compute CG coefficients (sketch)

$$|\hat{j}_1 \hat{j}_2 \hat{J} m\rangle = \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 m_1 m_2\rangle \, S^{\hat{j}_1 \hat{j}_2}_{m_1 m_2 \hat{J} m}$$

at $m = \hat{J}$

$$\underline{|\hat{j}_1 \hat{j}_2 \hat{J} \hat{J}\rangle = \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 m_1 m_2\rangle} \, \underbrace{S^{\hat{j}_1 \hat{j}_2}_{m_1 m_2 \hat{J} \hat{J}}}_{\equiv a_{m_1 m_2} \delta_{\hat{J}, m_1 + m_2}}$$

$$0 = \hat{J}_+ |\hat{j}_1 \hat{j}_2 \hat{J} \hat{J}\rangle = (\hat{J}_{1+} + \hat{J}_{2+}) |\hat{j}_1 \hat{j}_2 \hat{J} \hat{J}\rangle$$

$$= \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 m_1 + 1, m_2\rangle \sqrt{(\hat{j}_1 - m_1)(\hat{j}_1 + m_1 + 1)} \; a_{m_1 m_2} \delta_{\hat{J}\, m_1 + m_2}$$

$$+ \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 m_1 \, m_2 + 1\rangle \sqrt{(\hat{j}_2 - m_2)(\hat{j}_2 + m_2 + 1)} \; a_{m_1 m_2} \delta_{\hat{J}, m_1 + m_2}$$

1st term: $m_2 \to m_2' + 1$

2nd term: $m_1 \to m_1' + 1$

$$0 = \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 \, m_1 + 1 \; m_2' + 1\rangle \sqrt{(\hat{j}_1 - m_1)(\hat{j}_1 + m_1 + 1)} \; a_{m_1 m_2' + 1} \delta_{\hat{J}, m_1 + m_2' + 1}$$

$$+ \sum_{m_1 m_2} |\hat{j}_1 \hat{j}_2 \, m_1' + 1 \; m_2 + 1\rangle \sqrt{(\hat{j}_2 - m_2)(\hat{j}_2 + m_2 + 1)} \; a_{m_1 + 1 \, m_2} \delta_{\hat{J}, m_1' + m_2 + 1}$$

$$\Rightarrow \sqrt{(j_1-m_1)(j_1+m_1+1)}\ a_{m_1, m_2+1}\ \cancel{\delta_{j\, m_1+m_2+1}}$$

$$= -\sqrt{(j_2-m_2)(j_2+m_2+1)}\ a_{m_1+1, m_2}\ \cancel{\delta_{j\, m_1+m_2+1}}$$

$m_2 \to m_2 - 1$

$$\Rightarrow a_{m_1 m_2} = -\sqrt{\frac{(j_2-m_2+1)(j_2+m_2)}{(j_1-m_1)(j_1+m_1+1)}}\ a_{m_1+1\, m_2-1}$$

recursion relation for $a_{m_1 m_2}$

$$a_{m_1 m_2} = (-1)\sqrt{\frac{(j_2-m_2+1)(j_2+m_2)}{(j_1-m_1)(j_1+m_1+1)}}\ (-1)\sqrt{\frac{(j_2-m_2+2)(j_2+m_2-1)}{(j_1-m_1-1)(j_1+m_1+2)}}\ a_{m_1+2\, m_2-2}$$

$$= \cdots$$

$$= (-1)^{j_1-m_1}\sqrt{\frac{(j_1+m_1)!\,(j_2+m_2)!}{(j_1-m_1)!\,(j_2-m_2)!}}\sqrt{\frac{(j_1+j_2-j)!}{(j_2-j_1+j)!\,(2j)!}}$$

$$\times\ a_{j_1, j-j_1}$$

by normalization of $|\hat{j}_1 \hat{j}_2 \hat{j} \hat{j}\rangle$ $\qquad$ a only dep. on j

$$\Rightarrow a = \sqrt{\frac{(2\hat{j}+1)!\,(\hat{j}_1+\hat{j}_2-\hat{j})!}{(\hat{j}+\hat{j}_1+\hat{j}_2+1)!\,(\hat{j}+\hat{j}_1-\hat{j}_2)!\,(\hat{j}-\hat{j}_1+\hat{j}_2)!}}$$

$$S^{\hat{j}_1 \hat{j}_2}_{m_1 m_2 \hat{j} \underline{\underline{\hat{j}}}} = a_{m_1 m_2}\, \delta_{\hat{j}, m_1+m_2}.$$

$$= \delta_{\hat{j}, m_1+m_2} (-1)^{\hat{j}_1 - m_1} \sqrt{\frac{(2\hat{j}+1)!\,(\hat{j}_1+\hat{j}_2-\hat{j})!}{(\hat{j}+\hat{j}_1+\hat{j}_2+1)!\,(\hat{j}+\hat{j}_1-\hat{j}_2)!\,(\hat{j}-\hat{j}_1+\hat{j}_2)!}}$$

$$\times \sqrt{\frac{(\hat{j}_1+m_1)!\,(\hat{j}_2+m_2)!}{(\hat{j}_1-m_1)!\,(\hat{j}_2-m_2)!}}$$

general CG coefficients $S^{\hat{j}_1 \hat{j}_2}_{m_1 m_2 \hat{j} m}$:

$$S^{\hat{j}_1 \hat{j}_2}_{m_1 m_2 \hat{j} m} = \langle \hat{j}_1 \hat{j}_2 m_1 m_2 | \underline{\hat{j}_1 \hat{j}_2 \hat{j} m} \rangle$$

$$= \sqrt{\frac{(\hat{j}+m)!}{(2\hat{j})!\,(\hat{j}-m)!}} \langle \hat{j}_1 \hat{j}_2 m_1 m_2 | (\hat{J}_-)^{\hat{j}-m} | \hat{j}_1 \hat{j}_2 \hat{j} \hat{j} \rangle$$

$$\hat{J}_- = \hat{J}_{1-} + \hat{J}_{2-}$$

$$S^{j_1 j_2 \, *}_{m_1 m_2 j m} = \sqrt{\frac{(j+m)!}{(2j)!\,(j-m)!}} \, \underline{\underline{\langle j_1 j_2 j j |}} \underline{(\hat{J}_{1+} + \hat{J}_{2+})^{j-m}} \, \underline{| j_1 j_2 m_1 m_2 \rangle}$$

$$(\hat{J}_{1+} + \hat{J}_{2+})^{j-m} \, | j_1 j_2 m_1 m_2 \rangle$$

$$= \sum_s \frac{(j-m)!}{s!\,(j-m-s)!} \hat{J}_{1+}^{s} \, \hat{J}_{2+}^{j-m-s} \, | j_1 j_2 m_1 m_2 \rangle$$

$$= \sum_s \frac{(j-m)!}{s!\,(j-m-s)!} \underline{\underline{| j_1 j_2 \, m_1+s, \, m_2+j-m-s \rangle}}$$

$$\times \sqrt{\frac{(j_1-m_1)!\,(j_1+m_1+s)!}{(j_1-m_1-s)!\,(j_1+m_1)!}} \sqrt{\frac{(j_2-m_2)!\,(j_2+m_2+j-m-s)!}{(j_2-m_2-j+m+s)!\,(j_2+m_2)!}}$$

$$\langle j_1 j_2 j j | j_1 j_2 m_1 m_2 \rangle = \underline{S^{j_1 j_2}_{m_1 m_2 j j}}$$

$$S^{j_1 j_2}_{m_1 m_2 j m} = \delta_{m, m_1+m_2} \sqrt{(2j+1)\frac{(j_1+j_2-j)!\,(j_1-m_1)!\,(j_2-m_2)!\,(j+m)!\,(j-m)!}{(j+j_1+j_2+1)!\,(j+j_1-j_2)!\,(j-j_1+j_2)!\,(j_1+m_1)!\,(j_2+m_2)!}}$$

$$\times \sum_s (-1)^{j_1+m_1+s} \frac{(j_1+m_1+s)!\,(j+j_2-m_1-s)!}{s!\,(j-m-s)!\,(j_1-m_1-s)!\,(j_2-j+m_1+s)!}$$

Edmonds formula of CG coefficients.

$$(x)! = \begin{cases} x! & x \in \mathbb{N}_+ \\ 0 & \text{otherwise} \end{cases}$$

$\sum_s$ is a finite sum so that all $(\cdots)! \neq 0$

Relation between CG coefficients and D-matrix

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$$

rotation in $\mathcal{H}_1$ $\quad D_1(\vec{n}, \varphi)\,|j_1, m_1\rangle = e^{-\frac{i}{\hbar}\varphi \vec{n}\cdot\hat{\vec{J}}_1}\,|j_1, m_1\rangle$

$$= \sum_{m_1'} |j_1, m_1'\rangle D^{j_1}_{m_1' m_1}(\vec{n}, \varphi)$$

---, in $\mathcal{H}_2$ $\quad D_2(\vec{n},\varphi)\,|j_2 m_2\rangle = e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot\hat{\vec{J}}_2}\,|j_2 m_2\rangle$

$$= \sum_{m_2'} |j_2 m_2'\rangle\, D^{j_2}_{m_2' m_2}(\vec{n},\varphi)$$

in $\mathcal{H}_1\otimes\mathcal{H}_2$, $\quad D(\vec{n},\varphi) = D_1(\vec{n},\varphi)\otimes D_2(\vec{n},\varphi)$

$$= e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot(\hat{\vec{J}}_1+\hat{\vec{J}}_2)}$$

$$D(\vec{n},\varphi)\,\underline{|j_1 j_2 m_1 m_2\rangle} = e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot(\vec{J}_1+\vec{J}_2)}\,|j_1 j_2 m_1 m_2\rangle$$

$$= e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot\vec{J}_1}\,|j_1 m_1\rangle \otimes e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot\vec{J}_2}\,|j_2 m_2\rangle$$

$$= \sum_{m_1' m_2'} |j_1 j_2 m_1' m_2'\rangle\, \underline{D^{j_1}_{m_1' m_1}(\varphi,\vec{n})\, D^{j_2}_{m_2' m_2}(\varphi,\vec{n})}$$

$\underline{D(\vec{n},\varphi)\,|j_1 j_2 j m\rangle} = e^{-\frac{i}{\hbar}\varphi\vec{n}\cdot\underbrace{(\vec{J}_1+\vec{J}_2)}_{\vec{J}}}\,|j_1 j_2 j m\rangle$

fix $(j_1 j_2)$, fix j

$$= \underline{\sum_{m'} |j_1 j_2 j m\rangle\, \underline{D^{j}_{m' m}}(\varphi,\vec{n})}$$

$\{|j_1 j_2 j m\rangle\}_{m=-j}^{j}$

spans irrep of $SU(2)$

apply
$$|j_1 j_2 m_1 m_2\rangle = \sum_{jm} |j_1 j_2 j m\rangle \left(S^{j_1 j_2}\right)^{-1}_{\underline{jm},\, \underline{m_1 m_2}}$$

$$|j_1 j_2 j m\rangle = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle S^{j_1 j_2}_{m_1 m_2 j m}$$

$$D(Q) \, |j_1 j_2 \underline{\underline{jm}}\rangle = D(Q) \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle S^{j_1 j_2}_{m_1 m_2 j m}$$

$\uparrow$

$Q \in SU(2)$

$$= \sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \underbrace{|j_1 j_2 m_1' m_2'\rangle}_{\sum_{j'm'} |j_1 j_2 j' m'\rangle \left(S^{j_1 j_2}\right)^{-1}_{j'm'\, m_1' m_2'}} \underline{D^{j_1}_{m_1' m_1}(Q) \, D^{j_2}_{m_2' m_2}(Q)} \, S^{j_1 j_2}_{m_1 m_2 \underline{jm}}$$

$$= \sum_{j'm'} |j_1 j_2 j' m'\rangle \underbrace{\left[\sum_{\substack{m_1 m_2 \\ m_1' m_2'}} \left(S^{j_1 j_2}\right)^{-1}_{j'm'\, m_1' m_2'} D^{j_1}_{m_1' m_1}(Q) \, D^{j_2}_{m_2' m_2}(Q) \, S^{j_1 j_2}_{m_1 m_2 \underline{jm}} \right]}_{\underline{\underline{\left[S^{-1} \left(D^{j_1}(Q) \otimes D^{j_2}(Q) \right) S \right]_{j'm',\, jm}}}}$$

$$\left[\underset{=}{S}^{-1}\left(\underline{D^{j_1}(Q)\otimes D^{j_2}(Q)}\right)\underset{=}{S}\right]_{j'm',\,jm} = \delta_{jj'}\,\underline{D^{j}_{m'm}(Q)}$$

$\mathcal{H}$ is spanned by $\{|j_1 j_2 j m\rangle\}_{j=|j_1-j_2|}^{j_1+j_2}\,{}_{m=-j}^{j}$

$\uparrow$ reducible rep.

$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$

$|j_1 m_1\rangle$ $|j_2 m_2\rangle$

D^{j_1} D^{j_2}

D^{j_1}, D^{j_2} 2 irreps of $SU(2)$

$D^{j_1}\otimes D^{j_2}$ is also rep of $SU(2)$

(tensor product rep of $SU(2)$)

rep. matrix $D^{j}_{m_1' m_1}(Q)\, D^{j}_{m_2' m_2}(Q)$

$\forall\ Q \in SU(2)$

$$D^{j_1}\otimes D^{j_2} = \bigoplus_{j=|j_1-j_2|}^{j_1+j_2} D^{j}$$

decomposition of tensor product rep into irreps

How D-matrix in the irrep is expressed in terms of D-matrix in tensor product rep.

$$\sum_{j} \left(S\, D^{j}(Q)\, S^{-1} \right) = D^{j_1}(Q) \otimes D^{j_2}(Q)$$

multiply $D^{j}(Q)^*$ and integrate Q over $Q \in SU(2)$

$$S^{j_1 j_2}_{m_1' m_2' j' m'}\, S^{j_1 j_2\ -1}_{j m\, m_1 m_2}\ \frac{16\pi^2}{2j'+1},$$

$$= \int D^{j_1}_{m_1' m_1}(Q)\, D^{j}_{m_2' m_2}(Q)\, D^{j}_{m' m}(Q)^*\ dQ$$

$$dQ = \sin\beta\, d\alpha\, d\beta\, d\gamma$$

from this we can solve

$$S^{j_1 j_2}_{m_1 m_2 j m} = \delta_{m_1 + m_2\, m}$$

$$\sqrt{\frac{(2j+1)\,(j+j_1-j_2)!\,(j-j_1+j_2)!\,(j_1+j_2-j)!\,(j+m)!\,(j-m)!}{(j+j_1+j_2+1)!\,(j_1+m_1)!\,(j_1-m_1)!\,(j_2+m_2)!\,(j_2-m_2)!}}$$

$$\sum_{n} (-1)^{n+j_2+m_2}\ \frac{(j+j_2+m_1-n)!\,(j_1-m_1+n)!}{(j-j_1+j_2-n)!\,(j+m-n)!\,n!\,(n+j_1-j_2-m)!}$$

Wigner's formula of CG coefficients.

CG coefficients & 3j symbol

properties of $S^{j_1 j_2}_{m_1 m_2 j m} = \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$

1) $j_1 + j_2 + j \in$ integer , $j = j_1 + j_2 , j_1 + j_2 - 1$ $\cdots |j_1 - j_2|$

in order that $S^{j_1 j_2}_{m_1 m_2 j m} \neq 0$

triangle inequality $j_1 + j_2 - j \geq 0$

$\left.\begin{array}{l} j_1 - j_2 + j \geq 0 \\ -j_1 + j_2 + j \geq 0 \end{array}\right\}$ $j \geq |j_1 - j_2|$

$-j \leq j_1 - j_2 \leq j$

$m_1 + m_2 = m$

2) $S^{j_1 j_2}_{m_1 m_2 j m} \in \mathbb{R}$

3). unitarity $$S^{j_1 j_2}_{m_1 m_2 j m} \equiv \left(S^{j_1 j_2\, -1}\right)^*_{j m\, m_1 m_2}$$

$$S^\dagger S = S S^\dagger = 1$$

4) $$S^{j_1 j_2}_{m_1 m_2 j m} = (-1)^{j_1 + j_2 - j} S^{j_2 j_1}_{m_2 m_1 j m}$$

recurrence relation

$$\sqrt{j(j+1) - m(m+1)}\, S^{j_1 j_2}_{m_1 m_2 j m+1} = \sqrt{j_1(j_1+1) - m_1(m_1-1)}\, S^{j_1 j_2}_{m_1-1\, m_2 j m}$$
$$+ \sqrt{j_2(j_2+1) - m_2(m_2-1)}\, S^{j_1 j_2}_{m_1\, m_2-1\, j m}$$

$$\sqrt{j(j+1) - m(m-1)}\, S^{j_1 j_2}_{m_1 m_2 j m-1} = \sqrt{j_1(j_1+1) - m_1(m_1+1)}\, S^{j_1 j_2}_{m_1+1\, m_2 j m}$$
$$+ \sqrt{j_2(j_2+1) - m_2(m_2+1)}\, S^{j_1 j_2}_{m_1\, m_2+1\, j m}$$

Wigner's 3j-symbol

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \frac{(-1)^{j_1-j_2-m}}{\sqrt{2j+1}} \langle j_1 j_2 m_1 m_2 | j_1 j_2 j m \rangle$$

symmetry properties ;

- $$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}$$

- $$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_1 & j_2 & j_3 \\ m_3 & m_1 & m_2 \end{pmatrix}$$

- $$\begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix} = \begin{pmatrix} j_3 & j_2 & j_1 \\ m_3 & m_2 & m_1 \end{pmatrix}$$

$$= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

- $$\begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

change of basis

$$|j_1 j_2 j m\rangle = (-1)^{j_2 - j - m} \sum_{m_1 m_2} \sqrt{2j+1} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix}$$

$$|j_1 j_2 m_1 m_2\rangle = \sum_{jm} (-1)^{j_2 - j_1 - m} \sqrt{2j+1} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}$$

$|j_1 j_2 m_1 m_2\rangle$

$|j_1 j_2 j m\rangle$

unitarity

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = \frac{1}{2j_3+1} \delta_{j_3 j_3'} \delta_{m_3 m_3'}$$

$$\sum_{j_3 m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'}$$

Coupling 3 angular momenta

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \qquad \hat{\vec{J}}_i \circlearrowright \mathcal{H}_i$$

irrep of $SU(2)$ w/ $\hat{j}_i$

$$\vec{J} = \underline{\vec{J}_1 + \vec{J}_2} + \vec{J}_3$$

$$\vec{J} \circlearrowright \mathcal{H}$$

decoupled basis in $\mathcal{H}$

$$|\hat{j}_1 \hat{j}_2 \hat{j}_3 m_1 m_2 m_3\rangle = |\hat{j}_1 m_1\rangle \otimes |\hat{j}_2 m_2\rangle \otimes |\hat{j}_3 m_3\rangle$$

$J_i^2 \quad (J_i)_z$

$$\hat{J}_i^2 |\hat{j}_i m_i\rangle = \hbar^2 (\hat{j}_i + 1)\hat{j}_i |\hat{j}_i m_i\rangle$$

$$(\hat{J}_i)_z |\hat{j}_i m_i\rangle = \hbar m_i |\hat{j}_i m_i\rangle$$

recoupling schemes : Scheme 1 : firstly couple J_1 & J_2

$$\hat{\vec{J}}_{12} = \hat{\vec{J}}_1 + \hat{\vec{J}}_2$$

common eigenbasis $\hat{J}_1^2 \quad \hat{J}_2^2 \quad \hat{J}_{12}^2 \quad (\hat{J}_{12})_z$

$$\rightarrow \quad \underline{\underline{|j_1 j_2 \hat{j}_{12} m_{12}\rangle}} = \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle \underline{\langle \hat{j}_1 \hat{j}_2 m_1 m_2 | j_1 \hat{j}_2 \hat{j}_{12} m_{12}\rangle}$$

then couple J_{12} and J_3 : $\vec{J} = \vec{J}_{12} + \vec{J}_3$

$= J_1 + J_2 + J_3$

$|j_1 j_2 j_{12} j_3 m_{12} m_3\rangle$

$$|(j_1 j_2) j_{12} j_3 j m\rangle = \sum_{m_{12} m_3} |j_1 j_2 j_{12} m_{12}\rangle \otimes |j_3 m_3\rangle$$

common eigenbasis of $J_1^2\ J_2^2\ J_3^2\ J_{12}^2\ J^2\ J_z$

$$\langle (j_1 j_2) j_{12} j_3 m_{12} m_3 | (j_1 j_2) j_{12} j_3 j m\rangle$$

$$= \sum_{\substack{m_{12} m_3 \\ m_1 m_2}} |j_1 j_2 j_3 m_1 m_2 m_3\rangle \langle j_1 j_2 m_1 m_2 | j_1 j_2 j_{12} m_{12}\rangle \langle j_{12} j_3 m_{12} m_3 | j_{12} j_3 j m\rangle$$

Scheme 2 first $\vec{J}_{23} = \vec{J}_2 + \vec{J}_3$ then

$$\vec{J} = \vec{J}_1 + \vec{J}_{23}$$

common eigenbasis of $J_1^2\ J_2^2\ J_3^2\ J_{23}^2\ J^2\ J_z$

$$|\hat{j}_1(\hat{j}_2\hat{j}_3)\hat{j}_{23}\hat{j}m\rangle$$

$$= \sum_{\substack{m_1 m_2 m_3 \\ m_{23}}} |\hat{j}_1\hat{j}_2\hat{j}_3 m_1 m_2 m_3\rangle \langle \hat{j}_2\hat{j}_3 m_1 m_2 | \hat{j}_2\hat{j}_3\hat{j}_{23} m_{23}\rangle$$

$$\langle \hat{j}_1\hat{j}_{23} m_1 m_{23} | \hat{j}_1\hat{j}_{23}\hat{j}m\rangle$$

two orthonormal basis

$$|(\hat{j}_1\hat{j}_2)\hat{j}_3\hat{j}_{12}\hat{j}m\rangle \xleftrightarrow[\text{transf.}]{\text{unitary}} |\hat{j}_1(\hat{j}_2\hat{j}_3)\hat{j}_{23}\hat{j}m\rangle$$

$$|\hat{j}_1(\hat{j}_2\hat{j}_3)\hat{j}_{23}\hat{j}m\rangle = \sum_{\hat{j}_{12}} |(\hat{j}_1\hat{j}_2)\hat{j}_{12}\hat{j}_3\hat{j}m\rangle$$

$$\underbrace{\langle(\hat{j}_1\hat{j}_2)\hat{j}_{12}\hat{j}_3\hat{j}m|\hat{j}_1(\hat{j}_2\hat{j}_3)\hat{j}_{23}\hat{j}m\rangle}$$

$$\equiv \sqrt{(2\hat{j}_{12}+1)(2\hat{j}_{23}+1)}$$

$$W(\hat{j}_1\hat{j}_2\hat{j}\hat{j}_3;\hat{j}_{12}\hat{j}_{23})$$

$\uparrow$

Racah coefficients

explicite formula of Racah coefficients

$$W(a,b,c,d;e,f) = (-1)^{a+b+c+d} \Delta(abc)\Delta(acf) \Delta(bdf)\Delta(cde) \times$$

$$\times \sum_z \left[\frac{(-1)^z (z+1)!}{(z-a-b-c)!(z-c-d-e)!(z-a-c-f)!(z-b-d-f)!} \times \frac{1}{(a+b+c+d-z)!(a+d+e+f-z)!(b+c+e+f-z)!} \right]$$

$$\Delta(abc) = \sqrt{\frac{(a+b-c)!(a-b+c)!(b+c-a)!}{(a+b+c+1)!}}$$

6j symbol.

$$\begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} = (-1)^{a+b+c+d} W(abcd;ef)$$

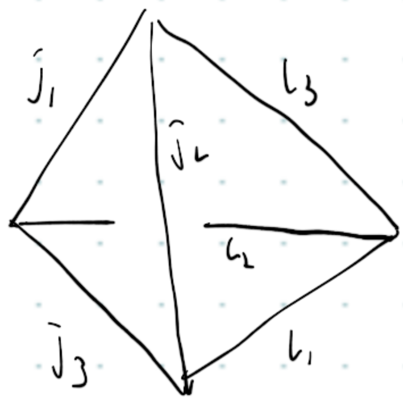
6 spins

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \quad j_i\ l_i = 0, \tfrac{1}{2}, 1, \cdots$$

(1) $\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \neq 0$ if $j_i\ l_i$ form a tetrahedron

s.t. $j_i\ l_i$ are edge lengths of

the tetrahedron



i.e. $j_1\ j_2\ j_3$ satisfy triangle inequality

$j_1\ l_2\ l_3$ ---

$j_3\ l_1\ l_2$ ---

$j_2\ l_1\ l_3$ ---

(2) inv. under permuting columns

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = \begin{Bmatrix} j_2 & j_1 & j_3 \\ l_2 & l_1 & l_3 \end{Bmatrix} = \cdots$$

(3) inv. under top-down flip in any pair of columns.

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = \begin{Bmatrix} l_1 & l_2 & j_3 \\ j_1 & j_2 & l_3 \end{Bmatrix} = \cdots$$

(4) orthogonality / unitarity

$$\sum_{j_3} (2j_3+1) \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3' \end{Bmatrix} = \frac{1}{2l_3+1} \delta_{l_3 l_3'}$$

$$\sum_{l_3} (-1)^{j_1+j_2+j_3} (2l_3+1) \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \begin{Bmatrix} j_1 & l_1 & j \\ j_2 & l_2 & l_3 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_2 & l_1 & j \end{Bmatrix}$$

(5) a formula to relate 3j symbols

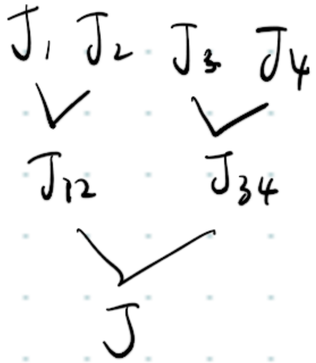
$$\sum_{\mu_1 \mu_2 \mu_3} (-1)^{l_1+l_2+l_3+\mu_1+\mu_2+\mu_3} \begin{pmatrix} j_1 & l_1 & l_2 \\ \mu_1 & \mu_2 & -\mu_3 \end{pmatrix} \begin{pmatrix} l_1 & j_2 & l_3 \\ -\mu_1 & m_2 & \mu_3 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & j_3 \\ \mu_1 & -\mu_2 & \mu_3 \end{pmatrix}$$

$$= \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix}$$

4-angular-momentum coupling & 9j symbol.

$\vec{J} = \vec{J}_1 + \vec{J}_2 + \vec{J}_3 + \vec{J}_4$ acting $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \mathcal{H}_4$ $\quad J_1^2\, J_{12}$

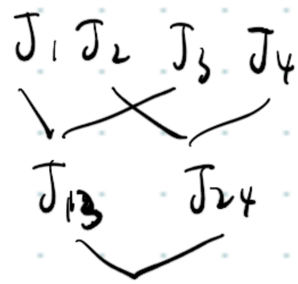
scheme 1



$J_1^2\ J_2^2\ J_{12}^2\ J_3^2\ J_4^2\ J_{34}^2\ J^2\ J_z$

$|(j_1 j_2) j_{12}\ (j_3 j_4) j_{34}\ j\ m\rangle$

scheme 2



$J_1^2\ J_3^2\ J_{13}^2\ J_2^2\ J_4^2\ J_{24}^2\ J^2\ J_z$

$|(j_1 j_3) j_{13}\ (j_2 j_4) j_{24}\ j\ m\rangle$

J

unitary transf. between 2 basis : 9j symbol.

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = \frac{1}{\sqrt{(2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1)}}$$

$$\langle (j_1 j_2) j_{12} (j_3 j_4) j_{34} j m \mid (j_1 j_3) j_{13} (j_2 j_4) j_{24} j m \rangle$$

$$= \sum_{j'} (-1)^{2j'} (2j'+1) \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_{34} & j & j' \end{Bmatrix} \begin{Bmatrix} j_3 & j_4 & j_{34} \\ j_2 & j' & j_{24} \end{Bmatrix} \begin{Bmatrix} j_{12} & j_{34} & j \\ j' & j_1 & j_3 \end{Bmatrix}$$

LS coupling & jj coupling

two electrons with obital angular momenta $\vec{L}_1, \vec{L}_2$

spin angular momenta $\vec{S}_1$ $\vec{S}_2$

total angular momentum : $\vec{J} = \vec{L}_1 + \vec{S}_1 + \vec{L}_2 + \vec{S}_2$

$$\mathcal{H} = \mathcal{H}_{L_1} \otimes \mathcal{H}_{S_1} \otimes \mathcal{H}_{L_2} \otimes \mathcal{H}_{S_2}$$

LS coupling

$$\vec{L}_1 \quad \vec{S}_1 \quad \vec{L}_2 \quad \vec{S}_2$$

$$\vec{L} \qquad \vec{S}$$

$$\vec{J}$$

$$|(l_1 l_2) L, (s_1 s_2) S\, j\, m\rangle$$

$$\equiv \underline{|L S j m\rangle}$$

jj coupling

$$\vec{L}_1 \quad \vec{S}_1 \quad \vec{L}_2 \quad \vec{S}_2$$

$$\vec{J}_1 \qquad \vec{J}_2$$

$$\vec{J}$$

$$|(l_1 s_1) j_1\, (l_2 s_2) j_2\, j\, m\rangle$$

$$\equiv |j_1 j_2\, j\, m\rangle$$

Hamiltonian

$$\hat{H} = \underline{\hat{H}_{01}} + \underline{\hat{H}_{02}} + \frac{e_1^2}{r_{12}} + \underbrace{f(r_1)\,\hat{\vec{S}}_1 \cdot \hat{\vec{L}}_1 + f(r_2)\,\hat{\vec{S}}_2 \cdot \hat{\vec{L}}_2}_{\text{spin-orbital interaction}}$$

$$r_{12} = |\vec{r}_1 - \vec{r}_2|$$

$$\hat{H}_{0i} = \frac{1}{2m}\hat{p}_i^2 + V_i(r_i)$$

$\hat{H}|\psi\rangle = E|\psi\rangle$

if $\hat{H} = \hat{H}_{01} + \hat{H}_{02} \equiv \hat{H}_0$ no interaction

commuting operators $\begin{cases} \hat{H}_0, L^2, S^2\ J^2\ J_z \rightarrow |\alpha\ \underline{LSjm}\rangle \\ \quad\quad \uparrow \text{label of radial-part wave function} \\ \hat{H}_0\ J_1^2\ J_2^2\ J^2\ J_z \rightarrow |\alpha\ j_1 j_2 j m\rangle \end{cases}$

- $\left(H_0 + \underline{\frac{e^2}{r_{12}}}\right)|\psi\rangle = E|\psi\rangle$ if $f(r_1)\ f(r_2)$ smaller than e^2

$\uparrow$ rotational inv. $\rightarrow$ commuting with $\vec{L} = \vec{L}_1 + \vec{L}_2$

commuting operators : $H_0 + \frac{e^2}{r_{12}}$, L^2, S^2, J^2, J_z

$|\psi\rangle$ is LS coupling state

$|\psi\rangle = |\alpha\ L S j m\rangle$

- $\left(H_0 + f(r_1)\vec{S}_1\cdot\vec{L}_1 + f(r_2)\vec{S}_2\cdot\vec{L}_2\right)|\psi\rangle = E|\psi\rangle$

if e^2 is smaller than $f(r_1)$, $f(r_2)$

$\vec{S}_i\cdot\vec{L}_i$ commutes with J_i^2

commuting operators ; $H = +f(r_1)\,\vec{S}_1\cdot\vec{L}_1 + f(r_2)\,\vec{S}_2\cdot\vec{L}_2$

$$= J_1^2,\ J_2^2,\ J^2,\ J_z$$

$|\psi\rangle$ is jj coupling state.

$$|\psi\rangle = |\alpha, j, j_1\, j\, m\rangle$$

Irreducible tensor operator :

tensor and tensor operator : Vector and transformation under rotation

$$v_k' = \sum_k Q(\alpha,\beta,\gamma)_{ki}\, v_i \qquad Q(\alpha,\beta,\gamma) \in SO(3)$$

$$k, i = 1,2,3$$

tensor product : $\vec{a}, \vec{b}$ vectors

rank-2 tensor : $\vec{a}\otimes\vec{b} \equiv ab$

$$(ab)_{k_1k_2} = a_{k_1} b_{k_2} \qquad \begin{pmatrix} a_1b_1 & a_1b_2 & a_1b_3 \\ a_2b_1 & a_2b_2 & a_2b_3 \\ a_3b_1 & a_3b_2 & a_3b_3 \end{pmatrix}$$

tensor transf. as :

$$\underline{(a'b')_{k_1k_2}} = a'_{k_1} b'_{k_2}$$

$$= \sum_{i_1 i_2} Q_{k_1 i_1} Q_{k_2 i_2} a_{i_1} b_{i_2}$$

$$= \sum_{i_1 i_2} Q_{k_1 i_1} Q_{k_2 i_2} \underline{(ab)_{i_1 i_2}}$$

in QM: vector operator

$$\hat{\vec{V}}' = D(Q)\,\hat{\vec{V}}\,D(Q)^{-1} = Q^{-1}\hat{\vec{V}}$$

$Q \in SO(3)$

$$D(Q)\,\hat{V}_i\,D(Q)^{-1} = \sum_j Q^{-1}_{ij}\,\hat{V}_j$$

$$= \sum_j \hat{V}_j\,Q_{ji}$$

rank-2 tensor operator $\quad D(Q)\,\hat{\tau}_{ij}\,D(Q)^{-1} = \sum_{kl} \hat{\tau}_{kl}\,Q_{ki}\,Q_{lj}$

$\hat{\tau}_{ij} = \hat{A}_i\hat{B}_j$ has $3\times3 = 9$ components,

but some linear combinations have simpler transformation rules.

- $\hat{A}_1\hat{B}_1 + \hat{A}_2\hat{B}_2 + \hat{A}_3\hat{B}_3$ is inv. under rotation

$$D(Q)\sum_i \hat{A}_i\hat{B}_i\,D(Q)^{-1} = \sum_i\sum_j \hat{A}_j Q_{ji}\sum_k \hat{B}_k Q_{ki}$$

$D(Q)^{-1}D(Q)$

$$= \sum_j \hat{A}_j\hat{B}_j$$

• $(\hat{A}_2\hat{B}_3 - \hat{A}_3\hat{B}_2,\ \hat{A}_3\hat{B}_1 - \hat{A}_1\hat{B}_3,\ \hat{A}_1\hat{B}_2 - \hat{A}_2\hat{B}_1)$

$= \hat{\vec{A}} \times \hat{\vec{B}}$ transf. as a vector.

there are parts in this tensor operator, transforming as scalar and vector.

we want to separate parts in $\hat{\tau}_{ij}$ that transf. differently.

$Q(\alpha,\beta,\gamma)$ is 3-dim irrep of $SO(3)$ carried by

$$\mathbb{R}^3 \ni \vec{v}, \vec{a}, \vec{b} \qquad \vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$$

$\cong$

$\mathcal{H}_{j=1}$

on $\mathcal{H}_{j=1}$ we have $D^{j=1}_{m'm}(\alpha,\beta,\gamma)$

$|j,m\rangle \quad m = -1, 0, 1$

unitary equivalent $\quad D^{j=1}(\alpha,\beta,\gamma) = U\, Q(\alpha,\beta,\gamma)\, U^{-1}$

$$U = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}$$

unitary transf. from x, y, z-basis to $|-1\rangle, |0\rangle, |1\rangle$

vector in $\mathbb{R}^3$ $\qquad \hat{V}'_k = \sum_i \hat{V}_i Q_{ik}$

in x, y, z basis $\rightarrow \hat{V}'_k U^{-1}_{km} = \sum_i \underline{\underline{\hat{V}_i U^{-1}_{in}}} \underbrace{U_{nl} Q_{lk}(\alpha,\beta,\gamma) U^{-1}_{km}}_{D^{j=1}_{nm}(\alpha,\beta,\gamma)}$

$$\hat{T}_m = \sum_k \hat{V}_k U^{-1}_{km}$$

$$\hat{T}'_m = \sum_k \hat{V}'_k U^{-1}_{km}$$

$$\hat{T}'_m = \sum_n T_n D^{j=1}_{nm}(\alpha,\beta,\gamma)$$

components of $\hat{\vec{V}}$ in $|-1\rangle$ $|0\rangle$, $|1\rangle$ basis

$$\left\{ \begin{aligned} \hat{T}_1 &= -\frac{1}{\sqrt{2}}(\hat{V}_1 + i\hat{V}_2) \equiv -\frac{1}{\sqrt{2}}\hat{V}_+ \\ \hat{T}_0 &= \hat{V}_3 \\ \hat{T}_{-1} &= \frac{1}{\sqrt{2}}(\hat{V}_1 - i\hat{V}_2) = \frac{1}{\sqrt{2}}\hat{V}_- \end{aligned} \right.$$

rank-2 tensor $\qquad \vec{A} \otimes \vec{B} \in \mathcal{H}_{j=1} \otimes \mathcal{H}_{j=1}$

$i, j = 1, 2, 3 \qquad \hat{A}'_i \hat{B}'_j = \sum_{kl} \hat{A}_k \hat{B}_l Q_{ki} Q_{lj}$

$$\vec{A} \to \hat{\vec{T}}_A \qquad (\hat{T}_A)_i = \sum_k \hat{A}_k U^{-1}_{ki}$$

$$(\hat{T}'_A)_m (\hat{T}'_B)_n = \sum_{kl} (\hat{T}_A)_k (\hat{T}_B)_l D^{j=1}_{km} D^{j=1}_{ln}$$

we know $D^{j_1} \otimes D^{j_2} = \bigoplus_{k=|j_1-j_2|}^{j_1+j_2} S^{-1} D^{k} S$

$$D^{j_1=1} \otimes D^{j_2=1} = D^{j=0} \oplus D^{j=1} \oplus D^{j=2}$$

scalar vector irreducible rank-2 tensor.

$$[S^{-1} D^1(Q) \otimes D^1(Q) S]_{jm', jm} = D^j_{m'm}(Q)$$

$$\sum_{m'n'} (\hat{T}_A \hat{T}_B)_{m'n'} S^{11}_{m'n' jm} \equiv [(\hat{T}_A \hat{T}_B) S]_{jm}$$

irreducible tensor opertor

$$j = 0, 1, 2$$

$$[T'_A T'_B S]_{jm} = \sum_{m'} [\hat{T}_A \hat{T}_B S]_{jm'} [\underbrace{S^{-1} (D^1 \otimes D^1) S]_{jm' jm}}$$

$D^{j}_{m'm}$

$$\underline{\hat{T}^{(j)}_{m} \equiv [\hat{T}_A \hat{T}_B S]_{jm}} \qquad j = 0, 1, 2$$

$m = -j \cdots j$

transf. of $\hat{T}^{(j)}_{m}$: $\hat{T}'^{(j)}_{m} = \sum_{m'} T^{(j)}_{m'} D^{j}_{m'm}(Q)$

irreducible transf.

$j=0$ inv. scalar 1

$$T'^{(0)}_{0} = T^{(0)}_{0}$$

$j=1$ vector 3 $T'^{(1)}_{m} = \sum_{m'} \hat{T}^{(1)}_{m'} D^{(1)}_{m'm}$

$j=2$ tensor 5 $T'^{(2)}_{m} = \sum_{m'} \hat{T}^{(2)}_{m'} D^{(2)}_{m'm}$.

$$\underline{1+3+5 = 9 = 3\times 3}$$

$$\hat{T}^{(j)}_{m} = [\hat{T}_A \hat{T}_B S]_{jm} = \sum_{i_1 i_2} \sum_{m_1 m_2} (\hat{A}\hat{B})_{i_1 i_2} (U^{-1} \otimes U^{-1})_{i_1 i_2 m_1 m_2}$$

$S^{11}_{m_1 m_2 j m}$

$$\hat{T}^{(0)} = -\frac{1}{\sqrt{3}} \hat{\vec{A}} \cdot \hat{\vec{B}}$$

$$\hat{T}^{(1)} = \begin{cases} T^{(1)}_{1} = \frac{i}{\sqrt{2}} \left(-\frac{1}{\sqrt{2}}\right) \left[(\vec{A} \times \vec{B})_x + i (\vec{A} \times \vec{B})_y\right] \\ T^{(1)}_{0} = \frac{i}{\sqrt{2}} (\vec{A} \times \vec{B})_z \\ T^{(1)}_{-1} = \frac{i}{\sqrt{2}} \frac{1}{\sqrt{2}} \left[(\vec{A} \times \vec{B})_x - i (\vec{A} \times \vec{B})_y\right] \end{cases}$$

$$\hat{T}^{(2)} = \begin{cases} T^{(2)}_{2} = \frac{1}{\sqrt{2}} A_+ B_+ \\ T^{(2)}_{1} = \frac{1}{2} (A_+ B_z + A_z B_+) \\ T^{(2)}_{0} = \frac{1}{2} \sqrt{\frac{2}{3}} (3 A_z B_z - \vec{A} \cdot \vec{B}) \\ T^{(2)}_{-1} = \frac{1}{2} (A_- B_z + A_z B_-) \\ T^{(2)}_{-2} = \frac{1}{2} A_- B_- \end{cases}$$

$$A_\pm = A_x \pm i A_y$$

Def: (irreducible tensor operators)

a rank-k irreducible tensor operator $\hat{T}^{(k)}$ is $2k+1$ operators $\hat{T}^{(k)}_{q=-k,-k+1,\dots,k-1,k}$ called the components of $\hat{T}^{(k)}$, s.t. under $SO(3)$ rotation

$$\left.\begin{aligned}\hat{T}'^{(k)}_{q} &\equiv \underline{D(Q)\,\hat{T}^{(k)}_{q}\,D(Q)^{-1}} \\ &= \sum_{q'} \hat{T}^{(k)}_{q'}\,D^{k}_{q'q}(Q)\end{aligned}\right\}$$

$\hat{T}^{(k)}_{q}$ is the tensor component in $|k, q\rangle$

- Any linear combination of $\hat{T}^{(k)}_{q}$ is still a rank-k tensor operator.

- Commutation relation with angular momentum

$$\begin{cases} [\hat{J}_{\pm}, \hat{T}^{(k)}_{q}] = \underline{\sqrt{(k\mp q)(k\pm q+1)}}\,\hbar\,\hat{T}^{(k)}_{q\pm 1} \\ [\hat{J}_{z}, T^{(k)}_{q}] = \underline{q}\hbar\, T^{(k)}_{q} \end{cases}$$

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$$

Pf infinitesimal rotation $Q(\delta\varphi, \vec{n})$

$$\hat{T}'^{(k)}_q = \underbrace{\left(1 - \frac{i}{\hbar}\delta\varphi\,\vec{n}\cdot\hat{\vec{J}}\right)\hat{T}^{(k)}_q\left(1 + \frac{i}{\hbar}\delta\varphi\,\vec{n}\cdot\hat{\vec{J}}\right)}_{D(Q)\hat{T}^{(k)}_q D(Q)^{-1}}$$

$$= \underline{\hat{T}^{(k)}_q - \frac{i}{\hbar}\delta\varphi\,\vec{n}\cdot\left[\hat{\vec{J}}, \hat{T}^{(k)}_q\right]}$$

$$\hat{T}'^{(k)}_q = \sum_{q} T^{(k)}_{q'} D^{k}_{q'q}(Q)$$

$$= \sum_{q'} \hat{T}^{(k)}_{q'} \langle kq' | e^{-\frac{i}{\hbar}\delta\varphi\,\vec{n}\cdot\hat{\vec{J}}} | kq\rangle$$

$$= \sum_{q'} \hat{T}^{(k)}_{q'}\left(\delta_{q'q} - \frac{i}{\hbar}\delta\varphi\,\vec{n}\cdot\langle kq'|\hat{\vec{J}}|kq\rangle\right)$$

$$= \underline{\hat{T}^{(k)}_q - \frac{i}{\hbar}\delta\varphi\,\vec{n}\sum_{q'}\hat{T}^{(k)}_{q'}\langle kq'|\vec{J}|kq\rangle}$$

$$[\hat{\vec{J}}, \hat{T}_q^{(k)}] = \sum_{q'} \hat{T}_{q'}^{(k)} \langle k\, q' | \hat{\vec{J}} | k\, q \rangle \quad \square$$

Direct product of irreducible tensor operators

Given 2 irreducible tensor operators $\hat{T}_{q_1}^{(k_1)}$ $\hat{U}_{q_2}^{(k_2)}$

$$\hat{X}_q^{(k)} := \sum_{q_1 q_2} \underbrace{\hat{T}_{q_1}^{(k_1)} \hat{U}_{q_2}^{(k_2)}}\, S_{q_1 q_2\, kq}^{k_1 k_2}$$

$$= \sum_{q_1 q_2} (-1)^{-k_1+k_2+q} \sqrt{2k+1}\, \hat{T}_{q_1}^{(k_1)} \hat{U}_{q_2}^{(k_2)} \times \begin{pmatrix} k_1 & k_2 & k \\ q_1 & q_2 & -q \end{pmatrix}$$

$$|k_1 - k_2| \leq k \leq k_1 + k_2$$

in short $X_q^{(k)} \equiv \left(T^{(k_1)} \otimes U^{(k_2)} \right)_q^{(k)}$

inverse formular

$$\hat{T}_{q_1}^{(k_1)} \hat{U}_{q_2}^{(k_2)} = \sum_k X_{q_1+q_2}^{(k)} S_{q_1 q_2\, k\, q_1+q_2}^{k_1 k_2}$$

check: $X^{(k)}_q$ is indeed irreducible $\quad D(Q)^{-1} D(Q)$ ✓

Pf $\underline{D(Q)\,\hat{X}^{(k)}_q\,D(Q)^{-1}} = \sum_{q_1 q_2} D(Q)\,\hat{T}^{(k_1)}_{q_1}\,U^{(k_2)}_{q_2}\,D(Q)^{-1}\; S^{k_1 k_2}_{q_1 q_2\, k q}$

since $\hat{T}, \hat{U}$ are irreducible

$$= \sum_{\substack{q_1 q_2 \\ q_1' q_2'}} \hat{T}^{(k_1)}_{q_1'}\,\hat{U}^{(k_2)}_{q_2'}\,D^{(k_1)}_{q_1' q_1}\,D^{(k_2)}_{q_2' q_2}\; S^{k_1 k_2}_{q_1 q_2\, k q}$$

$$= \sum_{q_1' q_2'} \underline{\hat{T}^{(k_1)}_{q_1'}\,\hat{U}^{(k_2)}_{q_2'}}\;\underbrace{\sum_{q_1 q_2} \underline{D^{(k_1)}_{q_1' q_1}\,D^{(k_2)}_{q_2' q_2}}\;\underline{S^{k_1 k_2}_{q_1 q_2\, k q}}}_{\sum_{q'} \underline{S^{k_1 k_2}_{q_1' q_2'\, k q}}\, D^{(k)}_{q' q}(Q)}$$

$$= \underline{\sum_{q'} X^{(k)}_{q'}\,D^{(k)}_{q' q}(Q)}$$

Invariant operator: when $\hat{T}^{(k_1)}_{q_1}$, $\hat{U}^{(k_2)}_{q_2}$ have the same rank, $k_1 = k_2 \equiv k$ $\quad 0 = |k_1 - k_2|$

We can have $\hat{X}^{(0)}_0 = \sum_{q_1 q_2} T^{(k)}_{q_1} U^{(k)}_{q_2} \underline{S^{kk}_{q_1 q_2 0 0}}$

$q_1 + q_2 = 0$

$$= \frac{1}{\sqrt{2k+1}} \sum_q (-1)^{k-q} T^{(k)}_q U^{(k)}_{-q}$$

$$\equiv \hat{T}^{(k)} \cdot \hat{U}^{(k)}$$

generalization of dot product of 3d vectors.

Wigner - Eckert Theorem

Thm suppose the eigenbasis of the Hamiltonian is

$$|\tau, j, m\rangle$$

other quantum numbers (for τ); total angular momentum (for j, m)

$\forall \ \hat{T}^{(k)}_q$ irreducible tensor operator

$$\langle \tau' j' m' | \hat{T}^{(k)}_q | \tau j m \rangle$$

$$= \underbrace{(-1)^{j'-m'} \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix}} \underbrace{\langle \tau' j' \| T^{(k)} \| \tau j \rangle}_{\text{reduced matrix element.}}$$

The result factorize the part of symmetry : 3j symbol

and the part relating to other physical properties, $\langle \tau' j' \| T^{(k)} \| \tau j \rangle$

Pf. $\underline{\langle \tau' j' m' | \underset{\downarrow\, D(\Omega)^{-1}D(\Omega)}{\hat{T}^{(k)}_q} | \underset{\downarrow\, D(\Omega)^{-1}D(\Omega)}{\tau j m} \rangle} \leftarrow \int d\Omega$

$$= \sum_{n'} \langle \tau' j' n' | D^{j'\,*}_{n'm'} \sum_{q'} \hat{T}^{(k)}_{q'} D^{(k)}_{q'q} \sum_{n} | \tau j n \rangle D^{j}_{nm}(\Omega)$$

$$= \sum_{n' n q} \underline{D^{j'\,*}_{n'm'} D^{j}_{nm}} D^{k}_{q'q} \langle \tau' j' n' | \hat{T}^{(k)}_{q'} | \tau j n \rangle$$

$$\sum_J S^{jk}_{nq'JM'} \underline{D^J_{M'M}} S^{jk}_{mqJ\underline{M}} \qquad \frac{M' = n+q'}{M = m+q}$$

the left is indep of Q, so is the right.

we integrate $Q \in SU(2)$ $\int_{SU(2)} dQ = 1$

$$\int_{SU(2)} dQ\, D^{j'}_{\mu'\nu'}(Q)\, D^{j}_{\mu\nu}(Q) = \delta_{j'j}\, \delta_{\mu'\mu}\, \delta_{\nu'\nu} \frac{1}{2j+1}$$

$$\langle \tau' j' m' | \hat{T}^{(k)}_q | \tau j m\rangle \qquad \langle \tau' j' n' | T^{(k)}_q | \tau j m\rangle$$

$$= \sum_{\substack{n'nq \\ J}} \delta_{j'J}\, \delta_{n'M'}\, \delta_{m'M} \frac{1}{2j'+1} S^{jk}_{n'q'Jn+q'} S^{jk}_{mqJm+q}$$

$M' = n+q'$, $M = m+q$, $J \to j'$

$$= \underbrace{\delta_{m'm+q} S^{jk}_{mqj'm'} \frac{1}{\sqrt{2j'+1}}}\ \boxed{\sum_{n'nq'} \delta_{n',n+q'} \frac{1}{\sqrt{2j'+1}} S^{jk}_{nq'j'n+q'} \langle \tau' j' n | T^{(k)}_{q'} | \tau j n\rangle}$$

$$= (-1)^{j'-m'} \begin{pmatrix} j' & k & j \\ -m' & q & m \end{pmatrix} \overbrace{\langle \tau' j' \| T^{(k)} \| \tau j \rangle}^{\text{indep of } m', m, q} \qquad \square$$

<u>selection rules</u> ; condition that $\langle \tau' j' m' | \hat{T}^{(k)}_q | \tau j m \rangle \neq 0$

come from $\underline{S^{jk}_{mq\, j'm'}} \neq 0$

(1) $m + q = m'$ (2) triangle inequality among $j \;\; k \;\; j'$

Example: $k = 0$ $\langle \tau' j' m' | T^{(0)}_0 | \tau j m \rangle \neq 0$

$$j' = j \quad m' = m$$

$k = 1$

$$\langle \tau' j' m' | T^{(1)}_q | \tau j m \rangle \neq 0$$

$$\Delta j \equiv j' - j = 0, \pm 1$$

$$q = m' - m = 0, \pm 1 \qquad \underline{j' + j \geq 1}$$

$k=2$

$$\langle \tau' j' m' | T^{(2)}_q | \tau j m \rangle \neq 0$$

$$\Delta j = 0, \pm 1, \pm 2$$

$$q = m' - m = 0, \pm 1, \pm 2$$

$$j' + j \geq 2$$

Given 2 irreducible tensor operators of the same rank

$$\hat{T}^{(k)}_q , \hat{U}^{(k)}_q$$

$$\frac{\langle \tau' j' m' | T^{(k)}_q | \tau j m \rangle}{\langle \tau' j' m' | U^{(k)}_q | \tau j m \rangle} = \frac{\langle \tau' j' \| T^{(k)} \| \tau j \rangle}{\langle \tau' j' \| U^{(k)} \| \tau j \rangle}$$

$$= C \quad \text{indep of } q, m, m'$$

Consider any vector operator $\hat{\vec{A}}$ and angular momentum operator $\hat{\vec{J}}$, both are irreducible.

$$\underline{\langle \tau' j' m' | \hat{\vec{A}} | \tau j m \rangle = C \langle \tau' j' m' | \hat{\vec{J}} | \tau j m \rangle}$$

to determine C :

$$\langle \tau j m | \hat{\vec{A}} \cdot \hat{\vec{J}} | \tau j m \rangle$$

$$= \sum_{\tau' m' j'} \langle \tau j m | \hat{\vec{A}} | \tau' j' m' \rangle \underbrace{\langle \tau' j' m' | \hat{\vec{J}} | \tau j m \rangle}_{\propto \delta_{\tau' \tau} \delta_{j' j}}$$

$$= \sum_{m'} \underbrace{\langle \tau j m | \hat{\vec{A}} | \tau j m' \rangle}_{C|_{\tau=\tau', j=j'} \langle \tau j m | \hat{\vec{J}} | \tau j m' \rangle} \langle \tau j m' | \hat{\vec{J}} | \tau j m \rangle$$

$$= C|_{\tau=\tau', j=j'} \underbrace{\sum_{m'} \langle \tau j m | \hat{\vec{J}} | \tau j m' \rangle \cdot \langle \tau j m' | \hat{\vec{J}} | \tau j m \rangle}_{\langle \tau j m | \hat{J}^2 | \tau j m \rangle = j(j+1)\hbar^2}$$

$$\Rightarrow C|_{\tau=\tau', j=j'} = \frac{\langle \tau j m | \vec{A} \cdot \vec{J} | \tau j m \rangle}{j(j+1)\hbar^2}$$

Landé 's formula

$$\langle \tau j m' | \vec{A} | \tau j m \rangle = \frac{\langle \tau j m | \vec{A} \cdot \vec{J} | \tau j m \rangle}{\hbar^2 j(j+1)} \langle \tau j m' | \vec{J} | \tau j m \rangle$$

Hydrogen atom in magnetic field

Hamiltonian : homogeneous magnetic field $\vec{B} = \text{const.}$

$$\vec{B} = B \hat{k}$$

vector potential $\vec{A} = \frac{1}{2} \vec{B} \times \vec{R}$

electron Hamiltonian

$$\hat{H} = -e\hat{V} + \frac{1}{2m} \hat{\pi}^2 + \frac{e}{m} \underline{\hat{\vec{S}} \cdot \hat{\vec{B}}} + \frac{e}{2m^2 c^2 r^3} \underline{\hat{\vec{S}} \cdot \hat{\vec{L}}}$$

$$\frac{1}{2m} \hat{\pi}^2 = \frac{1}{2m} (\hat{\vec{P}} + e\hat{\vec{A}})^2 = \frac{1}{2m} \hat{p}^2 + \frac{e}{m} \underline{\hat{\vec{A}} \cdot \hat{\vec{P}}} - \frac{i\hbar e}{2m} (\vec{\nabla} \cdot \vec{A}) + \frac{e^2}{2m} A^2$$

$$\underbrace{\vec{\nabla}\cdot\vec{A}=0}$$

coulomb gauge.

$$\frac{e}{m}\hat{\vec{A}}\cdot\hat{\vec{P}} = \frac{e}{2m}\hat{\vec{B}}\times\hat{\vec{R}}\cdot\hat{\vec{P}} = \frac{e}{2m}\hat{\vec{B}}\cdot\hat{\vec{R}}\times\hat{\vec{P}}$$

$$= \frac{e}{2m}\hat{\vec{B}}\cdot\hat{\vec{L}}$$

$$\vec{B} = (0, 0, B)$$

$$\hat{H} = \hat{H}_0 + \hat{H}' \qquad \hat{H}' = \hat{H}_a + \hat{H}_b$$

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e^2}{r}$$

$$\hat{H}_a = \underline{\xi(r)\,\hat{\vec{S}}\cdot\hat{\vec{L}}} \qquad \xi(r) = \frac{e}{2m^2c^2r^3}$$

$$\hat{H}_b = \frac{e}{2m}B\,(L_z + 2S_z)$$

$B=0$; fine structure of energy level. $[\vec{S}\cdot\vec{L}, L_z] \neq 0$

$[\vec{S}\cdot\vec{L}, S_z] \neq 0$

$$\hat{H} = \hat{H}_0 + \xi(r)\,\hat{\vec{S}}\cdot\hat{\vec{L}}$$

$\hat{H}_0$ commutes with $\hat{L}^2, \hat{S}^2, \hat{J}^2, \hat{L}_i\ \hat{S}_i\ \hat{J}_i$

$\hat{H}' = \xi(r)\,\hat{\vec{S}}\cdot\hat{\vec{L}}$ commutes with $\hat{S}^2, \hat{L}^2, \hat{J}^2, \hat{J}_z$

$\hat{H}, \hat{S}^2, \hat{L}^2, \hat{J}^2, \hat{J}_z$

common eigenbasis $\quad |n\, l\, s\, j\, m\rangle \quad \leftarrow$

n: radial quantum number.

perturbed eigenvalue

$$E_n' = \langle n l s j m | H' | n l s j m\rangle$$

$$= \underbrace{\langle n l | \xi(r) | n l\rangle}_{\xi_{nl}} \underbrace{\langle l s j m | \vec{S}\cdot\vec{L} | l s j m\rangle}$$

$$\vec{S}\cdot\vec{L} = \frac{1}{2}(J^2 - L^2 - S^2)$$

$$\rightarrow \frac{1}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]\hbar^2$$

$$\xi_{nl} = \frac{e^2}{2m^2c^2}\langle n l | \frac{1}{r^3} | n l\rangle$$

$$= \frac{e^2}{2m^2c^2a_0^3}\,\frac{1}{n^3(l+1)(l+\frac{1}{2})l}$$

$a_0 = \frac{\hbar^2}{me^2}$

Bohr radius.

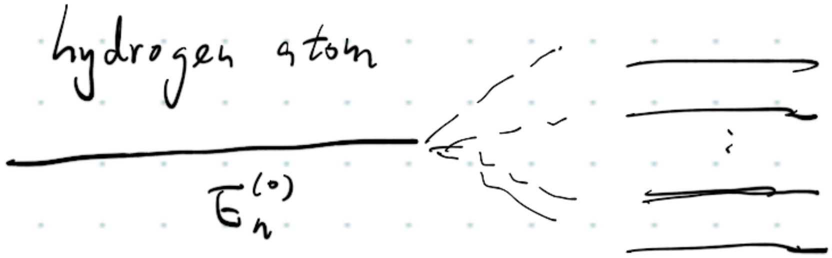
$$E_n' = \frac{\alpha^2}{n^3}\,\frac{me^4}{2\hbar^2}\,\frac{j(j+1) - l(l+1) - s(s+1)}{2l(l+1)(l+\frac{1}{2})\,l}$$

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

$\alpha = \dfrac{e^2}{\hbar c}$ fine structure const.

$= \dfrac{1}{137}$

$O(\alpha^2)$



$E_n^{(0)} + E_n'$

<u>$B \neq 0$</u> $\quad \vec{B} = B\hat{k}$

$$\hat{H} = \hat{H}_0 + \hat{H}' \qquad \hat{H}' = \xi(r)\,\hat{\vec{S}}\cdot\hat{\vec{L}} + \beta(L_z + 2S_z)$$

$$\beta = \frac{eB}{2m}$$

$$\vec{S}\cdot\vec{L} = S_z L_z - \frac{1}{2}(S_+L_- + S_-L_+)$$

$$\xi(r) = \frac{e^2}{2m^2c^2r^3}$$

$$L_\pm = L_x \pm iL_y$$

H' don't commute with J^2 $\quad [L_z, J^2] \neq 0$

$[S_z, J^2] \neq 0$

we choose to use the decoupled basis $|n l s m_l m_s\rangle$

$l = 0$

$m_l = 0$ $\quad \langle n l s \underset{0}{\underset{\shortparallel}{m_l}} m_s | H' | n l s \underset{0}{\underset{\shortparallel}{m_l'}} m_s' \rangle$

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

$m_s = \pm$

$$= \begin{pmatrix} \underline{\beta\hbar} & 0 \\ 0 & -\underline{\beta\hbar} \end{pmatrix}$$

$l = 1$ $\quad \zeta = \zeta_{nl}$

$s = \frac{1}{2}$ $\quad \langle n l s m_l m_s | H' | n l s m_l' m_s' \rangle$

$$\begin{array}{cccccc} 1+ & 1- & 0+ & 0- & -1+ & -1- \end{array}$$

$$= \begin{pmatrix} \frac{\hbar^2}{2}\zeta + 2\hbar\beta & & & & & \\ & -\frac{\hbar^2}{2}\zeta & \frac{\hbar^2}{\sqrt{2}}\zeta & & & \\ & \frac{\hbar^2}{\sqrt{2}}\zeta & \hbar\beta & & & \\ & & & \hbar\beta & \frac{\hbar^2}{\sqrt{2}}\zeta & \end{pmatrix}$$

$$\left|\begin{array}{ccc} & \frac{\hbar^2}{\sqrt{2}}\zeta & -\frac{\hbar^2}{2}\zeta \\ & & \frac{\hbar^2}{2}\zeta - 2\hbar\beta \end{array}\right|$$

Stationary Schrödinger eqn.

$$\hat{H}|\Psi\rangle = E|\Psi\rangle \qquad |\Psi\rangle = \sum_{m_l m_s} c_{m_l m_s} |n l s m_l m_s\rangle$$

$$(m_l, m_s) \equiv m$$

$$\equiv \sum_m c_m |m\rangle$$

$$\sum_m c_m \hat{H}|m\rangle = \sum_m E c_m |m\rangle$$

$$\rightarrow \sum_m c_m \langle \underbrace{m'|\hat{H}|m}_{\hat{H}_{m'm}}\rangle = \sum_m E c_m \overbrace{\langle m'|m\rangle}^{\delta_{m'm}}$$

$$\rightarrow \sum_m c_m \left(\underline{H_{m'm} - E\,\delta_{m'm}} \right) = 0$$

Secular eqn.

apply to our system: $\det\left(H_{m'm} - E\,\delta_{m'm}\right) = 0$

$$\Rightarrow \quad \frac{\hbar}{2}\mathfrak{z} - 2\beta - E = 0$$

$$\begin{vmatrix} -\frac{\hbar}{2}\mathfrak{z} - E & \frac{\hbar}{\sqrt{2}}\mathfrak{z} \\ \frac{\hbar}{\sqrt{2}}\mathfrak{z} & \beta - E \end{vmatrix} = 0$$

$$\begin{vmatrix} -\beta - E & \frac{\hbar}{\sqrt{2}}\mathfrak{z} \\ \frac{\hbar}{\sqrt{2}}\mathfrak{z} & \frac{\hbar}{\sqrt{2}}\mathfrak{z} - E \end{vmatrix} = 0$$

$$\frac{\hbar}{2}\mathfrak{z} - 2\beta - E = 0$$

solution ; perturbed energy level at $l=1$

$$E_1' = \hbar^2\mathfrak{z}\left(2\frac{\beta}{\hbar\mathfrak{z}} + \frac{1}{2}\right)$$

$$\left.\begin{matrix} E_2' \\ E_3' \end{matrix}\right\} = \frac{1}{2}\hbar^2\mathfrak{z}\left(\left[\frac{\beta}{\hbar\mathfrak{z}} - \frac{1}{2}\right] \pm \left[\left(\frac{\beta}{\hbar\mathfrak{z}}\right)^2 + \frac{\beta}{\hbar\mathfrak{z}} + \frac{9}{4}\right]^{1/2}\right.$$

$$\left.\begin{matrix} E_4' \\ E_5' \end{matrix}\right\} = \frac{1}{2}\hbar^2 \zeta \left(-\left[\frac{\beta}{\hbar\zeta} - \frac{1}{2}\right] \pm \left[\left(\frac{\beta}{\hbar\zeta}\right)^2 - \frac{\beta}{\hbar\zeta} + \frac{9}{4}\right]^{\frac{1}{2}} \right)$$

$$E_6' = \frac{1}{2}\hbar^2 \zeta \left(-\frac{\beta}{\hbar\zeta} + \frac{1}{2} \right)$$

$l \geq 2$ dimension of the matrix is very Larger

we find $[H', J_z] = 0$

m_j is a good quantum number
$\shortparallel$
$m_s + m_l$

$|n\, l\, s\, m_j - \frac{1}{2}\, \frac{1}{2}\rangle$

fix a generic m_j $\quad m_s = \frac{1}{2} \quad m_l = m_j - \frac{1}{2}$

$m_s = -\frac{1}{2} \quad m_l = m_j + \frac{1}{2}$

genenically

$|n\, l\, s\, m_j + \frac{1}{2}\, -\frac{1}{2}\rangle$

they span 2d Hilbert space $\mathcal{H}^{(n\, l\, s\, m_j)}$

$$|\psi\rangle = a_1 |n\, l\, s\, m_j - \tfrac{1}{2}\ \tfrac{1}{2}\rangle + a_2 |n\, l\, s\, m_j + \tfrac{1}{2}\ -\tfrac{1}{2}\rangle$$

$$H' = \xi\, \vec{S}\cdot\vec{L} + \beta(\hat{L}_z + 2\hat{S}_z)$$

secular eqn

$$\Rightarrow E'^{\pm}_{l m_j} = \hbar\left(\beta m_j - \frac{\hbar}{4}\xi\right) \pm \frac{\hbar}{2}\sqrt{\hbar^2 \xi (l+\tfrac{1}{2})^2 + 2\hbar\xi\beta m_j + \beta^2}$$

special case

- $m_j = l + \frac{1}{2}$ $\quad m_l \neq m_j + \frac{1}{2}$ $\qquad j = l+\frac{1}{2},\ l-\frac{1}{2}$

  only $|n\, l\, s\ m_j - \frac{1}{2}\ \ \frac{1}{2}\rangle$ $\quad \mathcal{H}^{(nlsm_j)}$ is 1d

  $$E' = \frac{\hbar}{2}\xi l + \hbar\beta(l+1)$$

- $m_j = -l - \frac{1}{2}$ $\quad m_l \neq m_j - \frac{1}{2}$

  only $|n\, l\, s\ m_j + \frac{1}{2}\ -\frac{1}{2}\rangle$ $\quad \mathcal{H}^{(nlsm_j)}$ is 1d

$$E' = -\frac{\hbar}{2}\zeta l - \hbar\beta(l+1)$$

all degeneracy of hydrogen atom disappear when $B \neq 0$ and finite

electron in external B field has no degeneracy

when magnetic field is strong $B \gg \hbar\zeta$

$$E'^{\pm} \sim \hbar\beta m_j \pm \frac{\hbar}{2}\beta$$

Example

$l=1$

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

$$\begin{cases} m_j = \frac{3}{2} & E' = 2\hbar\beta \\ m_j = \frac{1}{2} & E'^{+} = \hbar\beta \\ & E'^{-} = 0 \\ m_j = -\frac{1}{2} & E'^{+} = 0 \\ & E'^{-} = -\hbar\beta \\ m_j = -\frac{3}{2} & E' = -2\hbar\beta \end{cases}$$

$\Big\}$ degeneracy