CHEM 361B - Lecture 13 Activity

Spin

1. Consider a Hydrogen atom with an electron in the $\psi_{43-1}\alpha$ state. Apply the following operators and show that the value of their classical observable is.
   (a) $\hat{L}^2$ - Total extrinsic angular momentum is $\sqrt{12}\hbar$
   (b) $\hat{L}_z$ - z-component of the extrinsic angular momentum is $-\hbar$
   (c) $\hat{S}^2$ - Total intrinsic angular momentum is $\frac{\sqrt{3}}{2}\hbar$
   (d) $\hat{S}_z$ - z-component of the intrinsic angular momentum is $\frac{1}{2}\hbar$

2. The spin states, α and β, which represent spin up, and spin down, are normalised

$$\int \alpha^* \alpha \; d\sigma = \int \beta^* \beta \; d\sigma = 1$$

These two spin states are also orthogonal

$$\int \alpha^* \beta \; d\sigma = \int \beta^* \alpha \; d\sigma = 0$$

which means that the α and β states do not overlap. In general, testing if two states are orthogonal is a similar operation as normalisation, except the result of the integral is zero:

$$\int_{all\ space} \psi_m^* \psi_n \; d\Omega = 0 \quad \text{if } \psi_m \text{ and } \psi_n \text{ are orthogonal}$$

where $d\Omega$ is a generalised infinitesimal element that represents all dimensions that are being integrated.

   (a) Using the framework from above, let $\psi_m^* = \psi_{100}^* \alpha^*$, $\psi_n = \psi_{100}\beta$ and $d\Omega = r^2 \sin\theta \; dr \; d\theta \; d\phi \; d\sigma$. Show that the two states $\psi_{100}\alpha$ and $\psi_{100}\beta$ are orthogonal.
   (b) The Pauli Exclusion Principle states that no two electrons can be in the same state. What does the above result mean for the number of electrons in the 1s orbital?

3. Spin multiplicity is the number of ways a given state of a system can arrange their electrons in near-degenerate energy levels. It is calculated by adding the total spin from each electron:

$$S = \sum_i s_i$$

Note that s_i is a vector. S is the total spin for the atom and the atom's multiplicity is $2S + 1$. For the ground state of an atom, S can alternatively be found by adding up all the unpaired electrons and multiplying the result by $\frac{1}{2}$

(a) Show that the multiplicity of an atom in the ground state with all paired electrons (for example He) is 1. This is called a singlet state.

(b) Show that the spin multiplicity of carbon in the ground state is 3. This is called a triplet state. To get the proper multiplicity, first, fill the orbitals with highest m_ℓ value with one electron each, and assign a maximal m_s to them (i.e. $+\frac{1}{2}$). Once all orbitals in a subshell have one electron, add a second one (following the same order), assigning $m_s = -\frac{1}{2}$ to them.

(c) Show that the spin multiplicity of fluorine is 2. This is called a doublet state.