

Group Theory in Quantum Mechanics

Lecture 13 (3.12.13)

Smallest non-Abelian isomorphic groups $D_3 \sim C_{3v}$

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 5 Ch. 15)

(PSDS - Ch. 3)

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}
 D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

By nomograms based on $U(2)$ Hamilton-turns

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

All-commuting operators and D_3 -invariant class algebra

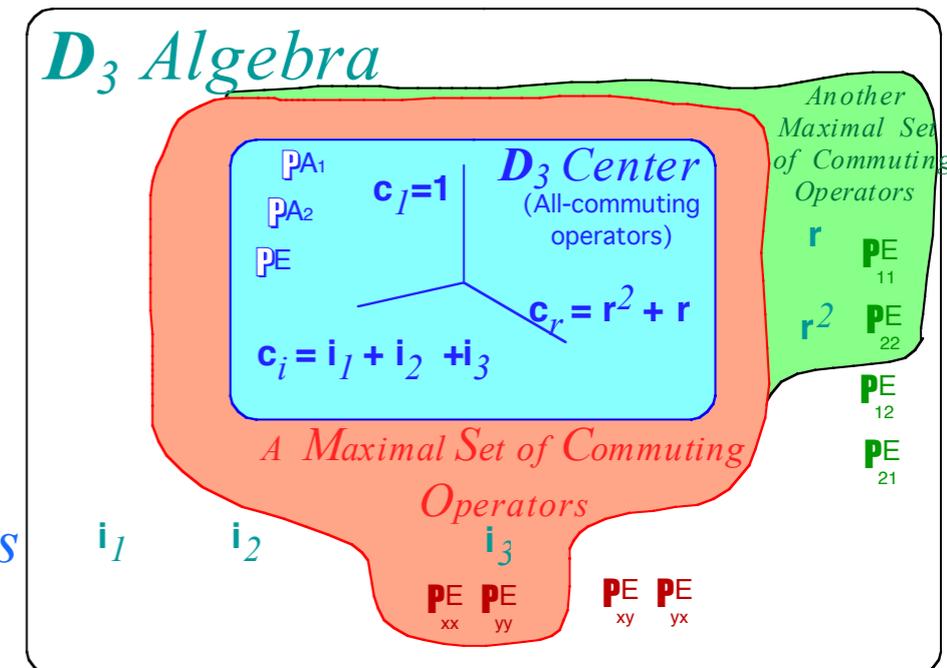
All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

Spectral resolution to irreducible representations (or "irreps") foretold by **characters** or traces

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^l \downarrow D_3$ splitting

D_3 Algebra



(Fig. 15.2.1 QTCA)



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Fig. 3.1.1 PSDS

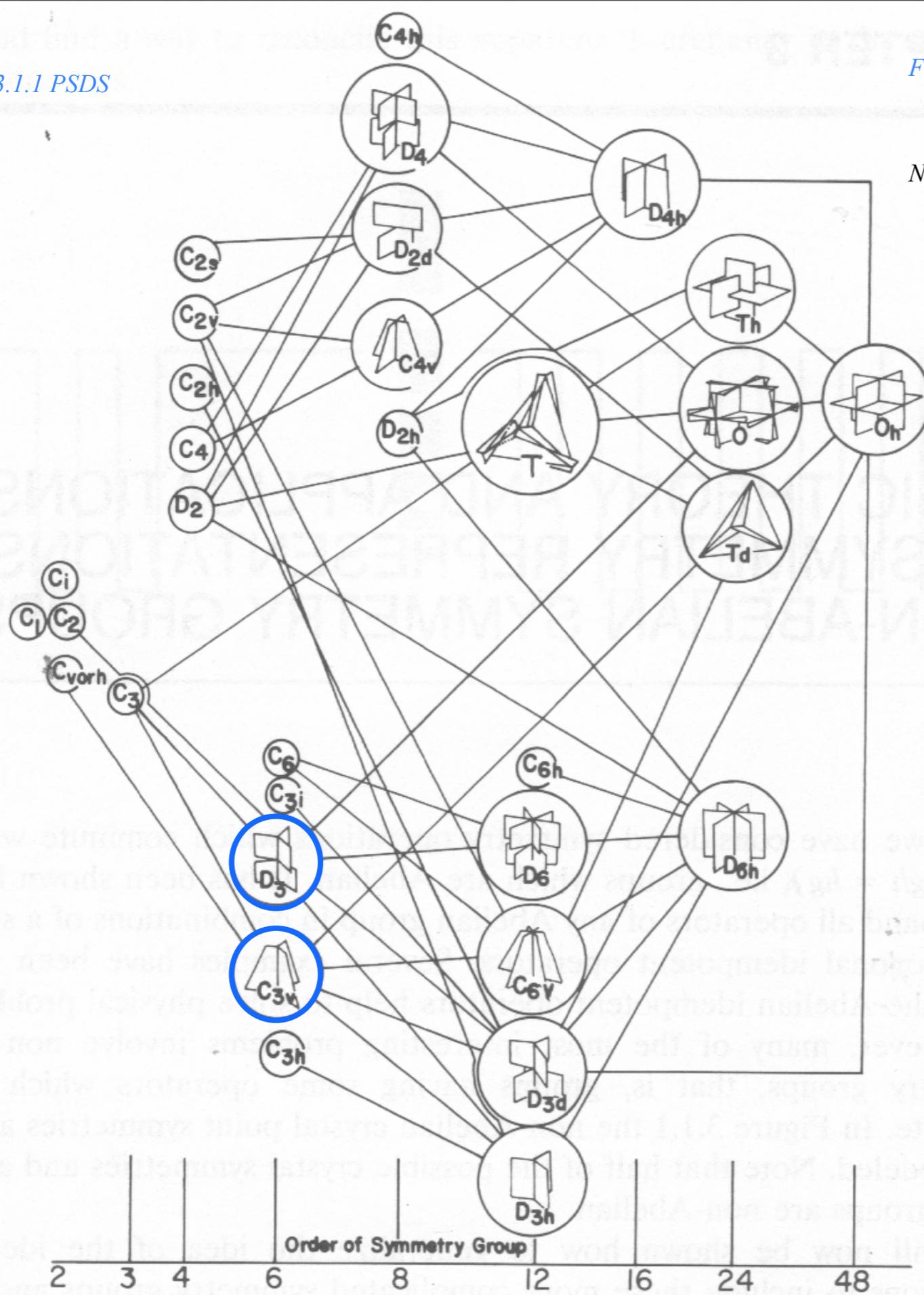
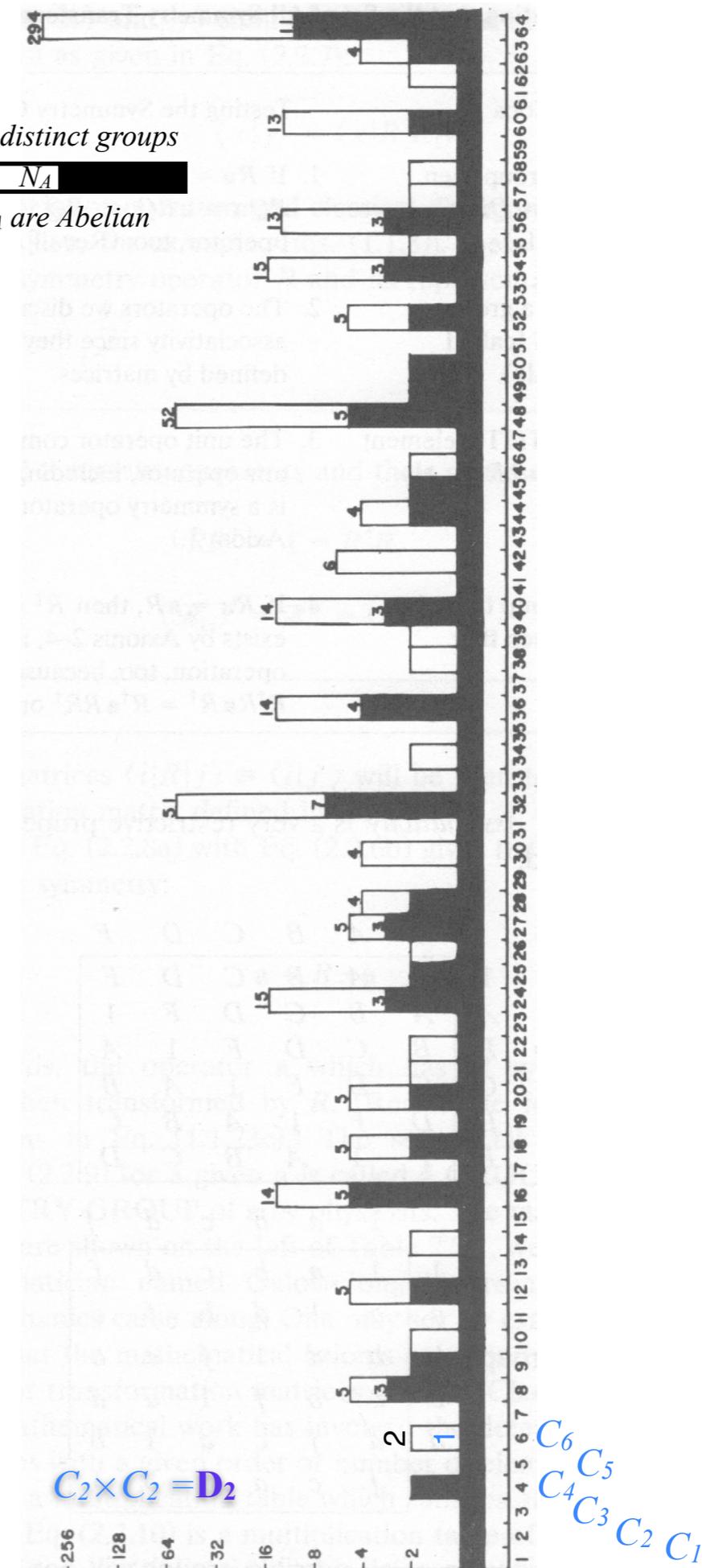


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

Fig. 2.2.2 PSDS

Total number N_g of distinct groups
 N_g N_A
 number N_A are Abelian



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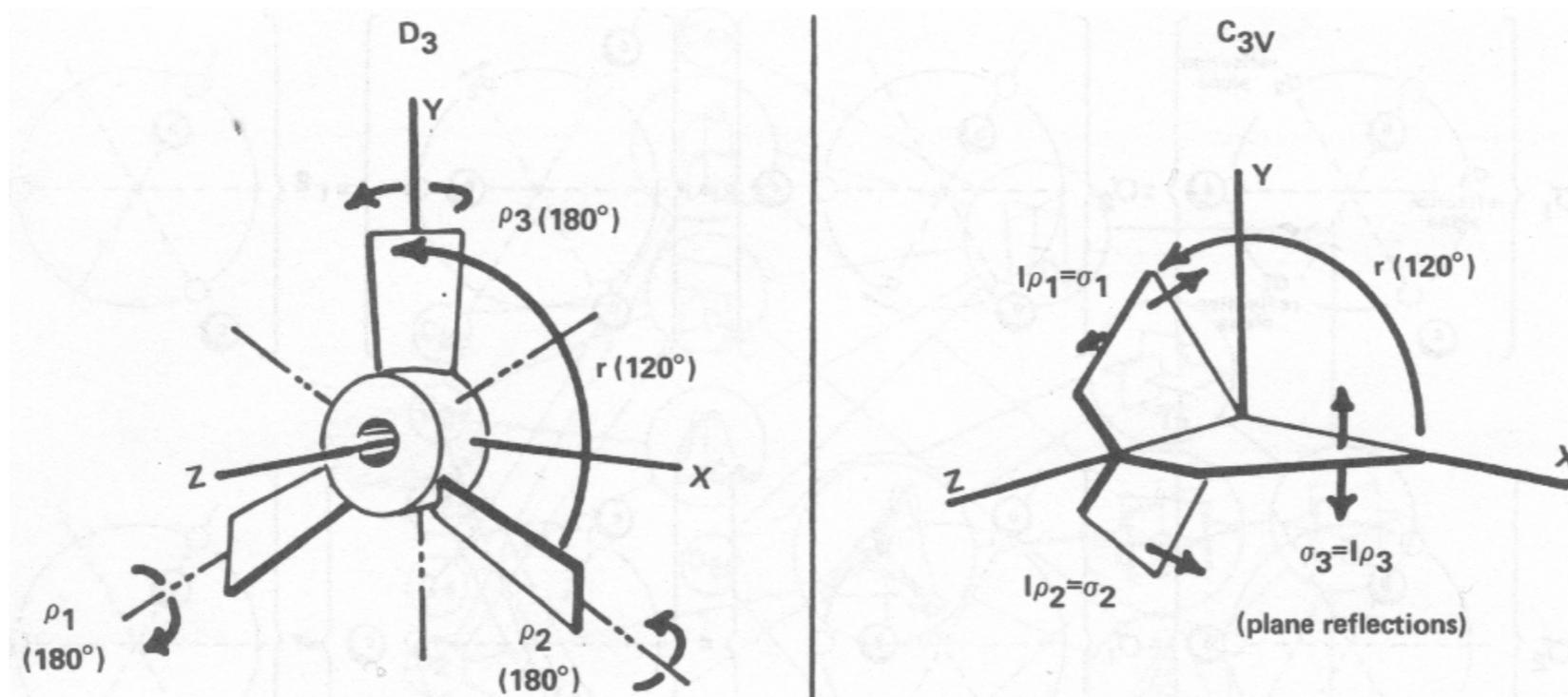


Figure 3.1.3 Pictorial comparison of D_3 and C_{3v} symmetry. A propeller having D_3 symmetry is shown next to a three-plane paddle having C_{3v} symmetry. The group operations are labeled by arrows, which indicate the effect they have. For example, ρ_3 is a 180° rotation around the y axis, while $I\rho_3 = \sigma_3$ is a reflection through the xz plane. (Here axes are fixed and the objects rotate.)

**isomorphic means mathematically the same abstract group even if physically different action.*

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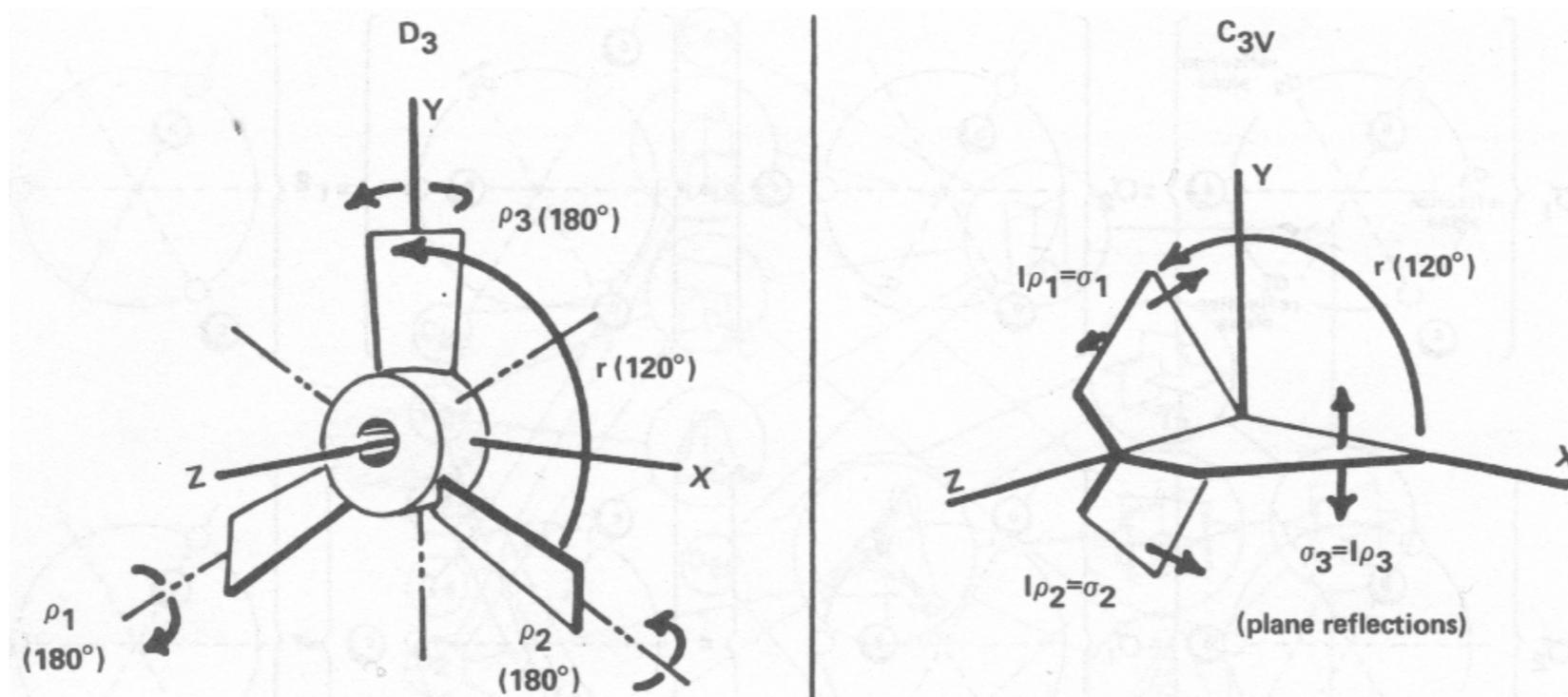


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$180^\circ D_3$ -Y-axis-rotation: $\rho_3 = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$ maps to : XZ-mirror-plane reflection: $\sigma_3 = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & +1 \end{pmatrix}$

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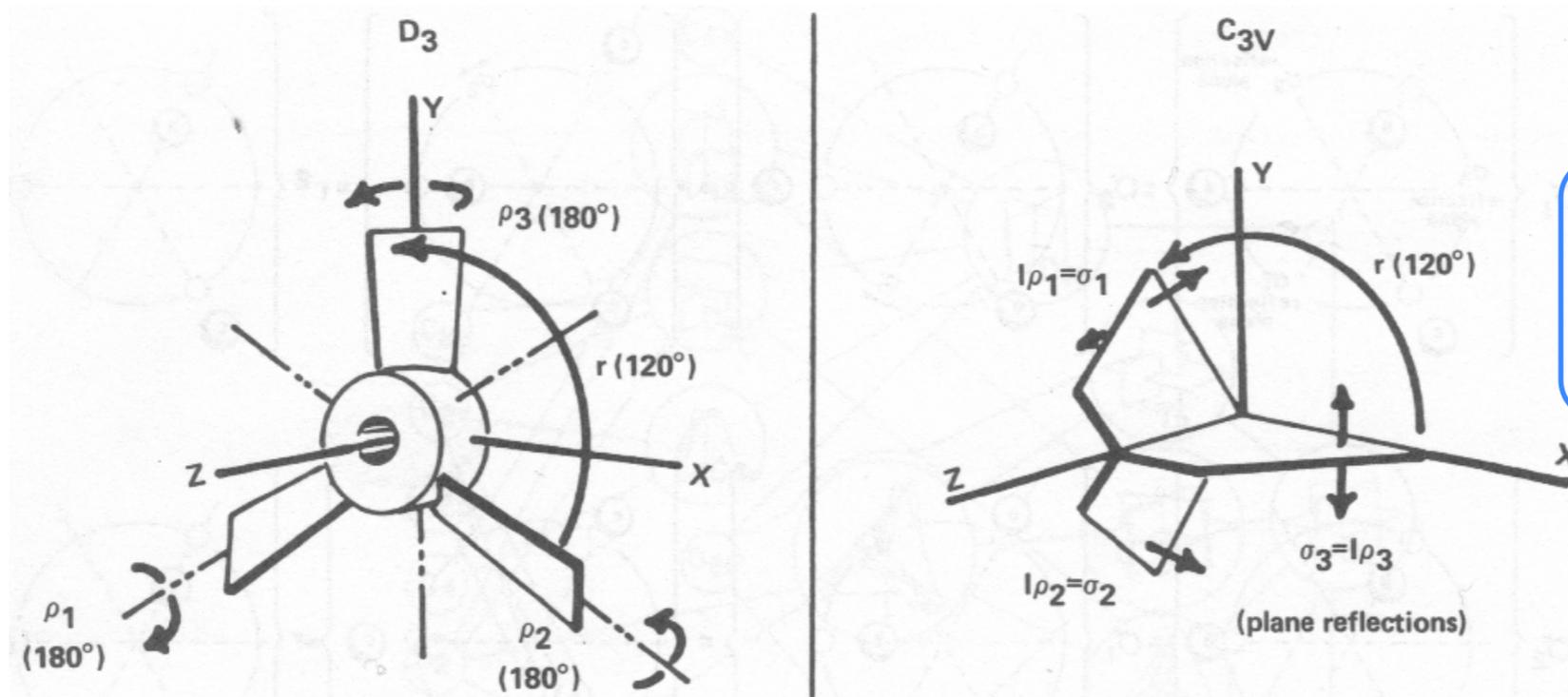


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Mirror-plane-reflection σ
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 $180^\circ \perp$ -axial-rotation-inversion
 $\sigma = \mathbf{R} \cdot \mathbf{I} = \mathbf{I} \cdot \mathbf{R}$

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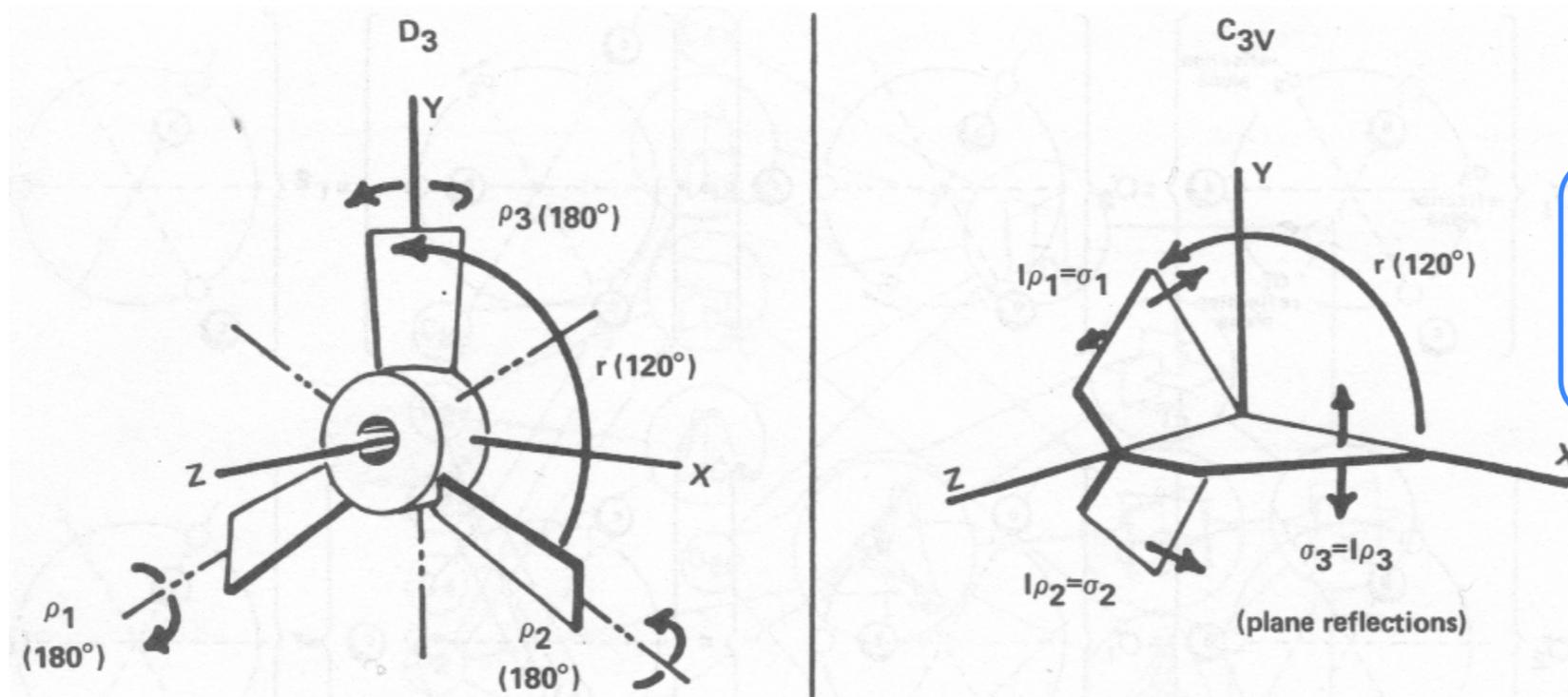


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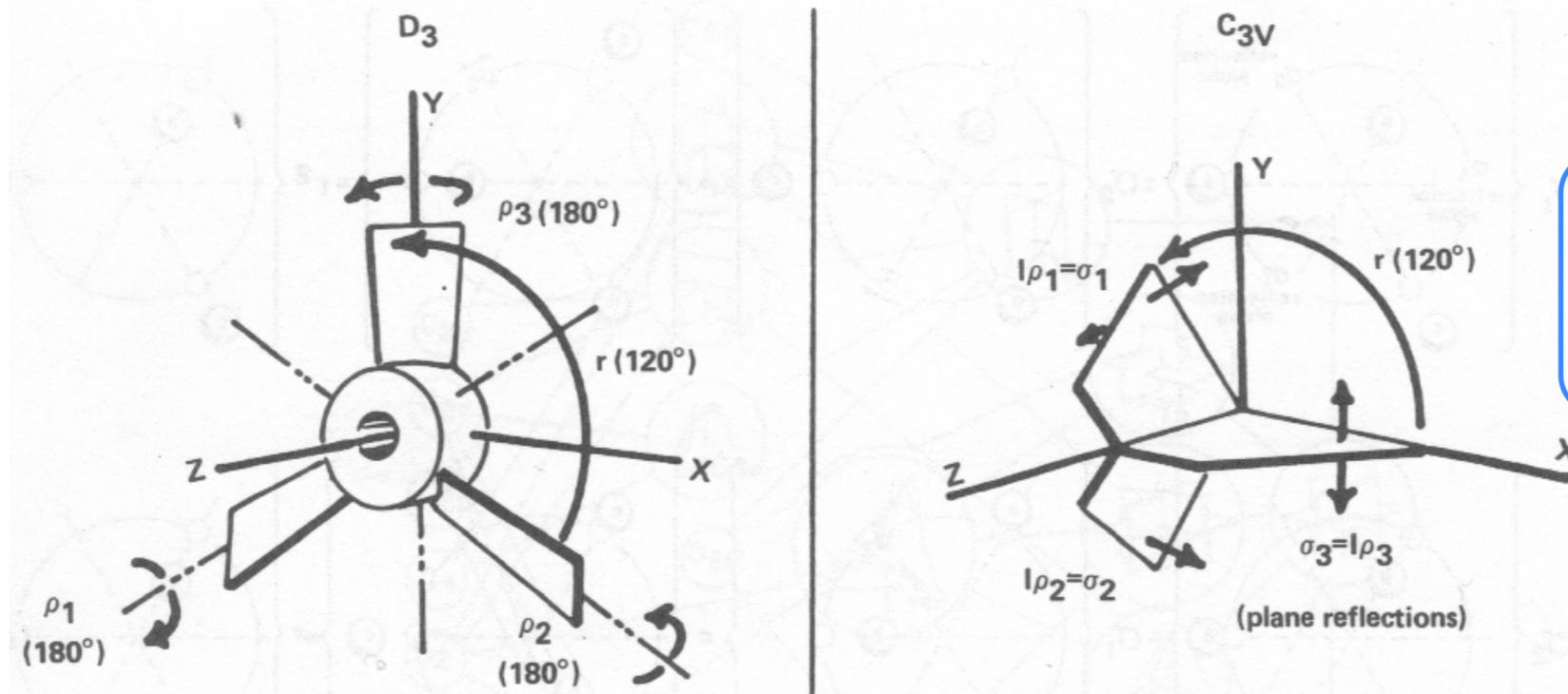


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$180^\circ D_3$ - ρ_2 -axis-rotation: ρ_2

maps to: $\perp \rho_2$ -mirror-plane reflection: $\sigma_2 = \rho_2 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_2$

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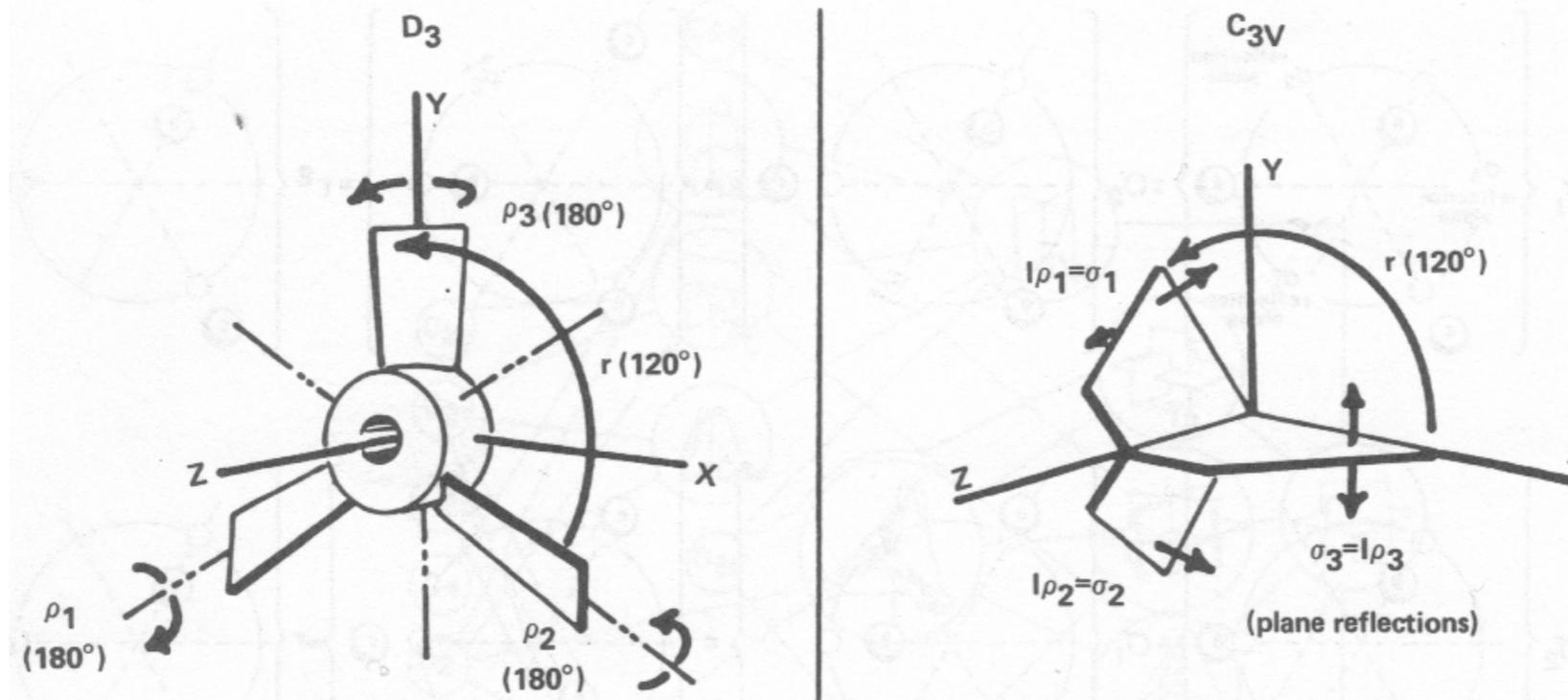


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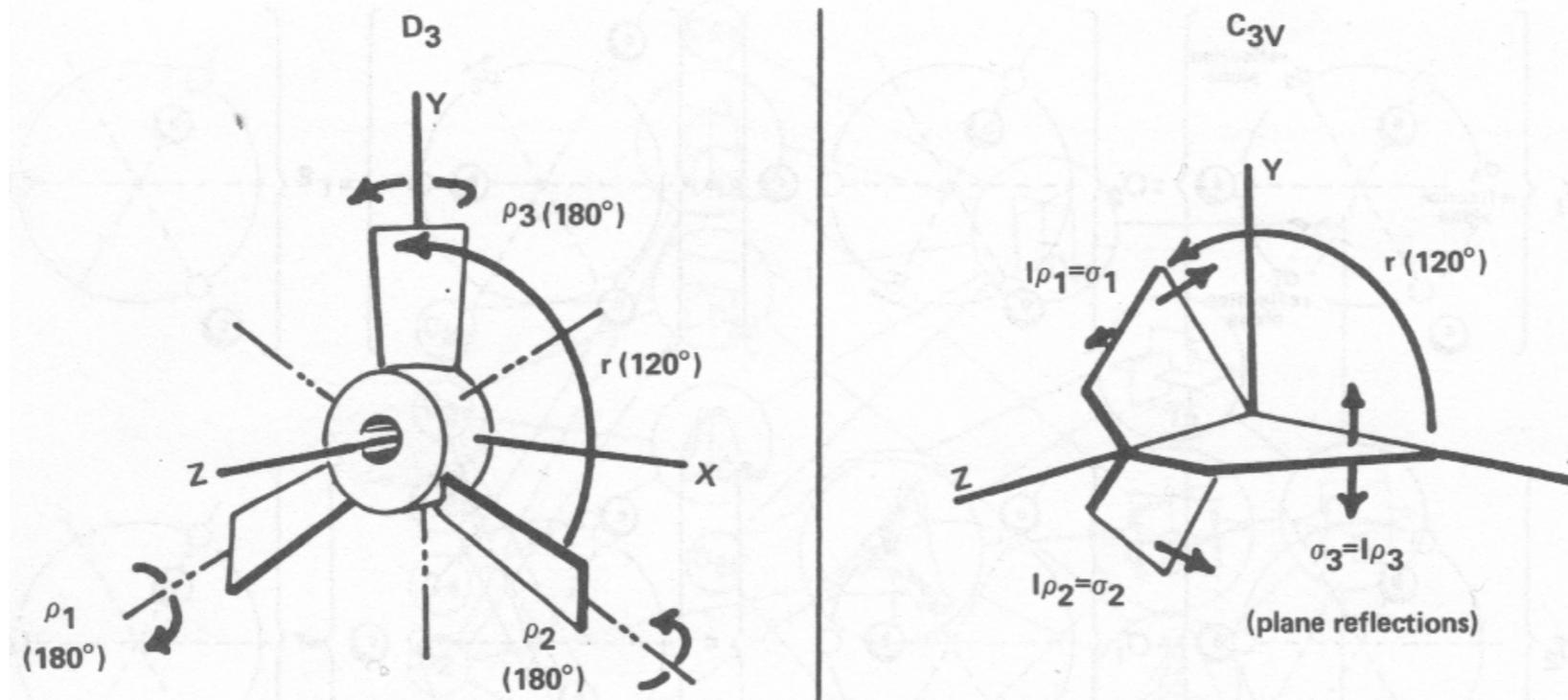


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D_3 -product: $\rho_1 \rho_2$

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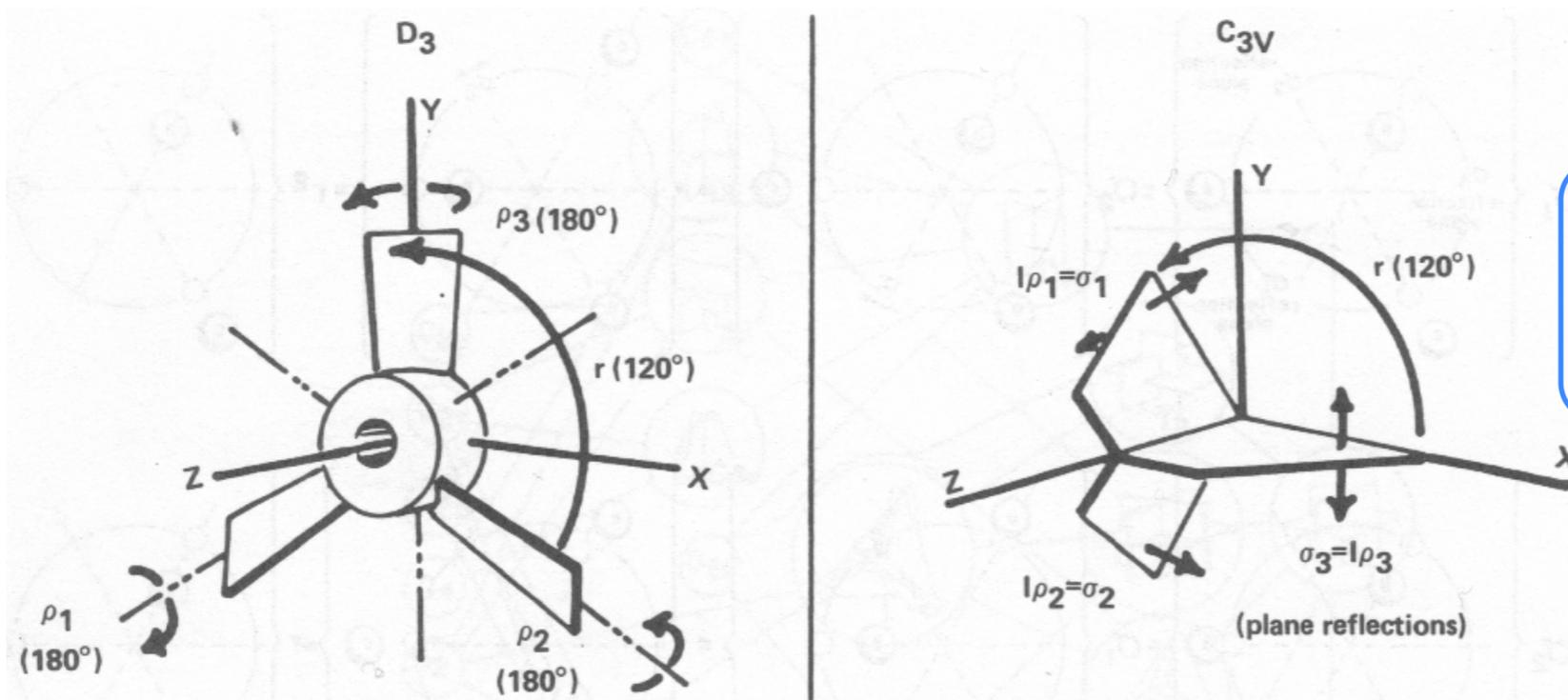


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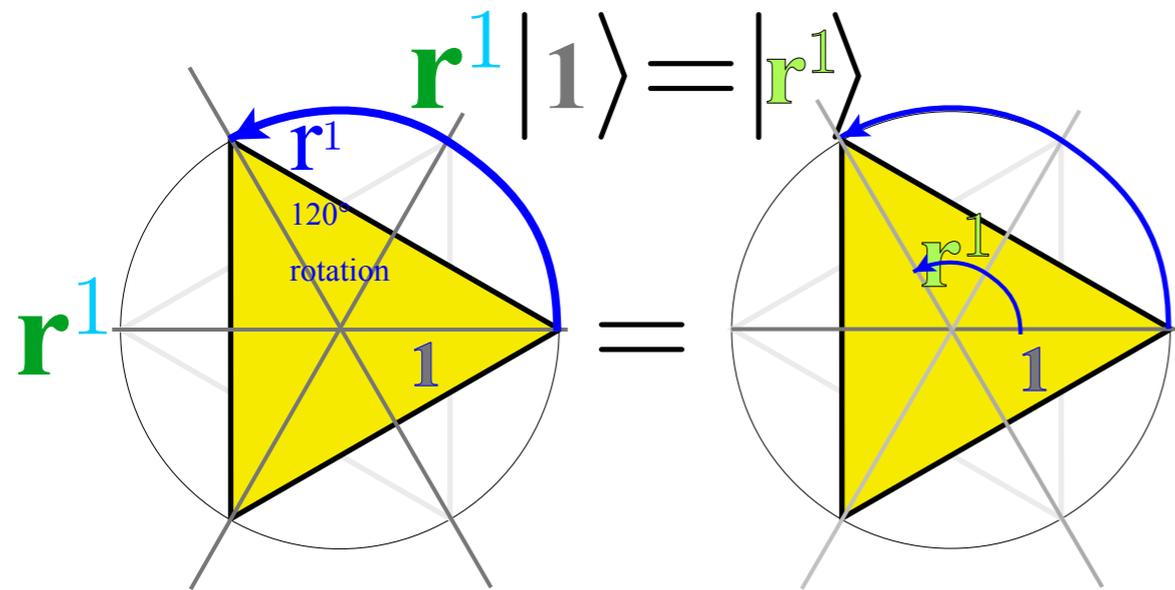
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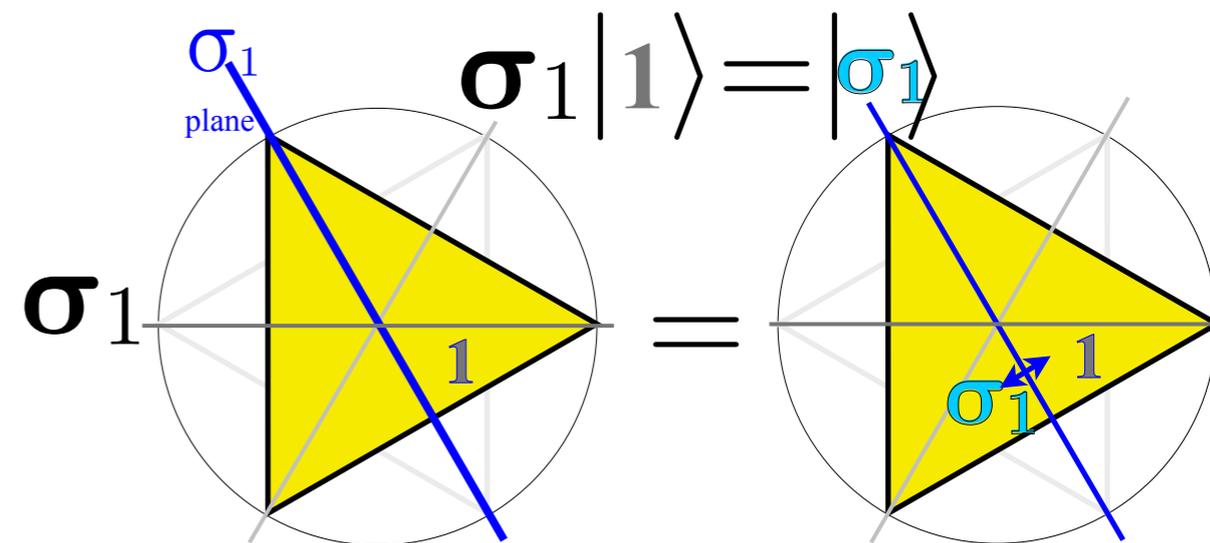
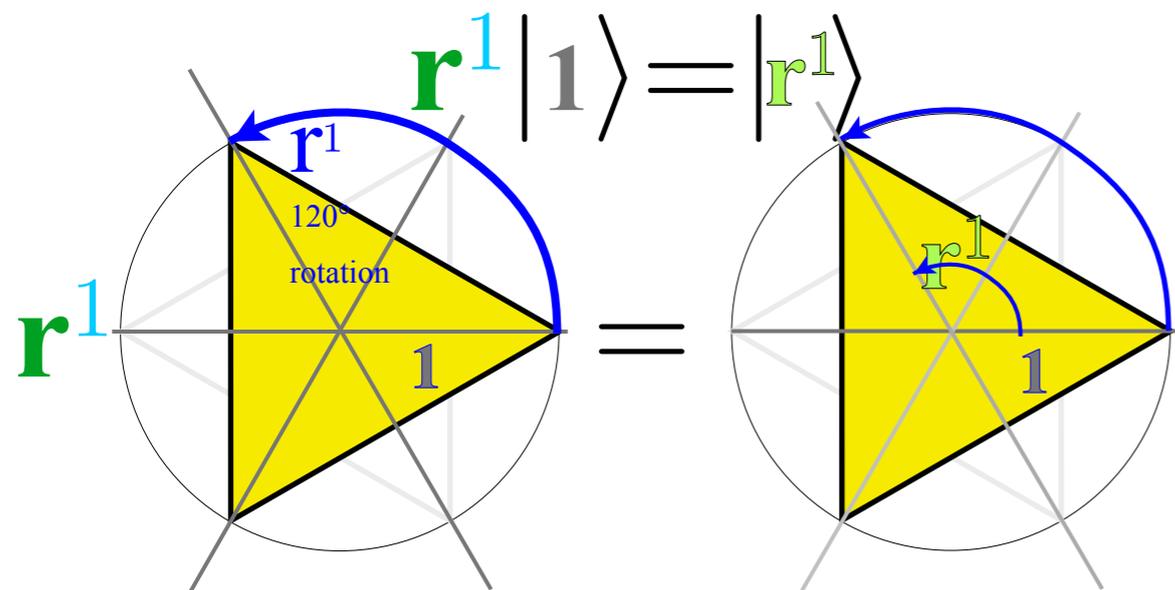
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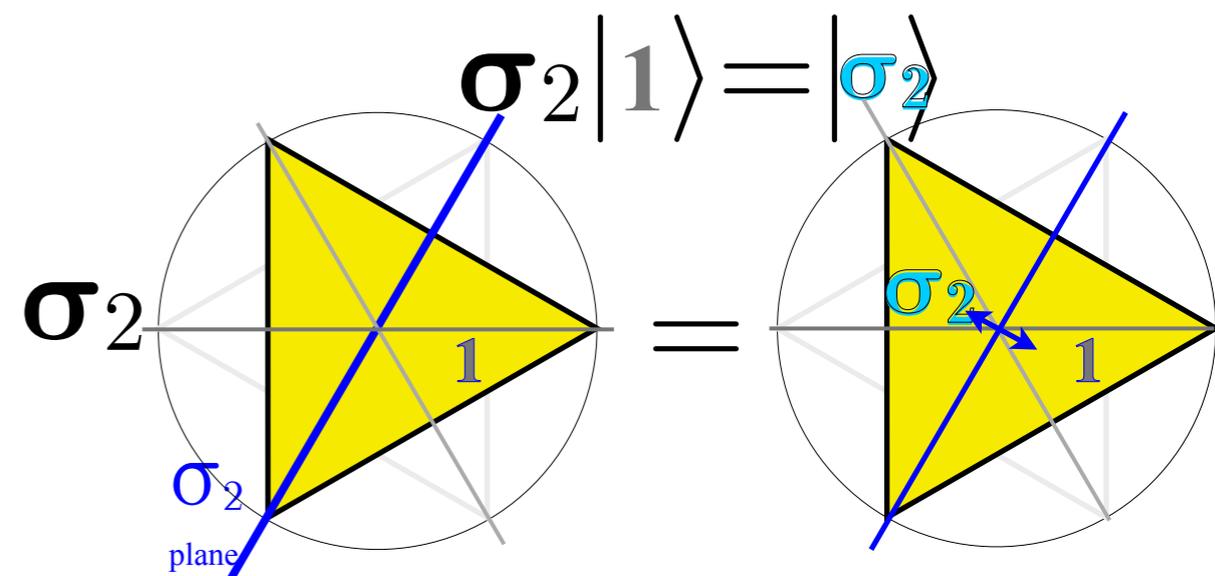
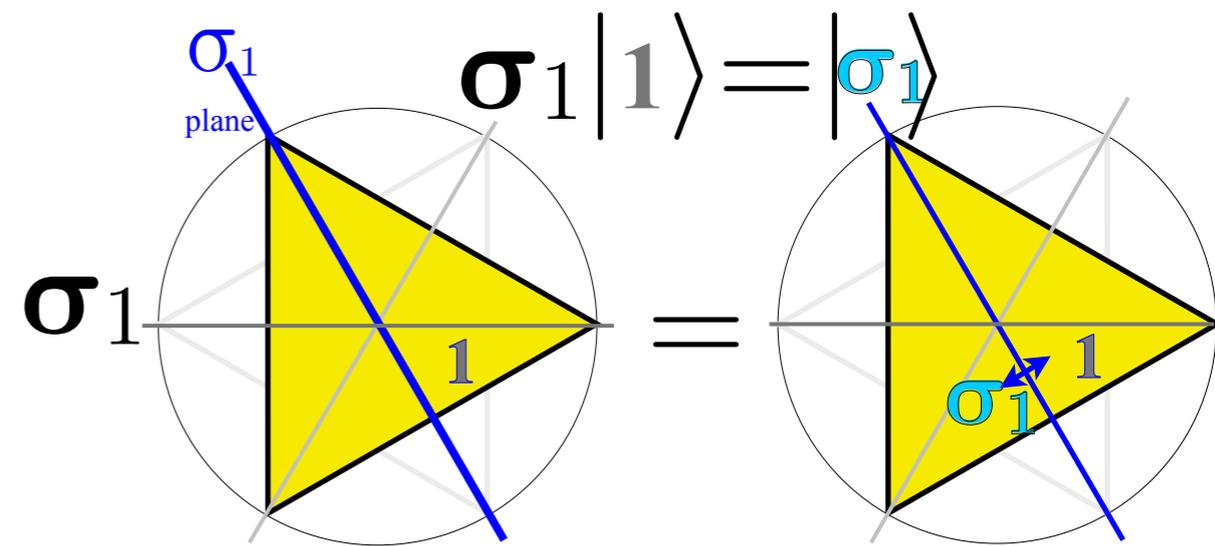
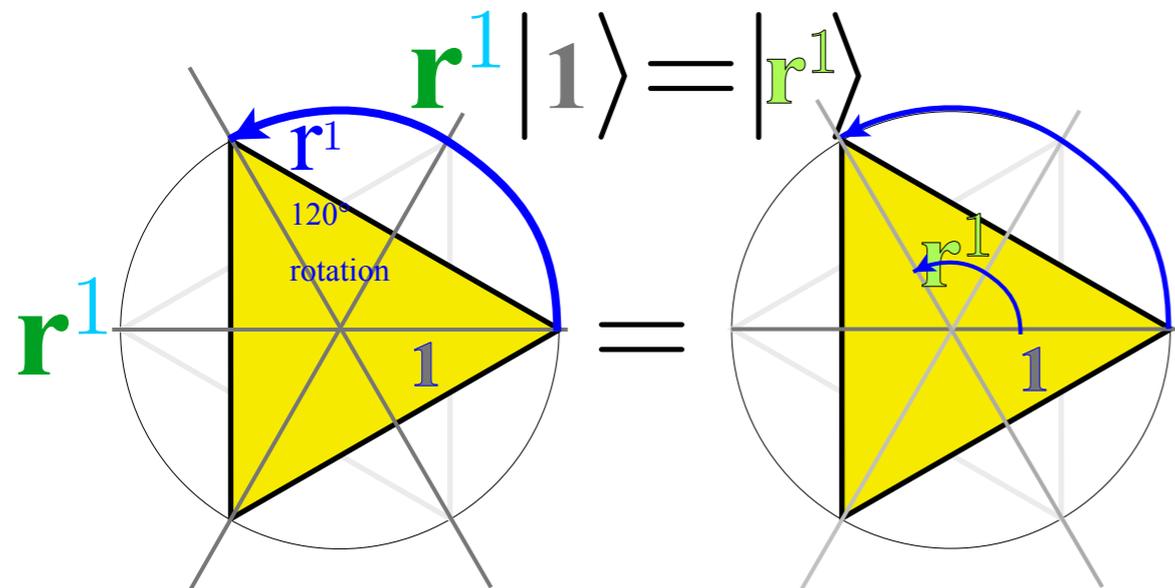
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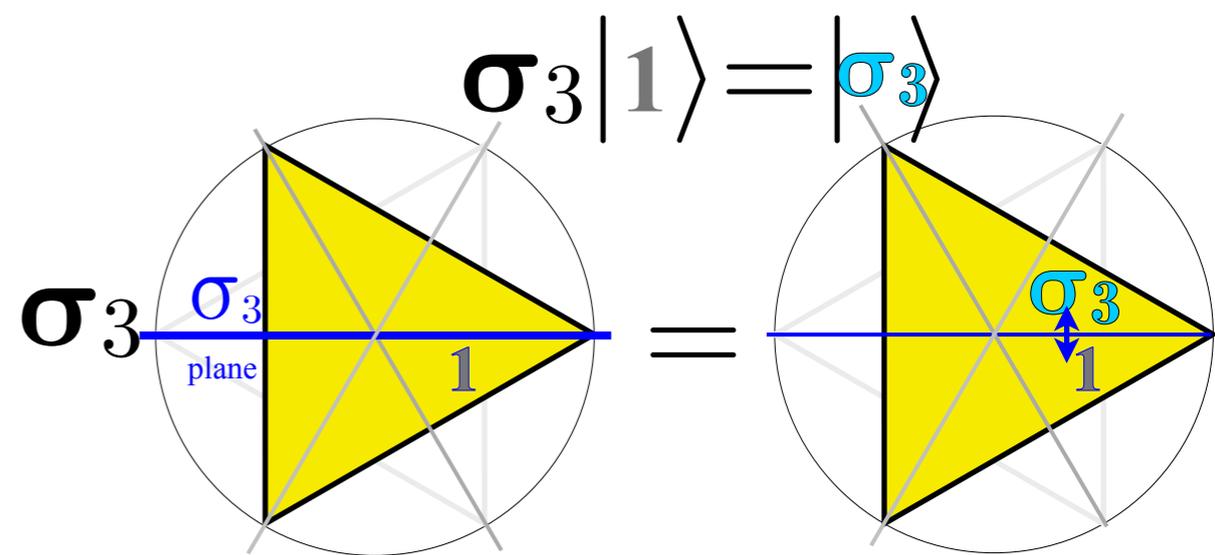
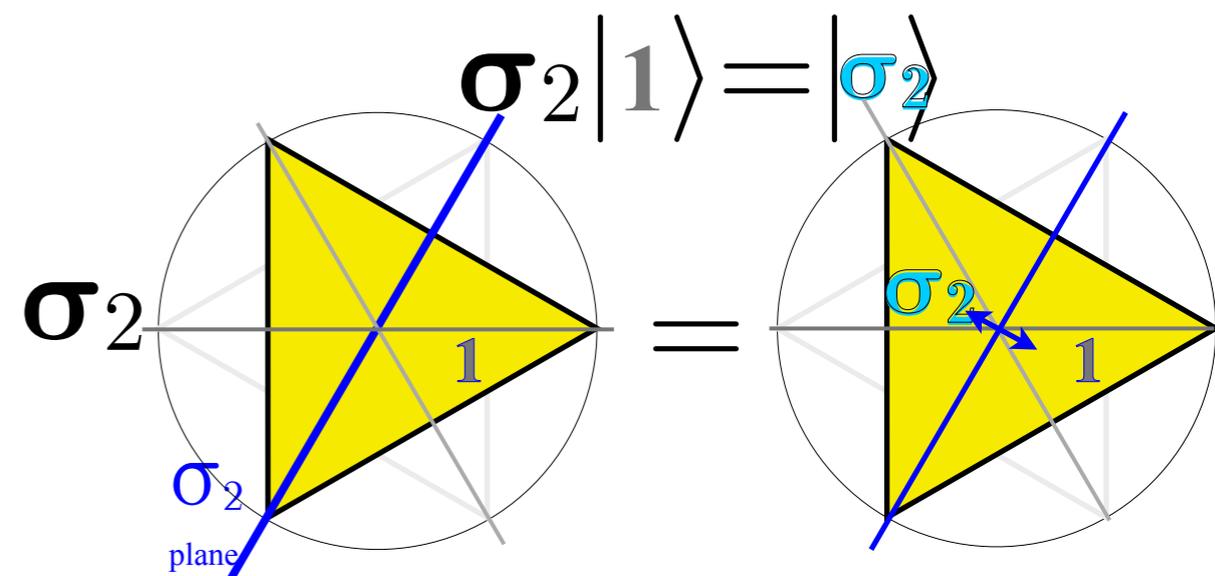
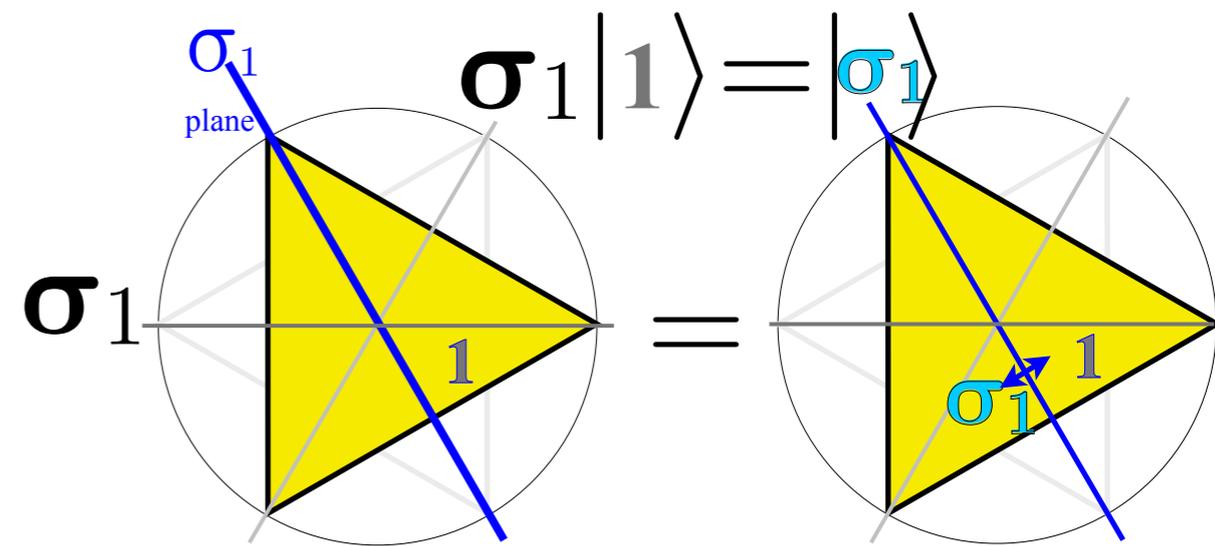
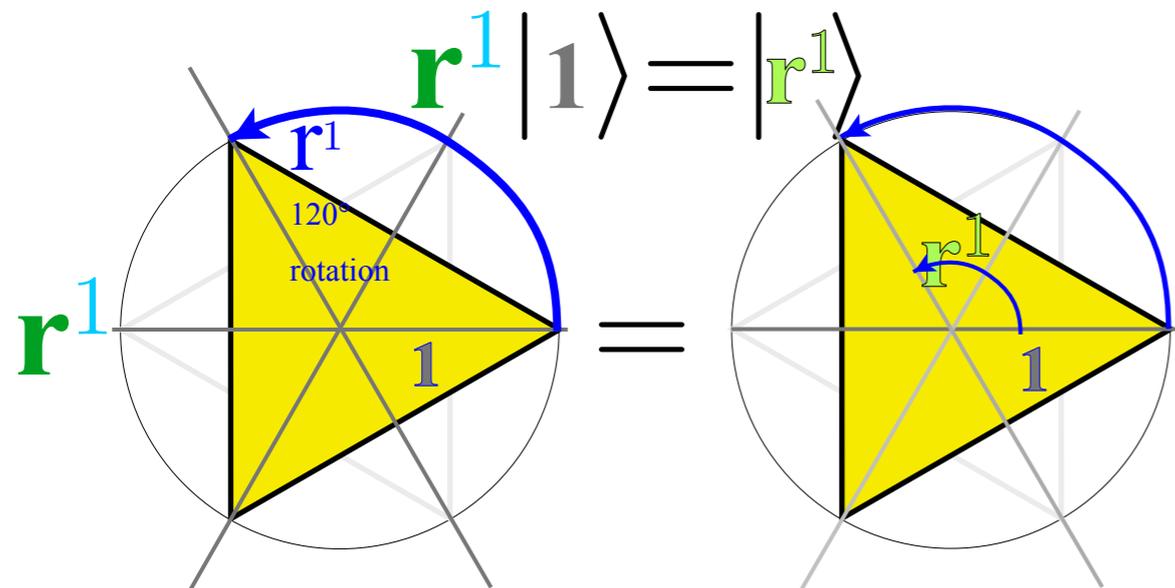
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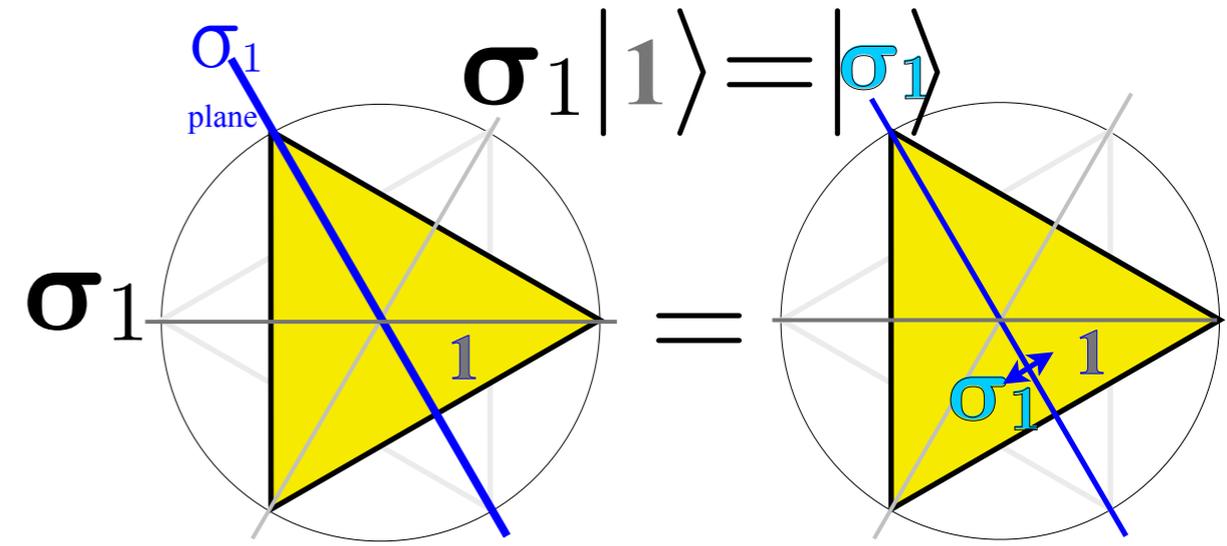
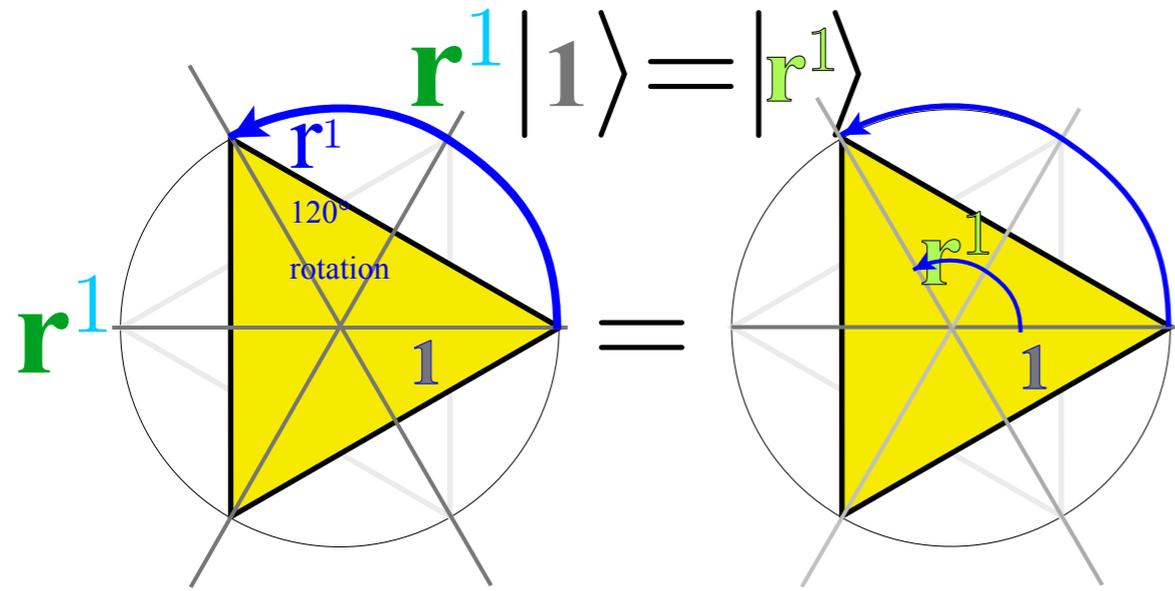
All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

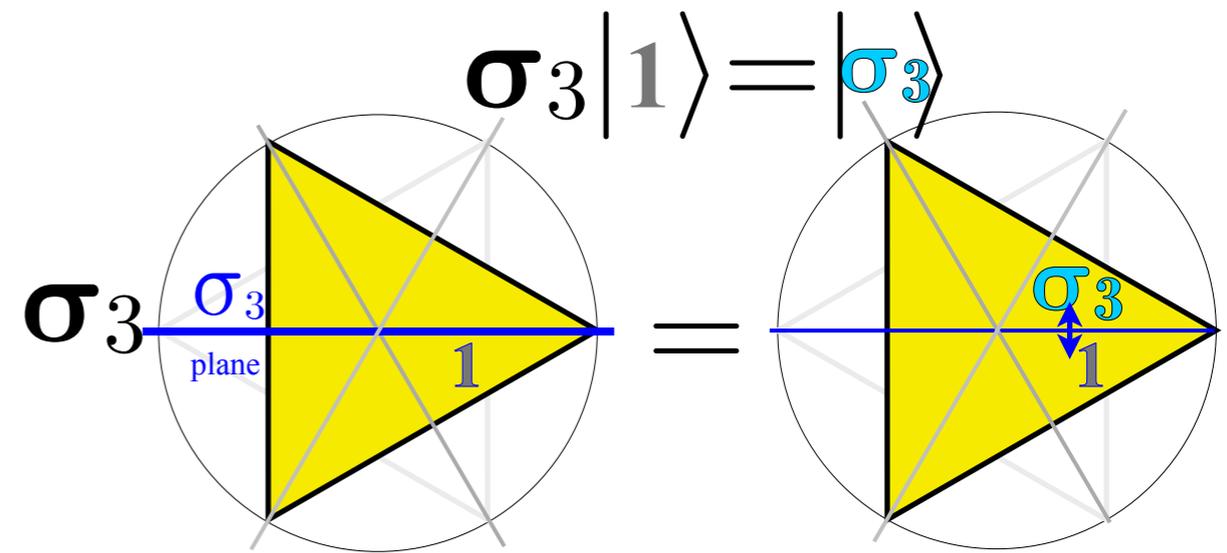
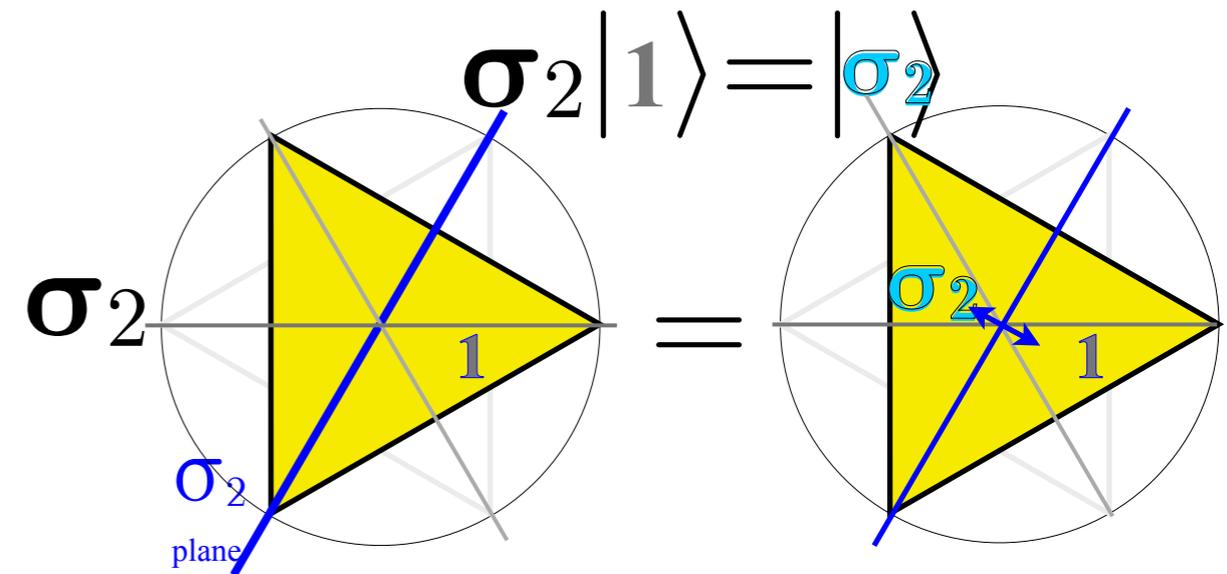
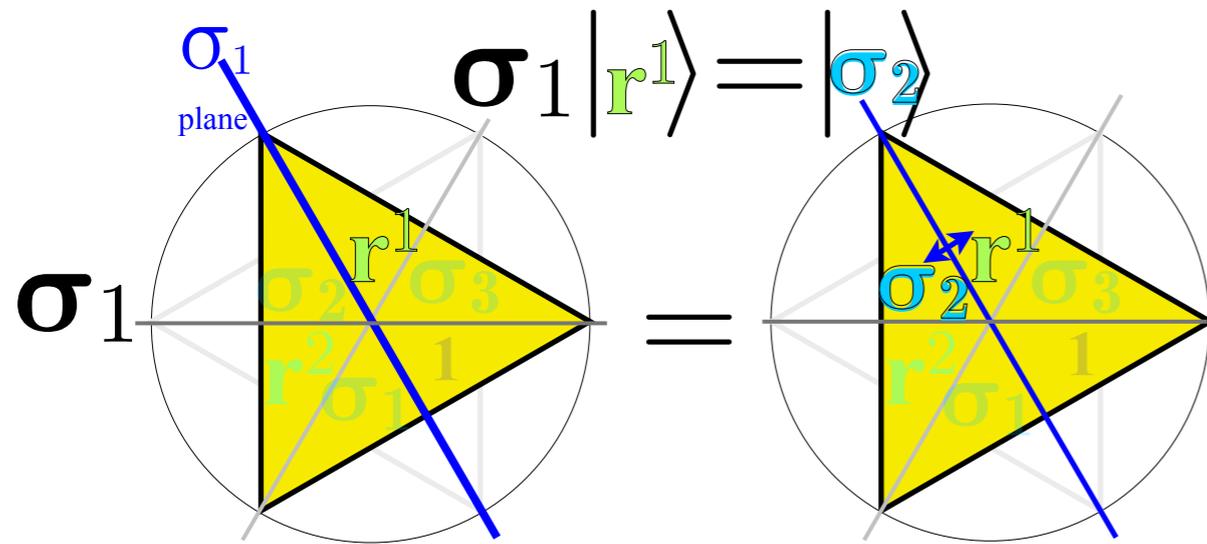
*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

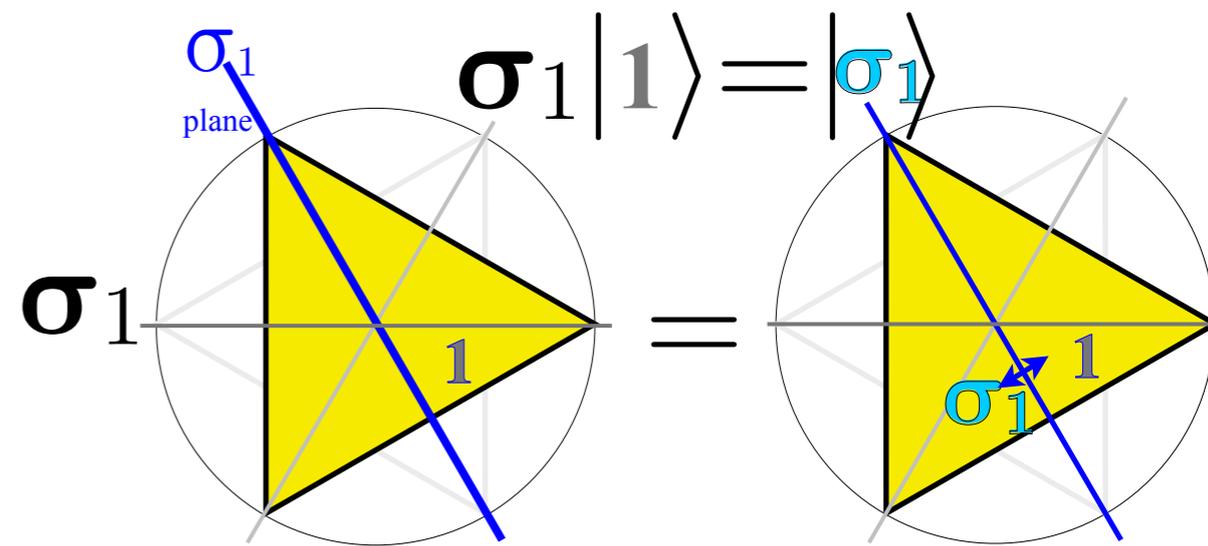
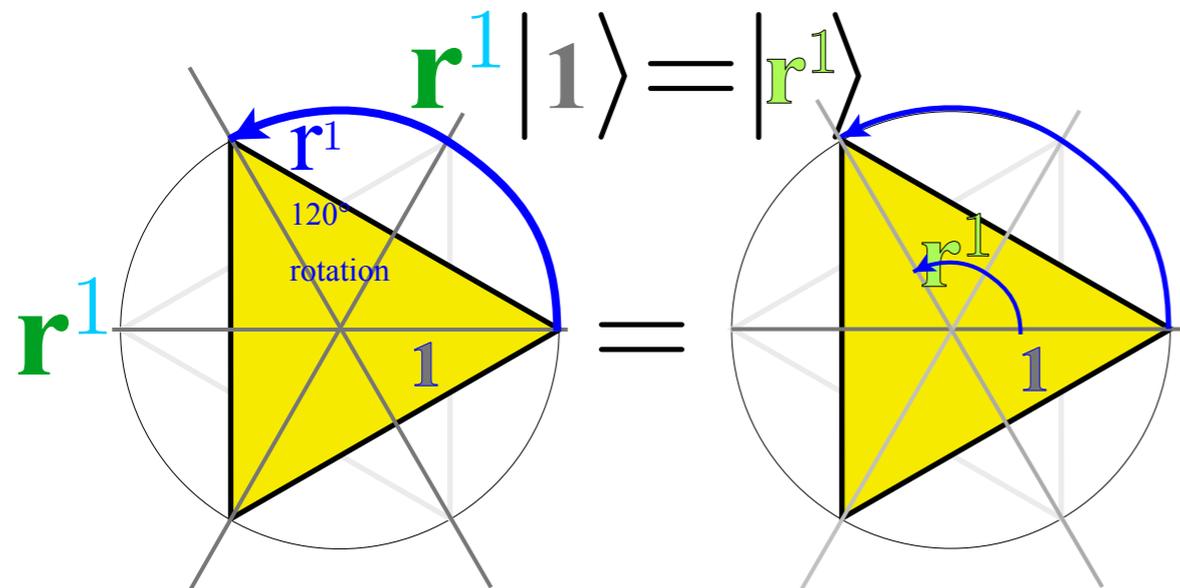


Example: Find C_{3v} product $\sigma_1 \mathbf{r}^1 |1\rangle = \sigma_1 |\mathbf{r}^1\rangle$

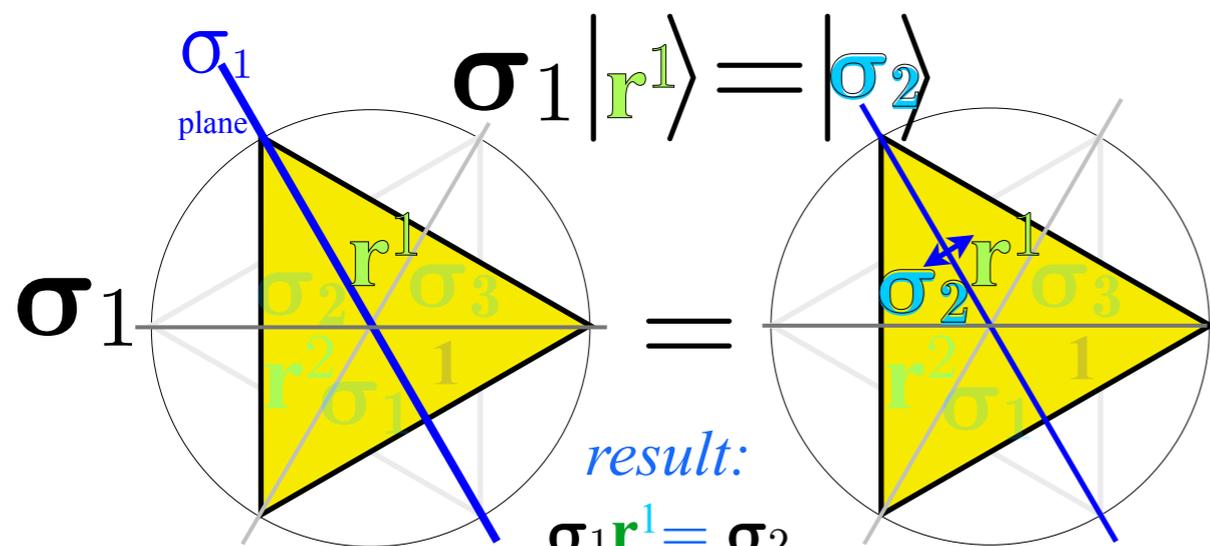


1

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

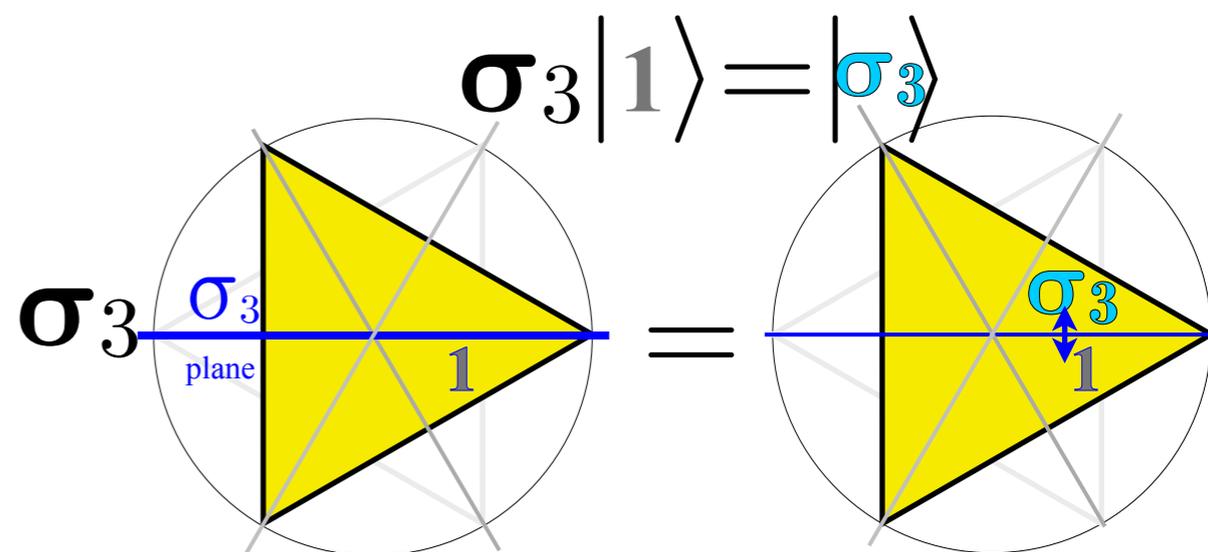
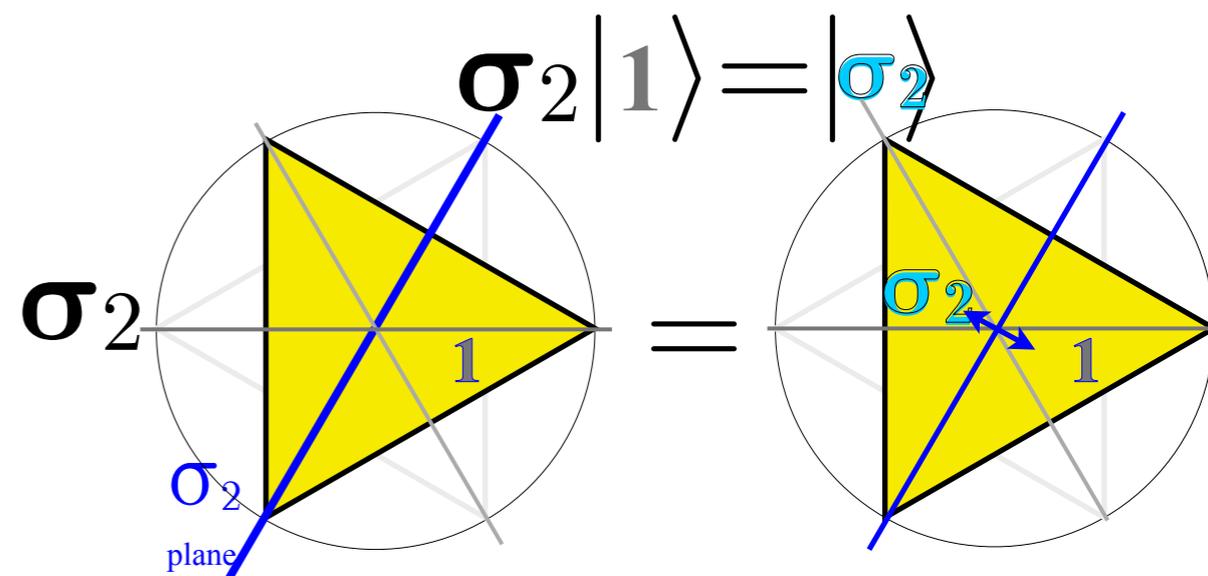


Example: Find C_{3v} product $\sigma_1 \mathbf{r}^1 |1\rangle = \sigma_1 |r^1\rangle$



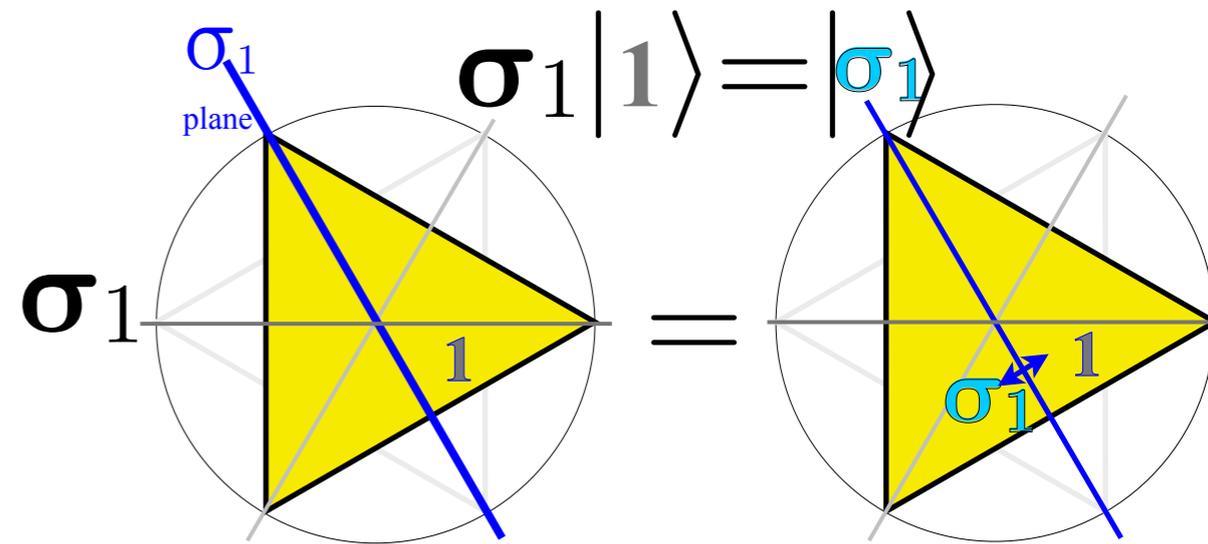
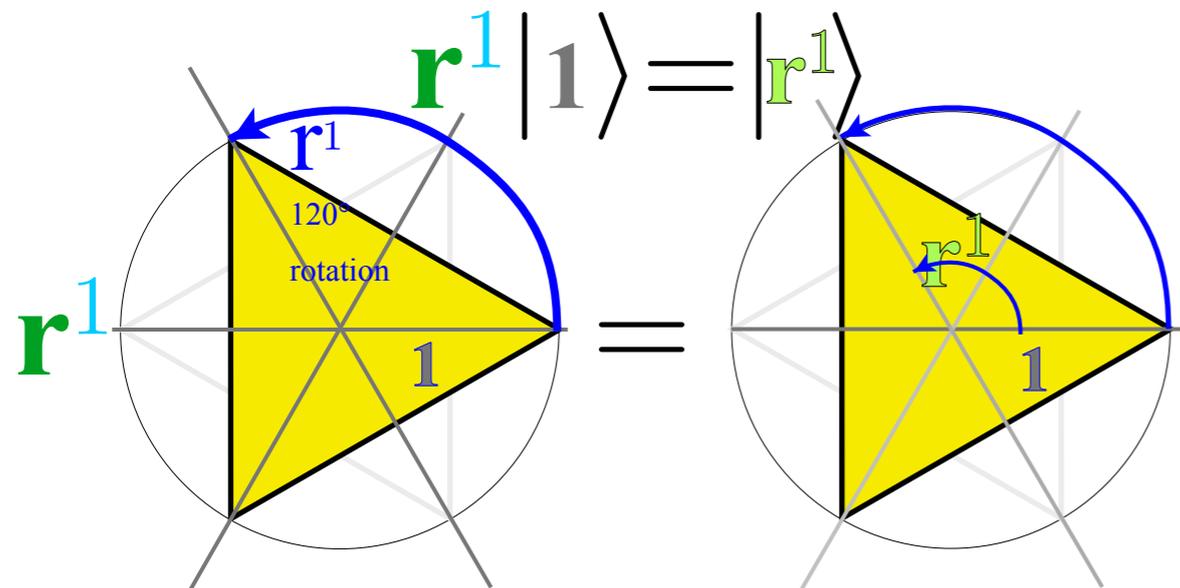
Factor \mathbf{r}^1
on right
acts first

left is last
(like Hebrew)

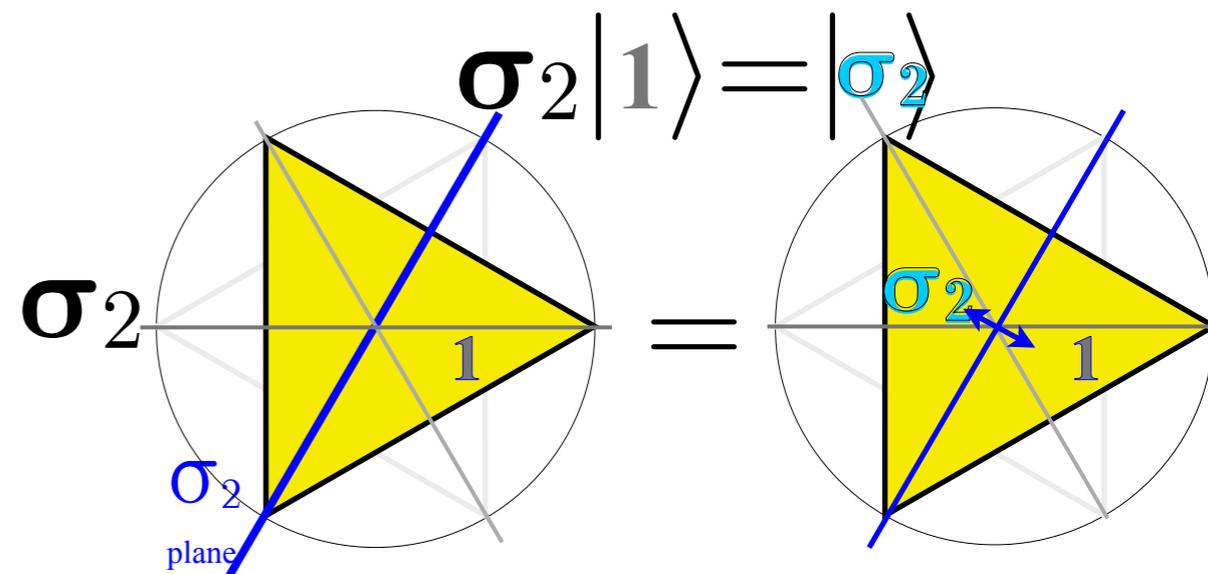
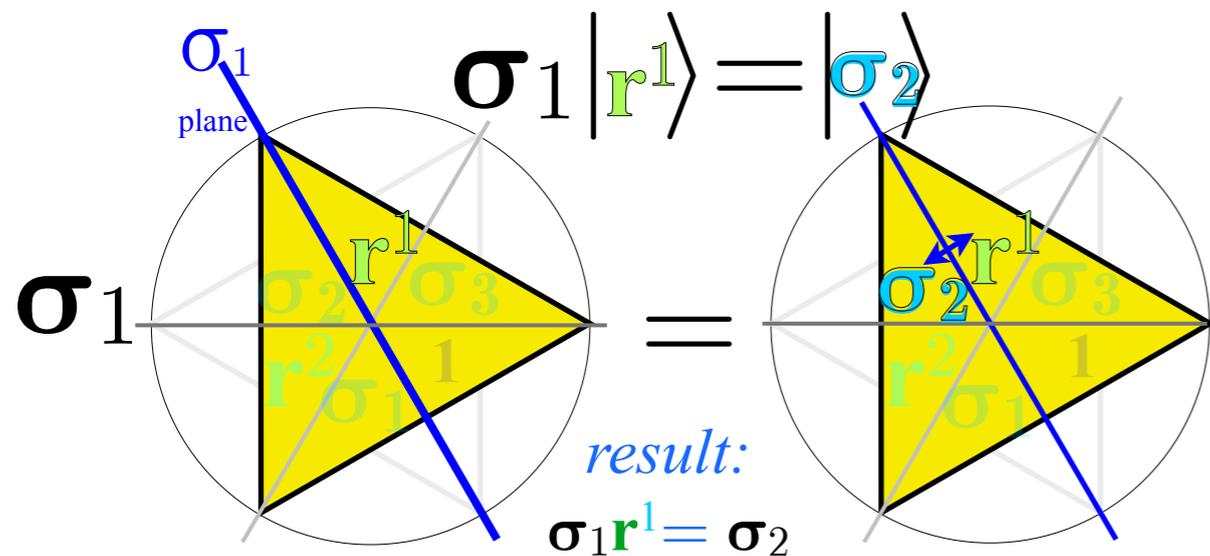


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Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

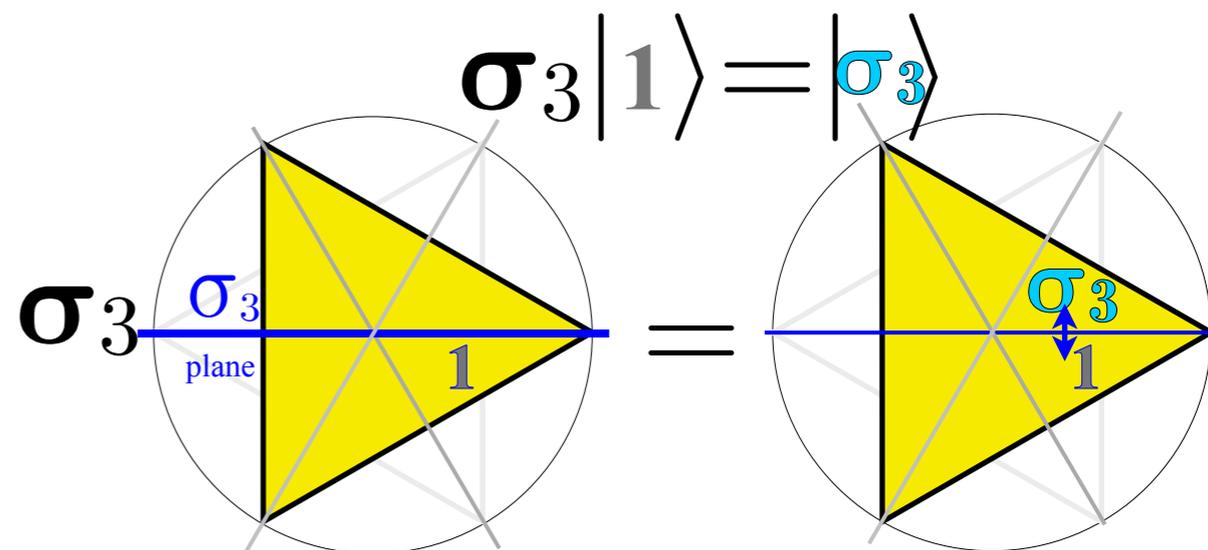


Example: Find C_{3v} product $\sigma_1 \mathbf{r}^1 |1\rangle = \sigma_1 |\mathbf{r}^1\rangle$



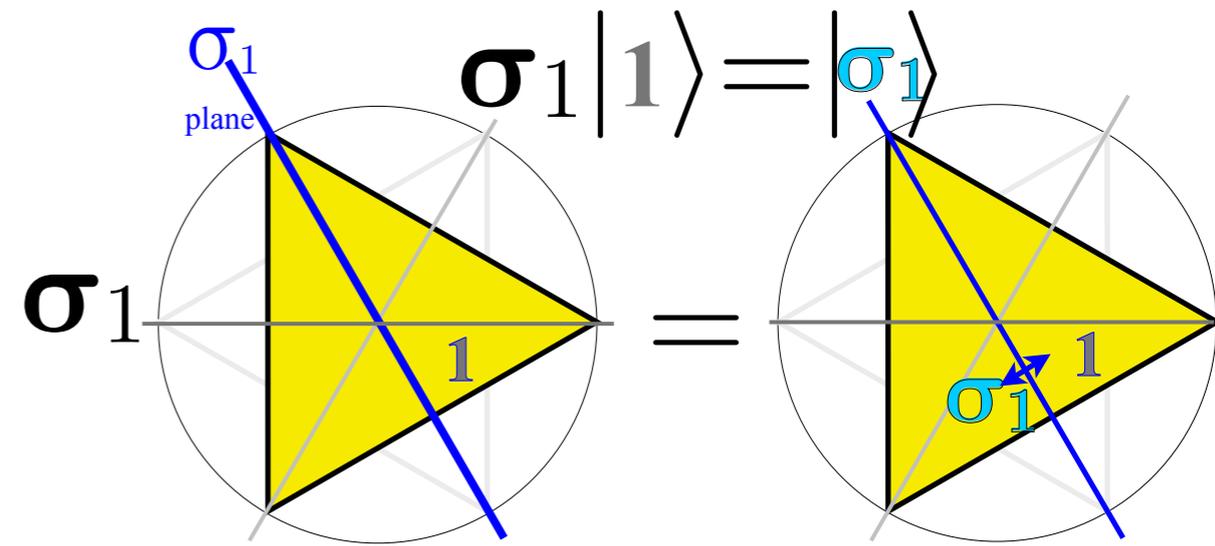
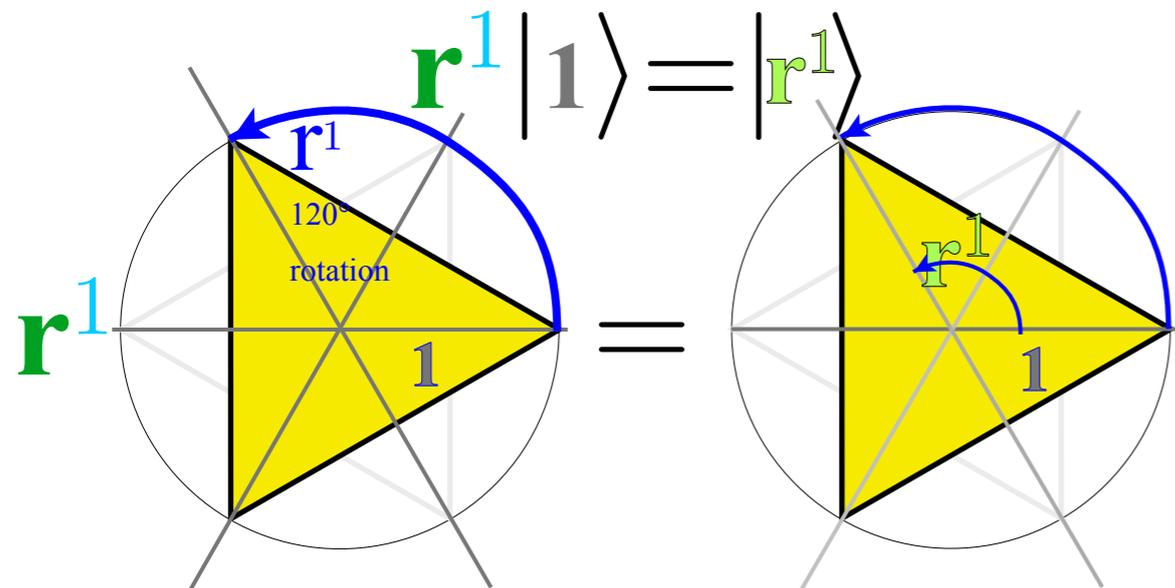
Other σ_1 results from graph:

$$\sigma_1 \{1, \mathbf{r}^1, \mathbf{r}^2, \sigma_1, \sigma_2, \sigma_3\} = \{\sigma_1, \sigma_2, \sigma_3, 1, \mathbf{r}^1, \mathbf{r}^2\}$$

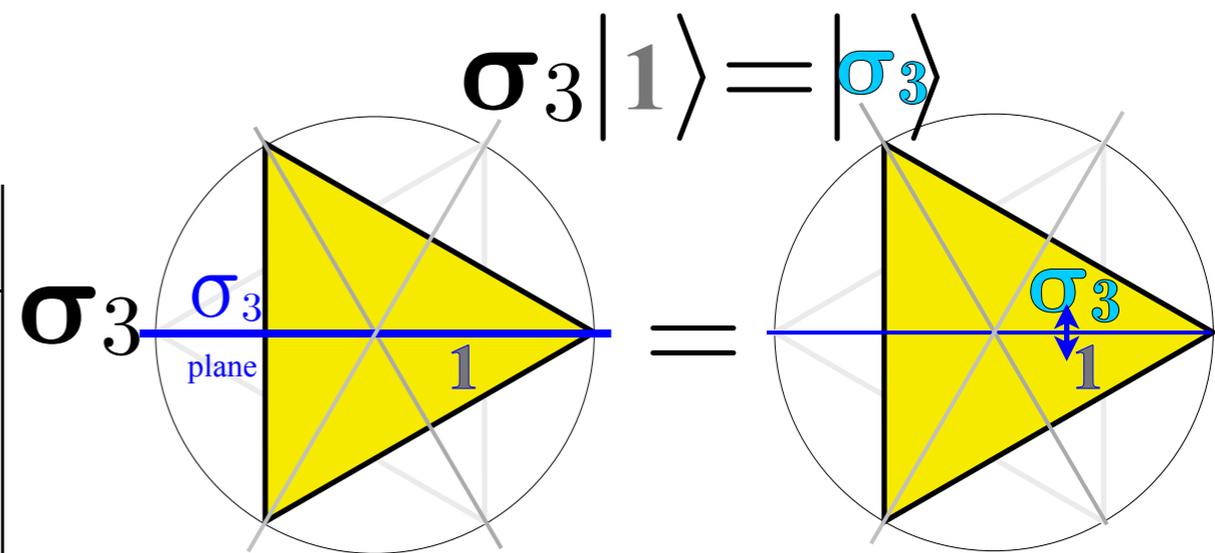
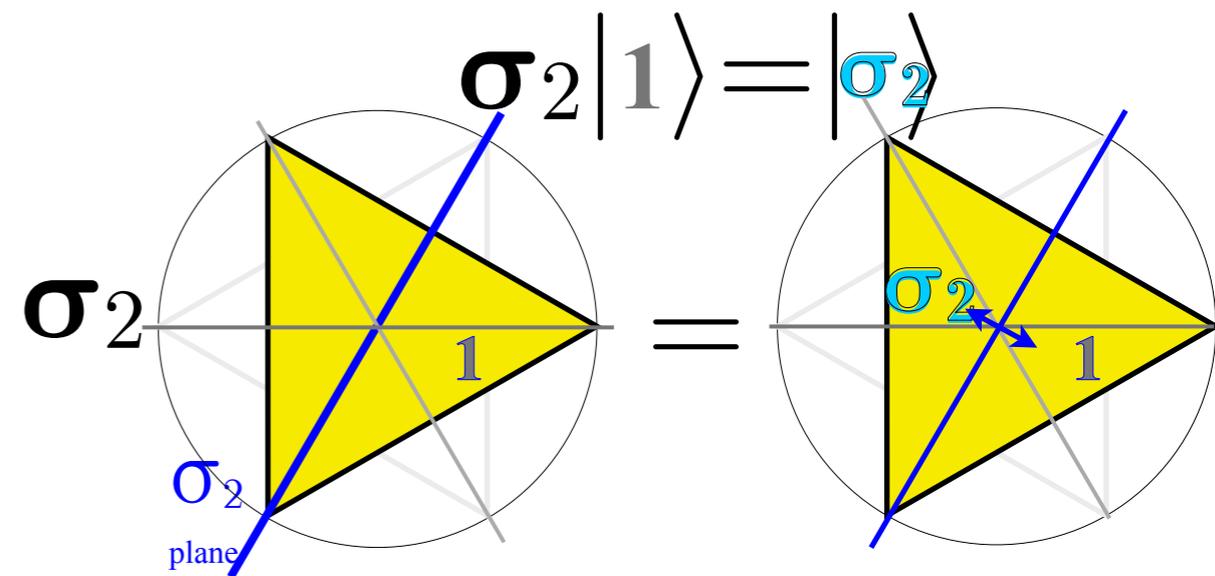
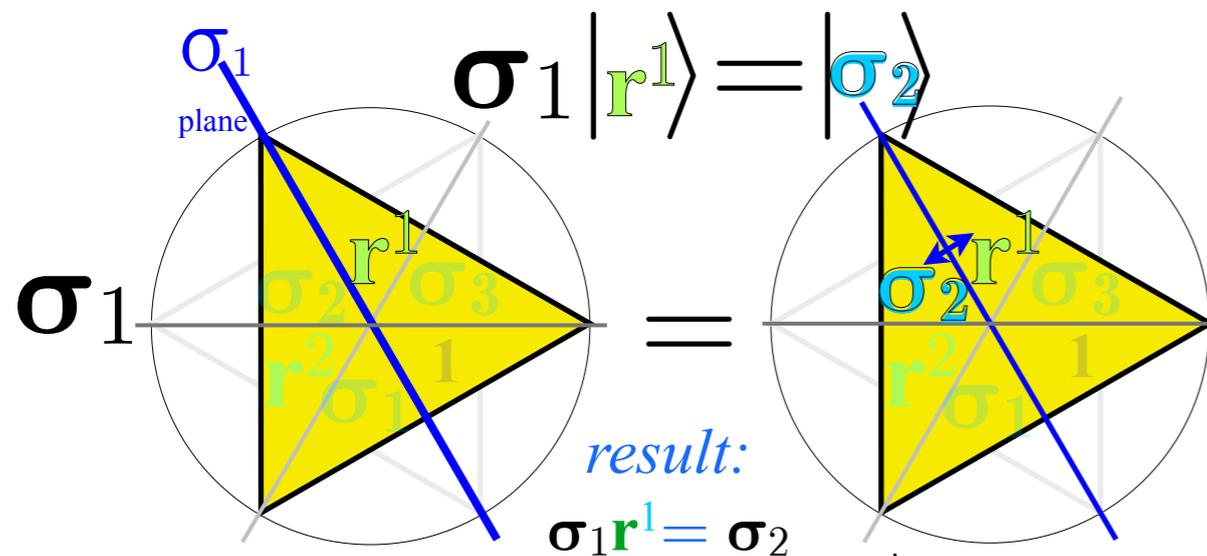


1

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$



Example: Find C_{3v} product $\sigma_1 \mathbf{r}^1 |1\rangle = \sigma_1 |\mathbf{r}^1\rangle$



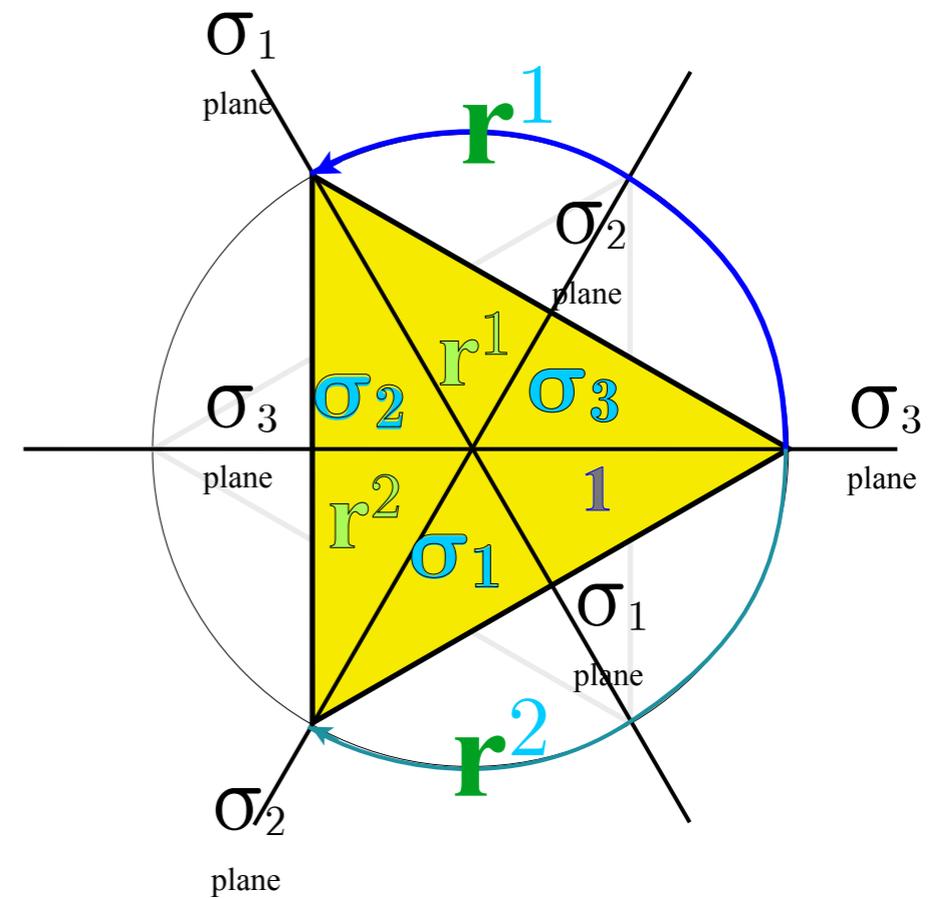
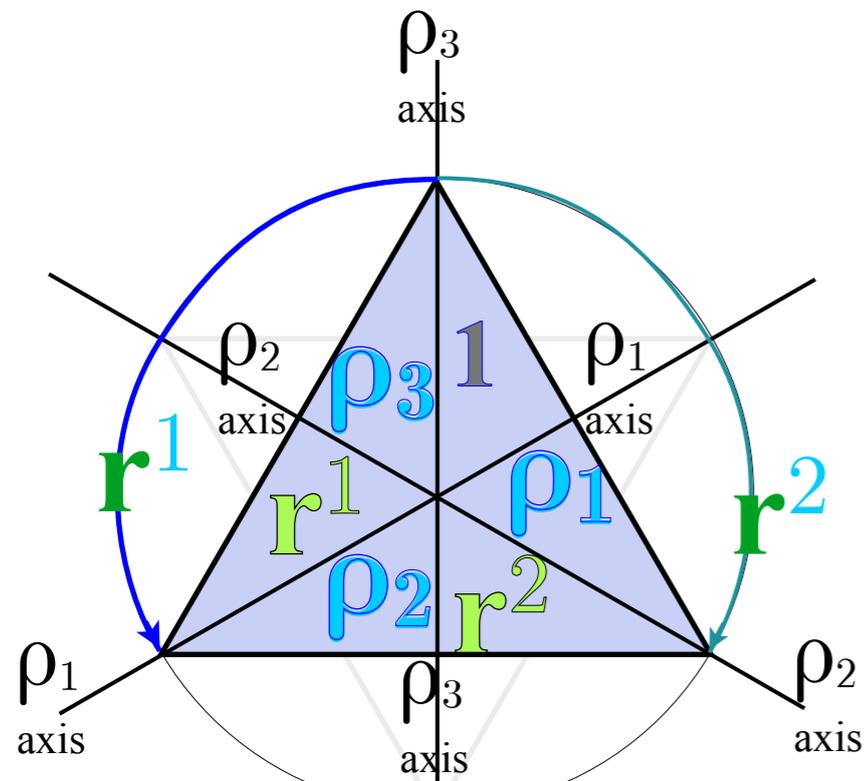
Other σ_1 results from graph:

$$\sigma_1 \{1, \mathbf{r}^1, \mathbf{r}^2, \sigma_1, \sigma_2, \sigma_3\} = \{\sigma_1, \sigma_2, \sigma_3, 1, \mathbf{r}^1, \mathbf{r}^2\}$$

...whole C_{3v} group table:

C_{3v} form	gg^\dagger	1	\mathbf{r}^2	\mathbf{r}^1	σ_1	σ_2	σ_3
1	1	1	\mathbf{r}^2	\mathbf{r}^1	σ_1	σ_2	σ_3
\mathbf{r}^1	\mathbf{r}^1	1	1	\mathbf{r}^2	σ_3	σ_1	σ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	1	1	σ_2	σ_3	σ_1
σ_1	σ_1	σ_3	σ_2	1	1	\mathbf{r}^1	\mathbf{r}^2
σ_2	σ_2	σ_1	σ_3	\mathbf{r}^2	1	1	\mathbf{r}^1
σ_3	σ_3	σ_2	σ_1	\mathbf{r}^1	\mathbf{r}^2	1	1

Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$



D_3 gg^\dagger form	1	r^2	r^1	ρ_1	ρ_2	ρ_3
1	1	r^2	r^1	ρ_1	ρ_2	ρ_3
r^1	r^1	1	r^2	ρ_3	ρ_1	ρ_2
r^2	r^2	r^1	1	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	1	r^1	r^2
ρ_2	ρ_2	ρ_1	ρ_3	r^2	1	r^1
σ_3	ρ_3	ρ_2	ρ_1	r^1	r^2	1

D_3 and C_{3v}
clearly are
isomorphic
 $D_3 \sim C_{3v}$
share
group table

...except for
notation
 $\rho_k \leftrightarrow \sigma_k$

C_{3v} gg^\dagger form	1	r^2	r^1	σ_1	σ_2	σ_3
1	1	r^2	r^1	σ_1	σ_2	σ_3
r^1	r^1	1	r^2	σ_3	σ_1	σ_2
r^2	r^2	r^1	1	σ_2	σ_3	σ_1
σ_1	σ_1	σ_3	σ_2	1	r^1	r^2
σ_2	σ_2	σ_1	σ_3	r^2	1	r^1
σ_3	σ_3	σ_2	σ_1	r^1	r^2	1

*3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}
 D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)*

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

By nomograms based on $U(2)$ Hamilton-turns

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

All-commuting operators and D_3 -invariant class algebra

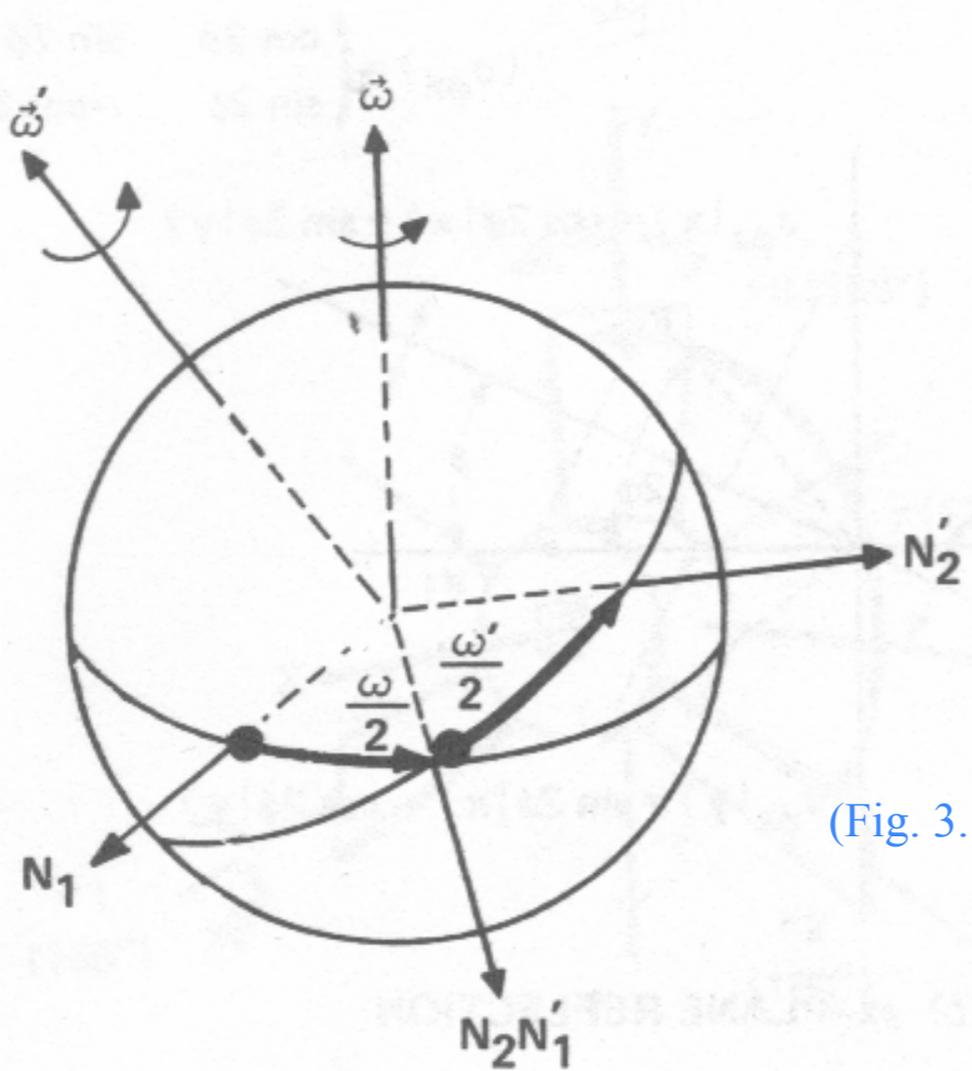
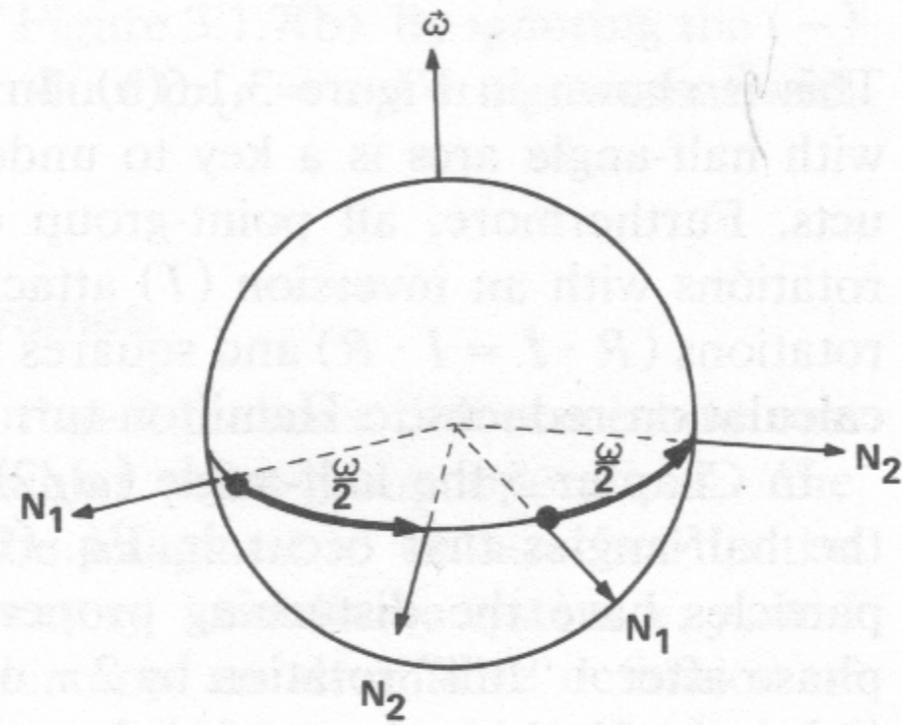
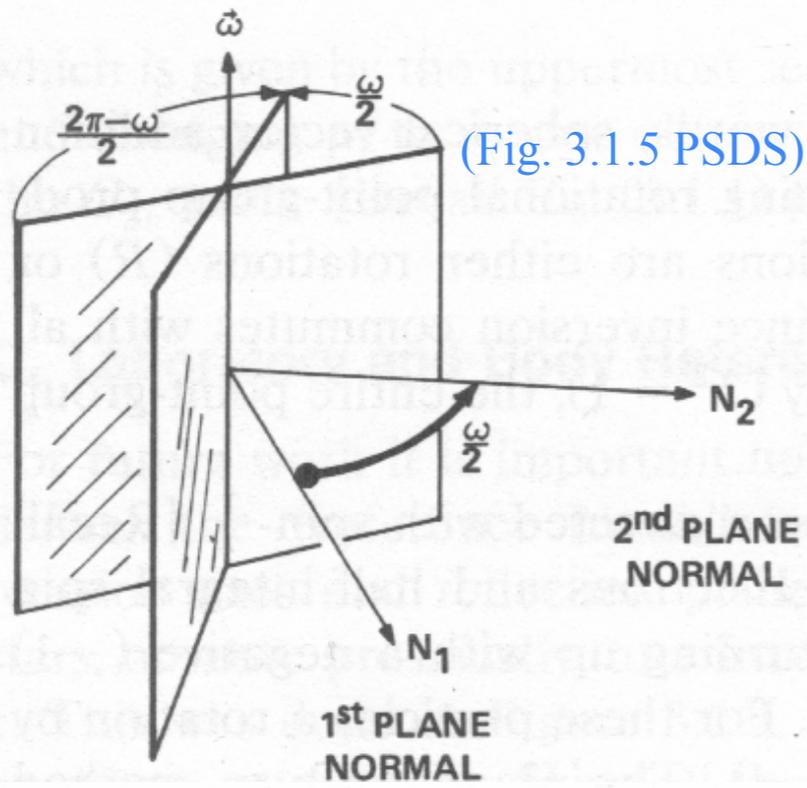
All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

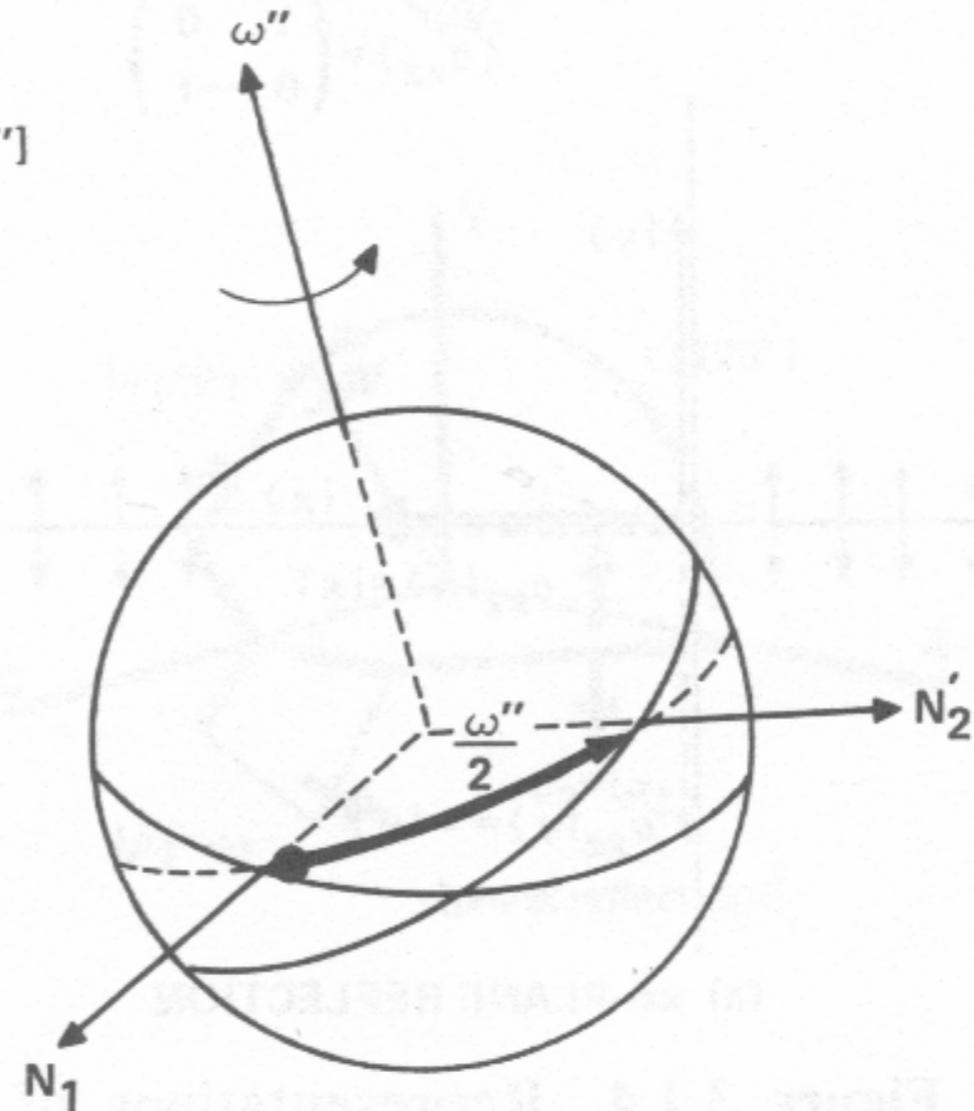
*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Deriving $D_3 \sim C_{3v}$ products by nomograms based on $U(2)$ Hamilton-turns

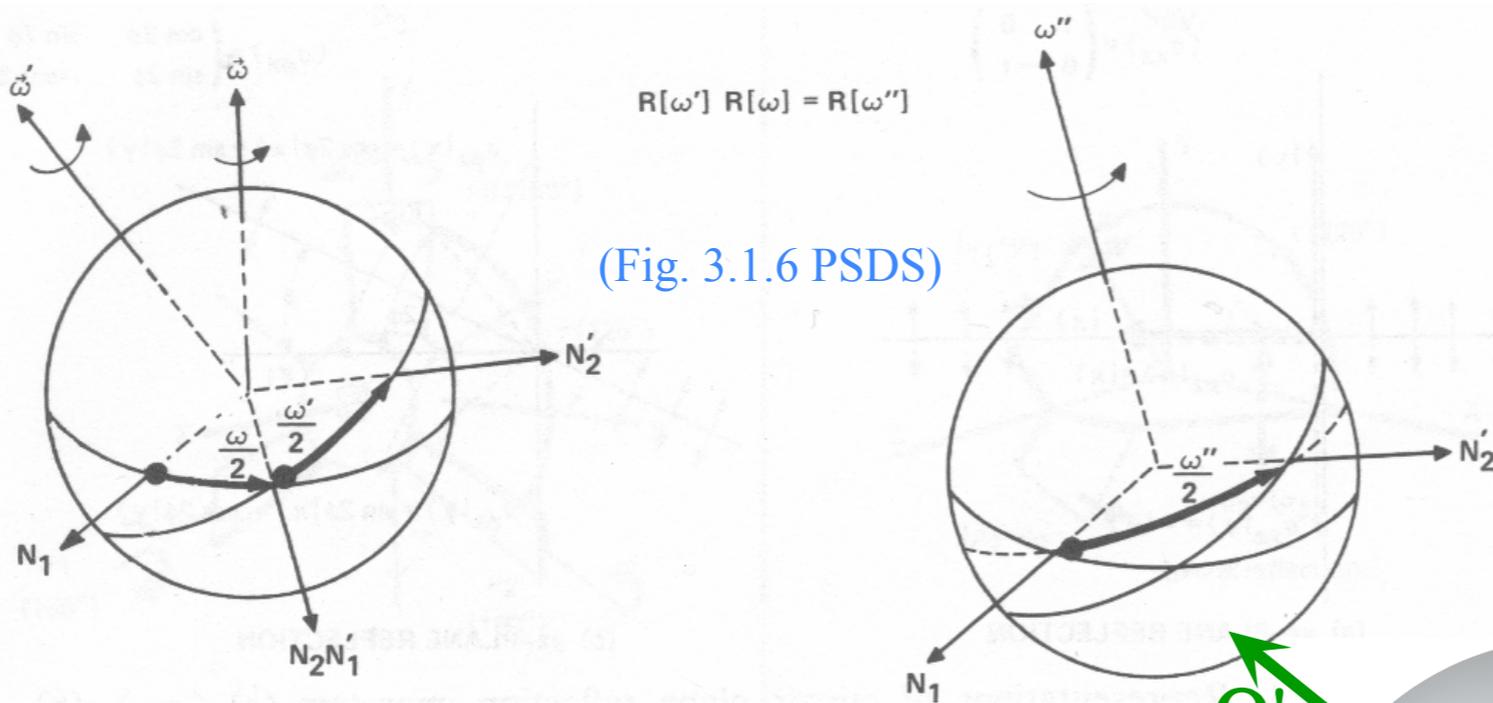
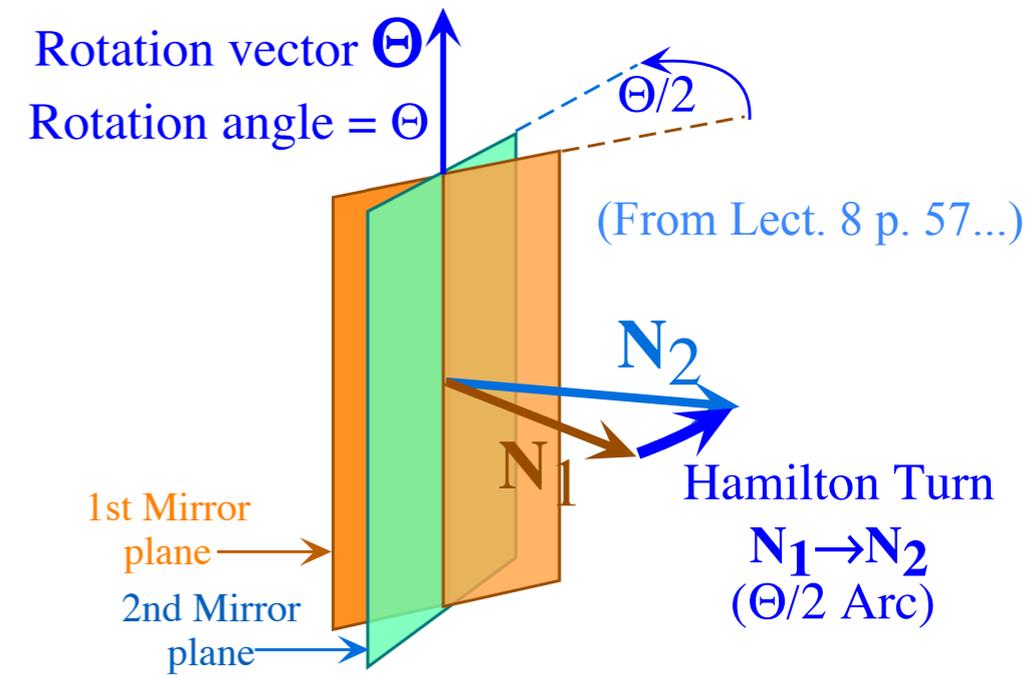
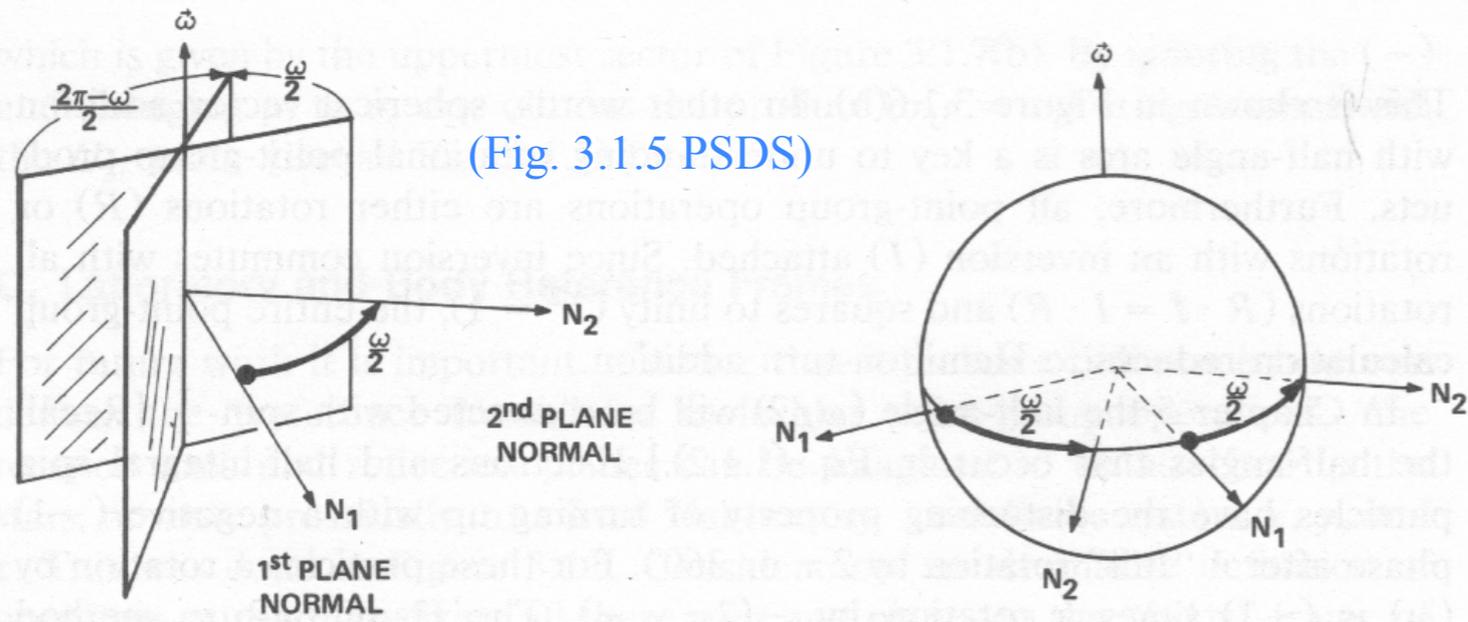


$$R[\omega'] R[\omega] = R[\omega'']$$

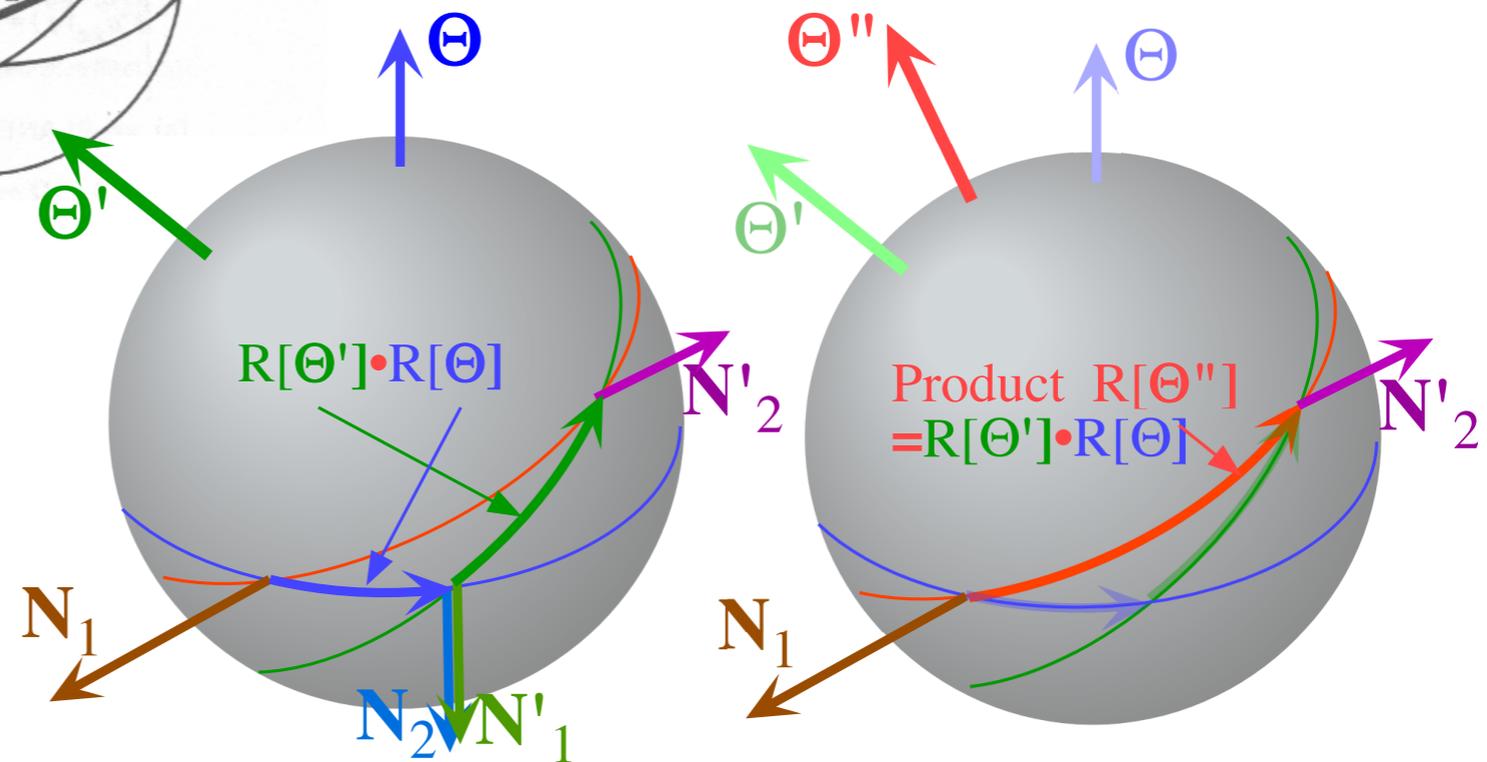


(Fig. 3.1.6 PSDS)

Deriving $D_3 \sim C_{3v}$ products by nomograms based on $U(2)$ Hamilton-turns



(Fig. 10.A.8 QTCA)



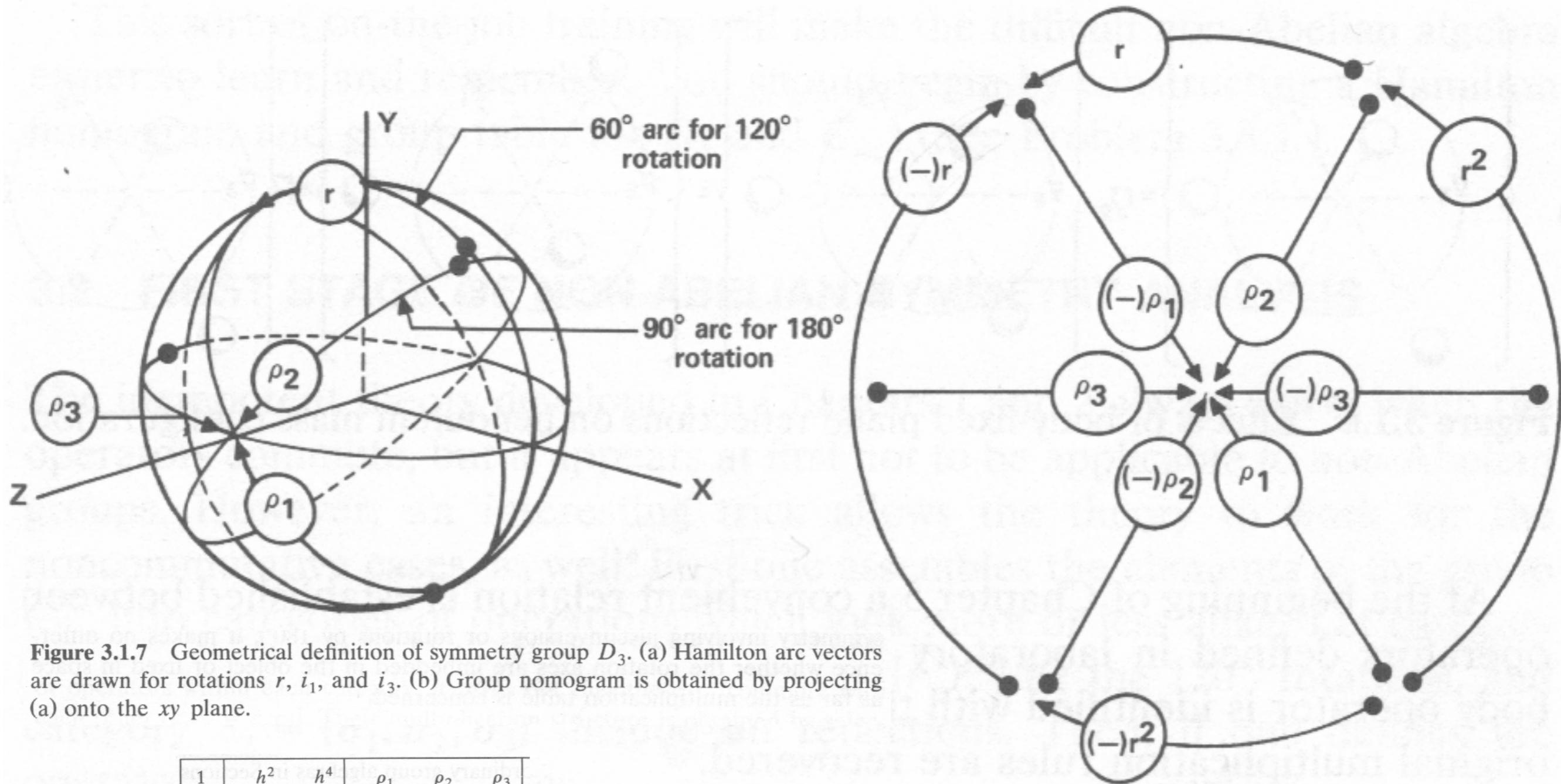


Figure 3.1.7 Geometrical definition of symmetry group D_3 . (a) Hamilton arc vectors are drawn for rotations r , i_1 , and i_3 . (b) Group nomogram is obtained by projecting (a) onto the xy plane.

1	h^2	h^4	ρ_1	ρ_2	ρ_3
h^4	-1	$-h^2$	$-\rho_2$	$-\rho_3$	ρ_1
h^2	h^4	-1	$-\rho_3$	ρ_1	ρ_2
ρ_1	ρ_2	ρ_3	-1	$-h^2$	$-h^4$
ρ_2	ρ_3	$-\rho_1$	h^4	-1	$-h^2$
ρ_3	$-\rho_1$	$-\rho_2$	h^2	h^4	-1

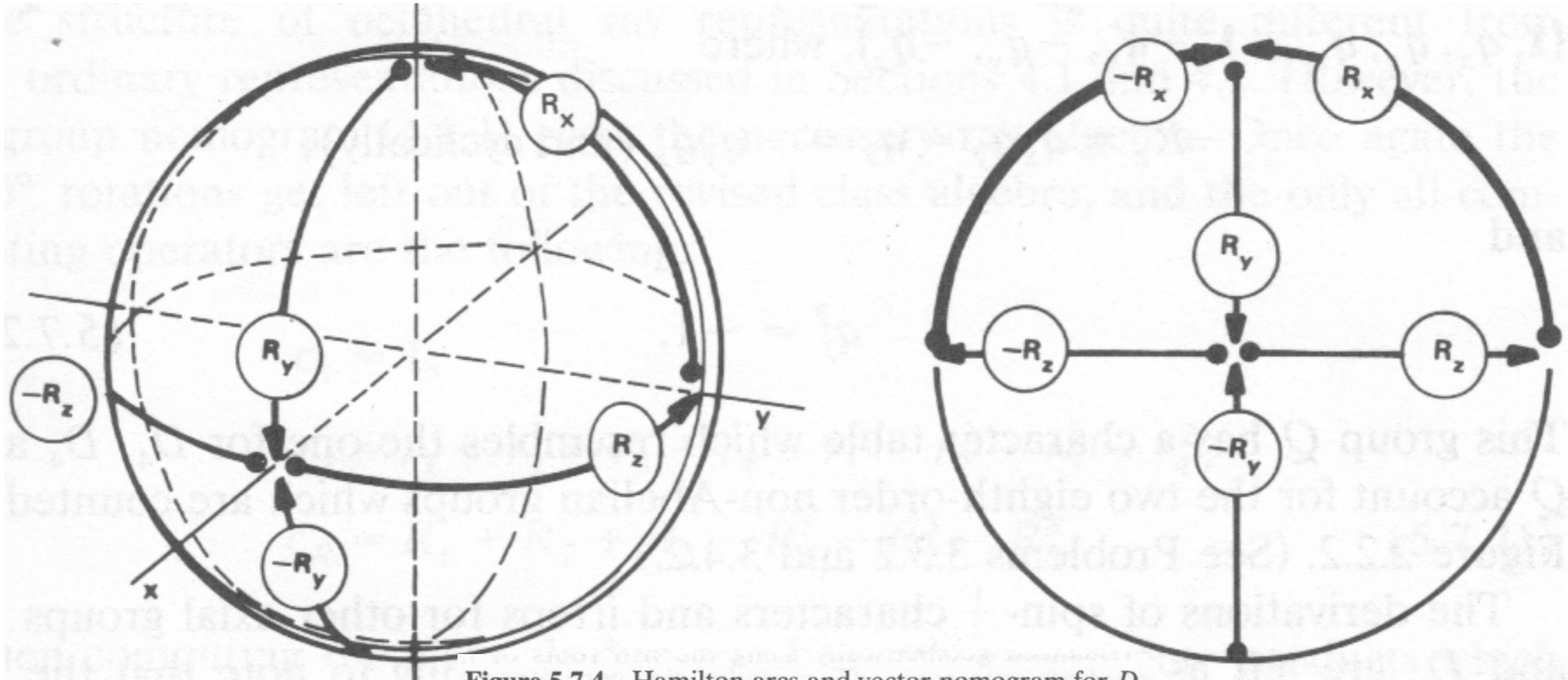
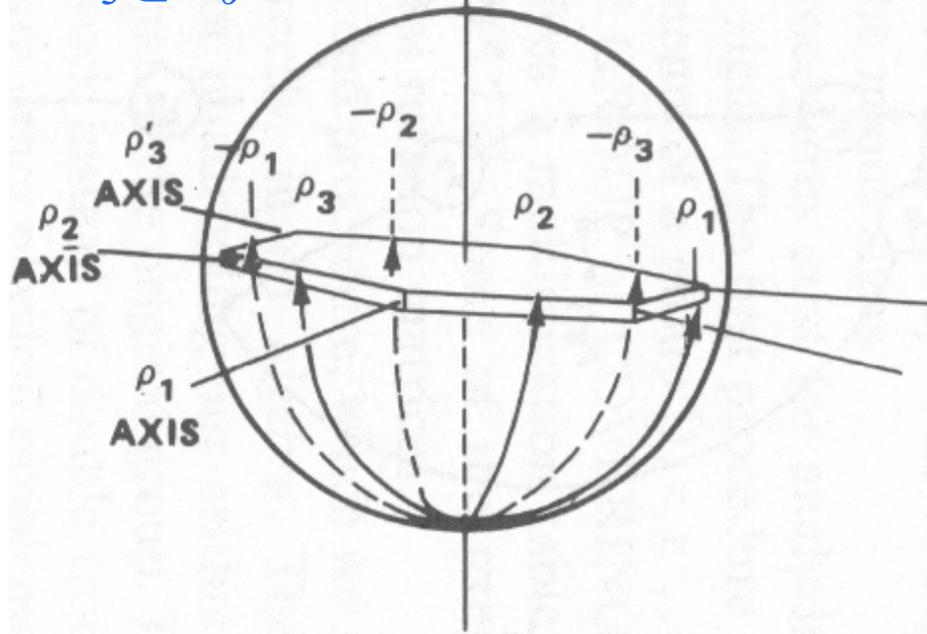


Figure 5.7.4 Hamilton arcs and vector nomogram for D_2

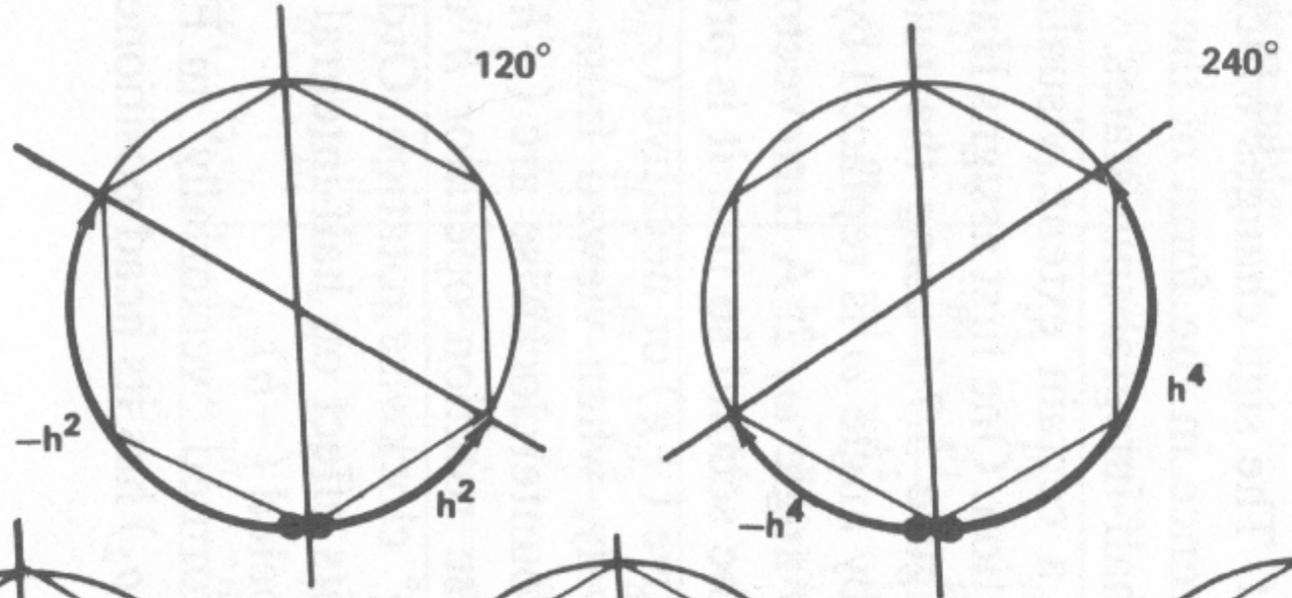
1	R_x	R_y	R_z
R_x	-1	R_z	$-R_y$
R_y	$-R_z$	-1	R_x
R_z	R_y	$-R_x$	-1

$$\mathcal{D}^E(R_x) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \quad \mathcal{D}^E(R_y) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathcal{D}^E(R_z) = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}.$$

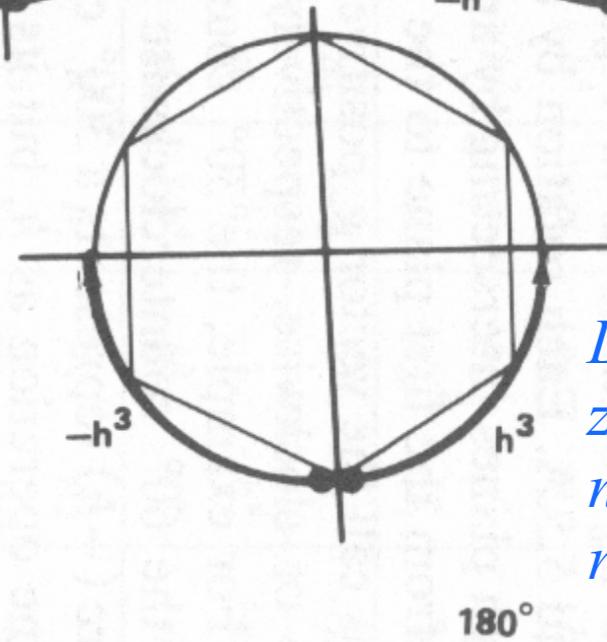
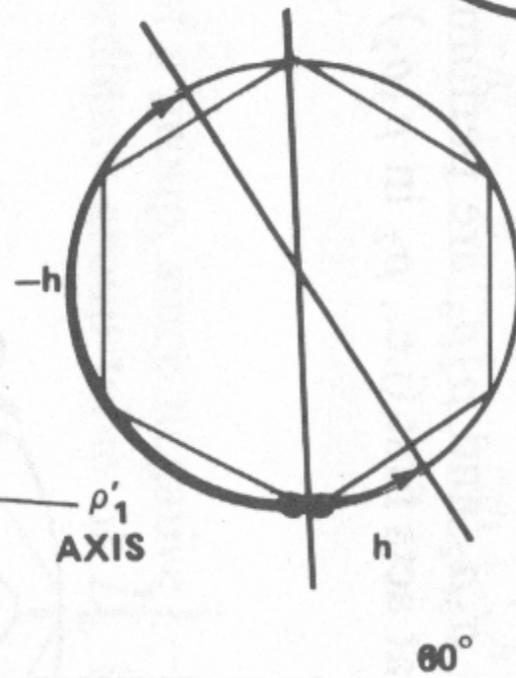
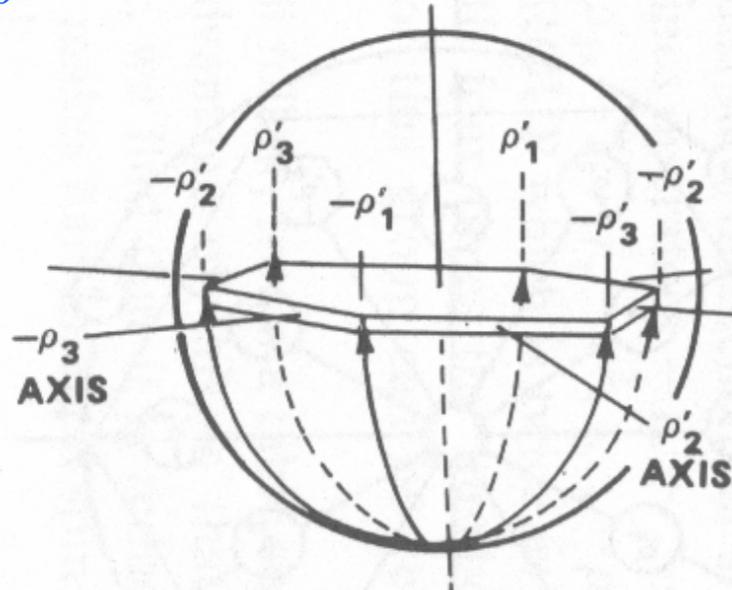
$D_3 \subset D_6$ Transverse 180° rotations



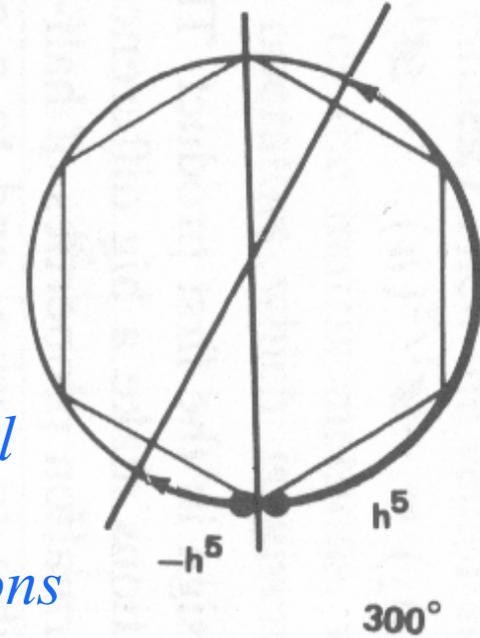
$D_3 \subset D_6$ z-Axial 120° rotations



D_6 Transverse 180° rotations



D_6 z-Axial $n(60^\circ)$ rotations



1	h^2	h^4	ρ_1	ρ_2	ρ_3	h^3	h	h^5	ρ'_1	ρ'_2	ρ'_3
h^4	-1	$-h^2$	$-\rho_2$	$-\rho_3$	ρ_1	-h	h^5	$-h^3$	$-\rho'_2$	$-\rho'_3$	ρ'_1
h^2	h^4	-1	$-\rho_3$	ρ_1	ρ_2	h^5	h^3	-h	$-\rho'_3$	ρ'_1	ρ'_2
ρ_1	ρ_2	ρ_3	-1	$-h^2$	$-h^4$	$-\rho'_1$	ρ'_3	$-\rho'_2$	h^3	h^5	-h
ρ_2	ρ_3	$-\rho_1$	h^4	-1	$-h^2$	$-\rho'_2$	$-\rho'_1$	$-\rho'_3$	h	h^3	h^5
ρ_3	$-\rho_1$	$-\rho_2$	h^2	h^4	-1	$-\rho'_3$	$-\rho'_2$	ρ'_1	$-h^5$	h	h^3
h^3	h^5	-h	ρ'_1	ρ'_2	ρ'_3	-1	h^4	$-h^2$	$-\rho_1$	$-\rho_2$	$-\rho_3$
h^5	-h	$-h^3$	$-\rho'_3$	ρ'_1	ρ'_2	$-h^2$	-1	$-h^4$	ρ_3	$-\rho_1$	$-\rho_2$
h	h^3	h^5	ρ'_2	ρ'_3	$-\rho'_1$	h^4	h^2	-1	$-\rho_2$	$-\rho_3$	ρ_1
ρ'_1	ρ'_2	ρ'_3	$-h^3$	$-h^5$	h	ρ_1	$-\rho_3$	ρ_2	-1	$-h^2$	$-h^4$
ρ'_2	ρ'_3	$-\rho'_1$	-h	$-h^3$	$-h^5$	ρ_2	ρ_1	ρ_3	h^4	-1	$-h^2$
ρ'_3	$-\rho'_1$	$-\rho'_2$	h^5	-h	$-h^3$	ρ_3	ρ_2	$-\rho_1$	h^2	h^4	-1

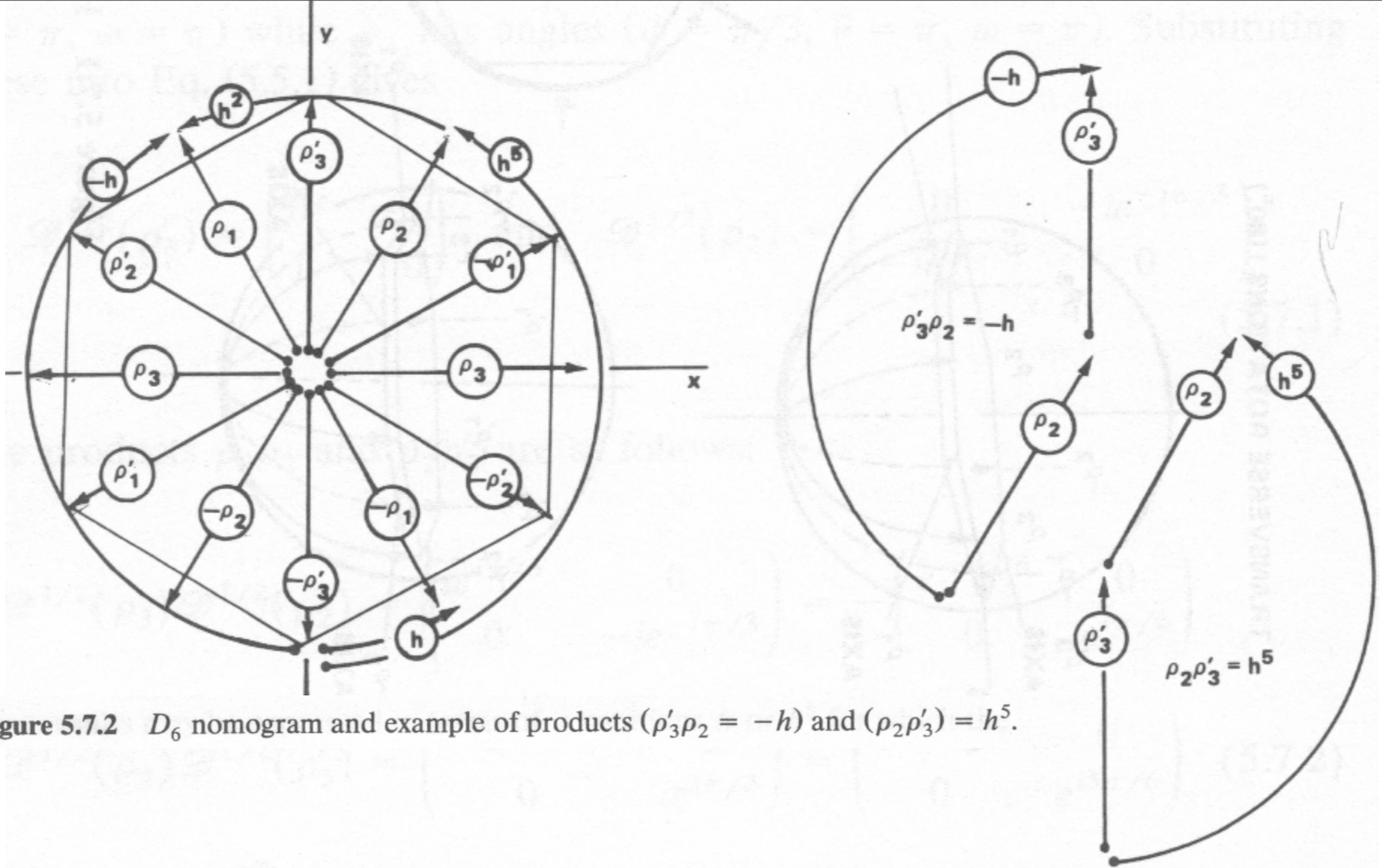


Figure 5.7.2 D_6 nomogram and example of products $(\rho'_3 \rho_2 = -h)$ and $(\rho_2 \rho'_3) = h^5$.

*3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}
 D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)*

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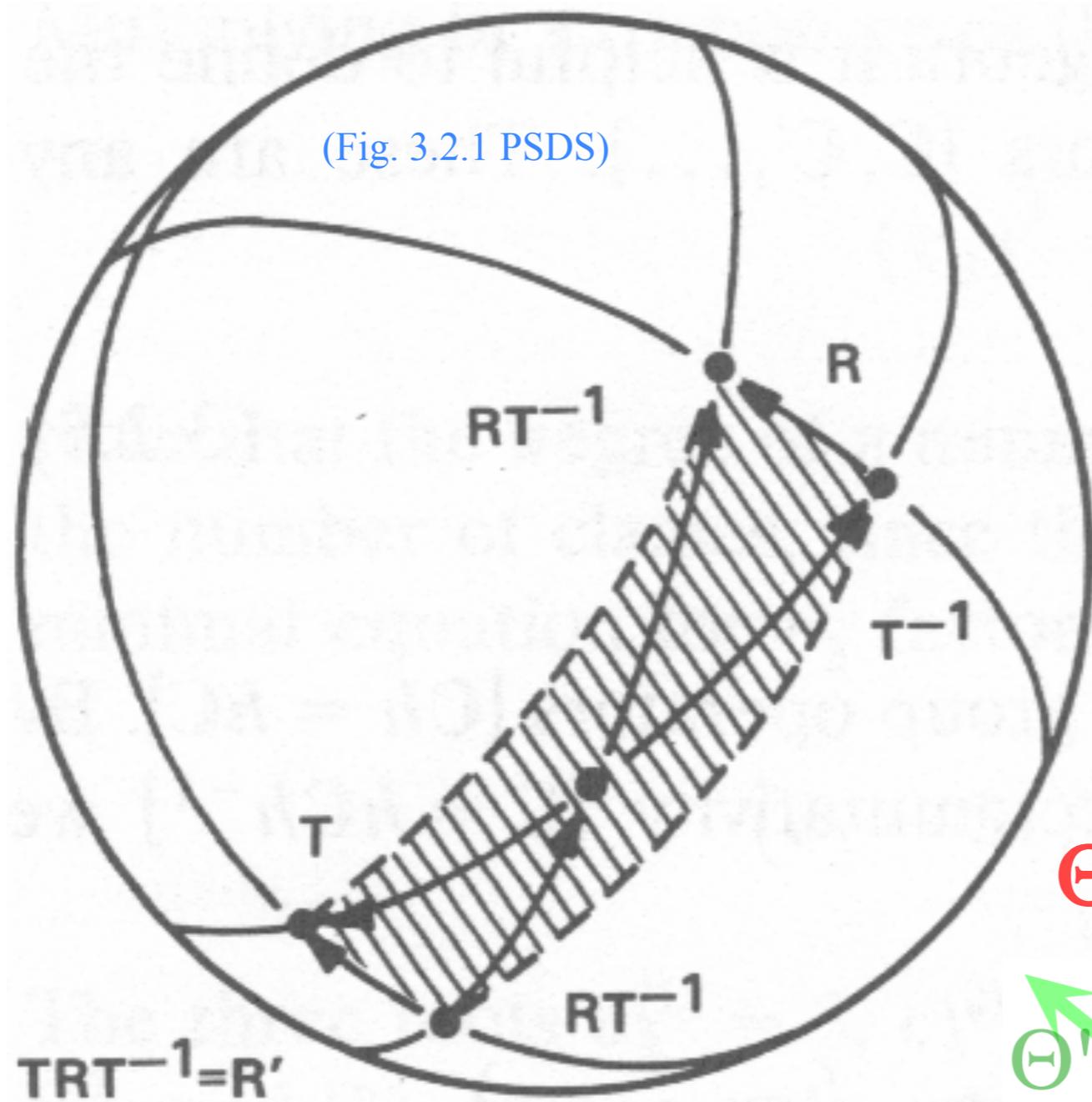
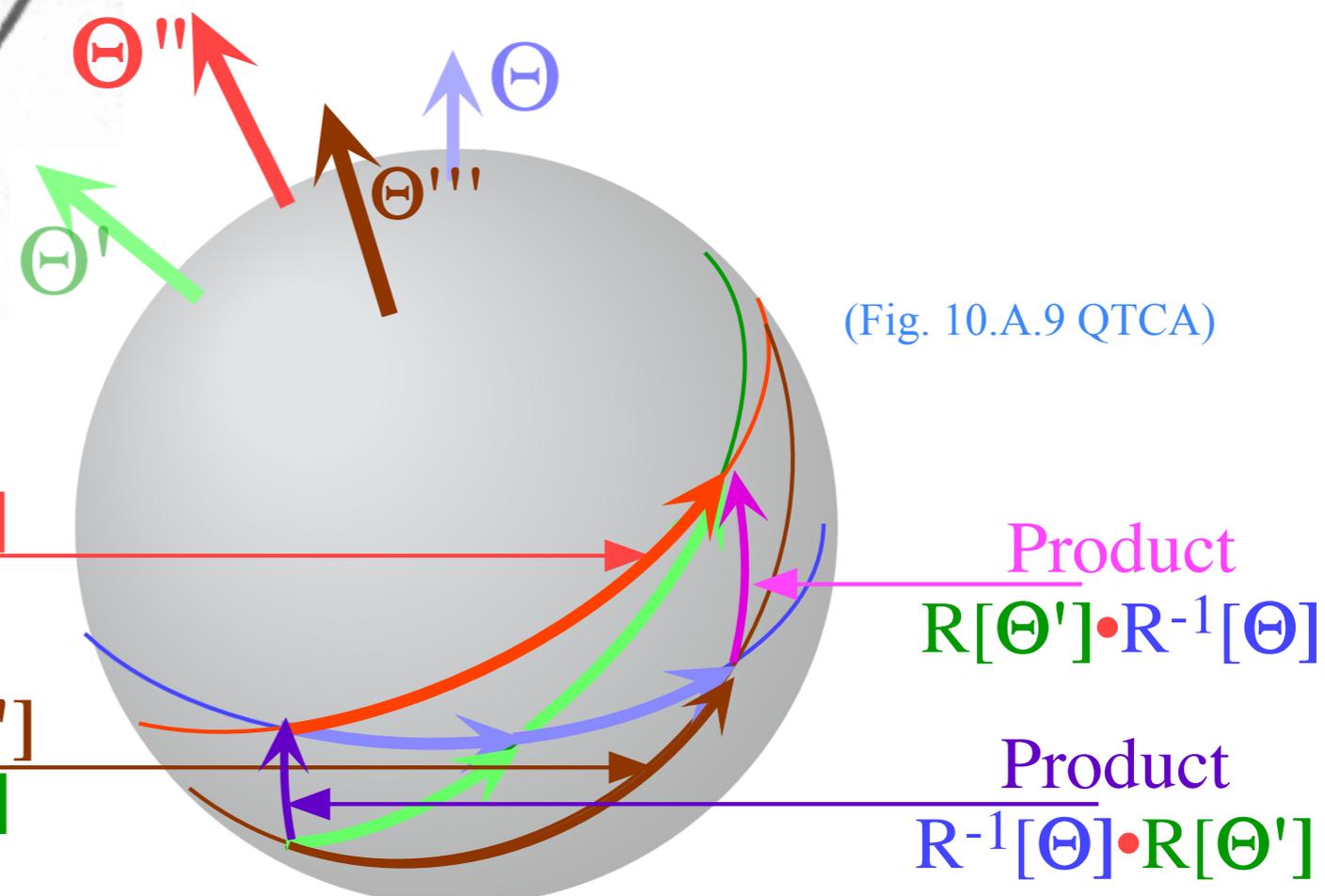


Figure 3.2.1 Showing class equivalence using Hamilton's vectors. Operation R is equivalent to $R' = TRT^{-1}$.

(From Lect. 8 p. 62...)



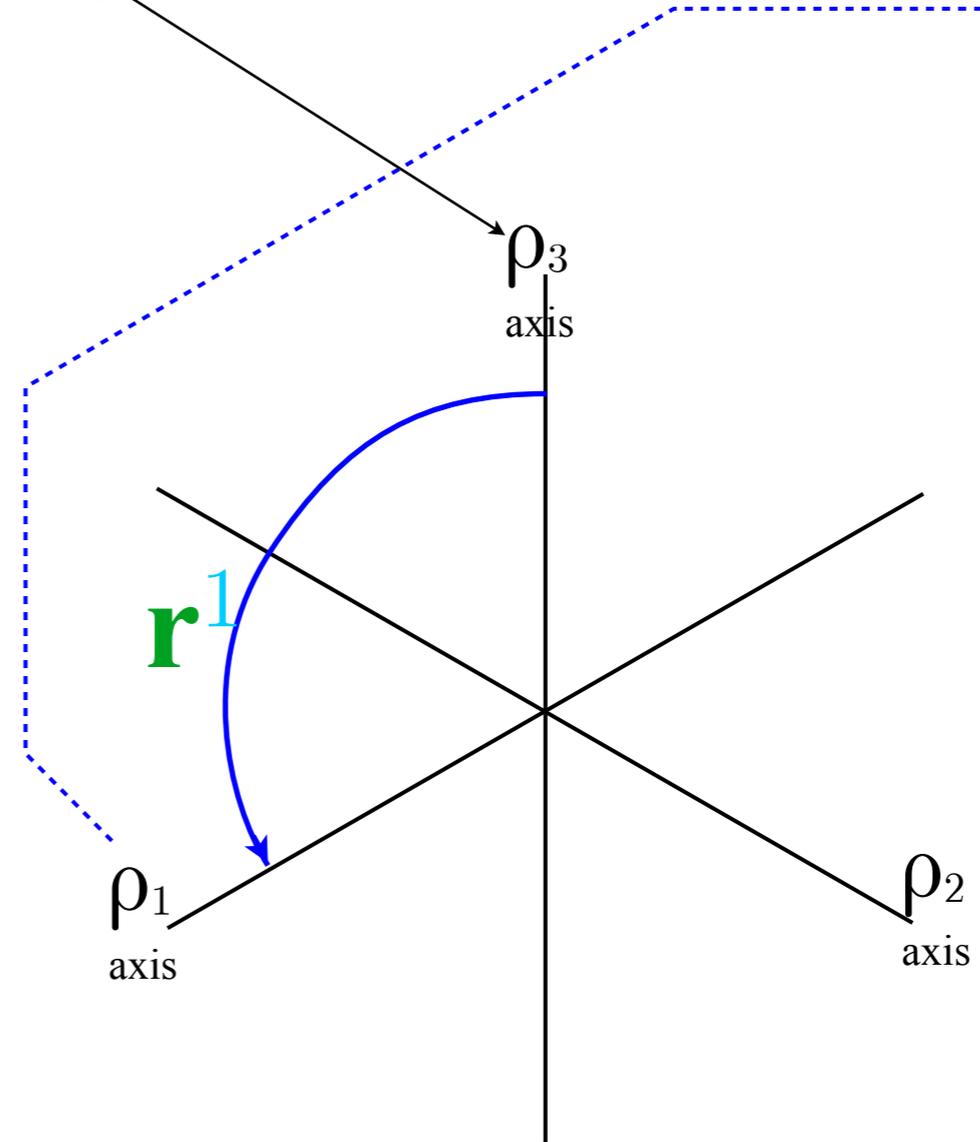
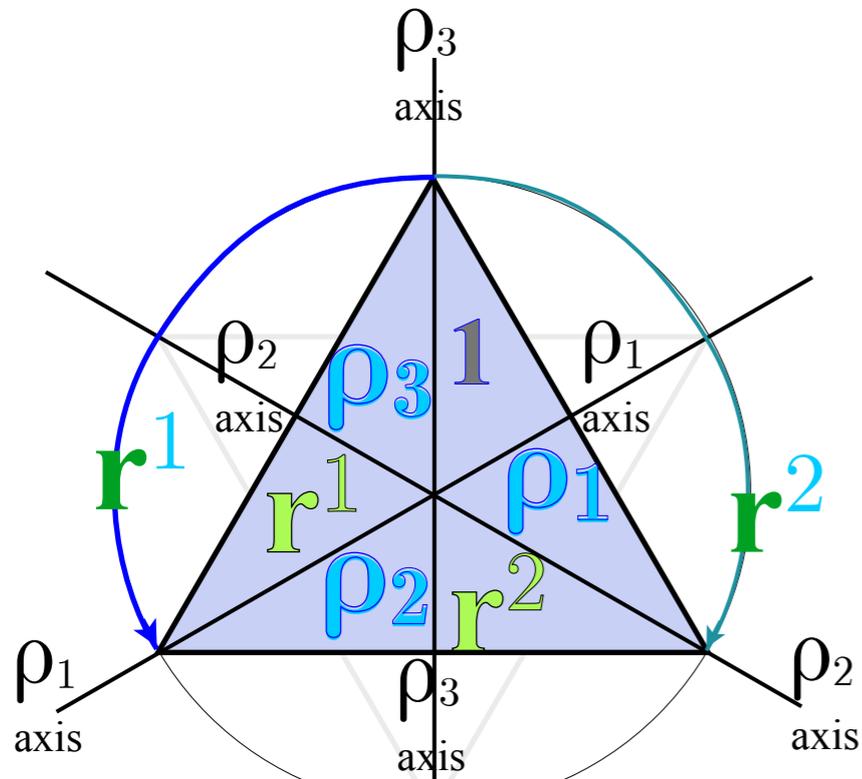
$$\text{Product } R[\Theta''] = R[\Theta'] \cdot R[\Theta]$$

$$\text{Product } R[\Theta'''] = R[\Theta] \cdot R[\Theta']$$

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Transforming D_3 operators using D_3 operators

Example 1: Rotating ρ_3 axis crank using r^1 puts it down onto ρ_1



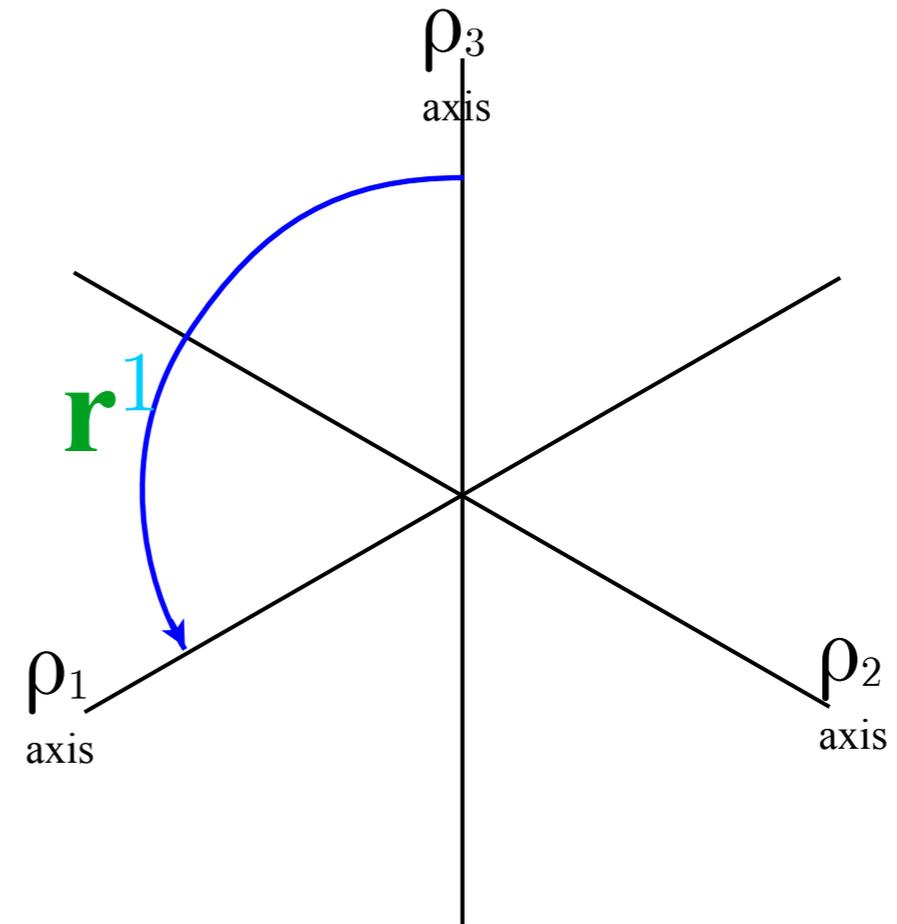
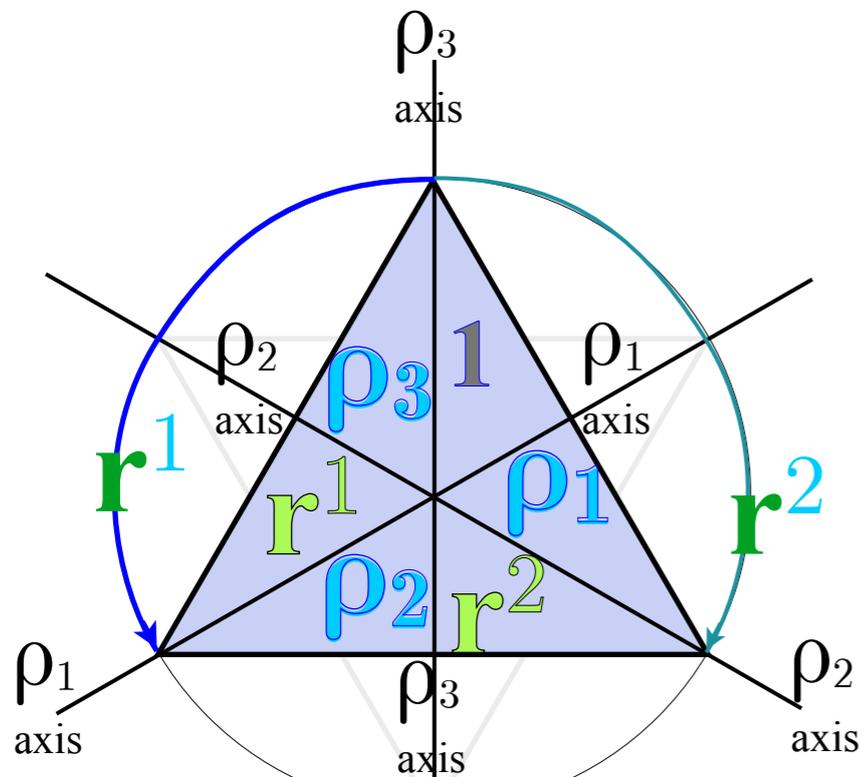
D_3 gg^\dagger form	$\mathbf{1}$	r^2	r^1	ρ_1	ρ_2	ρ_3
$\mathbf{1}$	$\mathbf{1}$	r^2	r^1	ρ_1	ρ_2	ρ_3
r^1	r^1	$\mathbf{1}$	r^2	ρ_3	ρ_1	ρ_2
r^2	r^2	r^1	$\mathbf{1}$	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	$\mathbf{1}$	r^1	r^2
ρ_2	ρ_2	ρ_1	ρ_3	r^2	$\mathbf{1}$	r^1
σ_3	ρ_3	ρ_2	ρ_1	r^1	r^2	$\mathbf{1}$

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Transforming D_3 operators using D_3 operators

Example 1: Rotating ρ_3 axis crank using \mathbf{r}^1 puts it down onto ρ_1

Seems to imply: $\mathbf{r}^1 \rho_3 (\mathbf{r}^1)^{-1} = \mathbf{r}^1 \rho_3 \mathbf{r}^2 = \rho_1$



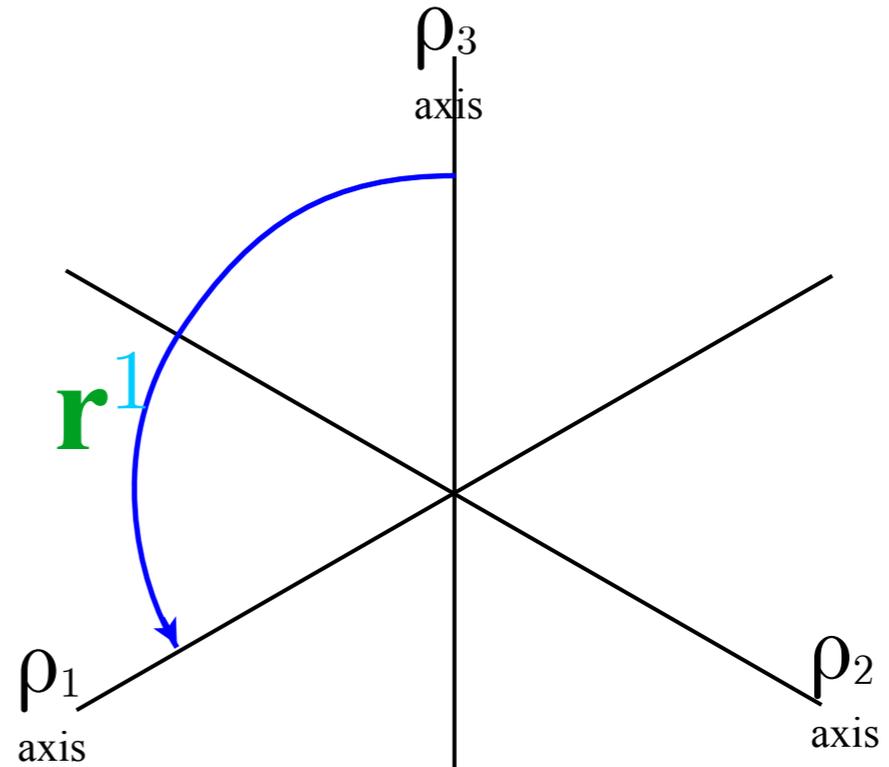
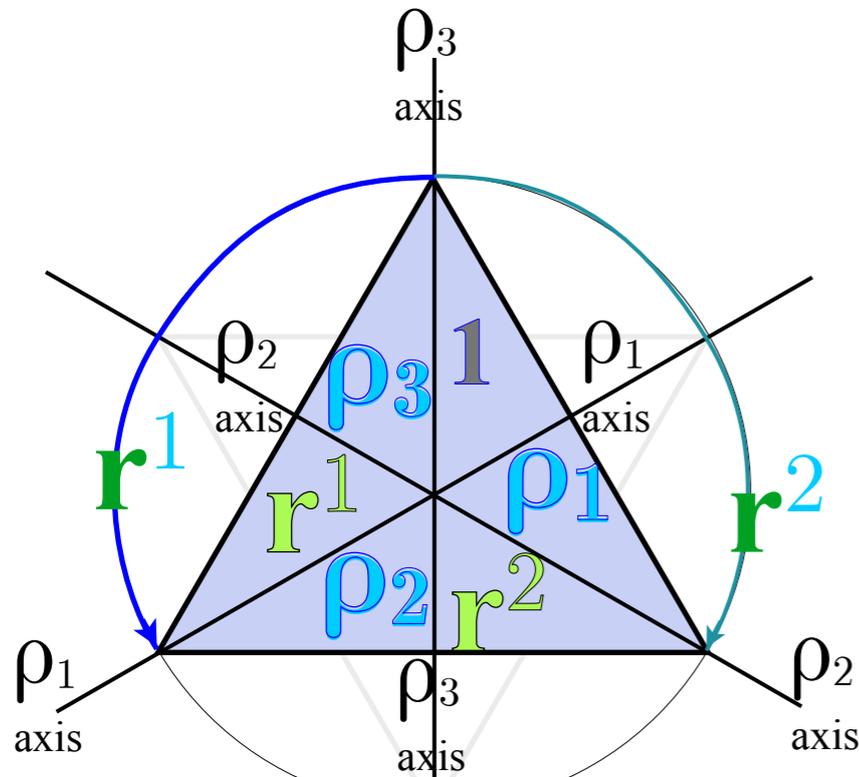
D_3 $g g^\dagger$ form	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
$\mathbf{1}$	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
\mathbf{r}^1	\mathbf{r}^1	$\mathbf{1}$	\mathbf{r}^2	ρ_3	ρ_1	ρ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	$\mathbf{1}$	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	$\mathbf{1}$	\mathbf{r}^1	\mathbf{r}^2
ρ_2	ρ_2	ρ_1	ρ_3	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}^1
σ_3	ρ_3	ρ_2	ρ_1	\mathbf{r}^1	\mathbf{r}^2	$\mathbf{1}$

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

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Example 1: Rotating ρ_3 axis crank using \mathbf{r}^1 puts it down onto ρ_1

Seems to imply: $\mathbf{r}^1 \rho_3 (\mathbf{r}^1)^{-1} = \mathbf{r}^1 \rho_3 \mathbf{r}^2 = \rho_1$



D_3 $g g^\dagger$ form	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
$\mathbf{1}$	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
\mathbf{r}^1	\mathbf{r}^1	$\mathbf{1}$	\mathbf{r}^2	ρ_3	ρ_1	ρ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	$\mathbf{1}$	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	$\mathbf{1}$	\mathbf{r}^1	\mathbf{r}^2
ρ_2	ρ_2	ρ_1	ρ_3	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}^1
σ_3	ρ_3	ρ_2	ρ_1	\mathbf{r}^1	\mathbf{r}^2	$\mathbf{1}$

Need to check that with table:

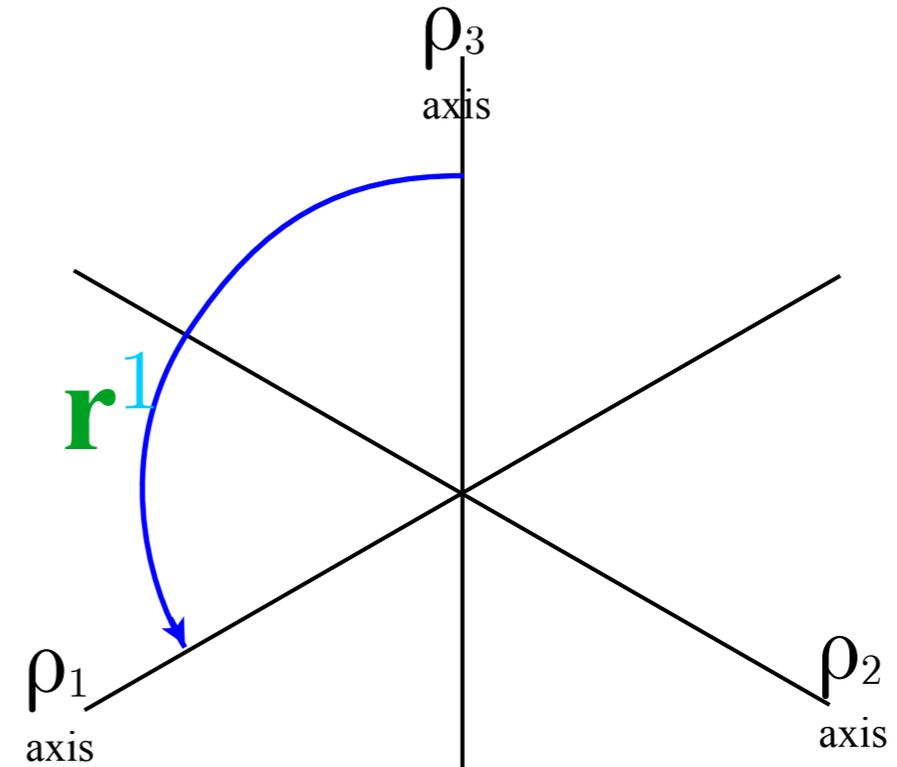
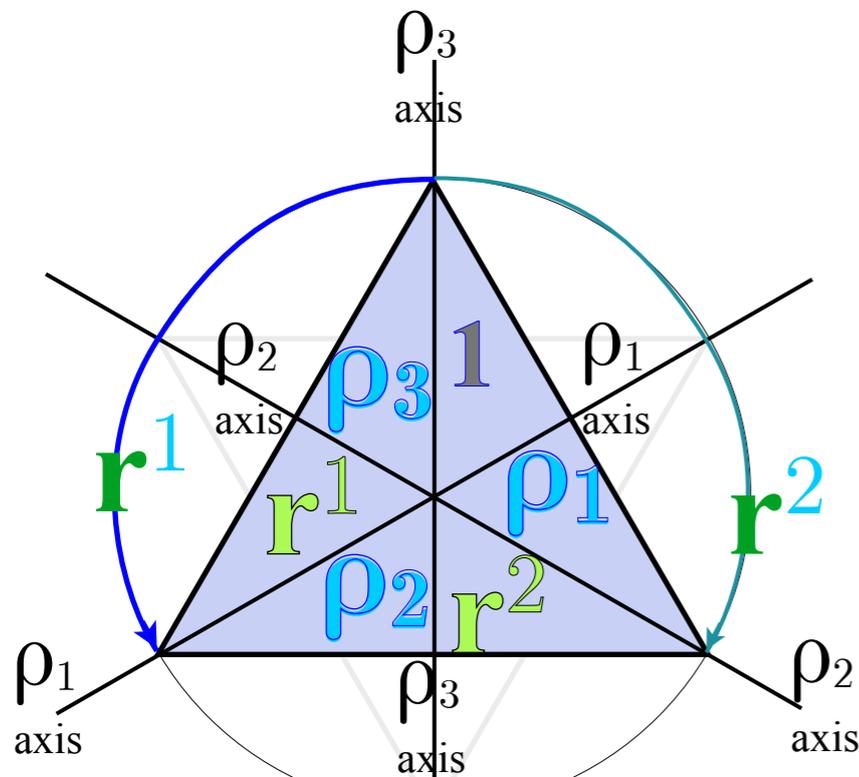
$$\mathbf{r}^1 \rho_3 \mathbf{r}^2 = \rho_2 \mathbf{r}^2$$

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Transforming D_3 operators using D_3 operators

Example 1: Rotating ρ_3 axis crank using \mathbf{r}^1 puts it down onto ρ_1

Seems to imply: $\mathbf{r}^1 \rho_3 (\mathbf{r}^1)^{-1} = \mathbf{r}^1 \rho_3 \mathbf{r}^2 = \rho_1$



D_3 $g g^\dagger$ form	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
$\mathbf{1}$	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
\mathbf{r}^1	\mathbf{r}^1	$\mathbf{1}$	\mathbf{r}^2	ρ_3	ρ_1	ρ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	$\mathbf{1}$	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	$\mathbf{1}$	\mathbf{r}^1	\mathbf{r}^2
ρ_2	ρ_2	ρ_1	ρ_3	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}^1
σ_3	ρ_3	ρ_2	ρ_1	\mathbf{r}^1	\mathbf{r}^2	$\mathbf{1}$

Need to check that with table:

$$\mathbf{r}^1 \rho_3 \mathbf{r}^2 = \rho_2 \mathbf{r}^2 = \rho_1$$

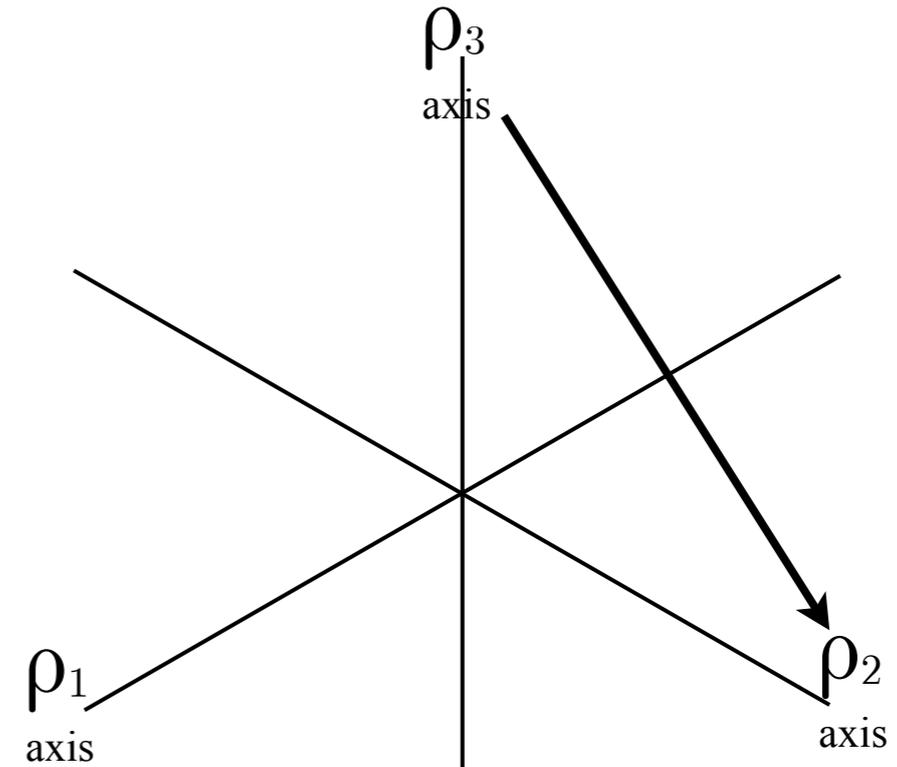
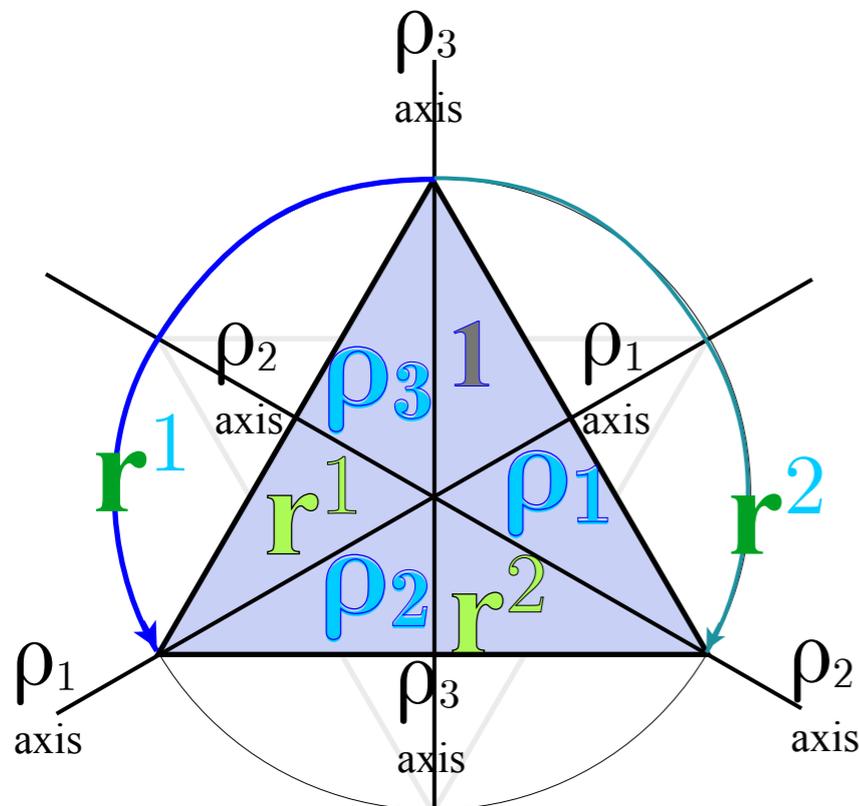
Checks out!

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Transforming D_3 operators using D_3 operators

Example 2: Rotating ρ_3 axis crank using ρ_1 puts it down onto ρ_2

Seems to imply: $\rho_1 \rho_3 (\rho_1)^{-1} = \rho_1 \rho_3 \rho_1 = \rho_2$



D_3 gg^\dagger form	1	r^2	r^1	ρ_1	ρ_2	ρ_3
1	1	r^2	r^1	ρ_1	ρ_2	ρ_3
r^1	r^1	1	r^2	ρ_3	ρ_1	ρ_2
r^2	r^2	r^1	1	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	1	r^1	r^2
ρ_2	ρ_2	ρ_1	ρ_3	r^2	1	r^1
σ_3	ρ_3	ρ_2	ρ_1	r^1	r^2	1

Need to check that with table:

$$\rho_1 \rho_3 \rho_1 = r^2 \rho_1 = \rho_2$$

Checks out!

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

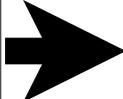
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By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

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Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

All-commuting operators and D_3 -invariant class algebra

All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

*Spectral resolution to **irreducible representations** (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Abelian (Commutative) $C_2, C_3, \dots, C_6 \dots$

H diagonalized by r^p symmetry operators that **COMMUTE**
with H ($r^p H = H r^p$),

and with each other ($r^p r^q = r^{p+q} = r^q r^p$).

Abelian (Commutative) $C_2, C_3, \dots, C_6 \dots$

H diagonalized by r^p symmetry operators that **COMMUTE**
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Non-Abelian (do not commute) D_3, O_h, \dots

While all H symmetry operations **COMMUTE**
with H ($\mathbf{U} H = H \mathbf{U}$)
most do not with each other ($\mathbf{U} \mathbf{V} \neq \mathbf{V} \mathbf{U}$).

Abelian (Commutative) $C_2, C_2, \dots, C_6 \dots$

H diagonalized by r^p symmetry operators that **COMMUTE**
with H ($r^p H = H r^p$),
and with each other ($r^p r^q = r^{p+q} = r^q r^p$).

Non-Abelian (do not commute) D_3, O_h, \dots

While all H symmetry operations **COMMUTE**
with H ($U H = H U$)
most do not with each other ($U V \neq V U$).

Q: So how do we write H in terms of non-commutative U ?

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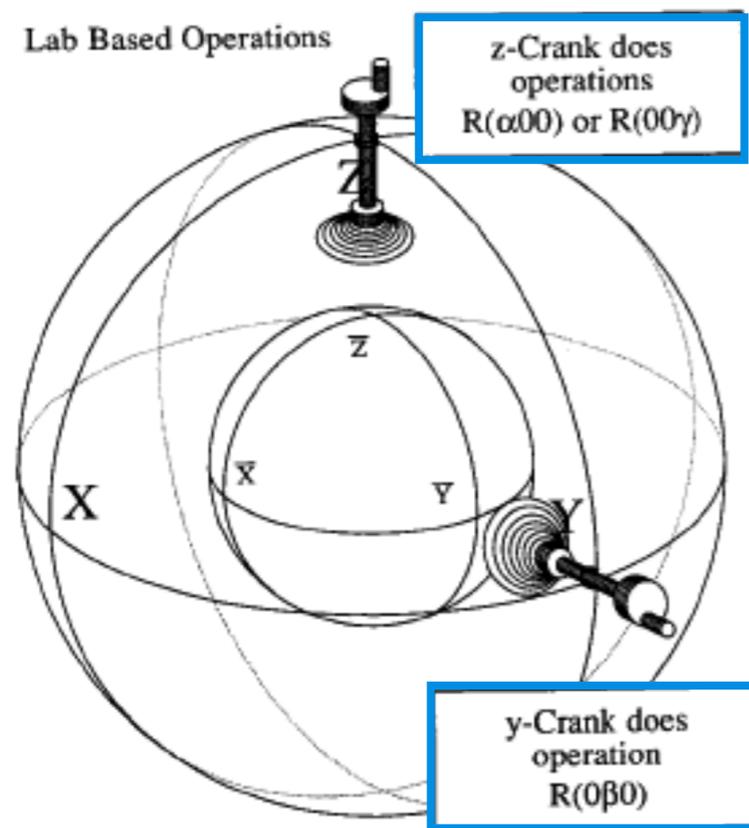
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*“Give me a place to stand...
and I will move the Earth”*

Archimedes 287-212 B.C.E

Ideas of duality/relativity go *way* back (... VanVleck, Casimir..., Mach, Newton, Archimedes...)

Lab-fixed (Extrinsic-Global)R

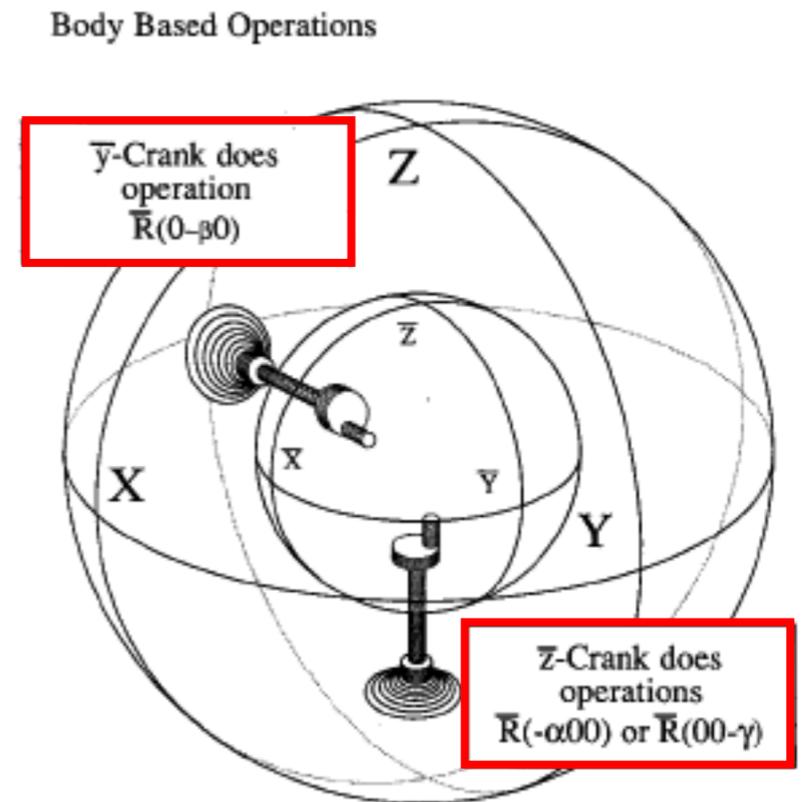
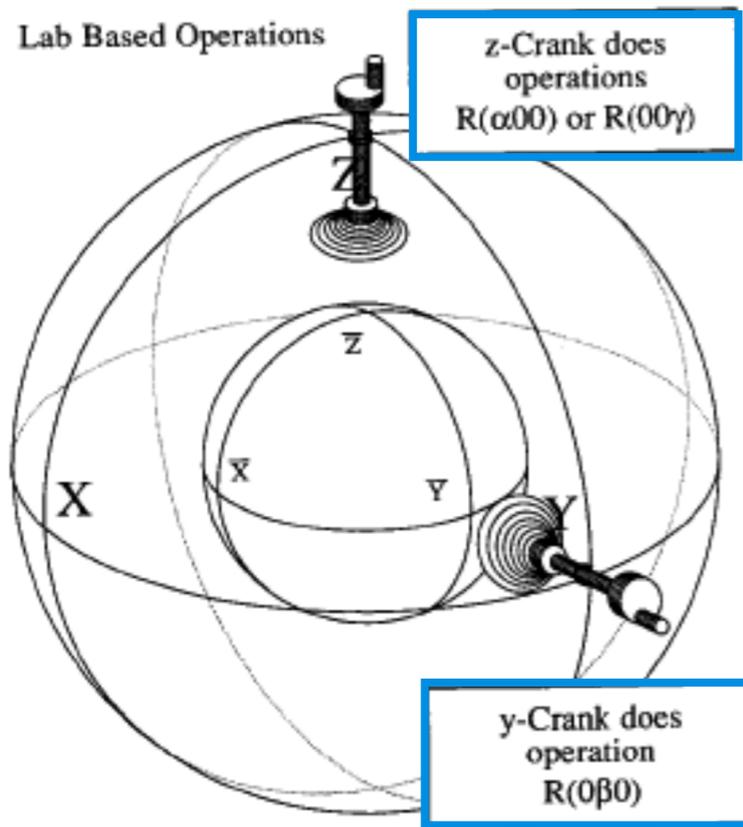


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Lab-fixed (Extrinsic-Global) \mathbf{R} vs. Body-fixed (Intrinsic-Local) $\bar{\mathbf{R}}$

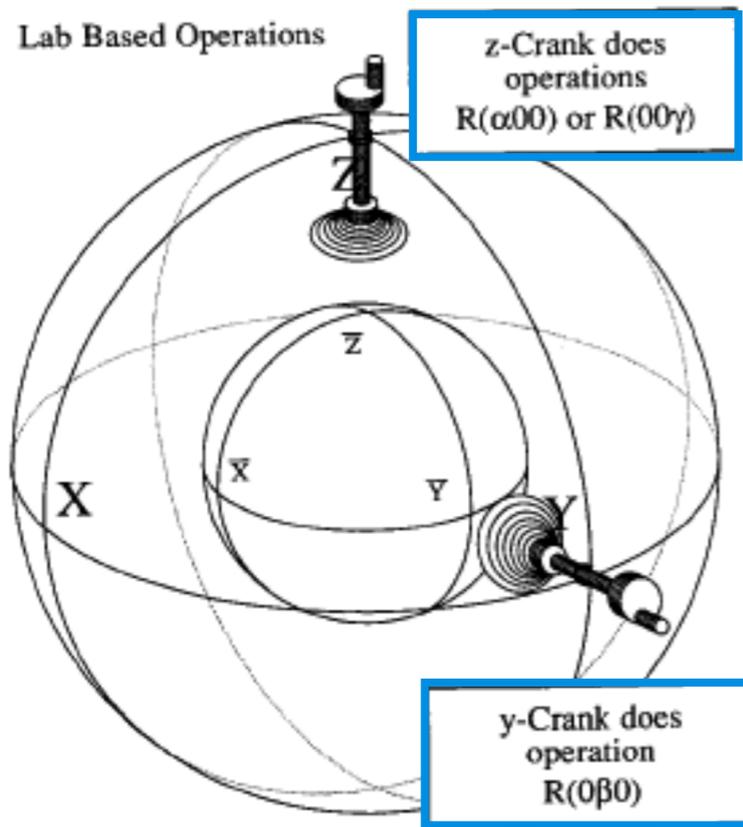


“Give me a place to stand...
and I will move the Earth”

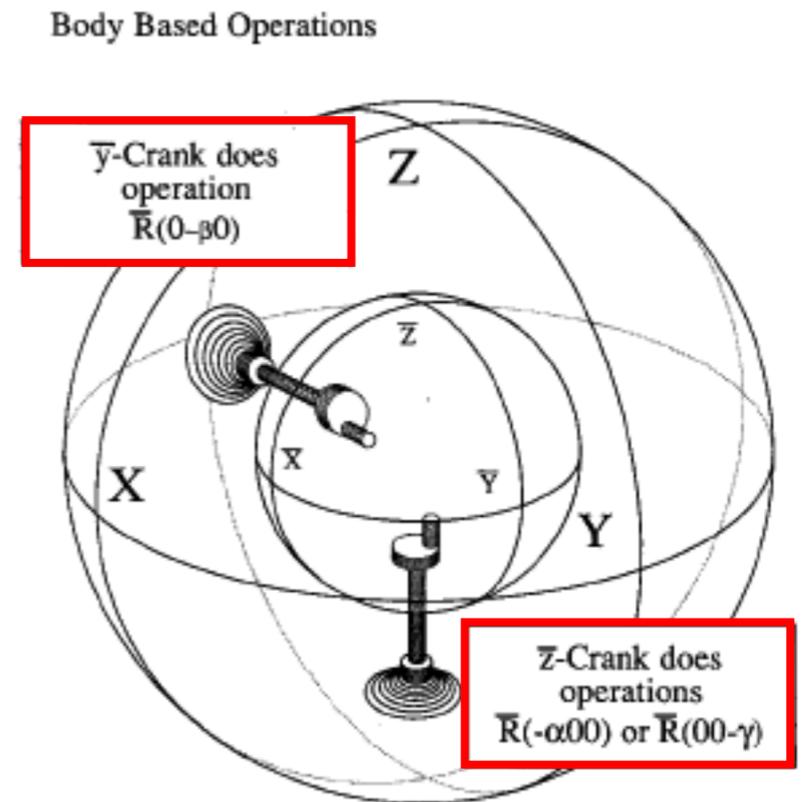
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\mathbf{R} commutes
with all $\bar{\mathbf{R}}$

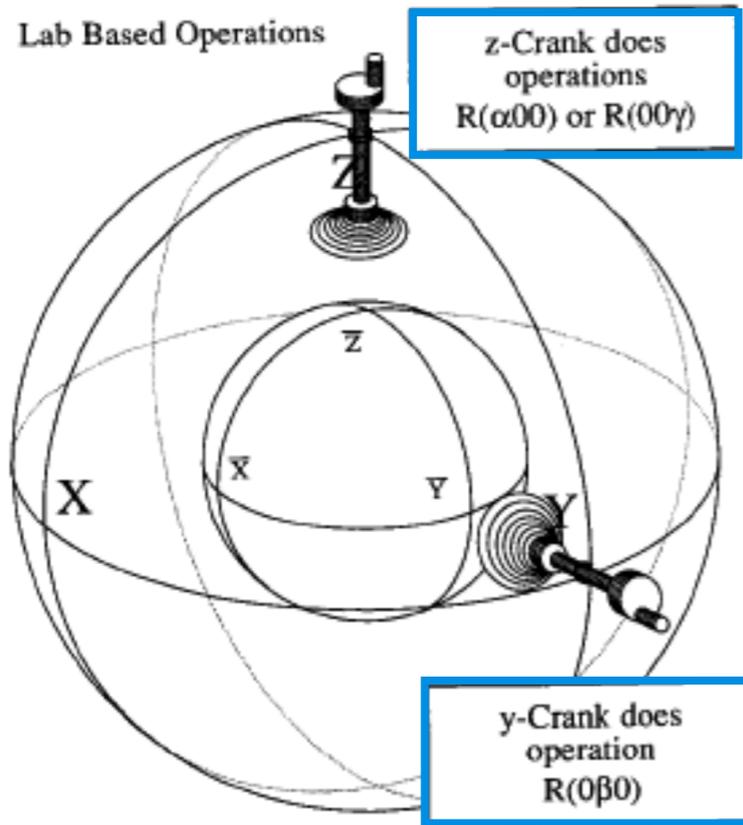


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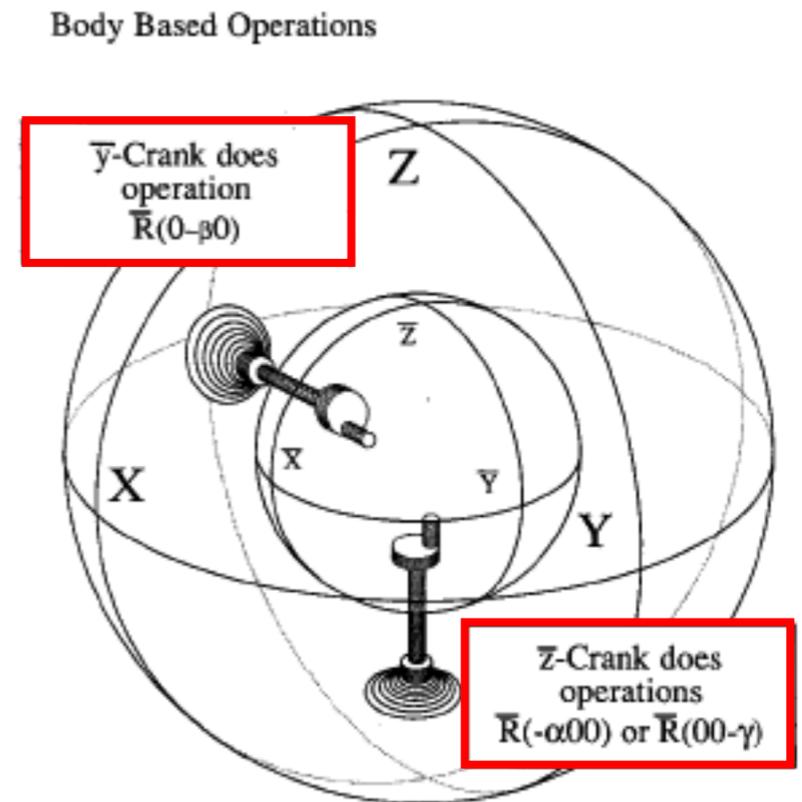


\mathbf{R} commutes
with all $\bar{\mathbf{R}}$

Mock-Mach
relativity principle

$$\mathbf{R}|1\rangle = \bar{\mathbf{R}}^{-1}|1\rangle$$

...for one state $|1\rangle$ only!

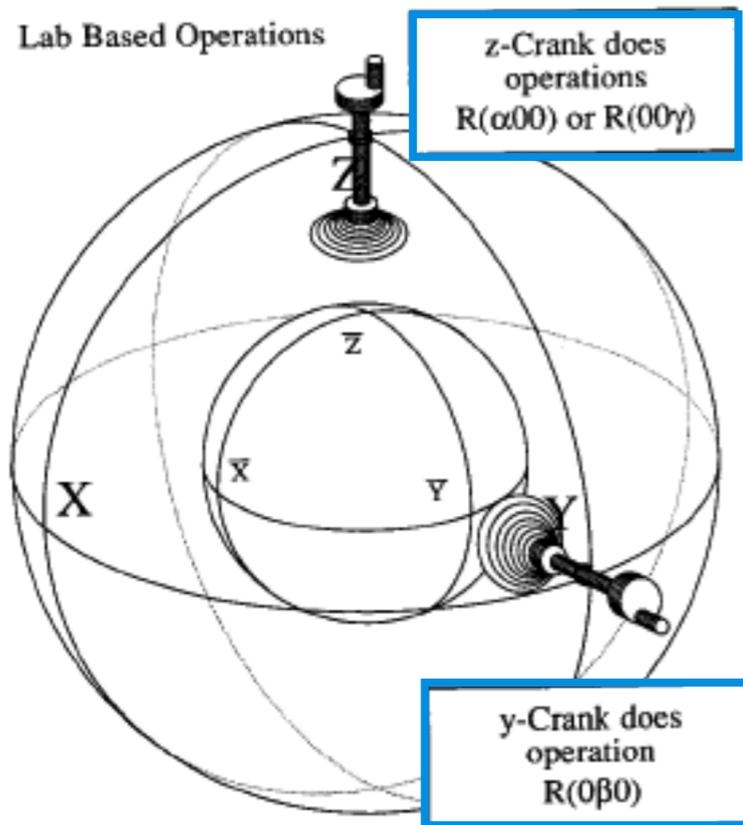


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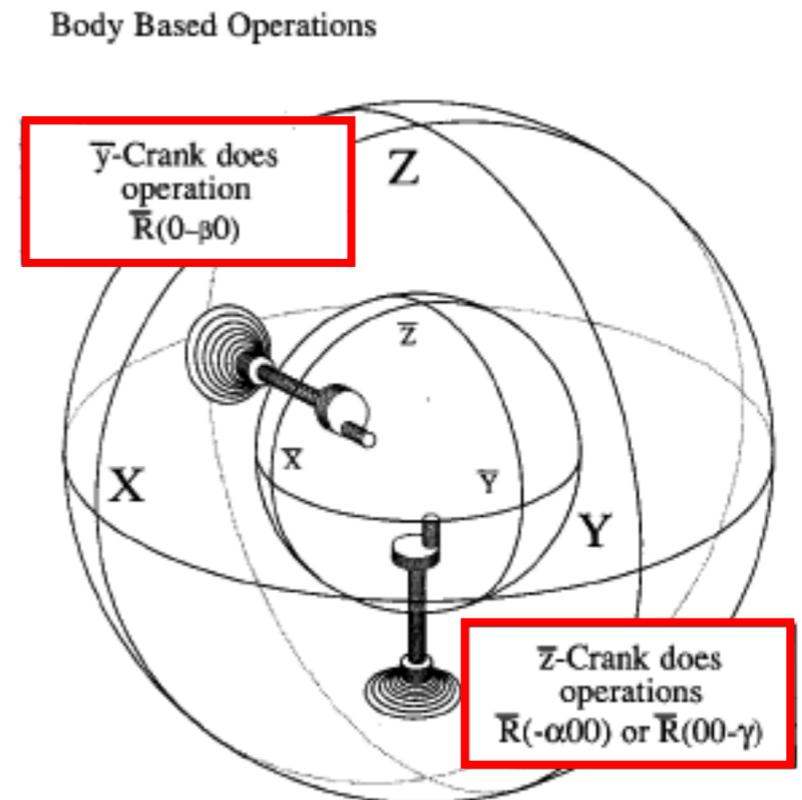


\mathbf{R} commutes
with all $\bar{\mathbf{R}}$

Mock-Mach
relativity principle

$$\mathbf{R}|1\rangle = \bar{\mathbf{R}}^{-1}|1\rangle$$

...for one state $|1\rangle$ only!



...But *how* do you actually *make* the \mathbf{R} and $\bar{\mathbf{R}}$ operations?

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

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Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

All-commuting operators and D_3 -invariant class algebra

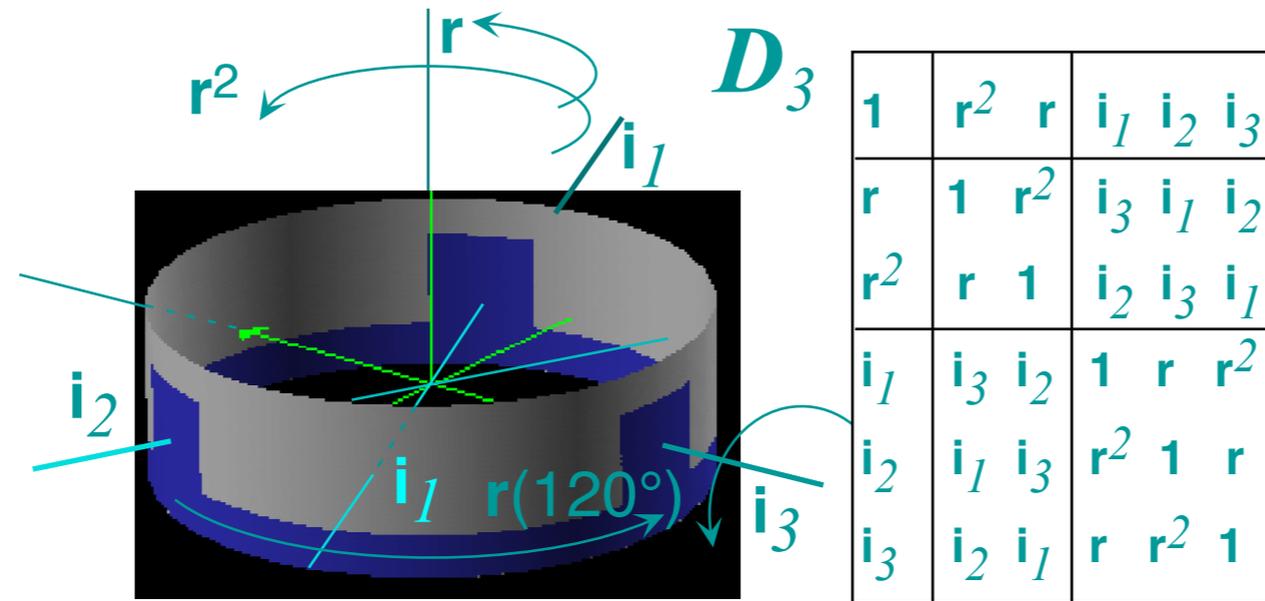
All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

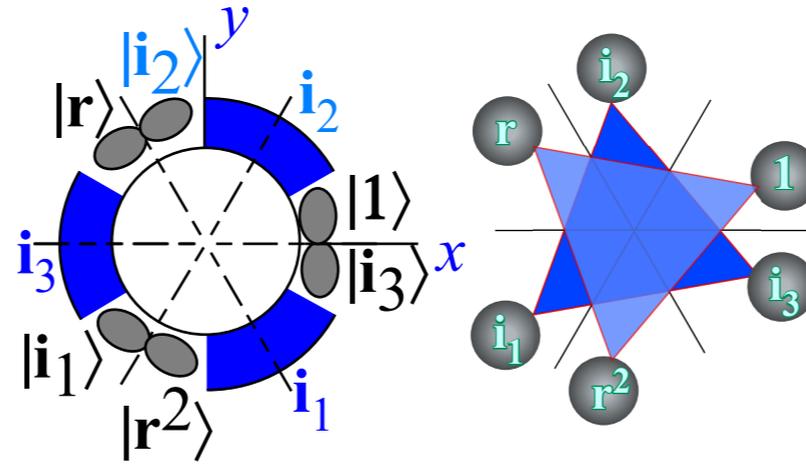
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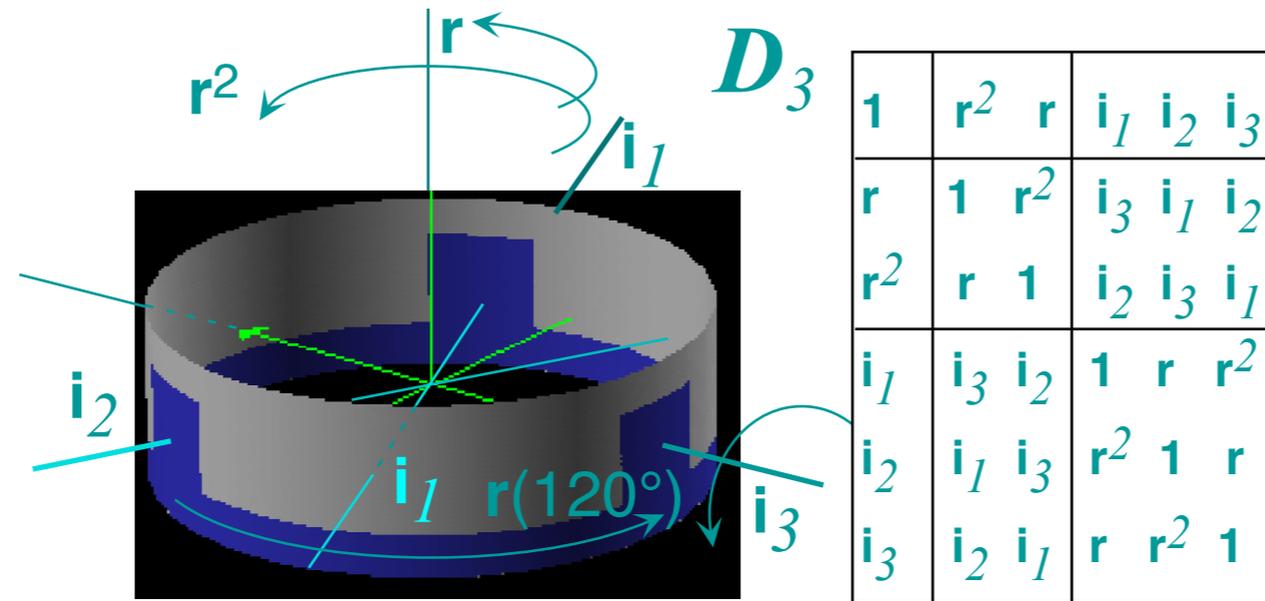
Example of GLOBAL vs LOCAL symmetry algebra for $D_3 \sim C_{3v}$



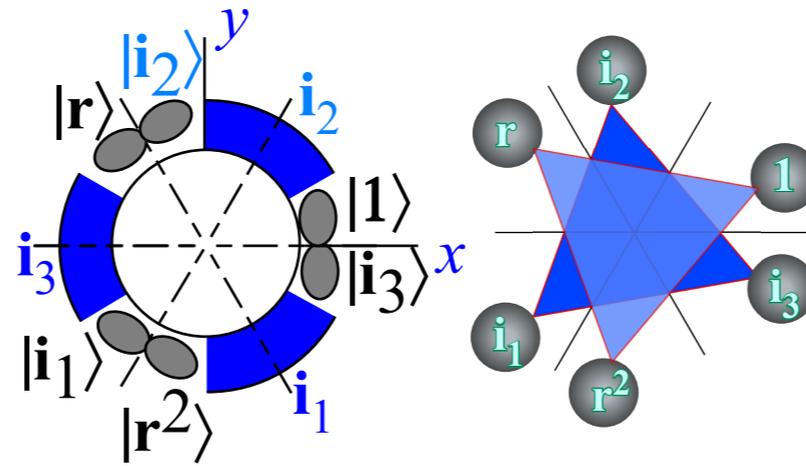
D_3 -defined
local-wave
bases



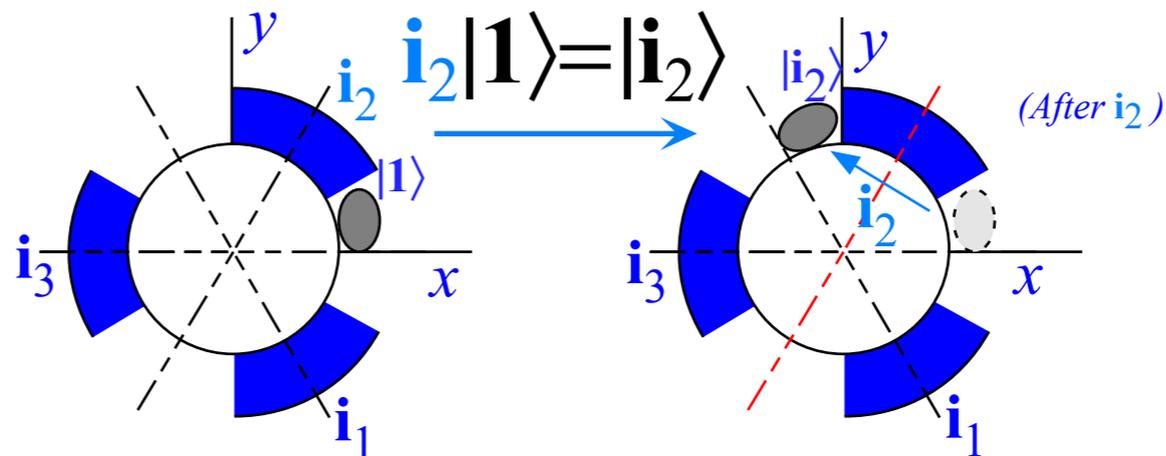
Example of GLOBAL vs LOCAL symmetry algebra for $D_3 \sim C_{3v}$



D_3 -defined
local-wave
bases



Lab-fixed (Extrinsic-Global) operations and rotation axes



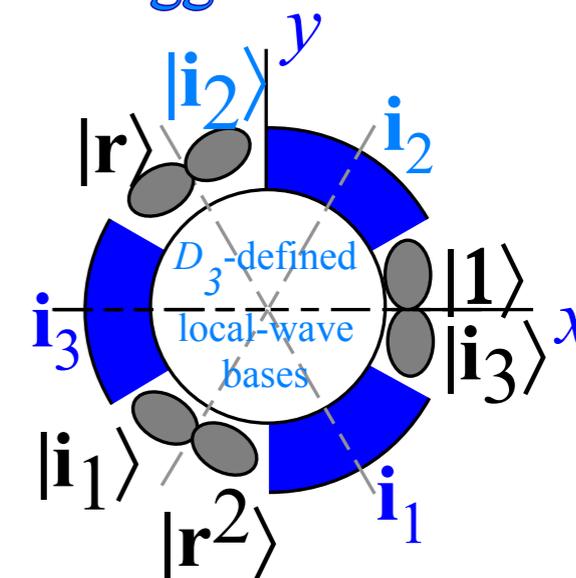
Example of RELATIVITY-DUALITY for $D_3 \sim C_{3v}$

To represent *external* {..**T,U,V**,... } switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on top of group table

$$\begin{aligned}
 R^G(\mathbf{1}) &= \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}, &
 R^G(\mathbf{r}) &= \begin{pmatrix} \cdot & \cdot & \mathbf{1} & \cdot & \cdot & \cdot \\ \mathbf{1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \mathbf{1} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \mathbf{1} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{1} \\ \cdot & \cdot & \cdot & \mathbf{1} & \cdot & \cdot \end{pmatrix}, &
 R^G(\mathbf{r}^2) &= \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}, &
 R^G(\mathbf{i}_1) &= \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix}, &
 R^G(\mathbf{i}_2) &= \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}, &
 R^G(\mathbf{i}_3) &= \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{1} \\ \cdot & \cdot & \cdot & \mathbf{1} & \cdot & \cdot \\ \cdot & \cdot & \mathbf{1} & \cdot & \cdot & \cdot \\ \cdot & \mathbf{1} & \cdot & \cdot & \cdot & \cdot \\ \mathbf{1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \mathbf{1} & \cdot \end{pmatrix}
 \end{aligned}$$

$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}	\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3
\mathbf{r}	$\mathbf{1}$	\mathbf{r}^2	\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2
\mathbf{r}^2	\mathbf{r}	$\mathbf{1}$	\mathbf{i}_2	\mathbf{i}_3	\mathbf{i}_1
\mathbf{i}_1	\mathbf{i}_3	\mathbf{i}_2	$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2
\mathbf{i}_2	\mathbf{i}_1	\mathbf{i}_3	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}
\mathbf{i}_3	\mathbf{i}_2	\mathbf{i}_1	\mathbf{r}	\mathbf{r}^2	$\mathbf{1}$

D_3 global gg^\dagger -table



Example of RELATIVITY-DUALITY for $D_3 \sim C_{3v}$

To represent *external* $\{.. \mathbf{T}, \mathbf{U}, \mathbf{V}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on top of group table

$$\begin{aligned}
 R^G(\mathbf{1}) &= \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} &
 R^G(\mathbf{r}) &= \begin{pmatrix} & & \mathbf{1} & & & \\ \mathbf{1} & & & & & \\ & \mathbf{1} & & & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \end{pmatrix} &
 R^G(\mathbf{r}^2) &= \begin{pmatrix} & \mathbf{1} & & & & \\ & & \mathbf{1} & & & \\ \mathbf{1} & & & & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \end{pmatrix} &
 R^G(\mathbf{i}_1) &= \begin{pmatrix} & & & \mathbf{1} & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ \mathbf{1} & & & & & \\ & \mathbf{1} & & & & \\ & & \mathbf{1} & & & \end{pmatrix} &
 R^G(\mathbf{i}_2) &= \begin{pmatrix} & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \\ & & & \mathbf{1} & & \\ & & \mathbf{1} & & & \\ & \mathbf{1} & & & & \end{pmatrix} &
 R^G(\mathbf{i}_3) &= \begin{pmatrix} & & & & & \mathbf{1} \\ & & & & \mathbf{1} & \\ & & & \mathbf{1} & & \\ & & \mathbf{1} & & & \\ & \mathbf{1} & & & & \\ \mathbf{1} & & & & & \end{pmatrix}
 \end{aligned}$$

$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}	\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3
\mathbf{r}	$\mathbf{1}$	\mathbf{r}^2	\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2
\mathbf{r}^2	\mathbf{r}	$\mathbf{1}$	\mathbf{i}_2	\mathbf{i}_3	\mathbf{i}_1
\mathbf{i}_1	\mathbf{i}_3	\mathbf{i}_2	$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2
\mathbf{i}_2	\mathbf{i}_1	\mathbf{i}_3	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}
\mathbf{i}_3	\mathbf{i}_2	\mathbf{i}_1	\mathbf{r}	\mathbf{r}^2	$\mathbf{1}$

D_3 global $g\mathbf{g}^\dagger$ -table

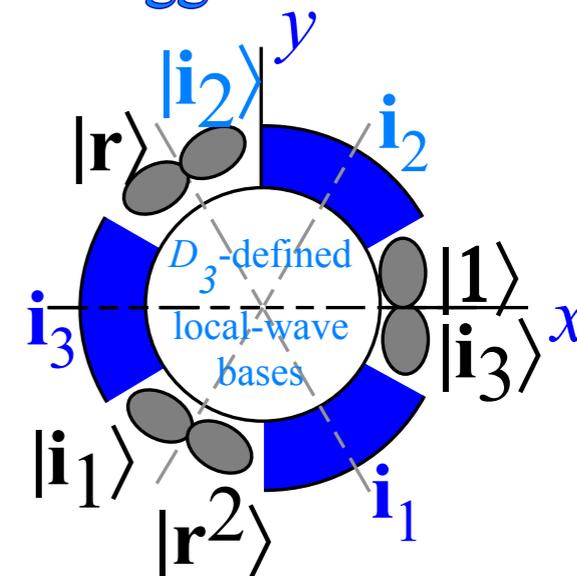
RESULT:

Any $R(\mathbf{T})$

commute (Even if \mathbf{T} and \mathbf{U} do not...)

with any $R(\bar{\mathbf{U}})$...

...and $\mathbf{T} \cdot \mathbf{U} = \mathbf{V}$ if & only if $\bar{\mathbf{T}} \cdot \bar{\mathbf{U}} = \bar{\mathbf{V}}$.



D_3 local $\mathbf{g}^\dagger \mathbf{g}$ -table

To represent *internal* $\{.. \bar{\mathbf{T}}, \bar{\mathbf{U}}, \bar{\mathbf{V}}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on side of group table

$$\begin{aligned}
 R^G(\bar{\mathbf{1}}) &= \begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & 1 \end{pmatrix} &
 R^G(\bar{\mathbf{r}}) &= \begin{pmatrix} & & \mathbf{1} & & & \\ \mathbf{1} & & & & & \\ & \mathbf{1} & & & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \end{pmatrix} &
 R^G(\bar{\mathbf{r}}^2) &= \begin{pmatrix} & \mathbf{1} & & & & \\ & & \mathbf{1} & & & \\ \mathbf{1} & & & & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \end{pmatrix} &
 R^G(\bar{\mathbf{i}}_1) &= \begin{pmatrix} & & & \mathbf{1} & & \\ & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ \mathbf{1} & & & & & \\ & \mathbf{1} & & & & \\ & & \mathbf{1} & & & \end{pmatrix} &
 R^G(\bar{\mathbf{i}}_2) &= \begin{pmatrix} & & & & \mathbf{1} & \\ & & & & & \mathbf{1} \\ & & & & & \mathbf{1} \\ & & & \mathbf{1} & & \\ & & \mathbf{1} & & & \\ & \mathbf{1} & & & & \end{pmatrix} &
 R^G(\bar{\mathbf{i}}_3) &= \begin{pmatrix} & & & & & \mathbf{1} \\ & & & & \mathbf{1} & \\ & & & \mathbf{1} & & \\ & & \mathbf{1} & & & \\ & \mathbf{1} & & & & \\ \mathbf{1} & & & & & \end{pmatrix}
 \end{aligned}$$

$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2	\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3
\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}	\mathbf{i}_2	\mathbf{i}_3	\mathbf{i}_1
\mathbf{r}	\mathbf{r}^2	$\mathbf{1}$	\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2
\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3	$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2
\mathbf{i}_2	\mathbf{i}_3	\mathbf{i}_1	\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}
\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2	\mathbf{r}	\mathbf{r}^2	$\mathbf{1}$

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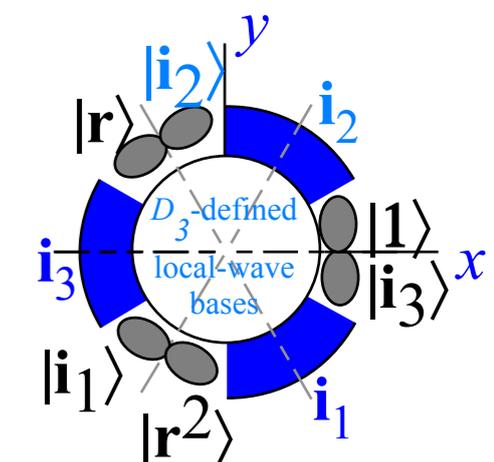
*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Example of RELATIVITY-DUALITY for $D_3 \sim C_{3v}$

To represent *external* $\{.. \mathbf{T}, \mathbf{U}, \mathbf{V}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on top of group table

$$\begin{matrix}
 R^G(\mathbf{1}) = & R^G(\mathbf{r}) = & R^G(\mathbf{r}^2) = & R^G(\mathbf{i}_1) = & R^G(\mathbf{i}_2) = & R^G(\mathbf{i}_3) = \\
 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$

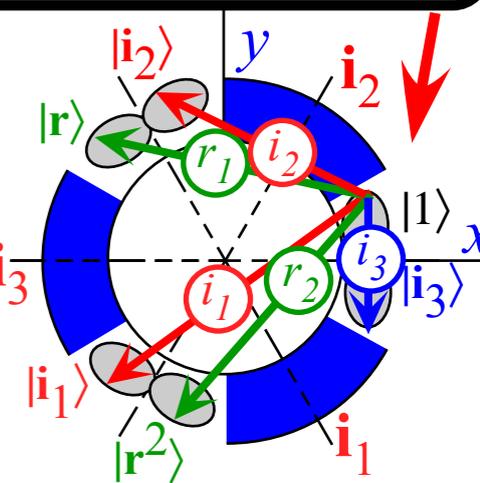


Local \mathbb{H} matrix parametrized by $\bar{\mathbf{g}}$'s

RESULT:
Any $R(\mathbf{T})$ commute (Even if \mathbf{T} and \mathbf{U} do not...)
with any $R(\bar{\mathbf{U}})$...
...and $\mathbf{T} \cdot \mathbf{U} = \mathbf{V}$ if & only if $\bar{\mathbf{T}} \cdot \bar{\mathbf{U}} = \bar{\mathbf{V}}$.

So an \mathbb{H} -matrix having *Global* symmetry D_3
 $\mathbb{H} = H\mathbf{1}^0 + r_1\bar{\mathbf{r}}^1 + r_2\bar{\mathbf{r}}^2 + i_1\bar{\mathbf{i}}_1 + i_2\bar{\mathbf{i}}_2 + i_3\bar{\mathbf{i}}_3$
is made from *Local* symmetry matrices

$$\begin{aligned}
 H &= \langle 1 | \mathbb{H} | 1 \rangle = H^* \\
 r_1 &= \langle \mathbf{r} | \mathbb{H} | 1 \rangle = r_2^* \\
 r_2 &= \langle \mathbf{r}^2 | \mathbb{H} | 1 \rangle = r_1^* \\
 i_1 &= \langle \mathbf{i}_1 | \mathbb{H} | 1 \rangle = i_1^* \\
 i_2 &= \langle \mathbf{i}_2 | \mathbb{H} | 1 \rangle = i_2^* \\
 i_3 &= \langle \mathbf{i}_3 | \mathbb{H} | 1 \rangle = i_3^*
 \end{aligned}$$



To represent *internal* $\{.. \bar{\mathbf{T}}, \bar{\mathbf{U}}, \bar{\mathbf{V}}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on side of group table

$$\begin{matrix}
 R^G(\bar{\mathbf{1}}) = & R^G(\bar{\mathbf{r}}) = & R^G(\bar{\mathbf{r}}^2) = & R^G(\bar{\mathbf{i}}_1) = & R^G(\bar{\mathbf{i}}_2) = & R^G(\bar{\mathbf{i}}_3) = \\
 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} &
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$

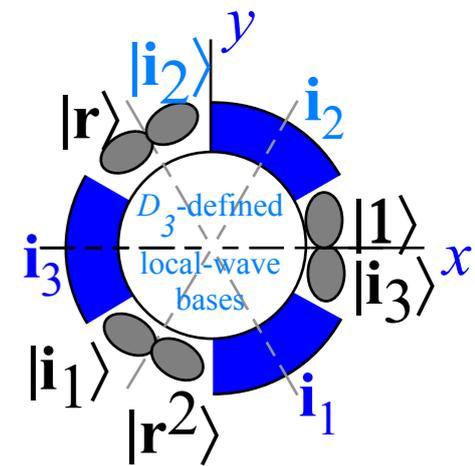
local D_3 defined Hamiltonian matrix

$$\mathbb{H} = \begin{matrix} & |1\rangle & |\mathbf{r}\rangle & |\mathbf{r}^2\rangle & |\mathbf{i}_1\rangle & |\mathbf{i}_2\rangle & |\mathbf{i}_3\rangle \\ \begin{matrix} \langle 1| \\ \langle \mathbf{r}| \\ \langle \mathbf{r}^2| \\ \langle \mathbf{i}_1| \\ \langle \mathbf{i}_2| \\ \langle \mathbf{i}_3| \end{matrix} & \begin{matrix} H \\ r_2 \\ r_1 \\ H \\ r_1 \\ r_2 \end{matrix} & \begin{matrix} r_1 \\ H \\ r_2 \\ i_2 \\ H \\ i_1 \end{matrix} & \begin{matrix} r_2 \\ r_1 \\ H \\ i_3 \\ i_1 \\ H \end{matrix} & \begin{matrix} i_1 \\ i_2 \\ i_3 \\ H \\ r_1 \\ r_2 \end{matrix} & \begin{matrix} i_2 \\ i_3 \\ i_1 \\ r_2 \\ H \\ r_1 \end{matrix} & \begin{matrix} i_3 \\ i_1 \\ i_2 \\ r_1 \\ r_2 \\ H \end{matrix} \end{matrix}$$

Example of RELATIVITY-DUALITY for $D_3 \sim C_{3v}$

To represent *external* $\{.. \mathbf{T}, \mathbf{U}, \mathbf{V}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on top of group table

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 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$



Local \mathbb{H} matrix parametrized by $\bar{\mathbf{g}}$'s

RESULT:

Any $R(\mathbf{T})$

commute (Even if \mathbf{T} and \mathbf{U} do not...)

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...and $\mathbf{T} \cdot \mathbf{U} = \mathbf{V}$ if & only if $\bar{\mathbf{T}} \cdot \bar{\mathbf{U}} = \bar{\mathbf{V}}$.

So an \mathbb{H} -matrix

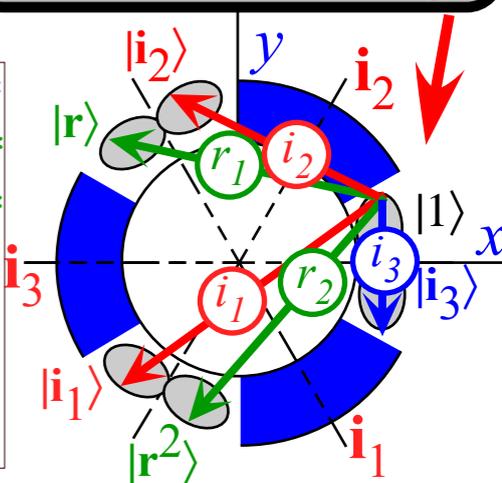
having *Global* symmetry D_3

$$\mathbb{H} = H\mathbf{1}^0 + r_1\bar{\mathbf{r}}^1 + r_2\bar{\mathbf{r}}^2 + i_1\bar{\mathbf{i}}_1 + i_2\bar{\mathbf{i}}_2 + i_3\bar{\mathbf{i}}_3$$

is made from

Local symmetry matrices

$$\begin{aligned}
 H &= \langle 1 | \mathbb{H} | 1 \rangle = H^* \\
 r_1 &= \langle r | \mathbb{H} | 1 \rangle = r_2^* \\
 r_2 &= \langle r^2 | \mathbb{H} | 1 \rangle = r_1^* \\
 i_1 &= \langle i_1 | \mathbb{H} | 1 \rangle = i_1^* \\
 i_2 &= \langle i_2 | \mathbb{H} | 1 \rangle = i_2^* \\
 i_3 &= \langle i_3 | \mathbb{H} | 1 \rangle = i_3^*
 \end{aligned}$$



All the global \mathbf{g} commute with general *local* \mathbb{H} matrix.

To represent *internal* $\{.. \bar{\mathbf{T}}, \bar{\mathbf{U}}, \bar{\mathbf{V}}, ... \}$ switch $\mathbf{g} \leftrightarrow \mathbf{g}^\dagger$ on side of group table

$$\begin{matrix}
 R^G(\bar{\mathbf{1}}) = & R^G(\bar{\mathbf{r}}) = & R^G(\bar{\mathbf{r}}^2) = & R^G(\bar{\mathbf{i}}_1) = & R^G(\bar{\mathbf{i}}_2) = & R^G(\bar{\mathbf{i}}_3) = \\
 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$

local D_3 defined Hamiltonian matrix

$$\mathbb{H} = \begin{matrix} & |1\rangle & |r\rangle & |r^2\rangle & |i_1\rangle & |i_2\rangle & |i_3\rangle \\ \begin{matrix} \langle 1| \\ \langle r| \\ \langle r^2| \\ \langle i_1| \\ \langle i_2| \\ \langle i_3| \end{matrix} & \begin{matrix} H & r_1 & r_2 & i_1 & i_2 & i_3 \\ r_2 & H & r_1 & i_2 & i_3 & i_1 \\ r_1 & r_2 & H & i_3 & i_1 & i_2 \\ i_1 & i_1 & i_2 & i_3 & H & r_1 & r_2 \\ i_2 & i_2 & i_3 & i_2 & r_2 & H & r_1 \\ i_3 & i_3 & i_1 & i_2 & r_1 & r_2 & H \end{matrix} \end{matrix}$$

Example of RELATIVITY-DUALITY for D

To represent *external* $\{..T, U, V, ... \}$...

$$R^G(\mathbf{1}) = \begin{pmatrix} 1 & \dots & \dots & \dots & \dots \\ \dots & 1 & \dots & \dots & \dots \\ \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & 1 \end{pmatrix}, \quad R^G(\mathbf{r}) = \begin{pmatrix} \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & \dots & 1 \end{pmatrix}, \quad R^G(\mathbf{r}^2) = \begin{pmatrix} \dots & \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & 1 \end{pmatrix}, \quad R^G(\mathbf{i}_1) = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & 1 \\ \dots & 1 \\ \dots & 1 \\ \dots & 1 \end{pmatrix}$$

$$H = \langle \mathbf{1} | \mathbf{H} | \mathbf{1} \rangle = H^*$$

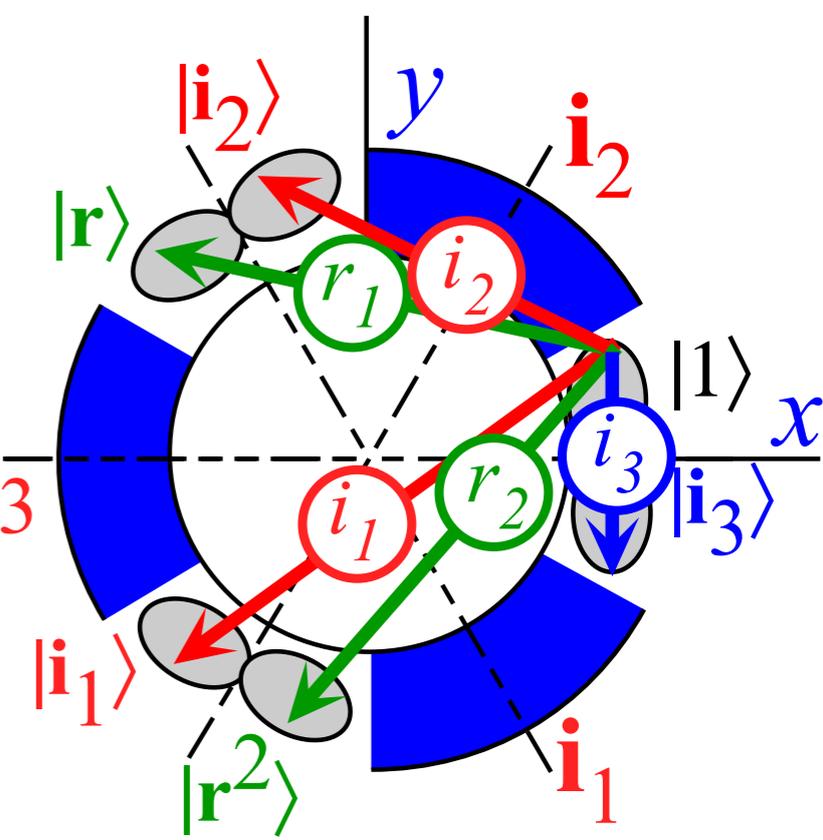
$$r_1 = \langle \mathbf{r} | \mathbf{H} | \mathbf{1} \rangle = r_2^*$$

$$r_2 = \langle \mathbf{r}^2 | \mathbf{H} | \mathbf{1} \rangle = r_1^*$$

$$i_1 = \langle \mathbf{i}_1 | \mathbf{H} | \mathbf{1} \rangle = i_1^*$$

$$i_2 = \langle \mathbf{i}_2 | \mathbf{H} | \mathbf{1} \rangle = i_2^*$$

$$i_3 = \langle \mathbf{i}_3 | \mathbf{H} | \mathbf{1} \rangle = i_3^*$$



RESULT:

Any $R(\mathbf{T})$ *commute* (Even if \mathbf{T} and \mathbf{U} do not...) with any $R(\bar{\mathbf{U}})$...
 ...and $\mathbf{T} \cdot \mathbf{U} = \mathbf{V}$ if & only if $\bar{\mathbf{T}} \cdot \bar{\mathbf{U}} = \bar{\mathbf{V}}$.

So an \mathbf{H} -matrix having *Global* symmetry D_3

$$\mathbf{H} = H\mathbf{1}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + i_1\mathbf{i}_1 + i_2\mathbf{i}_2 + i_3\mathbf{i}_3$$

is made from *Local* symmetry matrices

local-D -defined Hamiltonian matrix

$$\mathbf{H} = \begin{matrix} & | \mathbf{1} \rangle & | \mathbf{r} \rangle & | \mathbf{r}^2 \rangle & | \mathbf{i}_1 \rangle & | \mathbf{i}_2 \rangle & | \mathbf{i}_3 \rangle \\ \begin{matrix} (\mathbf{1} | \\ (\mathbf{r} | \\ (\mathbf{r}^2 | \\ (\mathbf{i}_1 | \\ (\mathbf{i}_2 | \\ (\mathbf{i}_3 | \end{matrix} & \begin{matrix} H & r_1 & r_2 & i_1 & i_2 & i_3 \\ r_2 & H & r_1 & i_2 & i_3 & i_1 \\ r_1 & r_2 & H & i_3 & i_1 & i_2 \\ H & r_1 & r_2 & i_1 & i_2 & i_3 \\ r_2 & H & r_1 & i_2 & i_3 & i_1 \\ r_1 & r_2 & H & i_3 & i_1 & i_2 \end{matrix} \end{matrix}$$

To represent *internal* $\{..T, U, V, ... \}$

$$R^G(\bar{\mathbf{1}}) = \begin{pmatrix} 1 & \dots & \dots & \dots & \dots \\ \dots & 1 & \dots & \dots & \dots \\ \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & 1 \end{pmatrix}, \quad R^G(\bar{\mathbf{r}}) = \begin{pmatrix} \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & \dots & 1 \end{pmatrix}, \quad R^G(\bar{\mathbf{r}}^2) = \begin{pmatrix} \dots & \dots & \dots & 1 & \dots & \dots \\ \dots & \dots & \dots & \dots & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & 1 \end{pmatrix}, \quad R^G(\bar{\mathbf{i}}_1) = \begin{pmatrix} \dots & \dots & \dots & \dots & \dots & \dots & 1 \\ \dots & 1 \\ \dots & 1 \\ \dots & 1 \\ \dots & 1 \end{pmatrix}$$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

By nomograms based on $U(2)$ Hamilton-turns

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

➔ All-commuting operators and D_3 -invariant class algebra ←

All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Spectral analysis of non-commutative “Group-table Hamiltonian”

1st Step: Spectral resolution of D_3 -Center (Class algebra of D_3)

1	r¹	r²	i₁	i₂	i₃
r²	1	r¹	i₂	i₃	i₁
r¹	r²	1	i₃	i₁	i₂
i₁	i₂	i₃	1	r¹	r²
i₂	i₃	i₁	r²	1	r¹
i₃	i₁	i₂	r¹	r²	1

Spectral analysis of non-commutative “Group-table Hamiltonian”

1st Step: Spectral resolution of D_3 -Center (Class algebra of D_3)

1	r¹	r²	i₁	i₂	i₃
r²	1	r¹	i₂	i₃	i₁
r¹	r²	1	i₃	i₁	i₂
i₁	i₂	i₃	1	r¹	r²
i₂	i₃	i₁	r²	1	r¹
i₃	i₁	i₂	r¹	r²	1

Each class-sum $\underline{\kappa}_k$ commutes with all of D_3 .

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

κ_g 's are *mutually commuting* with respect to themselves and *all-commuting* with respect to the whole group.

$$\mathbf{r} \kappa_i \mathbf{r}^{-1} = \mathbf{i}_2 + \mathbf{i}_3 + \mathbf{i}_1 = \kappa_i \quad \text{or:} \quad \mathbf{r} \kappa_i = \kappa_i \mathbf{r}$$

$$\sum_{\mathbf{h}=1}^{\circ G} \mathbf{h} \mathbf{g} \mathbf{h}^{-1} = v_g \kappa_g, \quad \text{where: } v_g = \frac{\circ G}{\circ \kappa_g} = \text{integer}$$

$\circ \kappa_g$ is order of class κ_g and must evenly divide group order $\circ G$.

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1	r¹	r²	i₁	i₂	i₃
r²	1	r¹	i₂	i₃	i₁
r¹	r²	1	i₃	i₁	i₂
i₁	i₂	i₃	1	r¹	r²
i₂	i₃	i₁	r²	1	r¹
i₃	i₁	i₂	r¹	r²	1

Each class-sum $\underline{\kappa}_k$ commutes with all of D_3 .

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

$$\kappa_3^2 = 3 \cdot \kappa_2 + 3 \cdot \mathbf{1}$$

Note also:

$$\kappa_2^2 - \kappa_2 - 2 \cdot \mathbf{1} = 0$$

Spectral analysis of non-commutative “Group-table Hamiltonian”

1st Step: Spectral resolution of D_3 -Center (Class algebra of D_3)

1	r¹	r²	i₁	i₂	i₃
r²	1	r¹	i₂	i₃	i₁
r¹	r²	1	i₃	i₁	i₂
i₁	i₂	i₃	1	r¹	r²
i₂	i₃	i₁	r²	1	r¹
i₃	i₁	i₂	r¹	r²	1

Each class-sum $\underline{\kappa}_k$ commutes with all of D_3 .

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

Class products give spectral polynomial and all-commuting projectors $\mathbf{P}^{(\alpha)}$

$$\leftarrow \kappa_3^2 = 3 \cdot \kappa_2 + 3 \cdot \mathbf{1}$$

Note also:

$$\kappa_2^2 - \kappa_2 - 2 \cdot \mathbf{1} = 0$$

$$0 = (\kappa_2 - 2 \cdot \mathbf{1})(\kappa_2 + \mathbf{1})$$

$$0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 + 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})$$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

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By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

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Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

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Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Stage spectral decomposition of global/local D_3 Hamiltonian

All-commuting operators and D_3 -invariant class algebra

➔ All-commuting projectors and D_3 -invariant characters ←

Group invariant numbers: Centrum, Rank, and Order

*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Spectral analysis of non-commutative “Group-table Hamiltonian”

1st Step: Spectral resolution of D_3 -Center (Class algebra of D_3)

1	r¹	r²	i₁	i₂	i₃
r²	1	r¹	i₂	i₃	i₁
r¹	r²	1	i₃	i₁	i₂
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Class products give spectral polynomial and all-commuting projectors $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, \mathbf{P}^{A_2} , and \mathbf{P}^E

Note also: $0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 + 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})$

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Spectral analysis of non-commutative “Group-table Hamiltonian”

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$$\mathbf{P}^E = \frac{(\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 + 3 \cdot \mathbf{1})}{(+0 - 3)(+0 + 3)}$$

Spectral analysis of non-commutative “Group-table Hamiltonian”

1st Step: Spectral resolution of D_3 -Center (Class algebra of D_3)

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Class resolution into sum of eigenvalue · Projector

$$\kappa_1 = 1 \cdot \mathbf{P}^{A_1} + 1 \cdot \mathbf{P}^{A_2} + 1 \cdot \mathbf{P}^E$$

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Note also:

$$\kappa_2^2 - \kappa_2 - 2 \cdot \mathbf{1} = 0$$

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$$0 = (\kappa_3 - 0 \cdot \mathbf{1})\mathbf{P}^E$$

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$$\kappa_1 = 1 \cdot \mathbf{P}^{A_1} + 1 \cdot \mathbf{P}^{A_2} + 1 \cdot \mathbf{P}^E$$

$$\kappa_2 = 2 \cdot \mathbf{P}^{A_1} - 2 \cdot \mathbf{P}^{A_2} - 1 \cdot \mathbf{P}^E$$

$$\kappa_3 = 3 \cdot \mathbf{P}^{A_1} - 3 \cdot \mathbf{P}^{A_2} + 0 \cdot \mathbf{P}^E$$

Inverse resolution gives D_3 Character Table

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3)/6$$

$$\mathbf{P}^E = (2\kappa_1 - \kappa_2 + 0)/3 = (2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)/3$$

$$\mathbf{P}^{A_1} = \frac{(\kappa_3 + 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})}{(+3 + 3)(+3 - 0)}$$

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χ_k^α	χ_1^α	χ_2^α	χ_3^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

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$$\mathbf{P}^E = \frac{(\kappa_3 - 3 \cdot 1)(\kappa_3 + 3 \cdot 1)}{(+0 - 3)(+0 + 3)}$$

Irreducible characters are traces of irreducible representations $D^{(\alpha)}(\mathbf{r}_\kappa)$

χ_k^α	χ_1^α	χ_2^α	χ_3^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

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Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Step in spectral analysis of D_3 “group-table” Hamiltonian: Algebra of D_3 Center (Classes)

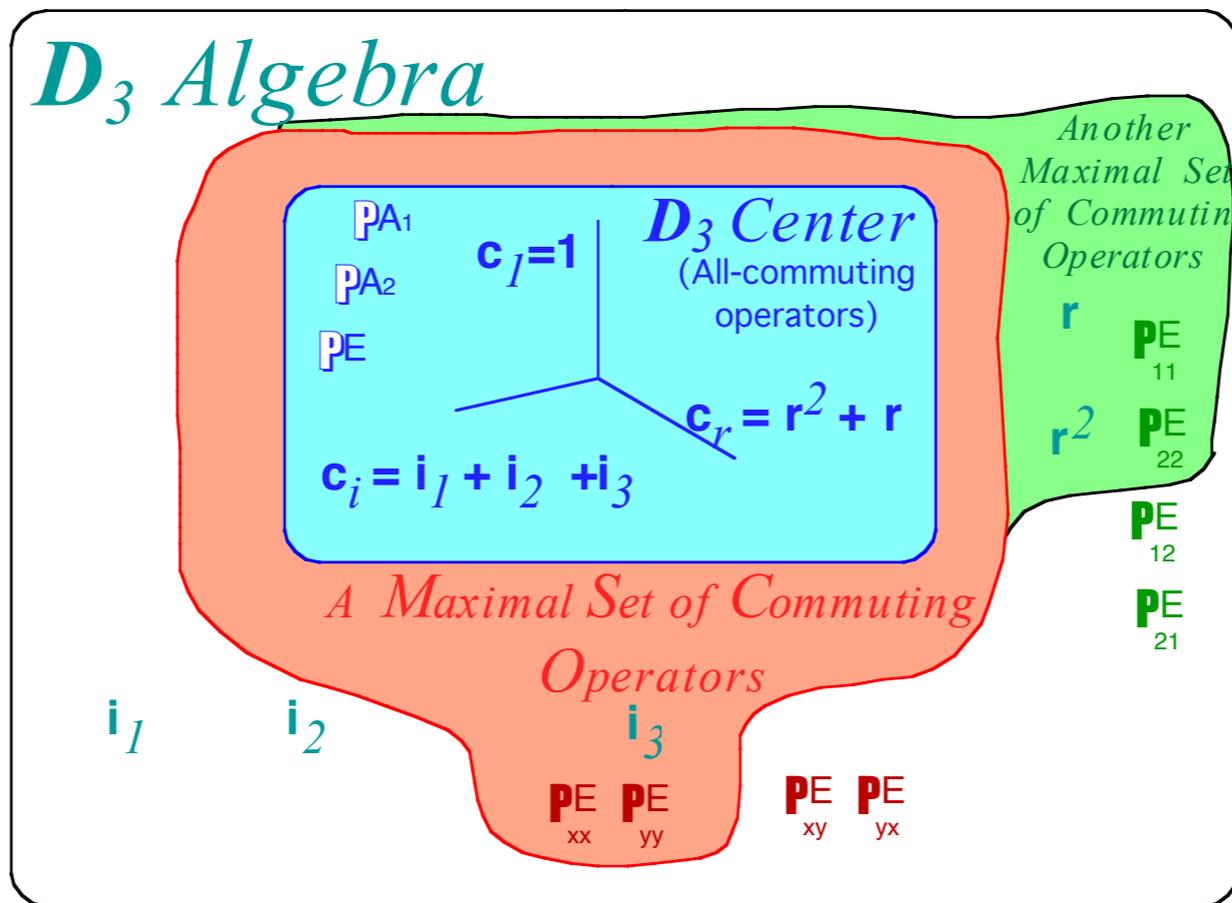
All-commuting operators and D_3 -invariant class algebra

All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order

*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting



(Fig. 15.2.1 QTCA)

Important invariant numbers or “characters”

ℓ^α = Irreducible representation (irrep) *dimension* or level *degeneracy*
For symmetry group or algebra G

Centrum: $\kappa(G) = \sum_{irrep(\alpha)} (\ell^\alpha)^0$ = Number of classes, invariants, irrep types, *all-commuting* ops

Rank: $\rho(G) = \sum_{irrep(\alpha)} (\ell^\alpha)^1$ = Number of irrep idempotents $\mathbf{P}_{n,n}^{(\alpha)}$, *mutually-commuting* ops

Order: $o(G) = \sum_{irrep(\alpha)} (\ell^\alpha)^2$ = *Total* number of irrep projectors $\mathbf{P}_{m,n}^{(\alpha)}$ or symmetry ops

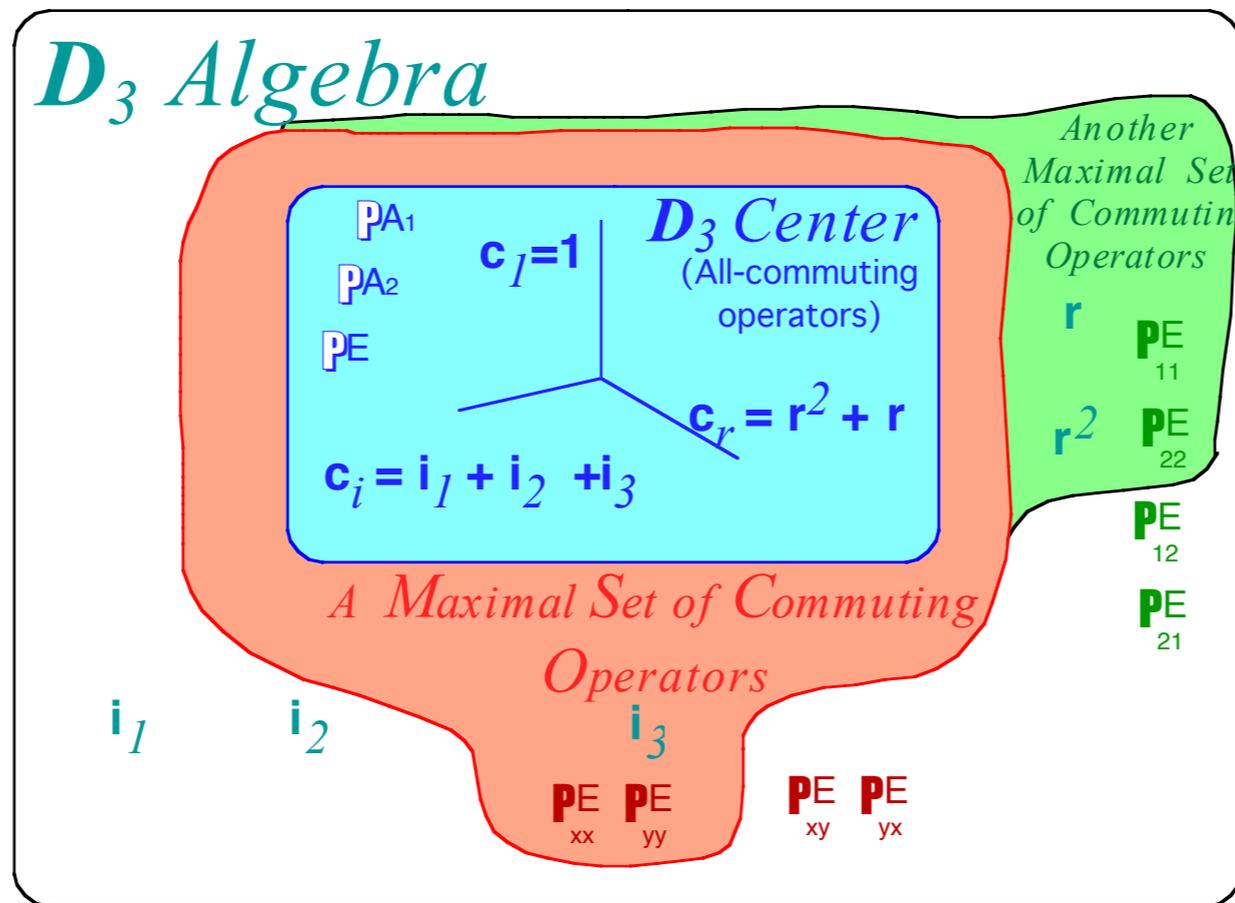
$$D_3 \quad \kappa = \boxed{1} \quad \boxed{r^1+r^2} \quad \boxed{i_1+i_2+i_3}$$

$$\mathbf{P}^{A_1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \end{bmatrix} / 6$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \end{bmatrix} / 6$$

$$\mathbf{P}^E = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \end{bmatrix} / 3$$

D_3 Algebra



Important invariant numbers or “characters”

ℓ^α = Irreducible representation (irrep) *dimension* or level *degeneracy*
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$$D_3 \quad \kappa = \boxed{1} \quad \boxed{r^1+r^2} \quad \boxed{i_1+i_2+i_3}$$

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$$\mathbf{P}^E = \begin{bmatrix} 2 & -1 & 0 \end{bmatrix} / 3$$

$$\kappa(D_3) = (1)^0 + (1)^0 + (2)^0 = 3$$

$$\rho(D_3) = (1)^1 + (1)^1 + (2)^1 = 4$$

$$\circ(D_3) = (1)^2 + (1)^2 + (2)^2 = 6$$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

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1st-Step in spectral analysis of D_3 “group-table” Hamiltonian: Algebra of D_3 Center (Classes)

All-commuting operators and D_3 -invariant class algebra

All-commuting projectors and D_3 -invariant characters

Group invariant numbers: Centrum, Rank, and Order



*Spectral resolution to **irreducible representations** (or “**irreps**”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

*Spectral resolution to irreducible representations (or “irreps”) foretold by **characters** or traces*

$$\begin{array}{c}
 R^G(\mathbf{1})= \\
 R^G(\mathbf{r})= \\
 R^G(\mathbf{r}^2)= \\
 R^G(\mathbf{i}_1)= \\
 R^G(\mathbf{i}_2)= \\
 R^G(\mathbf{i}_3)=
 \end{array}
 \begin{array}{c}
 \left(\begin{array}{cccccc}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{array} \right)
 \left(\begin{array}{cccccc}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{array} \right)
 \end{array}$$

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1}) = \left(\begin{array}{cccccc}
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1 \\
 1 & 1 & 1 & 1 & 1 & 1
 \end{array} \right) / 6 \quad \text{Trace}R(\mathbf{P}^{A_1}) = 1$$

*Spectral resolution to irreducible representations (or “irreps”) is foretold by **characters** or traces*

$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 r^1 \\
 r^2 \\
 i_1 \\
 i_2 \\
 i_3
 \end{array}
 \begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1}) = \frac{1}{6} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \quad \text{Trace} R(\mathbf{P}^{A_1}) = 1$$

So: $R(\mathbf{P}^{A_1})$ reduces to:

$$\begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$$\mathbf{P}^{A_2} = (\kappa_1 + \kappa_2 - \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_2}) = \frac{1}{6} \begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix} \quad \text{Trace} R(\mathbf{P}^{A_2}) = 1$$

So: $R(\mathbf{P}^{A_2})$ reduces to:

$$\begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

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$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 r^1 \\
 r^2 \\
 i_1 \\
 i_2 \\
 i_3
 \end{array}
 \begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1}) = \frac{1}{6} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \quad \text{Trace} R(\mathbf{P}^{A_1}) = 1$$

So: $R(\mathbf{P}^{A_1})$ reduces to:

$$\begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

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So: $R(\mathbf{P}^{A_2})$ reduces to:

$$\begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$$\mathbf{P}^E = (2\kappa_1 - \kappa_2 + 0)/3 = (2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + 0 + 0 + 0)/3 \Rightarrow R(\mathbf{P}^E) = \frac{1}{3} \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix} \quad \text{Trace} R(\mathbf{P}^E) = 4$$

So: $R(\mathbf{P}^E)$ reduces to:

$$\begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix}$$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

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Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

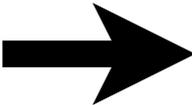
Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Step in spectral analysis of D_3 “group-table” Hamiltonian: Algebra of D_3 Center (Classes)

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$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 R^G(\mathbf{r}) = \\
 R^G(\mathbf{r}^2) = \\
 R^G(\mathbf{i}_1) = \\
 R^G(\mathbf{i}_2) = \\
 R^G(\mathbf{i}_3) =
 \end{array}
 \begin{array}{c}
 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},
 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix},
 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix},
 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix},
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix},
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{array}$$

$$R(\mathbf{P}^{A_1}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} / 6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_1}) = 1 \quad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to: } \begin{pmatrix} D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$R(\mathbf{P}^{A_2}) = \begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix} / 6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_2}) = 1$$

$$R(\mathbf{P}^E) = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix} / 3 \Rightarrow \text{Trace}R(\mathbf{P}^E) = 4$$

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$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 R^G(\mathbf{r}) = \\
 R^G(\mathbf{r}^2) = \\
 R^G(\mathbf{i}_1) = \\
 R^G(\mathbf{i}_2) = \\
 R^G(\mathbf{i}_3) =
 \end{array}
 \begin{array}{c}
 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}
 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}
 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix}
 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix}
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{array}$$

$$R(\mathbf{P}^{A_1}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} /6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_1}) = 1 \quad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to: } \begin{pmatrix} D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$R(\mathbf{P}^{A_2}) = \begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix} /6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_2}) = 1 \quad \text{So: } R(\mathbf{P}^{A_2}\mathbf{g}) \text{ reduces to: } \begin{pmatrix} D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$R(\mathbf{P}^E) = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix} /3 \Rightarrow \text{Trace}R(\mathbf{P}^E) = 4$$

*Spectral resolution to irreducible representations (or “irreps”) is foretold by **characters** or traces*

$$\begin{array}{c}
 R^G(\mathbf{1})= \\
 r^1 \\
 r^2 \\
 i_1 \\
 i_2 \\
 i_3
 \end{array}
 \begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r})= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}^2)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_1)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_2)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_3)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$$R(\mathbf{P}^{A_1}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} /6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_1}) = 1 \quad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to: } \begin{pmatrix} D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$R(\mathbf{P}^{A_2}) = \begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix} /6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_2}) = 1 \quad \text{So: } R(\mathbf{P}^{A_2}\mathbf{g}) \text{ reduces to: } \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$R(\mathbf{P}^E) = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix} /3 \Rightarrow \text{Trace}R(\mathbf{P}^E) = 4 \quad \text{So: } R(\mathbf{P}^E\mathbf{g}) \text{ reduces to: } \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D_{11}^E & D_{12}^E & \cdot & \cdot \\ \cdot & \cdot & D_{21}^E & D_{22}^E & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D_{11}^E & D_{12}^E \\ \cdot & \cdot & \cdot & \cdot & D_{21}^E & D_{22}^E \end{pmatrix}$$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

By nomograms based on $U(2)$ Hamilton-turns

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Step in spectral analysis of D_3 “group-table” Hamiltonian: Algebra of D_3 Center (Classes)

All-commuting operators and D_3 -invariant class algebra

All-commuting projectors and D_3 -invariant characters

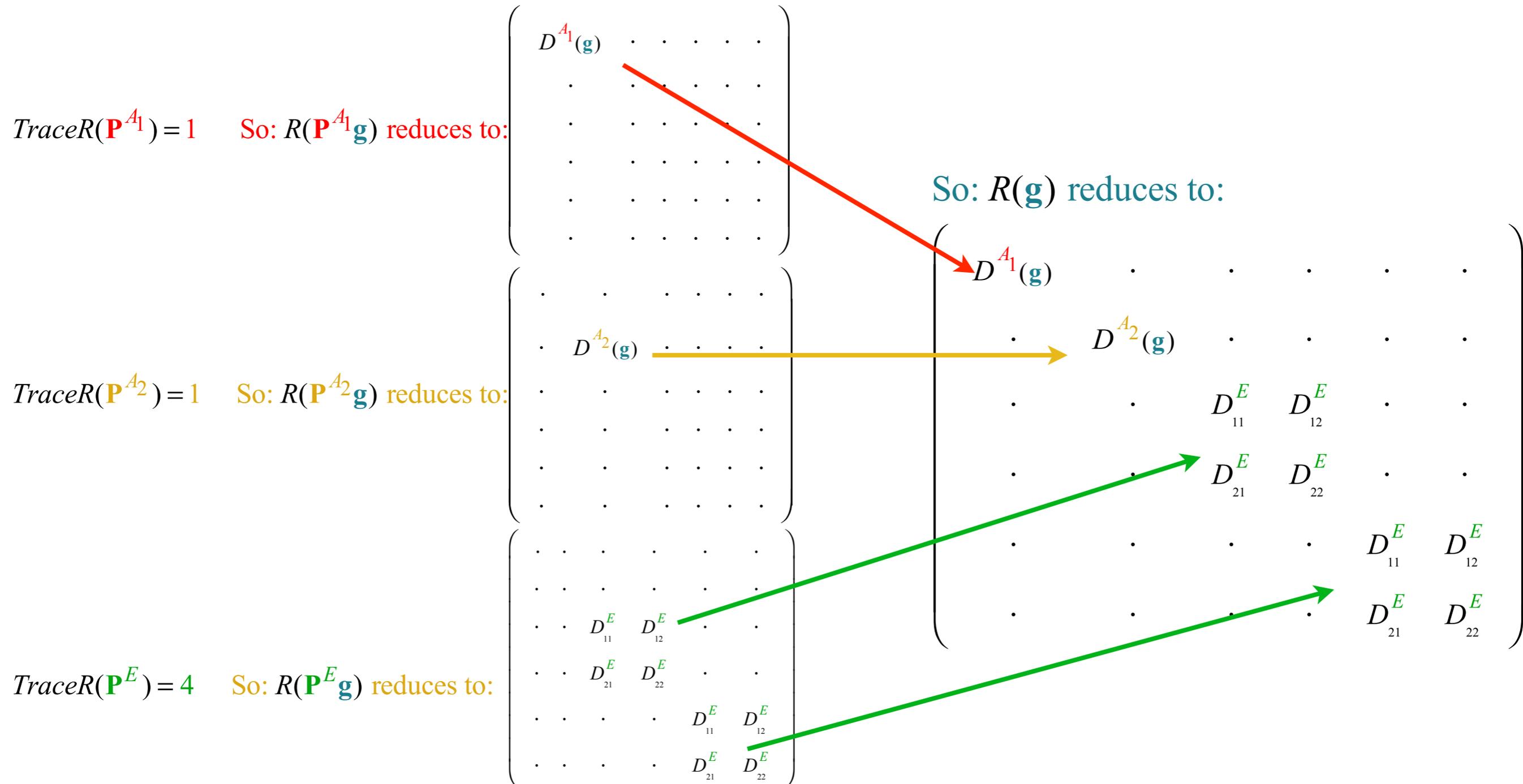
Group invariant numbers: Centrum, Rank, and Order

 *Spectral resolution to **irreducible representations** (or “**irreps**”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

Spectral resolution to irreducible representations (or "irreps") foretold by **characters** or traces

$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 r^1 \\
 r^2 \\
 i_1 \\
 i_2 \\
 i_3
 \end{array}
 \begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$



3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

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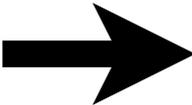
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 *Spectral resolution to **irreducible representations** (or “**irreps**”) foretold by **characters** or traces*

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting 

Spectral resolution to irreducible representations (or “ireps”) foretold by *characters* or *traces*

$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 r^1 \\
 r^2 \\
 i_1 \\
 i_2 \\
 i_3
 \end{array}
 \begin{pmatrix}
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix},
 \begin{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \begin{pmatrix}
 \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
 \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
 \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
 1 & \cdot & \cdot & \cdot & \cdot & \cdot
 \end{pmatrix}$$

$\{R^G(\mathbf{g})\}$ has lots of empty space and looks like it could be reduced.

But, $\{R^G(\mathbf{g})\}$ cannot be diagonalized all-at-once. (Not all \mathbf{g} commute.)

Nevertheless, $\{R^G(\mathbf{g})\}$ can be *block-diagonalized all-at-once* into “ireps” A_1 , A_2 , and E_1

$R(\mathbf{g})$ reduces to:

$$\begin{pmatrix}
 D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\
 \cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\
 \cdot & \cdot & D_{11}^E & D_{12}^E & \cdot & \cdot \\
 \cdot & \cdot & D_{21}^E & D_{22}^E & \cdot & \cdot \\
 \cdot & \cdot & \cdot & \cdot & D_{11}^E & D_{12}^E \\
 \cdot & \cdot & \cdot & \cdot & D_{21}^E & D_{22}^E
 \end{pmatrix}$$

Spectral resolution to irreducible representations (or "ireps") foretold by *characters* or *traces*

$$\begin{matrix}
 R^G(\mathbf{1}) = & R^G(\mathbf{r}) = & R^G(\mathbf{r}^2) = & R^G(\mathbf{i}_1) = & R^G(\mathbf{i}_2) = & R^G(\mathbf{i}_3) = \\
 \begin{matrix} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{matrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$

$\{R^G(\mathbf{g})\}$ has lots of empty space and looks like it could be reduced.

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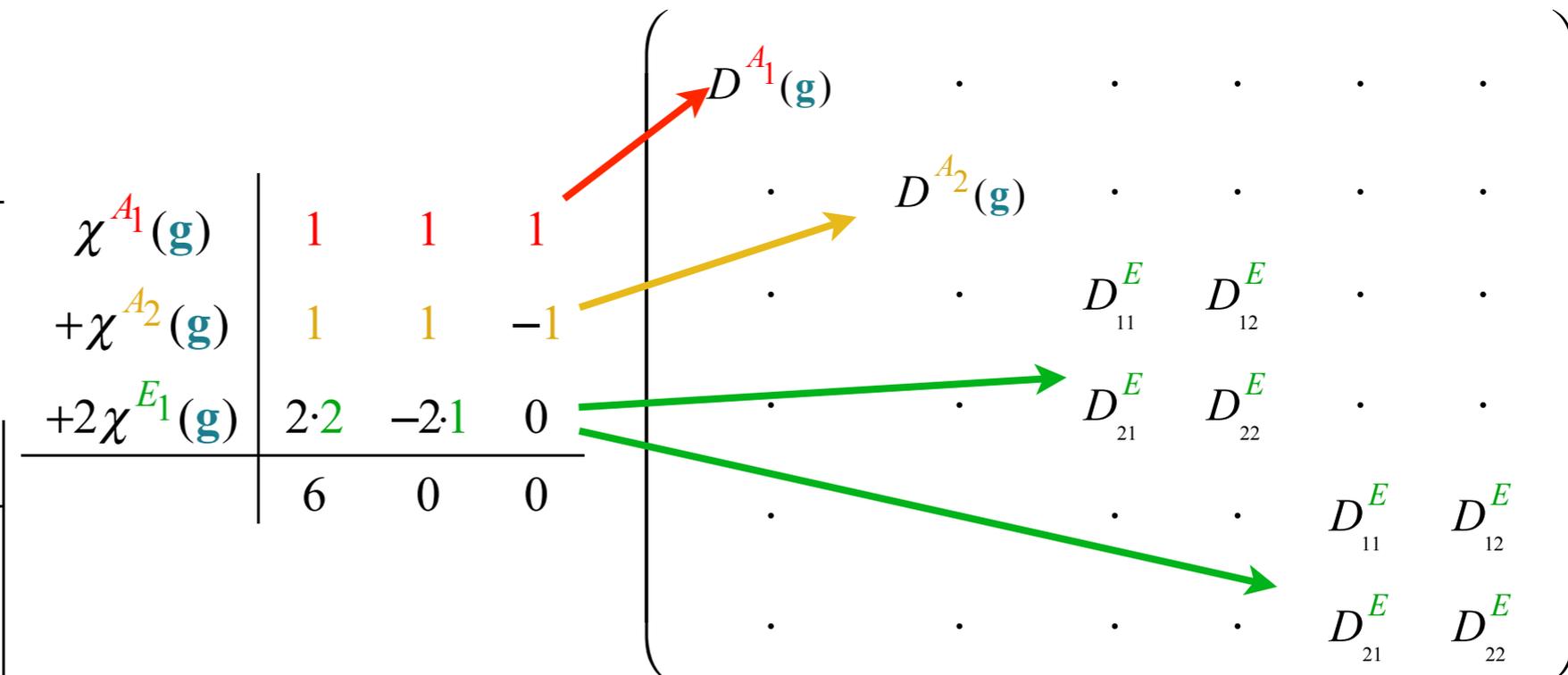
$R(\mathbf{g})$ reduces to:

We relate traces of $\{R^G(\mathbf{g})\}$:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\text{Trace } R^G(\mathbf{g}) =$	6	0	0

to D_3 character table:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0



Spectral resolution to irreducible representations (or "ireps") foretold by characters or traces

$$\begin{matrix}
 R^G(\mathbf{1}) = & R^G(\mathbf{r}) = & R^G(\mathbf{r}^2) = & R^G(\mathbf{i}_1) = & R^G(\mathbf{i}_2) = & R^G(\mathbf{i}_3) = \\
 \begin{matrix} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{matrix} \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} & \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}
 \end{matrix}$$

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Nevertheless, $\{R^G(\mathbf{g})\}$ can be *block-diagonalized all-at-once* into "ireps" A_1 , A_2 , and E_1

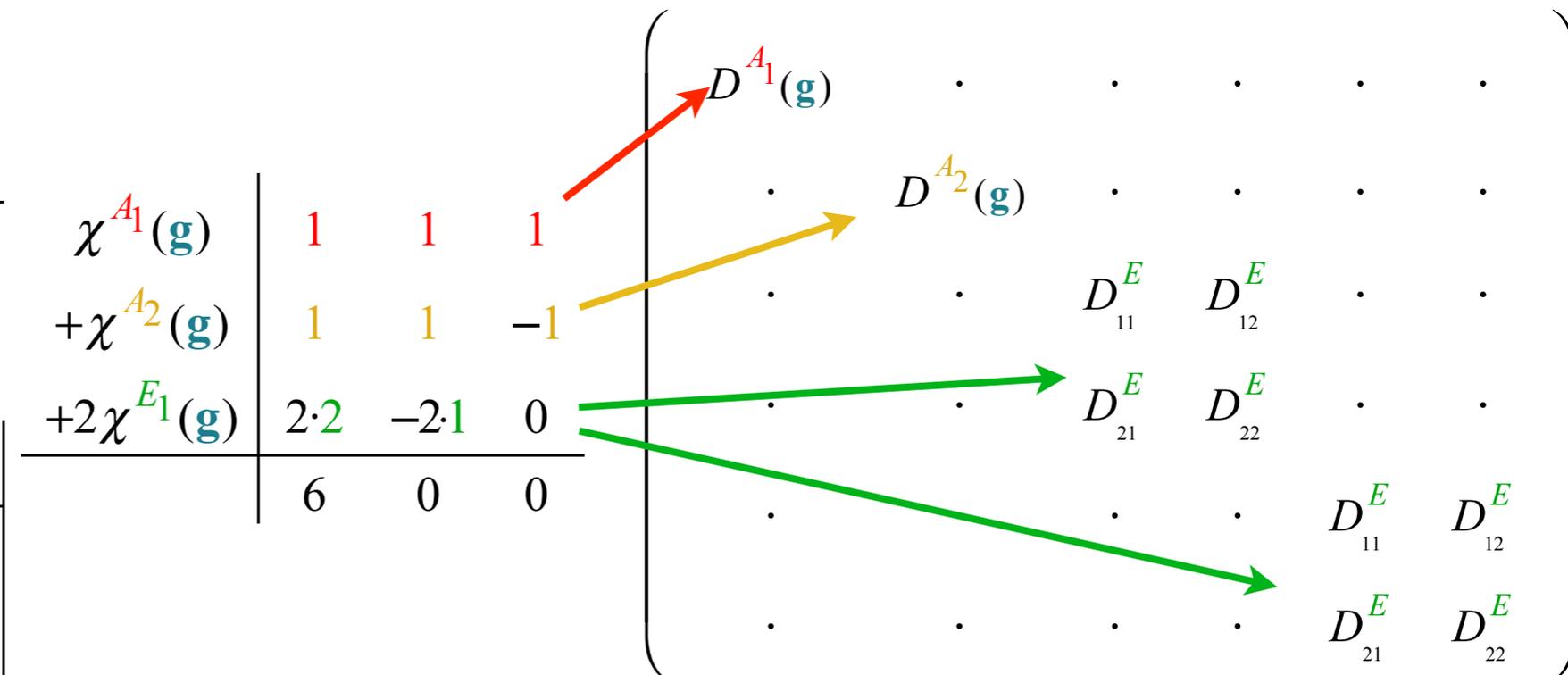
$R(\mathbf{g})$ reduces to:

We relate traces of $\{R^G(\mathbf{g})\}$:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\text{Trace } R^G(\mathbf{g}) =$	6	0	0

to D_3 character table:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0



So $\{R^G(\mathbf{g})\}$ can be *block-diagonalized* into a *direct sum* \oplus of "ireps" $R^G(\mathbf{g}) = D^{A_1}(\mathbf{g}) \oplus D^{A_2}(\mathbf{g}) \oplus 2D^{E_1}(\mathbf{g})$

3-Dihedral-axes group D_3 vs. 3-Vertical-mirror-plane group C_{3v}

D_3 and C_{3v} are isomorphic ($D_3 \sim C_{3v}$ share product table)

Deriving $D_3 \sim C_{3v}$ products:

By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$

By nomograms based on $U(2)$ Hamilton-turns

Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Non-commutative symmetry expansion and Global-Local solution

Global vs Local symmetry and Mock-Mach principle

Global vs Local matrix duality for D_3

Global vs Local symmetry expansion of D_3 Hamiltonian

1st-Step in spectral analysis of D_3 “group-table” Hamiltonian: Algebra of D_3 Center (Classes)

All-commuting operators and D_3 -invariant class algebra

All-commuting projectors and D_3 -invariant characters

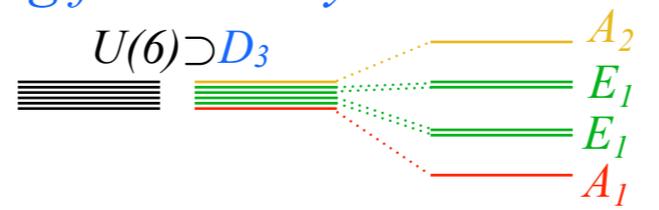
Group invariant numbers: Centrum, Rank, and Order

*Spectral resolution to **irreducible representations** (or “**irreps**”) foretold by **characters** or traces*



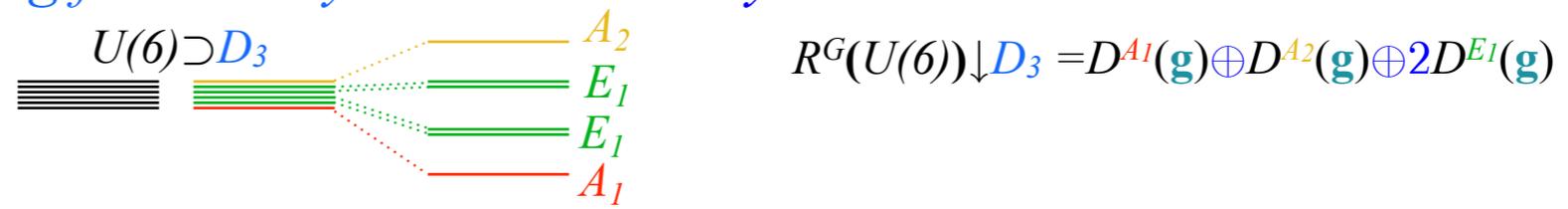
Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^l \downarrow D_3$ splitting

Spectral splitting in symmetry breaking foretold by character analysis

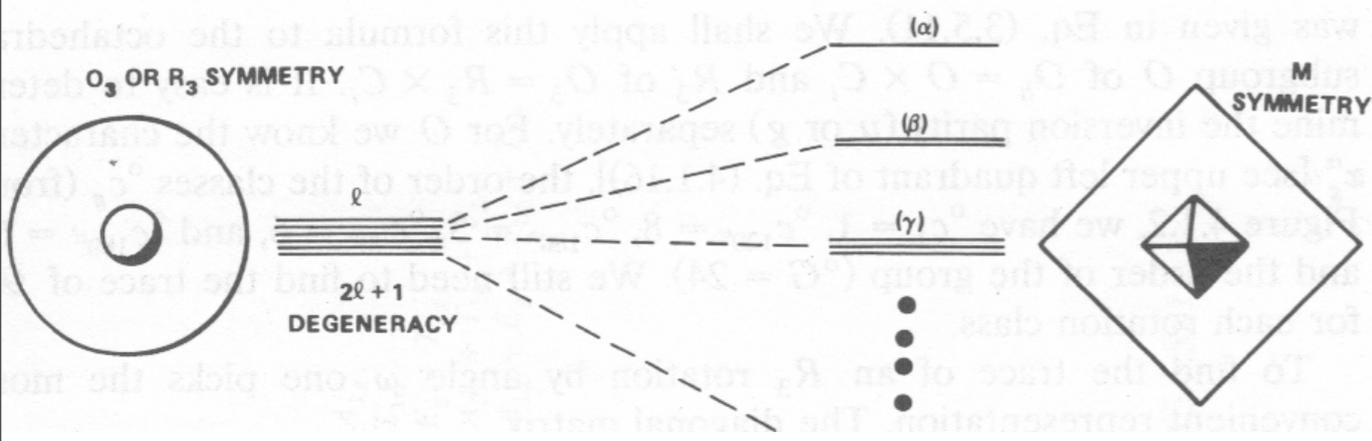


$$R^G(U(6)) \downarrow D_3 = D^{A_1}(\mathfrak{g}) \oplus D^{A_2}(\mathfrak{g}) \oplus 2D^{E_1}(\mathfrak{g})$$

Spectral splitting in symmetry breaking foretold by character analysis



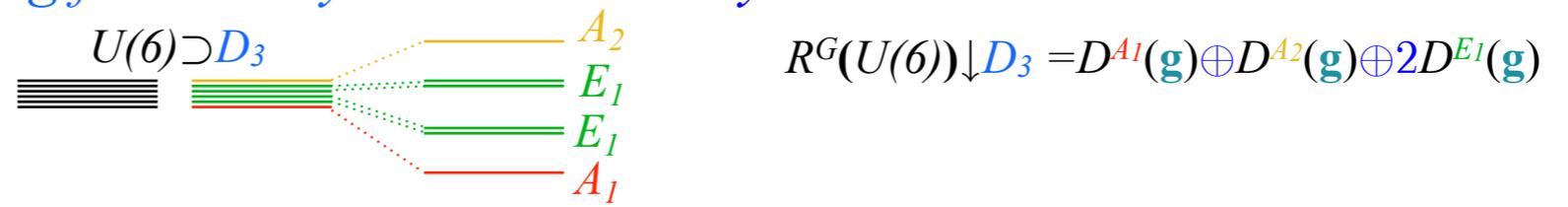
Crystal-field splitting: O(3) \supset D3 symmetry reduction and D^l \downarrow D3 splitting



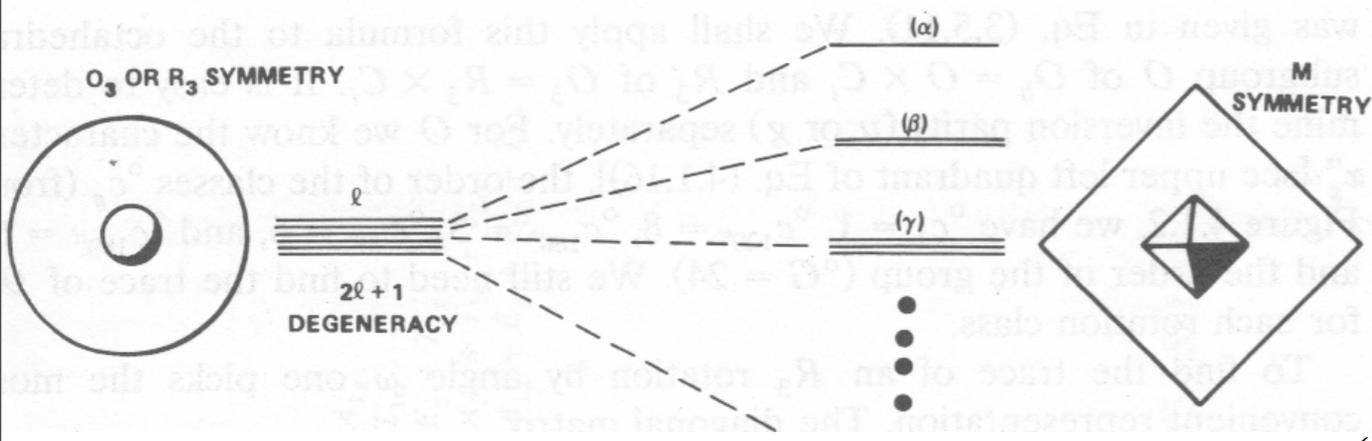
(Fig. 5.6.1 PSDS)

$$D^l(\mathbf{R}) = \begin{pmatrix} D_{l,l}^l(\mathbf{R}) & \dots & D_{l,-l}^l(\mathbf{R}) \\ D_{l-1,l}^l(\mathbf{R}) & & \\ \vdots & & \\ D_{-l,l}^l(\mathbf{R}) & \dots & D_{-l,-l}^l(\mathbf{R}) \end{pmatrix} \downarrow M \cong \begin{pmatrix} D^\alpha(\mathbf{R}) \\ D^\beta(\mathbf{R}) \\ D^\gamma(\mathbf{R}) \end{pmatrix}$$

Spectral splitting in symmetry breaking foretold by character analysis



Crystal-field splitting: O(3) \supset D3 symmetry reduction and D^l \downarrow D3 splitting



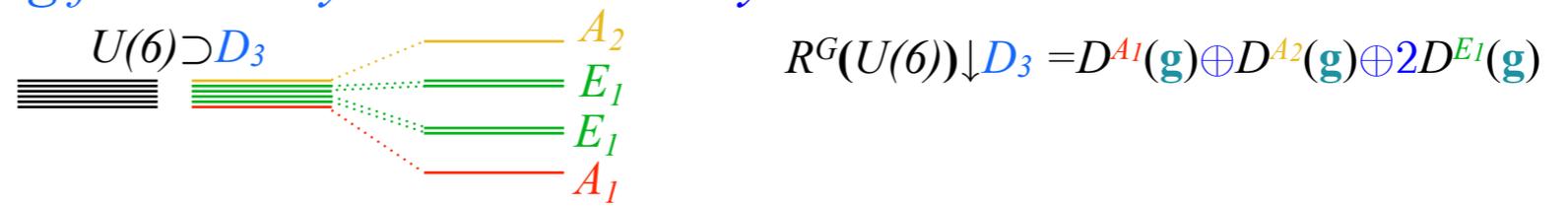
(Fig. 5.6.1 PSDS)

$$D^l(R) = \begin{pmatrix} D_{l,l}^l(R) & \dots & D_{l,-l}^l(R) \\ D_{l-1,l}^l(R) & & \\ \vdots & & \\ D_{-l,l}^l(R) & \dots & D_{-l,-l}^l(R) \end{pmatrix} \xrightarrow{M \cong} \begin{pmatrix} D^\alpha(R) \\ D^\beta(R) \\ D^\gamma(R) \end{pmatrix}$$

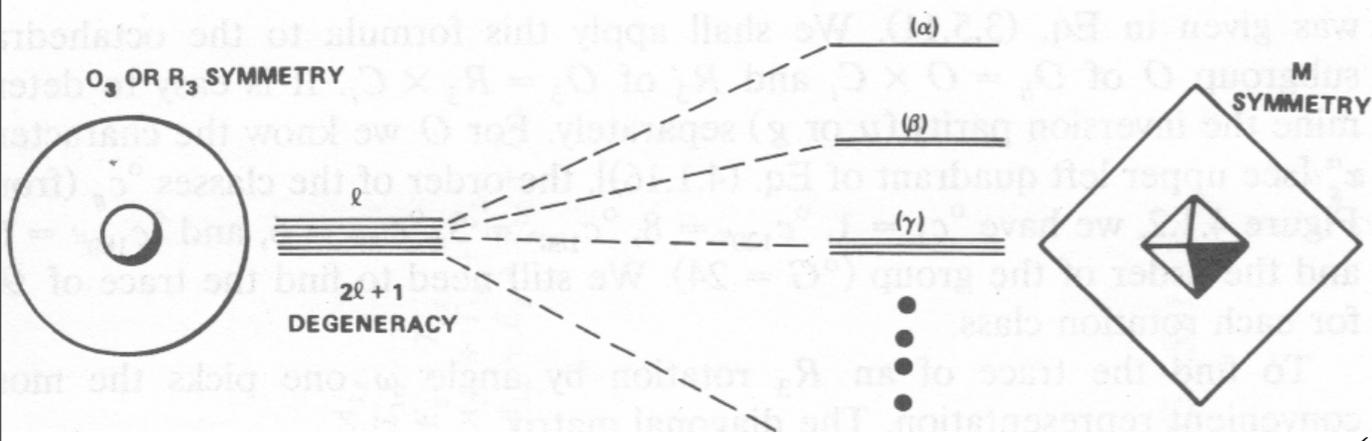
Use $R(3) \sim U(2)$ character formula: $\chi^l\left(\frac{2\pi}{n}\right) = \frac{\sin\left(\frac{(2l+1)\pi}{n}\right)}{\sin\left(\frac{\pi}{n}\right)}$

$R(3)$ character
 where: $2l+1$
 is l -orbital dimension
 (From Lect. 11 p. 11)

Spectral splitting in symmetry breaking foretold by character analysis



Crystal-field splitting: O(3) \supset D3 symmetry reduction and D^l \downarrow D3 splitting



(Fig. 5.6.1 PSDS)

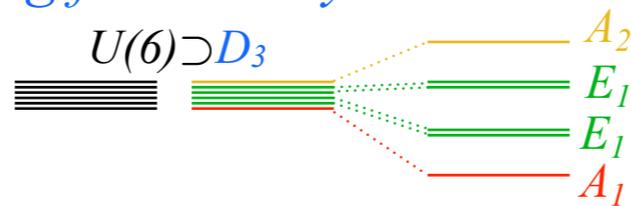
$$D^l(\mathbf{R}) = \begin{pmatrix} D_{l,l}^l(\mathbf{R}) & \dots & D_{l,-l}^l(\mathbf{R}) \\ D_{l-1,l}^l(\mathbf{R}) & & \\ \vdots & & \\ D_{-l,l}^l(\mathbf{R}) & \dots & D_{-l,-l}^l(\mathbf{R}) \end{pmatrix} \xrightarrow{M \cong} \begin{pmatrix} D^\alpha(\mathbf{R}) \\ D^\beta(\mathbf{R}) \\ D^\gamma(\mathbf{R}) \end{pmatrix}$$

Use $R(3) \sim U(2)$ character formula:
$$\chi^l\left(\frac{2\pi}{n}\right) = \frac{\sin\left(\frac{(2l+1)\pi}{n}\right)}{\sin\left(\frac{\pi}{n}\right)}$$

$R(3)$ character
 where: $2l+1$ is l -orbital dimension
 (From Lect. 11 p. 11)

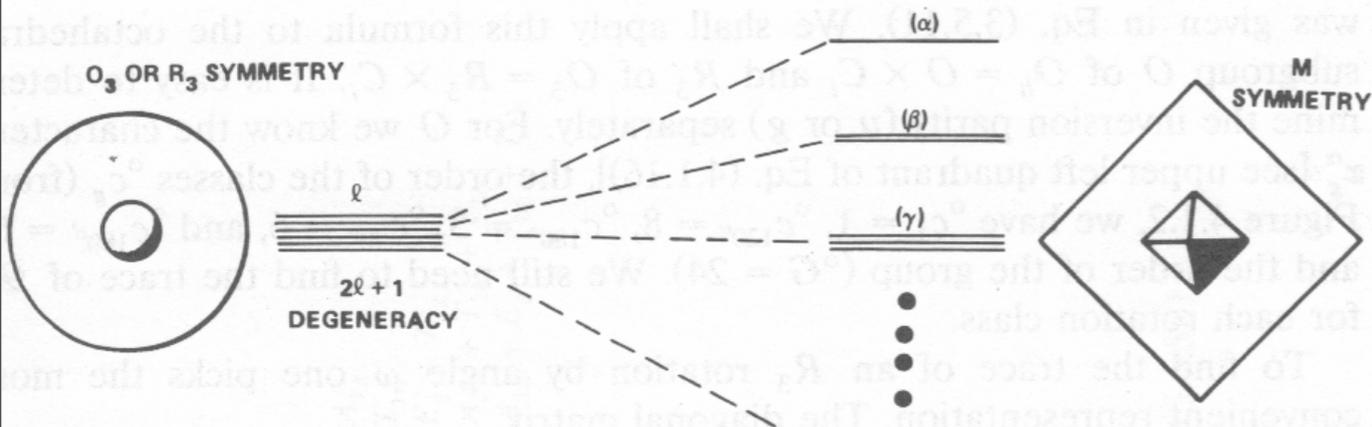
$$\chi^l(\Theta) = \frac{\sin\left(\left(l + \frac{1}{2}\right)\Theta\right)}{\sin\left(\frac{\Theta}{2}\right)}$$

Spectral splitting in symmetry breaking foretold by character analysis



$$R^G(U(6)) \downarrow D_3 = D^{A_1}(\mathbf{g}) \oplus D^{A_2}(\mathbf{g}) \oplus 2D^{E_1}(\mathbf{g})$$

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting



(Fig. 5.6.1 PSDS)

$$D^\ell(\mathbf{R}) = \begin{pmatrix} D_{\ell,\ell}^\ell(\mathbf{R}) & \dots & D_{\ell,-\ell}^\ell \\ D_{\ell-1,\ell}^\ell & & \\ \vdots & & \\ D_{-\ell,\ell}^\ell & \dots & D_{-\ell,-\ell}^\ell \end{pmatrix} \downarrow M \cong \begin{pmatrix} D^\alpha(\mathbf{R}) \\ D^\beta(\mathbf{R}) \\ D^\gamma(\mathbf{R}) \end{pmatrix}$$

Use $R(3) \sim U(2)$ character formula: $\chi^\ell\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$

$R(3)$ character

where: $2\ell+1$

(From Lect. 11 p. 11)

is ℓ -orbital dimension

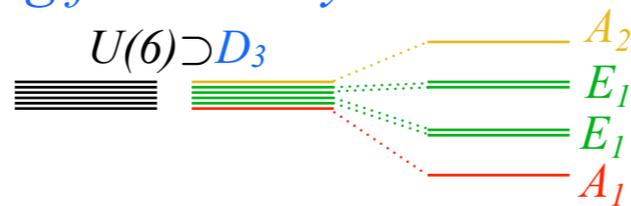
$$\chi^\ell(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and D_3 character table:

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

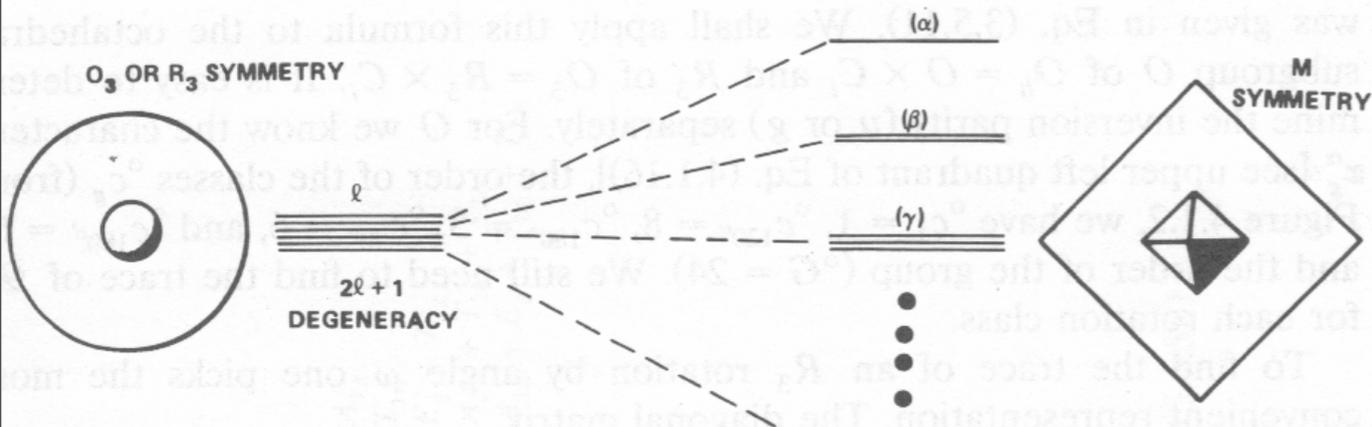
$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	-1
2	5	-1	1
3	7	1	-1
4	9	0	1
5	11	-1	-1
6	13	1	1
7	15	0	-1

Spectral splitting in symmetry breaking foretold by character analysis



$$R^G(U(6)) \downarrow D_3 = D^{A_1}(\mathbf{g}) \oplus D^{A_2}(\mathbf{g}) \oplus 2D^{E_1}(\mathbf{g})$$

Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting



(Fig. 5.6.1 PSDS)

$$D^\ell(\mathbf{R}) = \begin{pmatrix} D_{\ell,\ell}^\ell(\mathbf{R}) & \dots & D_{\ell,-\ell}^\ell(\mathbf{R}) \\ D_{\ell-1,\ell}^\ell(\mathbf{R}) & & \\ \vdots & & \\ D_{-\ell,\ell}^\ell(\mathbf{R}) & \dots & D_{-\ell,-\ell}^\ell(\mathbf{R}) \end{pmatrix} \xrightarrow{M \cong} \begin{pmatrix} D^\alpha(\mathbf{R}) \\ D^\beta(\mathbf{R}) \\ D^\gamma(\mathbf{R}) \end{pmatrix}$$

Use $R(3) \sim U(2)$ character formula: $\chi^\ell\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$

$R(3)$ character

where: $2\ell+1$

(From Lect. 11 p. 11)

is ℓ -orbital dimension

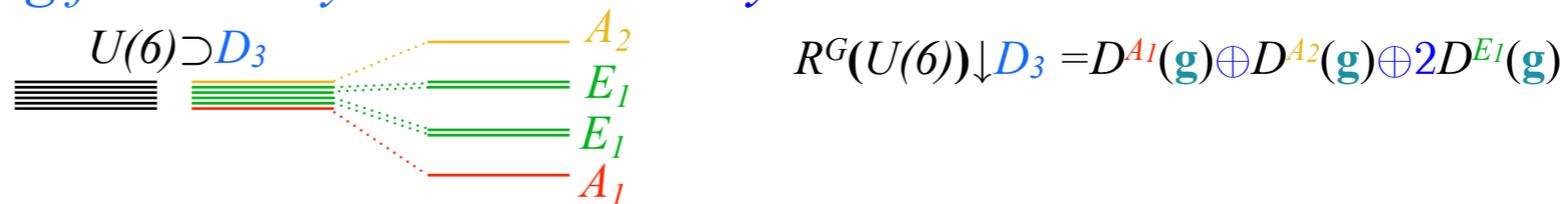
$$\chi^\ell(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

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$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

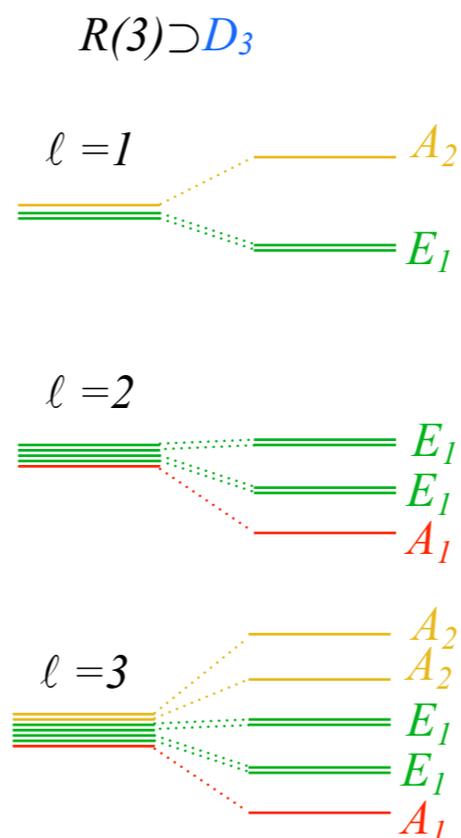
$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	.	.	$1A_1$
1	.	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	.	2	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	$1A_1 \oplus 2A_2 \oplus 3E_1$
5	2	1	3	$2A_1 \oplus A_2 \oplus 3E_1$
6	3	2	4	$3A_1 \oplus 2A_2 \oplus 4E_1$
7	2	3	5	$2A_1 \oplus 3A_2 \oplus 5E_1$

Spectral splitting in symmetry breaking foretold by character analysis



Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	.	.	$1A_1$
1	.	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	.	2	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	$1A_1 \oplus 2A_2 \oplus 3E_1$
5	2	1	3	$2A_1 \oplus A_2 \oplus 3E_1$
6	3	2	4	$3A_1 \oplus 2A_2 \oplus 4E_1$
7	2	3	5	$2A_1 \oplus 3A_2 \oplus 5E_1$



D_3 character table:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

