

PHY 742 Quantum Mechanics
1:00-1:50 AM MWF Olin 103

Plan for Lecture 16:

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**

2/19/2020 PHY 742 Spring 2020 -- Lecture 16 1

1

10	Wed: 02/05/2020	Chap. 2.6	H ₂ ⁺ molecular ion: Born Oppenheimer approximation	#10	02/12/2020
11	Fri: 02/07/2020	Chap. 15	Time-dependent perturbations	#11	02/14/2020
12	Mon: 02/10/2020	Chap. 15	Time-dependent perturbations	#12	02/14/2020
13	Wed: 02/12/2020	Chap. 15	Time-dependent perturbations	#13	02/17/2020
14	Fri: 02/14/2020	Chap. 16	The Dirac equation		
15	Mon: 02/17/2020	Chap. 16	The Dirac equation	#14	02/19/2020
16	Wed: 02/19/2020	Chap. 16	The Dirac equation	#15	02/21/2020
17	Fri: 02/21/2020				
18	Mon: 02/24/2020				
19	Wed: 02/26/2020				
20	Fri: 02/28/2020				
	Mon: 03/02/2020	No class	APS March Meeting		Take Home Exam
	Wed: 03/04/2020	No class	APS March Meeting		Take Home Exam
	Fri: 03/06/2020	No class	APS March Meeting		Take Home Exam
	Mon: 03/09/2020	No class	Spring Break		
	Wed: 03/11/2020	No class	Spring Break		
	Fri: 03/13/2020	No class	Spring Break		
21	Mon: 03/16/2020				
22	Wed: 03/18/2020				

2/19/2020 PHY 742 Spring 2020 -- Lecture 16 2

2

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:

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

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

2/19/2020 PHY 742 Spring 2020 -- Lecture 16 3

3

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:

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

4

4

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:

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

5

5

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:

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

More details about spin-angular functions:

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

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

6

6

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

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

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

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

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

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 7

7

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

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

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

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

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

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

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 8

8

More relationships between the operators

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

Relationships between the upper and lower component functions:

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

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

Algebraic relations --

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

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 9

9

Summary of allowed combinations of eigenvalues

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

Alternatively

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 10

10

Dirac equation for electron in the field of a H-like ion -- continued
 Note that for stationary state solutions to the Dirac equation
 $H\Psi_{EKJM} = E\Psi_{EKJM}$, the κ value is identified with ϕ^U .

$$\Psi_{EKJM} = \begin{pmatrix} \phi^U(\mathbf{r}) \\ \phi^L(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} g_{EKJ}(r)\chi_{\kappa JM}(\hat{\mathbf{r}}) \\ if_{EKJ}(r)\chi_{-\kappa JM}(\hat{\mathbf{r}}) \end{pmatrix}$$

Combinations:

$\kappa = -1$	$J = \frac{1}{2}$	$l_U = 0$	Possibilities:
+1	$\frac{1}{2}$	1	$J = l + \frac{1}{2} \quad \kappa = -l - 1 = -(J + \frac{1}{2})$
-2	$\frac{3}{2}$	1	$J = l - \frac{1}{2} \quad \kappa = l = (J + \frac{1}{2})$
+2	$\frac{5}{2}$	2	
-3	$\frac{7}{2}$	2	
+3	$\frac{9}{2}$	3	

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 11

11

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

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

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

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

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

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 12

12

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

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

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:

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

13

13

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:

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

Coupled differential equations for radial functions:

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

14

14

Coupled differential equations for radial functions:

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

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

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:

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

15

15

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

Coupled differential equations for radial functions:

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

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

Shift energy to non-relativistic convention:

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

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

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

2/19/2020

PHY 742, Spring 2020 – Lecture 16

16

16

Non-relativistic connections -- continued

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

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

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

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

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

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

2/19/2020

PHY 742, Spring 2020 – Lecture 16

17

17

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:

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

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

2/19/2020

PHY 742, Spring 2020 – Lecture 16

18

18

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

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

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

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

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

19

19

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

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

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

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

Linear equations for determining s :

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

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:

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

20

20

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 $n = n' + 1$:

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

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

Further conditions for this case:

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

21

21

Continued analysis of this case:

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

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

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

Bound state energy eigenvalues:

$$E = \frac{mc^2}{\sqrt{1 + \frac{Z^2\alpha^2}{(\kappa^2 - Z^2\alpha^2 + n'^2)}}}$$

where $n' = 0, 1, 2, \dots$

A more convenient accounting defines the principal quantum number n :

$$n' = n - |\kappa| = n - (J + \frac{1}{2}) \quad n = (J + \frac{1}{2}), (J + \frac{1}{2} + 1), (J + \frac{1}{2} + 2), \dots$$

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

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 22

22

Exact solution of Dirac equation for H-like ion:

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

for $n = (J + \frac{1}{2}), (J + \frac{1}{2} + 1), (J + \frac{1}{2} + 2), \dots$

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 23

23

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

Schroedinger equation Dirac equation

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

Schematic diagram:

<u>3s, 3p, 3d</u>	<u>3d_{5/2}</u>	$\kappa = -3$
	<u>3p_{3/2}, 3d_{3/2}</u>	$\kappa = -/+2$
	<u>3s_{1/2}, 3p_{1/2}</u>	$\kappa = -/+1$
<u>2s, 2p</u>	<u>2p_{3/2}</u>	$\kappa = -2$
	<u>2s_{1/2}, 2p_{1/2}</u>	$\kappa = -/+1$
<u>1s</u>	<u>1s_{1/2}</u>	$\kappa = -1$

2/19/2020 PHY 742, Spring 2020 -- Lecture 16 24

24

Some details

Exact solution of Dirac equation for H-like ion:

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

25

25

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

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

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

26

26

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:

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

Coupled differential equations for radial functions:

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

27

27

Practical solution of radial portions of Dirac equation

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

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

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

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

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

2/19/2020

PHY 742, Spring 2020 -- Lecture 16

28

28
