

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

Plan for Lecture 15:
The Dirac equation

Chap. 16 in Professor Carlson's textbook:

- 1. Dirac equation for a free particle**
- 2. Dirac equation for a hydrogen atom**


2/17/2020 PHY 742: Spring 2020 -- Lecture 15 1

1

8	Fri: 01/31/2020	Chap. 12	Variational and other approximation methods	#8	02/07/2020
9	Mon: 02/03/2020	Chap. 2.6	Single particle states of molecules and solids	#9	02/10/2020
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				
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		

2/17/2020 PHY 742: Spring 2020 -- Lecture 15 2

2



P. A. M Dirac 1902-1984
 Won Nobel Prize in Physics in 1933 together with Erwin Schrödinger

The quantum theory of the electron

Paul Adrien Maurice Dirac
 Published: 01 February 1928
<https://doi.org/10.1098/rspa.1928.0023>

PROCEEDINGS OF THE ROYAL SOCIETY A
 MATHEMATICAL, PHYSICAL AND ENGINEERING SCIENCES

2/17/2020 PHY 742: Spring 2020 -- Lecture 15 3

3

Energy \leftrightarrow Momentum relationships in classical and quantum mechanics
Focusing on treatment of Fermi particles

	Non-relativistic mechanics	Relativistic mechanics
Classical	$E = \frac{\mathbf{p}^2}{2m}$	$E^2 - \mathbf{p}^2 c^2 = (mc^2)^2$ \Downarrow (with some license)
Quantum	$i\hbar \frac{\partial}{\partial t} \Psi = H\Psi$	$(E - \mathbf{p} \cdot \boldsymbol{\sigma} c)(E + \mathbf{p} \cdot \boldsymbol{\sigma} c) = (mc^2)^2$ \Downarrow $\left(i\hbar \frac{\partial}{\partial t} - \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi = (mc^2)^2 \Psi$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 4

4

Relativistic relationships – continued
Ref: J. J. Sakurai, Advanced Quantum Mechanics

$$\left(i\hbar \frac{\partial}{\partial t} - \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi = (mc^2)^2 \Psi$$

Let $\left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi \equiv mc^2 \Psi^R \quad \Psi \equiv \Psi^L$

Factored equations:

$$\left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi^L = mc^2 \Psi^R$$

$$\left(i\hbar \frac{\partial}{\partial t} - \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi^R = mc^2 \Psi^L$$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 5

5

Relativistic relationships – continued
Ref: J. J. Sakurai, Advanced Quantum Mechanics

Factored equations:

$$\left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi^L = mc^2 \Psi^R$$

$$\left(i\hbar \frac{\partial}{\partial t} - \mathbf{p} \cdot \boldsymbol{\sigma} c \right) \Psi^R = mc^2 \Psi^L$$

Dirac's rearrangement: $\varphi^U = \Psi^R + \Psi^L$
 $\varphi^L = \Psi^R - \Psi^L$

$$\begin{pmatrix} i\hbar \frac{\partial}{\partial t} & -\mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -i\hbar \frac{\partial}{\partial t} \end{pmatrix} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = mc^2 \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 6

6

Relativistic relationships – continued

$$\begin{pmatrix} i\hbar \frac{\partial}{\partial t} & -\mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -i\hbar \frac{\partial}{\partial t} \end{pmatrix} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = mc^2 \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

Further rearrangements:

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = \begin{pmatrix} mc^2 & \mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -mc^2 \end{pmatrix} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

$$\Downarrow$$

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

2/17/2020

PHY 742, Spring 2020 – Lecture 15

7

7

Four component wavefunction of free Fermi particle

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = \begin{pmatrix} mc^2 & \mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -mc^2 \end{pmatrix} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

$$\text{Assume } \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = \begin{pmatrix} \chi^U(\mathbf{k}) \\ \chi^L(\mathbf{k}) \end{pmatrix} e^{i\mathbf{k}\cdot\mathbf{r} - iEt/\hbar}$$

$$\Rightarrow \chi^U(\mathbf{k}) = \frac{\hbar\mathbf{k} \cdot \boldsymbol{\sigma} c}{E - mc^2} \chi^L(\mathbf{k})$$

$$\chi^L(\mathbf{k}) = \frac{\hbar\mathbf{k} \cdot \boldsymbol{\sigma} c}{E + mc^2} \chi^U(\mathbf{k})$$

$$E^2 = \hbar^2 c^2 \mathbf{k}^2 + m^2 c^4$$

$$E = \pm \sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$$

2/17/2020

PHY 742, Spring 2020 – Lecture 15

8

8

$$\text{Pauli matrices: } \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathbf{k} \cdot \boldsymbol{\sigma} = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix} \quad \text{Define: } k_{\pm} \equiv k_x \pm ik_y$$

$$\chi^U(\mathbf{k}) = \frac{\hbar\mathbf{k} \cdot \boldsymbol{\sigma} c}{E - mc^2} \chi^L(\mathbf{k}) \quad \chi^L(\mathbf{k}) = \frac{\hbar\mathbf{k} \cdot \boldsymbol{\sigma} c}{E + mc^2} \chi^U(\mathbf{k})$$

$$\text{Positive energy solutions: } E = \sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$$

$$\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi^L_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} \quad \kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E + mc^2}$$

$$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \chi^L_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_+ \end{pmatrix} \quad \kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E + mc^2}$$

2/17/2020

PHY 742, Spring 2020 – Lecture 15

9

9

Pauli matrices: $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\mathbf{k} \cdot \boldsymbol{\sigma} = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix}$ Define: $k_{\pm} \equiv k_x \pm ik_y$

$\chi^U(\mathbf{k}) = \frac{\hbar \mathbf{k} \cdot \boldsymbol{\sigma} c}{E - mc^2} \chi^L(\mathbf{k})$ $\chi^L(\mathbf{k}) = \frac{\hbar \mathbf{k} \cdot \boldsymbol{\sigma} c}{E + mc^2} \chi^U(\mathbf{k})$

Negative energy solutions: $E = -\sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$

$\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_+ \\ \kappa_- \end{pmatrix}$ $\chi^L_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E - mc^2} = -\frac{\hbar k_{\pm} c}{|E| + mc^2}$

$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_+ \end{pmatrix}$ $\chi^L_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E - mc^2} = -\frac{\hbar k_{\pm} c}{|E| + mc^2}$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 10

10

What does this all mean?

Positive energy solutions: $E = \sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$

$\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\chi^L_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_+ \\ \kappa_- \end{pmatrix}$ $\kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E + mc^2}$

$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\chi^L_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_+ \end{pmatrix}$ $\kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E + mc^2}$

For $\hbar c|\mathbf{k}| \ll mc^2$ $E \approx mc^2 + \frac{\hbar^2 |\mathbf{k}|^2}{2m}$

$\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\chi^L_{\uparrow}(\mathbf{k}) \approx \mathcal{N} \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\chi^L_{\downarrow}(\mathbf{k}) \approx \mathcal{N} \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 11

11

Dirac equation for free particles – slightly more convenient notation

mc^2 $E = \sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$ $\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\chi^L_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \tilde{\kappa}_+ \\ \tilde{\kappa}_- \end{pmatrix}$ $\tilde{\kappa}_{\pm} \equiv \frac{\hbar k_{\pm} c}{|E| + mc^2}$

$-mc^2$ $E = -\sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4}$ $\chi^U_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} -\tilde{\kappa}_+ \\ -\tilde{\kappa}_- \end{pmatrix}$ $\chi^L_{\uparrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\tilde{\kappa}_{\pm} \equiv \frac{\hbar k_{\pm} c}{|E| + mc^2}$

$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ $\chi^L_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \tilde{\kappa}_- \\ -\tilde{\kappa}_+ \end{pmatrix}$

$\chi^U_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} -\tilde{\kappa}_- \\ \tilde{\kappa}_+ \end{pmatrix}$ $\chi^L_{\downarrow}(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

For free particle, $E>0$ and $E<0$ solutions represent distinct physical situations.

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 12

12

Dirac equation for a free particle

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = \begin{pmatrix} mc^2 & \mathbf{p} \cdot \boldsymbol{\sigma} c \\ \mathbf{p} \cdot \boldsymbol{\sigma} c & -mc^2 \end{pmatrix} \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

$$\Downarrow$$

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

Other convenient notations in terms of 4×4 matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad H = \mathbf{p} \cdot \boldsymbol{\alpha} c + mc^2 \boldsymbol{\beta}$$

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

13

13

Dirac equation for Fermi particle in a scalar potential field

For free particle: $H = \mathbf{p} \cdot \boldsymbol{\alpha} c + mc^2 \boldsymbol{\beta}$ where: $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ and where:

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

Dirac's suggestion for representing a scalar potential field:

$$H = \mathbf{p} \cdot \boldsymbol{\alpha} c + mc^2 \boldsymbol{\beta} + V(\mathbf{r}) I_4 \quad \text{where } I_4 = \begin{pmatrix} I_2 & 0 \\ 0 & I_2 \end{pmatrix}$$

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

14

14

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

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

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:

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

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

15

15

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

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

In order to find an efficient functional form for the eigenfunctions, it is helpful to determine the constants of the motion:

Total angular momentum: $\mathbf{J} = \mathbf{L} + \frac{\hbar}{2} \boldsymbol{\sigma}$ in terms of J_z and \mathbf{J}^2

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

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 16

16

Digression – useful identity for operator vectors \mathbf{A} and \mathbf{B}

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

$$\begin{pmatrix} A_z & A_x - iA_y \\ A_x + iA_y & -A_z \end{pmatrix} \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix} = \begin{pmatrix} \mathbf{A} \cdot \mathbf{B} + iC_z & iC_x + C_y \\ iC_x - C_y & \mathbf{A} \cdot \mathbf{B} - iC_z \end{pmatrix}$$

where

$\mathbf{A} \cdot \mathbf{B} = A_x B_x + A_y B_y + A_z B_z$ and $\mathbf{C} = \mathbf{A} \times \mathbf{B}$

$C_x = A_y B_z - A_z B_y$ $C_y = A_z B_x - A_x B_z$ $C_z = A_x B_y - A_y B_x$

Note that: $\frac{(\boldsymbol{\sigma} \cdot \mathbf{r})(\boldsymbol{\sigma} \cdot \mathbf{r})}{r^2} = I_2$

It follows that: $(\boldsymbol{\sigma} \cdot \mathbf{r})(\boldsymbol{\sigma} \cdot \mathbf{p}) = \frac{(\boldsymbol{\sigma} \cdot \mathbf{r})}{r^2} (\boldsymbol{\sigma} \cdot \mathbf{r})(\boldsymbol{\sigma} \cdot \mathbf{p}) = \frac{(\boldsymbol{\sigma} \cdot \mathbf{r})}{r^2} \left(-i\hbar r \frac{\partial}{\partial r} + i\boldsymbol{\sigma} \cdot \mathbf{L} \right)$

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 17

17

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

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

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

$$\mathbf{J}^2 = \begin{pmatrix} (\mathbf{L} + \frac{1}{2} \hbar \boldsymbol{\sigma})^2 & 0 \\ 0 & (\mathbf{L} + \frac{1}{2} \hbar \boldsymbol{\sigma})^2 \end{pmatrix} = \begin{pmatrix} L^2 + \frac{3\hbar^2}{4} I_2 + \hbar \boldsymbol{\sigma} \cdot \mathbf{L} & 0 \\ 0 & L^2 + \frac{3\hbar^2}{4} I_2 + \hbar \boldsymbol{\sigma} \cdot \mathbf{L} \end{pmatrix}$$

$$K = \begin{pmatrix} \boldsymbol{\sigma} \cdot \mathbf{L} + \hbar I_2 & 0 \\ 0 & -\boldsymbol{\sigma} \cdot \mathbf{L} - \hbar I_2 \end{pmatrix} \quad \text{Note that: } K^2 = \mathbf{J}^2 + \frac{1}{4} \hbar^2$$

Commutation relations:

$[H, \mathbf{J}^2] = 0$ $[K, \mathbf{J}^2] = 0$ $[K, J_z] = 0$ $[H, K] = 0$, etc.

2/17/2020 PHY 742, Spring 2020 -- Lecture 15 18

18

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 : $|JM\rangle$

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

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

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

19

19

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

Eigenvalues of K operator:

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

$$K \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = -\hbar \kappa \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

$$K^2 \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix} = \hbar^2 \left(J + \frac{1}{2} \right)^2 \begin{pmatrix} \varphi^U \\ \varphi^L \end{pmatrix}$$

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

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

20

20

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:

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

$$(\boldsymbol{\sigma} \cdot \mathbf{L} + \hbar) \varphi^U = -\kappa \varphi^U \quad \text{and} \quad (\boldsymbol{\sigma} \cdot \mathbf{L} + \hbar) \varphi^L = \kappa \varphi^L$$

After some algebra --

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

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

21

21

Summary of allowed combinations of eigenvalues

$$\begin{array}{ccc} & l_U & l_L \\ \kappa = -\left(j + \frac{1}{2}\right) & j - \frac{1}{2} & j + \frac{1}{2} \\ \kappa = +\left(j + \frac{1}{2}\right) & j + \frac{1}{2} & j - \frac{1}{2} \end{array}$$

Alternatively

$$\begin{array}{ccc} & j & l_L \\ \kappa = -(l_U + 1) & l_U + \frac{1}{2} & l_U + 1 \\ \kappa = +l_U & l_U - \frac{1}{2} & l_U - 1 \end{array}$$

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

22

22

Addition of angular momentum - orbital angular momentum and spin angular momentum

Clebsch-Gordon coefficients

$$|JM, j_1 j_2\rangle = \sum_{m_1, m_2} |j_1 m_1, j_2 m_2\rangle \langle j_1 m_1, j_2 m_2 | JM, j_1 j_2\rangle$$

$$j_1 m_1 \Rightarrow l m_l \quad J = l + \frac{1}{2}$$

$$j_2 m_2 \Rightarrow \frac{1}{2} m_s \quad \text{or } J = l - \frac{1}{2}$$

Clebsch-Gordon coefficients for this case:

$$j_1 = l \quad j_2 = s = \frac{1}{2}$$

$$|(l + \frac{1}{2})M; l \frac{1}{2}\rangle = \sqrt{\frac{l+M+\frac{1}{2}}{2l+1}} |l(M-\frac{1}{2}); \frac{1}{2} \frac{1}{2}\rangle + \sqrt{\frac{l-M+\frac{1}{2}}{2l+1}} |l(M+\frac{1}{2}); \frac{1}{2} -\frac{1}{2}\rangle$$

$$|(l - \frac{1}{2})M; l \frac{1}{2}\rangle = -\sqrt{\frac{l-M+\frac{1}{2}}{2l+1}} |l(M-\frac{1}{2}); \frac{1}{2} \frac{1}{2}\rangle + \sqrt{\frac{l+M+\frac{1}{2}}{2l+1}} |l(M+\frac{1}{2}); \frac{1}{2} -\frac{1}{2}\rangle$$

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

23

23

Another representation of the spin-angular function in terms of spherical harmonic functions and eigenvectors of σ_z

$$|(l + \frac{1}{2})M; l \frac{1}{2}\rangle = \sqrt{\frac{l+M+\frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l-M+\frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|(l - \frac{1}{2})M; l \frac{1}{2}\rangle = -\sqrt{\frac{l-M+\frac{1}{2}}{2l+1}} Y_{l(M-\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \sqrt{\frac{l+M+\frac{1}{2}}{2l+1}} Y_{l(M+\frac{1}{2})}(\hat{\mathbf{r}}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

24

24

Consider: $(\boldsymbol{\sigma} \cdot \mathbf{L} + \hbar l_2) |JM; l \frac{1}{2}\rangle = \hbar(J(J+1) - l(l+1) + \frac{1}{4}) |JM; l \frac{1}{2}\rangle$
 $= -\kappa |JM; l \frac{1}{2}\rangle$

Possibilities:

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

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

Combinations:

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

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

25

25

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

Next time, we will show that the coupled radial equations take the form:

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

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

Question:

- How do these results reduce to the Schrodinger equation in the non-relativistic limit
- What new physics is contained more generally?

2/17/2020

PHY 742, Spring 2020 -- Lecture 15

26

26
