Quantum Chemistry

Exercises 9

1. Just as electrons have intrinsic magnetic moments, nuclei do also, and the magnitude of a nuclear moment is given by

$$\boldsymbol{\mu} = g\frac{e}{2m_N}\mathbf{S}$$

where g is a factor characteristic of the particular nucleus, m_N is the mass of the nucleus, and **S** is the spin angular momentum of the nucleus. For example, a proton has a spin of 1/2 and g=5.5849. In a nuclear magnetic resonance experiment involving protons, the protons undergo transitions between the states m_s = -1/2 and m_s = 1/2. Calculate the frequency of radiation for such an experiment in a magnetic field of 2.0 Tesla.

2. The total z-component of the spin angular momentum for a n-electron system is

$$S_{z,Total} = \sum_{i=1}^{n} S_{zi}$$

Show that both

$$\psi = \frac{1}{\sqrt{2}}\begin{vmatrix} 1s\alpha(1) & 1s\beta(1) \\ 1s\alpha(2) & 1s\beta(2) \end{vmatrix}$$

and

$$\psi = \frac{1}{\sqrt{3!}}\begin{vmatrix} 1s\alpha(1) & 1s\beta(1) & 2s\alpha(1) \\ 1s\alpha(2) & 1s\beta(2) & 2s\alpha(2) \\ 1s\alpha(3) & 1s\beta(3) & 2s\alpha(3) \end{vmatrix}$$

are eigenfunctions of $\hat{S}_{z,Total}$

3. Consider the determinantal atomic wave function

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

where $\psi_{21\pm1}$ is a hydrogen-like wave function. Show that ⍰ is an eigenfunction of

$$\hat{L}_{z,Total} = \hat{L}_{z1} + \hat{L}_{z2}$$

and

$$\hat{S}_{z,Total} = \hat{S}_{z1} + \hat{S}_{z2}$$

What are the eigenvalues?