CHEM 2430 HW #8

1. Explain why $e^{-cr_1}e^{-cr_2}\left(r_1 - r_2\right)$ is not a suitable trial function for the He atom?

2. Write a proper wavefunction for the ground state of positronium (e^+, e^-) including spin.

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

4. For an atom with a …d^2 configuration (where… denotes a closed shell), what electronic states can result, indicating both angular momentum and spin?

What state do you expect to be in lowest energy?

5. The 2s → 2p excited states of the Be atom are relatively low-lying in energy. In light of that, write down a wavefunction for the ground state that includes s/p mixing.