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 $\mu = \frac{1}{2} m_e$

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

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

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

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

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

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

⇅ _ _ _ _ $\quad {}^1G$

2 1 0 -1 -2

↿ ↿ _ _ _ $\quad {}^3F$

_ ⇅ _ _ _ $\quad m_L = 2$

↿ _ ⇂ _ _ $\quad m_L = 2$ $\Big\}\ {}^1G, {}^1D$

singlet coupled

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

$9 + 21 + 5 = 35$ arrangements

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

↑ — ↑ — — ^3F

— ↑ ↑ — — } ^3F and ^3P
↑ — ↑ — — }

5. This suggests the following wave function for Be

$$c_1 \, |1s\,\overline{1s}\,2s\,\overline{2s}| + c_2 \{ |1s\,\overline{1s}\,2p_x\,\overline{2p_x}| + |1s\,\overline{1s}\,2p_y\,\overline{2p_y}| + |1s\,\overline{1s}\,2p_z\,\overline{2p_z}$$