CHEM 190 and CHEM 290

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Homework No. 1
Due Thursday April 12 in class

1. Textbook Chapter 8 No. 4
2. Textbook Chapter 8 No. 7
3. Textbook Chapter 8 No. 15

4. To represent the two possible orientations of the spin of a single electron or proton, only two functions need be considered. These two functions are written as $\alpha$ and $\beta$ (spin up and spin down, respectively) without ever specifying the independent variable, i.e., the form of these functions. The effect of spin operators $s_x$, $s_y$, and $s_z$ is as follows:

$$s_x \alpha = \frac{1}{2} \beta, \quad s_y \alpha = \frac{i}{2} \beta, \quad s_z \alpha = \frac{1}{2} \alpha,$$

$$s_x \beta = \frac{1}{2} \alpha, \quad s_y \beta = -\frac{i}{2} \alpha, \quad s_z \beta = -\frac{1}{2} \beta.$$

Further operators are defined by

$$s_+ = s_x + is_y, \quad s_- = s_x - is_y,$$

and

$$s^2 = s_x^2 + s_y^2 + s_z^2.$$

The operators $s_+$ and $s_-$ are respectively called raising and lowering operators.

(a) Find $s_+ \alpha$, $s_+ \beta$, $s_- \alpha$, and $s_- \beta$.

(b) Find $s^2 \alpha$ and $s^2 \beta$.

(c) Find $[s_x, s_y]$, $[s_y, s_z]$, and $[s_z, s_x]$. Hint: apply the first commutator to both $\alpha$ and $\beta$ and determine what other operator has the same effect. Figure the others out by symmetry.

(d) Relate $s_+ s_-$ to $s_z^2 + s_y^2$ and a commutator and use (c) to simplify your answer.

(e) Do the same as (d) for $s_- s_+$.

(f) Use the above results to express $s^2$ in two alternative forms, both involving $s_z$ and either $s_+ s_-$ or $s_- s_+$. 

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5. To describe the spin state of an $N$-electron system, a function of $N$ variables must be specified. Such a function may always be expressed as a linear combination of products of one-electron spin functions. Again, the independent variables are not mentioned except to indicate which electrons have $\alpha$ spin and which $\beta$. An example of such a function, with $N = 3$, is $\alpha(1)\beta(2)\alpha(3)$, which is often abbreviated $\alpha\beta\alpha$. The many-electron spin operators are defined as sums of one-electron spin operators, $s_{xi}$, etc., where $s_{xi}$ acts only on the spin function of the $ith$ electron:

$$S_x = \sum_i s_{xi}, \quad S_y = \sum_i s_{yi}, \quad S_z = \sum_i s_{zi},$$

$$S_{\pm} = S_x \pm tS_y = \sum_i s_{\pm i}, \quad S^2 = S_x^2 + S_y^2 + S_z^2 \neq \sum_i s_i^2.$$

(a) Find $S_{\pm}\alpha\alpha$, $S_{\pm}\alpha\beta$, $S_{\pm}\beta\alpha$, and $S_{\pm}\beta\beta$.

(b) Find $S^2\alpha\alpha$, $S^2\alpha\beta$, $S^2\beta\alpha$, and $S^2\beta\beta$.

6. Textbook Chapter 8 No. 27

7. Textbook Chapter 8 No. 29

8. Textbook Chapter 8 No. 31