**PHY 741 Quantum Mechanics**
**12-12:50 AM MWF Olin 103**

**Plan for Lecture 34:**

**Chap. 20 in Shankar: The Dirac equation for a hydrogen atom**

1. **Angular and spin components**
2. **Radial components**
3. **Comparison with non-relativistic results**



| | | | | | |
|---|---|---|---|---|---|
| 22 | Mon, 10/23/2017 | Chap. 15 | Multi-electron atoms | #13 | 10/25/2017 |
| 23 | Wed, 10/25/2017 | Chap. 15 | Multi-electron atoms | #14 | 10/30/2017 |
| 24 | Fri, 10/27/2017 | | Effects of nuclear motion | | |
| 25 | Mon, 10/30/2017 | Chap. 17 | Time-independent perturbation theory | #15 | 11/3/2017 |
| 26 | Wed, 11/01/2017 | Chap. 17 | Time-independent perturbation theory | | |
| 27 | Fri, 11/03/2017 | | Effects of a static magnetic field | | |
| 28 | Mon, 11/06/2017 | Chap. 18 | Time-dependent perturbation theory | #16 | 11/10/2017 |
| 29 | Wed, 11/08/2017 | Chap. 18 | Time-dependent perturbation theory | | |
| 30 | Fri, 11/10/2017 | Chap. 19 | Scattering theory | #17 | 11/15/2017 |
| | Mon, 11/13/2017 | | *Class cancelled* | | |
| 31 | Wed, 11/15/2017 | Chap. 19 | Scattering theory | | |
| 32 | Fri, 11/17/2017 | Chap. 20 | Dirac Equation | | |
| 33 | Mon, 11/20/2017 | Chap. 20 | Dirac Equation | | |
| | Wed, 11/22/2017 | | *Thanksgiving Holiday -- No class* | | |
| | Fri, 11/24/2017 | | *Thanksgiving Holiday -- No class* | | |
| 34 | Mon, 11/27/2017 | Chap. 20 | Dirac Equation | | |
| 35 | Wed, 11/29/2017 | Chap. 20 | Dirac Equation | | |
| 36 | Fri, 12/01/2017 | Chap. 1-20 | Review | | |
| | Mon, 12/04/2017 | | Presentations I | | |
| | Wed, 12/06/2017 | | Presentations II | | |
| | Fri, 12/08/2017 | | Presentations III | | |



Schedule for PHY 741 presentations

Monday Dec. 4, 2017

| Time | Presenter | Title |
|---|---|---|
| 12:00-12:15 PM | TJ Colvin | |
| 12:17-12:32 PM | Sajant Anand anans14@ | Numerical Simulations of a Quantum Particle in a Box |
| 12:34-12:49 PM | | |

Wednesday Dec. 6, 2017

| Time | Presenter | Title |
|---|---|---|
| 12:00-12:15 PM | Haardik Pandey | |
| 12:1712:32 PM | Yan Li | Numerical solutions for a finite square well problem |
| 12:34-12:49 PM | Ellie Alipour | |

Friday Dec. 8, 2017

| Time | Presenter | Title |
|---|---|---|
| 12:00-12:15 PM | Kevin Roebuck | Spin splitting of open shell atoms in a magnetic field |
| 12:17-12:32 PM | Matthew Waldrip | IR spectra of ____ |
| 12:34-12:49 PM | Nouf Alharbi | |

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:

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

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



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

$$K\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} \boldsymbol{\sigma}\cdot\mathbf{L}+\hbar I_2 & 0 \\ 0 & -\boldsymbol{\sigma}\cdot\mathbf{L}-\hbar I_2 \end{pmatrix}\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix}$$
$$= -\hbar\kappa\begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} -\hbar\kappa\varphi^U(\mathbf{r}) \\ +\hbar\kappa\varphi^L(\mathbf{r}) \end{pmatrix}$$
$$\Rightarrow \begin{pmatrix} \varphi^U(\mathbf{r}) \\ \varphi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{E\kappa J}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Possibilities:

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

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 $\kappa$ value is identified with $\varphi^U$.

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

Combinations:

| $\kappa$ | $j$ | $l$ |
|---|---|---|
| $\kappa=-1$ | $j=\frac{1}{2}$ | $l=0$ |
| $+1$ | $\frac{1}{2}$ | 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:

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

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



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

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

$$\Rightarrow (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})\left(\hat{\mathbf{r}}\cdot\mathbf{p} + \frac{i\boldsymbol{\sigma}\cdot\mathbf{L}}{r}\right)h_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})$$
$$= (\hat{\mathbf{r}}\cdot\boldsymbol{\sigma})\left(-i\hbar\frac{\partial}{\partial r} - i\hbar\frac{(\kappa+1)}{r}\right)h_{E\kappa J}(r)\chi_{\kappa JM}(\hat{\mathbf{r}})$$

It can also be shown that:

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

Further consideration of 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:

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

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

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

Fine structure constant: $\alpha\equiv\frac{e^2}{\hbar c}\sim\frac{1}{137.035999139}$

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

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

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

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

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

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

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



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

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

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

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

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 $\rho \rightarrow \infty$, 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:

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



Continued analysis of this case:

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

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

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

Bound state energy eigenvalues:

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

A more convenient accounting defines the principal quantum number $n$:

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

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



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

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

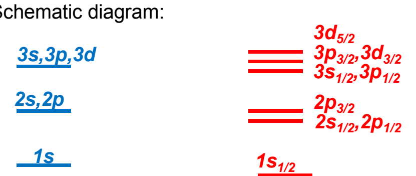
Schroedinger equation

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

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

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

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

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

where $\frac{D_0}{C_0}=\frac{1-s}{Z\alpha}$ 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 $f_{E\kappa J}(r)=F_{E\kappa J}(r)/r$

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

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