PHY 745 Group Theory
11-11:50 AM MWF Olin 102

Plan for Lecture 25:

Group theory and intrinsic spin; specifically, s=1/2

1. Dirac equation for hydrogen atom
2. Spin-orbit interaction
3. Double groups

	Fri: 03/17/2017		*APS Meeting - no class*		
23	Mon: 03/20/2017	Chap. 7.7	Jahn-Teller Effect	#15	03/24/2017
24	Wed: 03/22/2017	Chap. 7.7	Jahn-Teller Effect		
25	Fri: 03/24/2017		Spin 1/2	#16	03/27/2017
26	Mon: 03/27/2017				
27	Wed: 03/29/2017				
28	Fri: 03/30/2017				
29	Mon: 04/03/2017				
30	Wed: 04/05/2017				
31	Fri: 04/07/2017				
32	Mon: 04/10/2017				
33	Wed: 04/12/2017				
	Fri: 04/14/2017		*Good Friday Holiday -- no class*		
34	Mon: 04/17/2017				
35	Wed: 04/19/2017				
36	Fri: 04/21/2017				
	Mon: 04/24/2017		Presentations I		
	Wed: 04/26/2017		Presentations II		

Dirac equation for describing the quantum mechanics of an electron

Two component matrices --

Pauli spin matrices

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

Identity matrix

$$I \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Four-component Dirac Hamiltonian for an electron in a spherically symmetric scalar potential *V(r)*:

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

Other useful four-component matrices:

$$\mathbf{J} = \begin{pmatrix} \mathbf{L}I + \hbar\boldsymbol{\sigma}/2 & 0 \\ 0 & \mathbf{L}I + \hbar\boldsymbol{\sigma}/2 \end{pmatrix}$$

$$K = \begin{pmatrix} \mathbf{L}\cdot\boldsymbol{\sigma} + \hbar I & 0 \\ 0 & -\left(\mathbf{L}\cdot\boldsymbol{\sigma} + \hbar I\right) \end{pmatrix}$$

The following commutation relations can be shown:

$$\left[H,K\right]=0 \qquad \left[H,J^2\right]=0 \qquad \left[H,J_z\right]=0$$

Useful identity:

For two operators $\mathbf{A}$ and $\mathbf{B}$ and Pauli matrices $\boldsymbol{\sigma}$:

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

Eigenfunctions of Dirac Hamiltonian for spherical potential

$$H\Psi = \begin{pmatrix} \left(V(r)+mc^2\right)I & c\boldsymbol{\sigma}\cdot\mathbf{p} \\ c\boldsymbol{\sigma}\cdot\mathbf{p} & \left(V(r)-mc^2\right)I \end{pmatrix} \begin{pmatrix} \psi^{Upper}_{jml_U}(\mathbf{r}) \\ \psi^{Lower}_{jml_L}(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} \psi^{Upper}_{jml_U}(\mathbf{r}) \\ \psi^{Lower}_{jml_L}(\mathbf{r}) \end{pmatrix}$$

Relationships between eigenvalues

κ	l_U	l_L
$-(j+\frac{1}{2})$	$-\kappa-1$	$-\kappa$
$j+\frac{1}{2}$	κ	$\kappa-1$

$$\begin{pmatrix} \psi^{Upper}_{jml_U}(\mathbf{r}) \\ \psi^{Lower}_{jml_L}(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} (G(r)/r)\mathcal{Y}^{l_U}_{jm} \\ (iF(r)/r)\mathcal{Y}^{l_L}_{jm} \end{pmatrix}$$

$$\mathcal{Y}^{l}_{jm} = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}Y_{l(m-\frac{1}{2})}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}Y_{l(m+\frac{1}{2})}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix} \quad \text{for } j = l+\tfrac{1}{2}$$

$$\mathcal{Y}^{l}_{jm} = -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}}Y_{l(m-\frac{1}{2})}(\hat{\mathbf{r}})\begin{pmatrix}1\\0\end{pmatrix} + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}}Y_{l(m+\frac{1}{2})}(\hat{\mathbf{r}})\begin{pmatrix}0\\1\end{pmatrix} \quad \text{for } j = l-\tfrac{1}{2}$$

Radial differential equations:

$$\hbar c\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) = \left(E - V(r) + mc^2\right)F$$

$$\hbar c\left(\frac{dF}{dr} - \frac{\kappa}{r}F\right) = -\left(E - V(r) - mc^2\right)G$$

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Normalization of wavefunctions for bound states:

$$\int_0^\infty dr\left(|G(r)|^2 + |F(r)|^2\right) = 1$$

Non-relativistic limit:

Let $E^{NR} \equiv E - mc^2$

Radial differential equations:

$$\hbar c\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) = \left(E^{NR} - V(r) + 2mc^2\right)F$$

$$\hbar c\left(\frac{dF}{dr} - \frac{\kappa}{r}F\right) = -\left(E^{NR} - V(r)\right)G$$

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

$$\hbar c\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) \approx \left(2mc^2\right)F$$

$$\hbar c\left(\frac{d}{dr} - \frac{\kappa}{r}\right)\frac{\hbar c}{2mc^2}\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) = \frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} - \frac{\kappa(\kappa+1)}{r^2}\right)G$$

$$\approx -\left(E^{NR} - V(r)\right)G$$

$\Rightarrow$ In non-relativistic limit -- $E^{NR} - V(r) \ll 2mc^2$:
Upper component radial function satisfies
Schroedinger equation:

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

Lower component is related according to:

$$F(r) \approx \frac{\hbar}{2mc}\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right)$$

κ	l_U	l_L
$-(j+\frac{1}{2})$	$-\kappa-1$	$-\kappa$
$j+\frac{1}{2}$	κ	$\kappa-1$

κ	j	l_U	l_L
-1	$\frac{1}{2}$	0	1
1	$\frac{1}{2}$	1	0
-2	$\frac{3}{2}$	1	2
2	$\frac{3}{2}$	2	1
-3	$\frac{5}{2}$	2	3
3	$\frac{5}{2}$	3	2
-4	$\frac{7}{2}$	3	4

Example for the H atom

$$V(r) = -\frac{Ze^2}{r}$$

Define fine structure constant:

$$\alpha \equiv \frac{e^2}{\hbar c} = \frac{1}{137.035999679}$$

Radial differential equations:

$$\hbar c\left(\frac{dG}{dr} + \frac{\kappa}{r}G\right) = \left(E - V(r) + mc^2\right)F$$

$$\hbar c\left(\frac{dF}{dr} - \frac{\kappa}{r}F\right) = -\left(E - V(r) - mc^2\right)G$$

$$\left(\frac{d}{dr} + \frac{\kappa}{r}\right)G = \left(\frac{\alpha Z}{r} + \frac{mc}{\hbar}\left(1 + \frac{E}{mc^2}\right)\right)F$$

$$\left(\frac{d}{dr} - \frac{\kappa}{r}\right)F = \left(-\frac{\alpha Z}{r} + \frac{mc}{\hbar}\left(1 - \frac{E}{mc^2}\right)\right)G$$

In terms of Bohr radius:

$$a \equiv \frac{\hbar}{\alpha mc} \qquad r \rightarrow r/a$$

$$\left(\frac{d}{dr}+\frac{\kappa}{r}\right)G=\left(\frac{\alpha Z}{r}+\frac{1}{\alpha}\left(1+\frac{E}{mc^2}\right)\right)F$$

$$\left(\frac{d}{dr}-\frac{\kappa}{r}\right)F=\left(-\frac{\alpha Z}{r}+\frac{1}{\alpha}\left(1-\frac{E}{mc^2}\right)\right)G$$