Exchange Symmetry.

- The C.G. coefs have an important property in the coupling of identical particles.

$$\langle j\,j\,m\,m' | J M\rangle = (-1)^{J-2j} \langle j\,j\,m'\,m | J M\rangle$$

$$\therefore |j\,j\,J M\rangle = \frac{1}{2}\sum_{mm'} \left\{ |jm\rangle_1 |jm'\rangle_2 + (-1)^{J-2j} |jm'\rangle_1 |jm\rangle_2 \right. \langle j\,j\,m\,m' | J M\rangle$$

e.g. two spin ½ particles.

$$\alpha = |\tfrac{1}{2}\,\tfrac{1}{2}\rangle \qquad \beta = |\tfrac{1}{2}\,-\tfrac{1}{2}\rangle$$

$$\left.\begin{aligned} |\tfrac{1}{2}\,\tfrac{1}{2}\,1\,1\rangle &= \alpha_1\alpha_2 \\ |\tfrac{1}{2}\,\tfrac{1}{2}\,1\,0\rangle &= \tfrac{1}{\sqrt{2}}(\alpha_1\beta_2 + \beta_1\alpha_2) \\ |\tfrac{1}{2}\,\tfrac{1}{2}\,1\,-1\rangle &= \beta_1\beta_2 \end{aligned}\right\} \begin{aligned} &j_1 = j_2 = \tfrac{1}{2} \\ &J = 1 \text{ (triplet)} \\ &\text{symmetric.} \end{aligned}$$

$$|\tfrac{1}{2}\,\tfrac{1}{2}\,0\,0\rangle = \tfrac{1}{\sqrt{2}}(\alpha_1\beta_2 - \beta_1\alpha_2) \qquad J = 0 \text{ (singlet) antisym.}$$

2 equivalent p electrons.

$j_1 = j_2 = 1$

$J = 0, 1, 2$

$J = 0$	symmetric	^1S
$J = 1$	antisymmetric	^3P
$J = 2$	symmetric	^1D

^3S, ^1P, ^3D do not exist for equivalent p electrons

Coupling to form a Scalar.

The physical properties of an atom in free space are invariant under rotations and therefore transform as scalars. The construction of scalar quantities is therefore of particular importance. - i.e. quantities independent of choice of co-ordinate axes.

1. 2 Angular Momenta.

$$\overset{J\,M}{|0\,0\rangle} = \sum_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle \langle j_1 j_2 m_1 m_2 | 0\,0\rangle$$

Since $\langle j_1 j_2 m_1 m_2 | 0\,0\rangle = \delta_{j_1 j_2}\, \delta_{m_1,-m_2} \dfrac{(-1)^{j_1 - m_1}}{\sqrt{2j_1+1}}$

$$|0\,0\rangle = \frac{1}{\sqrt{2j_1+1}} \sum_{\substack{m_1\\ m_2}} |j_1 m_1\rangle |j_1 m_2\rangle \begin{pmatrix} j_1 \\ m_2\ m_1 \end{pmatrix}$$

$$\begin{pmatrix} j_1 \\ m_1\ m_2 \end{pmatrix} = (-1)^{j_1+m_1}\, \delta_{m_1,-m_2}$$

= metric tensor or 1-j symbol.

~~eg. for j = 1, $|00\rangle = \frac{-1}{\sqrt{4\pi}}(\sin^2\theta + \cos^2\theta) = \frac{-1}{\sqrt{4\pi}}$~~

eg. for $j = \frac{1}{2}$ $\quad |00\rangle = \frac{1}{\sqrt{2}} \left[\alpha(1)\beta(2) - \beta(1)\alpha(2)\right]$

$$\begin{pmatrix} j_1 \\ m_1\ m_2 \end{pmatrix} = (-1)^{2j_1} \begin{pmatrix} j_1 \\ m_2\ m_1 \end{pmatrix}$$

Since $\langle j_1, -m_1 | j_2\, m_2\rangle = \delta_{m_1,-m_2}$ (scalar), $\langle j_1, -m_1|$ transforms under rotations in the same way as $(-1)^{j_1+m_1} |j_1 m_1\rangle$

Coupling to Form a Scalar - 3D vector Analogy

- We know that quantities which are invariant under rotations are particularly important in angular momentum theory - e.g. vector recoupling calcs.

Tensors and their Transformation Properties

1st rank - vectors $x_i' = \sum_j a_{ij} x_j$

$$\sum_i a_{ij} a_{ik} = \delta_{jk} \quad \text{- orthogonality condition.}$$

2nd. rank $\quad T_{ij}' = \sum_{i',j'} a_{ii'} a_{jj'} T_{i'j'}$

Particular realization $T_{ij} = x_i y_j$ for two vectors $\vec{x}$ and $\vec{y}$.

3rd rank $\quad T_{ijk}' = \sum_{i'j'k'} a_{ii'} a_{jj'} a_{kk'} T_{i'j'k'}$

$$\text{e.g. } T_{ijk} = x_i y_j z_k$$

Formation of Scalars

$$\vec{x} \cdot \vec{y} = \sum_i x_i y_i \quad \text{in cartesian co-ords.}$$

In general $\vec{x} \cdot \vec{y} = \sum_{i,i'} x_i y_{i'} g_{ii'}$

$g_{ii'}$ = metric tensor.

In relativity, $\vec{x} = (x_1, x_2, x_3, ct)$

and $\quad \underset{\sim}{g} = \begin{pmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & -1 \end{pmatrix}$

so that $\vec{x} \cdot \vec{x} = x_1^2 + x_2^2 + x_3^2 - c^2 t^2$.

Consider $T_{ij} = x_i y_j$, $\quad U_{ji} = y_j' x_i'$

Then $\sum_{i,j} T_{ij} U_{ji} = (\vec{x}\cdot\vec{x}')(\vec{y}\cdot\vec{y}')$ is a scalar.

In general $T'_{ij} = \sum_{i'j'} a_{ii'} a_{jj'} T_{i'j'}$

$$\therefore \; T_{ij} = \sum_{i',j'} a^{-1}_{ii'} a^{-1}_{jj'} T'_{i'j'}$$

$$\therefore \; \sum_{i,j} T_{ij} U_{ji} = \sum_{\substack{i,j\\ i',j'\\ i'',j''}} a^{-1}_{ii'} a^{-1}_{jj'} T'_{i'j'} a^{-1}_{i''i} a^{-1}_{jj''} U'_{j''i''}$$

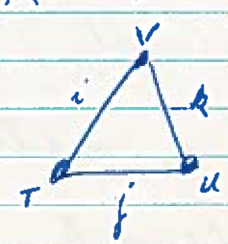
$$\delta_{i',i''} \qquad \delta_{j',j''}$$

$$= \sum_{i'j'} T'_{i'j'} U'_{j'i''}$$

Corresponds to

Similarly

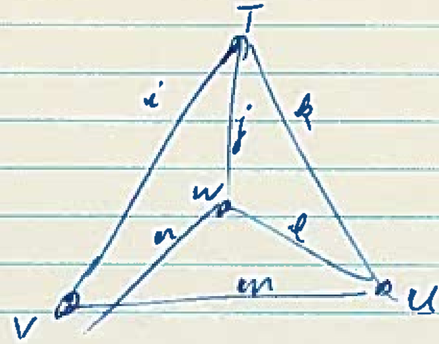
$$\sum_{i,j,k} T_{ij} U_{jk} V_{ki} = \sum_{i,j,k} T'_{ij} U'_{jk} V'_{ki}$$

$=$ 

and $\sum_{i,j,k} T_{i,j,k} U_{k,j,i} = \sum_{i,j,k} T'_{i,j,k} U'_{k,j,i}$

Products containing more than two factors are more difficult to construct.

$T_{i,j,k}\, U_{k,l,m}\, V_{m,\dots}$?



$T_{ijk}\, U_{klm}\, V_{mni}\, W_{n,l,j}$

<u>Forming scalars from vectors</u>

$\vec{x} \cdot \vec{y} \times \vec{z} = \sum_{ijk} x_i y_j z_k \, \epsilon_{ijk}$ = scalar.

3-j symbol.

Under rotations $x_i' = \sum_{i'} a_{ii'} x_{i'}$

$x_i = \sum_{i'} a_{ii'}^{-1} x_{i'}'$

$\therefore$ scalar $= \sum_{i'j'k'} x_{i'}' y_{j'}' z_{k'}' \underbrace{\sum_{ijk} a_{ii'}^{-1} a_{jj'}^{-1} a_{kk'}^{-1} \epsilon_{ijk}}_{\epsilon_{i'j'k'}'}$

transforms contragrad-iently to $x_i y_j z_k$

Except that $\underset{\sim}{a}$ is replaced by $\underset{\sim}{a}^{-1}$, $\underset{\sim}{\epsilon}$ satisfies the transformation law to be a third rank tensor. (a contragradient tensor).

1. 2 Angular Momenta

$$|00\rangle = \sum_{m_1, m_2} |j_1 m_1\rangle |j_2 m_2\rangle \langle j_1 j_2 m_1 m_2 | 00\rangle$$

Since $\langle j_1 j_2 m_1 m_2 | 00\rangle = \delta_{j_1 j_2} \delta_{m_1, -m_2} \frac{(-1)^{j_1 - m_1}}{\sqrt{2j_1+1}}$

$$|00\rangle = \frac{1}{\sqrt{2j_1+1}} \sum_{\substack{m_1\\m_2}} |j_1 m_1\rangle |j_1 m_2\rangle (-1)^{j_1 - m_1} \delta_{m_1, -m_2}$$

Define $\begin{pmatrix} j_1 \\ m_1 \quad m_2 \end{pmatrix} = (-1)^{j_1+m_1} \delta_{m_1, -m_2}$

= metric tensor or 1-j symbol.

Then $\underbrace{(-1)^{2j_1}|00\rangle}_{\text{invariant.}} = \frac{1}{\sqrt{2j_1+1}} \sum_{\substack{m_1\\m_2}} |j_1 m_1\rangle |j_1 m_2\rangle \begin{pmatrix} j_1 \\ m_1 \quad m_2 \end{pmatrix}$.

For example, in the spherical harmonic representation with $j=1$

$$|10\rangle = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$|1 \pm 1\rangle = \mp\sqrt{\frac{3}{8\pi}} \sin\theta \, e^{\pm i\varphi}$$

Then "invariant" $\propto$ $\cancel{-\frac{1}{4\pi}(\sin^2\theta + \cos^2\theta) = -\frac{1}{4\pi}}$

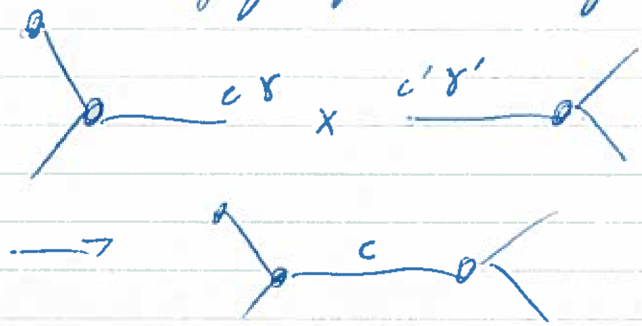
$$= -\frac{1}{4\pi}\left(\cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\varphi_1 - \varphi_2)\right)$$

$$= -\frac{1}{4\pi} \cos\theta_{12}$$

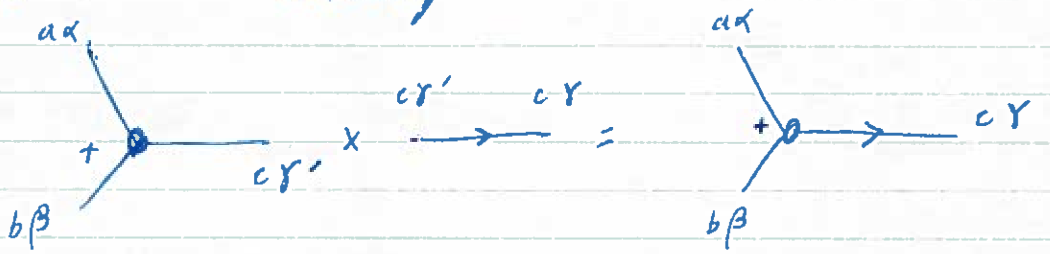
Note that $\begin{pmatrix} j_1 \\ m_1 \quad -m_1 \end{pmatrix} = (-1)^{2j_1} \begin{pmatrix} j_1 \\ -m_1 \quad m_1 \end{pmatrix}$

Examples.

- Pieces of graphs are joined together



by ~~xxx~~ setting $c' = c$, $\gamma' = \gamma$ and summing over γ. For example



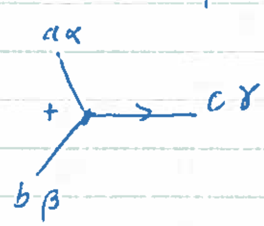
corresponds to the equation

$$\sum_{\gamma'} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma' \end{pmatrix} \begin{pmatrix} & c & \\ \gamma & & \gamma' \end{pmatrix} = (-1)^{c+\gamma} \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix}$$

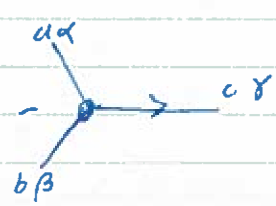
This gives a representation for the V.C. coef. since

$$\langle a b \alpha \beta | c \gamma \rangle = (-1)^{a-b+\gamma} (2c+1)^{1/2} \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix}$$

$$= (-1)^{a-b-c} (2c+1)^{1/2}$$



$$= (-1)^{2a} (2c+1)^{1/2}$$



2. 3 angular momenta

A state $|j_3, -m_3\rangle$ composed of angular momenta j_1, j_2 is represented as

$$|j_3 \, -m_3\rangle = \sum_{m_1 m_2} |j_1 m_1\rangle |j_2 m_2\rangle \langle j_1 j_2 m_1 m_2 | j_3 \, -m_3\rangle$$

But $|000\rangle = \frac{1}{\sqrt{2j_3+1}} \sum_{m_3} |j_3 m_3\rangle |j_3 \, -m_3\rangle \begin{pmatrix} & j_3 & \\ m_3 & & -m_3 \end{pmatrix}$

scalar invariant

$$= \frac{1}{\sqrt{2j_3+1}} \sum_{\substack{m_1 m_2 \\ m_3}} |j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle \langle j_1 j_2 m_1 m_2 | j_3 \, -m_3\rangle \begin{pmatrix} & j_3 & \\ m_3 & & -m_3 \end{pmatrix}$$

Define $\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 - j_2 - m_3} / \sqrt{2j_3+1} \times \langle j_1 j_2 m_1 m_2 | j_3 \, -m_3\rangle$

3-j symbol.

Then

$$\sum_{\substack{m_1 m_2 \\ m_3}} |j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$$

$$= \text{scalar invariant}$$

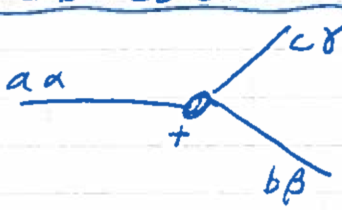
$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ is invariant under even permutations of columns and is multiplied by $(-1)^{j_1+j_2+j_3}$ for odd permutations.

- Satisfies triangular rule and $m_3 + m_1 + m_2 = 0$.

$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}$ can be regarded as the components of a tensor which transforms contragradiently to $|j_1 m_1\rangle |j_2 m_2\rangle |j_3 m_3\rangle$ under rotations.

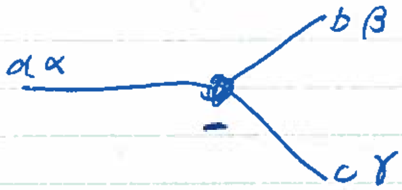
Graphical Representation

$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} =$



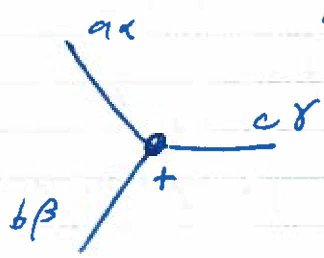
anticlockwise

$=$

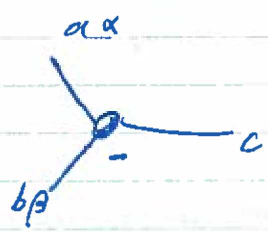


clockwise.

Sign change under odd permutations is represented by



$= (-1)^{a+b+c}$



The metric tensor is denoted by

$a\alpha \xleftarrow{\qquad} b\beta = \delta(a,b)\begin{pmatrix} a & \\ \alpha & \beta \end{pmatrix}$ | $a\alpha \xrightarrow{\qquad} b\beta = \delta_{a,b}\begin{pmatrix} a & \\ \beta & \alpha \end{pmatrix}$

$a\alpha \xleftarrow{\qquad} a,-\alpha = (-1)^{a+\alpha}$, $a\alpha \xrightarrow{\qquad} a,-\alpha = (-1)^{a-\alpha}$

also $a\alpha$ —— $b\beta$ $= \delta(ab)\delta(\alpha\beta)$

Example

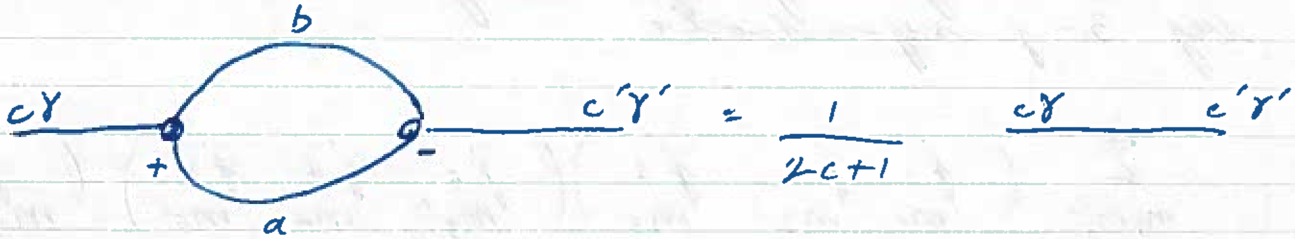
Recall that

$$\sum_{m_1m_2} \langle m_1 m_2 | JM \rangle \langle m_1 m_2 | J'M' \rangle = \delta(JJ')\delta(MM')$$

Since $\langle j_1 j_2 m_1 m_2 | J, M \rangle \times \dfrac{(-1)^{j_1-j_2-M}}{\sqrt{2J+1}} = \begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & M \end{pmatrix}$

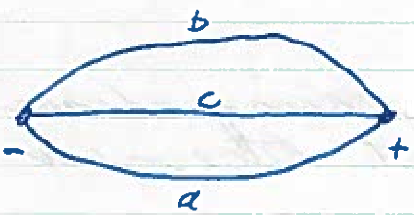
the corresponding sum rule for 3-j symbols is

$$\sum_{\alpha\beta} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} a & b & c' \\ \alpha & \beta & \gamma' \end{pmatrix} = \frac{1}{2c+1}\, \delta(cc')\, \delta(\gamma\gamma')$$



The lines a and b joining vertices imply summation over α and β. ie contractions.

Put γ′ = γ and sum over γ.

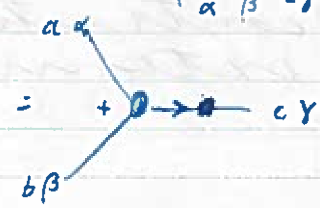


$= 1$.

contraction with the metric tensor is

$$\sum_{\gamma} \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma' \end{pmatrix} \begin{pmatrix} & c & \\ \gamma & & \gamma' \end{pmatrix} = (-1)^{c+\gamma} \begin{pmatrix} a & b & c \\ \alpha & \beta & -\gamma \end{pmatrix}$$

=



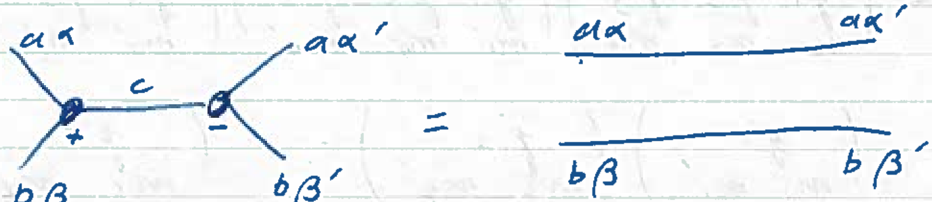
The sum rule

$$\sum_{JM} \langle m_1 m_2 | JM \rangle \langle m_1' m_2' | JM \rangle = \delta(m_1 m_1')\, \delta(m_2 m_2')$$

becomes

$$\sum_{c\gamma} (2c+1) \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma \end{pmatrix} = \delta(\alpha\alpha')\, \delta(\beta\beta')$$

$\sum_{c} (2c+1)$

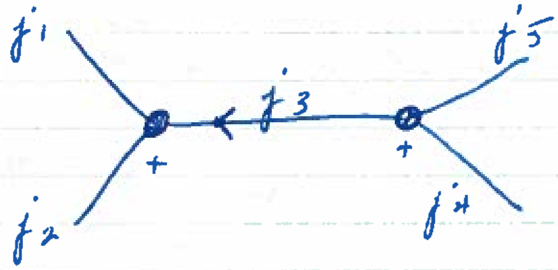


Recall that

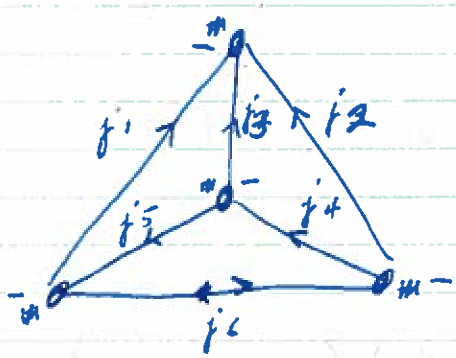
$$\sum_{m_1 m_2} |j_1 m_1\rangle\, |j_2 m_2\rangle \begin{pmatrix} & j_1 & \\ m_2 & & m_1 \end{pmatrix} = \text{scalar}.$$

Generalize by replacing state vectors by 3-j symbols.

$$\sum_{m_3 m_3'} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_3 & j_4 & j_5 \\ m_3' & m_4 & m_5 \end{pmatrix} \begin{pmatrix} & j_3 & \\ m_3 & & m_3' \end{pmatrix}$$



· Connect successively, using above contraction, so that there are no external lines.



$$= \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix}$$

$$= \sum \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_5 & j_6 \\ m_1' & m_5 & m_6' \end{pmatrix} \begin{pmatrix} j_4 & j_2 & j_6 \\ m_4' & m_2' & m_6 \end{pmatrix} \begin{pmatrix} j_4 & j_5 & j_3 \\ m_4 & m_5' & m_3' \end{pmatrix}$$

$$\begin{pmatrix} & j_1 & \\ m_1 & & m_1' \end{pmatrix} \begin{pmatrix} & j_2 & \\ m_2 & & m_2' \end{pmatrix} \cdots \begin{pmatrix} & j_6 & \\ m_6 & & m_6' \end{pmatrix}$$

Rules for Transforming Graphs.

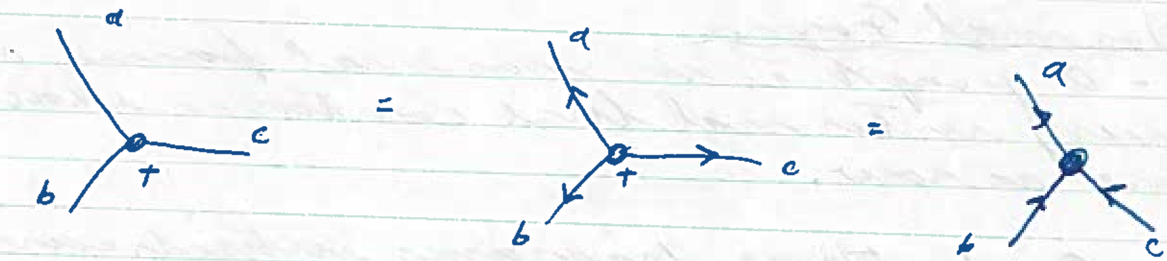
1. 

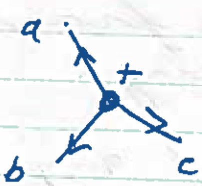
$$\sum_\beta \begin{pmatrix} a \\ \alpha' & \beta \end{pmatrix}\begin{pmatrix} a \\ \alpha & \beta \end{pmatrix} = \sum_\beta (-1)^{2a+\alpha+\alpha'}\delta(\alpha,-\beta)\delta(\alpha',-\beta)$$

$$= \delta(\alpha\alpha')$$

2. 

3. 

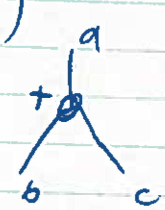
4. 



$$= \sum_{\alpha'\beta'\gamma'} \begin{pmatrix} a & b & c \\ \alpha' & \beta' & \gamma' \end{pmatrix}\begin{pmatrix} a \\ \alpha & \alpha' \end{pmatrix}\begin{pmatrix} b \\ \beta & \beta' \end{pmatrix}\begin{pmatrix} c \\ \gamma & \gamma' \end{pmatrix}$$

$$= (-1)^{a+b+c+\alpha+\beta+\gamma} \begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix}$$

$$= \begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} =$$



since $\alpha+\beta+\gamma = 0$,
$a+b+c$ = integer

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{a+b+c} \begin{pmatrix} a & b & c \\ -\alpha & -\beta & -\gamma \end{pmatrix}$$

5. Direction of all arrows or sign of all nodes may be changed in closed diagrams.

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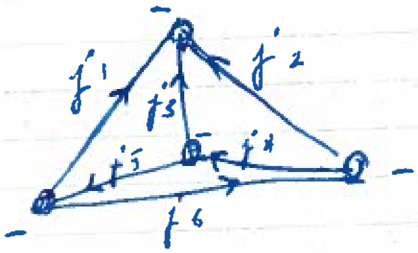
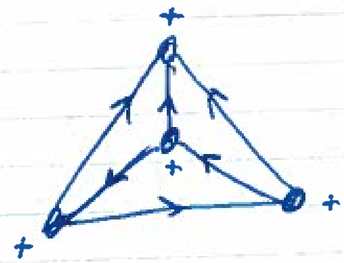
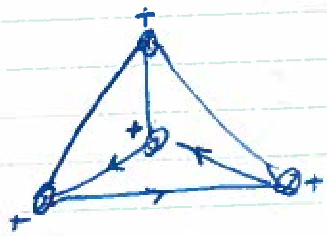
$$\therefore \begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix}$$

$=$ 

$=$ 

$=$ 

Normal Form

- A graph is in normal form if every internal line contains exactly one arrow.

Only those diagrams which can be put in normal form arise from angular momentum coupling.

- see p. 175 for graphical form of 9-j symbol.