

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

Plan for Lecture 33:

Chap. 20 in Shankar: The Dirac equation

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

1

22	Mon, 10/23/2017	Chap. 15	Multielectron atoms	<u>#13</u>	10/25/2017
23	Wed, 10/25/2017	Chap. 15	Multielectron atoms	<u>#14</u>	10/30/2017
24	Fri, 10/27/2017		Effects of nuclear motion		
25	Mon, 10/30/2017	Chap. 17	Time-independent perturbation theory	<u>#15</u>	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	<u>#16</u>	11/10/2017
29	Wed, 11/08/2017	Chap. 18	Time-dependent perturbation theory		
30	Fri, 11/10/2017	Chap. 19	Scattering theory	<u>#17</u>	11/15/2017
	Mon, 11/13/2017		Class canceled		
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		

11/17/2017

PHY 741 Fall 2017 – Lecture 33

2

How do these relationships effect quantum mechanics?

Focusing on treatment of Fermi particles

Non-relativistic mechanics

Relativistic mechanics

$$E = \frac{\mathbf{p}^2}{2m}$$

↓

$$\begin{aligned} E^2 - \mathbf{p}^2 c^2 &= (mc^2)^2 \\ \Downarrow \text{(with some license)} \\ (E - \mathbf{p} \cdot \mathbf{\sigma}c)(E + \mathbf{p} \cdot \mathbf{\sigma}c) &= (mc^2)^2 \\ \Downarrow \\ \left(i\hbar \frac{\partial}{\partial t} - \mathbf{p} \cdot \mathbf{\sigma}c \right) \left(i\hbar \frac{\partial}{\partial t} + \mathbf{p} \cdot \mathbf{\sigma}c \right) \Psi \\ = (mc^2)^2 \Psi \end{aligned}$$

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

3

Relativistic relationships – continued

Ref: J. J. Sakurai, Advanced Quantum Mechanics

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

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

Factored equations:

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

4

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: $\varphi^U = \Psi^R + \Psi^L$

$$\varphi^L = \Psi^R - \Psi^L$$

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

5

Relativistic relationships – continued

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

Further rearrangements:

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

6

Four component wavefunction of free Fermi particle

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

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

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

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

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

7

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

$$\mathbf{k} \cdot \boldsymbol{\sigma} = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix}$$

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

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

$$\chi_{\uparrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_{\uparrow}^L(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} \quad \kappa_z \equiv \frac{\hbar k_z c}{E + mc^2}$$

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

8

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

$$\mathbf{k} \cdot \boldsymbol{\sigma} = \begin{pmatrix} k_z & k_x - ik_y \\ k_x + ik_y & -k_z \end{pmatrix}$$

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

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

$$\chi_{\uparrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} \quad \chi_{\uparrow}^L(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \kappa_z \equiv \frac{\hbar k_z c}{E - mc^2}$$

$$\chi_{\downarrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_z \end{pmatrix} \quad \chi_{\downarrow}^L(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \kappa_{\pm} \equiv \frac{\hbar k_{\pm} c}{E - mc^2}$$

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

9

What does this all mean?

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

$$\chi_{\uparrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_{\uparrow}^L(\mathbf{k}) = \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} \quad \kappa_z \equiv \frac{\hbar k_z c}{E + mc^2}$$

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

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

$$\chi_{\uparrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \chi_{\uparrow}^L(\mathbf{k}) \approx \mathcal{N} \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\chi_{\downarrow}^U(\mathbf{k}) = \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \chi_{\downarrow}^L(\mathbf{k}) \approx \mathcal{N} \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

10

Dirac equation for free particles

$$\begin{aligned} \chi_{\uparrow}^U(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \chi_{\uparrow}^L(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} \\ E &= \sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4} & \chi_{\downarrow}^U(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \chi_{\downarrow}^L(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_z \end{pmatrix} \\ \hbar k_z c & \equiv \frac{\hbar k_z c}{E + mc^2} & \hbar k_{\pm} c & \equiv \frac{\hbar k_{\pm} c}{E + mc^2} \end{aligned}$$

$$\begin{aligned} -mc^2 & E = -\sqrt{\hbar^2 c^2 \mathbf{k}^2 + m^2 c^4} & \chi_{\uparrow}^U(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} \kappa_z \\ \kappa_+ \end{pmatrix} & \chi_{\uparrow}^L(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ & & \chi_{\downarrow}^U(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} \kappa_- \\ -\kappa_z \end{pmatrix} & \chi_{\downarrow}^L(\mathbf{k}) &= \mathcal{N} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \end{aligned}$$

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

11

Dirac equation for a free particle

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

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

Other convenient notations in terms of 4×4 matrices

$$\begin{aligned} \boldsymbol{\alpha} &= \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} & \beta &= \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} & H &= \mathbf{p} \cdot \boldsymbol{\alpha} c + mc^2 \beta \\ \boldsymbol{\sigma}_x &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} & \boldsymbol{\sigma}_y &= \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} & \boldsymbol{\sigma}_z &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} & I &\equiv I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

12

Dirac equation for Fermi particle in a scalar potential field

For free particle: $H = \mathbf{p} \cdot \mathbf{a}c + mc^2\beta$

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

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

Dirac's suggestion for representing a scalar potential field:

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

13

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

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

For H-like ion with nuclear charge Z :

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

Stationary state solutions:

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

14

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

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

H

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

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

15

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

Clebsch-Gordon coefficients

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

$$\begin{aligned} j_1 m_1 &\Rightarrow lm_l & J &= l + \frac{1}{2} \\ j_2 m_2 &\Rightarrow \frac{1}{2} m_s & \text{or } J &= l - \frac{1}{2} \end{aligned}$$

Clebsch-Gordon coefficients for this case:

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

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

19

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

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

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

20

$$\text{Consider: } (\boldsymbol{\sigma} \cdot \mathbf{L} + \hbar I_2) |JM; l\frac{1}{2}\rangle = \hbar(J(J+1) - l(l+1) + \frac{1}{4}) I_2 |JM; l\frac{1}{2}\rangle = -\kappa |JM; l\frac{1}{2}\rangle$$

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

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

21

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

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 Schrödinger equation in the non-relativistic limit
 - What new physics is contained more generally?

11/17/2017

PHY 741 Fall 2017 -- Lecture 33

22