

1. Show that the state

$$|J, M\rangle = \sum_{m_1 m_2} \begin{array}{c} \downarrow j_1 m_1 \\ \hline JM \\ \hline \downarrow j_2 m_2 \end{array} |j_1, m_1\rangle |j_2, m_2\rangle ,$$

is an eigenstate of $\mathbf{J}_1 \cdot \mathbf{J}_2$. What is the corresponding eigenvalue.

2. The interaction Hamiltonian for a one-electron atom in an external magnetic field directed along the z -axis is $H_I = -\mu_0 \sigma_z B$,

- (a) Express the energy shift of the state $|n, j, j\rangle$ in terms of a reduced matrix element of σ .
- (b) Show that the energy shift of the states $|n, j, m\rangle$ and $|n, j, j\rangle$ are related by

$$\Delta E_{njm} = \frac{m}{j} \Delta E_{njj} .$$

Note:

$$\begin{pmatrix} j & 1 & j \\ -m & 0 & m \end{pmatrix} = (-1)^{j-m} \frac{m}{\sqrt{j(j+1)(2j+1)}} .$$

3. Hartree-Fock:

- (a) Write down in detail the Hartree-Fock equations for the 3 closed subshells of the neon atom. (Give numerical values for the occupation numbers and exchange factors).
- (b) Write down in detail the Dirac-Fock equations for the 4 closed subshells of the neon atom. (Give numerical values for the occupation numbers and exchange factors).

4. Compile and run the program NRHF.F for Li using the data set LI.IN as input. How do the HF eigenvalues compare with experiment? Modify the data set to determine the $2p$ and $3s$ energies for boron, assuming a "frozen" Be-like core and a single valence electron. How do these energies compare with experiment. (A description of the input data file is given at the beginning of the program)