Fall 2011   CHEM 760: Introductory Quantum Chemistry

Homework 9   Due: Dec 13

1. textbook 10.3

2. textbook 10.7

3. Consider the determinantal atomic wave function

$$\Psi(1,2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_{211}\alpha(1) & \psi_{21-1}\beta(1) \\ \psi_{211}\alpha(2) & \psi_{21-1}\beta(2) \end{vmatrix}$$

where $\psi_{21\pm1}$ is a hydrogen-like wave function. Show that $\Psi(1,2)$ is an eigenfunction of

$$\hat{L}_{z,total} = \hat{L}_{z1} + \hat{L}_{z2} \text{ and } \hat{S}_{z,total} = \hat{S}_{z1} + \hat{S}_{z2}$$

What are the eigenvalues?

4. Why is distinguishing the two electrons in a helium atom impossible, but distinguishing the two electrons in separate hydrogen atoms possible? Do you think the electrons are distinguishable in the diatomic H_2 hydrogen? Explain your reasoning.

5. Considering a hypothetical universe, in which the electron has a spin of $s = 1$, and is therefore a boson. For an electron with $s = 1$, there are three spin functions, corresponding to $m_s = 1$, 0, and -1, which may be designated as α, β, and γ, respectively. The ground state configuration of helium in this universe is $1s^2$.

   a) Write out all of the acceptable trial functions for the helium in this hypothetical universe, written as the product of a 1s(1)1s(2) spatial function times acceptable spin functions. Make sure that the wave functions you write down obey the appropriate form of the generalized Pauli principle in this hypothetical universe. The spin portion of your wave function should be in terms of the spin functions $\alpha(m_s = 1)$, β ($m_s = 1$), and γ ($m_s = -1$).

   b) For each of the trial functions you wrote down above, what is the value of the projection of the total spin angular momentum vector onto the z-axis, M_s?

   c) Use the information you obtained in b) to deduce the term symbols that derive from the $1s^2$ configuration in this hypothetical universe. Be sure that your term symbol encodes the values of **L** and **S**, along with the behavior of the wave function under the inversion operation.

The following problems are not to be turned in for a grade. For practice only.

Textbook 10.5, 10.6, 10.9, 11.7, 11.11, 11.20, and 11.39