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

Plan for Lecture 19:

Chap. 16 in Professor Carlson's text:

The Dirac equation for a hydrogen-like ion

1. Solution of the analytic radial wave functions
2. 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 3/4/2022

Dirac equation for electron in the field of a nucleus with atomic number Z --

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

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:

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

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

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: $$H\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}=E\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$

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

Coupled differential equations for radial functions:

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

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

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

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

Note that: $\hat{\mathbf{r}} \cdot \boldsymbol{\sigma} = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix}$ and $\left(\hat{\mathbf{r}} \cdot \boldsymbol{\sigma}\right) \chi_{\kappa JM}(\hat{\mathbf{r}}) = -\chi_{-\kappa JM}(\hat{\mathbf{r}})$

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

Coupled differential equations for modified radial functions:

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

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

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: $\alpha \equiv \frac{e^2}{\hbar c} \sim \frac{1}{137.035999084}$

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

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

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

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:

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

Some details: Let $n = n'$

$$\begin{pmatrix} (s+\kappa+n')\sqrt{\epsilon_1\epsilon_2} & -Z\alpha\sqrt{\epsilon_1\epsilon_2} \\ Z\alpha\epsilon_1 & (s-\kappa+n')\epsilon_1 \end{pmatrix}\begin{pmatrix} C_{n'} \\ D_{n'} \end{pmatrix} = \begin{pmatrix} \sqrt{\epsilon_1\epsilon_2} & \epsilon_1 \\ \sqrt{\epsilon_1\epsilon_2} & \epsilon_1 \end{pmatrix}\begin{pmatrix} C_{n'-1} \\ D_{n'-1} \end{pmatrix}$$

$$\Rightarrow \left((s+\kappa+n')\sqrt{\epsilon_1\epsilon_2} - Z\alpha\epsilon_1\right)C_{n'} - \left((s-\kappa+n')\epsilon_1 + Z\alpha\sqrt{\epsilon_1\epsilon_2}\right)D_{n'} = 0$$

Note that: $C_{n'} = -\sqrt{\frac{\epsilon_1}{\epsilon_2}}D_{n'}$

$$\left(-(s+\kappa+n')\epsilon_1 + Z\alpha\epsilon_1\sqrt{\frac{\epsilon_1}{\epsilon_2}}\right) - \left((s-\kappa+n')\epsilon_1 + Z\alpha\sqrt{\epsilon_1\epsilon_2}\right) = 0$$

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

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:

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

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 --

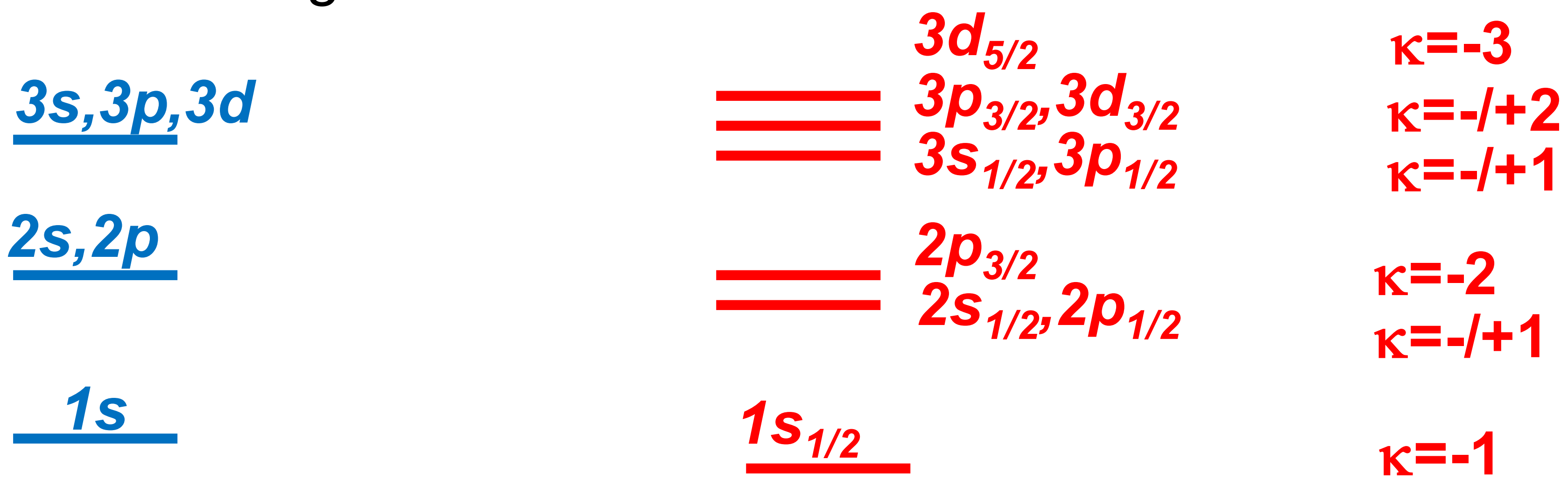
Schrödinger equation

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

Dirac equation

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

Schematic diagram:



Some details

Exact solution of Dirac equation for H-like ion:

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

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

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

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

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

$$\text{where } \frac{D_0}{C_0} = \frac{1 - \sqrt{1 - (Z\alpha)^2}}{Z\alpha} \qquad \text{Degenerate with } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Normalization: $\langle \Psi(\mathbf{r}) | \Psi(\mathbf{r}) \rangle = 1$

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

$$\mathcal{N}^2 4\pi \frac{Z^3}{\pi a_0^3} \left(1 + \left(\frac{1-\sqrt{1-(Z\alpha)^2}}{Z\alpha} \right)^2 \right) \int dr\ r^2 \left(\frac{Zr}{a_0} \right)^{2\sqrt{1-(Z\alpha)^2}-2} e^{-2Zr/a_0} = 1$$

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 $f_{E\kappa J}(r)=F_{E\kappa J}(r)/r$

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

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

Coupled radial equations, can be solved numerically