

Answers HW #8

1. $(r_1 - r_2) e^{-cr_1} e^{-cr_2}$ is antisymmetric with respect to exchange of r_1 and r_2 . Thus this would require a triplet spin function. A closed-shell ground state should have a singlet spin function.

Also this wave function has a node when $r_1 = r_2$, again unexpected behavior for the ground state wave function.

2. The positronium "atom" can exist as a singlet or triplet state.

In the former case we have for the wavefunction

$\psi(r)(\alpha\beta - \beta\alpha)$ where $\psi(r)$ is the hydrogenic wavefunction with the reduced mass $\mu = \frac{1}{2}me$

In the case of the triplet we have $\psi(r)$ times $\alpha\alpha$, $\alpha\beta + \beta\alpha$, or $\beta\beta$.

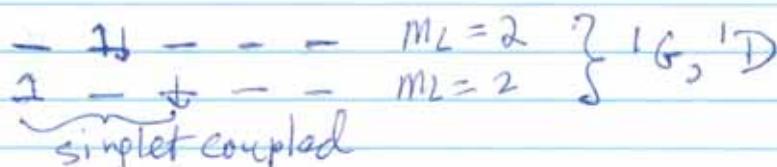
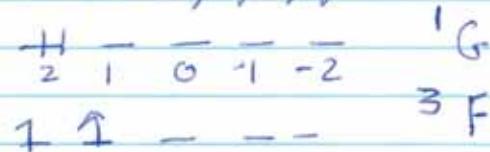
3. Show that $\hat{S}_z = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, $\hat{S}_y = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\hat{S}^2 = \frac{1}{4}\hbar^2 \begin{pmatrix} 3 & 0 \\ 0 & 0 \end{pmatrix}$

$$\hat{S}_z(\alpha) = \frac{1}{2}\hbar \begin{pmatrix} \alpha \\ 0 \end{pmatrix}, \quad \hat{S}_z(\beta) = -\frac{1}{2}\hbar \begin{pmatrix} 0 \\ \beta \end{pmatrix}$$

$$\hat{S}_y(\alpha) = \frac{i\hbar}{2} \begin{pmatrix} 0 \\ \beta \end{pmatrix}, \quad \hat{S}_y(\beta) = -\frac{i\hbar}{2} \begin{pmatrix} \alpha \\ 0 \end{pmatrix}$$

$$\hat{S}^2(\alpha) = \frac{3}{4}\hbar^2 \begin{pmatrix} \alpha \\ 0 \end{pmatrix}, \quad \hat{S}^2(\beta) = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ \beta \end{pmatrix}$$

4. d^2 : $L = 4, 3, 2, 1, 0$



So far we have 1G , 3F , 1D

$$9 + 2\downarrow + 5 = 35 \text{ arrangements}$$

This leaves 10 arrangements. These correspond to 3P and 1S



5. This suggests the following wave function for Be

$$c_1 |1s\bar{1s}2s\bar{2s}\rangle + c_2 \left\{ |1s\bar{1s}2p_x\bar{2p}_x\rangle + |1s\bar{1s}2p_y\bar{2p}_y\rangle + |1s\bar{1s}2p_z\bar{2p}_z\rangle \right\}$$