CH 107 Tutorial 5

Please solve these problems BEFORE the tutorial session

1. Write the general (complete) Hamiltonian for an n electron atom with nuclear charge Z.

2. What is orbital approximation? Does it involve neglect of the inter-electronic repulsion?

3. Why are 2-e spin-functions α(1)β(2) or β(1)α(2) not acceptable? Consider the following slater determinant for a two electron system. Comment, with proper justification, whether this is a valid wavefunction for He atom in one of it's excited states.

$$\psi = {}^{1}/_{\sqrt{2}} \begin{vmatrix} 2s(1)\alpha(1) & 3s(1)\beta(1) \\ 2s(2)\alpha(2) & 3s(2)\beta(2) \end{vmatrix}$$

4. Evaluate the spin wavefunctions of He atom in an excited state where the 2 electrons are in two different orbitals. Write the slater determinant for the total wavefunctions.

5. Consider an atom with two electrons, 1 and 2. The operator for the square of the total spins of these electrons is

$$\widehat{S^2_{total}} = (\widehat{S_1} + \widehat{S_2})^2 = \widehat{S_1^2} + \widehat{S_2^2} + 2(\widehat{S_{1x}} \cdot \widehat{S_{2x}} + \widehat{S_{1y}} \cdot \widehat{S_{2y}} + \widehat{S_{1z}} \cdot \widehat{S_{2z}})$$

Given:

$$\widehat{S_x}\alpha = \tfrac{\hbar}{2}\beta, \quad \widehat{S_x}\beta = \tfrac{\hbar}{2}\alpha, \quad \widehat{S_y}\alpha = \tfrac{\iota\hbar}{2}\beta, \quad \widehat{S_y}\beta = \tfrac{\iota\hbar}{2}\alpha, \quad \widehat{S_z}\alpha = \tfrac{\hbar}{2}\alpha, \quad \widehat{S_z}\beta = -\tfrac{\hbar}{2}\beta$$

and $\widehat{S_i^2} = \widehat{S_{ix}^2} + \widehat{S_{iy}^2} + \widehat{S_{iz}^2}$ for $i = 1, 2$

a) Write the spin wavefunction for the electronic part of the atom when both electrons have α spin

b) With appropriate proof, determine if this wavefunction is an eigenfunction of $\widehat{S^2_{total}}$