CHEM 190 and CHEM 290

K. Lindenberg and K. Baldridge — Spring 2001

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 α and β (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:

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

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

Further operators are defined by

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

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 α and β and determine what other operator has the same effect. Figure the others out by symmetry.

(d) Relate s_+s_- to $s_x^2 + s_y^2$ 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_+.

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 α spin and which β. 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:

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

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

   (a) Find $S_z\alpha\alpha$, $S_z\alpha\beta$, $S_z\beta\alpha$, and $S_z\beta\beta$.

   (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**