

Adding spins

$$S_1 \quad S_1 = \frac{1}{2} \quad |\vec{S}_1| = \sqrt{S_1(S_1+1)} \cdot \hbar = \frac{\sqrt{3}}{2} \hbar$$

and

$$S_2 \quad m_{S_1} = -\frac{1}{2} \text{ ; } +\frac{1}{2} \quad S_{1z} = m_{S_1} \cdot \hbar$$

S_2 : same

Question: $S_1 + S_2 = ?$

Answer :

$$S_1 + S_2 \left\{ \begin{array}{l} \uparrow \downarrow \quad S = S_1 + S_2 = 0 \\ \quad \quad m_s = 0 \end{array} \right\} \text{ singlet}$$
$$\left\{ \begin{array}{l} \uparrow \\ \uparrow \quad S = S_1 + S_2 = 1 \\ \quad \quad m_s = -1, 0, 1 \end{array} \right\} \text{ triplet}$$

$$\text{Multiplicity: } M = 2S + 1$$

Momentum addition generally

$$\vec{X}_1 : |\vec{X}_1| = \sqrt{X_1(X_1+1)} \cdot \hbar$$

$$m_{X_1} = -X_1, \dots, 0, \dots, X_1 \rightarrow \underbrace{(2X_1+1)}_{M_1}$$

$$\vec{X}_2 : |\vec{X}_2| = \sqrt{X_2(X_2+1)} \cdot \hbar$$

$$m_{X_2} = -X_2, \dots, 0, \dots, X_2 \rightarrow \underbrace{(2X_2+1)}_{M_2}$$

$$\vec{Y} = \vec{X}_1 + \vec{X}_2 : \text{yes, but how?}$$

$$Y = |X_1 - X_2|, \dots, \underbrace{(X_1 + X_2)}_{\text{sum}} \left. \vphantom{Y} \right\} \begin{array}{l} \text{a set of} \\ \text{possible} \\ \text{quantum} \\ \text{numbers} \end{array}$$

magnitude of the difference

$$|\vec{Y}_i| = \sqrt{Y_i(Y_i+1)} \cdot \hbar$$

$$m_{Y_i} = -Y_i, \dots, 0, \dots, Y_i$$

$$Y_{iz} = m_{Y_i} \cdot \hbar$$

Momentum addition examples

X	m_x	Y	m_Y
$\frac{1}{2}$	$+\frac{1}{2}$	0	0
$\frac{1}{2}$	$-\frac{1}{2}$	1	-1, 0, 1

X	m_x	Y	m_Y
$\frac{1}{2}$	$+\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}, \frac{1}{2}$
1	-1, 0, 1	$\frac{3}{2}$	$-\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}$

X	m_x	Y	m_Y
1	-1, 0, 1	0	0
1	-1, 0, 1	1	-1, 0, 1
		2	-2, -1, 0, 1, 2

Single electron states

$$(n, l, m_l, m_s)$$

$$L = |\vec{L}| = \sqrt{l(l+1)} \cdot \hbar ; \quad L_z = m_l \cdot \hbar$$

$$S = |\vec{S}| = \sqrt{s(s+1)} \cdot \hbar ; \quad S_z = m_s \cdot \hbar$$

$$\vec{J} = \vec{L} + \vec{S}$$

$$J = |\vec{J}| = \sqrt{j(j+1)} \cdot \hbar ; \quad J_z = m_j \cdot \hbar$$

$$(n, l, m_l, m_s) \quad \text{vs} \quad (n, l, j, m_j)$$

(j, m_j) are "better" quantum numbers than (m_l, m_s) because in magnetic spectroscopic experiments the measured or observed quantities are j and m_j .

Many electron atoms/states

$$(\vec{L}_1, \vec{S}_1), (\vec{L}_2, \vec{S}_2), \dots, (\vec{L}_n, \vec{S}_n)$$

LS-coupling (Russel-Saunders):

$$\left. \begin{aligned} \vec{L} &= \vec{L}_1 + \vec{L}_2 + \dots + \vec{L}_n \\ \vec{S} &= \vec{S}_1 + \vec{S}_2 + \dots + \vec{S}_n \end{aligned} \right\} \vec{J} = \vec{L} + \vec{S}$$

LS-coupling works better for lighter atoms with 2-3 valence electrons: the spin-orbit interaction is weak, the spin-spin correlation exchange is strong.

jj-coupling:

$$\left. \begin{aligned} \vec{J}_1 &= \vec{L}_1 + \vec{S}_1 \\ \vec{J}_2 &= \vec{L}_2 + \vec{S}_2 \\ &\vdots \\ \vec{J}_n &= \vec{L}_n + \vec{S}_n \end{aligned} \right\} \vec{J} = \vec{J}_1 + \vec{J}_2 + \dots + \vec{J}_n$$

The jj-coupling works better for heavier atoms, where the spin-orbit coupling is strong.

Spectroscopic symbols

$$n^M L_J$$

n : principal quantum number
(often dropped)

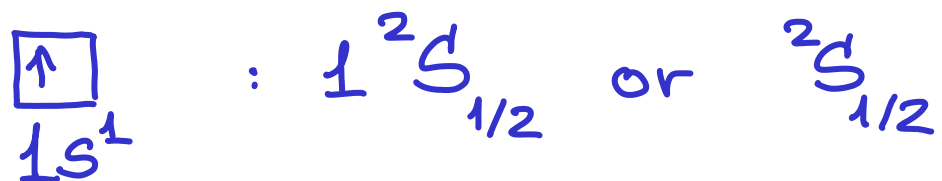
L : orbital angular momentum
(S, P, D, F, G, H)

M : multiplicity of the state
 $M = 2S + 1$; S : spin q.n.

J : total angular momentum
quantum number

Examples:

Hydrogen ground state:



Helium ground state:

