7. Spinor representations and double groups

We have already proved that the characters of a rotation associated to the irrep of the full rotational group [SO(3)] labelled by the natural number $l = 0, 1 ..$ is given by

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

A more detailed analysis of the group of rotations (left to the Lie group chapter) shows that (*) only depends on the commutation relations of the "angular momentum operators" (i.e. the basis of the associated Lie algebra su(2)). The irrep of SU(2) can be thus labelled by semi-integers $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ with associated characters

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

j semi-integer can be conceived as the maximum eigenvalue of the angular momentum operator $J_z = S_z + L_z$.

7.1 Pure double group approach

According to the formula above for "spinorial representations"

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

$$= (-1)^{2j}\chi\left(\Gamma^{j}(\phi)\right).$$

$\Rightarrow$ if $j = \frac{1}{2}, \frac{3}{2} \ldots$ $\chi\left(\Gamma^{j}(\phi+2\pi)\right) = -\chi\left(\Gamma^{j}(\phi)\right)$. In other words we can distinguish between rotations of an angle ϕ or $\phi + 2\pi$. This result suggests to introduce a new operator $\bar{E}$

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

$R(\phi, \vec{n})$ is the rotation of an angle ϕ around the axis $\vec{n}$.

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

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 $\bar{G}$ 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 if $n>2$

(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

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

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

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	$\begin{cases} 1 & j=1/2, 7/2, \ldots \\ -1 & j=3/2, 9/2, \ldots \\ 0 & j=5/2, 11/2 \ldots \end{cases}$	$\sqrt{2}$ $(j=1/2, 9/2, \ldots)$ 0 $(j=3/2, 9/2, \ldots)$ $-\sqrt{2}$ $(j=5/2, 11/2, \ldots)$
e.g.	$j=1/2$	2	0	1	$\sqrt{2}$
	$j=3/2$	4	0	-1	0
	$j=5/2$	6	0	0	$-\sqrt{2}$

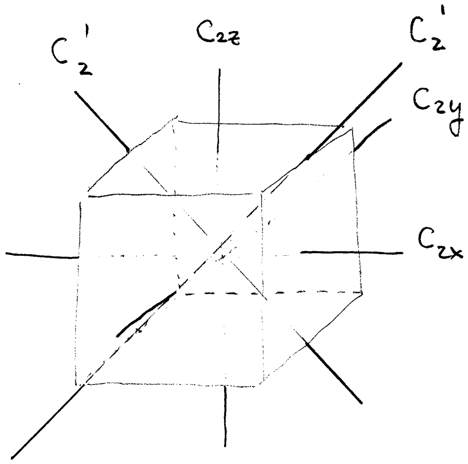
Dealing with <u>improper rotations</u> the following rules hold:

- if $i \in G \Rightarrow i\psi^j = \pm\psi^j$ $\quad G = \{H\} \oplus i\{H\} \quad \chi[\Gamma^{j\pm}(iR)] = \pm\chi[\Gamma^{j\pm}(R)]$
- if $i \notin G \Rightarrow G = \{H\} \oplus iR\{H\}$ is isomorphous with $P = \{H\} \oplus R\{H\}$ where R is a proper rotation and $\{H\}$ is a subgroup of proper rotations $\Rightarrow \chi[\Gamma^j(iR')] = \chi[\Gamma^j(R')]$ j integer or half-int

where $R' \in R\{H\}$ and $iR' \in G$

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

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 2 new classes.

Summarizing

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

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

(notice that the WOT is still valid!)

$\bar{O}$	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 F, G, H representation with dimensionality 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.

$$E_{1/2} = \Gamma_{1/2} \quad \sum_{T \in \bar{G}} |\chi_{1/2}(T)|^2 = 2[1(4) + 8\cdot(1) + 6\cdot(2)] = 48 = \bar{h} \leftarrow \text{IR}$$

$$F_{3/2} \quad \Gamma_{3/2} \quad \sum_{T} |\chi_{3/2}(T)|^2 = 2[1\cdot(16) + 8(1)] = 48 = \bar{h} \leftarrow \text{IR}$$

$$\Gamma_{5/2} \quad \sum_{T} |\chi_{5/2}(T)|^2 = 2[1\cdot(36) + 6(2) + 6(2)] = 96 > \bar{h} \leftarrow$$ This representation is reducible.

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

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

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

Derivation of the 3 new irreducible representations for $\bar{O}$.

[1] Consider spinorial representations of SU(2) which are naturally representation of any of its subgroups (e.g. $\Gamma_{1/2}$ or $\Gamma_{3/2}$, ... Γ_j) Start with $j=\frac{1}{2}$.

[2] Calculate the characters associated to the spinorial representation with the help of the formulas:

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

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

Notice that from the relations above and from the Opechowskij rules which assimilates into the same classes $C_{2\vec{n}}$ and $\bar{C}_{2\vec{n}}$ if $\exists\, C_{2\vec{n}'}$ with $\vec{n}' \perp \vec{n}$ in the group it follows $\chi(C_2) = \bar{\chi}(C_2) = 0$ j half integer.

$$\Gamma_{1/2} = \{2\ 0\ 1\ \sqrt{2}\ 0\ -2\ -1\ -\sqrt{2}\}$$

[3] Verify if the representation just introduced is irreducible: One can use the WOT in the form:

$$\frac{\cancel{\ell_j}}{h}\sum_{\nu\nu'}\sum_{R\in\bar{G}} \Gamma^{j*}_{\nu\nu'}(R)\,\Gamma^{j}_{\nu'\nu'}(R) = \sum_{\nu\nu'}\delta_{\nu\nu'} = \cancel{\ell_j} \quad \Rightarrow \quad \sum_k c_k\,|\chi^j(\mathcal{C}_k)|^2 = h$$

Since the only classes with characters $\neq 0$ are $E, 8C_3, 6C_4, \bar{E}, 8\bar{C}_3, 6\bar{C}_4$ and the characters of the double classes only differ by a sign, the relation to be checked is:

$$48 = 2\left[|\chi^j(E)|^2 + 8|\chi^j(C_3)|^2 + 6|\chi^j(C_4)|^2\right]$$

$j = 1/2$ $\quad 48 = 2\left[2^2 + 8\cdot 1^2 + 6\cdot 2\right]$ $\quad \checkmark \Rightarrow E_{1/2}$ is the first spinorial representation.

$\boxed{4}$ Consider $j = 3/2$

$$\Gamma_{3/2} = \{ 4 \ 0 \ -1 \ 0 \ 0 \ -4 \ 1 \ 0 \}$$

$$48 = 2\left[1 \cdot 4^2 + 8 \cdot (-1)^2 \right] \quad \checkmark \quad \Rightarrow \quad F_{3/2}$$

repres of dimension 4

Consider $j = 5/2$

$$\Gamma_{5/2} = \{ 6 \ 0 \ 0 \ -\sqrt{2} \ 0 \ -6 \ 0 \ \sqrt{2} \}$$

$$48 \neq 2\left[1 \cdot 6^2 + 6 \cdot 2 \right] \Rightarrow \Gamma_{5/2} \text{ is reducible}$$

$$\alpha_{E_{1/2}} = \frac{1}{48}\left[1 \cdot 6 \cdot 2 + 6 \cdot (-\sqrt{2}) \cdot (\sqrt{2}) + 1 \cdot (-6)(-2) + 6 \cdot \sqrt{2}(-\sqrt{2}) \right] = 0$$

$$\alpha_{F_{3/2}} = \frac{1}{48}\left[1 \cdot 6 \cdot 4 + 1 \cdot (-6)(-4) \right] = 1$$

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

For what concerns the irreducible spinorial representations of $\bar{O}$ the calculation is exhausted since we know $\bar{O}$ only contains IR $l_6 = 2$ $l_7 = 2$ $l_8 = 4$.

70 tn.

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 $-\pi \leq \phi < \pi$.

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.

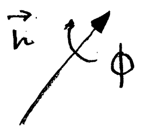
Def $\boxed{\text{POLE}}$ A pole of a rotation is the point of the unit sphere that is invariant under rotation and such that the rotation is seen as counterclockwise from outside the sphere.

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

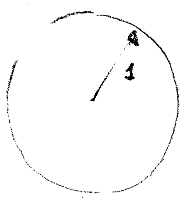
$$(xyz) \in h \text{ if } (xyz) \in \text{unit sphere and } \begin{cases} \text{(i)} & z > 0 \quad \text{or} \\ \text{(ii)} & z = 0,\ x > 0 \quad \text{or} \\ \text{(iii)} & z = 0,\ x = 0,\ y > 0 \end{cases}$$

- Parametrization of the rotations:



- $\vec{n}$ is the vector determining the rotation axis
- $0 \leq \phi < 2\pi$ (or $-\alpha \leq \phi < 2\pi - \alpha$) is the rotation angle.

- Visualization of the rotation



unit sphere

Rotation is the change of the positions in the points of a unit sphere

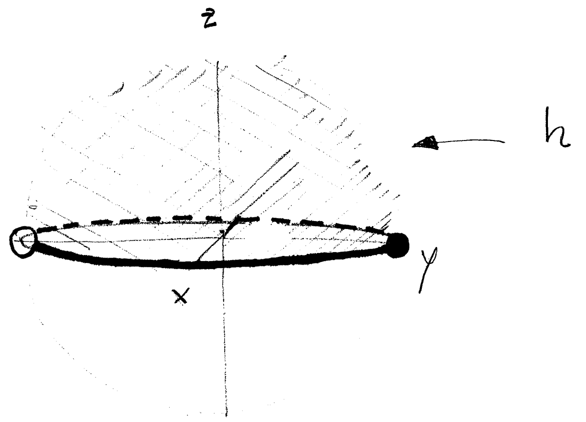
- Pole of a rotation: the point of the unit sphere which is invariant under rotation and from where the rotation is seen as counterclockwise when looking from outside the unit sphere.

Simbolically if g is a rotation $\Pi(g)$ is the pole

- If we define the rotation $R(\phi, \vec{n})$ it is clear that $R(\phi, \vec{n}) = R(-\phi,$

$\Rightarrow$ we can restrict to $0 \leq \phi \leq \pi$ and distinguish $R(\phi, \vec{n})$ and $R(\phi,$

- A careful definition of hemisphere allows to distinguish between positive and negative rotations. Positive (Negative) rotations have their poles in the positive (negative) hemisphere.



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

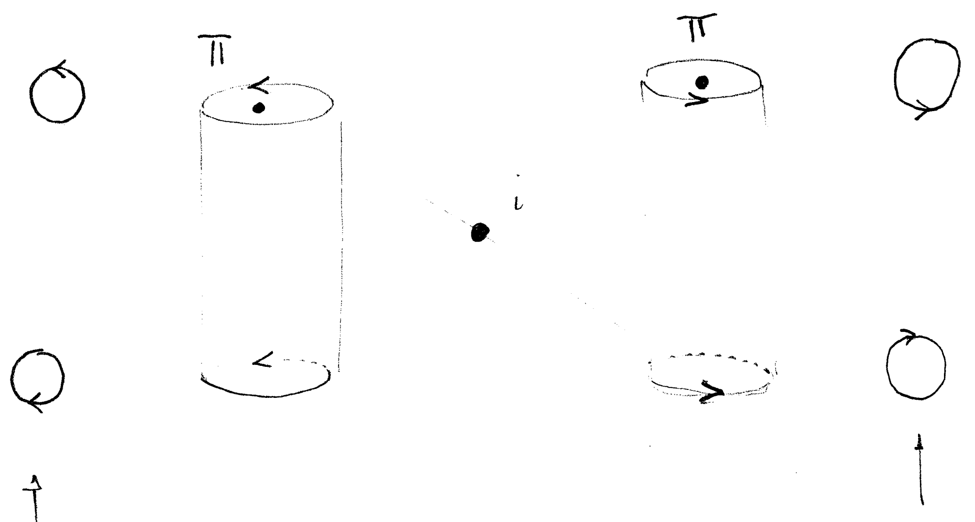
$$g_i\, \pi(g_i) = \pi(g_i)$$ the rotation does not influence its own pole.

We define $g\,\pi(g_i) \equiv \pi(g_i^g)$ the conjugated pole of $\pi(g)$ through g. As the rotation anticipates ($g_i^g = g g_i g^{-1}$ the conjugated of g_i through g)

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

-> $g\,\pi(g_i)$ is invariant under g_i^g => $g\,\pi(g_i) = \pi(g_i^g)$. 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°.

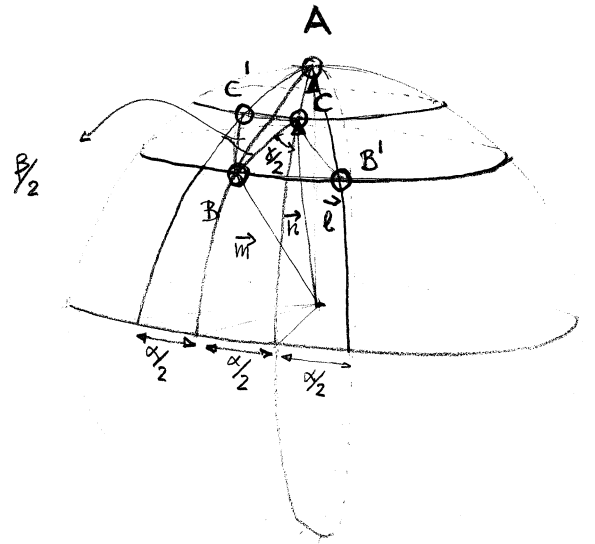
About improper rotations ig we limit ourself to say that $\pi(g) = \pi(ig)$



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 $\vec{n}_A = (0,0,1)$ => 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: $R(\gamma \vec{n}_C) \overset{def}{=} R(\alpha \vec{n}_A) R(\beta \vec{n}_B)$

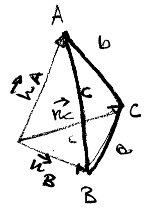
- If C is the pole of the composite rotation it should be left invariant under application of $R(\beta \vec{n}_B)$ and $R(\alpha \vec{n}_A)$ in the order. Now the rotation of β around $\vec{n}_B$ brings by construction $C \to C'$ and then $R(\alpha \vec{n}_A)$ back to C.

- 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

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

<u>proof</u>



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

- A, B, C are vertices and dihedral angles, i.e.: the angle of the curved polygon
- a, b, c indicates the arcs and the associated angles.

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

$\cos a = \vec{n}_B\cdot\vec{n}_C \qquad \cos b = \vec{n}_A\cdot\vec{n}_C \qquad \cos c = \vec{n}_A\cdot\vec{n}_B \qquad (|\vec{n}_\alpha| = 1)$

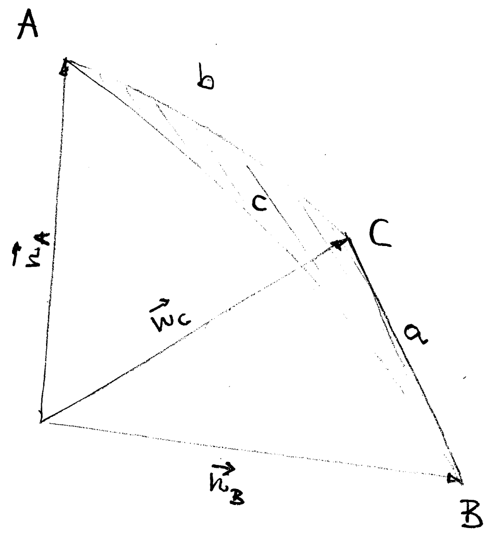
$\cos A = \vec{\tau}_b\cdot\vec{\tau}_c$ where $\vec{\tau}_b$ and $\vec{\tau}_c$ are unitary vectors tangent to c and b

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 $\vec{\tau}_c$

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

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

Notice $a, b, c < \pi \iff \sin a, \sin b, \sin c > 0$.



A
b
c
C
$\vec{w}_A$
$\vec{w}_C$
a
$\vec{w}_B$
B

proof of the sin theorem

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

as can be proven using the relations

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

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

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

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

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

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

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

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

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

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

see Fig. in the next page

$$\left.\begin{aligned} \sin c \sin A \sin b &= |(\vec{n}_A \times \vec{n}_B) \cdot \vec{n}_C| \\ \sin a \sin B \sin c &= |(\vec{n}_B \times \vec{n}_C) \cdot \vec{n}_A| \\ \sin b \sin C \sin a &= |(\vec{n}_C \times \vec{n}_A) \cdot \vec{n}_B| \end{aligned}\right\} \text{ these 3 are equal}$$

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

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

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

$\lrcorner$

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

$$A' + a = a' + A = \pi$$
$$B' + b = b' + B = \pi \qquad (2)$$
$$C' + c = c' + C = \pi$$

give figure of the polar triangle.

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

$(1) \mapsto \quad \cos a' = \cos b' \cos c' + \sin b' \sin c' \cos A'$ ⟵ cosine theorem applied to the polar triangle

$$\Downarrow (3)$$

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

Better, one can start directly from $\cos c' = \cos a' \cos b' + \sin a' \sin b' \cos C'$

Now by cycling

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

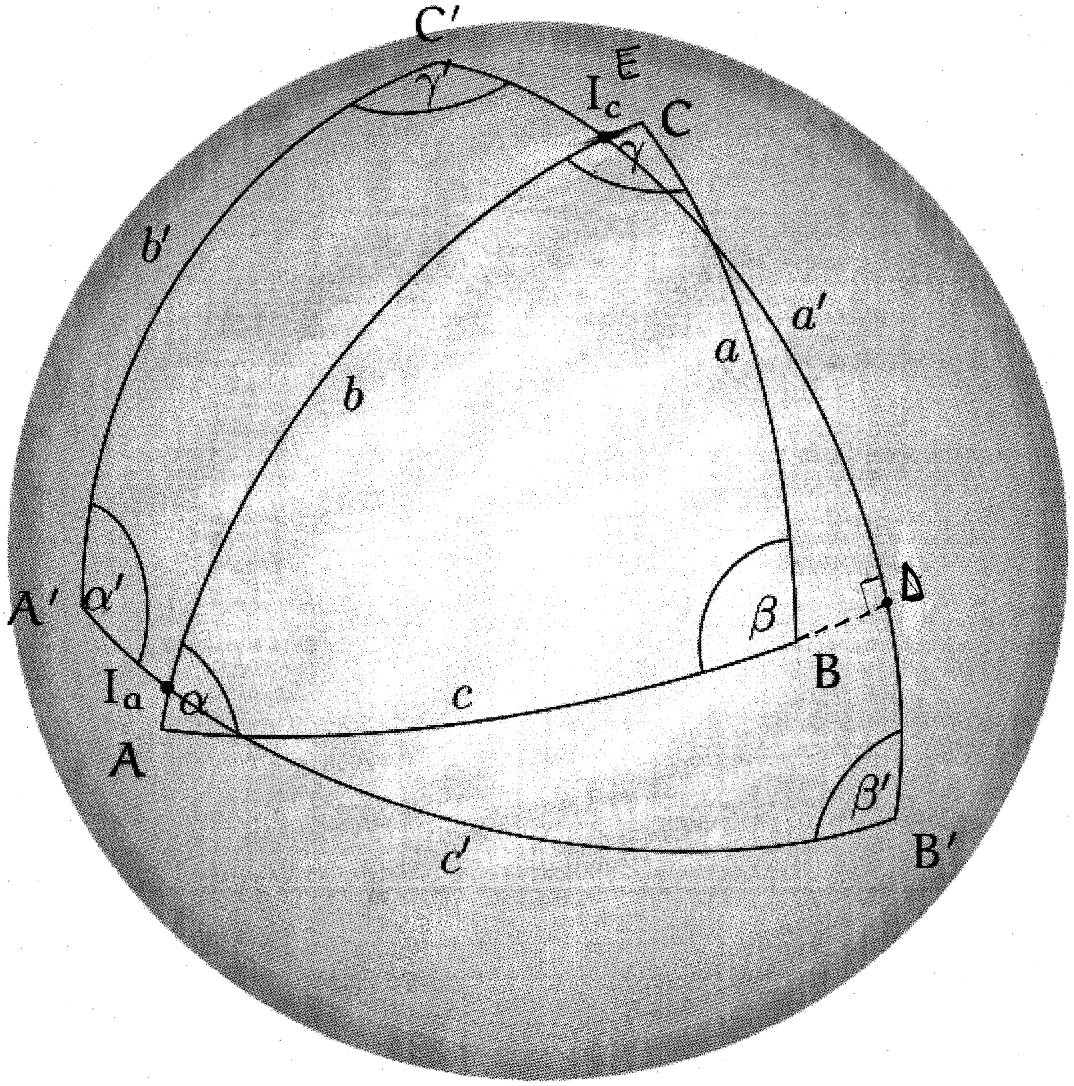
and inserting $\cos c = \vec{n}_A \cdot \vec{n}_B$

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

$C = \pi - \frac{\gamma}{2}$
$A = \frac{\alpha}{2}$
$B = \beta/2$

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:

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



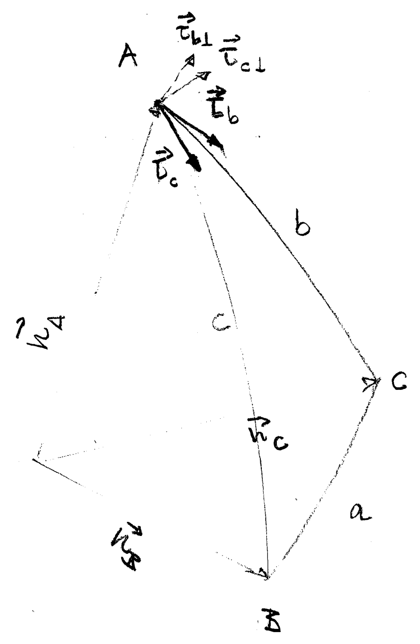
A', B', C' are the poles of the arcs BC, CA, AB which lie on the same side of the arcs as the opposite angles A, B, C respectively.
A'B'C' is the polar triangle of the (spherical) triangle ABC.

$C'\Delta = \pi/2$ since C' is the pole of AB => AD and A is the pole of B'C' => DC'

$B'E = \pi/2$ analogously

$$C'\Delta + B'E = \pi = C'E + 2ED + DB' = C'E + 2A + DB'$$

$$\Rightarrow \quad \pi - A = C'B' = a' \quad \Rightarrow \quad \boxed{A + a' = \pi}$$



$$\left.\begin{array}{l}(\vec{n}_A \times \vec{n}_B)\cdot \vec{n}_A = 0 \\ (\vec{n}_A \times \vec{n}_B)\cdot \vec{t}_c = 0 \\ \vec{t}_c \cdot \vec{n}_A = 0\end{array}\right\} \Rightarrow \quad \vec{t}_c,\ \frac{\vec{n}_A \times \vec{n}_B}{|\vec{n}_A \times \vec{n}_B|}\ \ \vec{n}_A$$ form an oriented orthonormal basis

$$\left.\begin{array}{l}(\vec{n}_A \times \vec{n}_C)\cdot \vec{n}_A = 0 \\ (\vec{n}_A \times \vec{n}_C)\cdot \vec{t}_b = 0 \\ \vec{t}_b \cdot \vec{n}_A = 0\end{array}\right\} \Rightarrow \quad \vec{t}_b,\ \frac{\vec{n}_A \times \vec{n}_C}{|\vec{n}_A \times \vec{n}_C|}\ \ \vec{n}_A$$ form an oriented orthonormal basis

$$\Rightarrow \quad \sin A = |\vec{t}_c \times \vec{t}_b| = \frac{|(\vec{n}_A \times \vec{n}_B) \times (\vec{n}_A \times \vec{n}_C)|}{|\vec{n}_A \times \vec{n}_B||\vec{n}_A \times \vec{n}_C|} = \frac{\times}{\sin c \sin b}$$

$\vec{n}_C$ 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

$$\left.\begin{aligned}
\vec{n}_A^{\,*} &= \frac{\vec{n}_B \times \vec{n}_\perp}{(\vec{n}_B \times \vec{n}_\perp)\cdot \vec{n}_A} \\
\vec{n}_B^{\,*} &= \frac{\vec{n}_\perp \times \vec{n}_A}{(\vec{n}_\perp \times \vec{n}_A)\cdot \vec{n}_B} \\
\vec{n}_\perp^{\,*} &= \frac{\vec{n}_A \times \vec{n}_B}{(\vec{n}_A \times \vec{n}_B)\cdot \vec{n}_\perp}
\end{aligned}\right\} \Rightarrow$$

$\vec{n}_A^{\,*}\cdot(\vec{n}_B \text{ or } \vec{n}_\perp) = 0$

$\vec{n}_A \cdot \vec{n}_A^{\,*} = 1$

and analogously for the others

Moreover we notice that

$\vec{n}_\perp^{\,*} = \vec{n}_\perp / |\vec{n}_\perp|^2$

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

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

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

$$[\vec{n}_B \times (\vec{n}_A \times \vec{n}_B)]_k = \sum_{ij} n_{Bi}\,(\vec{n}_A \times \vec{n}_B)_j\,\varepsilon_{ijk} = \sum_{\substack{ij\\lm}} n_{Bi}\, n_{Al}\, n_{Bm}\, \varepsilon_{lmj}\,\varepsilon_{ijk} =$$

$$= \sum_{ijlm} n_{Bi}\, n_{Al}\, n_{Bm}\, \varepsilon_{lmj}\,\varepsilon_{kij} = \sum_{ilm} n_{Bi}\, n_{Al}\, n_{Bm}\,(\delta_{lk}\delta_{mi} - \delta_{li}\delta_{mk})$$

$$= \sum_i n_{Bi}\, n_{Ak}\, n_{Bi} - \sum_i n_{Bi}\, n_{Ai}\, n_{Bk} = \left(|\vec{n}_B|^2\, \vec{n}_A - (\vec{n}_A \cdot \vec{n}_B)\,\vec{n}_B\right)_k$$

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

- $$g = \vec n_C \cdot \vec n_B^{\,*} = \frac{\vec n_C \cdot \left[(\vec n_A \times \vec n_B) \times \vec n_A \right]}{1 - (\vec n_A \cdot \vec n_B)^2} = \frac{\vec n_B \cdot \vec n_C - (\vec n_A \cdot \vec n_B)(\vec n_A \cdot \vec n_C)}{1 - (\vec n_A \cdot \vec n_B)^2}$$

$$\left[(\vec n_A \times \vec n_B) \times \vec n_A \right] = \left[\vec n_A \times (\vec n_B \times \vec n_A) \right] = \vec n_B - (\vec n_A \cdot \vec n_B)\, \vec n_A$$

- $$h = \frac{\vec n_C \cdot (\vec n_A \times \vec n_B)}{1 - (\vec n_A \cdot \vec n_B)^2}$$

$$\vec n_C = \frac{\left[\vec n_A \cdot \vec n_C - (\vec n_A \cdot \vec n_B)(\vec n_B \cdot \vec n_C) \right] \vec n_A + \left[\vec n_B \cdot \vec n_C - (\vec n_A \cdot \vec n_B)(\vec n_A \cdot \vec n_C) \right] \vec n_B + \left[\vec n_C \cdot (\vec n_A \times \vec n_B) \right] (\vec n_A \text{[illegible]}}{1 - (\vec n_A \cdot \vec n_B)^2}$$

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

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

$$\sin c\, \vec n_C = \frac{\cos b - \cos c \cos a}{\sin a \sin c} \sin a\, \vec n_A + \frac{\cos a - \cos c \cos b}{\sin c \sin b} \sin b\, \vec n_B + \sin b \sin A\, (\vec n_A \times \vec n_B) = \text{ due to the cosine theorem}$$

$$= \cos B \sin a\, \vec n_A + \cos A \sin b\, \vec n_B + \sin b \sin A\, (\vec n_A \times \vec n_B)$$

equivalently, due to the sin theorem

$$\text{(II)} \quad \boxed{\sin C\, \vec n_C = \cos B \sin A\, \vec n_A + \cos A \sin B\, \vec n_B + \sin B \sin A\, (\vec n_A \times \vec n_B)}$$

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.

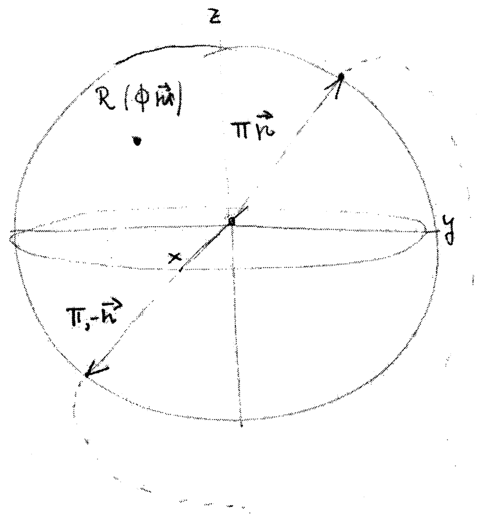
ii) On the other hand $\phi \longrightarrow \phi + 2\pi \quad (\lambda ; \vec{\Lambda}) \longrightarrow (-\lambda ; -\vec{\Lambda})$
this tells us that the Rodrigues parameters can distinguish the history of a rotation. (see later about this point)

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

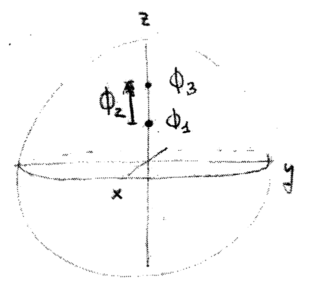
$$\lambda^2 + |\vec{\Lambda}|^2 = 1$$

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<->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)



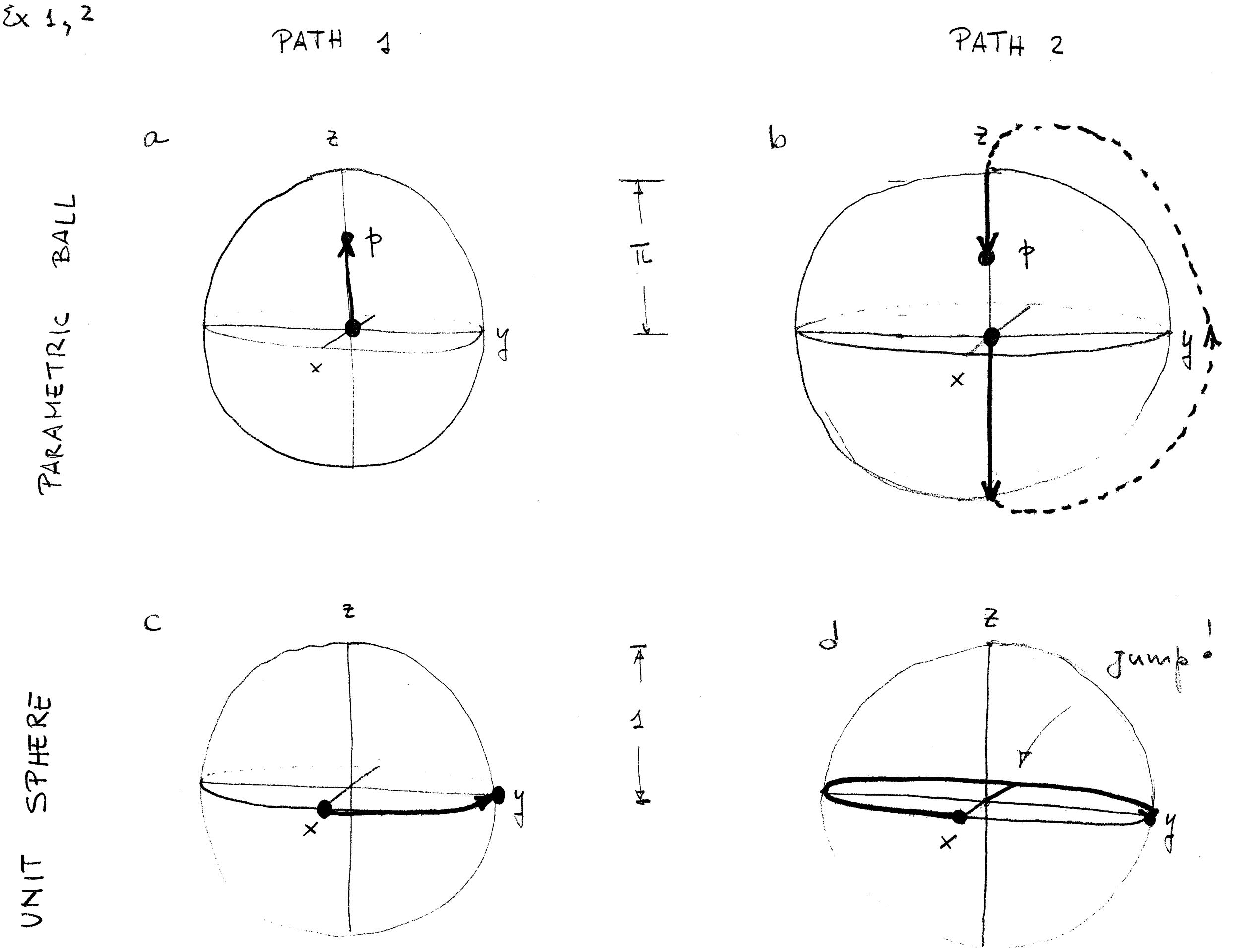
The composition of infinitesimal rotations generates paths in the parametric ball. As a simple example of path let us take 2 rotations around the z axis such that $\phi_1 + \phi_2 = \phi_3 < \pi$. We can represent the composition in the parametric ball as



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:

Ex 1, 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 d figures. In particular, path 2 has a "jump" between identified antipodal points while PATH 1 shows no "jump".

Ex. 3 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 **generic** angle α. Let's call $\phi, \vec{n}$ the parametrization of the composite rotation

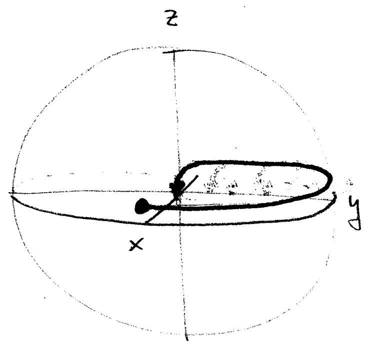
(ER) $$\cos\phi/2 = \cancel{\cos\tfrac{\alpha}{2}\cos\tfrac{\pi}{2}} - \sin\tfrac{\alpha}{2}\sin\tfrac{\pi}{2}\,(\hat{x}\cdot\hat{z}) = 0 \Rightarrow \phi = \pi$$

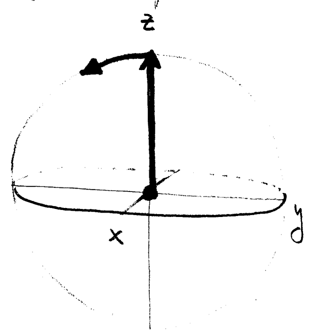
$$\overset{1}{\cancel{\sin\tfrac{\pi}{2}}}\,\vec{n} = \cancel{\sin\tfrac{\alpha}{2}\cos\tfrac{\pi}{2}\,\hat{x}} + \cos\tfrac{\alpha}{2}\,\overset{1}{\cancel{\sin\tfrac{\pi}{2}}}\,\hat{z} + \sin\tfrac{\alpha}{2}\,\overset{1}{\cancel{\sin\tfrac{\pi}{2}}}\,(\hat{x}\times\hat{z}) =$$

$$\vec{n} = \cos\tfrac{\alpha}{2}\,\hat{z} - \sin\tfrac{\alpha}{2}\,\hat{y}$$

(notice that the result is valid $\forall\, \alpha$)

Since $\phi = \pi$ 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 z and larger (negative) y.





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 $C_{\alpha z} C_{2x}$ without "jumps". We here taken for this purpose the same definition of h and $\bar{h}$ as in the unit sphere. (page 72)

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

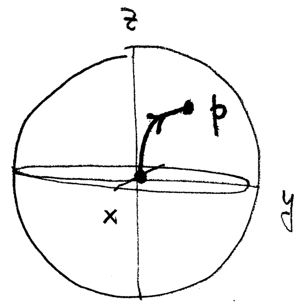
Def: homotopy: Two co-terminous paths in parameter space are said homotopic if they can be continuously deformed one into the other.

Def Class of homotopy: all paths homotopic to each other form a class of homotopy

Theorem: In the parametric ball (the parametric space of the proper rotation group - $SO(3)$ the group of the special ($\det \Gamma^{R^3}(g) = 1$) orthogonal matrices of dimension 3 -) there are only 2 classes of homotopy: paths without jumps and path with 1 jump.

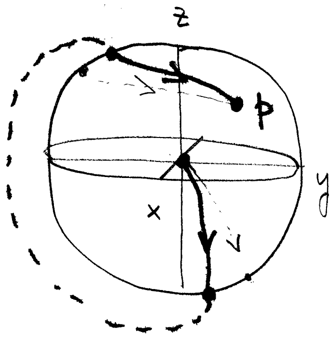
proof A path without a jump is all contained in a hemisphere => it does not contain antipodal points. A path containing a jump contains a pair of antipodal points. Antipodal points move "simultaneously" in infinitesimal transformation => remaining always in distinct hemispheres. It remains to be proven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

Path 1



path without jumps (class 0)

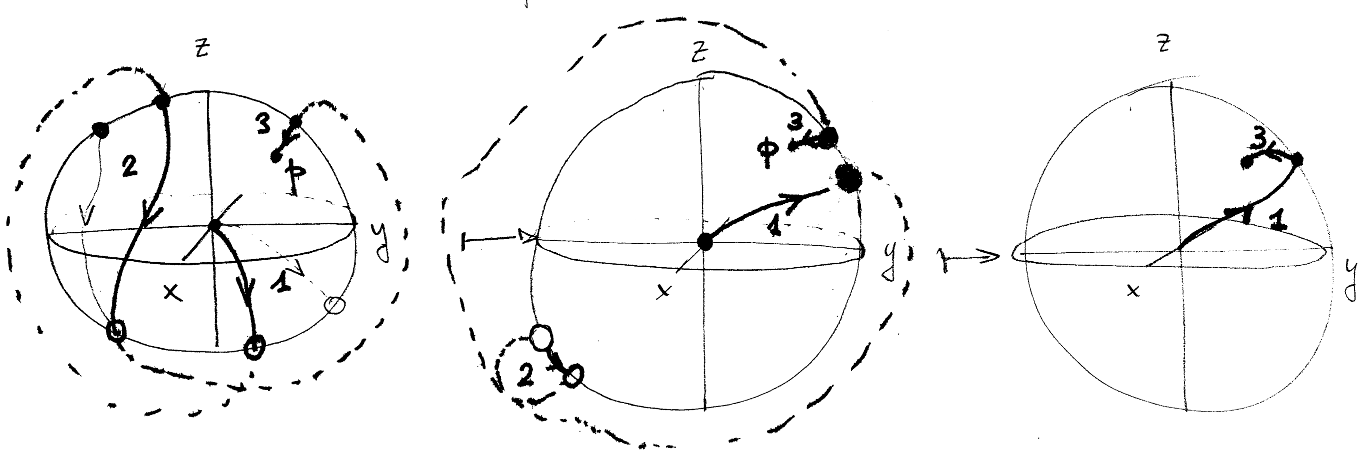
Path 2



path with a 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

projective factor

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

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 $\Rightarrow$ 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.

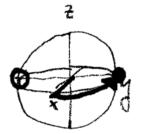
- SO(3) is not simply connected since not all loops in its parameter space can be continuously contracted to a point (it is doubly connected)

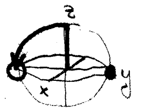
- $R(2\pi\vec{n}) = R(0\vec{n})$ as an operation in SO(3). Nevertheless, as all points in the parameter space, it can be reached from the origin by 2 classes of paths.

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

7.4 The spinor representations (an example of projective representation)

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 inside 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

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

$\bar{h}$ negative rotations

The standard ER parameters are the set

$$\lambda_g > 0 \qquad \text{or} \qquad \lambda_g = 0 \quad \vec{\Lambda} \in h \leftarrow \text{binary rotations.}$$

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

$R(-\lambda_g ; -\vec{\Lambda}_g)$ 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

- $\lambda_g > 0$ 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 $\vec{\Lambda}_3 \in h$

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

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

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

Examples of calculation of projective factors for a projective spinorial repr.

i) $[C_2, C_2] = -1 \quad \forall \vec{n}$ $\qquad \lambda_1 = \lambda_2 = 0, \; \vec{\Lambda}_1 = \vec{\Lambda}_2 = \vec{n} \qquad C_2^2 = \bar{E}$

$$\lambda_3 = \lambda_1\lambda_2 - \vec{\Lambda}_1 \cdot \vec{\Lambda}_2 = -1$$
$$\vec{\Lambda}_3 = \lambda_1 \vec{\Lambda}_2 + \lambda_2 \vec{\Lambda}_1 + \vec{\Lambda}_1 \times \vec{\Lambda}_2 = 0$$
$$\Rightarrow R(0, \vec{n}) R(0, \vec{n}) = R(-1, \vec{0})$$

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

$$\lambda_1 = \cos\frac{\pi}{3} = \frac{1}{2} \qquad \vec{\Lambda}_1 = \sin\frac{\pi}{3}\hat{e}_z = \frac{\sqrt{3}}{2}\hat{e}_z \qquad C_3^+ C_3^- = E$$
$$\lambda_2 = \cos\left(-\frac{\pi}{3}\right) = \frac{1}{2} \qquad \vec{\Lambda}_2 = \sin\left(-\frac{\pi}{3}\right)\hat{e}_z = -\frac{\sqrt{3}}{2}\hat{e}_z$$

$$\lambda_3 = \frac{1}{4} + \frac{3}{4} = 1$$
$$\vec{\Lambda}_3 = \frac{\sqrt{3}}{4}\hat{e}_z - \frac{\sqrt{3}}{4}\hat{e}_z - \frac{3}{4}\hat{e}_z \times \hat{e}_z = 0$$
$$\Rightarrow R\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\hat{e}_z\right) R\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\hat{e}_z\right) = R(1, \vec{0})$$

iii) $[\![C_3^+, C_3^+]\!] = -1$ $\qquad \lambda_1 = \lambda_2 = \frac{1}{2} \qquad \vec{\Lambda}_1 = \vec{\Lambda}_2 = \frac{\sqrt{3}}{2}\hat{e}_z$

$$\lambda_3 = \frac{1}{4} - \frac{3}{4} = -\frac{1}{2}$$
$$\vec{\Lambda}_3 = \frac{\sqrt{3}}{4}\hat{e}_z + \frac{\sqrt{3}}{4}\hat{e}_z + \frac{3}{4}\hat{e}_z \times \hat{e}_z = \frac{\sqrt{3}}{2}\hat{e}_z$$
$$\Rightarrow R\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\hat{e}_z\right) R\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\hat{e}_z\right) = R\left(-\frac{1}{2}, \frac{\sqrt{3}}{2}\hat{e}_z\right)$$

$$(C_3^+)^2 = \bar{C}_3^-.$$

iv) $[\![C_{2z}, C_{2x}]\!] = 1$

$$\lambda_1 = \cos\frac{\pi}{2} = 0 \qquad \vec{\Lambda}_1 = \sin\frac{\pi}{2}\,\hat{e}_x = \hat{e}_z$$

$$\lambda_2 = \cos\frac{\pi}{2} = 0 \qquad \vec{\Lambda}_2 = \sin\frac{\pi}{2}\,\hat{e}_z = \hat{e}_x$$

$$\lambda_3 = 0\,\hat{e}_x + 0\,\hat{e}_z - \hat{e}_x \cdot \hat{e}_z = 0$$

$$\vec{\Lambda}_3 = \hat{e}_z \times \hat{e}_x = \hat{e}_y \qquad \Rightarrow R(0, \hat{e}_z)\, R(0, \hat{e}_x) = R(0, \hat{e}_y) \quad \Rightarrow C_{2z} C_{2x} = C_{2y}$$

$\pi \hat{e}_y \in H$ northern hemisphere

$$\lambda_1 = \lambda_2 = 0 \qquad \vec{\Lambda}_1 = \hat{e}_x \quad \vec{\Lambda}_2 = \hat{e}_z$$

v) $[\![C_{2x}, C_{2z}]\!] = -1$

$$\lambda_3 = 0$$

$$\vec{\Lambda}_3 = \hat{e}_x \times \hat{e}_z = -\hat{e}_y \qquad \Rightarrow R(0, \hat{e}_x)\, R(0, \hat{e}_z) = R(0, -\hat{e}_y) \quad \Rightarrow C_{2x} C_{2z} = \bar{C}_{2y}$$

$-\pi \hat{e}_y \in \bar{H}$ southern hemisphere.

The <u>intertwining theorem</u> is fundamental to understand the characters of a spinor representation.

<u>Def</u>: g_i and g_j are intertwined by g if

(1) $g g_i = g_j g$

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

The conjugation g_i^g is intertwined with g_i by g: $g_i^g g = g g_i$

<u>Theorem</u> The following relations between spinorial projective factors hold

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

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

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

<u>proof</u> 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:

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

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

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

- $g_i^g = g g_i g^{-1}$ we perform the calculation step by step

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

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

$$(\cancel{\lambda\lambda_i} - \vec\Lambda\cdot\vec\Lambda_i)(-\vec\Lambda) + \lambda(\lambda\vec\Lambda_i + \cancel{\lambda_i\vec\Lambda} + \vec\Lambda\times\vec\Lambda_i) + (\lambda\vec\Lambda_i + \cancel{\lambda_i\vec\Lambda} + \vec\Lambda\times\vec\Lambda_i)\times(-\vec\Lambda)$$

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

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

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

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

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

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

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

A last composition is needed to obtain the (ER) of $g_i g g$.

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

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

$$\lambda_i\vec\Lambda + 2\lambda(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda + \lambda(1 - 2|\vec\Lambda|^2)\vec\Lambda_i + 2\lambda^2(\vec\Lambda\times\vec\Lambda_i)$$

$$+ (1 - 2|\vec\Lambda|^2)(\vec\Lambda_i\times\vec\Lambda) + 2\lambda(\vec\Lambda\times\vec\Lambda_i)\times\vec\Lambda\big]$$

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

$$+ 2\lambda^2(\vec\Lambda\times\vec\Lambda_i) + (\lambda^2 - |\vec\Lambda|^2)(\vec\Lambda_i\times\vec\Lambda) + \cancel{2\lambda|\vec\Lambda|^2\vec\Lambda_i} - \cancel{2\lambda(\vec\Lambda\cdot\vec\Lambda_i)\vec\Lambda}\big]$$

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

$\square$

ii) For coaxial rotations the operators commute

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

$$R(\lambda, p\sqrt{1-\lambda^2}\,\vec{n})\,R(\lambda_i, p_i\sqrt{1-\lambda_i^2}\,\vec{n}) = R\left(\lambda\lambda_i - pp_i\sqrt{1-\lambda^2}\sqrt{1-\lambda_i^2},\; pp_i(\lambda\sqrt{1-\lambda_i^2} + \lambda_i\sqrt{1-\lambda^2})\,\vec{n}\right)$$

the result is symmetric in the exchange λ and λ_i $\Rightarrow$ $[g, g_i] = [g_i, g]$

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 definition of regular and irregular rotations the first being the non-commuting or coaxial, the second being the bilateral binary (BB) rotations.

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

The characters are in general <u>not</u> <u>class functions</u> for projective representations (Schur, 1904). Theorem

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

proof

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

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

⌈ proof of the associativity condition

it must be a representation!

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

L

R

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

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

□ ⌋

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

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

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

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

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

Now we use associativity in the form $[\check{G}(gg_i)\check{G}(g^{-1})]\check{G}(g) = \check{G}(gg_i)[\check{G}(g^{-1})\check{G}(g)]$

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

$$[gg_i,g^{-1}]\,[g_i^g,g] = [g^{-1},g]$$ ← we introduce in (*) $[g^{-1},g]$

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

Once more the associativity in the form

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

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

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

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

From (4) 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 pairs of irregular rotations g_i and g

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

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

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

7.5 The algebra of rotations: quaternions

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

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

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

$\Rightarrow$ 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 $A = a + \mathbb{n}|\vec{A}|$.

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

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

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

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

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

$a \left\langle \begin{array}{l} \text{scalar} \\ \text{pseudoscalar} \Rightarrow ab = \text{scalar} \ ↯ \end{array} \right.$

$\vec{A} \left\langle \begin{array}{l} \text{vector} \Rightarrow \vec{A}\times\vec{B} = \text{pseudovector} \ ↯ \\ \text{pseudovector} \end{array} \right.$

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

Now let us deal with 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 parametrization:

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

* (Euler - Rodrigues) $[\![\cos\phi/2, \sin\phi/2\,\vec{n}]\!]$ 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 <u>devided</u>

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

Notice though that $\mathbb{A}\mathbb{B}^{*} \neq \mathbb{B}^{*}\mathbb{A}$!

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 $\mathcal{G}$, the associated double group is constructed by defining the "rotation by 2π" $= \bar{E}$ and constructing then $\bar{g}_i = \bar{E} g_i$ $\forall\, g_i \in \mathcal{G}$ $\Rightarrow$ 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 $\bar{\mathcal{G}}$ 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

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

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

we now have a one to one mapping between the elements of $\bar{\mathcal{G}}$ 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 $\overline{D}_2$ is now completely natural

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

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

Example of 2 elements of the new multiplication table

$$C_{2x}C_{2y} \mapsto [\![0,\hat{\imath}]\!]\,[\![0,\hat{\jmath}]\!] = \mathbb{i}\,\mathbb{j} = \mathbb{K} = [\![0,\hat{k}]\!] \mapsto C_{2z}$$

$$C_{2y}\,C_{2x} \mapsto [\![0,\hat{\jmath}]\!]\,[\![0,\hat{\imath}]\!] = \mathbb{j}\,\mathbb{i} = -\mathbb{K} = [\![0,-\hat{k}]\!] \mapsto \overline{C}_{2z}$$

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:

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

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

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

Now let us analyze the inverse and the conjugation in a double group sense, taking advantage of the quaternion representation.

$\boxed{\text{INVERSION}}$

Theorem: If $g \in \mathcal{G}$ it follows that

$$g^{\sim 1} \simeq g^{-1} \quad \text{if } g \text{ is not binary} \quad (*)$$
$$g^{\sim 1} \simeq \bar{g} \quad \text{if } g \text{ is binary.} \quad (**)$$

Moreover $\bar{g}^{\sim 1} \simeq \bar{E} g^{-1} \equiv \overline{(g^{-1})}$ if g is not binary and $\bar{g}^{\sim 1} \cong g$ if g is binary. A relation comprehensive of both cases reads $\bar{g}^{\sim 1} \simeq \bar{E}\, g^{\sim 1}$.

proof:

The inverse of a quaternion is easily given $A^{-1} = A^{*} |A|^{-2}$.

The quaternion associated to rotations are normalized quaternions

$\Rightarrow \quad \mathbb{R}^{-1} = \mathbb{R}^{*}$.

- For non-binary rotation $\mathbb{R} \leftrightarrow [\![\lambda, \vec{\Lambda}]\!] \Rightarrow \mathbb{R}^{-1} = \mathbb{R}^{*} = [\![\lambda, -\vec{\Lambda}]\!]$ $\lambda > 0$ which correspond to an inversion operation on the rotation pole

$$\Rightarrow \quad g^{\sim 1} \simeq g^{-1}.$$

- For binary rotation $\mathbb{R} \leftrightarrow [\![0, \vec{\Lambda}]\!] \Rightarrow \mathbb{R}^{-1} = \mathbb{R}^{*} = [\![0, -\vec{\Lambda}]\!] = -1\, [\![0, \vec{\Lambda}]\!]$

$$\Rightarrow \quad g^{\sim 1} \simeq \bar{E} g \equiv \bar{g}$$

- $\bar{g} \leftrightarrow [\![-\lambda, -\vec{\Lambda}]\!]$ whose quaternionic inverse is $[\![-\lambda, \vec{\Lambda}]\!] = [\![-1, 0]\!]\, [\![\lambda, -\vec{\Lambda}]\!]$

$\Rightarrow$ we conclude $\bar{g}^{\sim 1} \simeq \bar{E} g^{-1}$ if g is not binary.

- For a binary rotation $[\![0, \vec{\Lambda}]\!]\, [\![0, -\vec{\Lambda}]\!] = [\![1, 0]\!] \Leftrightarrow g\bar{g} = E \Leftrightarrow \bar{g}^{\sim 1} \simeq g \simeq \bar{E}\bar{E} g \simeq \bar{E}\bar{g} \simeq \bar{E} g^{\sim 1}$

$$\Rightarrow \text{ in general } \quad \bar{g}^{\sim 1} \simeq \bar{E}\, g^{\sim 1}$$

$\blacksquare$

CONJUGATION

Def: $g_i \tilde{c}\, g_j$ if $\exists\, g \in \mathcal{G}$ or $\bar{g} \in \bar{\mathcal{G}}$: $g g_i g^{-1} \simeq g_j$ or $\bar{g} g_i \bar{g}^{-1} \simeq g_j$.

Corollary: The definition of conjugation can be restricted to

$$g_i \tilde{c}\, g_j \quad \text{if } \exists\, g \in \mathcal{G} : \quad g g_i g^{-1} \simeq g_j$$

proof: $\bar{g} \simeq \bar{E} g \Rightarrow \bar{g}^{-1} \simeq \bar{E} g^{-1}$ from the inversion theorem. Moreover $[\bar{E}, g] = 0$ and $\bar{E}^2 = E$ (think in terms of quaternions)

$$\Rightarrow \bar{g} g_i \bar{g}^{-1} \simeq \bar{E} g g_i \bar{E} g^{-1} \simeq \bar{E}^2 g g_i g^{-1} \simeq g g_i g^{-1}.$$

The question is now about the connection $g_i c\, g_j$ and $g_i \tilde{c}\, g_j$. It is clear that

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

Let us proceed in steps:

A- Intertwining theorem (double group formulation). Given the relation $g g_i = g_j g$, it follows that: (recall the intertwining theorem for projective factors / page 37)

$g g_i \simeq g_j g$ if g and g_i are regular operations

$g g_i \simeq \bar{g}_j g$ if g and g_i are irregular operation.

proof: $g g_i = g_j g \Rightarrow$ ($g_j = g g_i g^{-1} = g_i^g$. If g and g_i are regular operations $[g, g_i] = [g_i^g, g]$ if g and g_i are not commuting, and $[g, g_i] = [g_i, g]$ if g, g_i are coaxial) $\Rightarrow$ in general $g g_i = g_j g$ has also validity in the double group sense since the projective factors coincide.

If g and g_i are irregular operations

$g g_i = g_j g$ but $[g, g_i] = -[g_j, g] \Rightarrow g g_i \simeq \bar{g}_j g$

B - First conjugation theorem.

Given the relation $g_i \tilde{c}\, \bar{g}_j$ it follows that

$$\exists\, g \in \mathcal{G} : \quad g g_i = g_j g \quad \text{but} \quad g g_i \not\simeq g_j g$$

proof

$$g_i \tilde{c}\, \bar{g}_j \iff g g_i g^{-1} \simeq \bar{g}_j \qquad g \in \bar{\mathcal{G}}$$

$$\Rightarrow \quad g g_i \simeq \bar{g}_j g \quad \Rightarrow \quad g g_i = g_j g$$

the last equality follows from $E = \bar{E}$ (but $E \simeq \bar{E}$).

For the proof of the second part of the theorem, let's assume $g g_i \simeq g_j g$

$$\Rightarrow \quad g_j g \simeq g g_i \simeq \bar{g}_j g \quad \Rightarrow \quad g_j \simeq \bar{g}_j \quad ⚡$$

C - Second conjugation theorem.

For any pair of operations g_i and g_j

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

Iff g_i and g (the operation needed for conjugation) are irregular

$\Rightarrow$ ADDITIONALLY

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

proof As a corollary of the intertwining theorem (double group formulation,

$$g_i g = g g_j \iff g_i c g_j \Rightarrow g g_i \simeq g_j g \iff g_i \tilde{c} g_j$$

for regular operations. For irregular operation $[g, g_i] = 0 \Rightarrow g_i = g_j \Rightarrow g_i \simeq g_j$ and "obviously $g_i \tilde{c}\, g_j \simeq g_i$. Moreover, as a corollary of the intertw.

$$g g_i \simeq \bar{g}_i g \Rightarrow g_i \tilde{c}\, \bar{g}_i \simeq \bar{g}_j .$$

We still have to prove the opposite direction

$\left(g_i \tilde{c} \bar{g}_j \text{ and } g_i \tilde{c} g_j \Rightarrow \bar{g}_i \tilde{c} \bar{g}_j\right) \Rightarrow g_i \tilde{c} \bar{g}_i \overset{Th 1}{\Rightarrow} \exists g \in \mathcal{G}$ such that $[g, g_i] = 0$

but $[\bar{g}, g_i] \neq 0$ Non coaxial rotations do not commute. Coaxial rotations commute in both cases. $\Rightarrow (g, \bar{g}_i)$ are irregular.

D - <u>Opechowski theorem</u> The class $C(g_i)$ of a regular operation $g_i \in \mathcal{G}$ gives 2 classes in $\bar{\mathcal{G}}$ which are $\bar{C}(g_i)$ and $\bar{C}(\bar{g}_i)$. If g_i is irregular, then $C(g_i)$ gives only one class in $\bar{\mathcal{G}}$, $\bar{C}(g_i)$ which coincides with $\bar{C}(\bar{g}_i)$.

<u>proof</u>:

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

  $\Rightarrow C(g_i) \subseteq \bar{C}(g_i)$. On the other hand $g_j \in \bar{C}(g_i) \Rightarrow g_j \tilde{c} g_i$

  $\Rightarrow g_i c g_j \Rightarrow C(g_i)$ and $\bar{C}(g_i)$ coincide.

  $g_i \tilde{c} g_j \Rightarrow \bar{g}_i \tilde{c} \bar{g}_j \Rightarrow$ all $\bar{g}_j : g_j \in C(g_i)$ form a class. The two classes are disjoint, otherwise $g_i \tilde{c} \bar{g}_j$ which is valid only if g_i is irregular.

- g_i irregular $g_i c g_j \Rightarrow g_i \tilde{c} g_j$ and $g_i c g_j \Rightarrow g_i \tilde{c} \bar{g}_j \simeq \bar{g}_i$

  $\Rightarrow \bar{C}(g_i)$ and $\bar{C}(\bar{g}_i)$ are the same class.

<u>Corollary</u>

N_c number of classes in $\mathcal{G}$
$\bar{N}_c$ number of classes in $\bar{\mathcal{G}}$
N_r number of regular classes
N_i number of irregular classes

The number of spinor irred representations coincide with the number of regular classes.

$N_c = N_r + N_i$ $\quad$ $\bar{N}_c = 2N_r + N_i = \bar{N}_{ir}$ $\quad$ $\bar{N}_c - N_c = N_r$
= number of spinor repr.