$$
(\boldsymbol{\sigma}\cdot\boldsymbol{L})\psi_A=-\hbar(\kappa+1)\psi_A, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=-y_{l_B}^{j,j_3}
$$

13. The operator $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})$

(a) $\{P,\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\}=0$

with $P=\beta\pi$

((**Proof**))

$$
\begin{aligned}
\{P,\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\} &= \{\beta\pi,\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\} \\
&= \beta\pi\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}+\boldsymbol{\Sigma}\cdot\hat{\boldsymbol{r}}\beta\pi \\
&= \beta\boldsymbol{\Sigma}\cdot\pi\hat{\boldsymbol{r}}+\boldsymbol{\Sigma}\cdot\beta\hat{\boldsymbol{r}}\pi \\
&= \beta\boldsymbol{\Sigma}\cdot\pi\hat{\boldsymbol{r}}-\boldsymbol{\Sigma}\cdot\beta\pi\hat{\boldsymbol{r}} \\
&= [\beta,\boldsymbol{\Sigma}]\cdot\pi\hat{\boldsymbol{r}} \\
&= 0
\end{aligned}
$$

or

$$
\begin{pmatrix} \pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})+(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi & 0 \\ 0 & -\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})-\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) \end{pmatrix}=0
$$

or

$$
\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})+(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi=0
$$

where, $P=\beta\pi$ and $\pi\hat{\boldsymbol{r}}+\hat{\boldsymbol{r}}\pi=0$. Thus we have

$\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}$ is odd under the parity.

(b) $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2 = 1$

((**Proof**))

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}) = \hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{r}} + i\boldsymbol{\sigma}\cdot(\hat{\boldsymbol{r}}\times\hat{\boldsymbol{r}}) = 1$$

(c) $[J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = 0$

((**Proof**))

$$J_3 = L_3 + S_3 = L_3 + \frac{\hbar}{2}\sigma_3$$

$$L_3 = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

$$\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}} = \sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta$$

Then we can evaluate the commutation relation

$$[J_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = [L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] + \frac{\hbar}{2}[\sigma_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]$$

$$\begin{aligned}
[L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]\psi &= L_3(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\psi - (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})L_3\psi \\
&= \frac{\hbar}{i}\frac{\partial}{\partial\phi}[(\sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta)\psi \\
&\quad - (\sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&= \frac{\hbar}{i}\psi\frac{\partial}{\partial\phi}(\sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta) \\
&\quad + (\sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&\quad - (\sigma_1 \sin\theta\cos\phi + \sigma_2 \sin\theta\sin\phi + \sigma_3\cos\theta)L_3\psi \\
&= -i\hbar\psi(-\sigma_1 \sin\theta\sin\phi + \sigma_2 \sin\theta\cos\phi)
\end{aligned}$$

or

$$[L_3, \boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] = i\hbar\sigma_1 \sin\theta\sin\phi - i\hbar\sigma_2 \sin\theta\cos\phi$$

We also have

$$\begin{aligned}[\frac{\hbar}{2}\sigma_3,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}] &= \frac{\hbar}{2}[\sigma_3,\sigma_1\sin\theta\cos\phi+\sigma_2\sin\theta\sin\phi+\sigma_3\cos\theta] \\ &= \frac{\hbar}{2}[\sigma_3,\sigma_1]\sin\theta\cos\phi-\frac{\hbar}{2}[\sigma_2,\sigma_3]\sin\theta\sin\phi \\ &= i\hbar\sigma_2\sin\theta\cos\phi-i\hbar\sigma_1\sin\theta\sin\phi\end{aligned}$$

Thus we have

$$[J_3,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]=0$$

14. Evaluation of $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$ and $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}$

(a)

$$[J_3,\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}}]y_{l_A}^{j,j_3}=0$$

or

$$[J_3(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})]y_{l_A}^{j,j_3} = (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})J_3 y_{l_A}^{j,j_3} = j_3(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$$

which means that $(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$ is the eigenfunction of J_3 with the eigenvalue j_3.

(b)

$$\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=-(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi y_{l_A}^{j,j_3}=(-1)^{l_A+1}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}$$

$$\pi(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=-(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})\pi y_{l_B}^{j,j_3}=(-1)^{l_B+1}(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}$$

leading to the relation

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3}=cy_{l_B}^{j,j_3}, \qquad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=cy_{l_A}^{j,j_3}$$

where c is constant. We note that

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2 y_{l_A}^{j,j_3}=c(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3}=c^2 y_{l_A}^{j,j_3}=y_{l_A}^{j,j_3}$$

since

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})^2=1$$

Then we get $c=\pm 1$. Here we choose c = -1.

$$(\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_A}^{j,j_3} = -y_{l_B}^{j,j_3}, \quad (\boldsymbol{\sigma}\cdot\hat{\boldsymbol{r}})y_{l_B}^{j,j_3} = -y_{l_A}^{j,j_3}$$

((**Note**)) In the non-relativistic quantum mechanics, it is well known that

$$\hat{\pi}\left|l,m\right\rangle = (-1)^l\left|l,m\right\rangle$$

15. Radial wave function in hydrogen atom

Now we solve the Dirac equation as

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B = (E - V(r) - mc^2)\psi_A,$$

or

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_B = -c\hbar\frac{df}{dr}y_{l_A}^{j,j_3} - \frac{(1-\kappa)c\hbar}{r}fy_{l_A}^{j,j_3} = (E - V(r) - mc^2)gy_{l_A}^{j,j_3}$$

or

$$-\hbar c\frac{df}{dr} - \frac{(1-\kappa)\hbar c}{r}f = (E - V(r) - mc^2)g$$

Similarly,

$$c(\boldsymbol{\sigma}\cdot\boldsymbol{p})\psi_A = (E - V(r) + mc^2)\psi_B$$

or

$$\hbar c\frac{dg}{dr} + \frac{(1+\kappa)\hbar c}{r}g = (E - V(r) + mc^2)f$$

Introducing

$$F(r) = rf(r), \qquad G(r) = rg(r)$$

then we have a radial equations,

$$\hbar c(\frac{dF}{dr} - \frac{\kappa}{r}F) = -(E - V(r) - mc^2)G$$

$$\hbar c(\frac{dG}{dr} + \frac{\kappa}{r}G) = (E - V(r) + mc^2)F$$

We assume that $V(r)$ is given by a Coulomb potential

$$V(r) = -\frac{Ze^2}{r}$$

We put

$$\alpha_1 = \frac{mc^2 + E}{\hbar c}, \qquad \alpha_2 = \frac{mc^2 - E}{\hbar c}$$

$$\gamma = \frac{Ze^2}{\hbar c} = Z\alpha, \qquad \rho = \sqrt{\alpha_1\alpha_2}\,r, \qquad \mu = \sqrt{\frac{\alpha_2}{\alpha_1}}$$

where α is the fine structure constant,

$$\alpha = \frac{e^2}{\hbar c} = 7.29735257 \text{ x } 10^{-3}, \qquad \frac{1}{\alpha} = 137.035999074(44).$$

Then we get the coupled equations we need to solve,

$$\left(\frac{d}{d\rho} - \frac{\kappa}{\rho}\right)F - \left(\mu - \frac{\gamma}{\rho}\right)G = 0$$

$$\left(\frac{d}{d\rho} + \frac{\kappa}{\rho}\right)G - \left(\frac{1}{\mu} + \frac{\gamma}{\rho}\right)F = 0$$

The analysis of the radial equation proceeds as usual.

$\rho \to \infty$,

$$\frac{dF}{d\rho} = \mu G, \qquad \frac{dG}{d\rho} = \sqrt{\frac{\alpha_1}{\alpha_2}}F$$

$$\frac{d^2F}{d\rho^2} = \sqrt{\frac{\alpha_2}{\alpha_1}}\frac{dG}{d\rho} = \sqrt{\frac{\alpha_2}{\alpha_1}}\sqrt{\frac{\alpha_1}{\alpha_2}}F = F$$

Similarly,

$$\frac{d^2G}{d\rho^2} = G$$

$$F = e^{-\rho}, \qquad G = e^{-\rho}$$

We assume that

$$F = e^{-\rho}\rho^{s}\sum_{m=0} a_m \rho^{m}$$

$$G = e^{-\rho}\rho^{s}\sum_{m=0} b_m \rho^{m}$$

We solve the problem using a series expansion method. These series forms are substituted into the coupled differential equation. We use the Mathematica to determine the value of *s* and the recursion relation. The results are as follows.

16. Indicial equation to determine the value of s

$$\begin{aligned} &(s-\kappa)a_0 + \gamma b_0 = 0 \\ &-\gamma a_0 + (s+\kappa)b_0 = 0 \end{aligned}$$

or

$$\begin{pmatrix} s-\kappa & \gamma \\ -\gamma & s+\kappa \end{pmatrix}\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Since a_0 and b_0 are not zero (non-trivial solution), the determinant of the matrix should be equal to zero.

$$s = \pm\sqrt{\kappa^2 - \gamma^2}$$

Note that

$$s^2 = \kappa^2 - \gamma^2 > \min(\kappa^2) - \gamma^2 = 1 - (Z\alpha)^2$$

So we get approximately $s > 1$, or $s<-1$. However, we must require that

$$\int |\psi(r)|^2 r^2 dr < \infty$$

The requirement amounts to

$$\int |f(r)|^2 r^2 dr = \int \frac{|F(r)|^2}{r^2} r^2 dr = \int |F(r)|^2 dr \approx \int |F(\rho)|^2 d\rho < \infty$$

$$\int |g(r)|^2 r^2 dr = \int \frac{|G(r)|^2}{r^2} r^2 dr = \int |G(r)|^2 dr \approx \int |G(\rho)|^2 d\rho < \infty$$

Around the origin,

$$F \approx \rho^s, \qquad G \approx \rho^s$$

Then we have

$$\int |F(\rho)|^2 d\rho \approx \int \rho^{2s} d\rho = \frac{\rho^{2s+1}}{2s+1}$$

$$\int |G(\rho)|^2 d\rho \approx \int \rho^{2s} d\rho = \frac{\rho^{2s+1}}{2s+1}$$

So in order to get the finite value of the probability near the origin, it is required that

$$s > -\frac{1}{2}$$

So we need to take

$$s = \sqrt{\kappa^2 - \gamma^2} = \sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2}$$

17. Mathematica (series expansion method)

```
Clear["Global`*"];

eq1 = D[F[ρ], ρ] - κ/ρ F[ρ] - (μ - γ/ρ) G[ρ];
eq2 = D[G[ρ], ρ] + κ/ρ G[ρ] - (1/μ + γ/ρ) F[ρ];

rule1 = {F → (Exp[-#] #^s (Sum[A[k] #^k, {k, 0, 10}]) &)};

rule2 = {G → (Exp[-#] #^s (Sum[B[k] #^k, {k, 0, 10}]) &)};

eq11 = eq1 /. rule1 /. rule2 // Expand;
eq21 = eq2 /. rule1 /. rule2 // Expand;
eq12 = eq11 Exp[ρ] ρ^(1-s) // Simplify;
eq22 = eq21 Exp[ρ] ρ^(1-s) // Simplify;
```

Determinastin of s

```
list1 = Table[{n, Coefficient[eq12, ρ, n]}, {n, 0, 2}] //
   Simplify;
list1 // TableForm
```

```
0     s A[0] - κ A[0] + γ B[0]
1     -A[0] + (1 + s - κ) A[1] - μ B[0] + γ B[1]
2     -A[1] + (2 + s - κ) A[2] - μ B[1] + γ B[2]
```

```
list2 = Table[{n, Coefficient[eq22, ρ, n]}, {n, 0, 2}] //
   Simplify;
list2 // TableForm
```

$$
\begin{array}{ll}
0 & -\gamma\, A[0] + (s + \kappa)\, B[0] \\
1 & -\frac{A[0]}{\mu} - \gamma\, A[1] - B[0] + B[1] + s\, B[1] + \kappa\, B[1] \\
2 & \frac{-A[1]+\mu\,(-\gamma\, A[2]-B[1]+(2+s+\kappa)\, B[2])}{\mu}
\end{array}
$$

Determination of recursion formula

$$\text{rule3} = \left\{F \to \left(\text{Exp}[-\#]\ \#^{s} \left(\sum_{n=q-3}^{q+3} A[n]\ \#^{n}\right) \&\right)\right\};$$

$$\text{rule4} = \left\{G \to \left(\text{Exp}[-\#]\ \#^{s} \left(\sum_{n=q-3}^{q+3} B[n]\ \#^{n}\right) \&\right)\right\};$$

```
eq13 = eq1 /. rule3 /. rule4 // Expand;
eq23 = eq2 /. rule3 /. rule4 // Expand;
```

$$\text{eq14} = \text{eq13}\ \text{Exp}[\rho]\ \rho^{4-q-s}\ //\ \text{Simplify};$$

$$\text{eq24} = \text{eq23}\ \text{Exp}[\rho]\ \rho^{4-q-s}\ //\ \text{Simplify};$$

```
list3 = Table[{n, Coefficient[eq14, ρ, n]}, {n, 2, 4}] //
   Simplify;
list3 // TableForm
```

```
2     -A[-2 + q] + (-1 + q + s - κ) A[-1 + q] - μ B[-2 + q] + γ B[-1 + q]
3     -A[-1 + q] + (q + s - κ) A[q] - μ B[-1 + q] + γ B[q]
4     -A[q] + (1 + q + s - κ) A[1 + q] - μ B[q] + γ B[1 + q]
```

```
list4 = Table[{n, Coefficient[ eq24, ρ, n]}, {n, 2, 4}] //
  Expand; list4 // TableForm
```

$$\begin{array}{ll}
2 & -\frac{A[-2+q]}{\mu} - \gamma A[-1+q] - B[-2+q] - B[-1+q] + q B[-1+q] + s B \\
3 & -\frac{A[-1+q]}{\mu} - \gamma A[q] - B[-1+q] + q B[q] + s B[q] + \kappa B[q] \\
4 & -\frac{A[q]}{\mu} - \gamma A[1+q] - B[q] + B[1+q] + q B[1+q] + s B[1+q] + \kappa
\end{array}$$

```
sq1 = Coefficient[eq12, ρ, 0];
sq2 = Coefficient[eq22, ρ, 0];
```

$$\mathtt{M1} = \begin{pmatrix} \mathtt{D[sq1, A[0]]} & \mathtt{D[sq1, B[0]]} \\ \mathtt{D[sq2, A[0]]} & \mathtt{D[sq2, B[0]]} \end{pmatrix}; \mathtt{Det[M1]}$$

$$s^2 + \gamma^2 - \kappa^2$$

18. Recursion relation

(i) The second recursion relations

$$(s+1-\kappa)a_1 - a_0 + \gamma b_1 - \mu b_0 = 0$$

$$(s+1+\kappa)b_1 - b_0 - \gamma a_1 - \frac{1}{\mu}a_0 = 0$$

(ii) The recursion relations (the general case)

$$(s+q-\kappa)a_q - a_{q-1} + \gamma b_q - \mu b_{q-1} = 0$$

$$(s+q+\kappa)b_q - b_{q-1} - \gamma a_q - \frac{1}{\mu}a_{q-1} = 0$$

The functions *F* and *G* would increase exponentially as $\rho \to \infty$ if the power series do not terminate. Assuming that the two series terminates with the same power, there must be exist n_r with the property. For $q = n_r$, we assume that

$$a_{n_r+1} = b_{n_r+1} = 0, \qquad a_{n_r} \neq 0, \qquad b_{n_r} \neq 0$$

Then we get

$$a_{n_r} = -\mu b_{n_r} \qquad (1)$$

From the recursion relation (in general)

$$(s+q-\kappa)a_q + \gamma b_q = a_{q-1} + \mu b_{q-1}$$

$$\mu[(s+q+\kappa)b_q - \gamma a_q] = a_{q-1} + \mu b_{q-1}$$

we get the relation

$$\mu[(s+q+\kappa)b_q - \gamma a_q] = (s+q-\kappa)a_q + \gamma b_q$$

or

$$[\mu(s+q+\kappa) - \gamma]b_q = (s+q-\kappa+\mu\gamma)a_q. \qquad (2)$$

or

$$C_q = \frac{a_q}{s+q+\kappa-\dfrac{\gamma}{\mu}} = \frac{b_q}{\dfrac{1}{\mu}(s+q-\kappa)+\gamma}$$

for $q = n_r, n_{r-1}, \ldots, 0$.

19. Derivation of the energy eigenvalue

From Eqs.(1) and (2) with $q = n_r$, we have

$$[\mu(s+n_r+\kappa) - \gamma]b_{n_r} = (s+n_r-\kappa+\mu\gamma)a_{n_r} = -\mu(s+n_r-\kappa+\mu\gamma)b_{n_r}$$

or

$$[\mu(s+n_r+\kappa) - \gamma] = -\mu(s+n_r-\kappa+\mu\gamma)$$

or

$$s+n_r = \gamma\frac{1-\mu^2}{2\mu} = \gamma\frac{(\alpha_1-\alpha_2)}{2\sqrt{\alpha_1\alpha_2}}$$

or

$$2\sqrt{\alpha_1\alpha_2}(s+n_r) = \gamma(\alpha_1-\alpha_2)$$

Noting that

$$\alpha_1 - \alpha_2 = \frac{2E}{\hbar c}, \qquad \sqrt{\alpha_1 \alpha_2} = \frac{\sqrt{m^2c^4 - E^2}}{\hbar c}$$

we have the energy eigenvalue as

$$\sqrt{m^2c^4 - E^2}\,(s + n_r) = \gamma E$$

or

$$E = \frac{mc^2}{\sqrt{1 + \frac{\gamma^2}{(n_r + s)^2}}} = \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{[n - (j + \frac{1}{2}) + \sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2}\,]^2}}}$$

This is famous fine structure formula for the hydrogen atom. The quantum numbers j and n_r assume the values

$$j = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots . \qquad n_r = 0,\ 1,\ 2,\ 3, \dots$$

The principal quantum number n of the nonrelativistic theory of the hydrogen atom is related to n_r and j by

$$n = j + \frac{1}{2} + n_r$$

$n = 1$

$n_r = 0, \quad j = \frac{1}{2}$

($l = 0$, $s = 1/2$)	$j = 1/2$	$1\ {}^2S_{1/2}$	$\kappa = -1$

$n = 2$

$n_r = 0, \quad j = \frac{3}{2}$

($l = 1$, $s = 1/2$)	$j = 3/2$	$2\ {}^2P_{3/2}$	$\kappa = -2$

$n_r = 1, \quad j = \frac{1}{2}$

($l = 0$, $s = 1/2$)	$j = 1/2$	$2\ {}^2S_{1/2}$	$\kappa = -1$
($l = 1$, $s = 1/2$)	$j = 1/2$	$2\ {}^2P_{1/2}$	$\kappa = 1$

$n = 3$

$n_r = 0, \quad j = \dfrac{5}{2}$

($l = 2$, $s = 1/2$ $\quad j = 5/2$ $\quad 3\,{}^2\mathrm{D}_{5/2}$) $\kappa = -3$

$n_r = 1, \quad j = \dfrac{3}{2}$

($l = 1$, $s = 1/2$ $\quad j = 3/2$ $\quad 3\,{}^2\mathrm{P}_{3/2}$) $\quad \kappa = -2$
($l = 2$, $s = 1/2$ $\quad j = 3/2$ $\quad 3\,{}^2\mathrm{D}_{3/2}$) $\quad \kappa = 2$

$n_r = 2, \quad j = \dfrac{1}{2}$

($l = 0$, $s = 1/2$ $\quad j = 1/2$ $\quad 3\,{}^2\mathrm{S}_{1/2}$) $\quad \kappa = -1$
($l = 1$, $s = 1/2$ $\quad j = 1/2$ $\quad 3\,{}^2\mathrm{P}_{1/2}$) $\quad \kappa = 1$

Table-2

$j = \dfrac{1}{2}$

$\kappa = 1, \quad l = 1$
$\kappa = -1, \quad l = 0$

$j = \dfrac{3}{2}$

$\kappa = 2, \quad l = 2$
$\kappa = -2, \quad l = 1$

$j = \dfrac{5}{2}$

$\kappa = 3, \quad l = 3$
$\kappa = -3, \quad l = 2$

Table 3 Notation in the nonrelativistic case

$n = 1$				
	$l = 0$,	$s = 1/2$	$j = 1/2$	$1\,{}^2\mathrm{S}_{1/2}$
$n = 2$				
	$l = 0$,	$s = 1/2$	$j = 1/2$	$2\,{}^2\mathrm{S}_{1/2}$
	$l = 1$,	$s = 1/2$	$j = 3/2$	$2\,{}^2\mathrm{P}_{3/2}$
	$l = 1$,	$s = 1/2$	$j = 1/2$	$2\,{}^2\mathrm{P}_{1/2}$
$n = 3$				
	$l = 0$,	$s = 1/2$	$j = 1/2$	$3\,{}^2\mathrm{S}_{1/2}$
	$l = 1$,	$s = 1/2$	$j = 3/2$	$3\,{}^2\mathrm{P}_{3/2}$

$l = 1$,	$s = 1/2$	$j = 1/2$	$3\ ^2P_{1/2}$
$l = 2$,	$s = 1/2$	$j = 5/2$	$3\ ^2D_{5/2}$
$l = 2$,	$s = 1/2$	$j = 3/2$	$3\ ^2D_{3/2}$

20. Energy levels

The energy ΔE

$$\Delta E = \frac{mc^2}{\sqrt{1 + \dfrac{Z^2\alpha^2}{(n - j - \frac{1}{2} + \sqrt{(j + \frac{1}{2})^2 - Z^2\alpha^2})^2}}} - mc^2$$

can be expanded by using a Taylor expansion in a power of $Z^2\alpha^2$.

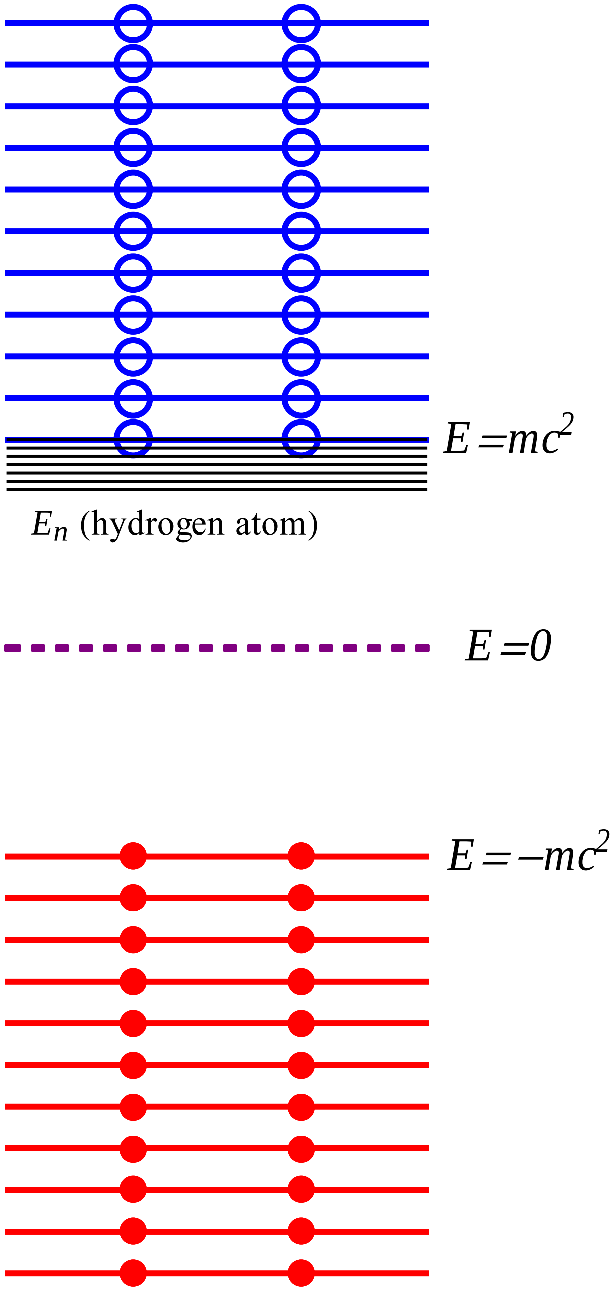

Fig. The energy levels of electron in the hydrogen atom (in the relativistic quantum mechanics)

Using the Mathematica, we have

$$\begin{aligned}\Delta E &= E - mc^2 \\ &= -\frac{mc^2}{2n^2}(Z\alpha)^2 + \frac{mc^2(6j+3-8n)}{8(1+2j)n^4}(Z\alpha)^4 + ... \\ &= -\frac{mc^2}{2n^2}(Z\alpha)^2 - \frac{mc^2}{2n^3}(Z\alpha)^4\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right) + ...\end{aligned}$$

The first tem is the non-relativistic limit

$$-\frac{mc^2}{2n^2}(Z\alpha)^2 = -\frac{13.6057Z^2}{n^2}\ [\text{eV}]$$

The second term is the relativistic correction to ΔE.

The principal quantum number n are n = 1, 2, 3, 4, … and $j+1/2 \le n$. There is the degeneracy between 2 $^2S_{1/2}$ ans 2 $^2P_{1/2}$.states (similarly 3 $^2S_{1/2}$ ans 3 $^2P_{1/2}$, 3 $^2P_{3/2}$ ans 3 $^2D_{3/2}$) persists in the eaxct solution to the Dirac equation. This degeneracy is lifted by the Lamb shift due to the coupling of electron to the zero-point fluctuation of the radiation field.

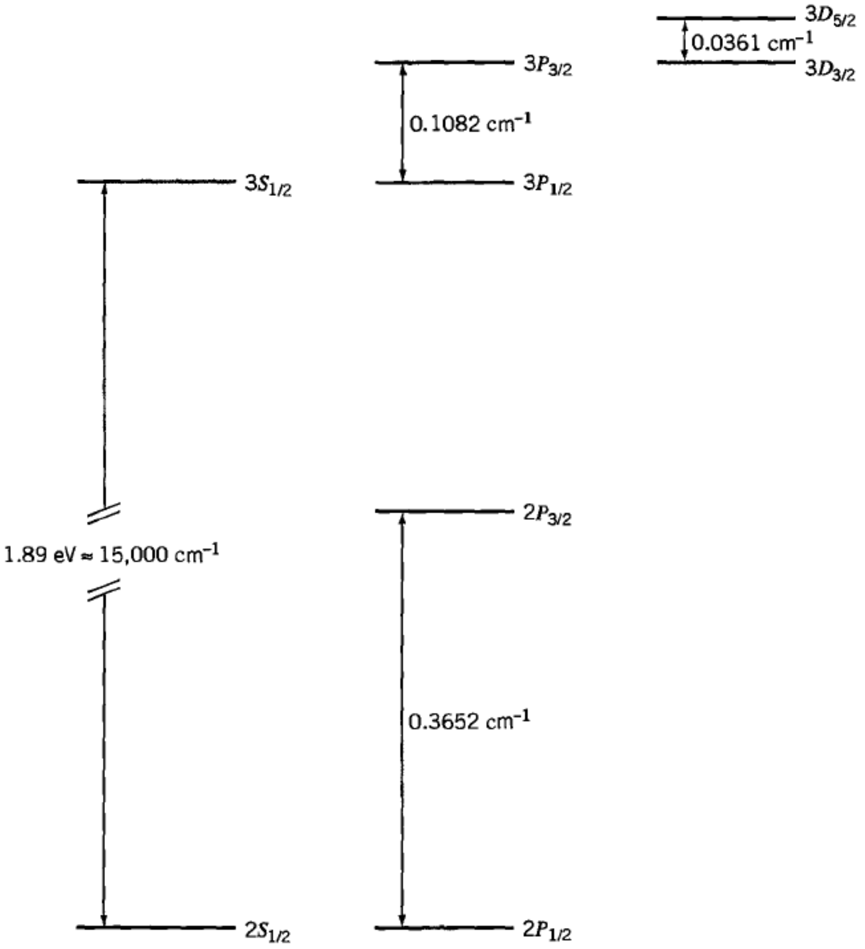

Fig. Detail of an energy-level diagram for the hydrogen atom. The manifolds of the n = 2 and n = 3 levels are shown, based on the Dirac theory, without radiative corrections (Lamb shifts) or hyperfine splittings. The energy differences are given in the units of cm^{-1}. 1eV = 8065.56 cm^{-1}. ((**Merzbacher, Quantum Mechanics**)

((**Mathematica**))
The energy is in the units of cm^{-1}; $E(erg)/(2\pi\hbar c)$.
1 eV = 8065.56 cm^{-1}

```
Clear["Global`*"];
```

$$\text{rule1} = \{c \to 2.99792\times 10^{10},\ \hbar \to 1.054571628\ 10^{-27},\ \text{me} \to 9.10938215\ 10^{-28},\ \text{eV} \to 1.602176487\times 10^{-12},\ \alpha \to 7.2973525376\times 10^{-3},\ Z \to 1\};$$

$$\text{E0} = \frac{\text{me}\, c^2}{\sqrt{1+\frac{Z^2\ \alpha^2}{\left(\text{n1}-\text{j1}-\frac{1}{2}+\sqrt{\left(\text{j1}+\frac{1}{2}\right)^2-Z^2\ \alpha^2}\right)^2}}} - \text{me}\, c^2;$$

$$\frac{1\ \text{eV}}{2\,\pi\,\hbar\, c}\ \text{//. rule1}$$

```
8065.56
```

```
Series[E0, {α, 0, 4}] //
 FullSimplify[#, {j1 > 0, n1 > 0}] &
```

$$-\frac{\left(c^2\ \text{me}\ Z^2\right)\ \alpha^2}{2\ \text{n1}^2}+\frac{c^2\ \text{me}\ (3+6\ \text{j1}-8\ \text{n1})\ Z^4\ \alpha^4}{8\ (1+2\ \text{j1})\ \text{n1}^4}+O[\alpha]^5$$

```
E1[n_, j_] := E0 / (2 π ħ c) /. {n1 → n, j1 → j} //. rule1
```

```
E1[3, 5 / 2] - E1[3, 3 / 2]
```

```
0.0360719
```

```
E1[3, 3 / 2] - E1[3, 1 / 2]
```

```
0.108219
```

```
E1[2, 3 / 2] - E1[2, 1 / 2]
```

```
0.365241
```

```
E1[3, 1 / 2] - E1[2, 1
   / 2]
```

```
15 241.6
```

21. Wave function for the ground state

Suppose that $n_r = 0$. Then we have

$$a_1 = b_1 = 0, \qquad a_0 \neq 0, \qquad b_0 \neq 0$$

From the recursion relation,

$$-a_0 - \mu b_0 = 0$$

or

$$a_0 = -\mu b_0 \tag{1}$$

From the indicial equation

$$-\gamma a_0 + (s+\kappa) b_0 = 0 \tag{2}$$

Using these two equations, we have

$$\frac{a_0}{b_0} = \frac{s+\kappa}{\gamma} = -\mu < 0$$

where

$$s = \sqrt{\kappa^2 - \gamma^2} < |\kappa|$$

Then we have

$$s + \kappa < 0 \qquad \text{and} \qquad 0 < s < |\kappa|$$

or

$$\kappa < -s < 0$$

The absence of the $\kappa > 0$ state for $n_r = 0$ corresponds to the familiar rule in relativistic quantum mechanics.

<u>Ground state:</u>

$$n = j + \frac{1}{2} + n_r$$

with $n = 1$. $n_r = 0$, $j = 1/2$.

$$E = \frac{mc^2}{\sqrt{1+\frac{Z^2\alpha^2}{1-Z^2\alpha^2}}} = \frac{mc^2}{\sqrt{\frac{1}{1-Z^2\alpha^2}}} = mc^2\sqrt{1-Z^2\alpha^2} \qquad \text{(ground state energy)}$$

$$\frac{a_0}{b_0} = -\mu = -\sqrt{\frac{mc^2+E}{mc^2-E}} = -\frac{1+\sqrt{1-Z^2\alpha^2}}{Z\alpha} \approx -\frac{2}{Z\alpha}$$

$$\rho = \frac{\sqrt{\alpha_1\alpha_2}\,r}{\hbar c} = \frac{mc}{\hbar}(Z\alpha)r\ .$$

with

$$\sqrt{\alpha_1\alpha_2} = \sqrt{(mc^2-E)(mc^2+E)} = \sqrt{m^2c^4-E^2} = mc^2(Z\alpha)$$

$$\kappa = -(j+\frac{1}{2}) = -1 \qquad \text{since } j = 1/2.$$

$$s = \sqrt{\kappa^2-\gamma^2} = \sqrt{1-Z^2\alpha^2} \approx 1-\frac{1}{2}Z^2\alpha^2$$

Then the radial wave function of the ground state are given by

$$\begin{aligned} f(r) &= a_0\frac{\sqrt{\alpha_1\alpha_2}}{\rho}e^{-\rho}\rho^s \\ &= a_0\sqrt{\alpha_1\alpha_2}e^{-\rho}\rho^{s-1} \\ &= a_0mc^2(Z\alpha)e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\ &= A_0e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \end{aligned}$$

and

$$
\begin{aligned}
g(r) &= b_0 \frac{\sqrt{\alpha_1\alpha_2}}{\rho} e^{-\rho}\rho^{s} \\
&= b_0\sqrt{\alpha_1\alpha_2} e^{-\rho}\rho^{s-1} \\
&= b_0 mc^2 (Z\alpha) e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\
&= -\frac{1}{2} a_0 mc^2 (Z\alpha)^2 e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2} \\
&= -\frac{1}{2}(Z\alpha) A_0 e^{-\rho}\rho^{-\frac{1}{2}Z^2\alpha^2}
\end{aligned}
$$

with

$$A_0 = a_0(mc^2)Z\alpha, \qquad b_0 = -\frac{Z\alpha}{2}a_0$$

The upper component *f*(*r*) is very similar to the non-relativistic wave function except for an enhanced (singular) part at small ρ which goes like $\rho^{-\frac{1}{2}Z^2\alpha^2}$. This singularity is very weak, and the solution is still integrable near the origin. The lower component g(r) is very much smaller (by a factor of $\frac{1}{2}Z\alpha$) than the upper component. Thus the relativistic solution differs from the non-relativistic solution only to the order of *Za*, or at very short distances.

((**Note**)) The radial function for the ground state in the non-relativistic theory

$$R_{10} = \frac{2Z^{3/2}}{a^{3/2}} e^{-\frac{rZ}{a}} = 2(\frac{mc}{\hbar})^{3/2}(Z\alpha)^{3/2} e^{-\rho}$$

with

$$\rho = \frac{rZ}{a} = \frac{rZ}{\hbar^2}me^2 = r(Z\alpha)\frac{mc}{\hbar}$$

where

$$a = \frac{\hbar^2}{me^2} \text{ (Bohr radius)} \qquad ,$$

$$\frac{Z}{a} = \frac{mc}{\hbar}Z\alpha .$$

22. Heisenberg's principle of uncertainty

In the Dirac theory,

$$H = c\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta mc^2 - \frac{Ze^2}{r}$$

From the Heisenberg's equation of motion, we get the relations,

$$\boldsymbol{\alpha} = \frac{1}{c}\boldsymbol{v}$$

$$\beta H + H\beta = 2mc^2$$

When

$$2\beta < H >= 2mc^2, \qquad \beta = \frac{mc^2}{E} = \frac{1}{\gamma} = \sqrt{1-\frac{v^2}{c^2}}$$

The Heisenberg's principle of uncertainty:

$$\Delta p_r \Delta r \approx \hbar$$

((**Special relativity**))

$$\boldsymbol{p} = \gamma m\boldsymbol{v}, \qquad E = \gamma mc^2 = c\sqrt{m^2c^2 + \boldsymbol{p}^2}$$

with

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}$$

So we get the Hamiltonian

$$\begin{aligned} H &\approx \boldsymbol{v}\cdot\boldsymbol{p} + mc^2\frac{1}{\gamma} - \frac{Ze^2}{r} \\ &= \gamma mv^2 + mc^2\frac{1}{\gamma} - \frac{Ze^2}{r} \\ &= c\sqrt{\boldsymbol{p}^2 + m^2c^2} - \frac{Ze^2}{r} \end{aligned}$$

Note that

$$\boldsymbol{v}\cdot\boldsymbol{p}+mc^2\frac{1}{\gamma}=\boldsymbol{v}\cdot\gamma m\boldsymbol{v}+mc^2\frac{1}{\gamma}$$

$$=\frac{mv^2}{\sqrt{1-\frac{v^2}{c^2}}}+mc^2\sqrt{1-\frac{v^2}{c^2}}$$

$$=\frac{mc^2}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$=\sqrt{m^2c+cp}$$

We now consider the Hamiltonian given by

$$H=c\sqrt{(\Delta p_r)^2+m^2c^2}-\frac{Ze^2}{\hbar}\Delta p_r$$

We take a derivative of H with respect to Δp_r

$$\frac{\partial}{\partial(\Delta p_r)}H=\frac{c\Delta p_r}{\sqrt{(\Delta p_r)^2+m^2c^2}}-\frac{Ze^2}{\hbar}=0$$

Then we get

$$\frac{c\Delta p_r}{\sqrt{(\Delta p_r)^2+m^2c^2}}=\frac{Ze^2}{\hbar}$$

or

$$\frac{(\Delta p_r)^2}{(\Delta p_r)^2+m^2c^2}=(Z\alpha)^2$$

From this, $(\Delta p_r)^2$ can be obtained as

$$(\Delta p_r)^2=m^2c^2\frac{(Z\alpha)^2}{1-(Z\alpha)^2}$$

or

$$\Delta p_r=\frac{mcZ\alpha}{\sqrt{1-(Z\alpha)^2}}$$

From the relation $\Delta p_r \Delta r \approx \hbar$ we get

$$\Delta r \approx \frac{\hbar}{\Delta p_r} = \frac{\hbar}{mcZ\alpha}\sqrt{1-(Z\alpha)^2} \approx \frac{\hbar}{mcZ\alpha}$$

Then the local minimum of H is given by

$$H = mc^2\sqrt{1-(Z\alpha)^2}$$

which is exactly the same as the value of E_{ground} in the relativistic theory.

23. Determination of C_q (a_q, b_q)

We derive the recursion relation for C_q fro the relation

$$(s+q-\kappa)a_q + \gamma b_q = a_{q-1} + \mu b_{q-1}$$

$$C_q = \frac{a_q}{s+q+\kappa-\frac{\gamma}{\mu}} = \frac{b_q}{\frac{1}{\mu}(s+q-\kappa)+\gamma}$$

From these equations we get

$$C_q = \frac{\gamma(\mu-\frac{1}{\mu})+2(s+q-1)}{q(2s+q)}C_{q-1}$$

where

For $q = n_r+1$, $C_q = 0$. Then we have

$$\gamma(\mu-\frac{1}{\mu})+2(s+n_r)=0$$

Finally we get the recursion formula,

$$C_q = \frac{2(s+q-1)-2(s+n_r)}{q(q+2s)}C_{q-1}$$
$$= \frac{2(q-1-n_r)}{q(q+2s)}C_{q-1}$$

For $q = 1$,

$$C_1 = \frac{2(-n_r)}{1(1+2s)} C_0 ,$$

For $q = 2$,

$$\begin{aligned} C_2 &= \frac{2(1-n_r)}{2(2+2s)} C_1 \\ &= \frac{2(1-n_r)}{2(2+2s)} \frac{2(-n_r)}{1(1+2s)} C_0 \\ &= \frac{2^2(-1)^2 n_r(n_r-1)}{2!(1+2s)(2+2s)} C_0 \end{aligned}$$

For $q = 3$,

$$\begin{aligned} C_3 &= \frac{2(2-n_r)}{3(3+2s)} C_2 \\ &= \frac{2^3(-1)^3 n_r(n_r-1)(n_r-2)}{3!(1+2s)(2+2s)(3+2s)} C_0 \end{aligned}$$

In general

$$C_k = \frac{2^k(-1)^k[n_r!/(n_r-k)!]}{k!(1+2s)(2+2s)...(k+2s)} C_0$$

where

$$C_q = \frac{a_q}{s+q+\kappa-\dfrac{\gamma}{\mu}} = \frac{b_q}{\dfrac{1}{\mu}(s+q-\kappa)+\gamma}$$

REFERENCES

E. Fermi, Notes on Quantum Mechanics (The University of Chicago Press, 1961).

J.D. Bjorken and S.D. Drell, Relativistic Quantum Mechanics (McGraw-Hill, New York, 1964)

J.J. Sakurai, Advanced Quantum Mechanics (Addison-Wesley, New York, 1967).

M.E. Rose, Relativistic Electron Theory (John Wiley & Sons, New York, 1961).

A. Das, Lectures on Quantum mechanics, second edition (World Scientific, 2012).

F.J, Dyson, Advanced Quantum Mechanics (World Scientific, 2007).

S.S. Schweber, An Introduction to Relativistic Quantum Field Theory (Row, Peterson, 1961).
F. Schwabl, Advanced *Quantum Mechanics* (Springer Verlag, Berlin, 2005).
F. Gross, Relativistic Quantum Mechanics and Field Theory (Wiley-VCH, 1993).
Eugen Merzbacher, *Quantum Mechanics*, third edition (John Wiley & Sons, New York, 1998).
Ramamurti Shankar, *Principles of Quantum Mechanics*, second edition (Springer, New York, 1994).
Leonard Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc, New York, 1955).
B.R. Holstein, Topics in ADVANCED Quantum Mechanics (Addison-Wesley, 1992).
H. Bethe and E.E. Salpeter, Quantum Mechanics of one and two-electron atoms

APPENDIX I

Klein-Gordon equation

((Problem))

The relativistic wave equation for bosons of rest mass *m* may be obtained by the relation

$$E^2 = \boldsymbol{p}^2 c^2 + m^2 c^4$$

through the identifications

$$E \to i\hbar \frac{\partial}{\partial t}, \qquad \boldsymbol{p} \to \frac{\hbar}{i}\nabla$$

(a) Obtain the wave equation relevant to bosons of rest mass *m*. This equation is called the Klein-Gordon equation.
(b) What form does this equation assume for photons?
(c) Suppose that the wavefunction is independent of time *t*. It depends only on *r*. Using the spherical co-ordinates; $\{r, \theta, \phi\}$, find the differential equation for the wavefunction $\psi(r)$. Show that $\psi(r)$ has the form of $\psi(r) = A\dfrac{e^{-r/a}}{r}$, where *A* and *a* are constants. We assume that $l = 0$.
(d) Find the expression for the characteristic length *a*.
(e) Use this equation to show that there is a local conservation law of the form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{j} = 0$$

with

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^* \nabla \psi - \psi \nabla \psi^*) .$$

Determine the form of $\rho(\boldsymbol{r},t)$. From this form for ρ, give an argument for why the Klein-Gordon equation is not a good candidate for a one-particle relativistic wave equation in plane of the Schrodinger equation, for which $\rho = \psi^{*}\psi$

((**Solution**))

(a)

We start with

$$E^2\psi = (\boldsymbol{p}^2c^2 + m^2c^4)\psi\,,$$

with

$$E \to i\hbar\frac{\partial}{\partial t}, \qquad \boldsymbol{p} \to \frac{\hbar}{i}\nabla$$

Then we have

$$-\hbar^2\frac{\partial^2}{\partial t^2}\psi = -\hbar^2c^2\nabla^2\psi + m^2c^4\psi$$

or

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = \frac{m^2c^2}{\hbar^2}\psi \qquad \text{(Klein-Gordon equation)}$$

(b) For photon, the mass *m* is equal to zero. Then we have the wave equation as

$$\nabla^2\psi - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi = 0$$

(c) Suppose that the wavefunction is independent of time *t*. It depends only on *r*.

$$\frac{1}{r}\frac{\partial}{\partial r}(\frac{\partial}{\partial r}r)\psi(r) = \frac{m^2c^2}{\hbar^2}\psi$$

We assume that $\psi = \dfrac{u}{r}$.

$$\frac{d^2}{dr^2}u(r) = \frac{m^2c^2}{\hbar^2}u(r) = \frac{1}{a^2}u(r)\,.$$

Then we have the

$$u = Ae^{-r/a}$$

or

$$\psi = A\frac{e^{-r/a}}{r}$$

(d)

a is the characteristic length and is defined by

$$a = \frac{\hbar}{mc}.$$

(e) The current density is given by

$$\boldsymbol{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

$$\begin{aligned}
\nabla\cdot\boldsymbol{j} &= \frac{\hbar}{2mi}[\nabla\cdot(\psi^*\nabla\psi) - \nabla\cdot(\psi\nabla\psi^*)) \\
&= \frac{\hbar}{2mi}(\nabla\psi^*\cdot\nabla\psi + \psi^*\nabla^2\psi - \nabla\psi\nabla\psi^* - \psi\nabla^2\psi^*) \\
&= \frac{\hbar}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)
\end{aligned}$$

Using the equation of continuity, we have

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot\boldsymbol{j} = -\frac{\hbar}{2mi}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*)$$

We use the Klein-Gordon equation

$$\nabla^2\psi = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi + \frac{m^2c^2}{\hbar^2}\psi, \qquad \nabla^2\psi^* = \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi^* + \frac{m^2c^2}{\hbar^2}\psi^*$$

Then we get

$$\frac{\partial\rho}{\partial t} = -\frac{\hbar}{2mi}[\psi^*(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi + \frac{m^2c^2}{\hbar^2}\psi) - \psi(\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\psi^* + \frac{m^2c^2}{\hbar^2}\psi^*)]$$

$$= -\frac{\hbar}{2mc^2 i}(\psi^*\frac{\partial^2}{\partial t^2}\psi - \psi\frac{\partial^2}{\partial t^2}\psi^*)$$

$$= -\frac{\hbar}{2mc^2 i}\frac{\partial}{\partial t}(\psi^*\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^*)$$

Thus we have

$$\rho = \frac{i\hbar}{2mc^2}(\psi^*\frac{\partial}{\partial t}\psi - \psi\frac{\partial}{\partial t}\psi^*)$$

Suppose that

$$\psi^*\frac{\partial}{\partial t}\psi = \alpha + i\beta$$

where α and β are real. Then we have

$$\psi\frac{\partial}{\partial t}\psi^* = \alpha - i\beta$$

Then we have

$$\rho = \frac{i\hbar}{2mc^2}[\alpha + i\beta - (\alpha - i\beta)] = \frac{i\hbar}{2mc^2}2i\beta = -\frac{\beta\hbar}{mc^2}$$

When $\beta > 0$, the probability density could be negative, which is inconsistent with the requirement that ρ should be positive. In this sense, the Klein-Gordon equation is not a good candidate for a one-particle relativistic wave equation in plane of the Schrodinger equation, for which $\rho = \psi^*\psi$