

Problem: Find CG coefficients for $\frac{1}{2} \otimes 1 = \frac{3}{2} \oplus \frac{1}{2}$ [1]

$$\begin{array}{l|l} s_1 \otimes s_2 & s \oplus s \\ \hline 2s_1 + 1 = 2 & 2s + 1 = 4 \\ 2s_2 + 1 = 3 & 2s + 1 = 2 \\ 3 \times 2 = 6 & 4 + 2 = 6 \end{array}$$

$$s_1 \otimes s_1 = s \oplus s$$

dim. of Hilbert space: 6

direct product states

$$|s_1 m_1 s_2 m_2\rangle$$

$$\underbrace{|\frac{1}{2}, \pm\frac{1}{2}\rangle}_{s_1}, \underbrace{|1, \pm 1\rangle, |1, 0\rangle}_{s_2}$$

$$\left. \begin{array}{l} |\frac{1}{2}, \frac{1}{2}; 1, -1\rangle \\ |\frac{1}{2}, \frac{1}{2}; 1, 0\rangle \\ |\frac{1}{2}, \frac{1}{2}; 1, 1\rangle \end{array} \right\} \left. \begin{array}{l} |\frac{1}{2}, -\frac{1}{2}; 1, -1\rangle \\ |\frac{1}{2}, -\frac{1}{2}; 1, 0\rangle \\ |\frac{1}{2}, -\frac{1}{2}; 1, 1\rangle \end{array} \right\} \text{Product states}$$

$$\text{Coupled states} \left\{ \begin{array}{l} |\frac{3}{2}, \frac{3}{2}\rangle \\ |\frac{3}{2}, \frac{1}{2}\rangle \\ |\frac{3}{2}, -\frac{1}{2}\rangle \\ |\frac{3}{2}, -\frac{3}{2}\rangle \end{array} \right. \left\{ \begin{array}{l} |\frac{1}{2}, \frac{1}{2}\rangle \\ |\frac{1}{2}, -\frac{1}{2}\rangle \end{array} \right.$$

$$|\frac{3}{2}, \frac{3}{2}\rangle = |\frac{1}{2}, \frac{1}{2}; 1, 1\rangle$$

$$|\frac{3}{2}, \frac{1}{2}\rangle = \sqrt{\frac{2}{3}} |\frac{1}{2}, \frac{1}{2}; 1, 0\rangle + \sqrt{\frac{1}{3}} |\frac{1}{2}, -\frac{1}{2}; 1, 1\rangle$$

$$|\frac{3}{2}, -\frac{1}{2}\rangle = \alpha \sqrt{\frac{1}{3}} |\frac{1}{2}, \frac{1}{2}; 1, -1\rangle + \beta \sqrt{\frac{2}{3}} |\frac{1}{2}, -\frac{1}{2}; 1, 0\rangle$$

$$|\frac{3}{2}, -\frac{3}{2}\rangle = |\frac{1}{2}, -\frac{1}{2}; 1, -1\rangle$$

Coupled states

$$|s m; s_1 s_2\rangle$$

$$\begin{aligned} s &= s_1 - s_2 \text{ to } s_1 + s_2 \\ &= 1 - \frac{1}{2} \text{ to } 1 + \frac{1}{2} \\ &= \frac{1}{2} \text{ to } \frac{3}{2} \end{aligned}$$

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

$$\begin{array}{cc} \swarrow & \searrow \\ m & \\ -\frac{1}{2}, \frac{1}{2} & -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2} \end{array}$$

$$|\frac{1}{2}, \frac{1}{2}\rangle = -\sqrt{\frac{1}{3}} |\frac{1}{2}, \frac{1}{2}; 1, 0\rangle + \sqrt{\frac{2}{3}} |\frac{1}{2}, -\frac{1}{2}; 1, 1\rangle$$

$$|\frac{1}{2}, -\frac{1}{2}\rangle = \alpha_1 |\frac{1}{2}, \frac{1}{2}; 1, -1\rangle + \beta_1 |\frac{1}{2}, -\frac{1}{2}; 1, 0\rangle$$

Lower half to be determined using the relation

$$\langle j_1 m_1, j_2 m_2 | j m \rangle = (-1)^{j_1 + j_2 - j} \langle j_1 -m_1, j_2 -m_2 | j -m \rangle$$

For example: For $|\frac{3}{2}, -\frac{1}{2}\rangle$

$$j_1 = \frac{1}{2}, m_1 = \frac{1}{2}, j_2 = 1, m_2 = -1$$

$$j = \frac{3}{2}, m = -\frac{1}{2}$$

$$\langle \frac{1}{2} \frac{1}{2}, 1 -1 | \frac{3}{2} -\frac{1}{2} \rangle = (-1)^{1 + \frac{1}{2} - \frac{3}{2}} \langle \frac{1}{2} -\frac{1}{2}, 1 1 | \frac{3}{2} \frac{1}{2} \rangle$$

$$= \sqrt{\frac{1}{3}}$$

Now, assemble all the relation between product states and coupled states in matrix-vector form. Elements of matrix are CG coefficients.

Addition rules for angular momentum l

Let's say N electrons with ang. mom. values

$$l_1, l_2, l_3, \dots, l_N$$

$$l_1, l_2$$

$$l_1 \leq l_2$$

ordered

$$l_1 \leq l_2 \leq \dots \leq l_N$$

$$\text{Let } l_{\text{sum}} = \sum_{i=1}^{N-1} l_i$$

$$\text{Rule is: } l_{\min} = \max(0, l_N - l_{\text{sum}})$$

$$|l_2 - l_1|$$

$$l_{\max} = \sum_{i=1}^N l_i$$

$$l_1 + l_2$$

Possible Total ang mom (squared) values

$$L^2 = \hbar^2 l(l+1)$$

$$l = |l_{\max}|, |l_{\max} - 1|, \dots, l_{\min}$$

How many states: $\sum_{l_{\min}}^{l_{\max}} 2l + 1$. You can calculate possible values of L .

Example: 2 p orbital electrons, one forbitad electron

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Symbol	s	p	d	f	g	h	...
l	0	1	2	3	4	5	...

Spectroscopic notation

$$l_1 = 1, \quad l_2 = 1, \quad l_3 = 3$$

$$l_{\text{sum}} = 1 + 1 = 2$$

$$l_{\text{min}} = \max(0, 3 - 2) = 1$$

$$l_{\text{max}} = 5$$

$$\therefore l = 1, 2, 3, 4, 5$$

$$\text{Dim. of Hilbert Space: } 3 + 5 + 7 + 9 + 11 = 35$$

Curse of dimensionality.

• Thankfully $Y_l^m(\theta, \varphi)$ are still the solution.

$l=1$ $m=-1, 0, 1$
In position representation, $Y_l^m(\theta, \varphi)$ are the solution

$$\text{ex: } \langle \theta, \varphi | l, m, l_1, l_2 \rangle = Y_l^m(\theta, \varphi) \rightarrow \text{spherical harmonics.}$$