Answers to Exam I **Physics 607** **Oct. 3, 2001**

1. The state $|JM\rangle$ is an eigenstate of J^2, J_1^2, and J_2^2. Since $J^2 = J_1^2 + J_2^2 + 2(\mathbf{J}_1 \cdot \mathbf{J}_2)$, we have
$$(\mathbf{J}_1 \cdot \mathbf{J}_2)\,|JM\rangle = \lambda|JM\rangle,$$
with
$$\lambda = \frac{1}{2}\left[J(J+1) - J_1(J_1+1) - J_2(J_2+1)\right]$$

2. The energy shift is
$$\begin{aligned}\Delta E_{njm} &= -\mu_0 B\,(-1)^{j-m}\begin{pmatrix} j & 1 & j \\ -m & 0 & m\end{pmatrix}\langle j||\sigma||j\rangle \\ &= -\mu_0\,B\,\frac{m}{\sqrt{j(j+1)(2j+1)}}\langle j||\sigma||j\rangle \\ &= \frac{m}{j}\,\Delta E_{njj}\end{aligned}$$

3. Hartree-Fock Equations:

   (a) Nonrelativistic:
$$h_0P_{1s} + V_{\rm dir}P_{1s} - \Big[v_0(1s,r)P_{1s} + v_0(2s,1s,r)P_{2s} + v_1(2p,1s,r)P_{2p}\Big] = \epsilon_{1s}P_{1s}$$
$$h_0P_{2s} + V_{\rm dir}P_{2s} - \Big[v_0(1s,2s,r)P_{1s} + v_0(2s,r)P_{2s} + v_1(2p,2s,r)P_{2p}\Big] = \epsilon_{2s}P_{2s}$$
$$\begin{aligned}h_0P_{2p} + V_{\rm dir}P_{2p} - \Big[\frac{1}{3}v_1(1s,2p,r)P_{1s} + \frac{1}{3}v_1(2s,2p,r)P_{2s} + \ v_0(2p,r)P_{2p} \\ + \ \frac{2}{5}v_2(2p,r)P_{2p}\Big] = \epsilon_{2p}P_{2p}\end{aligned}$$

   Here,
$$h_0P_{nl} = \left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} - \frac{Z}{r}\right)P_{nl}$$

   and
$$V_{\rm dir} = 2v_0(1s,r), +2v_0(2s,r) + 6v_0(2p,r)$$

(b) Relativistic: $R_{n\kappa} = (P_{n\kappa}, Q_{n\kappa})$

$$\begin{aligned}
h_0 R_{1s} + V_{\rm dir} R_{1s} - \Big[& v_0(1s,r) R_{1s} + v_0(2s,1s,r) R_{2s} + \frac{1}{3} v_1(2p_{1/2},1s,r) R_{2p_{1/2}} \\
& + \frac{2}{3} v_1(2p_{3/2},1s,r) R_{2p_{3/2}} \Big] = \epsilon_{1s} R_{1s} \\
h_0 R_{2s} + V_{\rm dir} R_{2s} - \Big[& v_0(1s,2s,r) R_{1s} + v_0(2s,r) R_{2s} + \frac{1}{3} v_1(2p_{1/2},2s,r) R_{2p_{1/2}} \\
& + \frac{2}{3} v_1(2p_{3/2},2s,r) R_{2p_{3/2}} \Big] = \epsilon_{2s} R_{2s} \\
h_0 R_{2p_{1/2}} + V_{\rm dir} R_{2p_{1/2}} - \Big[& \frac{1}{3} v_1(1s,2p_{1/2},r) R_{1s} + \frac{1}{3} v_1(2s,2p_{1/2},r) R_{2s} \\
& + v_0(2p_{1/2},r) R_{2p_{1/2}} + \frac{2}{5} v_2(2p_{1/2},2p_{3/2},r) R_{2p_{3/2}} \Big] = \epsilon_{2p_{1/2}} R_{2p_{1/2}} \\
h_0 R_{2p_{3/2}} + V_{\rm dir} R_{2p_{3/2}} - \Big[& \frac{1}{3} v_1(1s,2p_{3/2},r) R_{1s} + \frac{1}{3} v_1(2s,2p_{3/2},r) R_{2s} \\
& + v_0(2p_{3/2},r) R_{2p_{3/2}} + \frac{1}{5} v_2(2p_{3/2},2p_{1/2},r) R_{2p_{1/2}} \\
& + \frac{1}{5} v_2(2p_{3/2},2p_{1/2},r) R_{2p_{1/2}} \Big] = \epsilon_{2p_{3/2}} R_{2p_{3/2}}
\end{aligned}$$

Here,

$$h_0 R_{n\kappa} = \begin{pmatrix} -\frac{Z}{r} + c^2 & c\left(\frac{d}{dr} - \frac{\kappa}{r}\right) \\ -c\left(\frac{d}{dr} + \frac{\kappa}{r}\right) & -\frac{Z}{r} - c^2 \end{pmatrix} R_{n\kappa}$$

and

$$V_{\rm dir} = 2v_0(1s,r), +2v_0(2s,r) + 2v_0(2p_{1/2},r) + 4v_0(2p_{3/2},r)$$

4. Hartree-Fock Energies

Shell	Energy	Expt.
Lithium		
$1s$	-2.792364	
$2s$	-0.196304	-0.198142
$2p$	-0.128637	-0.130235
$3s$	-0.073797	-0.074182
Boron		
$1s$	-8.185922	
$2s$	-0.873823	
$2p$	-0.275903	-0.304947
$3s$	-0.114517	-0.122513