Paper: Quantum Mechanics & Applications (CBCS)

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Unit-VI (Many Electron Atoms)

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<u>Solved problems</u>

1. Find the value of Lande g-factor for $^3S_1$ and $^3P_1$ levels.

Solution: For the $^3S_1$ level, we have

$$L = 0, \quad S = 1, \quad J = 1$$

Lande g-factor is given by

$$g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

So
$$g = 1 + \frac{1(1+1) - 0(0+1) + 1(1+1)}{2 \times 1(1+1)}$$

$$= 1 + \frac{2 - 0 + 2}{4}$$

$$= 1 + \frac{4}{4}$$

$$= 2$$

For the $^3P_1$ level, we have

$$L = 1, \quad S = 1, \quad J = 1$$

Lande g-factor is given by

$$g = 1 + \frac{J(J+1) - L(L+1) + S(S+1)}{2J(J+1)}$$

So
$$g = 1 + \frac{1(1+1) - 1(1+1) + 1(1+1)}{2 \times 1(1+1)}$$

$$= 1 + \frac{2 - 2 + 2}{4}$$

$$= 1 + \frac{2}{4}$$

$$= \frac{3}{2}$$

2. Find the term symbol for the electronic ground state of oxygen atom.

Solution: The ground state electronic configuration of oxygen atom is

$$^8O : 1s^2 2s^2 2p^4$$

For p^4

	↑↓	↑	↑
m_l =	+1	0	−1

Here S = 1; thus (2S + 1) = 3

L = 1

So J = L + S (According to Hund's rule, when a subshell is more than half filled then highest J lies deepest)

= 1 + 1

= 2

Thus the ground state term symbol for oxygen atom is

$^{2S+1}L_J = {}^3P_2$

3. Find the terms $\{\boldsymbol{j_1},\ \boldsymbol{j_2}\}_J$ arising from $2s^1 3d^1$ electronic configuration in j-j coupling scheme.

Solution: For the s- electron: $l_1 = 0, s_1 = \frac{1}{2}\ , j_1 = \ \frac{1}{2}$

For the d- electron: $l_2 = 2, s_2 = \frac{1}{2}\ , j_2 = \ \frac{3}{2}, \frac{5}{2}$

It gives two possible (j_1, j_2) combinations: $\left(\frac{1}{2}, \frac{3}{2}\right)$ and $\left(\frac{1}{2}, \frac{5}{2}\right)$.

These combinations give the following J-values:

$\left(\frac{1}{2}, \frac{3}{2}\right)$ gives J = 1, 2

$\left(\frac{1}{2}, \frac{5}{2}\right)$ gives J = 2, 3

So the terms $\{j_1,\ j_2\}_J$ are $\left(\frac{1}{2}, \frac{3}{2}\right)_{1,2}$ and $\left(\frac{1}{2}, \frac{5}{2}\right)_{2,3}$.

4. Determine the possible terms of a one-electron atom corresponding to n = 3 and compute the angle between $\vec{L}$ and $\vec{S}$ for the term $^2D_{5/2}$.

Solution: For n = 3,

l = 0, 1, 2

and $s = \frac{1}{2}$.

So multiplicity $(2S + 1) = 2$.

The possible values of j are

$j = l \pm s$

For $l = 0,\ s = \frac{1}{2},$ $j = \frac{1}{2}$

For $l = 1,\ s = 1/2,$ $j = \frac{3}{2}, \frac{1}{2}$

For $l = 2,\ s = \frac{1}{2},$ $j = \frac{5}{2}, \frac{3}{2}$

The possible terms are

$$^2S_{1/2},\ ^2P_{3/2},\ ^2P_{1/2},\ ^2D_{5/2},\ ^2D_{3/2}$$

For the state $^2D_{5/2}$,

$$l = 2, \quad s = \frac{1}{2}\ , \quad j = \frac{5}{2}$$

So the angle between $\vec{L}$ and $\vec{S}$ is

$$\text{angle } (\vec{L}, \vec{S}) = \cos^{-1}\left[\frac{j(j+1) - l(l+1) + s(s+1)}{2\sqrt{l(l+1)}\sqrt{s(s+1)}}\right]$$

$$= \cos^{-1}\left[\frac{\frac{35}{4} - 6 - \frac{3}{4}}{2\sqrt{6 \times \frac{3}{4}}}\right]$$

$$= \cos^{-1}[0.47]$$

$$= 61.9^\circ$$

5. Which one of the following is the correct order of energies of the terms of the carbon atom in the ground state electronic configuration $s^2 2s^2 2p^2$?

(a) $^3P < {}^1D < {}^1S$

(b) $^3P < {}^1S < {}^1D$

(c) $^3P < {}^1F < {}^1S$

(d) $^3P < {}^1D < {}^1F$

Solution: The ground state electronic configuration of carbon atom is $1s^2 2s^2 2p^2$. This gives rise to the following terms:

$$^1S_0,\ ^1D_2,\ ^3P_0,\ ^3P_1,\ ^3P_2$$

According to Hund's rule, out all of the terms arising from equivalent electrons, those with largest multiplicity lie deepest. Of the terms, that with highest L value lies deepest.

Hence, the correct order of energies of the terms is

(a) $^3P < {}^1D < {}^1S$

6. The quantum numbers of the two optically active electrons in a two-valence electron atom are

$$\boldsymbol{n_1 = 6}, \qquad \boldsymbol{l_1 = 3}, \qquad \boldsymbol{s_1 = \frac{1}{2}}$$

$$\boldsymbol{n_2 = 5}, \qquad \boldsymbol{l_2 = 1}, \qquad \boldsymbol{s_2 = \frac{1}{2}}$$

Assuming $L - S$ coupling, find the possible values of L and hence of J.

Solution:

Given that for the two optical electrons, $l_1 = 3$ and $l_2 = 1$

Hence, $L = |3 - 1|$ to $|3 + 1|$

$= 2, 3, 4$

Again, it is given that $s_1 = \frac{1}{2}$ and $s_2 = \frac{1}{2}$

Hence, $S = \left|\frac{1}{2} - \frac{1}{2}\right|$ to $\left|\frac{1}{2} + \frac{1}{2}\right|$

$= 0, 1$

The possible J values are

$$J = |L - S| \text{ to } |L + S|$$

For $S = 0$ and $L = 2$, we have, $J = 2$

For $S = 0$ and $L = 3$, we have, $J = 3$

For $S = 0$ and $L = 4$, we have, $J = 4$

and

For $S = 1$ and $L = 2$, we have, $J = 1, 2, 3$

For $S = 1$ and $L = 3$, we have, $J = 2, 3, 4$

For $S = 1$ and $L = 4$, we have, $J = 3, 4, 5$