3. **The quantum numbers of two electrons in a two-valence electron atom are :**

$$n_1=6,\ l_1=3,\ s_1=\tfrac{1}{2}.$$
$$n_2=5,\ l_2=1,\ s_2=\tfrac{1}{2}.$$

(a) Assuming *L-S* coupling, find the possible values of *L* and hence of *J*. (a) Assuming *j-j* coupling, find the possible values of *J*

(Meerut 44, 79)

Solution. (a) Given that :

$$l_1=3,\ l_2=1$$

$$\therefore\quad L=|l_1-l_2|,\ |l_1-l_2|+1,\ldots\ldots\ldots(l_1+l_2)$$
$$=\mathbf{2,\ 3,\ 4.}$$

Again, $s_1=\frac{1}{2},\ s_2=\frac{1}{2}.$

$$\therefore\quad S=|s_1-s_2|,\ |s_1-s_2|+1,\ldots\ldots\ldots(s_1+s_2)$$
$$=0,\ 1.$$

Hence the J-values are :

$$J=|L-S|,\ldots\ldots\ldots(L+S)$$

For $S=0$ and $L=2, 3, 4$, we have

$$J=\mathbf{2,\ 3,\ 4.}$$

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

$$J=\mathbf{1,\ 2,\ 3\ ;\ \ 2,\ 3,\ 4\ \ and\ \ 3,\ 4,\ 5.}$$

(b) $l_1=3,\ s_1=\frac{1}{2}.$

$$\therefore\quad j_1=|l_1-s_1|,\ |l_1-s_1|+1,\ldots\ldots(l_1+s_1)$$
$$=\frac{5}{2},\ \frac{7}{2}.$$

Again, $l_2=1,\ s_2=\frac{1}{2}.$

$$\therefore\quad j_2=\frac{1}{2},\ \frac{3}{2}.$$

These give four j_1, j_2 combinations :

$$\left(\frac{1}{2},\frac{5}{2}\right);\ \left(\frac{1}{2},\frac{7}{2}\right);\ \left(\frac{3}{2},\frac{5}{2}\right);\ \left(\frac{3}{2},\frac{7}{2}\right).$$

These combinations give the following J-values :

$$\left(\frac{1}{2},\frac{5}{2}\right)\text{ gives } J=\mathbf{2,\ 3.}$$
$$\left(\frac{1}{2},\frac{7}{2}\right)\text{ gives } J=\mathbf{3,\ 4.}$$
$$\left(\frac{3}{2},\frac{5}{2}\right)\text{ gives } J=\mathbf{1,\ 2,\ 3,\ 4.}$$
$$\left(\frac{3}{2},\frac{7}{2}\right)\text{ gives } J=\mathbf{2,\ 3,\ 4,\ 5.}$$

We see that *J* values are the *same* in both cases.

4. Compute the possible terms and energy levels for a configuration with three optically active electrons 2p 3p 4d.

Solution. The configuration 2p 3p 4d is even. Let us first compute spin combinations. We have

$$s_1 = \frac{1}{2}, \; s_2 = \frac{1}{2}, \; s_3 = \frac{1}{2}.$$

On combining s_1 and s_2, we obtain $S' = 0, 1$. Then on combining s_3 with each of these S' values, we obtain

$$S = \frac{1}{2}, \frac{1}{2}, \frac{3}{2}$$

so that $$2S + 1 = 2, 2, 4,$$
which correspond to two sets of doublet terms and one set of quartet terms.

Let us now compute orbital momenta combinations. We have

$$l_1 = 1, \; l_2 = 1, \; l_3 = 2.$$

On combining l_1 and l_2, we obtain

$$L' = 0, 1, 2.$$

Combining $l_3 = 2$ to each of these L' values, we obtain

$$L = 2 \,;\, 1, 2, 3 \,;\, 0, 1, 2, 3, 4$$

which correspond to

$$D \,;\, P, D, F \,;\, S, P, D, F, G \text{ states.}$$

The possible terms are

$$^2D, {}^2D, {}^4D \,;\; {}^2P, {}^2P, {}^4P, {}^2D, {}^2D, {}^4D, {}^2F, {}^2F, {}^4F \,;$$
$$^2S, {}^2S, {}^4S, {}^2P, {}^2P, {}^4P, {}^2D, {}^2D, {}^4D, {}^2F, {}^2F, {}^4F, {}^2G, {}^2G, {}^4G$$

that is,

$^2S\,(2)$, $^2P\,(4)$, $^2D\,(6)$, $^2F\,(4)$, $^2G\,(2)$, $^4S\,(1)$, $^4P\,(2)$, $^4D\,(3)$, $^4F\,(2)$, $^4G\,(1)$
where the numbers in parentheses indicate the number of the corresponding terms.

Including spin-orbit splitting, we can write

$$^2S_{1/2}\,(2),\; {}^2P_{1/2,\,3/2}\,(4),\; {}^2D_{3/2,\,5/2}\,(6),\; {}^2F_{5/2,\,7/2}\,(4)\,;\; {}^2G_{7/2,\,9/2}\,(2),$$
$$^4S_{3/2}\,(1),\; {}^4P_{1/2,\,3/2,\,5/2}\,(2),\; {}^4D_{1/2,\,3/2,\,5/2,\,7/2}\,(3),\; {}^4F_{3/2,\,5/2,\,7/2,\,9/2}\,(2),$$
$$^4G_{5/2,\,7/2,\,9/2,\,11/2}\,(1) \,;\text{ a total of 65 levels.}$$