PHY 742 Quantum Mechanics
12:00-12:50 AM MWF Olin 103

Plan for Lecture 18:

Chap. 16 in Professor Carlson's text:

The Dirac equation for a hydrogen-like ion

1. Angular and spin components
2. Radial components
3. Comparison with non-relativistic hydrogen-like ion

16	Wed: 02/23/2022	Chap. 16	The Dirac equation	#14	02/25/2022
17	Fri: 02/25/2022	Chap. 16	The Dirac equation	#15	02/28/2022
18	Mon: 02/28/2022	Chap. 16	The Dirac equation	#16	03/02/2022
19	Wed: 03/02/2022	Chap. 16	The Dirac equation		
20	Fri: 03/04/2022	Chap. 16	The Dirac equation		
	Mon: 03/07/2022	No class	*Spring Break*		
	Wed: 03/09/2022	No class	*Spring Break*		
	Fri: 03/11/2022	No class	*Spring Break*		
	Mon: 03/14/2022	No class	*APS March Meeting*	Prepare Project	
	Wed: 03/16/2022	No class	*APS March Meeting*	Prepare Project	
	Fri: 03/18/2022	No class	*APS March Meeting*	Prepare Project	
	Mon: 03/21/2022		Project presentations I		
	Wed: 03/23/2022		Project presentations II		
21	Fri: 03/25/2022				

Note: Project topic needed by Friday 3/5/2022

PHY 742 -- Assignment #16

February 28, 202

Continue reading Chapter 16 in **Professor Carlson's QM textbook.**.

1. Consider a H-like ion with $Z=5$ as represented by the Dirac equation. Numerically evaluate all of the eigenstate energies for principal quantum numbers n=1,2 and 3. Compare each of the results with corresponding eigenstate energies of the Schrödinger equation.

Additional references –

J. J. Sakurai, Advanced Quantum Mechanics

Hans A. Bethe and Edwin E. Salpeter, Quantum Mechanics of one and two electron atoms

Dirac equation for Fermi particle in a scalar potential field

$$H = \mathbf{p}\cdot\boldsymbol{\alpha}c + mc^2\beta + V(\mathbf{r})I_4$$

where: $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}$ $\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ and where:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad I \equiv I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$I_4 = \begin{pmatrix} I_2 & 0 \\ 0 & I_2 \end{pmatrix}$$

Dirac equation for electron in the field of a H-like ion

$$H = \mathbf{p} \cdot \boldsymbol{\alpha} c + mc^2 \beta + V(\mathbf{r}) I_4$$

For H-like ion with nuclear charge Z :

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

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

Stationary state solutions:

$$\Psi(\mathbf{r},t) = \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} e^{-iEt/\hbar}$$

$$\begin{pmatrix} mc^2 + V(r) & \mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -mc^2 + V(r) \end{pmatrix} \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

Dirac equation for electron in the field of a H-like ion -- continued

$$H = \begin{pmatrix} mc^2 + V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2 + V(r) \end{pmatrix}$$

Note that the following operators commute with the Hamiltonian and have simultaneous eigenvalues:

$$J_z = \begin{pmatrix} L_z + \frac{1}{2}\hbar\sigma_z & 0 \\ 0 & L_z + \frac{1}{2}\hbar\sigma_z \end{pmatrix}$$

$$\mathbf{J}^2 = \begin{pmatrix} \mathbf{L}^2 + \frac{3\hbar^2}{4}I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} & 0 \\ 0 & \mathbf{L}^2 + \frac{3\hbar^2}{4}I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} \end{pmatrix}$$

$$K = \begin{pmatrix} \boldsymbol{\sigma}\cdot\mathbf{L} + \hbar I_2 & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\mathbf{L} - \hbar I_2 \end{pmatrix}$$

Dirac equation for electron in the field of a H-like ion -- continued

$$\begin{pmatrix} mc^2 + V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2 + V(r) \end{pmatrix} \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

We can show that:

$$\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g_{\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

More details about spin-angular functions:

Eigenfunctions of $\mathbf{J}^2$ and J_z : $\left|JM\right\rangle$

$$\mathbf{J}^2\left|JM\right\rangle = \hbar^2 J(J+1)\left|JM\right\rangle$$

$$J_z\left|JM\right\rangle = \hbar M\left|JM\right\rangle$$

$$K^2\left|JM\right\rangle = \hbar^2\left(J(J+1)+\tfrac{1}{4}\right)\left|JM\right\rangle = \hbar^2\left(J+\tfrac{1}{2}\right)^2\left|JM\right\rangle$$

Dirac equation for electron in the field of a H-like ion -- continued

$$J_z \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} L_z + \frac{1}{2}\hbar\sigma_z & 0 \\ 0 & L_z + \frac{1}{2}\hbar\sigma_z \end{pmatrix} \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \hbar M \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

$$\mathbf{J}^2 \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \mathbf{L}^2 + \frac{3\hbar^2}{4} I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} & 0 \\ 0 & \mathbf{L}^2 + \frac{3\hbar^2}{4} I_2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} \end{pmatrix} \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

$$= \hbar^2 J(J+1) \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

$$K \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \boldsymbol{\sigma}\cdot\mathbf{L} + \hbar I_2 & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\mathbf{L} - \hbar I_2 \end{pmatrix} \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

$$= -\hbar\kappa \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} -\hbar\kappa\varphi^U(\mathbf{r}) \\ +\hbar\kappa\varphi^L(\mathbf{r}) \end{pmatrix}$$

Dirac equation for electron in the field of a H-like ion -- continued

$$K\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}=\begin{pmatrix}\boldsymbol{\sigma}\cdot\mathbf{L}+\hbar I_2 & 0\\ 0 & -\boldsymbol{\sigma}\cdot\mathbf{L}-\hbar I_2\end{pmatrix}\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}$$

$$=-\hbar\kappa\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}=\begin{pmatrix}-\hbar\kappa\varphi^U(\mathbf{r})\\ +\hbar\kappa\varphi^L(\mathbf{r})\end{pmatrix}$$

$$\Rightarrow\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}=\begin{pmatrix}g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})\\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})\end{pmatrix}$$

It can also be shown that φ^U and φ^L are eigenvectors of $\mathbf{L}^2$:

$$\mathbf{L}^2\varphi^U=\hbar^2 l_U(l_U+1)\varphi^U \quad \text{and} \quad \mathbf{L}^2\varphi^L=\hbar^2 l_L(l_L+1)\varphi^L$$

$$\Rightarrow \mathbf{L}^2\chi_{\kappa JM}(\hat{\mathbf{r}})=\hbar^2 l_U(l_U+1)\chi_{\kappa JM}(\hat{\mathbf{r}}) \quad \text{and} \quad \mathbf{L}^2\chi_{-\kappa JM}(\hat{\mathbf{r}})=\hbar^2 l_L(l_L+1)\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

More relationships between the operators

$$\mathbf{L}^2 = \mathbf{J}^2 - \hbar\boldsymbol{\sigma}\cdot\mathbf{L} - \tfrac{3}{4}\hbar^2 = \mathbf{J}^2 + \tfrac{1}{4}\hbar^2 - \hbar\left(\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar\right)$$

Relationships between the upper and lower component functions:

$$\mathbf{L}^2\chi_{\kappa JM}(\hat{\mathbf{r}}) = \hbar^2 l_U(l_U+1)\chi_{\kappa JM}(\hat{\mathbf{r}}) \quad \text{and} \quad \mathbf{L}^2\chi_{-\kappa JM}(\hat{\mathbf{r}}) = \hbar^2 l_L(l_L+1)\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

$$\left(\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar\right)\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\kappa\chi_{\kappa JM}(\hat{\mathbf{r}}) \quad \text{and} \quad \left(\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar\right)\chi_{-\kappa JM}(\hat{\mathbf{r}}) = \kappa\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

Algebraic relations --

$$l_L(l_L+1) = l_U(l_U+1) - 2\kappa$$

$$l_U(l_U+1) = J(J+1) + \kappa + \tfrac{1}{4}$$

Summary of allowed combinations of eigenvalues

	l_U	l_L
$\kappa = -\left(J + \frac{1}{2}\right)$	$J - \frac{1}{2}$	$J + \frac{1}{2}$
$\kappa = +\left(J + \frac{1}{2}\right)$	$J + \frac{1}{2}$	$J - \frac{1}{2}$

Alternatively

	J	l_L
$\kappa = -\left(l_U + 1\right)$	$l_U + \frac{1}{2}$	$l_U + 1$
$\kappa = +l_U$	$l_U - \frac{1}{2}$	$l_U - 1$

Dirac equation for electron in the field of a H-like ion -- continued

Note that for stationary state solutions to the Dirac equation

$H\Psi_{E\kappa JM} = E\Psi_{E\kappa JM}$, the κ value is identified with φ^U.

$$\Psi_{E\kappa JM} = \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Combinations:

$\kappa = -1$	$J = \frac{1}{2}$	$l_U = 0$
$+1$	$\frac{1}{2}$	1
-2	$\frac{3}{2}$	1
$+2$	$\frac{3}{2}$	2
-3	$\frac{5}{2}$	2
$+3$	$\frac{5}{2}$	3

Possibilities:

$J = l + \frac{1}{2} \qquad \kappa = -l - 1 = -\left(J + \frac{1}{2}\right)$

$J = l - \frac{1}{2} \qquad \kappa = l = \left(J + \frac{1}{2}\right)$

Evaluating the spin-orbital functions in terms of Clebsch-Gordan coefficients:

For $J = l + \frac{1}{2}$ and $\kappa = -l - 1 = -\left(J + \frac{1}{2}\right)$

$$\chi_{\kappa JM}(\hat{\mathbf{r}}) = \sqrt{\frac{l + M + \frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l - M + \frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

For $J = l - \frac{1}{2}$ and $\kappa = l = +\left(J + \frac{1}{2}\right)$:

$$\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\sqrt{\frac{l - M + \frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l + M + \frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Now considering the full Hamiltonian:

$$H = \begin{pmatrix} mc^2 + V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2 + V(r) \end{pmatrix} = \begin{pmatrix} mc^2 + V(r) & \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)^2 \left(\mathbf{p}\cdot\boldsymbol{\sigma}\right)c \\ \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)^2 \left(\mathbf{p}\cdot\boldsymbol{\sigma}\right)c & -mc^2 + V(r) \end{pmatrix}$$

Recall that: $\left(\boldsymbol{\sigma}\cdot\mathbf{A}\right)\left(\boldsymbol{\sigma}\cdot\mathbf{B}\right) = \mathbf{A}\cdot\mathbf{B} + i\boldsymbol{\sigma}\cdot\left(\mathbf{A}\times\mathbf{B}\right)$

Some details -- Stationary state solutions:

$$\Psi(\mathbf{r},t)=\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}e^{-iEt/\hbar}$$

$$\begin{pmatrix} mc^2+V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2+V(r)\end{pmatrix}\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}=E\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}$$

Let $\begin{pmatrix}\varphi^U(\mathbf{r})\\ \varphi^L(\mathbf{r})\end{pmatrix}=\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})\\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})\end{pmatrix}$

$$\Rightarrow\left(mc^2+V(r)-E\right)g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})+\mathbf{p}\cdot\boldsymbol{\sigma}cif_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})=0$$

$$\mathbf{p}\cdot\boldsymbol{\sigma}cg_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})+\left(-mc^2+V(r)-E\right)if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})=0$$

Some tricks -- recall that $\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)^2 = I_2$

$$\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)^2\left(\mathbf{p}\cdot\boldsymbol{\sigma}\right) = \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(\mathbf{p}\cdot\boldsymbol{\sigma}\right)$$

$$= \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(\hat{\mathbf{r}}\cdot\mathbf{p} + \frac{i\boldsymbol{\sigma}\cdot\mathbf{L}}{r}\right)$$

$$= \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(-i\hbar\frac{\partial}{\partial r} + \frac{i\boldsymbol{\sigma}\cdot\mathbf{L}}{r}\right)$$

Also note that: $\left(\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar I_2\right)\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\hbar\kappa\chi_{\kappa JM}(\hat{\mathbf{r}})$

so that: $\boldsymbol{\sigma}\cdot\mathbf{L}\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\hbar\left(\kappa+1\right)\chi_{\kappa JM}(\hat{\mathbf{r}})$

$$\boldsymbol{\sigma}\cdot\mathbf{L}\chi_{-\kappa JM}(\hat{\mathbf{r}}) = -\hbar\left(-\kappa+1\right)\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

More tricks --

$$\left(mc^2+V(r)-E\right)g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})+\mathbf{p}\cdot\boldsymbol{\sigma}cif_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})=0$$

$$\mathbf{p}\cdot\boldsymbol{\sigma}cg_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})+\left(-mc^2+V(r)-E\right)if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})=0$$

$$\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(-i\hbar\frac{\partial}{\partial r}+\frac{i\boldsymbol{\sigma}\cdot\mathbf{L}}{r}\right)$$

What about $\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\chi_{\kappa JM}\left(\hat{\mathbf{r}}\right)$?

Recall:

For $\kappa = -\left(J + \frac{1}{2}\right) \qquad l = -\kappa - 1 \quad \text{and} \quad J = l + \frac{1}{2}$

$$\chi_{\kappa JM}(\hat{\mathbf{r}}) = \sqrt{\frac{l + M + \frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l - M + \frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

For $\kappa = +\left(J + \frac{1}{2}\right) \quad l = \kappa \text{ and } J = l - \frac{1}{2}$

$$\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\sqrt{\frac{l - M + \frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l + M + \frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\hat{\mathbf{r}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix}$$

For example, consider the example κ=-1:

In this case: For $\kappa=-1 \qquad l=0$ and $J=\frac{1}{2}=l+\frac{1}{2}$

$$\chi_{\kappa JM}(\hat{\mathbf{r}})=\chi_{-1\frac{1}{2}\frac{1}{2}}(\hat{\mathbf{r}})=Y_{00}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix} \qquad \chi_{-1\frac{1}{2}-\frac{1}{2}}(\hat{\mathbf{r}})=Y_{00}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix}$$

$$\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\chi_{-1\frac{1}{2}\frac{1}{2}}(\hat{\mathbf{r}})=Y_{00}(\hat{\mathbf{r}})\begin{pmatrix}\cos\theta\\ \sin\theta e^{i\varphi}\end{pmatrix} \qquad \hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\chi_{-1\frac{1}{2}-\frac{1}{2}}(\hat{\mathbf{r}})=Y_{00}(\hat{\mathbf{r}})\begin{pmatrix}\sin\theta e^{-i\varphi}\\ -\cos\theta\end{pmatrix}$$

Note that for $\kappa=+1 \quad l=1$ and $J=\frac{1}{2}=l-\frac{1}{2}$

$$\chi_{\kappa JM}(\hat{\mathbf{r}})=\chi_{1\frac{1}{2}\frac{1}{2}}(\hat{\mathbf{r}})=-\sqrt{\frac{1}{3}}Y_{10}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix}+\sqrt{\frac{2}{3}}Y_{11}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix}=-\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\chi_{-1\frac{1}{2}\frac{1}{2}}(\hat{\mathbf{r}})$$

$$\chi_{1\frac{1}{2}-\frac{1}{2}}(\hat{\mathbf{r}})=-\sqrt{\frac{2}{3}}Y_{1-1}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix}+\sqrt{\frac{1}{3}}Y_{10}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix}=-\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\chi_{-1\frac{1}{2}-\frac{1}{2}}(\hat{\mathbf{r}})$$

The example showed the following results which can be proved more generally --

$$\left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

Also, recall -- --

$$\mathbf{p}\cdot\boldsymbol{\sigma} = \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\left(-i\hbar\frac{\partial}{\partial r} + \frac{i\boldsymbol{\sigma}\cdot\mathbf{L}}{r}\right)$$

Returning to our coupled equations:

$$\left(mc^2 + V(r) - E\right)g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) + \mathbf{p}\cdot\boldsymbol{\sigma}cif_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) = 0$$

$$\mathbf{p}\cdot\boldsymbol{\sigma}cg_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) + \left(-mc^2 + V(r) - E\right)if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) = 0$$

$$\left(\mathbf{p}\cdot\boldsymbol{\sigma}\right)cif_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) = \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\hbar c\left(\frac{\partial}{\partial r} + \frac{\kappa+1}{r}\right)f_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) = -\hbar c\left(\frac{\partial}{\partial r} + \frac{-\kappa+1}{r}\right)f_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})$$

$$\left(\mathbf{p}\cdot\boldsymbol{\sigma}\right)cg_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) = \left(\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\right)\hbar c\left(\frac{\partial}{\partial r} + \frac{\kappa+1}{r}\right)g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) = -\hbar c\left(\frac{\partial}{\partial r} + \frac{\kappa+1}{r}\right)g_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}})$$

Summary of results for the full Hamiltonian:

$$H=\begin{pmatrix} mc^2+V(r) & (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})^2(\mathbf{p}\cdot\boldsymbol{\sigma})c \\ (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})^2(\mathbf{p}\cdot\boldsymbol{\sigma})c & -mc^2+V(r) \end{pmatrix}$$

$$=\begin{pmatrix} mc^2+V(r) & (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})(\hat{\mathbf{r}}\cdot\mathbf{p}+i\boldsymbol{\sigma}\cdot\mathbf{L}/r)c \\ (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})(\hat{\mathbf{r}}\cdot\mathbf{p}+i\boldsymbol{\sigma}\cdot\mathbf{L}/r)c & -mc^2+V(r) \end{pmatrix}$$

Eigenvalue problem:

$$H\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}=E\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Coupled differential equations for radial functions:

$$\left(V(r)+mc^2-E\right)g_{E\kappa J}(r)=\hbar c\left(\frac{d}{dr}+\frac{-\kappa+1}{r}\right)f_{E\kappa J}(r)$$

$$\left(V(r)-mc^2-E\right)f_{E\kappa J}(r)=-\hbar c\left(\frac{d}{dr}+\frac{\kappa+1}{r}\right)g_{E\kappa J}(r)$$

Coupled differential equations for radial functions:

$$\left(V(r)+mc^2-E\right)g_{E\kappa J}(r)=\hbar c\left(\frac{d}{dr}+\frac{-\kappa+1}{r}\right)f_{E\kappa J}(r)$$

$$\left(V(r)-mc^2-E\right)f_{E\kappa J}(r)=-\hbar c\left(\frac{d}{dr}+\frac{\kappa+1}{r}\right)g_{E\kappa J}(r)$$

Let $g_{E\kappa J}(r)\equiv\frac{G_{E\kappa J}(r)}{r}$ and $f_{E\kappa J}(r)\equiv\frac{F_{E\kappa J}(r)}{r}$

Coupled differential equations for radial functions:

$$\left(V(r)+mc^2-E\right)G_{E\kappa J}(r)=\hbar c\left(\frac{d}{dr}+\frac{-\kappa}{r}\right)F_{E\kappa J}(r)$$

$$\left(V(r)-mc^2-E\right)F_{E\kappa J}(r)=-\hbar c\left(\frac{d}{dr}+\frac{\kappa}{r}\right)G_{E\kappa J}(r)$$

Digression – how are these equations related to non-relativistic limit?

Coupled differential equations for radial functions:

$$\left(V(r)+mc^2-E\right)G_{E\kappa J}(r)=\hbar c\left(\frac{d}{dr}+\frac{-\kappa}{r}\right)F_{E\kappa J}(r)$$

$$\left(V(r)-mc^2-E\right)F_{E\kappa J}(r)=-\hbar c\left(\frac{d}{dr}+\frac{\kappa}{r}\right)G_{E\kappa J}(r)$$

Shift energy to non-relativistic convention:

$$E^{NR}=E-mc^2$$

$$\left(V(r)-E^{NR}\right)G_{E\kappa J}(r)=\hbar c\left(\frac{d}{dr}+\frac{-\kappa}{r}\right)F_{E\kappa J}(r)$$

$$\left(V(r)-2mc^2-E^{NR}\right)F_{E\kappa J}(r)=-\hbar c\left(\frac{d}{dr}+\frac{\kappa}{r}\right)G_{E\kappa J}(r)$$

Non-relativistic connections -- continued

$$\left(V(r) - E^{NR}\right) G_{E\kappa J}(r) = \hbar c \left(\frac{d}{dr} + \frac{-\kappa}{r} \right) F_{E\kappa J}(r)$$

$$\left(V(r) - 2mc^2 - E^{NR}\right) F_{E\kappa J}(r) = -\hbar c \left(\frac{d}{dr} + \frac{\kappa}{r} \right) G_{E\kappa J}(r)$$

For $2mc^2 \gg V(r) - E^{NR}$:

$$F_{E\kappa J}(r) \approx \frac{\hbar c}{2mc^2} \left(\frac{d}{dr} + \frac{\kappa}{r} \right) G_{E\kappa J}(r)$$

$$\Rightarrow \left(V(r) - E^{NR}\right) G_{E\kappa J}(r) = \frac{\hbar^2 c^2}{2mc^2} \left(\frac{d}{dr} + \frac{-\kappa}{r} \right)\left(\frac{d}{dr} + \frac{\kappa}{r} \right) G_{E\kappa J}(r)$$

$$\left(-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r} \right) + V(r) \right) G_{E\kappa J}(r) = E^{NR} G_{E\kappa J}(r)$$

Non-relativistic connections -- continued

For $2mc^2 \gg V(r) - E^{NR}$:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r}\right) + V(r)\right) G_{E\kappa J}(r) \approx E^{NR} G_{E\kappa J}(r)$$

$$cF_{E\kappa J}(r) \approx \frac{\hbar}{2mc}\left(\frac{d}{dr} + \frac{\kappa}{r}\right) G_{E\kappa J}(r)$$

Note that $\frac{\hbar}{mc}$ has the units of length. In units of the Bohr radius:

$$a_0 = \frac{\hbar^2}{me^2} \qquad \frac{\hbar}{mca_0} = \frac{e^2}{\hbar c} \equiv \alpha \quad \text{(fine structure constant)}$$

$$\alpha = \frac{1}{137.035999084}$$

2/28/2022 lecture ran out of time at this slide.

Resuming analysis of solution of Dirac equation for H-like ion:

Analysis of radial solutions following J. J. Sakuri, Advanced Quantum Mechanics (1967)

Fine structure constant: $\alpha \equiv \frac{e^2}{\hbar c} \sim \frac{1}{137.035999}$

Let $\epsilon_1 \equiv \frac{mc^2 + E}{\hbar c} \qquad \epsilon_2 \equiv \frac{mc^2 - E}{\hbar c} \qquad \rho \equiv \sqrt{\epsilon_1 \epsilon_2}\, r$

Let $\quad g(r) = \mathcal{N} G(\rho)/\rho \qquad f(r) = \mathcal{N} F(\rho)/\rho$

$$\left(\frac{d}{d\rho} + \frac{\kappa}{\rho}\right) G(\rho) = \left(\sqrt{\frac{\epsilon_1}{\epsilon_2}} + \frac{Z\alpha}{\rho}\right) F(\rho)$$

$$\left(\frac{d}{d\rho} - \frac{\kappa}{\rho}\right) F(\rho) = \left(\sqrt{\frac{\epsilon_2}{\epsilon_1}} - \frac{Z\alpha}{\rho}\right) G(\rho)$$

Power series solutions in terms of unknowns s, C_n, D_n:

Assume $\quad G(\rho) = e^{-\rho} \rho^s \sum_{n=0}^{\infty} C_n \rho^n$

$$F(\rho) = e^{-\rho} \rho^s \sum_{n=0}^{\infty} D_n \rho^n$$

$$\left(\frac{d}{d\rho}+\frac{\kappa}{\rho}\right)G(\rho)=\left(\sqrt{\frac{\epsilon_1}{\epsilon_2}}+\frac{Z\alpha}{\rho}\right)F(\rho)$$

$$\left(\frac{d}{d\rho}-\frac{\kappa}{\rho}\right)F(\rho)=\left(\sqrt{\frac{\epsilon_2}{\epsilon_1}}-\frac{Z\alpha}{\rho}\right)G(\rho)$$

Assume $G(\rho)=e^{-\rho}\rho^s\sum_{n=0}^{\infty}C_n\rho^n$

$$F(\rho)=e^{-\rho}\rho^s\sum_{n=0}^{\infty}D_n\rho^n$$

Linear equations for determining s:

$$\begin{pmatrix} s+\kappa & -Z\alpha \\ Z\alpha & s-\kappa \end{pmatrix}\begin{pmatrix} C_0 \\ D_0 \end{pmatrix}=0 \qquad s=\pm\sqrt{\kappa^2-Z^2\alpha^2}$$

For physical solution, $s=\sqrt{\kappa^2-Z^2\alpha^2}$ $\qquad D_0=\frac{\kappa+\sqrt{\kappa^2-Z^2\alpha^2}}{Z\alpha}C_0$

More generally, the relationships between the coefficients are:

$$\begin{pmatrix} s+\kappa+n & -Z\alpha \\ Z\alpha & s-\kappa+n \end{pmatrix}\begin{pmatrix} C_n \\ D_n \end{pmatrix}=\begin{pmatrix} 1 & \sqrt{\frac{\epsilon_1}{\epsilon_2}} \\ \sqrt{\frac{\epsilon_2}{\epsilon_1}} & 1 \end{pmatrix}\begin{pmatrix} C_{n-1} \\ D_{n-1} \end{pmatrix}$$

Relationships between the coefficients:

$$\begin{pmatrix} s+\kappa+n & -Z\alpha \\ Z\alpha & s-\kappa+n \end{pmatrix}\begin{pmatrix} C_n \\ D_n \end{pmatrix} = \begin{pmatrix} 1 & \sqrt{\frac{\epsilon_1}{\epsilon_2}} \\ \sqrt{\frac{\epsilon_2}{\epsilon_1}} & 1 \end{pmatrix}\begin{pmatrix} C_{n-1} \\ D_{n-1} \end{pmatrix}$$

In order to satisfy boundary condition as $\rho \to \infty,$ the series has to truncate.

Condition for series truncating at $n = n'+1$:

$$\begin{pmatrix} s+\kappa+n'+1 & -Z\alpha \\ Z\alpha & s-\kappa+n'+1 \end{pmatrix}\begin{pmatrix} C_{n'+1} \\ D_{n'+1} \end{pmatrix} = 0$$

$$\begin{pmatrix} 1 & \sqrt{\frac{\epsilon_1}{\epsilon_2}} \\ \sqrt{\frac{\epsilon_2}{\epsilon_1}} & 1 \end{pmatrix}\begin{pmatrix} C_{n'} \\ D_{n'} \end{pmatrix} = 0 \qquad \Rightarrow C_{n'} = -\sqrt{\frac{\epsilon_1}{\epsilon_2}} D_{n'}$$

Further conditions for this case:

$$2\sqrt{\epsilon_1\epsilon_2}\left(s+n'\right) = Z\alpha\left(\epsilon_1 - \epsilon_2\right)$$

Continued analysis of this case:

$$2\sqrt{\epsilon_1\epsilon_2}\left(s+n'\right)=Z\alpha\left(\epsilon_1-\epsilon_2\right)$$

Recall: $\epsilon_1 \equiv \frac{mc^2+E}{\hbar c} \qquad \epsilon_2 \equiv \frac{mc^2-E}{\hbar c}$

$$s=\sqrt{\kappa^2-Z^2\alpha^2}$$

Bound state energy eigenvalues:

$$E=\frac{mc^2}{\sqrt{1+\frac{Z^2\alpha^2}{\left(\sqrt{\kappa^2-Z^2\alpha^2}+n'\right)^2}}} \quad \text{where } n'=0,1,2..$$

A more convenient accounting defines the principal quantum number n:

$$n'=n-|\kappa|=n-\left(J+\tfrac{1}{2}\right) \qquad n=\left(J+\tfrac{1}{2}\right),\left(J+\tfrac{1}{2}+1\right),\left(J+\tfrac{1}{2}+2\right)....$$

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

Exact solution of Dirac equation for H-like ion:

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

for $n = \left(J+\frac{1}{2}\right), \left(J+\frac{1}{2}+1\right), \left(J+\frac{1}{2}+2\right), \ldots$

Dirac equation for electron in the field of a H-like ion

Comparison with Schrödinger equation --

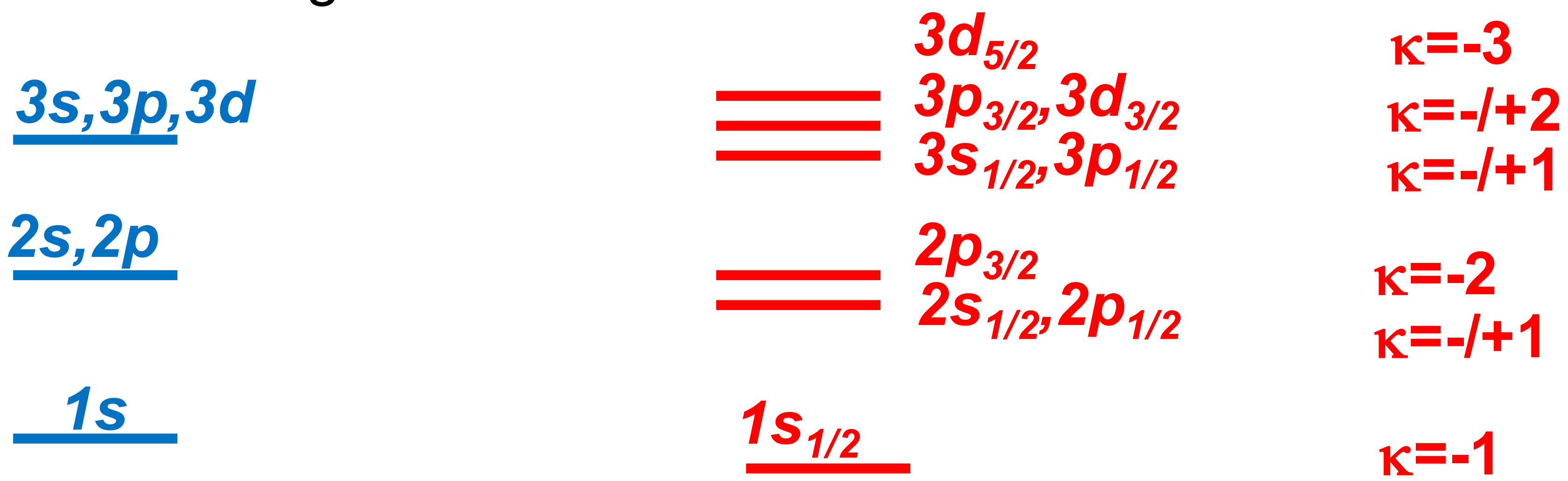
Schrödinger equation

$$E_n^{Sch} = -\frac{Z^2\alpha^2 mc^2}{2n^2}$$

Dirac equation

$$E_n^{Dir} - mc^2 \approx -\frac{Z^2\alpha^2 mc^2}{2n^2}\left(1 + \frac{Z^2\alpha^2}{n}\left(\frac{1}{J+\frac{1}{2}} - \frac{3}{4n}\right)....\right)$$

Schematic diagram:



Some details

Exact solution of Dirac equation for H-like ion:

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

for $n = 1$ and $J = \frac{1}{2}$:

$$E_1 = mc^2\sqrt{1 - Z^2\alpha^2}$$

More details about ground state of H-like ion from Dirac equation

$$n=1 \quad J=\tfrac{1}{2} \qquad \kappa=-1$$

$$E_1 = mc^2\sqrt{1-Z^2\alpha^2} \qquad s=\sqrt{1-Z^2\alpha^2} \qquad \sqrt{\epsilon_1\epsilon_2}=\frac{Z\alpha mc^2}{\hbar c}=\frac{Z}{a_0}$$

$$\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \mathcal{N}\left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0} r^{s-1} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ i\frac{D_0}{C_0}(\boldsymbol{\sigma}\cdot\hat{\mathbf{r}})\begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix}$$

$$\text{where } \frac{D_0}{C_0}=\frac{1-s}{Z\alpha} \qquad \text{Degenerate with } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

More general treatment of bound states of Fermi particle within spherical potential *V(r)*

$$H = \begin{pmatrix} mc^2 + V(r) & \mathbf{p}\cdot\boldsymbol{\sigma}c \\ \mathbf{p}\cdot\boldsymbol{\sigma}c & -mc^2 + V(r) \end{pmatrix}$$

Eigenvalue problem:

$$H\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix} = E\begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Coupled differential equations for radial functions:

$$\left(V(r) + mc^2 - E\right) g_{E\kappa J}(r) = \hbar c\left(\frac{d}{dr} + \frac{-\kappa+1}{r}\right) f_{E\kappa J}(r)$$

$$\left(V(r) - mc^2 - E\right) f_{E\kappa J}(r) = -\hbar c\left(\frac{d}{dr} + \frac{\kappa+1}{r}\right) g_{E\kappa J}(r)$$

Practical solution of radial portions of Dirac equation

$$\left(V(r) + mc^2 - E\right) g_{E\kappa J}(r) = \hbar c \left(\frac{d}{dr} + \frac{-\kappa + 1}{r} \right) f_{E\kappa J}(r)$$

$$\left(V(r) - mc^2 - E\right) f_{E\kappa J}(r) = -\hbar c \left(\frac{d}{dr} + \frac{\kappa + 1}{r} \right) g_{E\kappa J}(r)$$

Let $g_{E\kappa J}(r) = G_{E\kappa J}(r) / r$ and $f_{E\kappa J}(r) = F_{E\kappa J}(r) / r$

$$\left(\frac{d}{dr} + \frac{\kappa}{r} \right) G_{E\kappa J}(r) = \frac{1}{\hbar c} \left(E + mc^2 - V(r) \right) F_{E\kappa J}(r)$$

$$\left(\frac{d}{dr} - \frac{\kappa}{r} \right) F_{E\kappa J}(r) = -\frac{1}{\hbar c} \left(E - mc^2 - V(r) \right) G_{E\kappa J}(r)$$