PHY 742 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 17:

The Dirac equation

Chap. 16 in Professor Carlson's textbook:

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

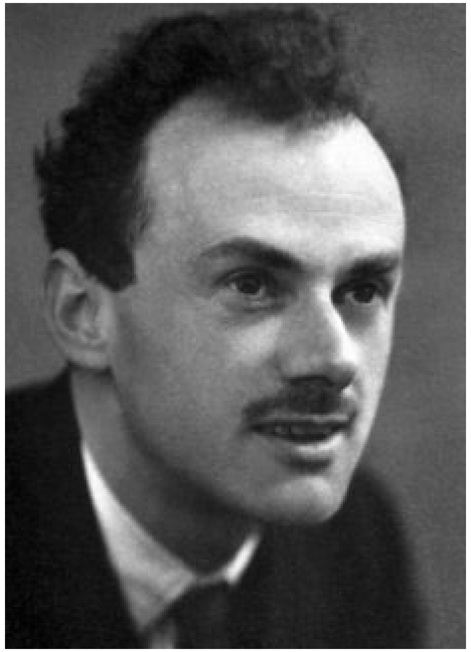
10	Mon: 02/07/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals	#9	02/09/2022
11	Wed: 02/09/2022	Chap. 11 (A-C)	Time evolution and Feynman path integrals	#10	02/11/2022
12	Fri: 02/11/2022	Chap. 15 A	Approximation methods for time evolution of quantum systems	#11	02/14/2022
13	Mon: 02/14/2022	Chap. 15	Approximate time evolution	#12	02/16/2022
14	Wed: 02/16/2022	Chap. 15	Fermi Golden Rule	#13	02/18/2022
15	Fri: 02/18/2022	Chap. 15	Matrix elements and selection rules		
	Mon: 02/21/2022	Chaps. (11-15)	Homework review & presentations		
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		

PHY 742 -- Assignment #15

February 25, 2022

Continue reading Chapter 16 in **Professor Carlson's QM textbook.**.

1. From the 4 × 4 matrix represenations of the operators $\mathbf{J}^2$ and K, show that both $\mathbf{J}^2$ and K^2 are constant matrices and their values are related by $K^2=\mathbf{J}^2+\hbar^2/4$. Alternatively, in terms of the quantum number J, the eigenvalues of K^2 can be written $K^2=J(J+1)\hbar^2+\hbar^2/4$.



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

Energy ←→ Momentum relationships in classical and quantum mechanics

Focusing on treatment of Fermi particles

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

Relativistic relationships – continued

Ref: J. J. Sakurai, Advanced Quantum Mechanics

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

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

Factored equations:

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

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

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

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

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

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:

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

$$\Downarrow$$

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

Four component wavefunction of free Fermi particle

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

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

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

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

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

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

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

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

Define: $k_\pm \equiv k_x \pm ik_y$

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

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

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

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

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

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

Define: $k_\pm \equiv k_x \pm ik_y$

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

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

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

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

What does this all mean?

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

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

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

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

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

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

Dirac equation for free particles – slightly more convenient notation

mc^2

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

$$\chi_\uparrow^U(\mathbf{k}) = \mathcal{N}\begin{pmatrix}1\\0\end{pmatrix} \qquad \chi_\uparrow^L(\mathbf{k}) = \mathcal{N}\begin{pmatrix}\tilde{\kappa}_z\\ \tilde{\kappa}_+\end{pmatrix}$$

$$\chi_\downarrow^U(\mathbf{k}) = \mathcal{N}\begin{pmatrix}0\\1\end{pmatrix} \qquad \chi_\downarrow^L(\mathbf{k}) = \mathcal{N}\begin{pmatrix}\tilde{\kappa}_-\\ -\tilde{\kappa}_z\end{pmatrix}$$

$$\tilde{\kappa}_z \equiv \frac{\hbar k_z c}{|E| + mc^2}$$

$$\tilde{\kappa}_\pm \equiv \frac{\hbar k_\pm c}{|E| + mc^2}$$

-mc^2

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

$$\chi_\uparrow^U(\mathbf{k}) = \mathcal{N}\begin{pmatrix}-\tilde{\kappa}_z\\ -\tilde{\kappa}_+\end{pmatrix} \qquad \chi_\uparrow^L(\mathbf{k}) = \mathcal{N}\begin{pmatrix}1\\0\end{pmatrix}$$

$$\chi_\downarrow^U(\mathbf{k}) = \mathcal{N}\begin{pmatrix}-\tilde{\kappa}_-\\ \tilde{\kappa}_z\end{pmatrix} \qquad \chi_\downarrow^L(\mathbf{k}) = \mathcal{N}\begin{pmatrix}0\\1\end{pmatrix}$$

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

Dirac equation for a free particle

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

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

Other convenient notations in terms of 4×4 matrices

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

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

Note: This notation is not entirely consistent with your textbook and is problematic because of other common usages of α and β.

Dirac equation for Fermi particle in a scalar potential field

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

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

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

Dirac's suggestion for representing a scalar potential field:

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

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:

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

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

Preview –

Non-relativistic spherical atom --

Eigenstate quantum numbers $|nlm_l>$; independent of electron spin

Relativistic spherical atom

Eigenstate quantum numbers $|n\kappa\, jm_j>$; electron spin included

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

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

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

Digression – useful identity for operator vectors **A** and **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

$$\mathbf{A}\cdot\mathbf{B}=A_xB_x+A_yB_y+A_zB_z \quad \text{and} \quad \mathbf{C}=\mathbf{A}\times\mathbf{B}$$

$$C_x=A_yB_z-A_zB_y \qquad C_y=A_zB_x-A_xB_z \qquad C_z=A_xB_y-A_yB_x$$

Note: You might like to verify these relationships!

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

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

Digression – useful identity for operator vectors **A** and **B** -- continued

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

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

where

$$\mathbf{A}\cdot\mathbf{B} = A_xB_x + A_yB_y + A_zB_z \quad \text{and} \quad \mathbf{C} = \mathbf{A}\times\mathbf{B}$$

$$C_x = A_yB_z - A_zB_y \qquad C_y = A_zB_x - A_xB_z \qquad C_z = A_xB_y - A_yB_x$$

$$(\boldsymbol{\sigma}\cdot\mathbf{L})(\boldsymbol{\sigma}\cdot\mathbf{L}) = \mathbf{L}^2 + i\boldsymbol{\sigma}\cdot(\mathbf{L}\times\mathbf{L}) = \mathbf{L}^2 - \hbar\boldsymbol{\sigma}\cdot\mathbf{L}$$

What is $(\boldsymbol{\sigma}\cdot\mathbf{L})(\boldsymbol{\sigma}\cdot\mathbf{L})$?

$$\mathbf{L}\times\mathbf{L} = \begin{pmatrix} \hat{\mathbf{x}} & \hat{\mathbf{y}} & \hat{\mathbf{z}} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{pmatrix} = i\hbar L_x\hat{\mathbf{x}} + i\hbar L_y\hat{\mathbf{y}} + i\hbar L_z\hat{\mathbf{z}}$$

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

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

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

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

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

Note that:

$$K^2 = \mathbf{J}^2 + \frac{1}{4}\hbar^2$$

Commutation relations:

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

Note that: $K^2 = \mathbf{J}^2 + \frac{1}{4}\hbar^2$

Some details --

$$\left(\boldsymbol{\sigma}\cdot\mathbf{L}+\hbar I_2\right)^2 = \mathbf{L}^2 - \hbar\boldsymbol{\sigma}\cdot\mathbf{L} + 2\hbar\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar^2 I_2$$

$$= \mathbf{L}^2 + \hbar\boldsymbol{\sigma}\cdot\mathbf{L} + \hbar^2 I_2 = \left(\mathbf{L}+\tfrac{1}{2}\hbar\boldsymbol{\sigma}\right)^2 + \tfrac{1}{4}\hbar^2 I_2$$

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

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

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

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

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

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

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

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

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

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

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

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

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

More relationships between the operators

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

Relationships between the upper and lower component functions:

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

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

After some algebra --

$$l_L(l_L+1) = l_U(l_U+1) - 2\kappa \qquad \kappa = \pm\left(j + \frac{1}{2}\right)$$

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

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

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

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

Eigenvalues of K operator:

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

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

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

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

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

Summary of allowed combinations of eigenvalues

	l_U	l_L
$\kappa = -\left(j + \frac{1}{2}\right)$	$j - \frac{1}{2}$	$j + \frac{1}{2}$
$\kappa = +\left(j + \frac{1}{2}\right)$	$j + \frac{1}{2}$	$j - \frac{1}{2}$

Alternatively

	j	l_L
$\kappa = -\left(l_U + 1\right)$	$l_U + \frac{1}{2}$	$l_U + 1$
$\kappa = +l_U$	$l_U - \frac{1}{2}$	$l_U - 1$

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

Clebsch-Gordon coefficients

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

$$j_1 m_1 \Rightarrow l m_l \qquad\qquad J = l + \tfrac{1}{2}$$

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

Clebsch-Gordon coefficients for this case:

$$j_1 = l \qquad j_2 = s = \tfrac{1}{2}$$

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

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

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

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

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

Consider: $\left(\boldsymbol{\sigma}\cdot\mathbf{L}+\hbar I_2\right)\left|JM;l\,\tfrac{1}{2}\right\rangle=\hbar\left(J(J+1)-l(l+1)+\tfrac{1}{4}\right)I_2\left|JM;l\,\tfrac{1}{2}\right\rangle$

$$=-\kappa\left|JM;l\,\tfrac{1}{2}\right\rangle$$

Possibilities:

$J=l+\tfrac{1}{2}\qquad \kappa=-l-1$

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

Combinations:

$\kappa=-1$	$j=\tfrac{1}{2}$	$l=0$
$+1$	$\tfrac{1}{2}$	1
-2	$\tfrac{3}{2}$	1
$+2$	$\tfrac{3}{2}$	2
-3	$\tfrac{5}{2}$	2
$+3$	$\tfrac{5}{2}$	3

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

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

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

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

Questions:

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