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

### Plan for Lecture 26:

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

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

***Chapter 14 in DDJ**



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|---|---|---|---|---|---|
| | 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 | | Dirac equation for H-like atoms | #17 | 03/29/2017 |
| 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

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

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

In terms of two component matrices --

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

Other useful four-component matrices:

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

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

The following commutation relations can be shown:

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

In principle, it is possible to have eigenstates that are simultaneously diagonal in $H$, $K$, $J^2$, and $J_z$, but $K$ and $J^2$ are closely related.



Suppose that the simultaneous eigenvectors:

$$H\Psi = E\Psi \qquad K\Psi = -\hbar\kappa\Psi \qquad J^2\Psi = \hbar^2 j(j+1)\Psi \qquad J_z\Psi = \hbar m\Psi$$

Take the form:

$$\Psi = \begin{pmatrix} \frac{G(r)}{r}\mathcal{Y}^{Upper} \\ \frac{iF(r)}{r}\mathcal{Y}^{Lower} \end{pmatrix}$$

$$K\Psi = -\hbar\kappa\Psi \quad K^2\Psi = \hbar^2\kappa^2\Psi$$



$$K = \begin{pmatrix} \mathbf{L}\cdot\boldsymbol{\sigma} + \hbar I & 0 \\ 0 & -(\mathbf{L}\cdot\boldsymbol{\sigma} + \hbar I) \end{pmatrix} \qquad K^2 = (\mathbf{L}\cdot\boldsymbol{\sigma} + \hbar I)^2 \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}$$

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

$$K^2\Psi = \hbar^2\kappa^2\Psi = \left(J^2 + \frac{\hbar^2}{4}\right)\Psi = \hbar^2\left(j + \frac{1}{2}\right)^2\Psi$$

$$\Rightarrow \kappa^2 = \left(j + \frac{1}{2}\right)^2$$

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

Either: $\Psi = \begin{pmatrix} \frac{G(r)}{r}\mathcal{Y}^{Upper}\left(\kappa = -j - \frac{1}{2}\right) \\ \frac{iF(r)}{r}\mathcal{Y}^{Lower}\left(\kappa = j + \frac{1}{2}\right) \end{pmatrix}$ or $\Psi = \begin{pmatrix} \frac{G(r)}{r}\mathcal{Y}^{Upper}\left(\kappa = j + \frac{1}{2}\right) \\ \frac{iF(r)}{r}\mathcal{Y}^{Lower}\left(\kappa = -j - \frac{1}{2}\right) \end{pmatrix}$

Also note that

$$\mathbf{J}=\mathbf{L}+\frac{\hbar}{2}\boldsymbol{\sigma}$$

$$\hbar\mathbf{L}\cdot\boldsymbol{\sigma}+\hbar^2 I = J^2 I - L^2 I - \frac{\hbar^2}{4}\sigma^2 + \hbar^2 I$$

$$\left(\hbar\mathbf{L}\cdot\boldsymbol{\sigma}+\hbar^2 I\right)\mathcal{Y} = \hbar^2\left(j(j+1)-l(l+1)+\frac{1}{4}\right)\mathcal{Y}$$

$$\Rightarrow\left(j(j+1)-l_U(l_U+1)+\frac{1}{4}\right) = -\kappa$$

$$\left(j(j+1)-l_L(l_L+1)+\frac{1}{4}\right) = \kappa$$

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

$$\left(j(j+1)-l_L(l_L+1)+\frac{1}{4}\right) = \kappa$$

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

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

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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

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

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

| $\kappa$ | $j$ | $l_U$ | $l_L$ |
|---|---|---|---|
| $-1$ | $\frac{1}{2}$ | 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 |



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

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

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

Radial differential equations:

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

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



Radial differential equations:

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Normalization of wavefunctions for bound states:

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

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:

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

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

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

Behavior for $r \to \infty$:

$G(r) \approx G_\infty e^{-\lambda r} \qquad F(r) \approx F_\infty e^{-\lambda r}$

$$\begin{pmatrix} -\lambda & \frac{1}{\alpha}\left(1 + \frac{E}{mc^2}\right) \\ \frac{1}{\alpha}\left(1 - \frac{E}{mc^2}\right) & -\lambda \end{pmatrix}\begin{pmatrix} G_\infty \\ F_\infty \end{pmatrix} = 0$$

$$\lambda = \frac{1}{\alpha}\sqrt{1 - \left(\frac{E}{mc^2}\right)^2} \equiv \frac{1}{\alpha}\sqrt{1 - \varepsilon^2}$$



Polynomial expansion:

$$G(r) = e^{-\lambda r} r^s \sum_{j=0}^{N} a_j r^j \qquad F(r) = e^{-\lambda r} r^s \sum_{j=0}^{N} b_j r^j$$

Assuming that the series truncates at $j = N,\ N = 0,1,...$

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

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

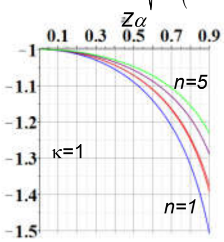
Equating terms of order $\left(\frac{1}{r}\right)$:

$$\begin{pmatrix} s+\kappa & \alpha Z \\ -\alpha Z & s-\kappa \end{pmatrix}\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = 0 \qquad s = \sqrt{\kappa^2 - \alpha^2 Z^2} \qquad \frac{b_0}{a_0} = -\frac{\kappa + \sqrt{\kappa^2 - \alpha^2 Z^2}}{\alpha Z}$$

Evaluating the coefficients of the polynomial of order *N*

Let $n = N + |\kappa|$, find

$$\frac{E}{mc^2} \equiv \varepsilon = \frac{1}{\sqrt{1 + \frac{Z^2\alpha^2}{\left(n - |\kappa| + \sqrt{\kappa^2 - Z^2\alpha^2}\right)^2}}}$$






Eigenstate energies of H atom for principal quantum number $n$ :

$$\frac{E}{mc^2} \equiv \varepsilon = \frac{1}{\sqrt{1 + \frac{Z^2\alpha^2}{\left(n - |\kappa| + \sqrt{\kappa^2 - Z^2\alpha^2}\right)^2}}}$$

For $n = |\kappa|$ $\quad \frac{E}{mc^2} \equiv \varepsilon = \sqrt{1 - \frac{Z^2\alpha^2}{n^2}}$

Note that for a given principal quantum number *n*, the energies for $+\kappa$ and $-\kappa$ are degenerate.

For *n=1*, *κ=-1:* $\quad \Psi_{1s_{1/2}} = \frac{Ce^{-Zr}r^{\sqrt{1-Z^2\alpha^2}}}{r} \begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\ i\frac{1-\sqrt{1-Z^2\alpha^2}}{Z\alpha} \boldsymbol{\sigma}\cdot\hat{\mathbf{r}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix}$



Paul Strange, "Relativistic Quantum Mechanics", Cambridge U. Press (1998), pg. 241

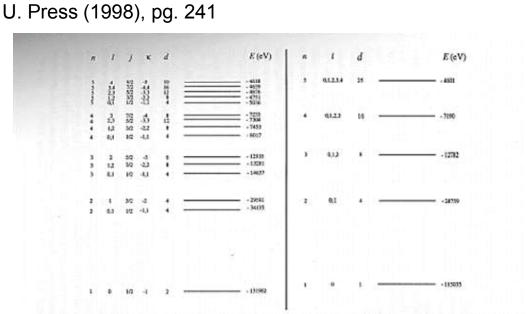



Fig. 8.3. The energy levels of the one-electron atom with $Z = 92$. The left hand side shows relativistic energy levels calculated using equation (8.43). They are labelled by the quantum numbers $n$, $l$, $j$, $\kappa$ and their degeneracy $d$, up to $l = 5$. Also shown is the energy of each level in electronvolts. On the right hand side for comparison we show the equivalent non-relativistic energy levels with their quantum numbers and degeneracies.

Summary of results for solution of Dirac equation for H-like ion

$$\frac{E}{mc^2} \equiv \varepsilon = \frac{1}{\sqrt{1+\frac{Z^2\alpha^2}{\left(n-|\kappa|+\sqrt{\kappa^2-Z^2\alpha^2}\right)^2}}}$$

where $\kappa = \pm\left(j+\frac{1}{2}\right)$

For $Z\alpha << 1$, $\frac{E}{mc^2} \approx 1 - \frac{Z^2\alpha^2}{2n^2}$

Spin-orbit splitting

$$\frac{\Delta E_{SO}}{mc^2} = \varepsilon(n,|\kappa|+1) - \varepsilon(n,|\kappa|)$$