7. Spin-orbit and double groups

7.1 Pure double group approach

We have already proved that the character of a rotation can be written

$$\chi\left(\Gamma^{l}(\phi)\right) = \frac{\sin\left[(2l+1)\,\phi/2\right]}{\sin(\phi/2)} \qquad (*)$$

A more detailed analysis of the group of rotation (left to the continuous groups chapter) shows that (*) depends only on the commutation relations between the components of the generators of rotations.
$\Rightarrow$ the same result is valid for L, S and $J = L + S$

$$\chi\left(\Gamma^{j}(\phi)\right) = \frac{\sin\left[(2j+1)\,\phi/2\right]}{\sin \phi/2}$$

Now, since l is an integer and s is an integer or an half integer, j can be integer or half integer.

$$\chi\left(\Gamma^{j}(\phi+2\pi)\right) = \frac{\sin\left[(2j+1)\,\phi/2 + (2j+1)\pi\right]}{\sin\left[(\phi+2\pi)/2\right]} =$$

$$= \frac{\sin\left[(2j+1)\,\phi/2\right]\cos\left[(2j+1)\pi\right]}{-\sin(\phi/2)} = (-1)^{2j}\,\chi\left(\Gamma^{j}(\phi)\right)$$

$\Rightarrow$ if j is half integer $\chi\left(\Gamma^{j}(\phi+2\pi)\right) = -\Gamma^{j}(\phi)$. In other words we can distinguish the rotation of an angle ϕ or $\phi + 2\pi$. In config. space this is not possible but we are dealing with SPINORBITAL!

This result suggests to introduce a new operator $\bar{E}$

$$\bar{E}R = \bar{R} = R\left((\phi + 2\pi)\,n\right)$$

Def: A <u>DOUBLE GROUP</u>: Given a group $G = \{R\}$ we define DOUBLE GROUP the group obtained by the direct sum $\bar{G} = G \oplus \bar{E}G$. $= \{R\} \cdot \bar{E}\{R\}$.

One should notice that $\bar{G}$ contains twice as many elements as G but NOT necessarily twice the number of classes.
The number of new classes in $\bar{C}$ is given by Opechowski's rules:

(1) $\bar{C}_{2\vec{n}} = \bar{E}C_{2\vec{n}}$ and $C_{2\vec{n}}$ are in the same class

iff there is in G a (proper or improper) rotation about another C_2 axis normal to $\vec{n}$.

(2) $\bar{C}_n = \bar{E}C_n$ and C_n are always in different classes $n \neq 2$

(3) For $n>2$ $\bar{C}_n^{k}$ and $\bar{C}_n^{-k}$ are in the same class as are C_n^k and C_n^{-k}

Thus now we can more conveniently write

$$\chi[R(\phi\vec{n})] = \chi^j(\phi) = \frac{\sin[(2j+1)\phi/2]}{\sin(\phi/2)}$$

$$\chi[\bar{R}(\phi\vec{n})] = \bar{\chi}^j(\phi) = (-1)^{2j}\chi^j(\phi).$$

Examples the rotations in O: C_2, C_3, C_4

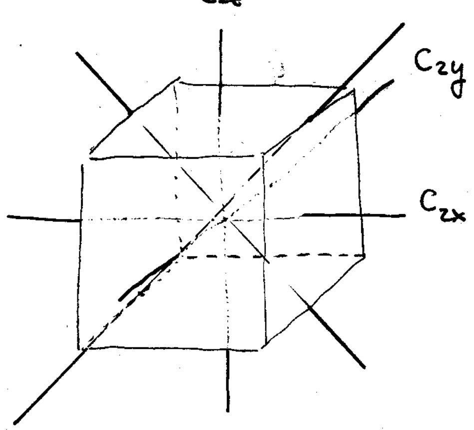
	E	C_2	C_3	C_4
ϕ	0	π	$2\pi/3$	$\pi/2$
χ^j	$2j+1$	0	$\begin{cases} 1 & j=1/2, 7/2, \dots \\ -1 & j=3/2, 9/2, \dots \\ 0 & j=5/2, 11/2 \dots \end{cases}$	$\sqrt{2}$ $(j=1/2, 9/2, \dots)$ 0 $(j=3/2, 7/2, \dots)$ $-\sqrt{2}$ $(j=5/2, 13/2, \dots)$
$j=1/2$	2	0	1	$\sqrt{2}$
$j=3/2$	4	0	-1	0
$j=5/2$	6	0	0	$-\sqrt{2}$

Dealing with improper rotations the following rules hold:

- if $I \in G \Rightarrow I\psi^j = \pm\psi^j$ ∴ $G = \{H\} \oplus I\{H\}$ $\quad \chi[\Gamma^{j\pm}(IR)] = \pm\chi[\Gamma^{j\pm}(R)]$
- if $I \notin G \Rightarrow G = \{H\} \oplus IR\{H\}$ is isomorphous with $P = \{H\} + R\{H\}$ where R is a proper rotation and $\{H\}$ is a subgroup of proper rotations $\Rightarrow$ $\chi[\Gamma^j(IR')] = \chi[\Gamma^j(R')]$
  where $R' \in R\{H\}$ and $IR' \in G$ $\quad$ (C_{3h} is an example)

<u>Examples</u> $\quad \bar{O} = \{O\} + \bar{E}\{O\}$

The classes of O are $\{E, 3C_2, 8C_3, 6C_4, 6C_2'\}$



From the Opechowski rules we know that $\bar{C}_2$ belongs to the same class of C_2 since there is C_{2x}, C_{2y}, C_{2z} which are orthogonal. The same happens to the $6\bar{C}_{2'}$. The (2) Opechowski's rule ensures instead that $8\bar{C}_3$ and $6\bar{C}_4$ are a new classes.

Summarizing

$$\bar{O} = \{E, \underset{3\bar{C}_2}{3C_2}, 8C_3, 6C_4, \underset{6\bar{C}_2'}{6C_2'}, \bar{E}, 8\bar{C}_3, 6\bar{C}_4\}$$

We have 3 new classes $\Rightarrow$ 3 new representations should appear.

$\bar{O}$	E	$3C_2$, $3\bar{C}_2$	$8C_3$	$6C_4$	$6C_2'$, $6\bar{C}_2'$	$\bar{E}$	$8\bar{C}_3$	$6\bar{C}_4$	
A_1	1	1	1	1	1	1	1	1	vector representations
A_2	1	1	1	1	-1	1	1	-1	
E	2	2	-1	0	0	2	-1	0	
T_1	3	-1	0	1	-1	3	0	-1	
T_2	3	-1	0	-1	1	3	0	-1	
$E_{1/2}$	2	0	1	$\sqrt{2}$	0	-2	-1	$-\sqrt{2}$	spinor representations
$E_{5/2}$	2	0	1	$-\sqrt{2}$	0	-2	-1	$\sqrt{2}$	
$F_{3/2}$	4	0	-1	0	0	-4	1	0	

The characters of the table are derived as follows. From the Opechowski's rules we obtain 3 further IR. From the order of $\bar{O}$ we get $l_6^2 + l_7^2 + l_8^2 = 24 \Rightarrow l_6 = 2 \quad l_7 = 2 \quad l_8 = 4$. The Mulliken notation has been extended by Herzberg including E, F, G, H representation with dimensionality 2, 4, 6, 8. The subscript is the value of j which corresponds to the representation Γ_j in which that IR first occurs. First occurs means that one uses the following argument.

$$E_{1/2} = \Gamma_{1/2} : \sum_T |\chi_{1/2}(T)|^2 = 1(4) + 8\cdot(1) + 6\cdot(2) = 24 = \bar{g}/2 \leftarrow \text{IR}$$

$$F_{3/2} \quad \Gamma_{3/2} \quad \sum_T |\chi_{3/2}(T)|^2 = 1\cdot(16) + 8(1) = 24 = \bar{g}/2 \leftarrow \text{IR}$$

$$\Gamma_{5/2} \quad \sum_T |\chi_{5/2}(T)|^2 = 1\cdot(36) + 6(2) + 6(2) = 48 > \bar{g}/2 \leftarrow \text{This representation is reducible.}$$

$\Gamma_{5/2}$ is reducible. Using the reduction formula one obtains

$$c(\Gamma_{1/2}) = 0 \qquad c(\Gamma_{3/2}) = 1$$

$$\Gamma_{5/2} - \Gamma_{3/2} = \{2\ 1\ 0\ -\sqrt{2}\ 0\ -2\ -1\ \sqrt{2}\} = E_{5/2}.$$

7.2 The geometry of rotations

(following Altmann
Rotations, Quaternions and Double Groups
Oxford 1986)

We start by saying that a generic rotation can be parametrized by an **axis** $\vec{n}$ of rotation and a rotation **angle** ϕ. It is thus conventionally taken $0 \leq \phi < 2\pi$. In reality one can shift the interval of an arbitrary angle and thus, for example assume $-\pi < \phi \leq \pi$.

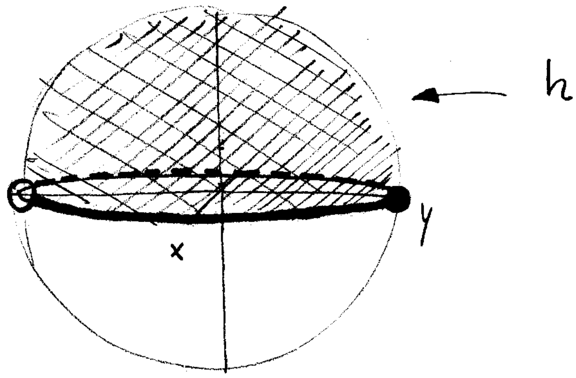
Somehow it is convenient to introduce the concept of **pole** (Sylvester 1850). Let us take a **unit sphere** (a sphere of radius 1 in coordinate space) and represent the rotations as rotations of the points of this sphere.

Def $\boxed{\text{POLE}}$ A pole of a rotation is the point of the unit sphere that is invariant under rotation and such that the rotation is seen as counterclockwise from outside the sphere.

Symbolically, for each rotation g we identify with $\Pi(g)$ the pole.

If we define the rotation with $R(\phi, \vec{n})$ it is clear that $R(\phi, \vec{n}) = R(-\phi, -\vec{n})$ and the distinction between positive and negative angles is arbitrary. Now having introduced the concept of pole $R(\phi, \vec{n})$ and $R(-\phi, \vec{n})$ have antipodal poles. More consistently we can define $R(\phi, \vec{n})$ and $R(\phi, -\vec{n})$ and take ϕ always positive. $\Pi(g)$ can belong to the positive or negative hemisphere (disjoint areas of the unit sphere) and $0 \leq \phi \leq \pi$. Let's call h the positive hemisphere and $\bar{h}$ the negative one. One possible definition:

$$(xyz) \in h \text{ if } (xyz) \in \text{unit sphere and } \begin{cases} \text{(i) } z > 0 & \text{or} \\ \text{(ii) } z = 0,\ x > 0 & \text{or} \\ \text{(iii) } z = 0,\ x = 0,\ y > 0 \end{cases}$$



The usefullness of the concept of poles can be seen for example in the calculation of conjugation classes. By definition

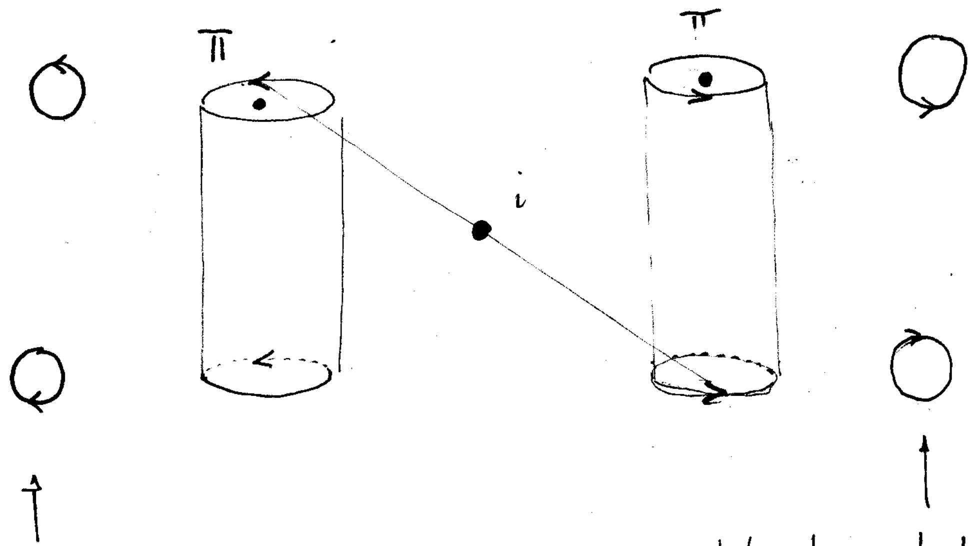
$$g_i \, \Pi(g_i) = \Pi(g_i)$$

We define $g\,\Pi(g_i) = \Pi(g_i^g)$ the conjugated pole of $\Pi(g)$ through g. As the notation anticipates

$$g_i^g \, g\,\Pi(g_i) = g g_i g^{-1} g\,\Pi(g_i) = g g_i \Pi(g_i) = g\,\Pi(g_i)$$

$\Rightarrow$ $g\,\Pi(g_i)$ is invariant under g_i^g $\Rightarrow$ $g\,\Pi(g_i) = \Pi(g_i^g)$. Let us take for example $D_3 = \{E \; 3C_2' \; 2C_3\}$ It is now clear that the 3 C_2' dihedral axis are connected by the C_3^+ and C_3^- which rotate their poles by 120°.

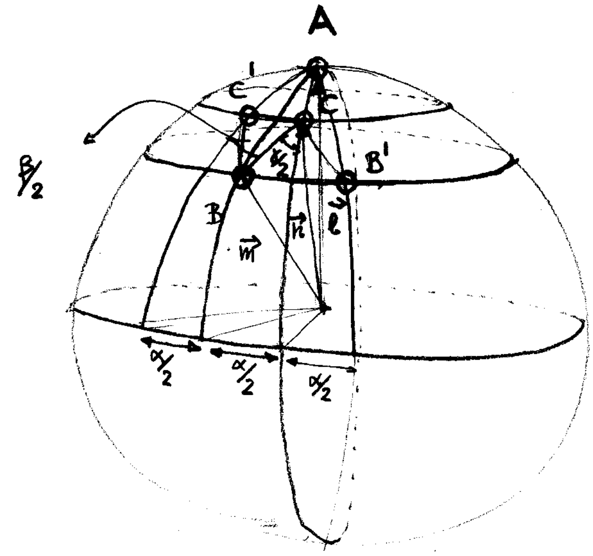
About improper rotations ig we limit ourself to say that $\Pi(g) = \Pi(ig)$



the rotation seen from outside the solid does not change under inversion.

With the concept of poles it is now also easier to understand the <u>Euler construction</u> for the product of 2 rotations:

$$R(\alpha\,\vec{n}_A)\,R(\beta\,\vec{n}_B)$$



We assume without loss of generality that $\vec{n}_A = (0,0,1) \Rightarrow$ the pole of $R(\alpha\,\vec{n}_A)$ is the north pole. Being B the pole of $R(\beta,\vec{n}_B)$ one has:

1) Join A and B with the great circle passing through both (in our case a meridian, easier to visualize)

2) Sweep the great circle left and right around each pole by half the rotation angle corresponding to the pole!

3) The four arcs cross at the points C and C'. C is the pole of the composite rotation. The angle γ of the composite rotation is twice the angle $\gamma/2$ indicated in the figure.

The proof of 3) goes as follow: $R(\gamma\,\vec{n}_C) \overset{\text{def}}{=} R(\alpha\,\vec{n}_A)\,R(\beta\,\vec{n}_B)$

- If C is the pole of the composite rotation it should be left invariant under application of $R(\beta\,\vec{n}_B)$ and $R(\alpha\,\vec{n}_A)$ in the order. Now the rotation of β around $\vec{n}_B$ brings by construction $C \to C'$ and then $R(\alpha\,\vec{n}_A)$ back to C.

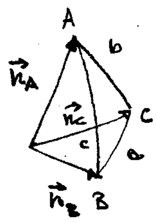
- About the angle γ let's consider the transformation of the composite rotation on the pole B. $R(\beta \vec{n}_B)$ leaves it invariant while $R(\alpha \vec{n}_A)$ takes it from B to B'. It is clear from the construction that the same effect is obtained by a rotation of γ around C.

This is the geometrical construction of the composite rotation. Using concept of spherical trigonometry it is possible to prove the following relation

$$(ER) \quad \boxed{\begin{aligned} \cos\tfrac{\gamma}{2} &= \cos\tfrac{\alpha}{2}\cos\tfrac{\beta}{2} - \sin\tfrac{\alpha}{2}\sin\tfrac{\beta}{2}\,(\vec{n}_A\cdot\vec{n}_B) \\ \sin\tfrac{\gamma}{2}\,\vec{n}_C &= \sin\tfrac{\alpha}{2}\cos\tfrac{\beta}{2}\,\vec{n}_A + \cos\tfrac{\alpha}{2}\sin\tfrac{\beta}{2}\,\vec{n}_B + \sin\tfrac{\alpha}{2}\sin\tfrac{\beta}{2}\,(\vec{n}_A\times\vec{n}_B) \end{aligned}}$$

proof

$$(*) \quad A = \frac{\alpha}{2} \qquad B = \frac{\beta}{2} \qquad C := \pi - \gamma/2$$



The proof starts with the cosine theorem of spherical trigonometry

$$\cos a = \cos b \cos c + \sin b \sin c \cos A \qquad (1)$$

[proof of the cosine theorem

$$\cos a = \vec{n}_B\cdot\vec{n}_C \qquad \cos b = \vec{n}_A\cdot\vec{n}_C \qquad \cos c = \vec{n}_A\cdot\vec{n}_B$$

$\cos A = \vec{\tau}_b\cdot\vec{\tau}_c$ where $\vec{\tau}_b$ and $\vec{\tau}_c$ are unitary vectors tangent to a and b by construction $\vec{\tau}_b$ belongs to the plane defined by $\vec{n}_A$ and $\vec{n}_c$ and it is $\perp$ to $\vec{n}_A$. Analogously for $\vec{\tau}_c$

$$\vec{\tau}_b = \frac{\vec{n}_c - (\vec{n}_c\cdot\vec{n}_A)\,\vec{n}_A}{|\vec{n}_c - (\vec{n}_c\cdot\vec{n}_A)\,\vec{n}_A|} = \frac{\vec{n}_c - \vec{n}_A\cos b}{\sqrt{(\vec{n}_c - \vec{n}_A\cos b)(\vec{n}_c - \vec{n}_A\cos b)}} = \frac{\vec{n}_c - \vec{n}_A\cos b}{\sqrt{1 - 2\cos^2 b + \cos^2 b}} = \frac{\vec{n}_c - \vec{n}_A\cos b}{\sin b}.$$

$$\vec{\tau}_c = \frac{\vec{n}_B - (\vec{n}_B\cdot\vec{n}_A)\,\vec{n}_A}{|\vec{n}_B - (\vec{n}_B\cdot\vec{n}_A)\,\vec{n}_A|} = \frac{\vec{n}_B - \cos c\,\vec{n}_A}{\sin c}$$

$$\Rightarrow \quad \cos A = \frac{\vec{n}_C - \vec{n}_A \cos b}{\sin b} \cdot \frac{\vec{n}_B - \cos c\, \vec{n}_A}{\sin c} = \frac{\cos a + \cos b \cos c - \cos b \cos c - \cos b \cos c}{\sin b \sin c}$$

$$= \frac{\cos a - \cos b \cos c}{\sin b \sin c} \qquad \square$$

First consider the supplementary triangle with dihedral angles A', B', C' and sides a', b', c' such that

$$\begin{aligned} A' + a &= a' + A = \pi \\ B' + b &= b' + B = \pi \\ C' + c &= c' + C = \pi \end{aligned} \qquad (2)$$

$$\Rightarrow \quad \cos a' \mapsto -\cos A \qquad \sin a' \mapsto \sin A \qquad \cos A' \mapsto -\cos a \qquad (3)$$

$$(1) \mapsto \quad \cos a' = \cos b' \cos c' + \sin b' \sin c' \cos A'$$

$$\Downarrow (3)$$

$$\cos A = -\cos B \cos C + \sin B \sin C \cos a$$

Now by cycling

$$\cos C = -\cos A \cos B + \sin A \sin B \cos c$$

and inserting $\cos c = \vec{n}_A \cdot \vec{n}_B$

$$(\mathrm{I}) \quad \boxed{\cos C = -\cos A \cos B + \sin A \sin B (\vec{n}_A \cdot \vec{n}_B)}$$

The task of finding $\vec{n}_C$ from A, B and $\vec{n}_A\ \vec{n}_B$ is harder. First of all one needs to get to the sin theorem:

$$\frac{\sin A}{\sin a} = \frac{\sin B}{\sin b} = \frac{\sin C}{\sin c}$$

proof of the sin theorem

$$\left(\vec{n}_A \times \vec{n}_B\right) \times \left(\vec{n}_A \times \vec{n}_C\right) = \left(\vec{n}_A \times \vec{n}_B \cdot \vec{n}_C\right)\vec{n}_A$$

as can be proven using the relations

$$\left(\vec{n}_A \times \vec{n}_B\right)_k = \sum_{ij} \varepsilon_{ijk}\, n_{Ai}\, n_{Bj} \qquad \sum_k \varepsilon_{ijk}\,\varepsilon_{nmk} = \left(\delta_{in}\delta_{jm} - \delta_{im}\delta_{jn}\right)$$

$$\left(\vec{n}_A \times \vec{n}_C\right)_n = \sum_{lm} \varepsilon_{lmn}\, n_{Al}\, n_{Cm} \qquad \varepsilon_{ijk} = \varepsilon_{kij} = \varepsilon_{jki} \qquad \varepsilon_{ijk} = -\varepsilon_{jik}$$

$$\left[\left(\vec{n}_A \times \vec{n}_B\right) \times \left(\vec{n}_A \times \vec{n}_C\right)\right]_r = \sum_{kn} \varepsilon_{knr} \sum_{ij} \varepsilon_{ijk} \sum_{lm} \varepsilon_{lmn}\, n_{Ai}\, n_{Bj}\, n_{Al}\, n_{Cm} =$$

$$= \sum_{knijlm} \varepsilon_{nrk}\,\varepsilon_{ijk}\,\varepsilon_{lmn}\, n_{Ai}\, n_{Bj}\, n_{Al}\, n_{Cm} = \sum \left(\delta_{ni}\delta_{rj} - \delta_{nj}\delta_{ri}\right)\varepsilon_{lmn}\, n_{Ai}\, n_{Bj}\, n_{Al}\, n_{Cm} =$$

$$= \underbrace{\sum_{ijlm} \varepsilon_{lmi}\, n_{Ai}\, n_{Br}\, n_{Al}\, n_{Cm}}_{=0} - \sum_{ijlm} \varepsilon_{lmj}\, n_{Ar}\, n_{Bj}\, n_{Al}\, n_{Cm} =$$

$$n_{Ai}\, n_{Br}\, n_{Al}\, n_{Cm} = n_{Al}\, n_{Br}\, n_{Ai}\, n_{Cm}$$

but $\varepsilon_{lmi} = -\varepsilon_{iml}$

$$= \sum_{ijlm} \left(\varepsilon_{ljm}\, n_{Al}\, n_{Bj}\right) n_{Cm}\, n_{Ar} = \left(\left(\vec{n}_A \times \vec{n}_B\right) \cdot \vec{n}_C\right)\vec{n}_A$$

using the fact that $|\vec{n}_A| = 1$

$$\left|\left(\vec{n}_A \times \vec{n}_B\right) \times \left(\vec{n}_A \times \vec{n}_C\right)\right| = \left|\vec{n}_A \times \vec{n}_B \cdot \vec{n}_C\right| = \left|\sum_{ijk} \varepsilon_{ijk}\, n_{Ai}\, n_{Bj}\, n_{Ck}\right|$$

$$\sin c \,\sin A\, \sin b = \left|\vec{n}_A \times \vec{n}_B \cdot \vec{n}_C\right|$$

$$\sin a\, \sin B\, \sin c = \left|\vec{n}_B \times \vec{n}_C \cdot \vec{n}_A\right|$$

$$\sin b\, \sin C\, \sin a = \left|\vec{n}_C \times \vec{n}_A \cdot \vec{n}_B\right|$$

divide by $\sin a \sin b \sin c$ end of the proof of the sin theorem. ∎

$\vec{n}_C$ can be expressed in the form

$$\vec{n}_C = f\,\vec{n}_A + g\,\vec{n}_B + h\,\underbrace{(\vec{n}_A \times \vec{n}_B)}_{\vec{n}_\perp}$$

f, g, and h can be obtained by introducing the reciprocal vectors

$$\left.\begin{aligned}
\vec{n}_A^{\,*} &= \frac{\vec{n}_B \times \vec{n}_\perp}{(\vec{n}_B \times \vec{n}_\perp)\cdot \vec{n}_A} \\
\vec{n}_B^{\,*} &= \frac{\vec{n}_\perp \times \vec{n}_A}{(\vec{n}_\perp \times \vec{n}_A)\cdot \vec{n}_B} \\
\vec{n}_\perp^{\,*} &= \frac{\vec{n}_A \times \vec{n}_B}{(\vec{n}_A \times \vec{n}_B)\cdot \vec{n}_\perp}
\end{aligned}\right\} \Rightarrow
\begin{aligned}
&\vec{n}_A^{\,*} \cdot (\vec{n}_B \text{ or } \vec{n}_\perp) = 0 \\
&\vec{n}_A \cdot \vec{n}_A^{\,*} = 1 \\
&\text{and analogously for the others} \\
&\vec{n}_\perp^{\,*} = \vec{n}_\perp
\end{aligned}$$

The normalization of the three reciprocal vectors is the same (as proven on page 76) $\Rightarrow$ we can use the one of $\vec{n}_\perp^{\,*}$

$$(\vec{n}_A \times \vec{n}_B)\cdot \vec{n}_\perp = |\vec{n}_\perp|^2 = |\vec{n}_A \times \vec{n}_B|^2 = \sin c^2 = 1 - \cos c^2 = 1 - (\vec{n}_A \cdot \vec{n}_B)^2$$

- $$f = \vec{n}_C \cdot \vec{n}_A^{\,*} = \frac{\vec{n}_C \cdot [\vec{n}_B \times (\vec{n}_A \times \vec{n}_B)]}{1 - (\vec{n}_A \cdot \vec{n}_B)^2}$$

$$\begin{aligned}
[\vec{n}_B \times (\vec{n}_A \times \vec{n}_B)]_k &= \sum_{ij} n_{Bi}\,(\vec{n}_A \times \vec{n}_B)_j\, \varepsilon_{ijk} = \sum_{\substack{ij\\lm}} n_{Bi}\, n_{Al}\, n_{Bm}\, \varepsilon_{lmj}\, \varepsilon_{ijk} = \\
&= \sum_{ijlm} n_{Bi}\, n_{Al}\, n_{Bm}\, \varepsilon_{lmj}\, \varepsilon_{kij} = \sum_{ilm} n_{Bi}\, n_{Al}\, n_{Bm}\, (\delta_{lk}\delta_{mi} - \delta_{li}\delta_{mk}) \\
&= \sum_i n_{Bi}\, n_{Ak}\, n_{Bi} - \sum_i n_{Bi}\, n_{Ai}\, n_{Bk} = \cancel{|\vec{n}_B|}\left(\vec{n}_A - (\vec{n}_A \cdot \vec{n}_B)\,\vec{n}_B\right)_k
\end{aligned}$$

$$f = \frac{\vec{n}_A \cdot \vec{n}_C - (\vec{n}_A \cdot \vec{n}_B)(\vec{n}_B \cdot \vec{n}_C)}{1 - (\vec{n}_A \cdot \vec{n}_B)^2}$$

• $g = \vec{n}_C \cdot \vec{n}_B^{\,*} = \dfrac{\vec{n}_C \cdot \left[(\vec{n}_A \times \vec{n}_B) \times \vec{n}_A \right]}{1 - (\vec{n}_A \cdot \vec{n}_B)^2} = \dfrac{\vec{n}_B \cdot \vec{n}_C - (\vec{n}_A \cdot \vec{n}_B)(\vec{n}_A \cdot \vec{n}_C)}{1 - (\vec{n}_A \cdot \vec{n}_B)^2}$

$$\left[(\vec{n}_A \times \vec{n}_B) \times \vec{n}_A \right] = \left[\vec{n}_A \times (\vec{n}_B \times \vec{n}_A) \right] = \vec{n}_B - (\vec{n}_A \cdot \vec{n}_B)\, \vec{n}_A$$

• $h_C = \dfrac{\vec{n}_C \cdot (\vec{n}_A \times \vec{n}_B)}{1 - (\vec{n}_A \cdot \vec{n}_B)^2}$

$$\vec{n}_C = \frac{\left[\vec{n}_A \cdot \vec{n}_C - (\vec{n}_A \cdot \vec{n}_B)(\vec{n}_B \cdot \vec{n}_C) \right] \vec{n}_A + \left[\vec{n}_B \cdot \vec{n}_C - (\vec{n}_A \cdot \vec{n}_B)(\vec{n}_A \cdot \vec{n}_C) \right] \vec{n}_B + \left[\vec{n}_C \cdot (\vec{n}_A \times \vec{n}_B) \right] (\vec{n}_A \times \vec{n}_B)}{1 - (\vec{n}_A \cdot \vec{n}_B)^2}$$

$$= \frac{(\cos b - \cos c \cos a)\, \vec{n}_A + (\cos a - \cos c \cos b)\, \vec{n}_B + \sin c \sin b \sin A\, (\vec{n}_A \times \vec{n}_B)}{\sin c^2}$$

$\Downarrow$ multiplying on both sides by $\sin c$.

$$\sin c\, \vec{n}_C = \frac{\cos b - \cos c \cos a}{\sin a \sin c} \sin a\, \vec{n}_A + \frac{\cos a - \cos c \cos b}{\sin c \sin b} \sin b\, \vec{n}_B +$$

$$+ \sin b \sin A\, (\vec{n}_A \times \vec{n}_B) =$$

$$= \cos B \sin a\, \vec{n}_A + \cos A \sin b\, \vec{n}_B + \sin b \sin A\, (\vec{n}_A \times \vec{n}_B)$$

equivalently, due to the sin theorem

(II) $\boxed{\sin C\, \vec{n}_C = \cos B \sin A\, \vec{n}_A + \cos A \sin B\, \vec{n}_B + \sin B \sin A\, (\vec{n}_A \times \vec{n}_B)}$

by inserting in (I) and (II) the conditions (*) on the angles A, B, C one obtains the Euler Rodrigues formulas (ER)

From the (ER) it is clear that it is most convenient to replace the ϕ and $\vec{n}$ by the new parameters

$$\lambda = \cos \phi/2 \qquad \vec{\Lambda} = \sin \phi/2 \ \vec{n}$$

The composition of rotation can thus be written in the form

$$R(\lambda_1; \vec{\Lambda}_1) R(\lambda_2; \vec{\Lambda}_2) = R(\lambda_3; \vec{\Lambda}_3)$$

where

$$\lambda_3 = \lambda_1 \lambda_2 - \vec{\Lambda}_1 \cdot \vec{\Lambda}_2$$
$$\vec{\Lambda}_3 = \lambda_1 \vec{\Lambda}_2 + \lambda_2 \vec{\Lambda}_1 + \vec{\Lambda}_1 \times \vec{\Lambda}_2$$

Remarks

i) $\left.\begin{matrix} R(\phi, \vec{n}) \\ R(-\phi; -\vec{n}) \end{matrix}\right\rangle R(\lambda, \vec{\Lambda})$ the Rodrigues parameters correctly assign the same rotation to the 2 cases.

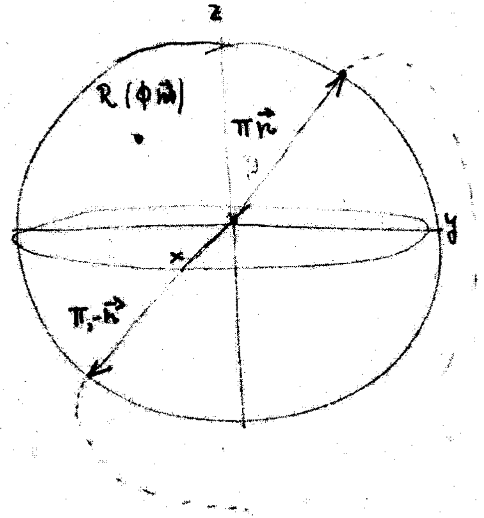
ii) On the other hand $\phi \to \phi + 2\pi$ $(\lambda; \vec{\Lambda}) \to (-\lambda; -\vec{\Lambda})$ this tells us that the Rodrigues parameters can distinguish the history of a rotation. (see later about this point)

iii) The Rodrigues parameters are 4 while a rotation can be identified by 3 parameters (example ϕ and direction of $\vec{n}$). Notice that

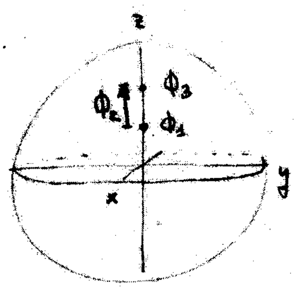
$$\lambda^2 + |\vec{\Lambda}|^2 = 1$$

7.3 The topology of rotations

From the definition of pole and the parametrization of the rotations using the unit sphere with positive and negative hemispheres it is now natural to introduce the PARAMETRIC BALL as the set of points contained inside a sphere of radius π. The points of this ball are in $1 \leftrightarrow 1$ correspondence with the full group of rotations. To be more precise one should peel off from the parametric ball one of the hemispheres to avoid a double counting of $R(\pi \vec{n}) = R(\pi, -\vec{n})$. An alternative way consists in taking the entire parametric ball with identification of all antipodal points: $R(\pi\vec{n})$ is a binary rotation (C_2)

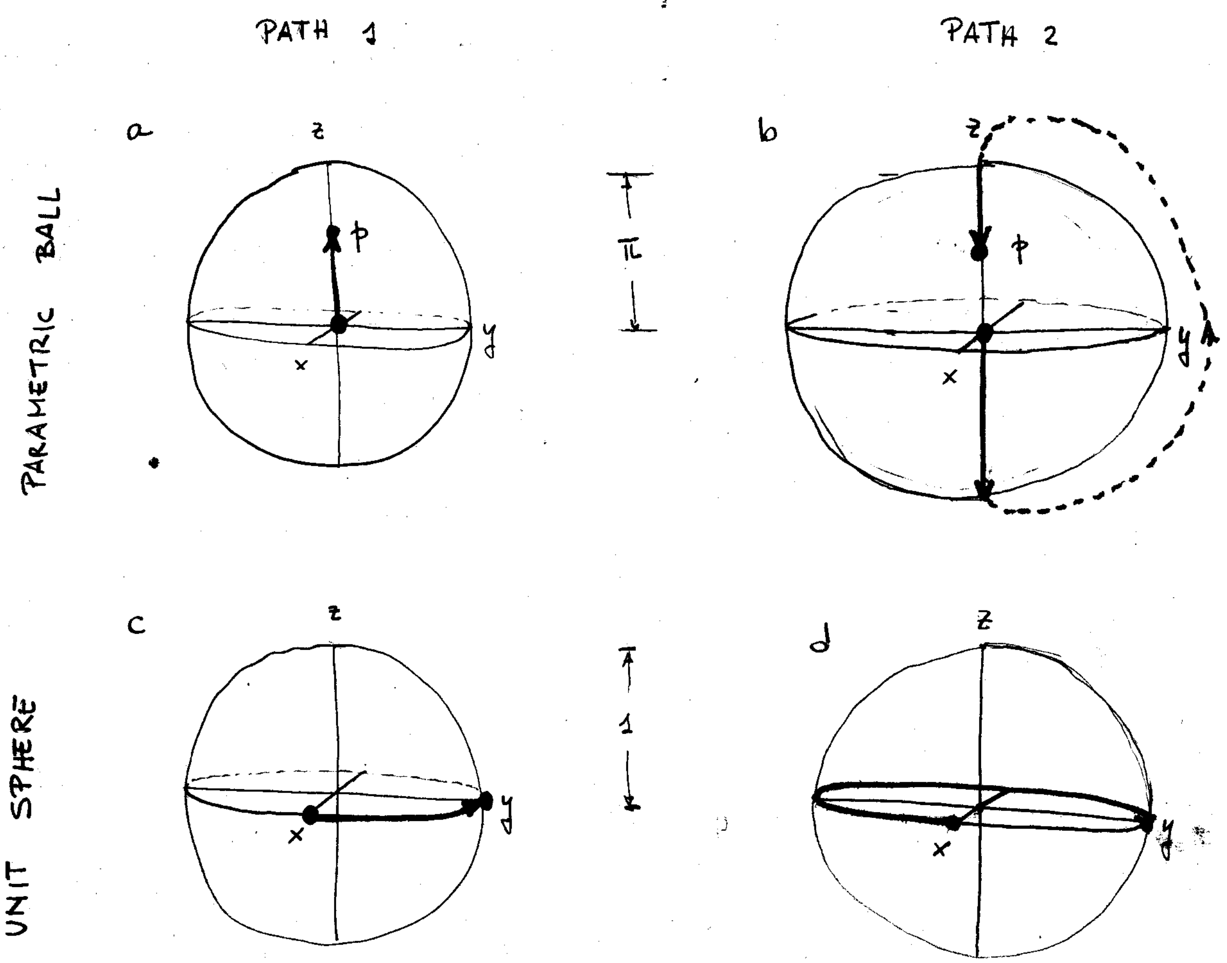


The composition of infinitesimal rotations generates paths in the parametric ball. As a simple example of path let us take 2 rotations around the z axis such that $\phi_1 + \phi_2 = \phi_3 < \pi$. We can represent the composition in the parametric ball as



In general a PATH is a line in the parametric ball that describes the change of the parametric point as a succession of rotations is effected.

There are infinite different paths connecting the origin to the parametric point p. Let's analyse the following 2:



$p = \frac{\pi}{2}\hat{z}$ is the same in a and b $\Rightarrow$ the rotations are the same, but the path is different as clearly seen in a) figures. In particular, path 2 has 1 "jump" between identified antipodal points while PATH 1 shows no "jump".

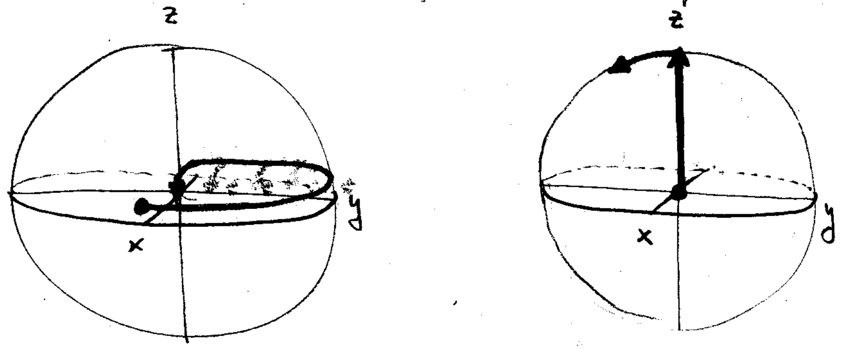
The paths can be easily calculated using the Euler construction and/or the (ER). Let us consider the rotation composed by $C_{\alpha x} C_{2z}$ where the rotation around $\hat{x}$ is of an infinitesimal angle α. Let's call $\phi \vec{n}$ the parametrization of the composite rotation

(ER) $$\cos \phi/2 = \cancel{\cos \alpha/2 \cos \pi/2} - \sin \alpha/2 \sin \pi/2 \, (\hat{x} \cdot \hat{z}) = 0 \Rightarrow \gamma = \pi$$

$$\underbrace{\sin \pi/2}_{1} \vec{n} = \cancel{\sin \tfrac{\alpha}{2} \cos \pi/2 \, \hat{x}} + \cos \alpha/2 \underbrace{\sin \pi/2}_{1} \hat{z} + \sin \alpha/2 \underbrace{\sin \pi/2}_{1} (\hat{x} \times \hat{z}) =$$

$$\vec{n} = \cos \alpha/2 \, \hat{z} - \sin \alpha/2 \, \hat{y}$$ (notice that the result is valid $\forall\, \alpha$)

Since $\gamma = \pi$ the parameter point moves on the surface of the parameter ball. The expression for $\vec{n}$ indicates that the pole moves in the $\hat{z}, \hat{y}$ plane towards smaller $\hat{z}$ and larger (negative) y.



UNIT SPHERE PARAMETER BALL

It should be noticed that, as $\alpha \to \pi$ the path approches the point $(0, -\pi, 0)$ where the surface has a "jump" to $(0, \pi, 0)$ since $(0, -\pi, 0)$ belongs to the negative hemisphere. The same point $(0, \pi, 0)$ can be reached also through the path $C_{2x} C_{\alpha z}$ without "jumps". We have taken for this purpose the same definition of h and $\bar{h}$ as in the unit sphere.

Idea: paths can be deformed continuously both on the unit sphere and in the parameter ball.

<u>Def</u>: homotopy: Two co-terminous paths in parameter space are said homotopic if they can be continuously deformed one into the other.

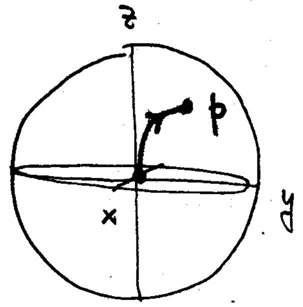
<u>Def</u> Class of homotopy: all paths homotopic to each other form a class of homotopy

<u>Theorem</u>: In the parametric ball (the parametric space of the proper rotation group - SO(3) the group of the special ($\det M_g = 1$) orthogonal matrices of dimension 3 -) there are only 2 class of homotopy: paths without jumps and path with 1 jump.

[redacted]

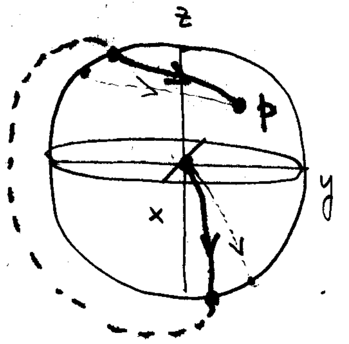
proof A path without a jump is all contained in a hemisphere => it does not contain antipodal point. A path containing 1 jump contains 1 pair of antipodal points. Antipodal points move "together" in infinitesimal transformation => remaining always in distinct hemispheres. It remains to be proven that 2 pairs of antipodal points can always be eliminated: graphically:

Path 1



path without jumps (class 0)

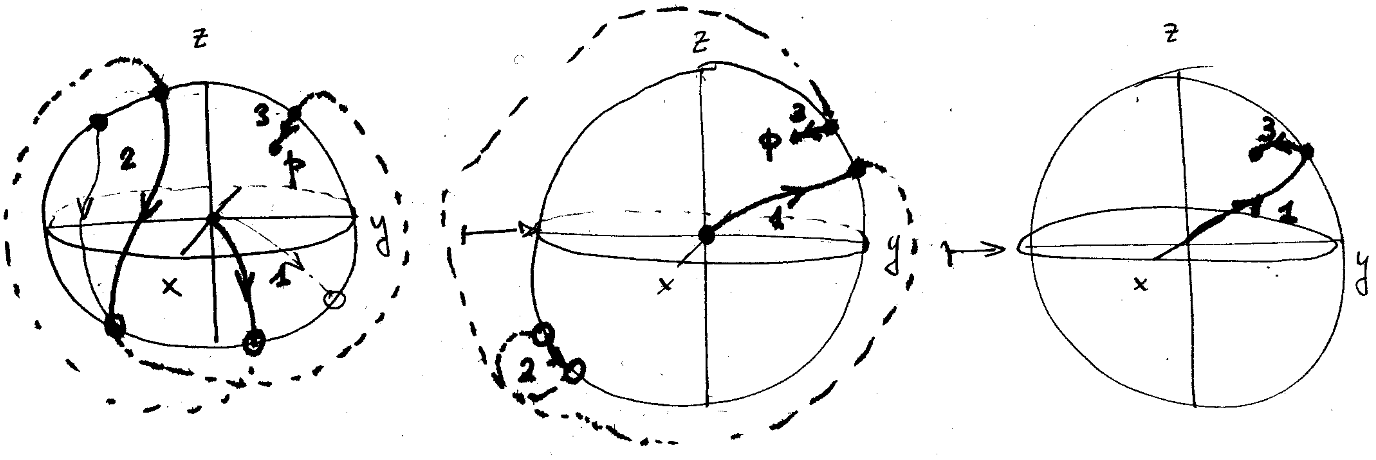
Path 2



path with 1 jump (class 1)

the depicted deformation of the path shows the impossibility to deform path 2 into path 1.

Path



the next step in the deformation is already PATH 1.

We can define a <u>projective representation</u> of SO(3) in the following way. Let's take 3 elements g_i, g_j, g_k of SO(3) such that $g_i g_j = g_k$. ~~A~~ projective representation

$$\check{G}(g_i)\check{G}(g_j) = [g_i, g_j]\,\check{G}(g_i g_j)$$

where $[g_i, g_j] = +1$ if the path g_i, g_j is of class 0

-1 if the path g_i, g_j is of class 1

$\check{G}(g_i g_j)$ is fixed but the sign is determined by the class of homotopy of the path g_i, g_j. If $g_i' g_j' = g_k$ and g_i', g_k' has the same class of homotopy of g_i, g_j => the sign does not change.

- Every element $g \in SO(3)$ is mapped in a parametric point p_g by a path of class 0 starting in the origin ($0\vec{n}$ map of the identity E) and ending in p_g.

- SO(3) is not simply connected since not all loops in its parameter space can be continuously contracted to a point (it is doubly connected)

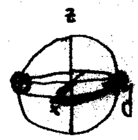
- $R(2\pi\vec{n}) = R(0\vec{n})$ as an operation in SO(3). Nevertheless, as all points in the parameter space, it can be reached from the origin by 2 classes of loops.

- The idea of a turn by 2π is handy to classify different classes of homotopy.

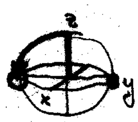
7.4 The spinor representations

First we want to determine the class of homotopy associated to the path g_i, g_j. Let us take as example C_{2z}, C_{2x} and C_{2x}, C_{2z}

$[C_{2z}, C_{2x}] = +1$ the entire path in h



$[C_{2x}, C_{2z}] = -1$ the path ends in $\bar{h}$



projective factors

For large groups it is more convenient an algebraic method based on the (ER).

- The standard parametric points are either in the parametric ball or on h. $\Rightarrow$ all standard parametric points are reached by path of class 0 from the origin.

- Standard ER parameters are deduced from the previous point

$$0 \leq \phi \leq \pi \quad \Rightarrow \quad \lambda = \cos \phi/2 \geq 0 \qquad \vec{\Lambda} = \sin \phi/2 \, \vec{n} \in h$$

positive rotations; $\bar{h}$ negative rotations

The standard ER parameters are the set

$$\lambda_g > 0 \quad \text{or} \quad \lambda_g = 0 \quad \Lambda \in h$$

$\leftarrow$ binary rotations.

$$g \in SO(3) \longleftrightarrow p_g \ \text{standard parametric point} \longleftrightarrow (\lambda_g ; \vec{\Lambda}_g) \ \text{standard ER parameters}$$

$R(-\lambda_g ; -\vec{\Lambda}_g)$ correspond to the same p_g but reached via a path of class 1. The path from $R(\lambda_g, \vec{\Lambda}_g)$ to $R(-\lambda_g, \vec{\Lambda}_g)$ is obtained

- $\lambda_g \neq 0$ as a 2π rotation of $\phi \to \phi + 2\pi$
- $\lambda_g = 0$ as a pure "jump" between antipodal points

$$R(\lambda_1; \vec{\Lambda}_1) R(\lambda_2; \vec{\Lambda}_2) = R(\lambda_1\lambda_2 - \vec{\Lambda}_1 \cdot \vec{\Lambda}_2 ; \lambda_1 \vec{\Lambda}_2 + \lambda_2 \vec{\Lambda}_1 + \vec{\Lambda}_1 \times \vec{\Lambda}_2)$$
$$= R(\lambda_3 ; \vec{\Lambda}_3)$$

if $\lambda_3 > 0$ or $\lambda_3 = 0$ and $\vec{\Lambda}_3 \in h$

$\Rightarrow \quad [g_1, g_2] = 1$

if $\lambda_3 < 0$ or $\lambda_3 = 0$ and $\vec{\Lambda}_3 \in \bar{h}$

$\Rightarrow \quad [g_1, g_2] = -1$

Examples:

i) $[C_2, C_2] = -1 \quad \forall \vec{n}$

$$R(0; \vec{n}) R(0; \vec{n}) = R(-1, \vec{0}) \qquad \lambda < 0$$

ii) $[C_3^+, C_3^+] = -1$

$C_3^+ : \lambda = \frac{1}{2}, \quad \vec{\Lambda} = \frac{\sqrt{3}}{2}(001)$

$C_3^- : \lambda' = \frac{1}{2} \quad \vec{\Lambda}' = \frac{\sqrt{3}}{2}(00\bar{1})$

$$\lambda_3 = \frac{1}{4} - \frac{3}{4} = -\frac{1}{2} \qquad \vec{\Lambda}_3 = \left(\frac{\sqrt{3}}{4} + \frac{\sqrt{3}}{4}\right)(001) = \frac{\sqrt{3}}{2}(001)$$

$$\lambda_3 = -\lambda' \qquad \vec{\Lambda}_3 = -\vec{\Lambda}'$$

The intertwining theorem is fundamental to understand the characters of a spinor representation.

Def: g_i and g_j are intertwined by g if

$$(1) \quad g g_i = g_j g$$

- if $i=j$ $\Rightarrow$ g_i intertwined with g $\Leftrightarrow$ $[g, g_i] = 0$ g and g_i commute
- if $i \neq j$ $\rightarrow$ $g_j = g_i^g$ the conjugate of g_i through g.

By using (1) we can state that $\boxed{g g_i = g_i^g g}$ {that is g_i and g_i^g are intertwined

Theorem: The following relations between projective factors hold

i) $[g, g_i] = [g_i^g, g]$ (non-commuting rotations)

ii) $[g, g_i] = [g_i, g]$ (coaxial rotations)

iii) $[g, g_i] = -[g_i, g]$ (bilateral binary, C_{2n} C_{2m} $n \perp m$)

proof i) $g \leftrightarrow (\lambda, \vec{\Lambda})$ $g_i \leftrightarrow (\lambda_i, \vec{\Lambda}_i)$

the ER parameters for the composite rotation $g g_i$ are

$$(\lambda\lambda_i - \vec{\Lambda}\vec{\Lambda}_i, \ \lambda\vec{\Lambda}_i + \lambda_i\vec{\Lambda} + \vec{\Lambda} \times \vec{\Lambda}_i)$$

In order to proceed we need to know the ER parameters for inverse or conjugate rotation. We do both:

- $g g^{-1} = E$ $\quad g \leftrightarrow \lambda, \vec{\Lambda}$ $\quad g^{-1} \leftrightarrow \lambda', \vec{\Lambda}'$ $\quad E \leftrightarrow 1, \vec{0}$

$$g g^{-1} \leftrightarrow \lambda\lambda' - \vec{\Lambda}\cdot\vec{\Lambda}', \ \lambda\vec{\Lambda}' + \lambda'\vec{\Lambda} + \vec{\Lambda} \times \vec{\Lambda}'$$

$\lambda' = \lambda$ $\quad \vec{\Lambda}' = -\vec{\Lambda}$ as it was to be expected (same angle, opposite pole)

- $g_i^g = g g_i g^{-1}$ one has to do it in pieces

$$g g_i g^{-1} = (g g_i) g^{-1} = R(\lambda\lambda_i - \vec\Lambda\cdot\vec\Lambda_i,\ \lambda\vec\Lambda_i + \lambda_i\vec\Lambda + \vec\Lambda\times\vec\Lambda_i)\, R(\lambda, -\vec\Lambda)$$

$$= R\Big[(\lambda\lambda_i - \cancel{\vec\Lambda\cdot\vec\Lambda_i})\lambda - (\cancel{\lambda\vec\Lambda_i} + \lambda_i\vec\Lambda + \cancel{\vec\Lambda\times\vec\Lambda_i})\cdot(-\vec\Lambda),$$
$$(\cancel{\lambda\lambda_i} - \vec\Lambda\cdot\vec\Lambda_i)(-\vec\Lambda) + \lambda(\lambda\vec\Lambda_i + \cancel{\lambda_i\vec\Lambda} + \vec\Lambda\times\vec\Lambda_i) + (\lambda\vec\Lambda_i + \cancel{\lambda_i\vec\Lambda} + \vec\Lambda\times\vec\Lambda_i)\times(-\vec\Lambda)\Big]$$

$$= R\Big[\lambda_i\overset{1}{\cancel{(\lambda^2 + |\vec\Lambda|^2)}},\ (\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + \lambda^2\vec\Lambda_i + 2\lambda\vec\Lambda\times\vec\Lambda_i - (\vec\Lambda\times\vec\Lambda_i)\times\vec\Lambda\Big]$$

$$= R\Big[\lambda_i,\ 2(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + 2\lambda\vec\Lambda\times\vec\Lambda_i + (\lambda^2 - |\vec\Lambda|^2)\vec\Lambda_i\Big] =$$

$$\Big[(\vec v\times\vec w)\times\vec v\Big]_k = \sum_{\substack{ij\\lm}} v_i w_j \varepsilon_{ijl}\varepsilon_{lmk} v_m = \sum_{ijm} v_i w_j v_m \sum_l \varepsilon_{ijl}\varepsilon_{mkl}$$

$$= \sum_{ijm} v_i w_j v_m (\delta_{im}\delta_{jk} - \delta_{ik}\delta_{jm}) = \sum_i v_i^2 w_k - v_k \sum_j w_j v_j$$

$$= \Big[|\vec v|^2\vec w - (\vec w\cdot\vec v)\vec v\Big]_k$$

$$= R\Big[\lambda_i,\ 2(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + 2\lambda\vec\Lambda\times\vec\Lambda_i + (1 - 2|\vec\Lambda|^2)\vec\Lambda_i\Big]$$

as expected the angle is invariant under conjugation. The other ER parameter represent the rotated pole of g_i (verify).

Now we must perform the last composition

$$R\Big[\lambda_i,\ 2(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + (1 - 2|\vec\Lambda|^2)\vec\Lambda_i + 2\lambda(\vec\Lambda\times\vec\Lambda_i)\Big]\, R(\lambda, \vec\Lambda) =$$

$$= R\Big[\lambda_i\lambda - \cancel{2(\vec\Lambda\cdot\vec\Lambda_i)|\vec\Lambda|^2} - (1 - \cancel{2|\vec\Lambda|^2})(\vec\Lambda_i\cdot\vec\Lambda) - \cancel{2\lambda(\vec\Lambda\times\vec\Lambda_i)\cdot\vec\Lambda},$$
$$\lambda_i\vec\Lambda + 2\lambda(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + \lambda(1 - 2|\vec\Lambda|^2)\vec\Lambda_i + 2\lambda^2(\vec\Lambda\times\vec\Lambda_i)$$
$$+ (1 - 2|\vec\Lambda|^2)(\vec\Lambda_i\times\vec\Lambda) + 2\lambda(\vec\Lambda\times\vec\Lambda_i)\times\vec\Lambda\Big]$$

$$= R\Big[\lambda_i\lambda - \vec\Lambda_i\cdot\vec\Lambda,\ \lambda_i\vec\Lambda + \cancel{2\lambda(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda} + \lambda\vec\Lambda_i - \cancel{2\lambda|\vec\Lambda|^2\vec\Lambda_i}$$
$$+ 2\lambda^2(\vec\Lambda\times\vec\Lambda_i) + (\lambda^2 - |\vec\Lambda|^2)(\vec\Lambda_i\times\vec\Lambda) + \cancel{2\lambda|\vec\Lambda|^2\vec\Lambda_i} - \cancel{2\lambda(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda}\Big]$$

$$= R\Big[\lambda_i\lambda - \vec\Lambda_i\cdot\vec\Lambda,\ \lambda_i\vec\Lambda + \lambda\vec\Lambda_i + \vec\Lambda\times\vec\Lambda_i\Big)$$ the same ER parameters as L_i)

□

ii] For coaxial rotations the operators commute

$$g \leftrightarrow (\lambda \,;\, \sqrt{1-\lambda^2}\,\vec{n})$$
$$g_i \leftrightarrow (\lambda_i \,;\, \pm\sqrt{1-\lambda_i^2}\,\vec{n})$$

$$R(\lambda, \sqrt{1-\lambda^2}\,\vec{n})\, R(\lambda_i, \pm\sqrt{1-\lambda_i^2}\,\vec{n}) = R(\lambda\lambda_i \mp \sqrt{1-\lambda^2}\sqrt{1-\lambda_i^2}, (\lambda\sqrt{1-\lambda_i^2} + \lambda_i\sqrt{1-\lambda^2})\,\vec{n})$$

the result is symmetric in the exchange λ and λ_i

iii]

$$g \leftrightarrow (0, \vec{n})$$
$$g_i \leftrightarrow (0, \vec{n}_i) \qquad \text{and} \qquad \vec{n}_i \perp \vec{n}$$

$$R(0,\vec{n})\, R(0,\vec{n}_i) = R(0, \vec{n}\times\vec{n}_i)$$
$$R(0,\vec{n}_i)\, R(0,\vec{n}) = R(0, \vec{n}_i\times\vec{n}) = R(0, -(\vec{n}\times\vec{n}_i))$$

the resulting composite rotations have antipodal poles. $\Rightarrow$ the projective factors differ by a sign. ■

The theorem can be rephrased by the introduction of regular and irregular rotations the first being the non-commuting or coaxial, the second being the bilateral binary (BB) rotations.

$$\text{for } g \text{ and } g_i \text{ regular} \qquad [g, g_i] = [g_i^c, g]$$
$$\text{for } g \text{ and } g_i \text{ irregular} \qquad [g, g_i] = -[g_i^c, g] = -[g_i, g].$$

The characters are in general not class functions for projective representations (Schur, 1904)

$$\chi(g_i^g \,|\, \check{G}) = [g_i^g, g]\,[g, g_i]^{-1}\,\chi(g_i \,|\, \check{G}) \qquad (1)$$

<u>proof</u>

the proof of (1) is based on the associativity condition for the factor system.

$$[g_i, g_j]\,[g_i g_j, g_k] = [g_i, g_j g_k]\,[g_j, g_k] \quad \text{(associativity condition)}$$

⌈ proof of the associativity condition

$$\check G(g_i)\{\check G(g_j)\check G(g_k)\} = \{\check G(g_i)\check G(g_j)\}\check G(g_k)$$

L: $$\check G(g_i)\,[g_j, g_k]\,\check G(g_j g_k) = [g_i, g_j g_k]\,[g_j, g_k]\,\check G(g_i g_j g_k)$$

R: $$[g_i, g_j]\,\check G(g_i g_j)\,\check G(g_k) = [g_i g_j, g_k]\,[g_i, g_j]\,\check G(g_i g_j g_k)$$

□ ⌋

$$\chi(g_i^g \mid \check G) = \mathrm{Tr}\,\check G(g g_i g^{-1}) = \mathrm{Tr}\{[g, g_i g^{-1}]^{-1}\,\check G(g)\,\check G(g_i g^{-1})\}$$

$$= [g, g_i g^{-1}]^{-1}\,[g_i, g^{-1}]\;\mathrm{Tr}\{\check G(g)\,\check G(g_i)\,\check G(g^{-1})\}$$

$$= [g, g_i g^{-1}]^{-1}\,[g_i, g^{-1}]^{-1}\;\mathrm{Tr}\{\check G(g^{-1})\,\check G(g)\,\check G(g_i)\} =$$

$$= [g, g_i g^{-1}]^{-1}\,[g_i, g^{-1}]^{-1}\,[g^{-1}, g]\;\mathrm{Tr}\{\check G(e)\,\check G(g_i)\}$$

$$= [g, g_i g^{-1}]^{-1}\,[g_i, g^{-1}]^{-1}\,[g^{-1}, g]\;\underbrace{[e, g_i]}_{1}\;\underbrace{\mathrm{Tr}\{\check G(g_i)\}}_{\chi(g_i \mid \check G)} \qquad (*)$$

Now we use associativity in the form

$$[g g_i, g^{-1}]\,[g g_i g^{-1}, g] = \underset{[g', e]}{\overset{1}{\cancel{[g g_i, g^{-1} g]}}}\,[g^{-1}, g]$$

$$[g g_i, g^{-1}]\,[g_i^g, g] = [g^{-1}, g] \leftarrow \text{we introduce in } (*) \quad [g^{-1}, g]$$

$$\chi(g_i^g \mid \check G) = [g, g_i g^{-1}]^{-1}\,[g_i, g^{-1}]^{-1}\,[g g_i, g^{-1}]\,[g_i^g, g]\;\chi(g_i \mid \check G)$$

Once more the associativity in the form

$$[g, g_i]\,[g g_i, g^{-1}] = [g, g_i g^{-1}]\,[g_i, g^{-1}]$$

$$\Rightarrow \; [g g_i, g^{-1}] = [g, g_i g^{-1}]\,[g_i, g^{-1}]\,[g, g_i]^{-1}$$

$$\Rightarrow \quad \chi(g_i^g|\check{G}) = \cancel{[\![g, g_i g]\!]^{-1}}\, \cancel{[\![g_i, g^{-1}]\!]^{-1}}\, \cancel{[\![g, g_i g^{-1}]\!]}\, \cancel{[\![g_i, g^{-1}]\!]}\, \underline{[\![g, g_i]\!]^{-1}}\, \underline{[\![g_i^g, g]\!]}$$

$$\chi(g_i|\check{G})$$

From (*) of page 89 and i) – iii) of page 87 it follows that $\square$

i) For all regular rotations

$$\chi(g_i^g|\check{G}) = \chi(g_i|\check{G})$$

ii) For all irregular rotations

$$\chi(g_i^g|\check{G}) = -\chi(g_i|\check{G}) \quad \text{but } [g_i, g] = 0$$

$$\Rightarrow \chi(g_i|\check{G}) = -\chi(g_i|\check{G}) = 0$$

Summarizing: the character is a class function of spinorial representations and it vanishes for irregular classes.

7.5 The algebra of rotations: quaternions

Def: A quaternion $\mathbb{A}$ is a set of 4 real numbers combined as $[\![a, \vec{A}]\!]$ with the non-commutative multiplication rule:

$$\mathbb{A}\mathbb{B} = [\![a, \vec{A}]\!][\![b, \vec{B}]\!] = [\![ab - \vec{A}\cdot\vec{B},\ a\vec{B} + b\vec{A} + \underbrace{\vec{A}\times\vec{B}}]\!]$$

for this reason it is non commutative.

The product of quaternions is associative (verify)

Def: real quaternion $[\![a, \vec{0}]\!]$ since $[\![a, \vec{0}]\!][\![b, \vec{0}]\!] = [\![ab, \vec{0}]\!]$ and $[\![a, \vec{0}]\!] \equiv a \in \mathbb{R}$.

moreover $a[\![b, \vec{B}]\!] = [\![a, \vec{0}]\!][\![b, \vec{B}]\!] = [\![ab, a\vec{B}]\!]$

Def: <u>pure</u> quaternion $[\![0,\vec{A}]\!]$.

Notice that the product of 2 pure quaternions is expressed in terms of scalar and vector product $[\![0,\vec{A}]\!][\![0,\vec{B}]\!] = [\![-\vec{A}\cdot\vec{B}, \vec{A}\times\vec{B}]\!]$

Def: <u>unit</u> quaternion is a pure quaternion $[\![0,\vec{n}]\!]$ with $|\vec{n}|^2=1$.

=> a pure quaternion can be written as

$[\![0,\vec{A}]\!] = |\vec{A}|\,[\![0,\vec{n}]\!]$. we give the symbol $\mathbb{n} := [\![0,\vec{n}]\!]$

Now we want to establish an additive form for quaternions.

$$[\![a,\vec{A}]\!] = [\![a,\vec{0}]\!] + [\![0,\vec{A}]\!]$$
$$[\![b,\vec{B}]\!] = [\![b,\vec{0}]\!] + [\![0,\vec{B}]\!]$$

the prove that this makes sense is given by:

$$[\![a,\vec{A}]\!][\![b,\vec{B}]\!] = \left([\![a,\vec{0}]\!] + [\![0,\vec{A}]\!]\right)\left([\![b,\vec{0}]\!] + [\![0,\vec{B}]\!]\right) =$$
$$= [\![ab,\vec{0}]\!] + [\![0,a\vec{B}]\!] + [\![0,b\vec{A}]\!] + [\![-\vec{A}\cdot\vec{B}, \vec{A}\times\vec{B}]\!] =$$
$$= [\![ab-\vec{A}\cdot\vec{B},\ a\vec{B}+b\vec{A}+\vec{A}\times\vec{B}]\!].$$

It follows that $[\![a,\vec{A}]\!] = a + \mathbb{n}A$ which resembles the complex numbers. An even closer analogy to the complex numbers is given by: $\mathbb{n}^2 = [\![0,\vec{n}]\!][\![0,\vec{n}]\!] = [\![-|\vec{n}|^2, 0]\!] = [\![-1,0]\!] = -1$.

Def binary form of a quaternion $\mathbb{A} = a + \mathbb{n}A$.

A pure quaternion can be easily identified with a binary rotation if thought in terms of ER parameters

$$R(\lambda,\Lambda) \longleftrightarrow [\![\cos\phi/2,\ \sin\phi/2\,\vec{n}]\!]$$

$$\Rightarrow [\![0,\vec{n}]\!] \leftrightarrow \phi = \pi.$$

The hystorical association $[\![0, \vec{A}]\!]$ with the vector $\vec{A}$ has serious limitations (it was through associated to the invention of the term "vector").

The $\boxed{\text{inversion}}$ of a quaternion helps us in the identification of its components:

$$i\vec{r} = -\vec{r} \Rightarrow \text{vector (polar vector)}$$
$$i\vec{r} = \vec{r} \Rightarrow \text{pseudovector (axial vector)}$$

Analogously for scalar (fields) they can be

$$A(\vec{r}) = \pm A(i\vec{r}) = \pm A(-\vec{r}) \quad \begin{cases} + & \text{scalar} \\ - & \text{pseudoscalar} \end{cases}$$

$\Rightarrow$ for example: $\vec{r} = r_x\vec{i} + r_y\vec{j} + r_z\vec{k}$

r_x, r_y, r_z = pseudoscalars
$\vec{i}, \vec{j}, \vec{k}$ = pseudovectors
$\vec{r}$ = vector.

Now we can return to the definition of quaternion product

$$[\![a, \vec{A}]\!]\,[\![b, \vec{B}]\!] = [\![ab - \vec{A}\cdot\vec{B},\ a\vec{B} + b\vec{A} + \vec{A}\times\vec{B}]\!]$$

$a \begin{cases} \text{scalar} \\ \text{pseudoscalar} \Rightarrow ab = \text{scalar} \ ϟ \end{cases}$

$\vec{A} \begin{cases} \text{vector} \Rightarrow \vec{A}\times\vec{B} = \text{pseudovector} \ ϟ \\ \text{pseudovector} \end{cases}$

$\Rightarrow$ $\boxed{\begin{array}{ll} a & \text{scalar} \\ \vec{A} & \text{pseudovector} \end{array}}$

Now let us deal wit conjugation

$$A^* \overset{\text{def}}{=} [\![a, -\vec{A}]\!]$$

It follows immediately $AA^* = [\![a^2 + A^2, \vec{0}]\!] = a^2 + A^2 \overset{\text{def}}{=} |A|^2$

A <u>normalized quaternion</u> $\mathbb{A}$: $|\mathbb{A}|^2 = a^2 + A^2 = 1$. (different from the unit quaternion $[\![0, \vec{n}]\!]$ which is a pure normalized quaternion)

The normalized quaternions have at least 2 famous parametrizations

* (Hamilton) $[\![\cos\alpha, \sin\alpha\,\vec{n}]\!]$

* (Euler - Rodriguez) $[\![\cos \phi/2, \sin \phi/2\,\vec{n}]\!]$ ϕ is the rotation angle!

The inverse quaternion $\mathbb{A}^{-1}$ is defined by

$$\mathbb{A}\mathbb{A}^{-1} = [\![1, 0]\!] = 1$$

but $\mathbb{A}\mathbb{A}^{*}|\mathbb{A}|^{-2} = 1 \Rightarrow \mathbb{A}^{-1} = \mathbb{A}^{*}|\mathbb{A}|^{-2}$ if $|\mathbb{A}| \neq 0$

Thus two quaternions can always be divided

$$\mathbb{A}/\mathbb{B} = \mathbb{C} \qquad \mathbb{C} = \mathbb{A}\mathbb{B}^{-1} = \mathbb{A}\mathbb{B}^{*}|\mathbb{B}|^{-2}$$

We conclude this introduction to the quaternion algebra with the following intuitive extension to the additive notation

$$\mathbb{A} = a[\![1, \vec{0}]\!] + A[\![0, \vec{n}]\!]$$

if $\vec{A} = A_x\vec{i} + A_y\vec{j} + A_z\vec{k}$ it can be proven that

$$\mathbb{A} = a[\![1, \vec{0}]\!] + A_x\underbrace{[\![0, \vec{i}]\!]}_{\mathbb{i}} + A_y\underbrace{[\![0, \vec{j}]\!]}_{\mathbb{j}} + A_z\underbrace{[\![0, \vec{k}]\!]}_{\mathbb{k}}$$

It follows: $\mathbb{i}^2 = \mathbb{j}^2 = \mathbb{k}^2 = -1 \qquad \mathbb{i}\mathbb{j} = \mathbb{k} \qquad \mathbb{j}\mathbb{i} = -\mathbb{k}$

These are the famous equations involving quaternion units that Hamilton carved on Monday 16 October 1843 on Brougham Bridge.

7.6 Double groups in terms of quaternions

Given a group G, the associated double group is constructed by defining the "rotation by 2π" = $\tilde{e}$ and constructing then $\tilde{g}_i = \tilde{e} g_i$ $\forall\, g_i \in G$ => the order of the group is doubled. ~~Here~~ ends the easy part and start the troubles without the quaternion formulation since even $g_1 g_2 = ?$ in the $\tilde{G}$ group and the construction of the multiplication table is cumbersome. Let us now use quaternions

• Proper rotation $\longrightarrow R(\lambda, \vec{\Lambda})$ in the Euler Rodriguez parametrization. The STANDARD parametrization takes paths of class 0 from the origin of the parameter ball.

[notice: improper rotations are associated to the same $R(\lambda, \vec{\Lambda})$ since i does not change the pole]

$R(\lambda, \vec{\Lambda}) \rightarrow$ quaternion $[\![\lambda, \vec{\Lambda}]\!]$ In fact the composition rule for (ER) is identical to the definition of the quaternion product

$$\tilde{e} \leftrightarrow [\![\cos\tfrac{2\pi}{2}, \sin\tfrac{2\pi}{2}\,\vec{n}]\!] = [\![-1, 0]\!] = -1$$

$$\Rightarrow \quad \tilde{g} = [\![\lambda, \vec{\Lambda}]\!]\,[\![-1, 0]\!] = [\![-\lambda, -\vec{\Lambda}]\!] \leftarrow \text{element of the double group.}$$

we now have a one to one mapping between the elements of $\tilde{G}$ and the associated quaternions. Example let us consider D_2

	E	C_{2x}	C_{2y}	C_{2z}
E	E	C_{2x}	C_{2y}	C_{2z}
C_{2x}	C_{2x}	E	C_{2z}	C_{2y}
C_{2y}	C_{2y}	C_{2z}	E	C_{2x}
C_{2z}	C_{2z}	C_{2y}	C_{2x}	E

The extension to $\tilde{D}_2$ is now completely natural

$$\begin{array}{cccc} E & C_{2x} & C_{2y} & C_{2z} \\ [1,(000)] & [0,(100)] & [0,(010)] & [0,(001)] \end{array}$$

$$\begin{array}{cccc} \tilde{E} & \tilde{C}_{2x} & \tilde{C}_{2y} & \tilde{C}_{2z} \\ [-1,(000)] & [0\ (\bar{1}00)] & [0,(0\bar{1}0)] & [0,(00\bar{1})] \end{array}$$

Example of 2 elements of the new multiplication table

$$C_{2x}C_{2y} \mapsto [0,i][0,j] = [0,\vec{k}] \to C_{2z}$$

$$C_{2y}C_{2x} \mapsto [0,j][0,i] = [0,-\vec{k}] \to \tilde{C}_{2z}$$

Now we are ready to study the general properties of products and conjugates in the double group and determine its class structure (Key to the number and dimension of the irreducible representations)

One has to be carefull with notation:

$$C_{2y}C_{2x} = C_{2z} \qquad C_{2x}^{-1} = C_{2x} \qquad \text{in } D_2$$

$$C_{2y}C_{2x} = \tilde{C}_{2z} \qquad C_{2x}^{-1} = \tilde{C}_{2x} \qquad \text{in } \tilde{D}_2$$

in G	in $\tilde{G}$	
$g_i = g_j$	$g_i \simeq g_j$	equality
g^{-1}	$g^{\sim 1}$	inverse
$g_i \, c \, g_j$	$g_i \, \tilde{c} \, g_j$	conjugation
$c(g_i)$	$\tilde{c}(g_i)$	class
rotations irrespective of the homotopy class	rotations with homotopy class (in the quaternions sense).	

Let us exercise the notation

$$g_i g_j = g_k \Rightarrow \text{ either } g_i g_j \simeq g_k$$
$$\text{or } g_i g_j \simeq \tilde{g}_k$$

By applying $\tilde{e}$ on the last equation $g_i \tilde{g}_j \simeq g_k$ and $\tilde{g}_i g_j \simeq g_k$

$$g_i g_j \simeq g_k \Rightarrow g_i g_j = g_k$$
$$g_i g_j \simeq \tilde{g}_k \Rightarrow g_i g_j = g_k$$

Products in $\tilde{G}$ must reduce to the ones in G if $\tilde{e} = e$.

For the inverses the following rules hold

(*) $g^{\sim 1} \simeq g^{-1}$ (g not binary)

(**) $g^{\sim 1} \simeq \tilde{g}$ (g binary)

proof

(*) follow from $gg^{-1} \simeq e$ as can be proven using quaternion algebra

$$(\Delta) \quad gg^{-1} \simeq [\![\lambda, \vec{\Lambda}]\!][\![\lambda, -\vec{\Lambda}]\!] \simeq [\![\lambda^2 + \Lambda^2, \vec{0}]\!] \simeq [\![1, \vec{0}]\!] \simeq e$$

(**) can also be proven using quaternions binary rotations $[\![0, \vec{n}]\!]$

$$(\square) \quad g\tilde{g} \simeq [\![0, \vec{n}]\!][\![0, -\vec{n}]\!] \simeq [\![1, \vec{0}]\!] \simeq e$$

As for the inverses of $\tilde{g}$:

$\tilde{g}^{\sim 1} \simeq \tilde{g}^{-1} \overset{\text{def}}{\simeq} \tilde{e} g^{-1}$ (non-binary) [from (Δ) multiplying by $\tilde{e}\tilde{e}$]

$\tilde{g}^{\sim 1} \simeq g$ (binary) [simply new reading of ($\square$)]

Putting all together $\forall \tilde{g} \in \tilde{G} \quad \tilde{g}^{\sim 1} \simeq \tilde{e} g^{\sim 1}$

Conjugation:

First we start with the definition

$g_i \tilde{c} g_j$ if either $g g_i g^{\sim 1} \simeq g_i$ or $\tilde{g} g_i \tilde{g}^{\sim 1} \simeq g_j$ but, using the fact that $\tilde{g}^{\sim 1} \simeq \tilde{e} g^{\sim 1}$ => the relation reduces to

$$g_i \tilde{c} g_j \quad \text{means} \quad g g_i g^{\sim 1} \simeq g_j$$

Now we want to correlate the conjugation in G with the one in $\tilde{G}$.

$g_i \, c \, g_j$ means $g g_i g^{-1} = g_j$ since a factor $\tilde{e}$ can always reappear passing from $=$ to $\simeq$

$$g_i \, c \, g_j \Longrightarrow \begin{cases} g_i \tilde{c} g_j & \text{either} \\ g_i \tilde{c} \tilde{g}_j & \text{or} \end{cases}$$

The point now is to determine when one or the other case are happening. We do it by steps.

(1) Intertwining theorem for double groups. If

$$g g_i = g_i g \quad \Rightarrow \quad g g_i \simeq g_i g$$

except when g and g_i are irregular operations => $g g_i \simeq \tilde{g}_i g$. Notice that if g and g_i are irregular => $[g, g_i] = 0$ -> $g_i = g_j$ => the relation is $g g_i \simeq \tilde{g}_i g$.

The proof is based on $g g_i = g_i g \Leftrightarrow g g_i g^{-1} = g_i = g_i^{g} \Leftrightarrow g g_i = g g_i^{g}$ and the calculation of the factors $[g, g_i] = \pm [g, g_i^{g}]$.

The consequences for double group conjugation are then

$$g g_i = g_i g \iff g_i \, c \, g_j$$

$$\Downarrow$$

1) $g g_i \simeq g_j g$ in general $\Rightarrow g g_i g^{-1} \simeq g_j \quad = \quad g_i \tilde{c} g_j$ the theorem considers $g_i g_i$!

2) $g g_i \simeq \tilde{g}_i g$ when g and g_i irregular $\Rightarrow \quad g_i \tilde{c} \tilde{g}_i$

(2) Theorem 1 for conjugation: Let us assume $g_i \tilde{c} \tilde{g}_j \Rightarrow \exists \, g \in G$ such that

$$g g_i = g_i g \qquad \text{but} \qquad g g_i \not\simeq g_i g$$

proof

- $g_i \tilde{c} \tilde{g}_j \iff g g_i g^{-1} \simeq \tilde{g}_j \Rightarrow g g_i \simeq \tilde{g}_j g \Rightarrow g g_i = g_j g$ since in G $\tilde{E} = E$
- let us assume $g g_i \simeq g_j g$, by comparison with $g g_i \simeq \tilde{g}_j g \Rightarrow g_i \simeq \tilde{g}_j$ ↯

∎

(3) Theorem 2 for conjugation: For any pair of operations g_i and g_j

$$g_i \, c \, g_j \Rightarrow g_i \tilde{c} g_j$$

but iff g_i is irregular $\Rightarrow$ the following additional relation also holds:

$$g_i \, c \, g_j \Rightarrow g_i \tilde{c} \tilde{g}_j$$

if g_i is irregular $\Rightarrow \quad g_i \tilde{c} \tilde{g}_i$ (consequence of intertwining theorem) but if $g_i \tilde{c} g_j \Rightarrow \tilde{g}_i \tilde{c} \tilde{g}_j \qquad g_i \tilde{c} \tilde{g}_i \tilde{c} \tilde{g}_j \Rightarrow g_i \tilde{c} \tilde{g}_j$.

∎

We still have to prove the reverse

$g_i \tilde{c} g_j$ but $\tilde{g}_i \tilde{c} \tilde{g}_j$ $\Rightarrow$ $g_i \tilde{c} \tilde{g}_i$ $\overset{\text{Th1}}{\Rightarrow}$ $\exists\, g \in G$ such that $[g, g_i] = 0$ but $[g, g_i] \neq 0$. The only operations that commute in both cases are the coaxial rotations $\Rightarrow$ g_i is irregular.

④ Theorem 3 (Opechowski) The class $C(g_i)$ of a regular operation $g_i \in G$ gives two classes in $\tilde{G}$ which are $\tilde{C}(g_i)$ and $\tilde{C}(\tilde{g}_i)$. If g_i is irregular, then $C(g_i)$ gives only one class in $\tilde{G}$, $\tilde{C}(g_i)$ which coincides with $\tilde{C}(\tilde{g}_i)$

proof

g_i regular $\Rightarrow$ $g_i c g_j \Rightarrow g_i \tilde{c} g_j \Rightarrow g_j \in C(g_i) \Rightarrow g_j \in \tilde{C}(g_i)$.

$C(g_i) \subseteq \tilde{C}(g_i)$. $g_j \in \tilde{C}(g_i)$ $g_i \tilde{c} g_i \Rightarrow g_i c g_i \Rightarrow C(g_i) = \tilde{C}(g_i)$.

$g_i \tilde{c} g_j \Rightarrow \tilde{g}_i \tilde{c} \tilde{g}_j \Rightarrow \tilde{C}(\tilde{g}_i)$ forms a second class. The two classes are disjoined since $g_i \tilde{c} \tilde{g}_j$ is valid iff g_i is irregular.

g_i irregular $\begin{cases} g_i c g_j \Rightarrow g_i \tilde{c} g_j & C(g_i) \\ g_i c g_j \Rightarrow g_i \tilde{c} \tilde{g}_j & \Rightarrow g_i \tilde{c} \tilde{g}_j \end{cases}$

■

Corollary: $|C_G|$ number of classes in G
$|C_{\tilde{G}}|$ number of classes in $\tilde{G}$

$|r|$ number of regular classes
$|i|$ number of irregular classes

$|C_G| = |r| + |i|$
$|C_{\tilde{G}}| = 2|r| + |i|$ = # irreducible representations

$|C_{\tilde{G}}| - |C_G| = |r|$ = # spinor representations.