

AMOP 2.21.18 class 12.0: *Symmetry Principles for*
reference links *Advanced Atomic-Molecular-Optical-Physics*
on following page
William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators

32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups

Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3

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Global vs Local symmetry expansion of D_3 Hamiltonian

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D_3 -invariant irep characters $\chi_k^{(\alpha)}$

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Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors

...and classes

3rd-Stage spectral decomposition of ALL of D_3

...and of Hamiltonian \mathbf{H}

GLOBAL vs LOCAL symmetry of states

...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$

AMOP reference links (Updated list given on 2nd page of each class presentation)

[Web Resources - front page](#)

[UAF Physics UTube channel](#)

[Quantum Theory for the Computer Age](#)

[Principles of Symmetry, Dynamics, and Spectroscopy](#)

[Classical Mechanics with a Bang!](#)

[Modern Physics and its Classical Foundations](#)

[2014 AMOP](#)

[2017 Group Theory for QM](#)

[2018 AMOP](#)

[Frame Transformation Relations And Multipole Transitions In Symmetric Polyatomic Molecules - RMP-1978](#)

[Rotational energy surfaces and high- J eigenvalue structure of polyatomic molecules - Harter - Patterson - 1984](#)

[Galloping waves and their relativistic properties - ajp-1985-Harter](#)

[Asymptotic eigensolutions of fourth and sixth rank octahedral tensor operators - Harter-Patterson-JMP-1979](#)

[Nuclear spin weights and gas phase spectral structure of 12C60 and 13C60 buckminsterfullerene -Harter-Reimer-Cpl-1992 - \(Alt1, Alt2 Erratum\)](#)

Theory of hyperfine and superfine levels in symmetric polyatomic molecules.

I) [Trigonal and tetrahedral molecules: Elementary spin-1/2 cases in vibronic ground states - PRA-1979-Harter-Patterson \(Alt scan\)](#)

II) [Elementary cases in octahedral hexafluoride molecules - Harter-PRA-1981 \(Alt scan\)](#)

[Rotation-vibration scalar coupling zeta coefficients and spectroscopic band shapes of buckminsterfullerene - Weeks-Harter-CPL-1991 \(Alt scan\)](#)

[Fullerene symmetry reduction and rotational level fine structure/ the Buckyball isotopomer 12C 13C59 - jcp-Reimer-Harter-1997 \(HiRez\)](#)

[Molecular Eigensolution Symmetry Analysis and Fine Structure - IJMS-harter-mitchell-2013](#)

Rotation–vibration spectra of icosahedral molecules.

I) [Icosahedral symmetry analysis and fine structure - harter-weeks-jcp-1989](#)

II) [Icosahedral symmetry, vibrational eigenfrequencies, and normal modes of buckminsterfullerene - weeks-harter-jcp-1989](#)

III) [Half-integral angular momentum - harter-reimer-jcp-1991](#)

[QTCA Unit 10 Ch 30 - 2013](#)

[AMOP Ch 32 Molecular Symmetry and Dynamics - 2019](#)

[AMOP Ch 0 Space-Time Symmetry - 2019](#)

RESONANCE AND REVIVALS

I) [QUANTUM ROTOR AND INFINITE-WELL DYNAMICS - ISMSLi2012 \(Talk\) OSU knowledge Bank](#)

II) [Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 \(Talks\)](#)

III) [Quantum Resonant Beats and Revivals in the Morse Oscillators and Rotors - \(2013-Li-Diss\)](#)

[Rovibrational Spectral Fine Structure Of Icosahedral Molecules - Cpl 1986 \(Alt Scan\)](#)

[Gas Phase Level Structure of C60 Buckyball and Derivatives Exhibiting Broken Icosahedral Symmetry - reimer-diss-1996](#)

[Resonance and Revivals in Quantum Rotors - Comparing Half-integer Spin and Integer Spin - Alva-ISMS-Ohio2013-R777 \(Talk\)](#)

[Quantum Revivals of Morse Oscillators and Farey-Ford Geometry - Li-Harter-cpl-2013](#)

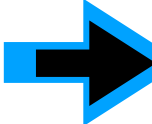

[Wave Node Dynamics and Revival Symmetry in Quantum Rotors - harter - jms - 2001](#)

**In development - a web based A.M.O.P. oriented reference page, with thumbnail/previews, greater control over the information display, and eventually full on Apache-SOLR Index and search for nuanced, whole-site content/metadata level searching. This bad boy will be a sure force multiplier.*

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Crystal-Point Group Zoo
 having 32 groups
 (Showing
 16 Abelian
 Crystal Groups)

Fig. 2.11.1 PSDS

The other 16
 crystal-point groups
 are
Non-Abelian

Abelian
 means
 all its elements
 commute

Non-Abelian
 means
 some elements
 do not commute

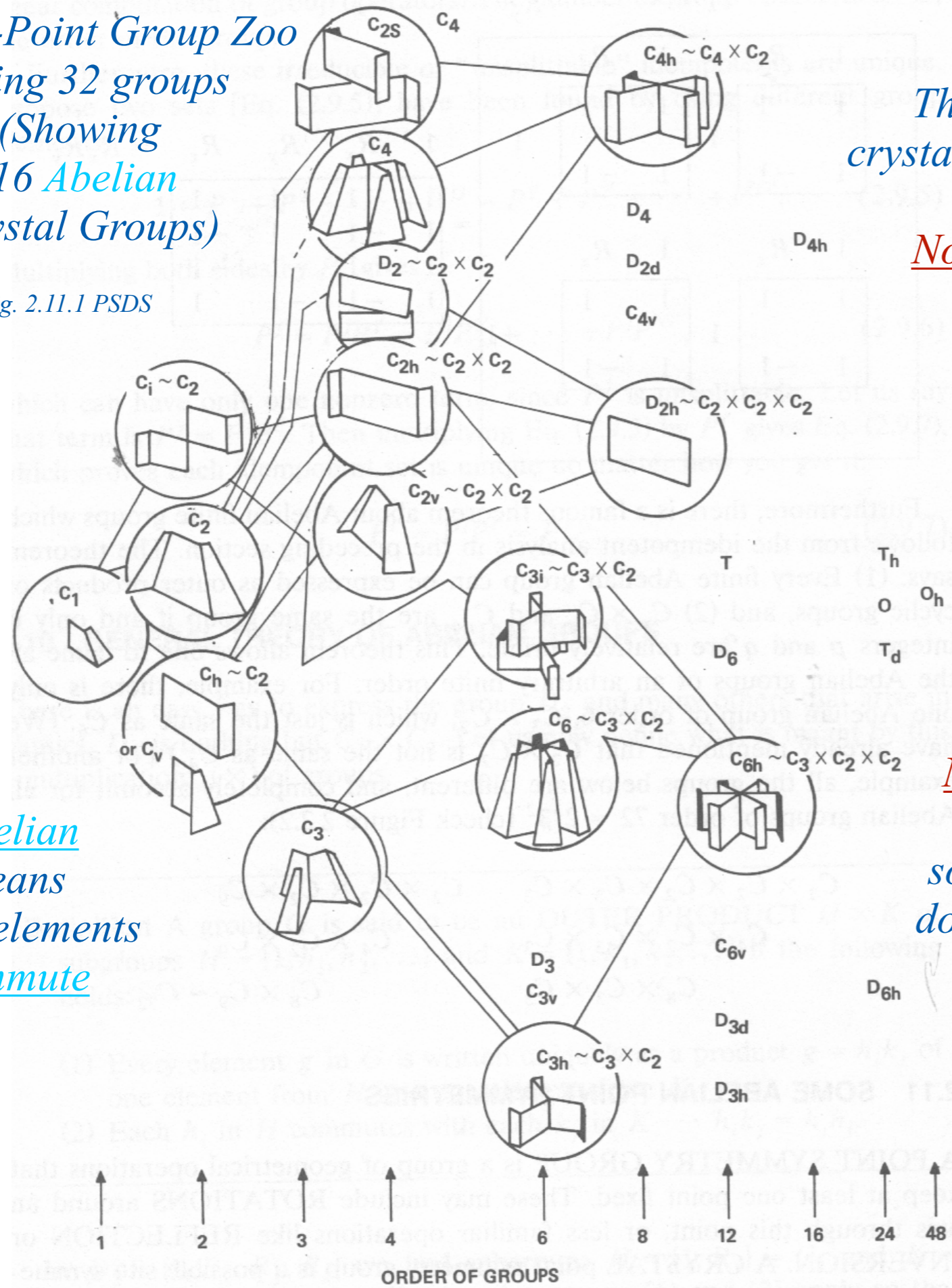
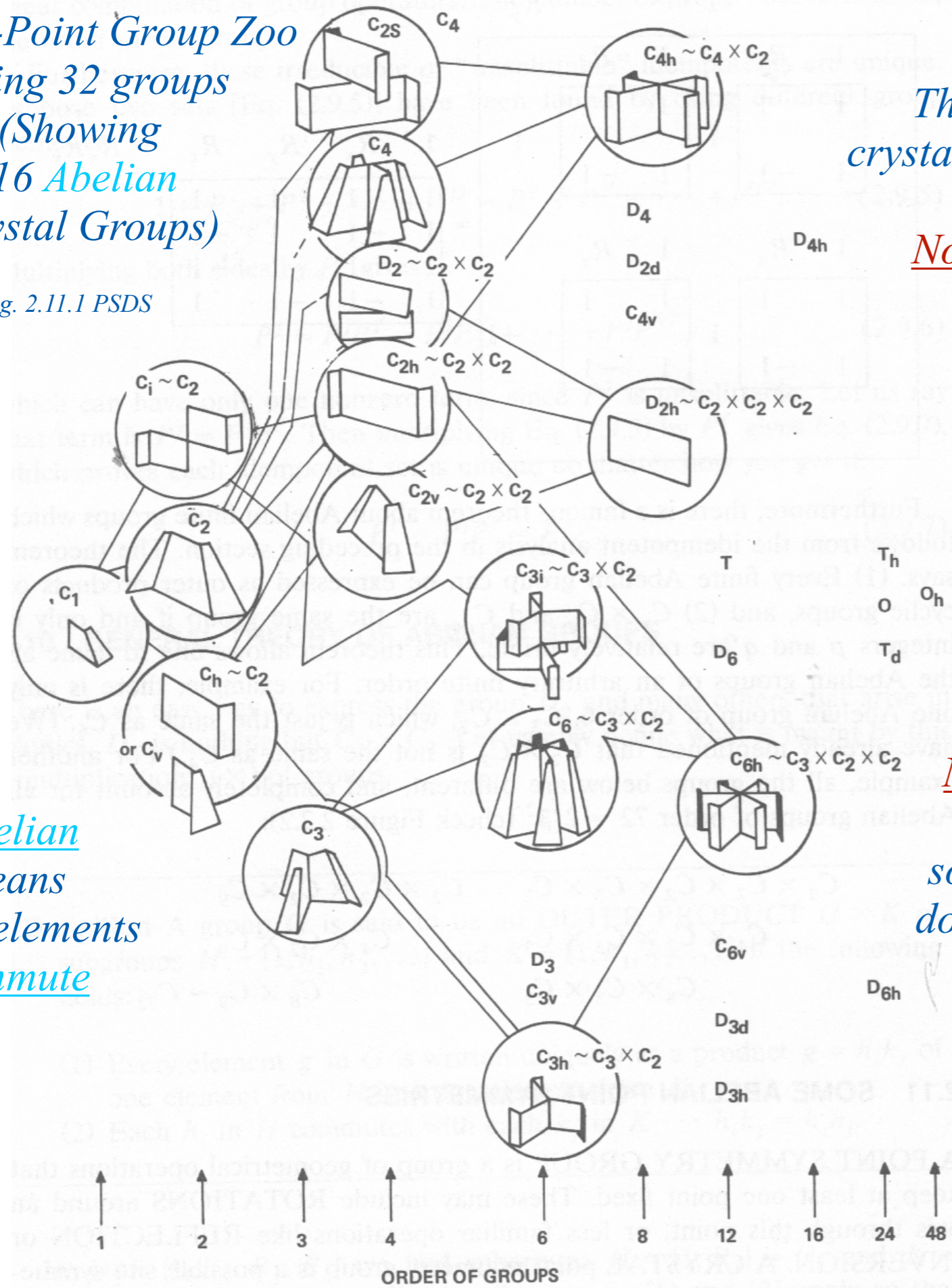


Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

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The other 16
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From GTQM Lecture 12.6 p. 134
 Character Trace of
 n-fold rotation
 where: $\ell^j = 2j+1$
 is U(2) irrep dimension

$$\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

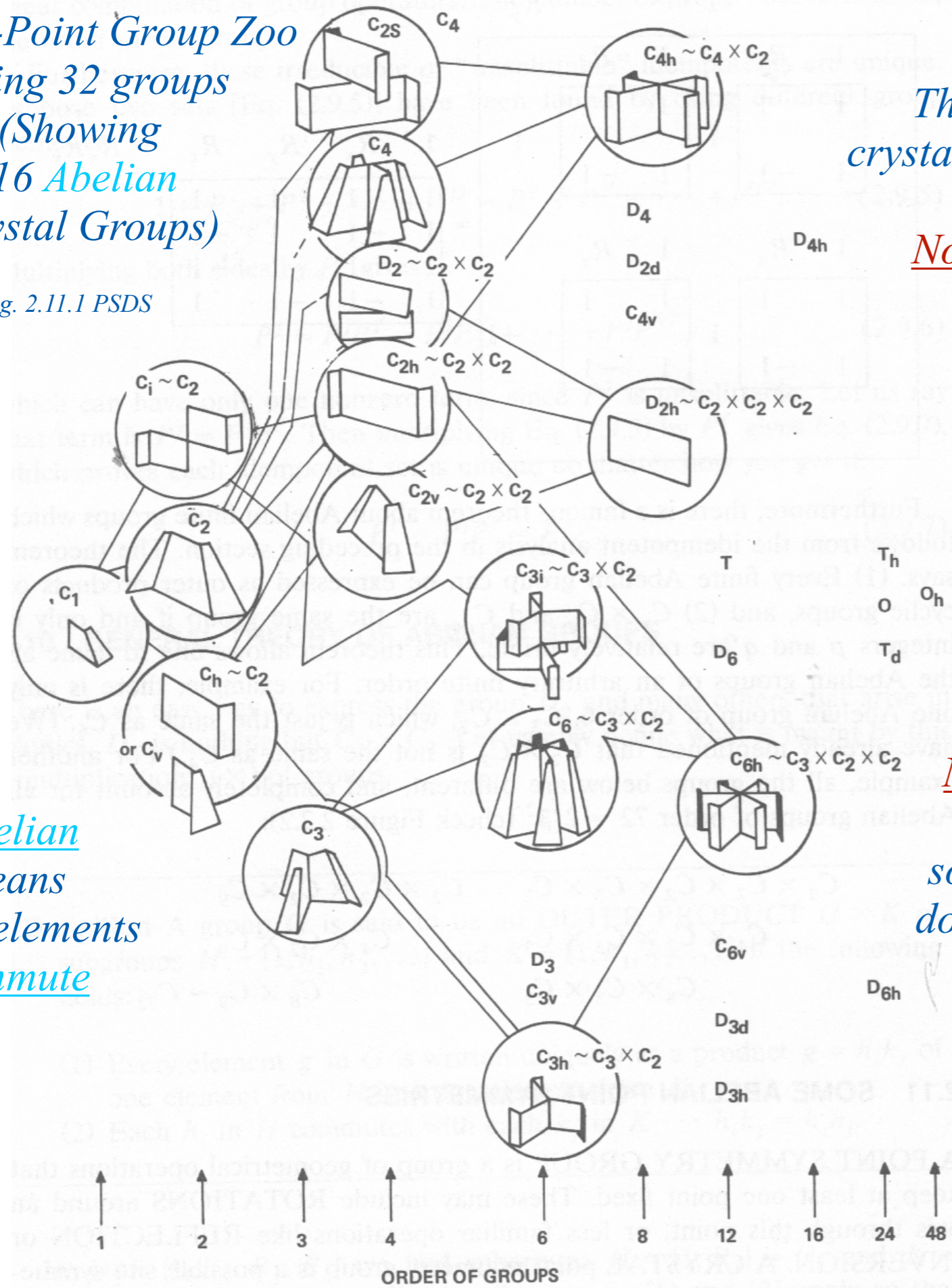
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To be a crystal-point group
 the Character Trace of
 n-fold vector rotation
 for: $\ell^1 = 2+1=3$
 must be an integer

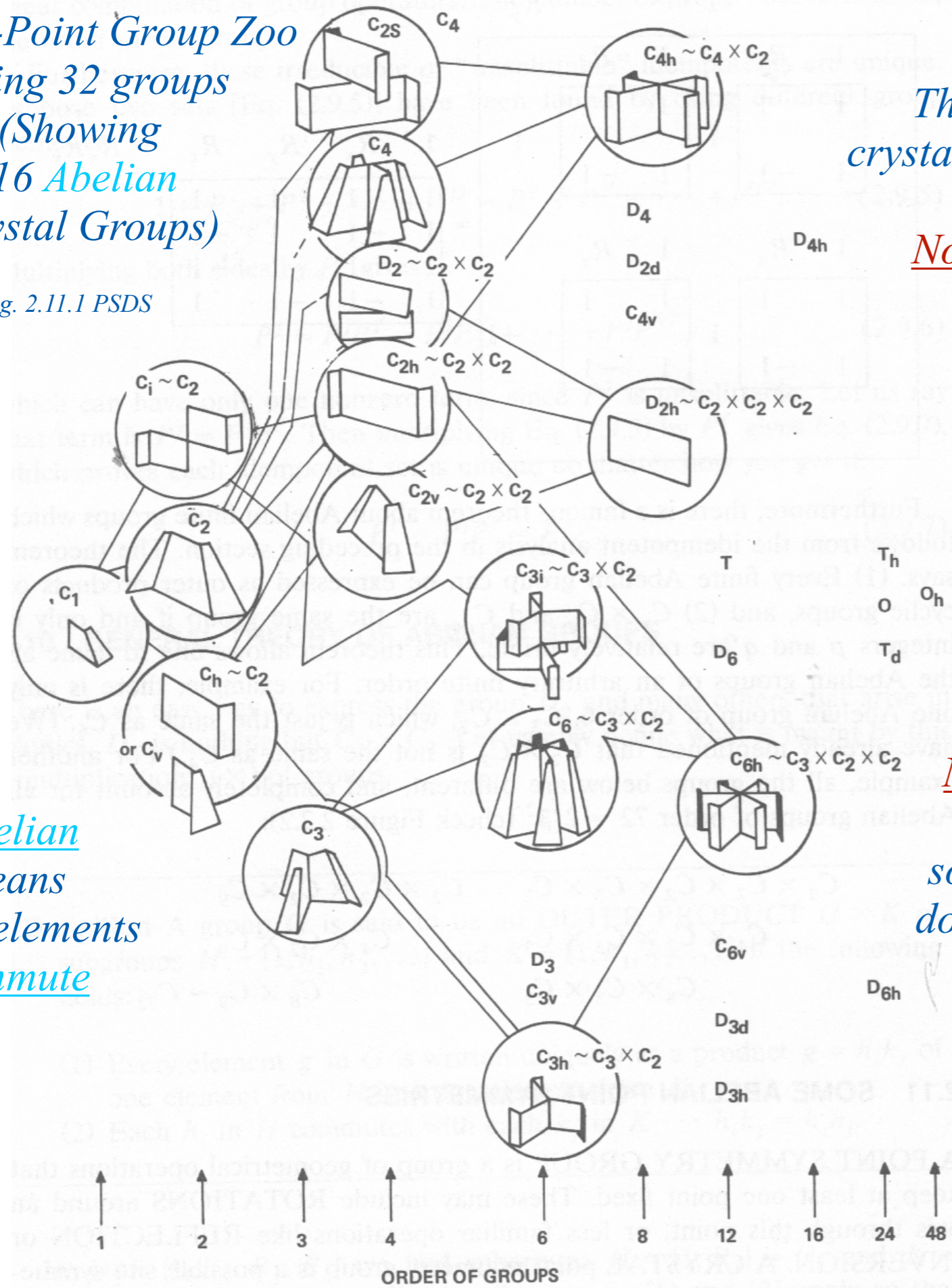
$$\chi^1\left(\frac{2\pi}{n}\right) = \frac{\sin \frac{\pi}{n} (2j+1)}{\sin \frac{\pi}{n}} = \frac{\sin \frac{3\pi}{n}}{\sin \frac{\pi}{n}} = \text{integer}$$

- $\frac{\sin \frac{3\pi}{2}}{\sin \frac{\pi}{2}} = -1$ (n=2 ok)
- $\frac{\sin \frac{3\pi}{3}}{\sin \frac{\pi}{3}} = +1$ (n=3 ok)
- $\frac{\sin \frac{3\pi}{4}}{\sin \frac{\pi}{4}} = +1$ (n=4 ok)
- $\frac{\sin \frac{3\pi}{5}}{\sin \frac{\pi}{5}} = G^+$ (n=5 NO!)
- $\frac{\sin \frac{3\pi}{6}}{\sin \frac{\pi}{6}} = +2$ (n=6 ok)

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*Crystal-Point Group Zoo
having 32 groups
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Abelian
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The other 16
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Log-histogram of
all groups of order
 $^{\circ}G=1$ to 64
Abelian shown in **Black**
Non-Abelian in White

Group "census"

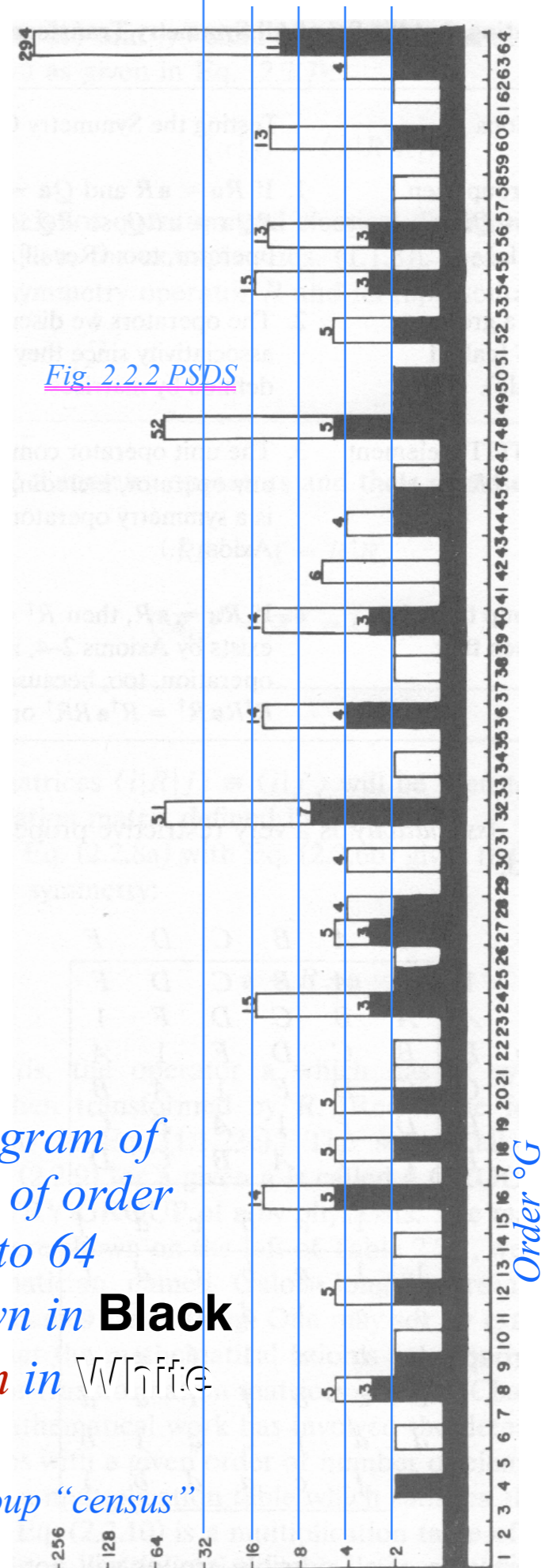
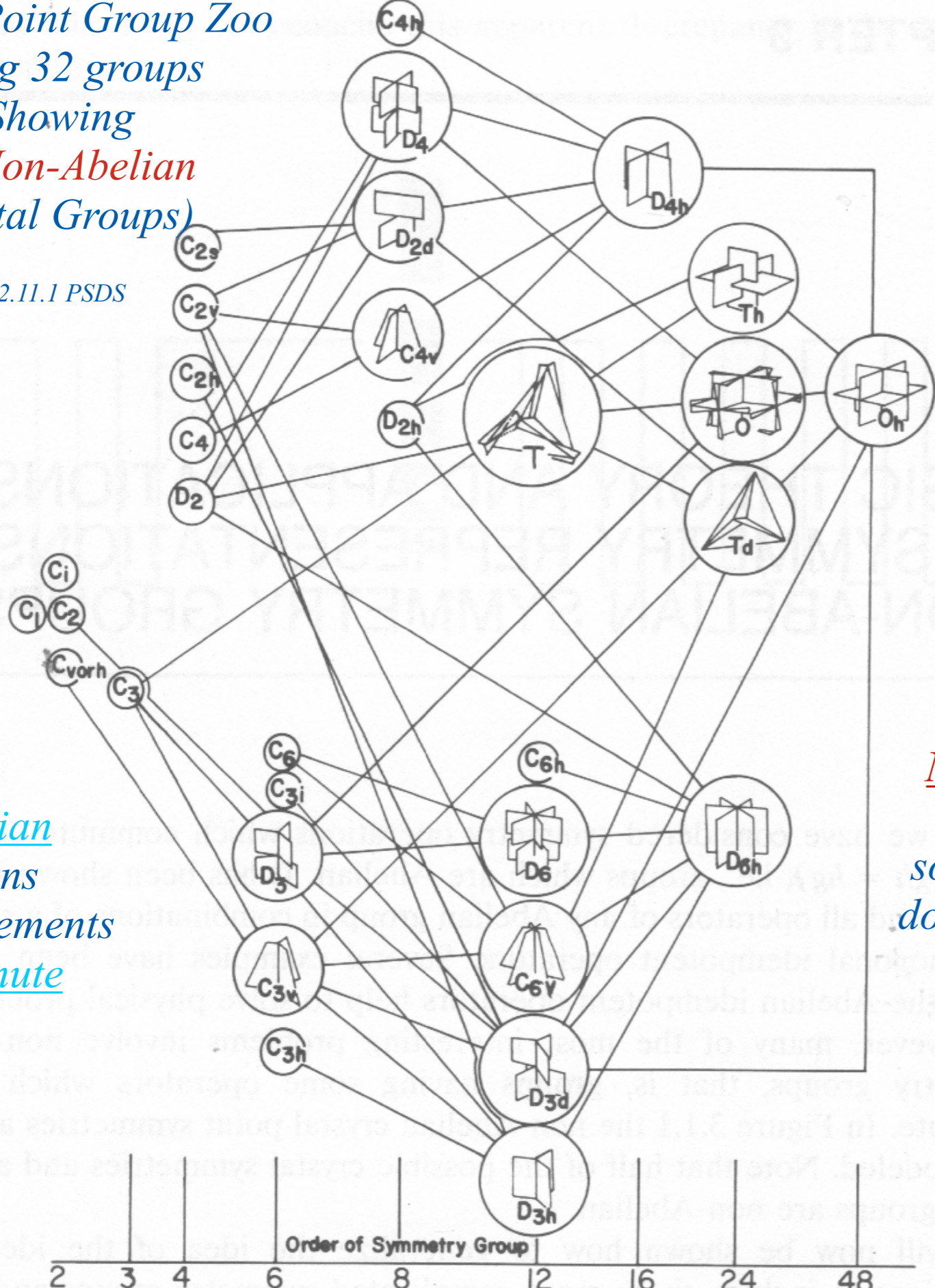


Fig. 2.2.2 PSDS

Figure 2.11.1 Abelian crystal point groups. Sixteen of the 32 crystal point groups are Abelian and are illustrated by models drawn in circles.

*Crystal-Point Group Zoo
having 32 groups
(Showing
16 Non-Abelian
Crystal Groups)*

Fig. 2.11.1 PSDS



Abelian
means
all its elements
commute

Clearly
most groups are
Non-Abelian

and
most groups are
unknown to physicists

Non-Abelian
means
some elements
do not commute

Log-histogram of
all groups of order
 $^{\circ}G=1$ to 64

Abelian shown in **Black**
Non-Abelian in **White**

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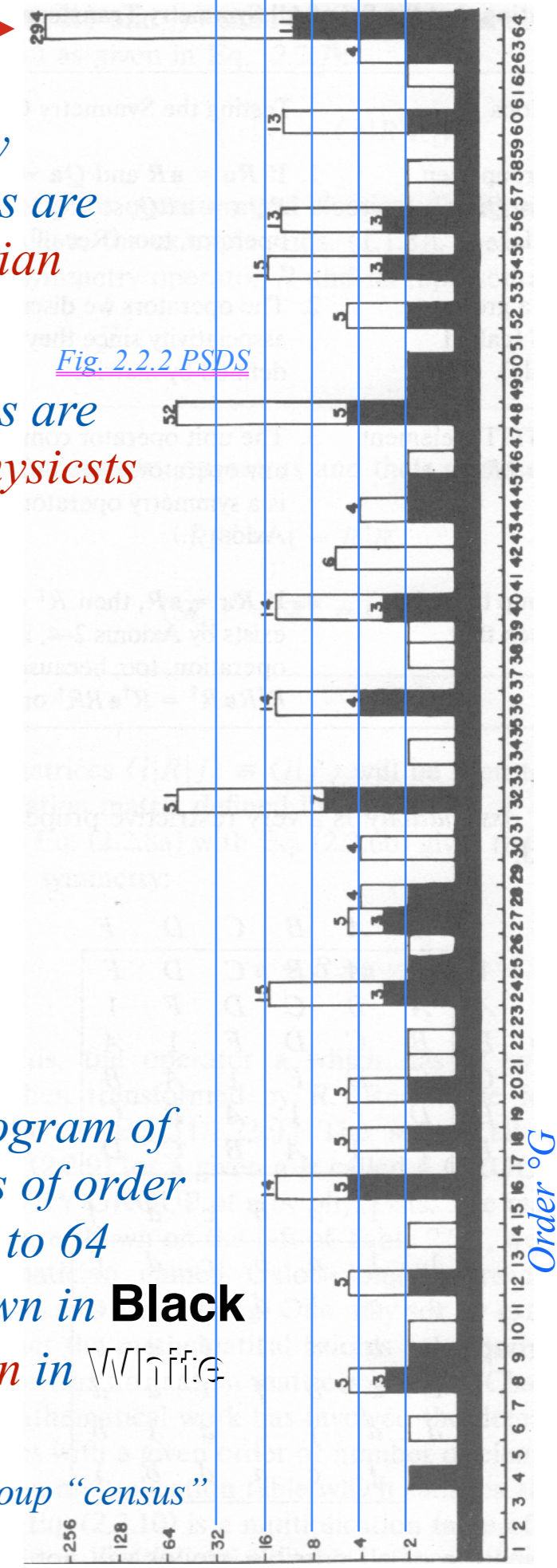


Figure 3.1.1 Crystal point symmetry groups. Models are sketched in circles for the 16 non-Abelian groups. (See also Figure 2.11.1.)

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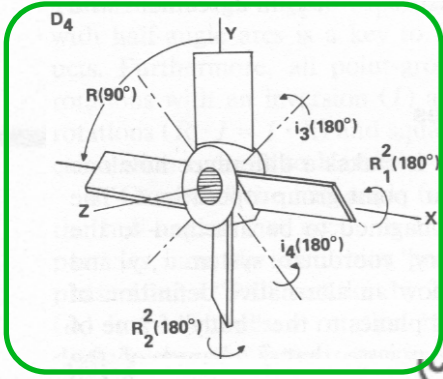
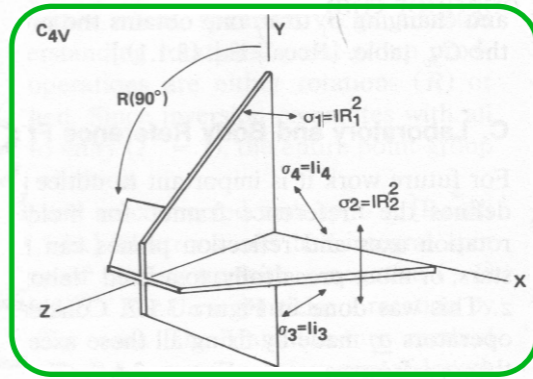
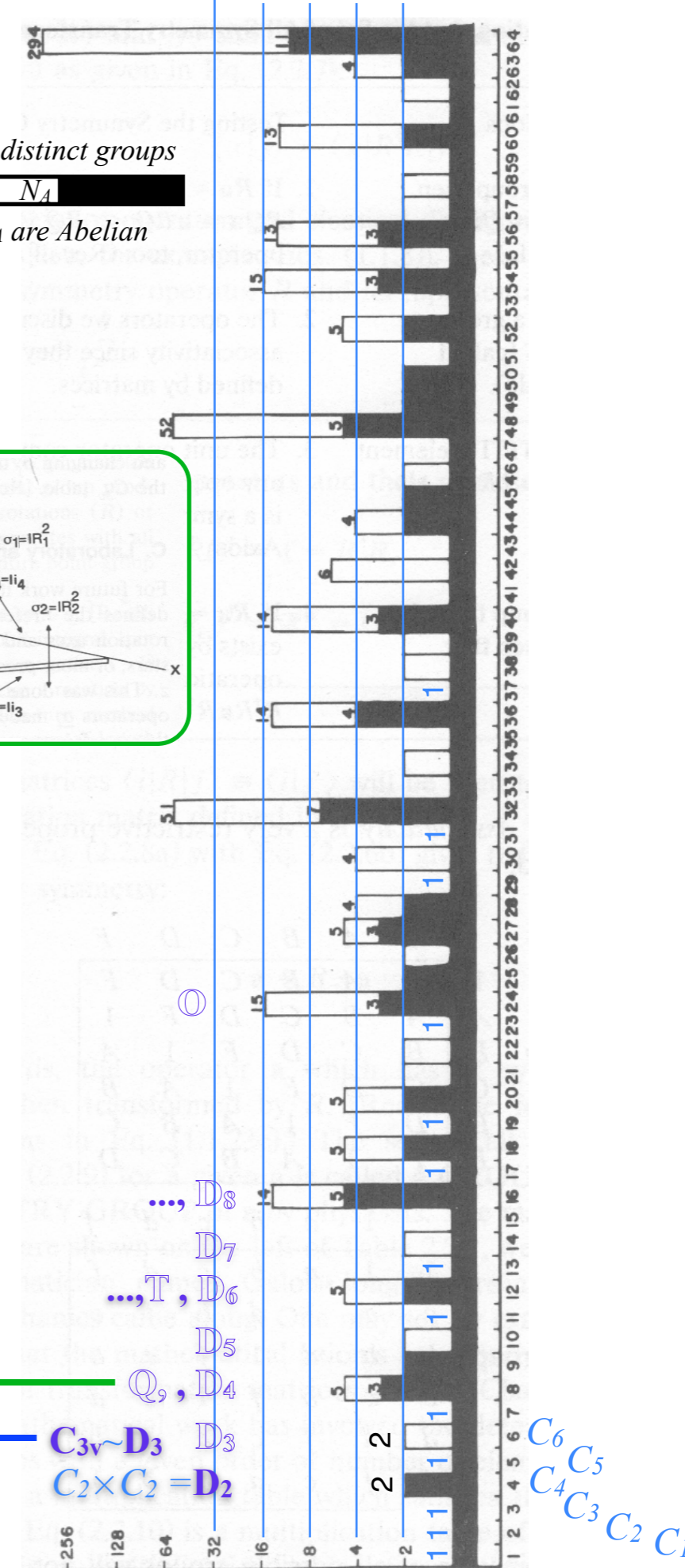


Fig. 2.2.2 PSDS

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



D_4 and C_{4v}
 are related
 similarly to
 D_3 and C_{3v}

Fig. 3.1.1 PSDS

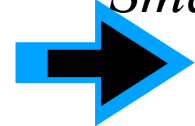
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$C_6, C_5, C_4, C_3, C_2, C_1$

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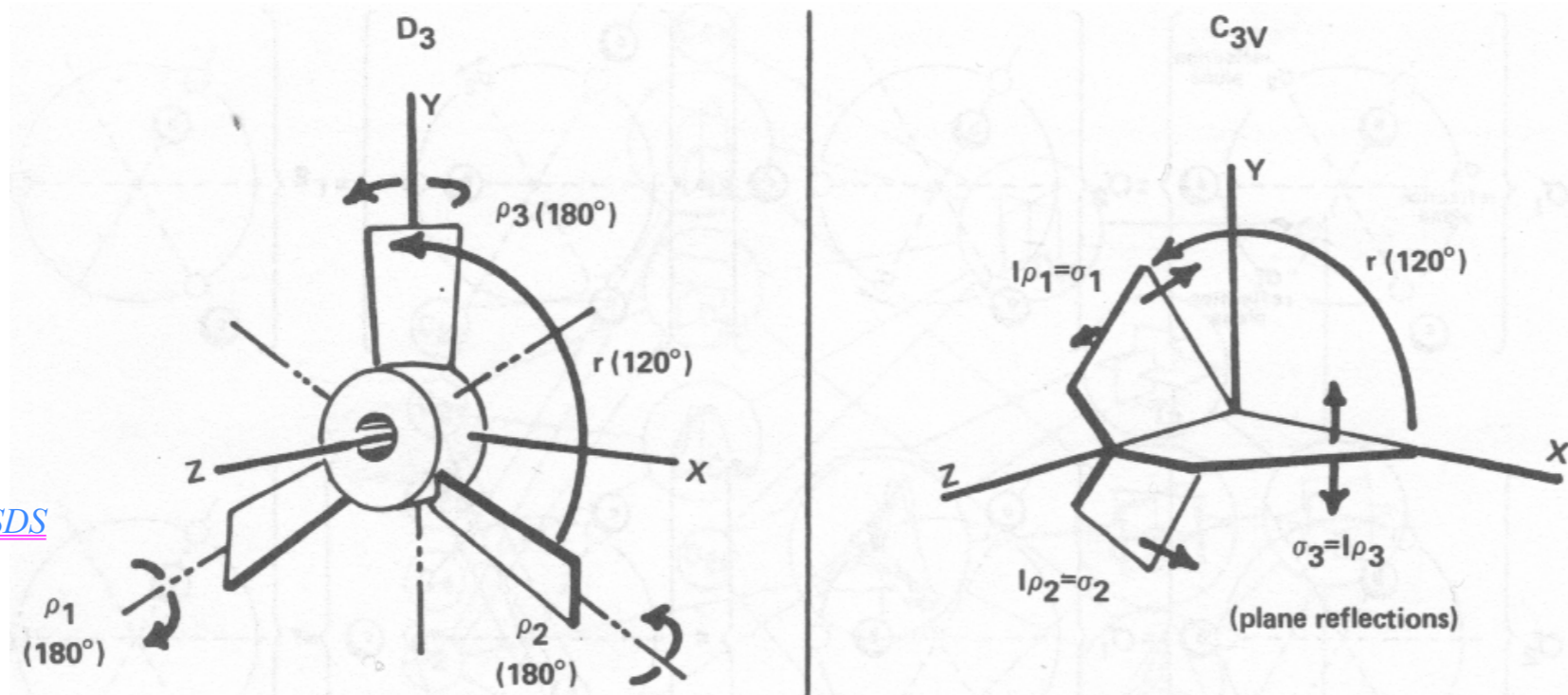
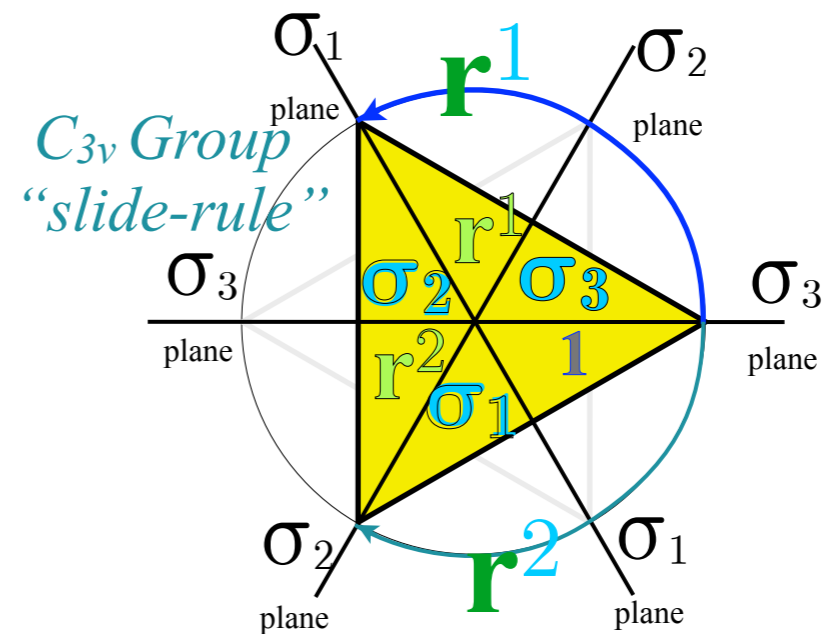
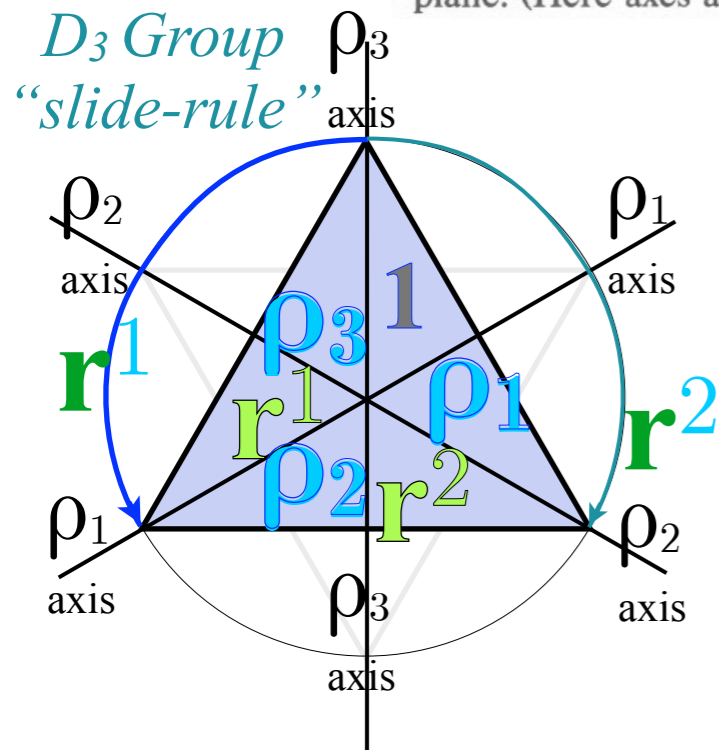


Fig. 3.1.3 PSDS

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.*

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

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

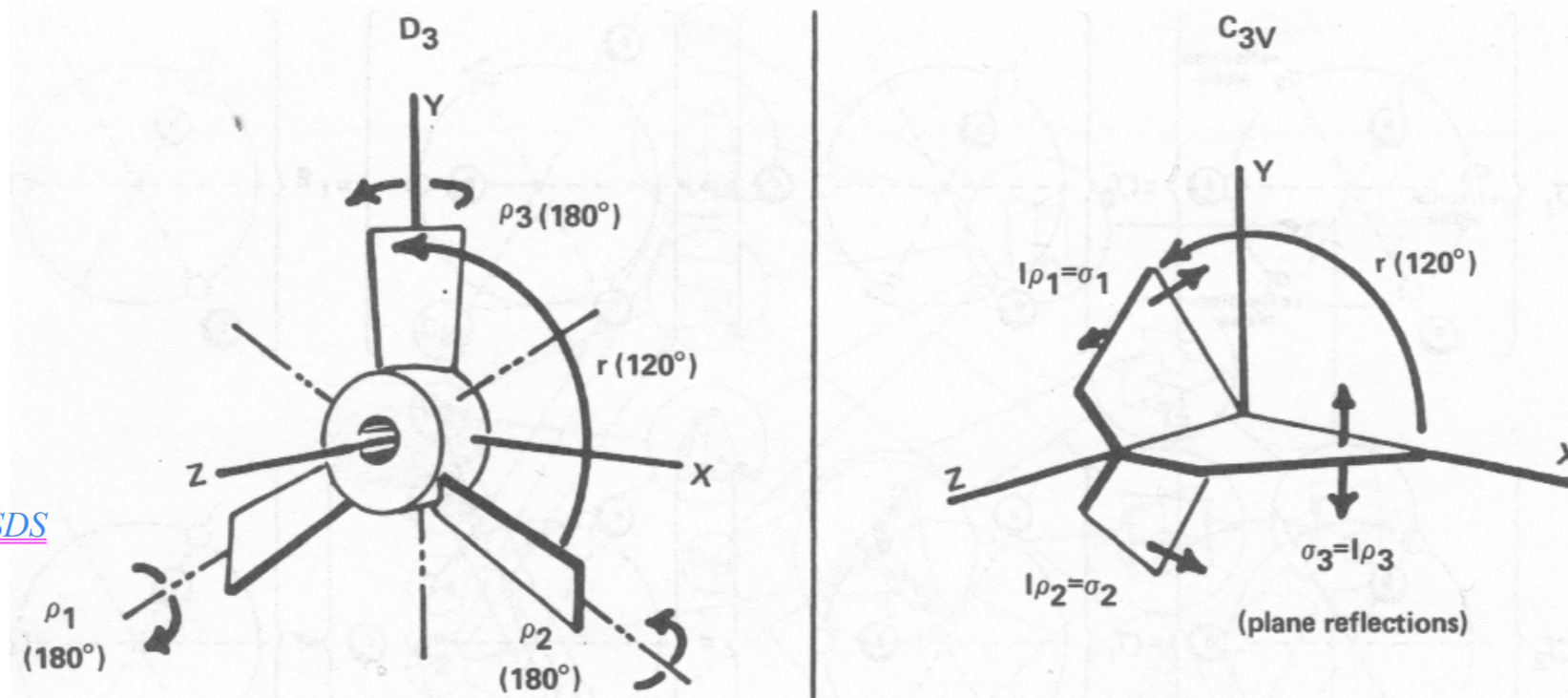


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$180^\circ D_3$ -Y-axis-rotation: $\rho_3 = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$ maps to: XZ-mirror-plane reflection: $\sigma_3 = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot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

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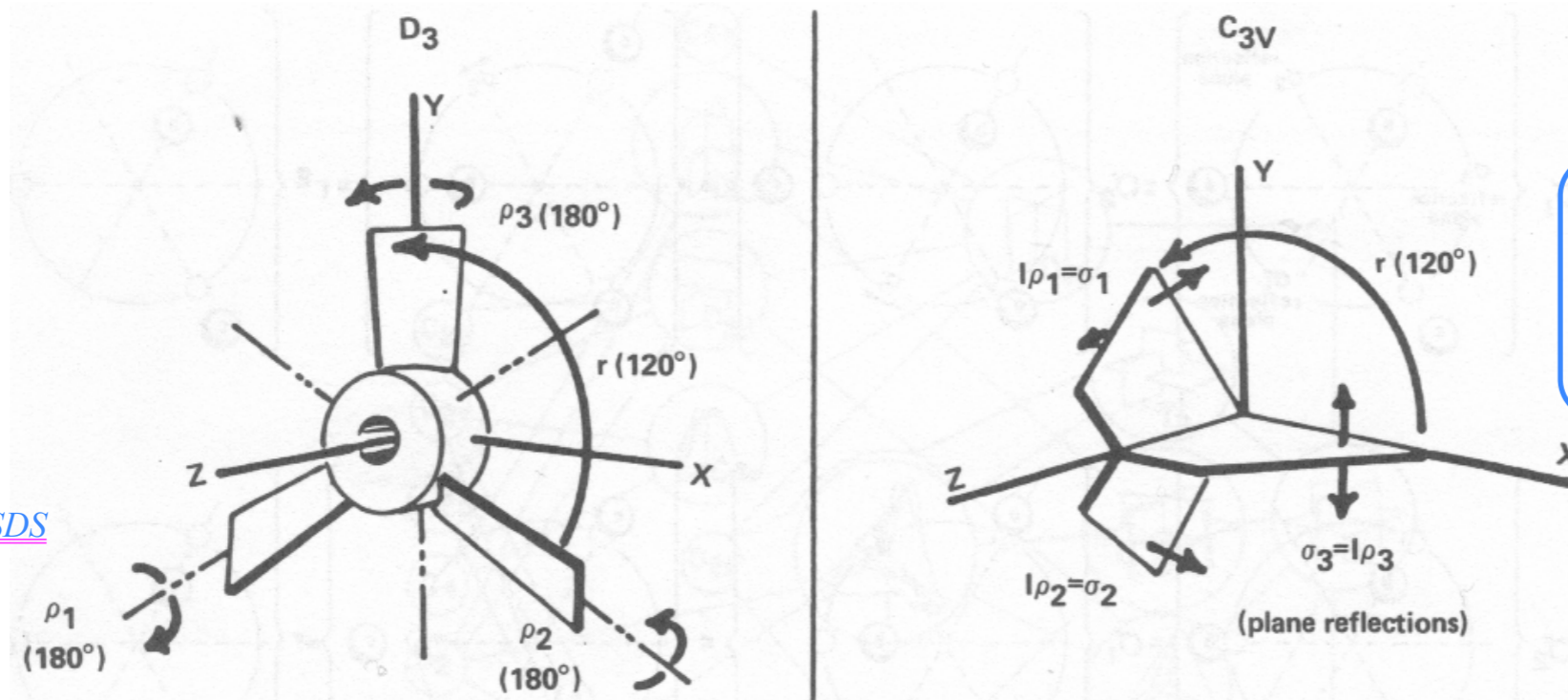


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Mirror-plane-reflection σ
equals
 $180^\circ \perp$ -axial-rotation-inversion
 $\sigma = \mathbf{R} \cdot \mathbf{I} = \mathbf{I} \cdot \mathbf{R}$

$$\sigma_3 = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & +1 \end{pmatrix}$$

$$= \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

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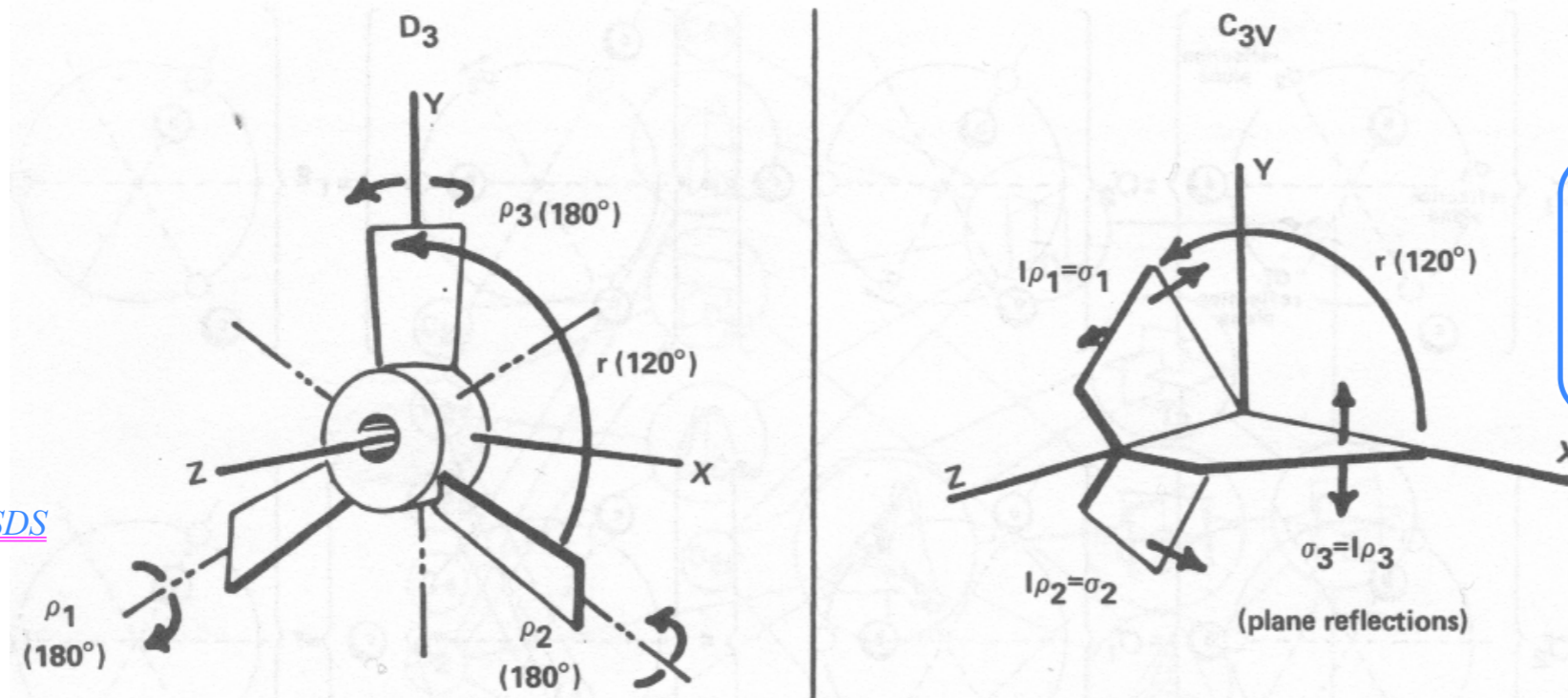


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Inversion
 $\mathbf{I} = -\mathbf{1}$
commutes
with
all \mathbf{R}

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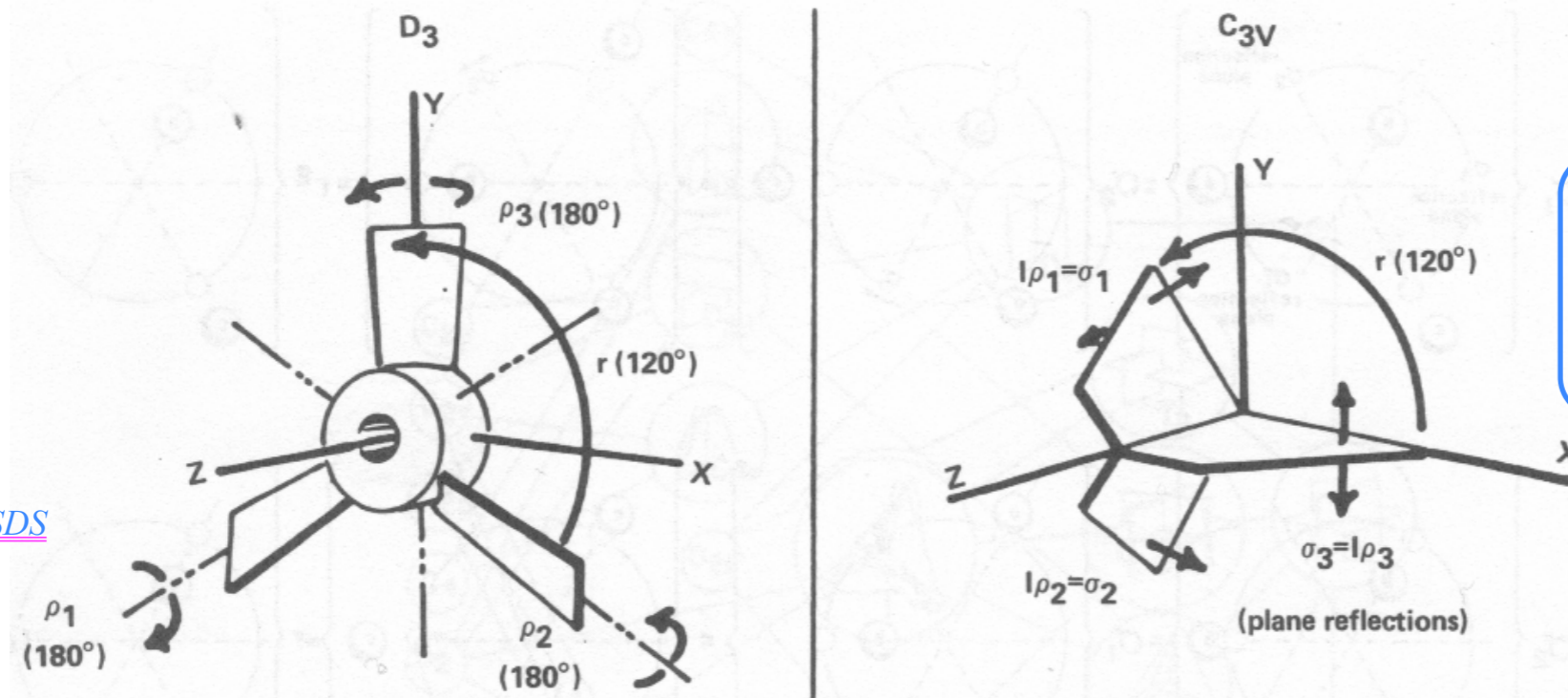


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Mirror-plane-reflection σ
equals
 $180^\circ \perp$ -axial-rotation-inversion
 $\sigma = \mathbf{R} \cdot \mathbf{I} = \mathbf{I} \cdot \mathbf{R}$

$$\sigma_3 = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & +1 \end{pmatrix} = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} = \rho_3 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_3$$

$180^\circ D_3$ -Y-axis-rotation: $\rho_3 = \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$

maps to: XZ-mirror-plane reflection: $\sigma_3 = \begin{pmatrix} +1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & +1 \end{pmatrix}$

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

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

Inversion
 $\mathbf{I} = -\mathbf{1}$
commutes
with
all \mathbf{R}

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

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

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

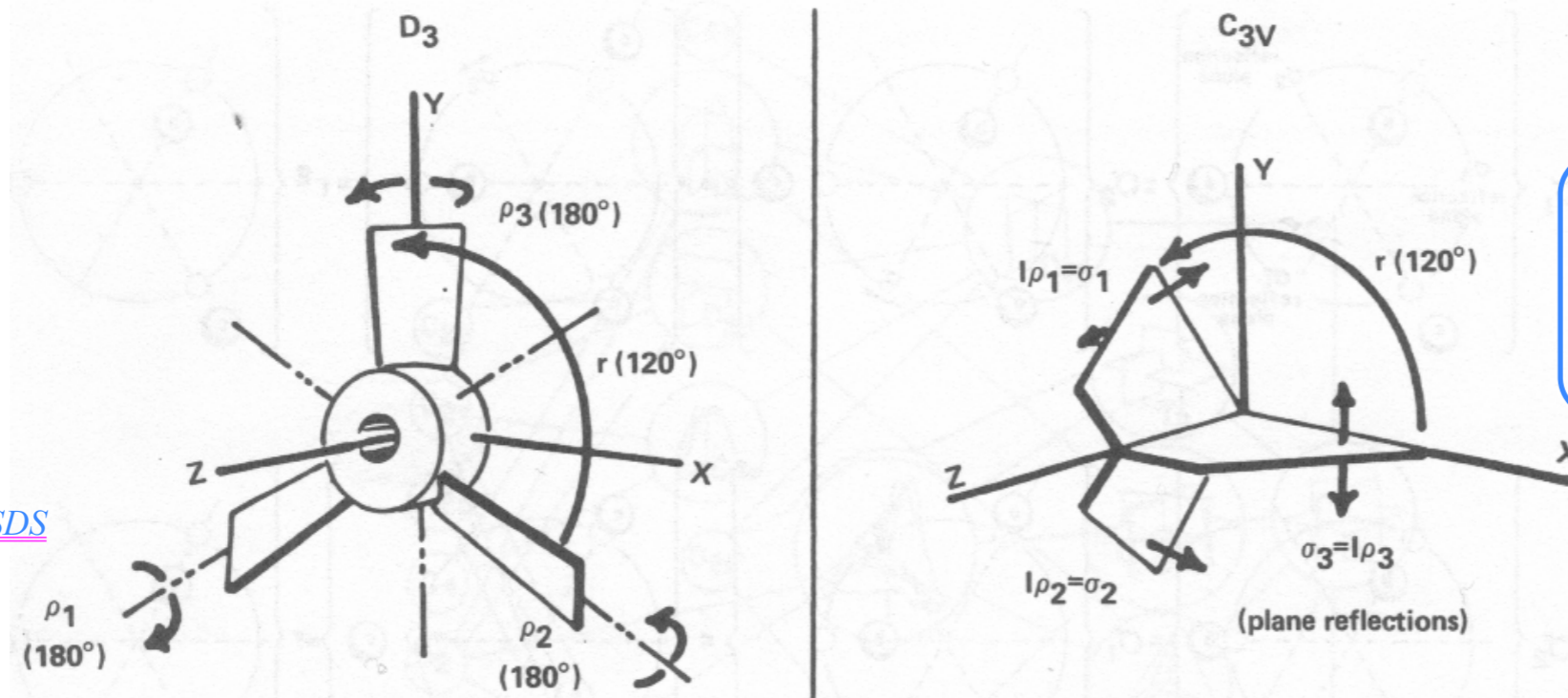


Fig. 3.1.3 PSDS

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$$= \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & +1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix} \begin{pmatrix} -1 & \cdot & \cdot \\ \cdot & -1 & \cdot \\ \cdot & \cdot & -1 \end{pmatrix}$$

$$= \rho_3 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_3$$

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

$180^\circ D_3$ - ρ_1 -axis-rotation: ρ_1

maps to: $\perp \rho_1$ -mirror-plane reflection: $\sigma_1 = \rho_1 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_1$

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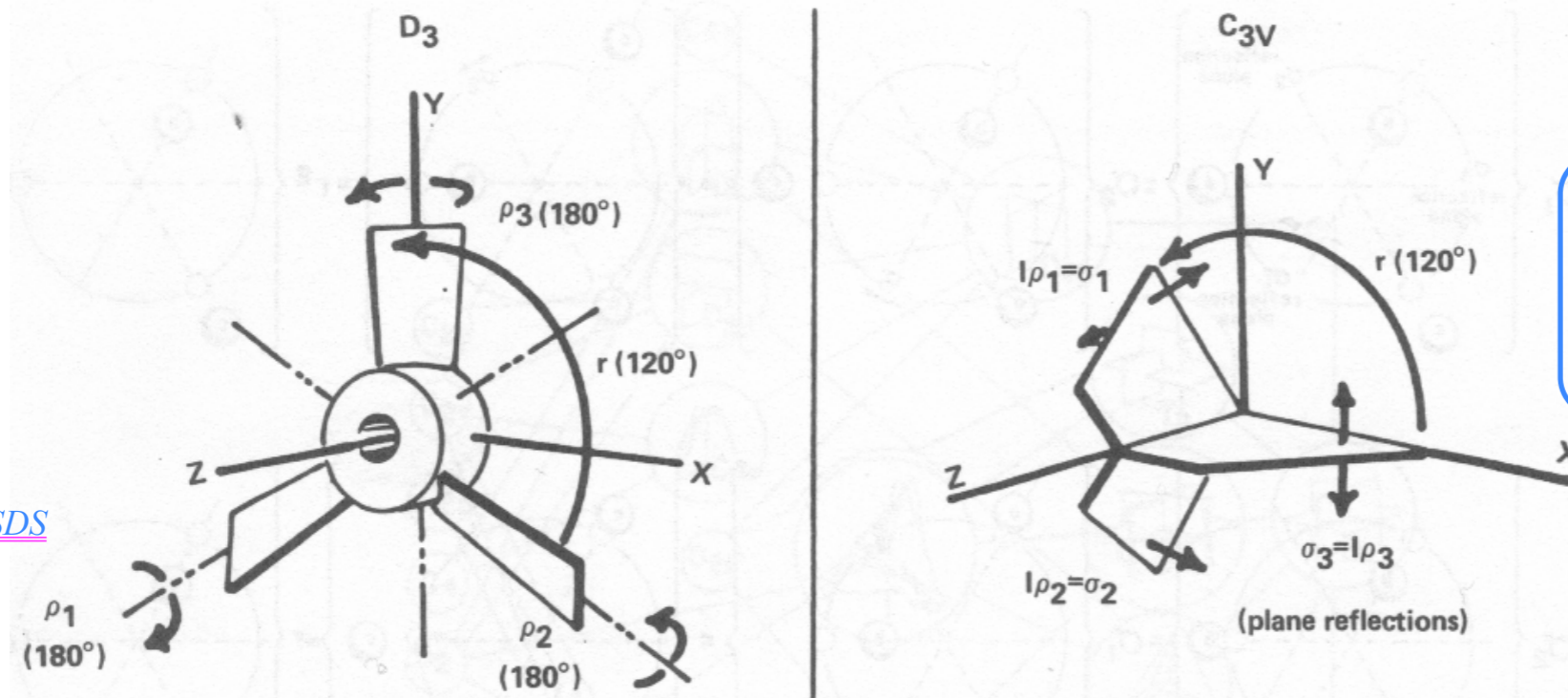


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$180^\circ D_3$ - ρ_1 -axis-rotation: ρ_1

maps to: $\perp \rho_1$ -mirror-plane reflection: $\sigma_1 = \rho_1 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_1$

D_3 -product: $\rho_1 \rho_2$

maps to: C_{3v} -product: $\sigma_1 \sigma_2 = \rho_1 \mathbf{I} \rho_2 = \rho_1 \rho_2$

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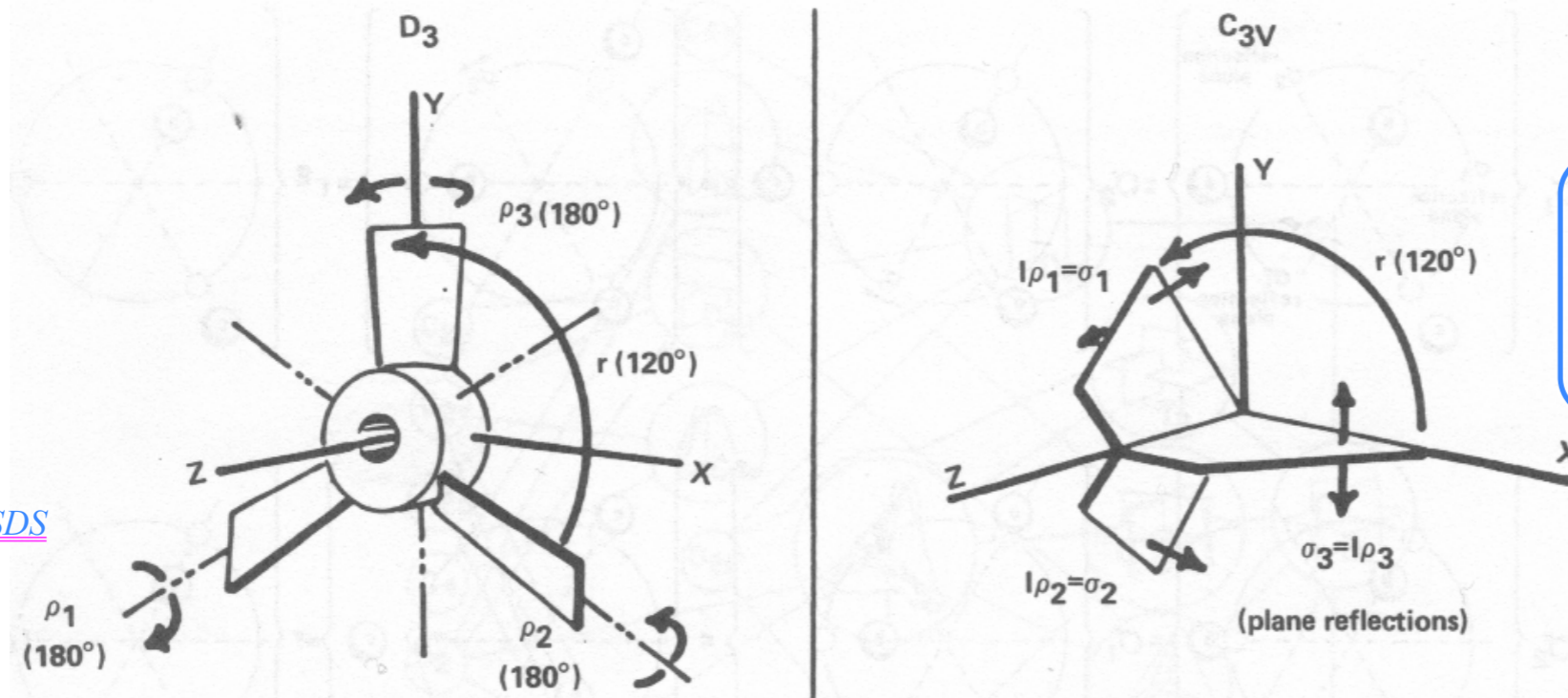


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$180^\circ D_3$ - ρ_2 -axis-rotation: ρ_2

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

$180^\circ D_3$ - ρ_1 -axis-rotation: ρ_1

maps to: $\perp \rho_1$ -mirror-plane reflection: $\sigma_1 = \rho_1 \cdot \mathbf{I} = \mathbf{I} \cdot \rho_1$

D_3 -product: $\rho_1 \rho_2$

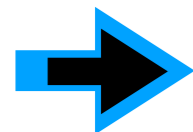
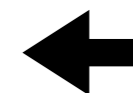
maps to: C_{3v} -product: $\sigma_1 \sigma_2 = \rho_1 \mathbf{I} \rho_2 = \rho_1 \rho_2$

D_3 -product: $\rho_1 \mathbf{r}^p$

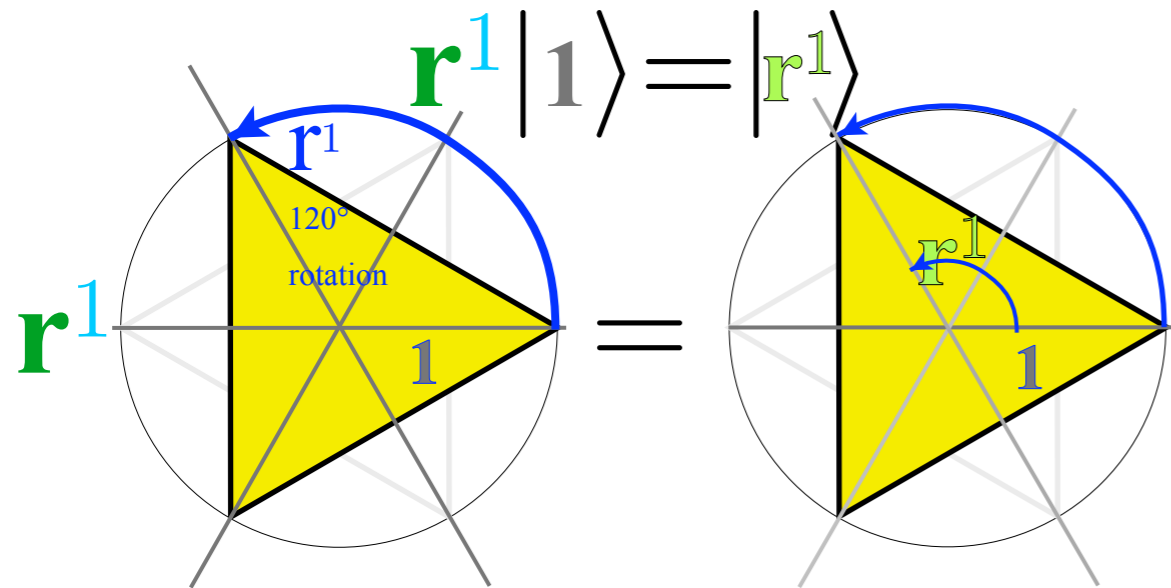
maps to: C_{3v} -product: $\sigma_1 \mathbf{r}^p = \rho_1 \mathbf{I} \mathbf{r}^p = \rho_1 \mathbf{r}^p \mathbf{I} = \mathbf{I} \rho_1 \mathbf{r}^p$

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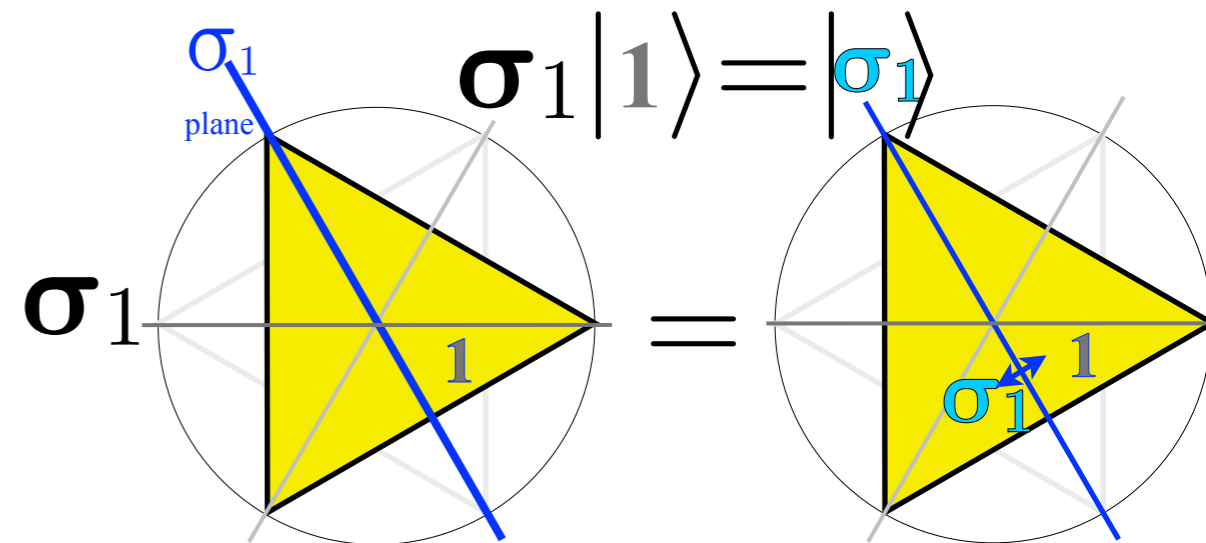
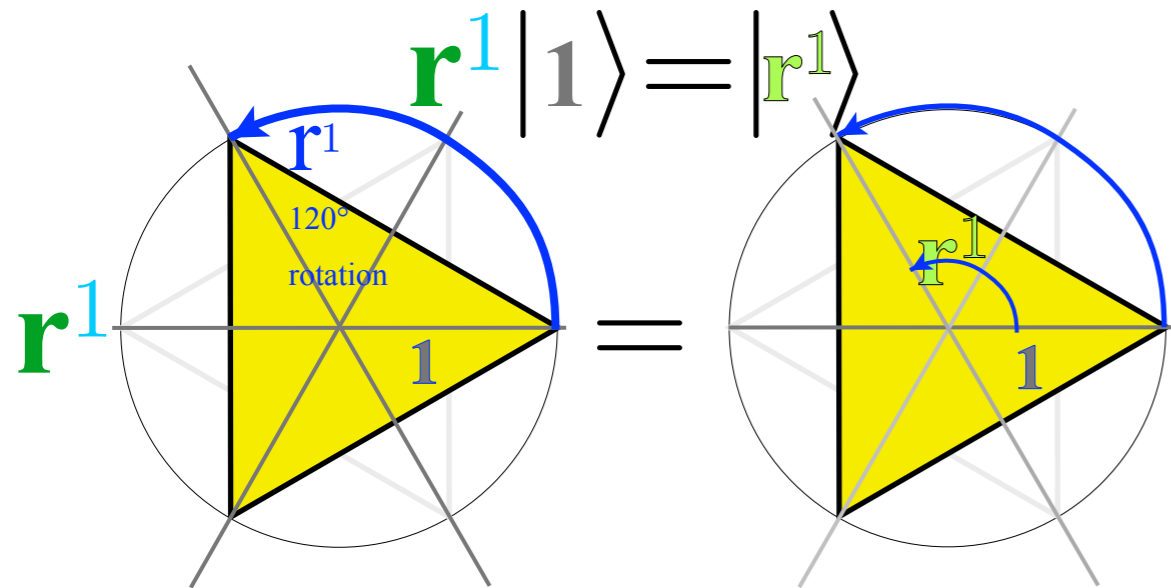
Showing that D_3 and C_{3v} are isomorphic* ($D_3 \sim C_{3v}$ share product table)

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$* *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**Group theory and algebra of D_3 Center (Class algebra)**Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes**1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

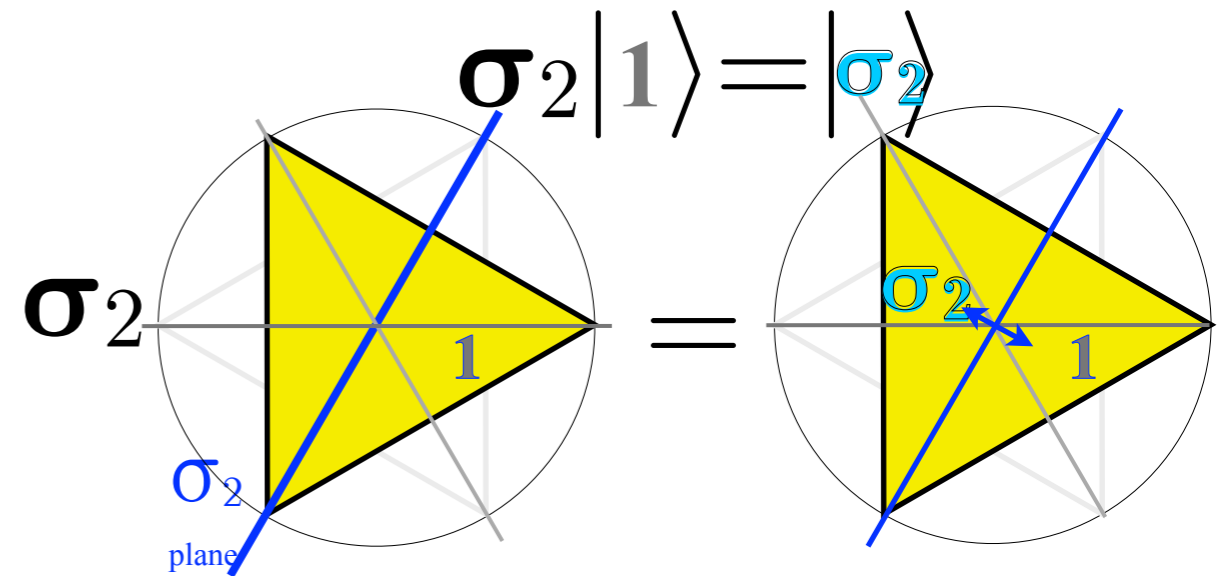
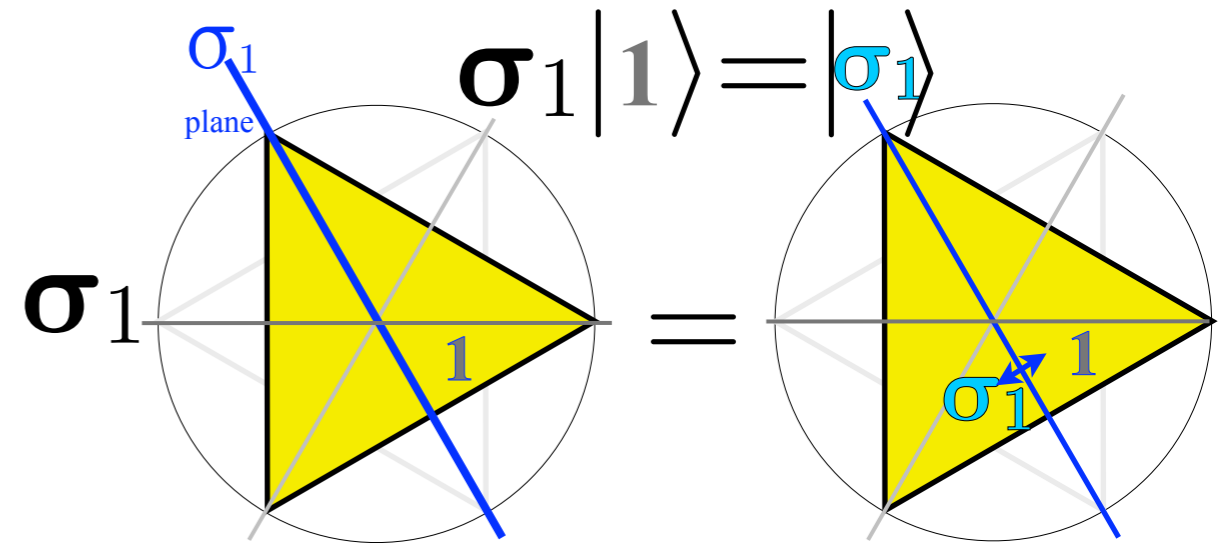
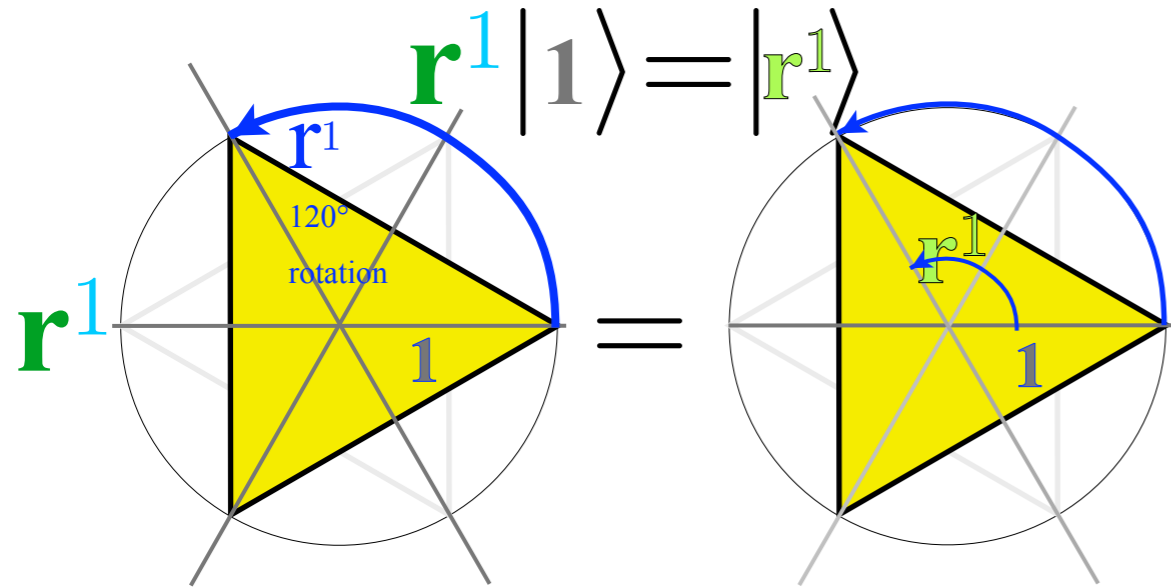
Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$



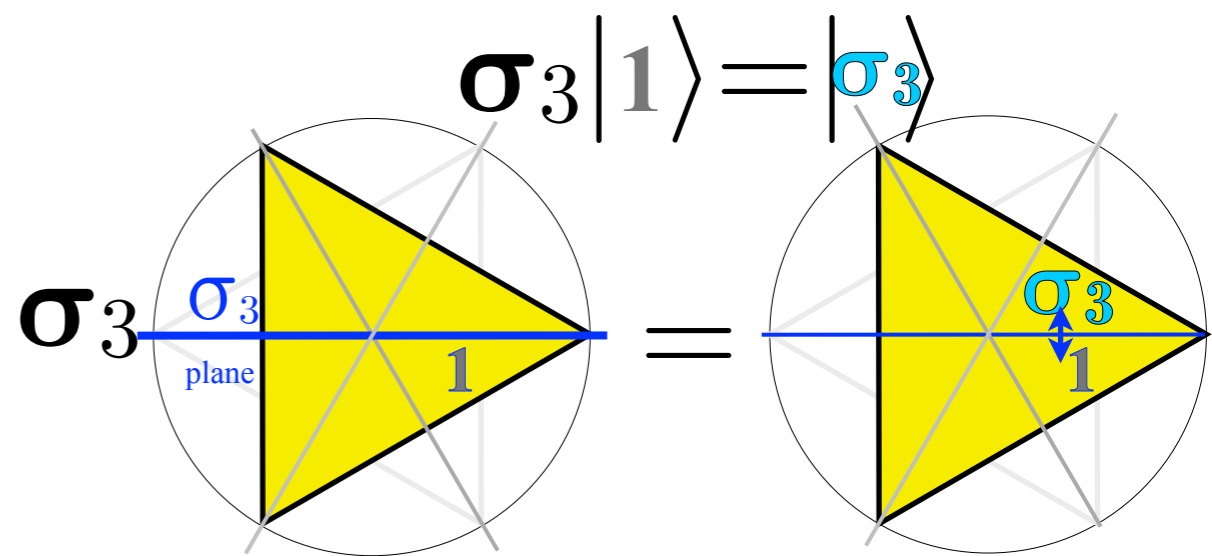
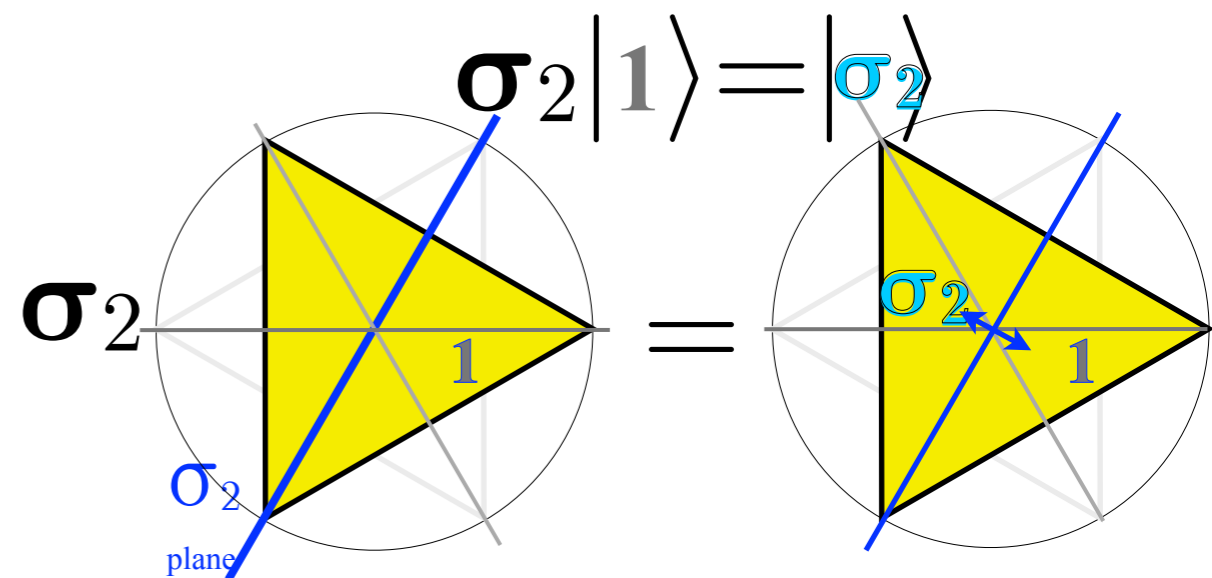
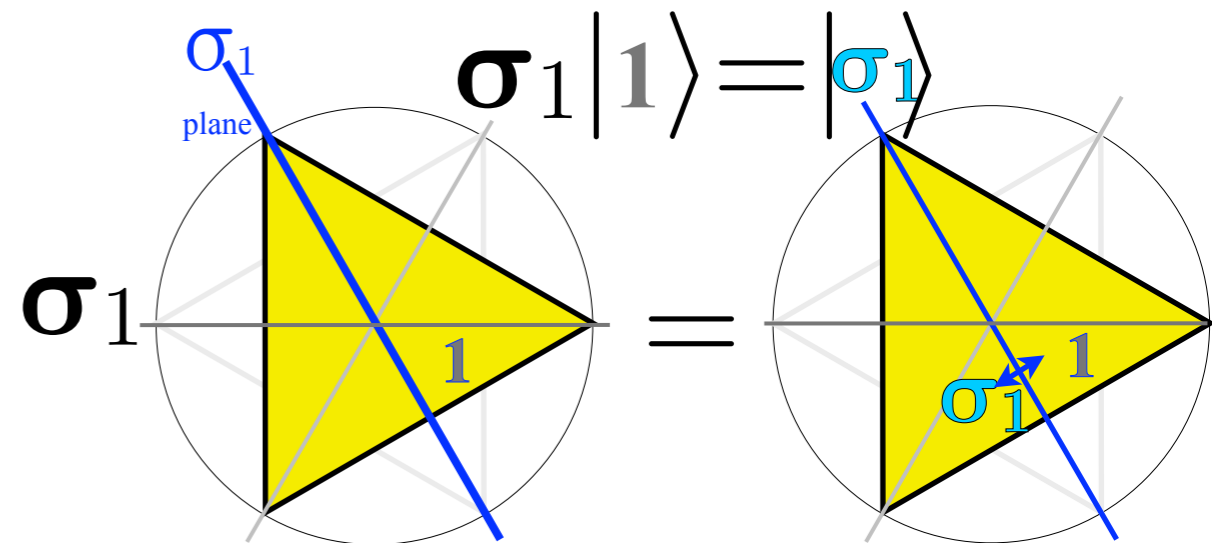
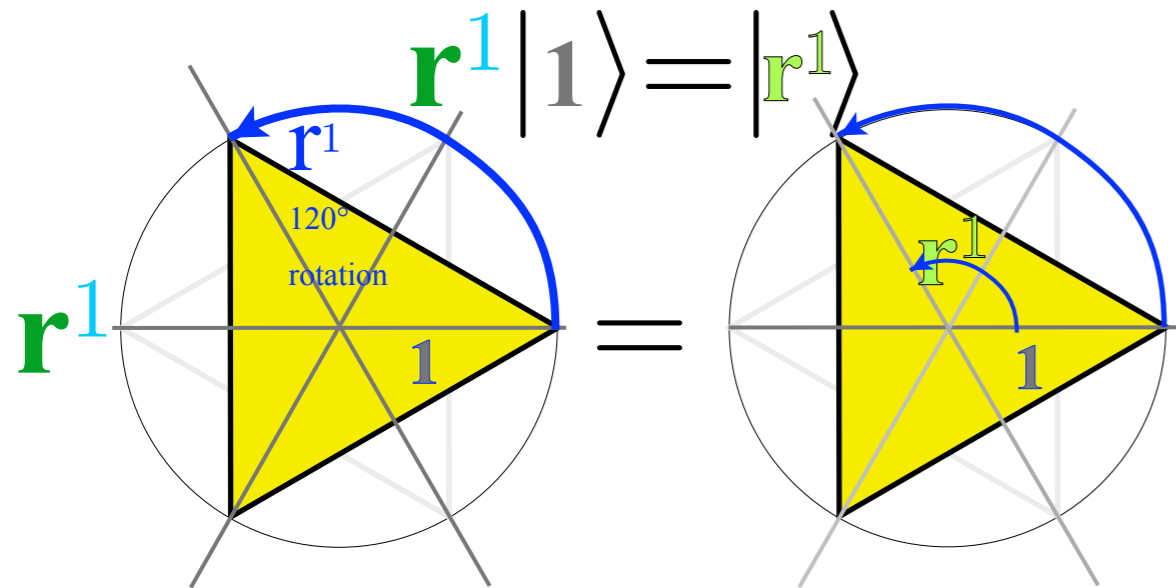
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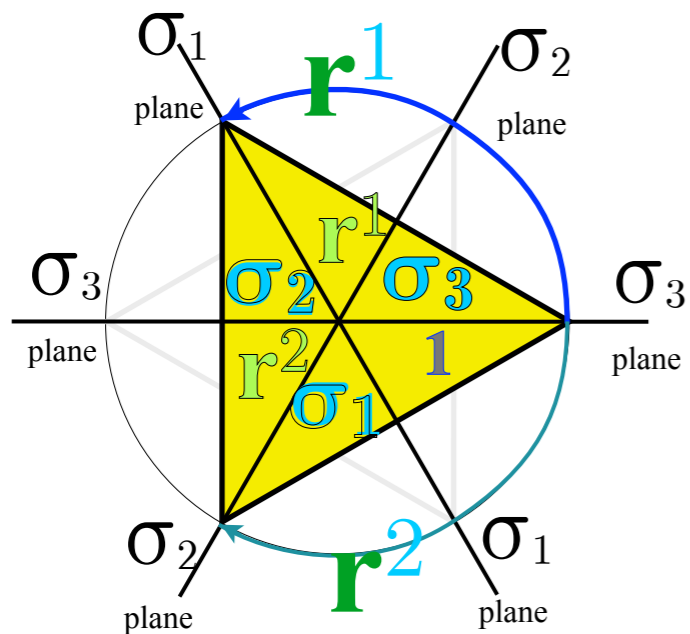


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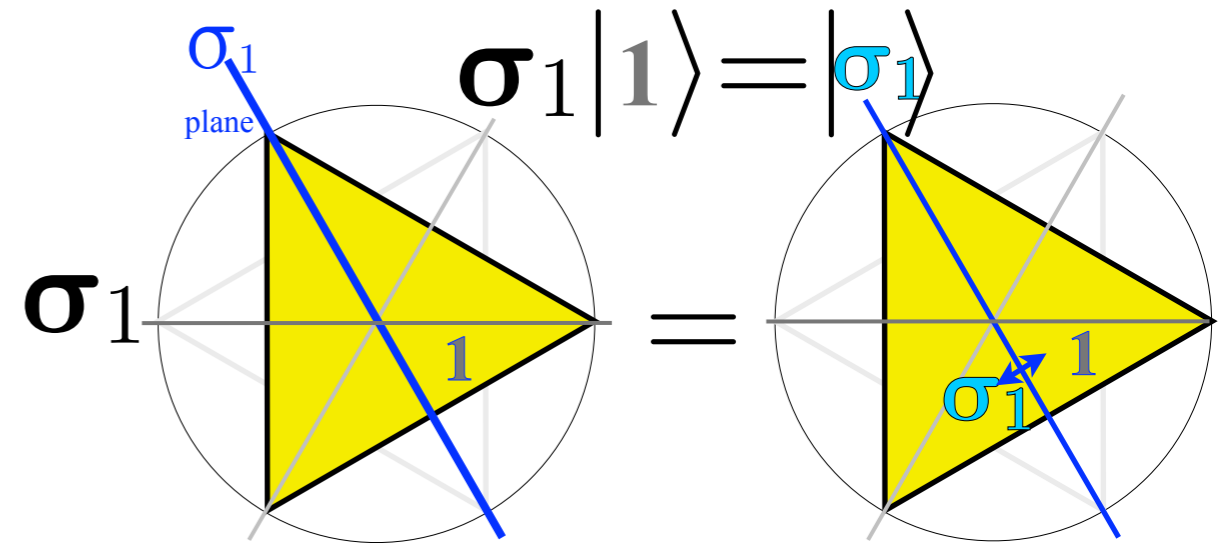
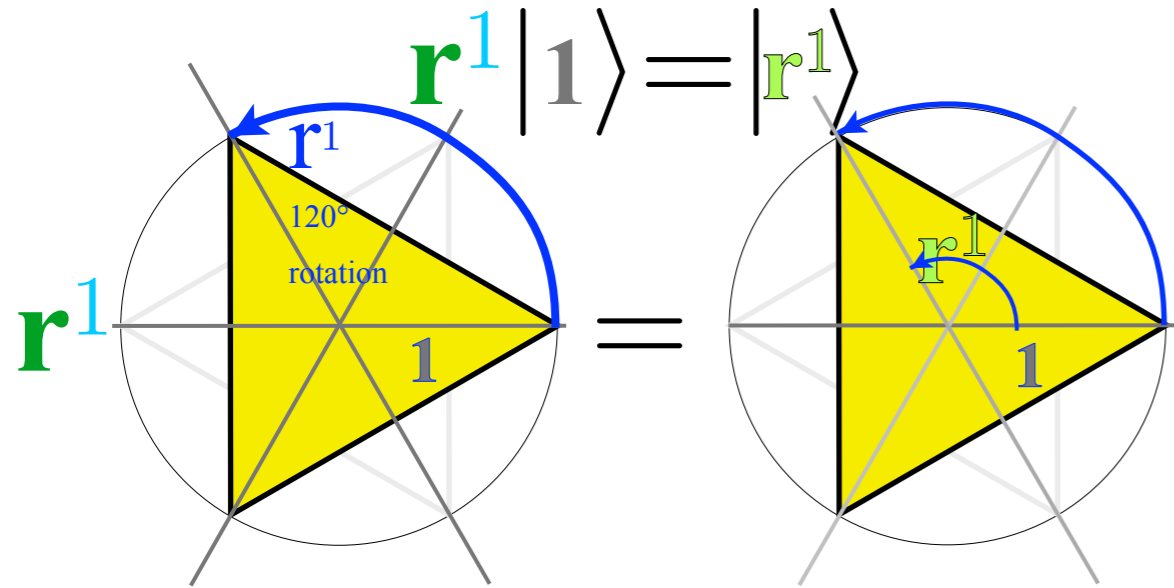


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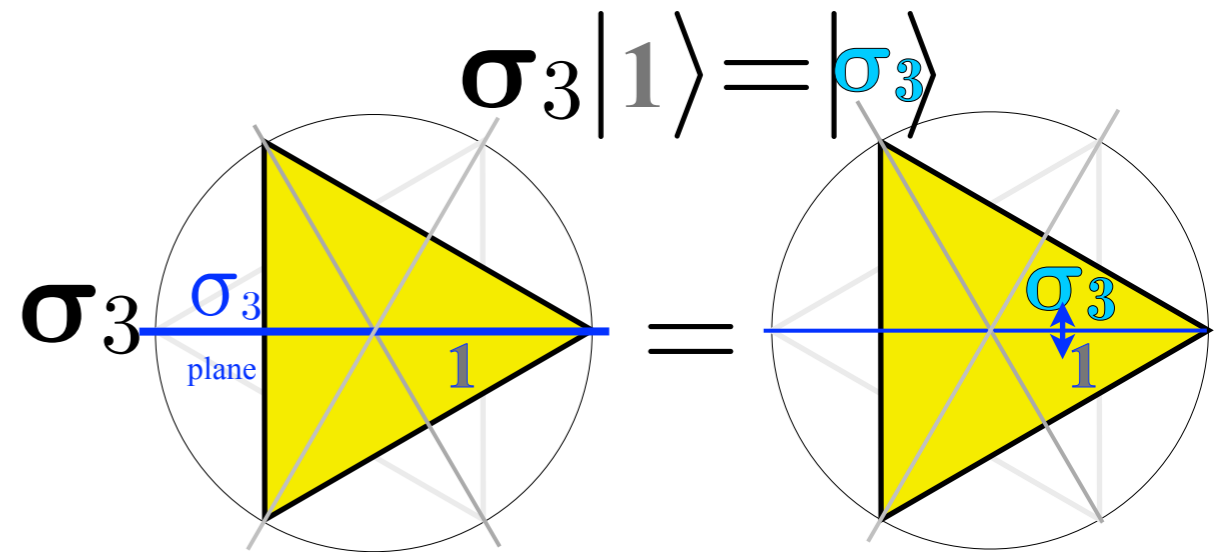
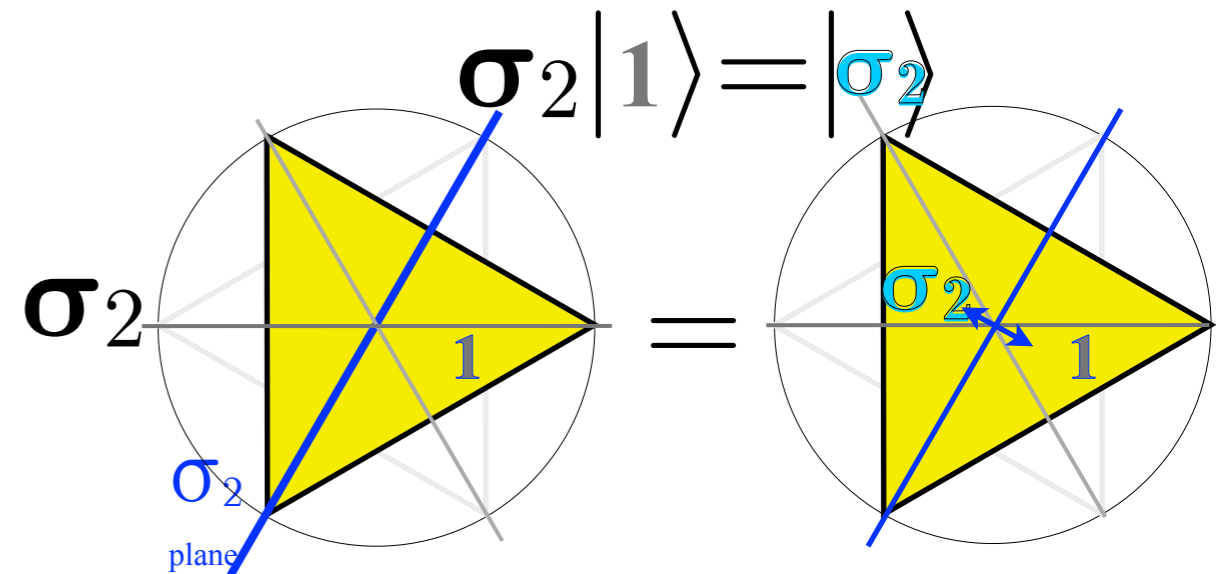
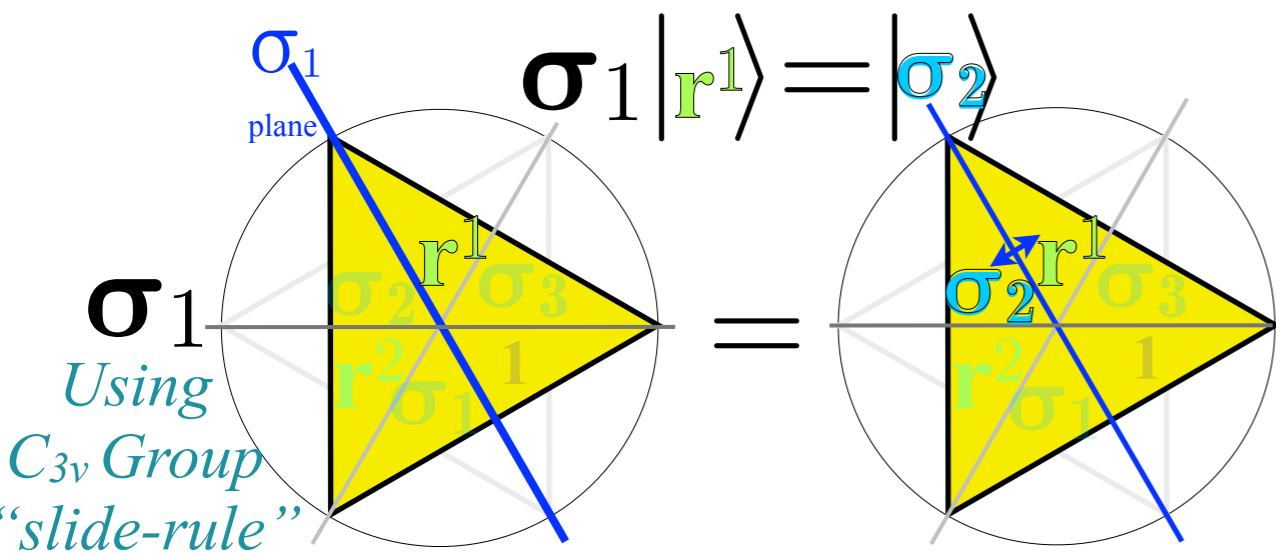
Building C_{3v} Group "slide-rule"



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

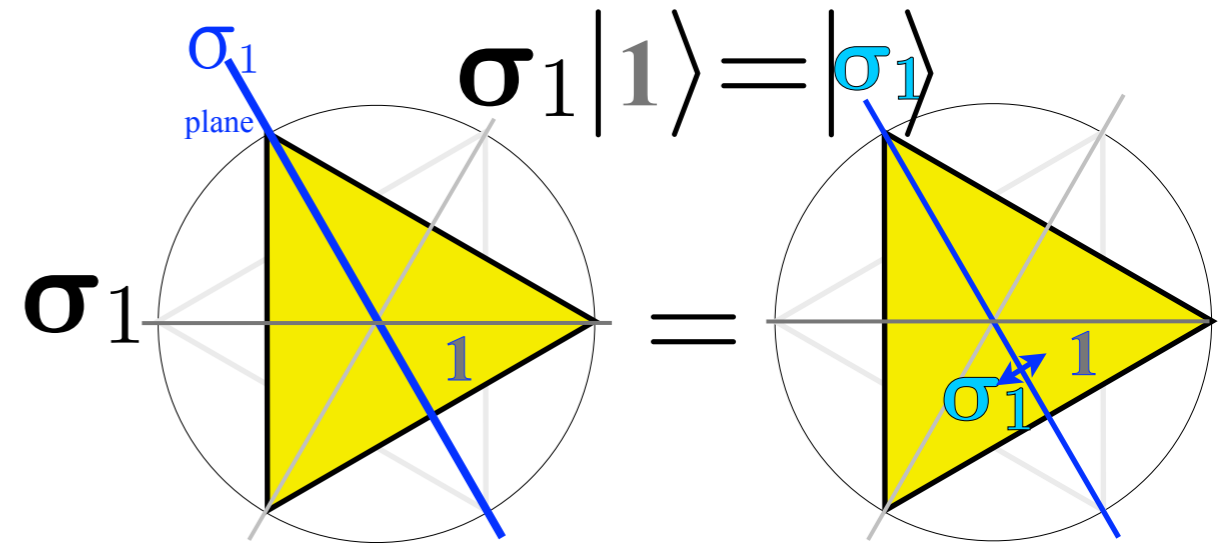
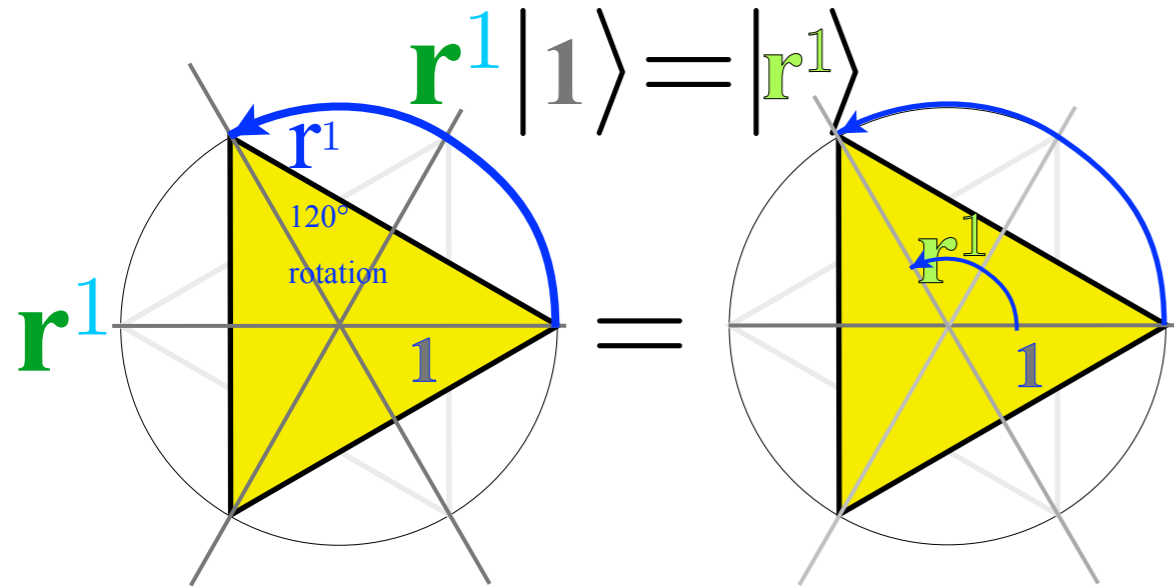


Example: Find C_{3v} product $\boldsymbol{\sigma}_1 \mathbf{r}^1 |1\rangle = \boldsymbol{\sigma}_1 |\mathbf{r}^1\rangle$

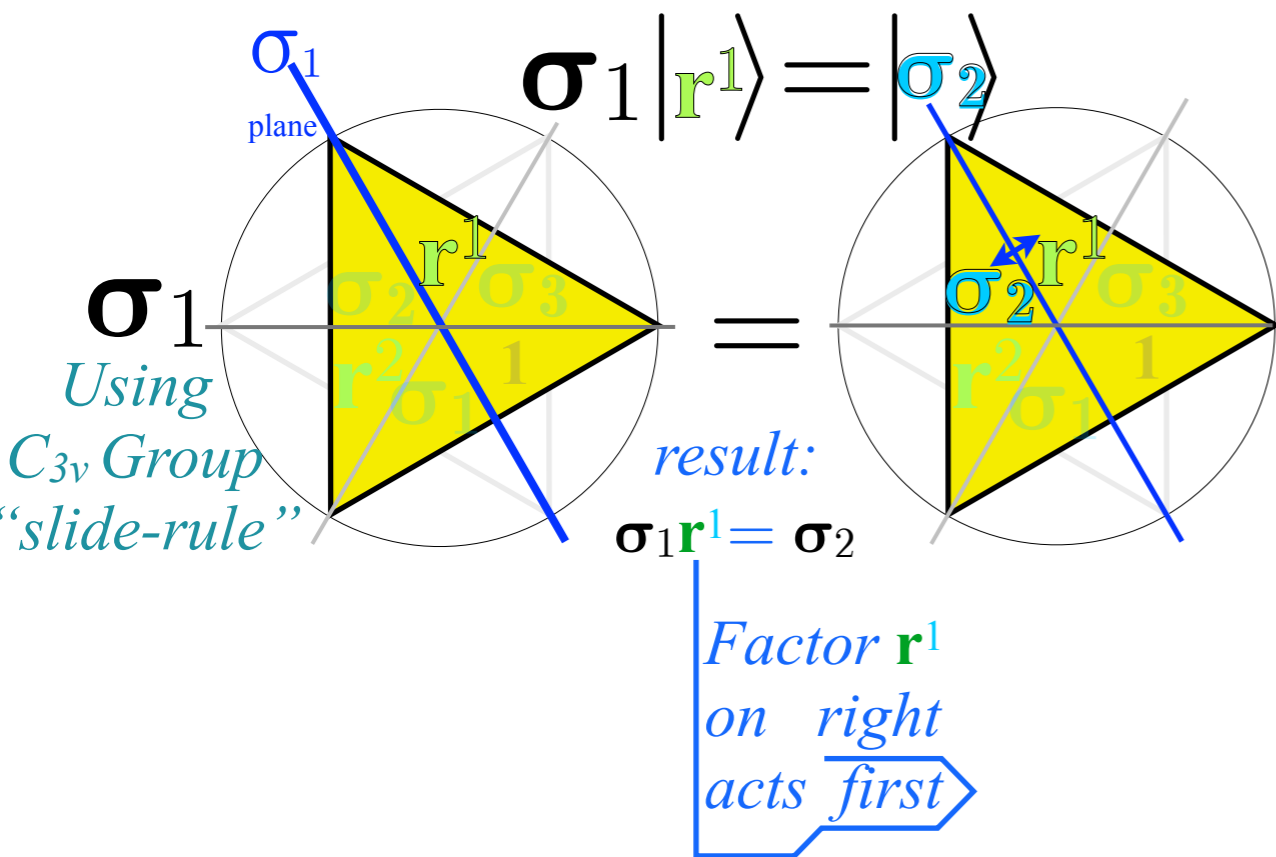


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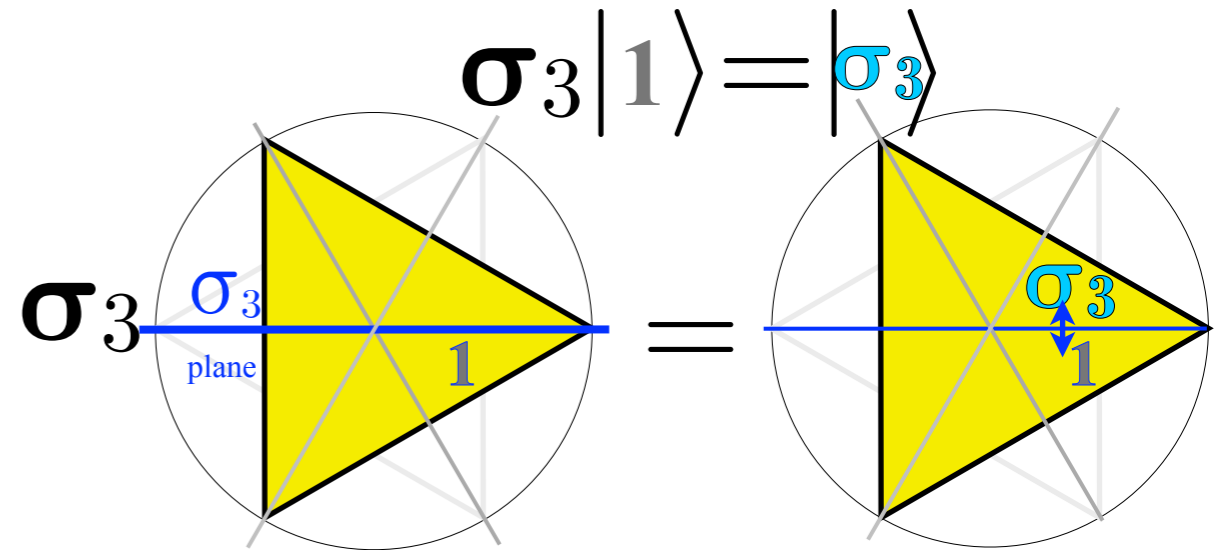
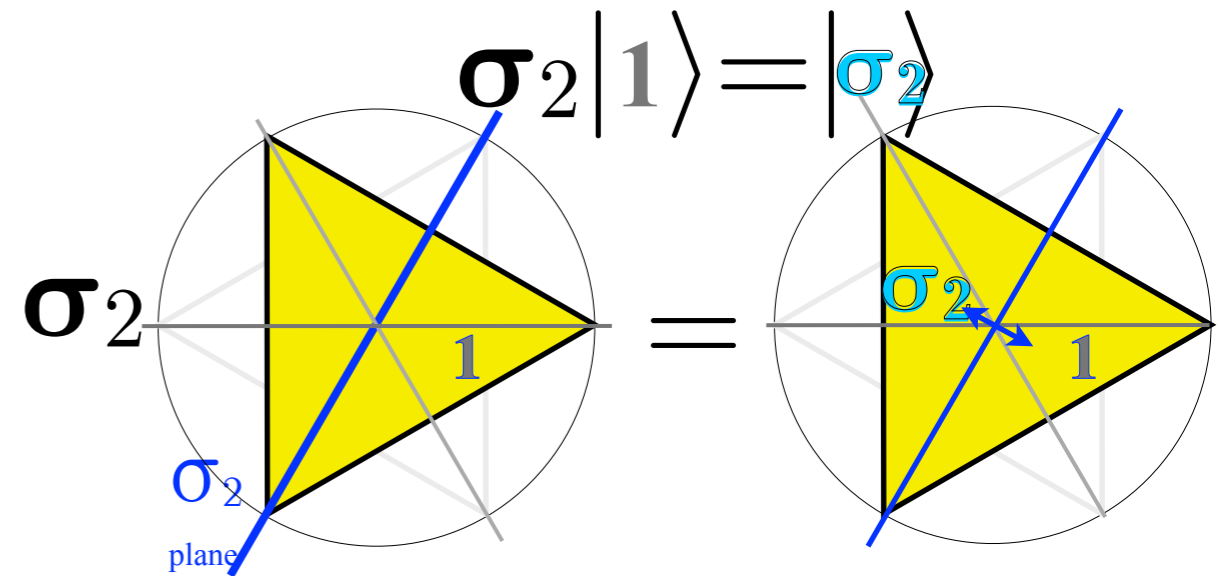
Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$



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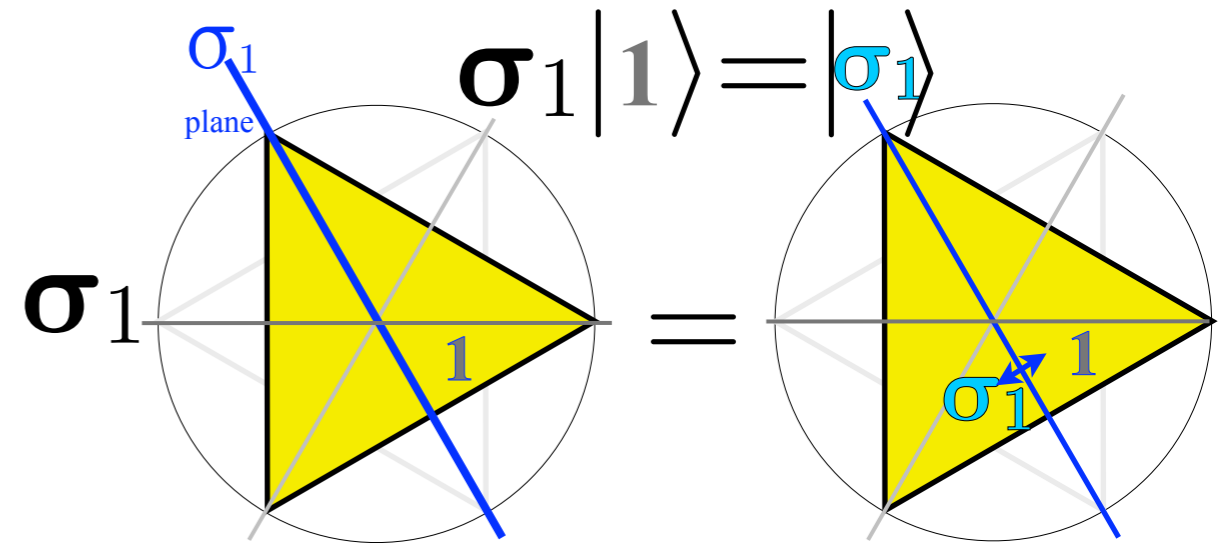
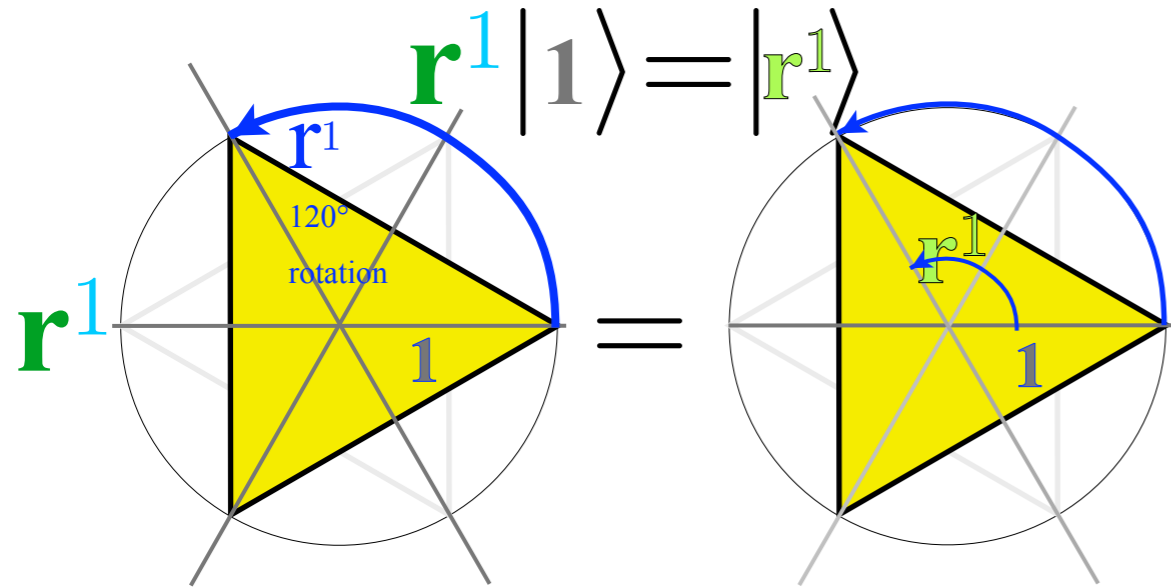


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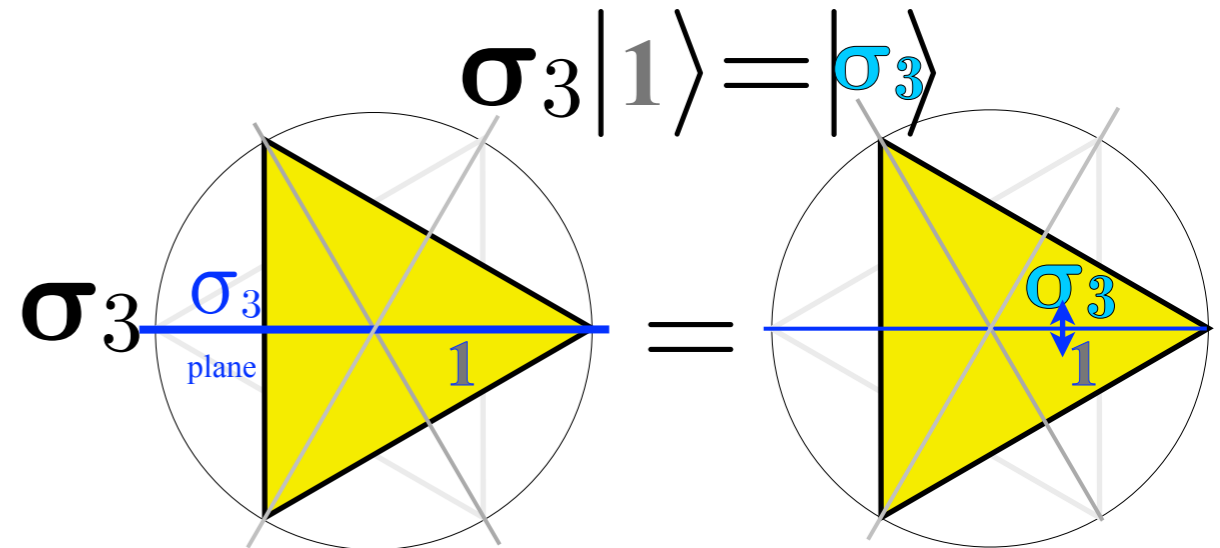
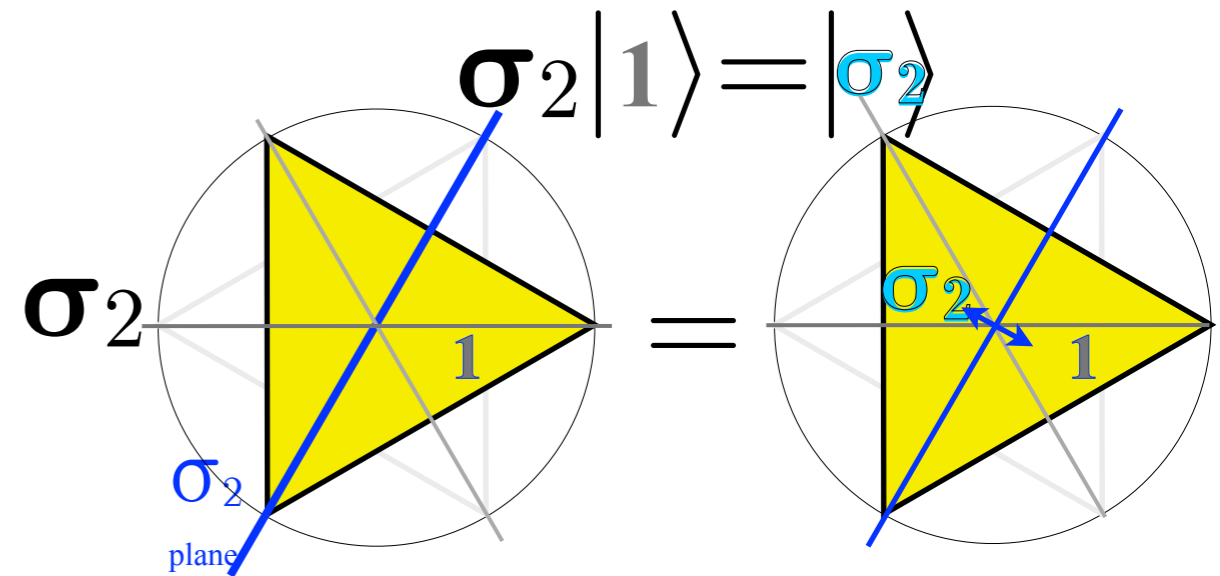
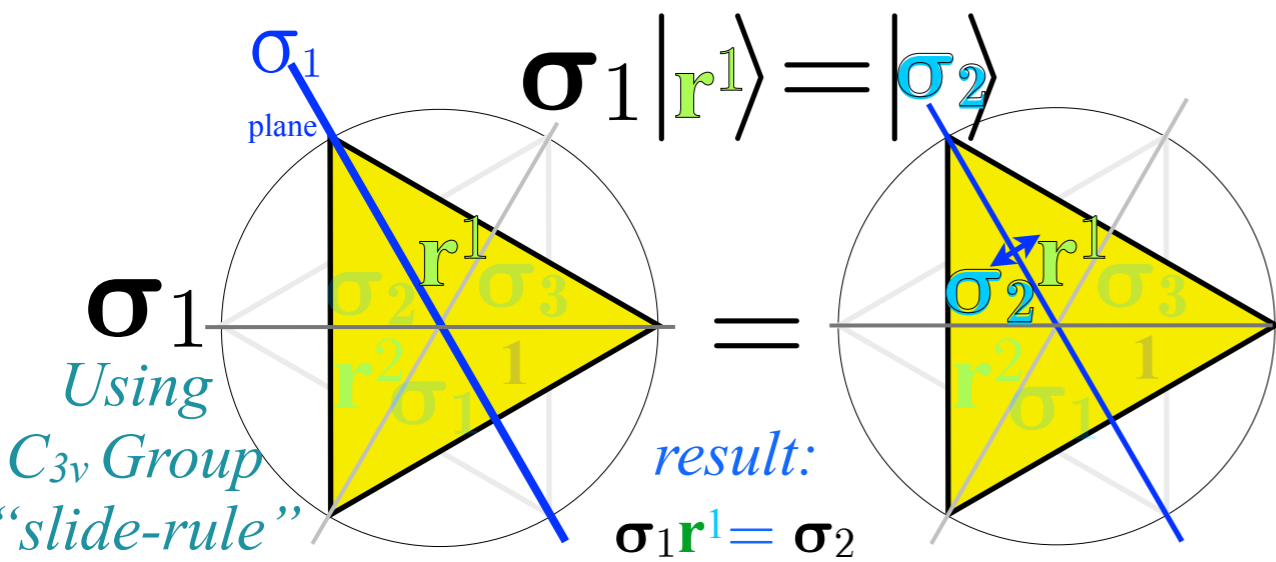


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Deriving $D_3 \sim C_{3v}$ products - By group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$



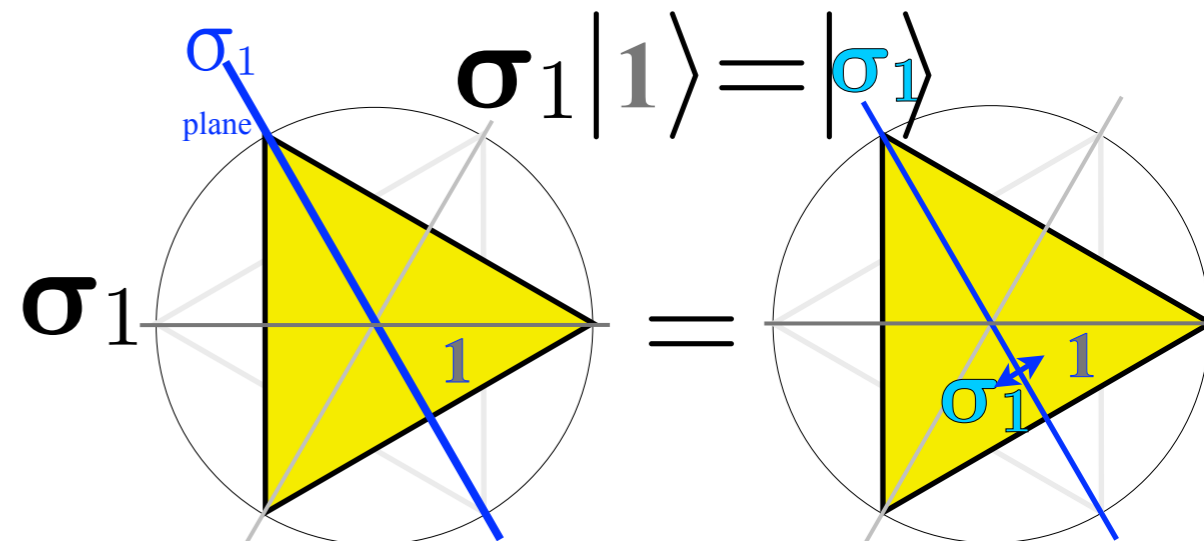
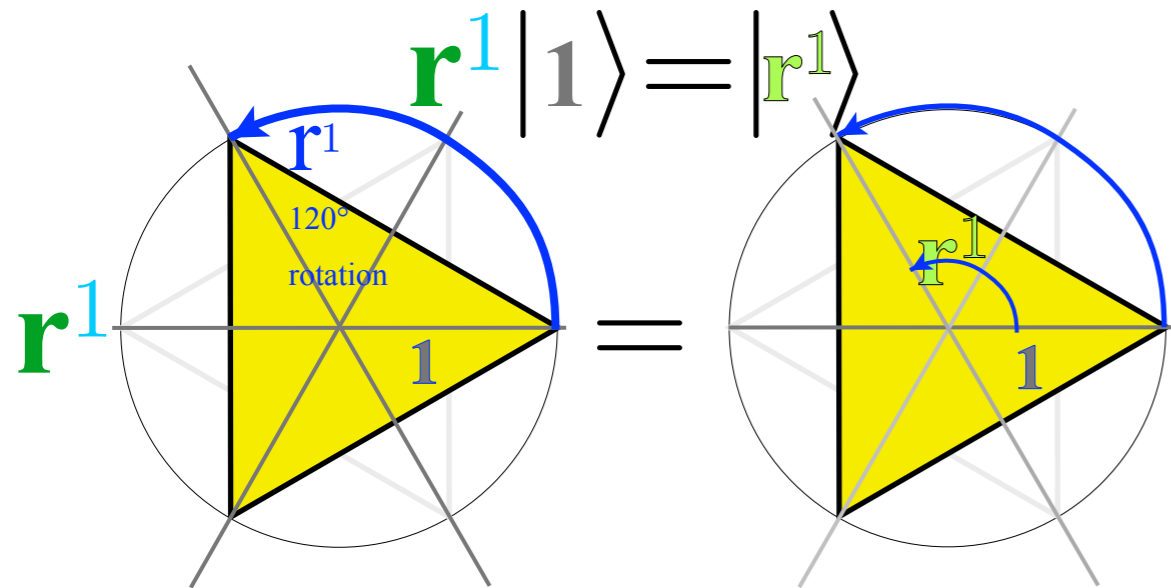
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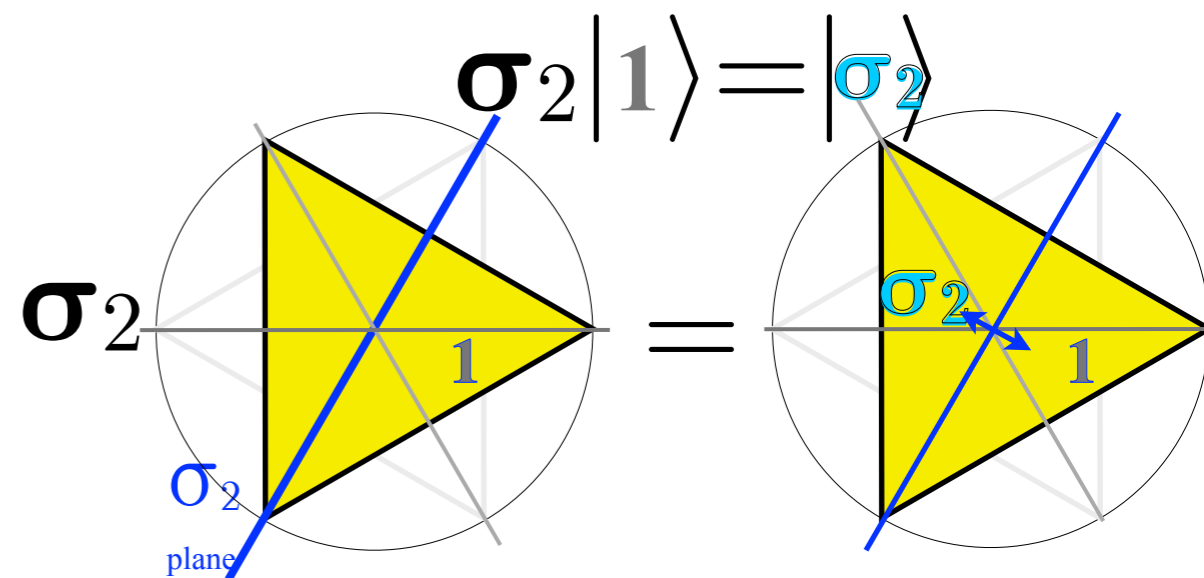
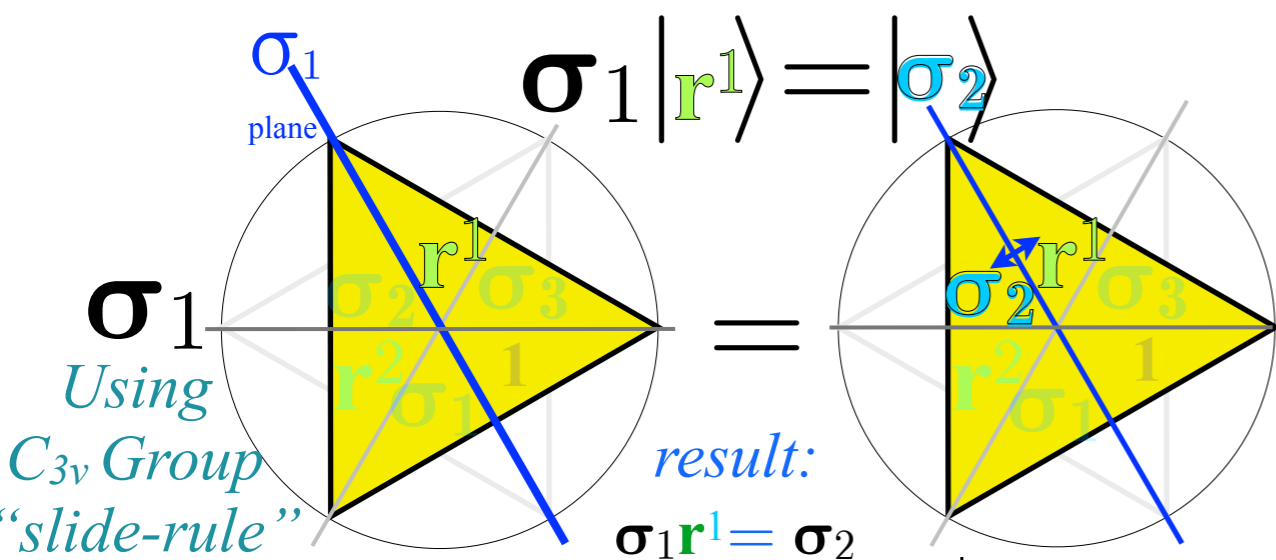
Other $\boldsymbol{\sigma}_1$ results from graph:

$$\boldsymbol{\sigma}_1 \{1, \mathbf{r}^1, \mathbf{r}^2, \boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3\} = \{\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3, 1, \mathbf{r}^1, \mathbf{r}^2\}$$

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 $\sigma_1 \mathbf{r}^1 |1\rangle = \sigma_1 |r^1\rangle$

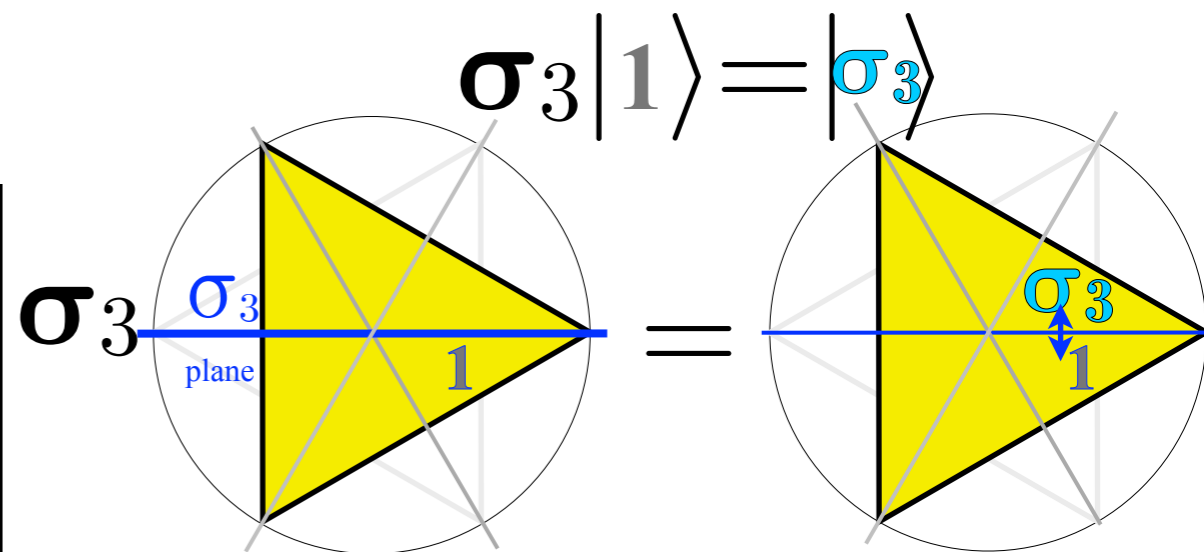


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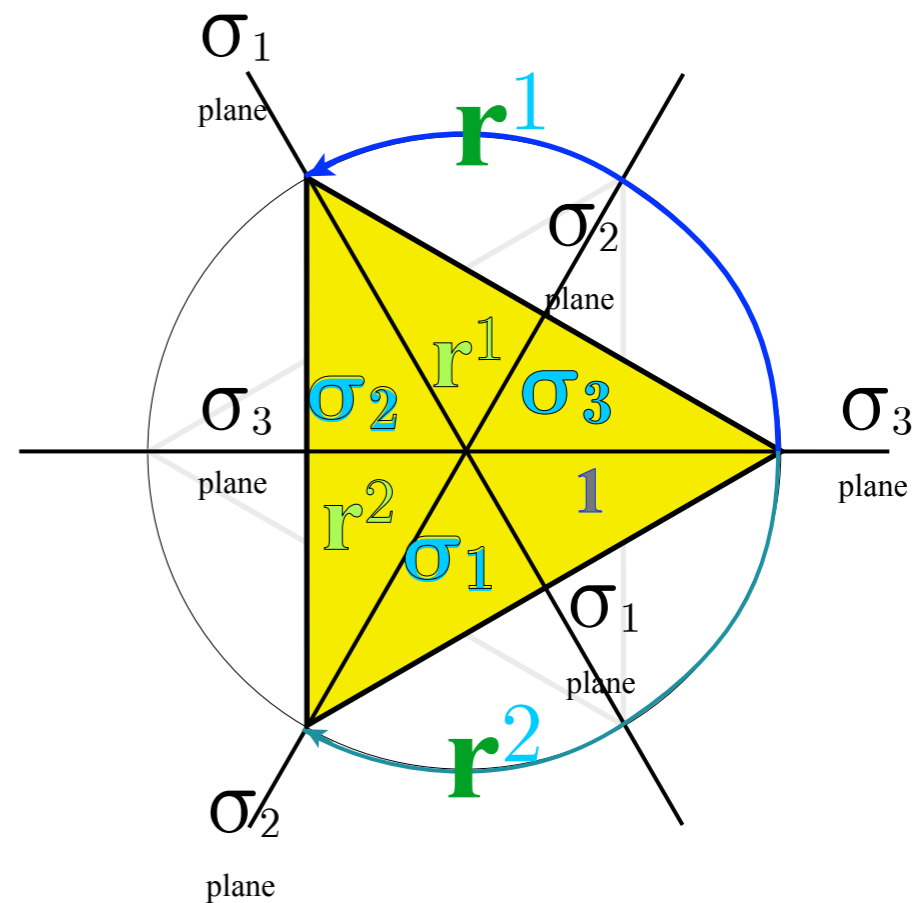
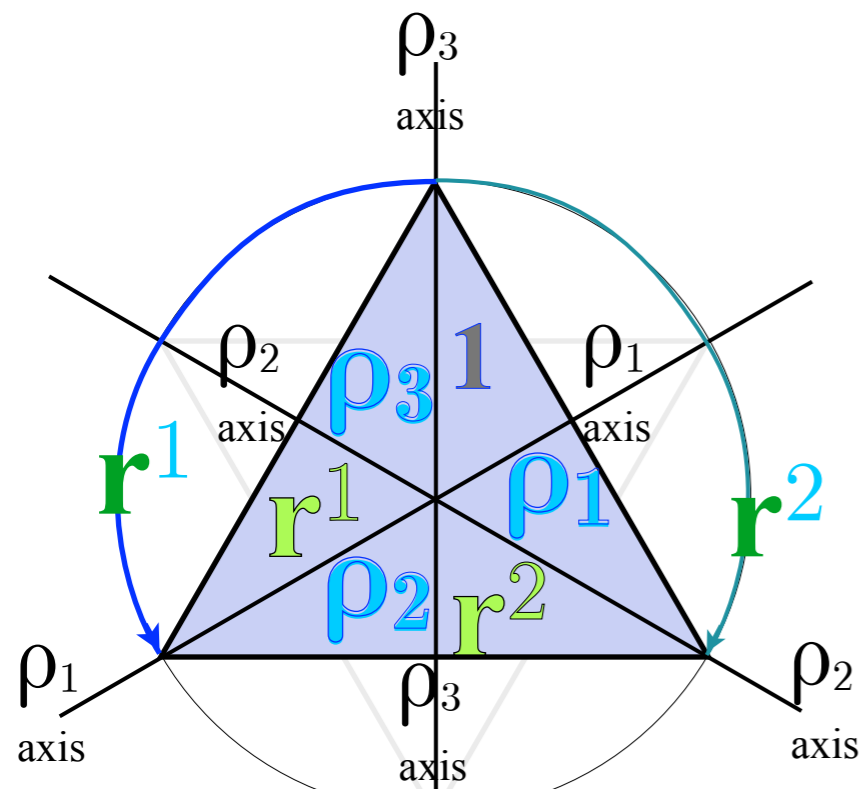
$$\sigma_1 \{1, \mathbf{r}^1, \mathbf{r}^2, \sigma_1, \sigma_2, \sigma_3\} = \{\sigma_1, \sigma_2, \sigma_3, 1, \mathbf{r}^1, \mathbf{r}^2\}$$

...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 $|g\rangle$



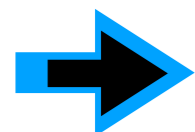
D_3 gg^\dagger form	1	r^2	r^1	ρ_1	ρ_2	ρ_3
1	1	r^2	r^1	ρ_1	ρ_2	ρ_3
r^1	r^1	1	r^2	ρ_3	ρ_1	ρ_2
r^2	r^2	r^1	1	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	1	r^1	r^2
ρ_2	ρ_2	ρ_1	ρ_3	r^2	1	r^1
ρ_3	ρ_3	ρ_2	ρ_1	r^1	r^2	1

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



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

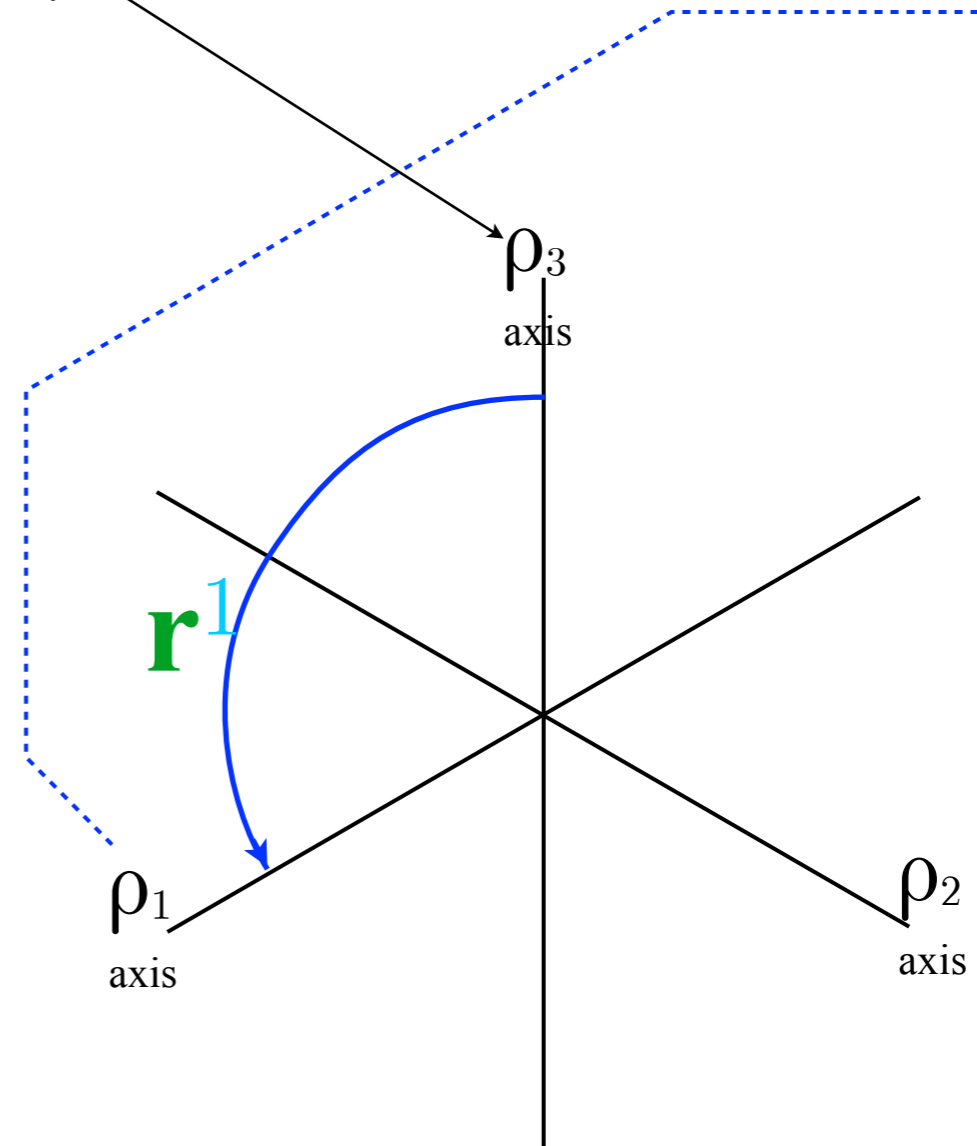
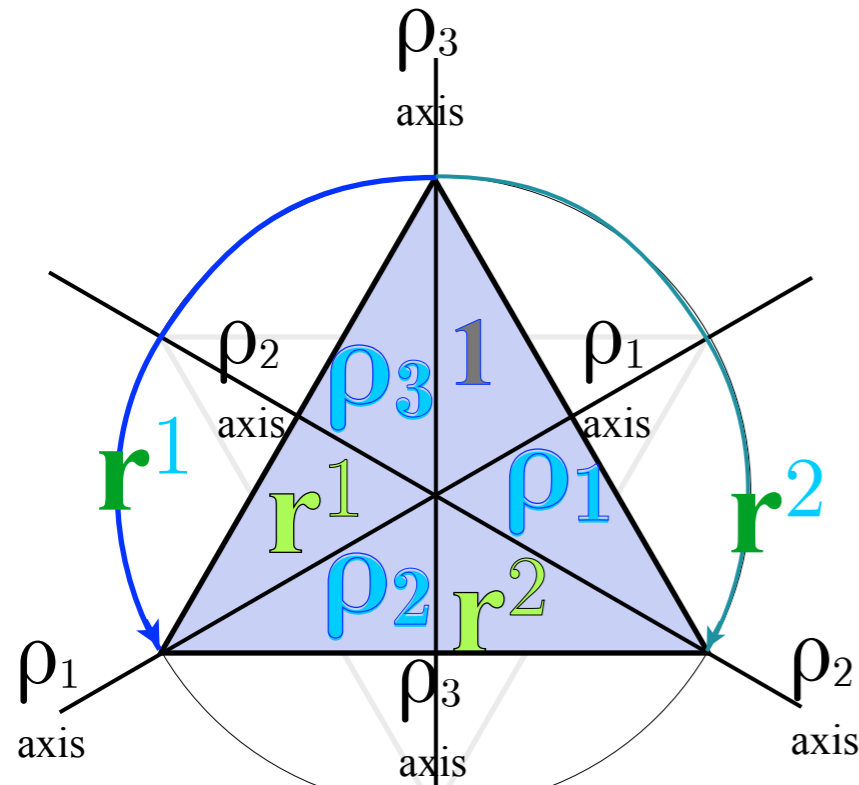
C_{3v} gg^\dagger form	1	r^2	r^1	σ_1	σ_2	σ_3
1	1	r^2	r^1	σ_1	σ_2	σ_3
r^1	r^1	1	r^2	σ_3	σ_1	σ_2
r^2	r^2	r^1	1	σ_2	σ_3	σ_1
σ_1	σ_1	σ_3	σ_2	1	r^1	r^2
σ_2	σ_2	σ_1	σ_3	r^2	1	r^1
σ_3	σ_3	σ_2	σ_1	r^1	r^2	1

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
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Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

Transforming D_3 operators using D_3 operators

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



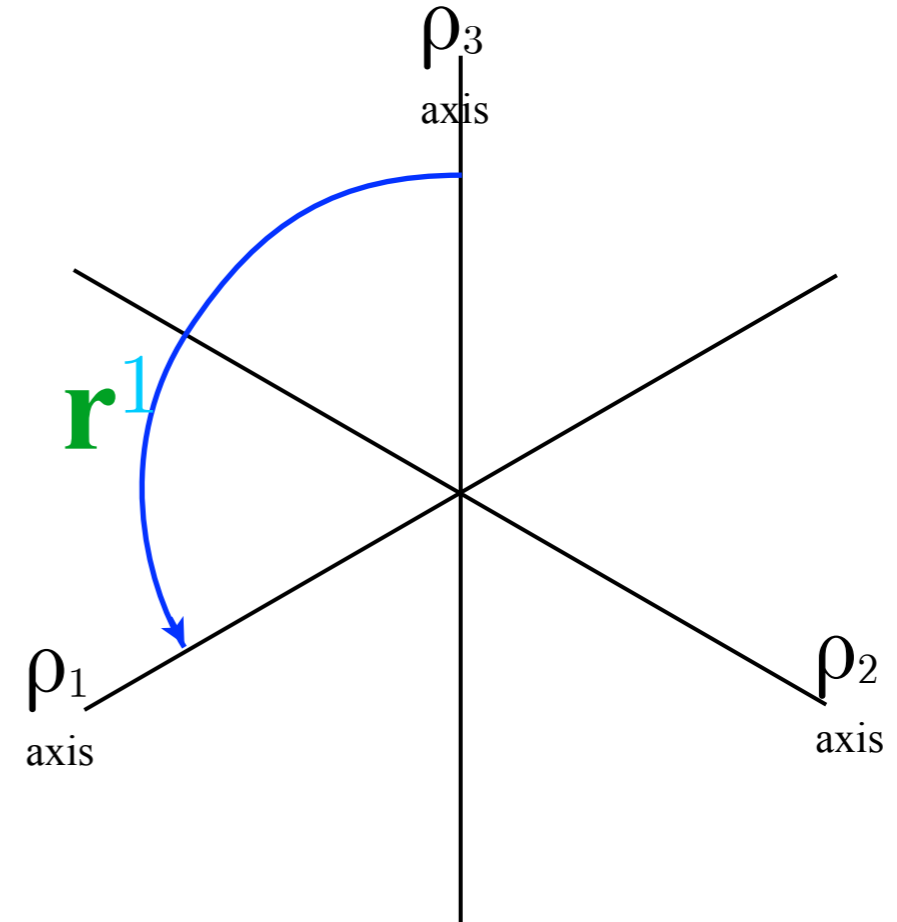
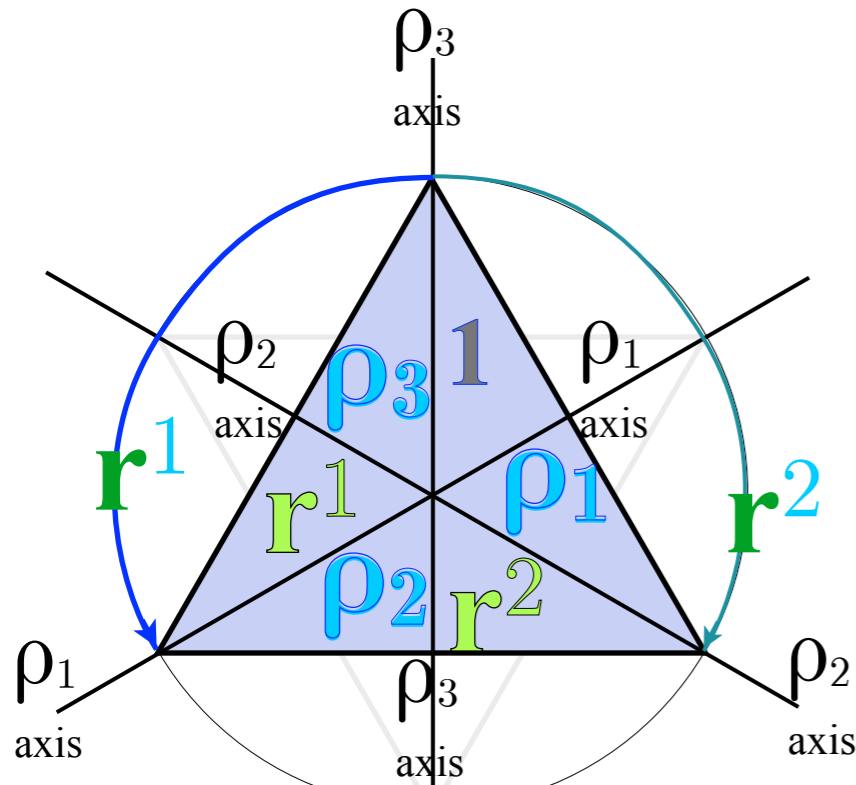
D_3 $g g^\dagger$ form	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
$\mathbf{1}$	$\mathbf{1}$	\mathbf{r}^2	\mathbf{r}^1	ρ_1	ρ_2	ρ_3
\mathbf{r}^1	\mathbf{r}^1	$\mathbf{1}$	\mathbf{r}^2	ρ_3	ρ_1	ρ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	$\mathbf{1}$	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	$\mathbf{1}$	\mathbf{r}^1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

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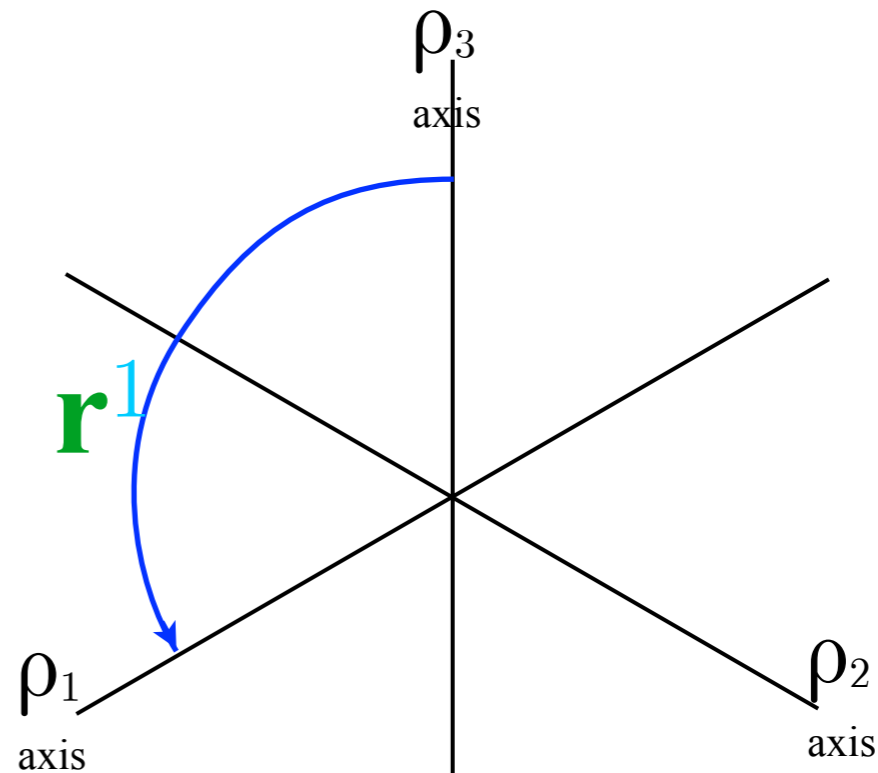
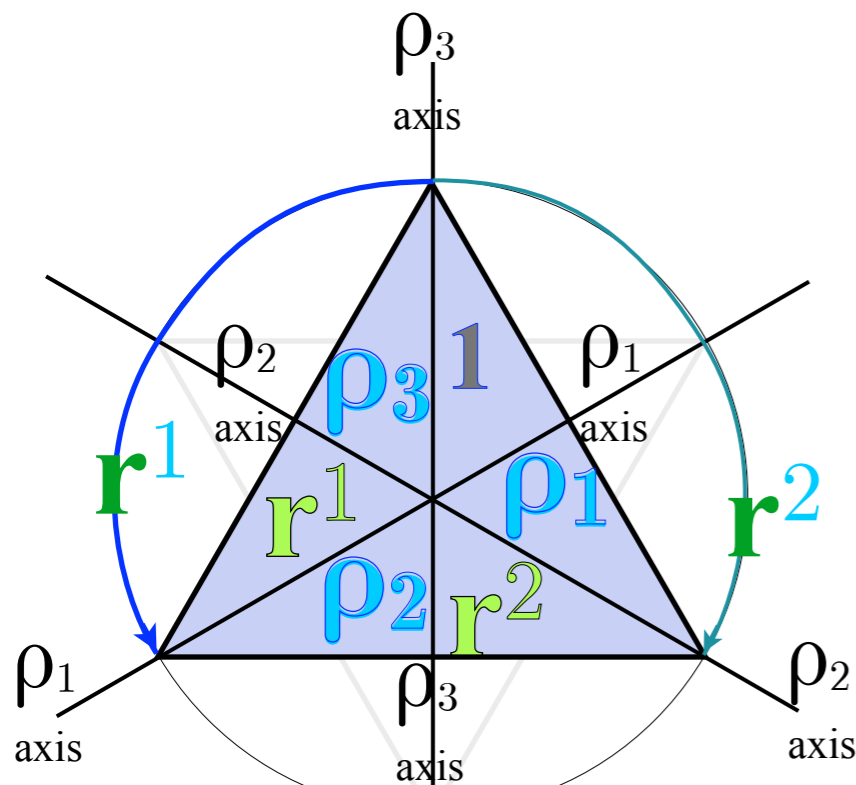
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\mathbf{r}^1	\mathbf{r}^1	1	\mathbf{r}^2	ρ_3	ρ_1	ρ_2
\mathbf{r}^2	\mathbf{r}^2	\mathbf{r}^1	1	ρ_2	ρ_3	ρ_1
ρ_1	ρ_1	ρ_3	ρ_2	1	\mathbf{r}^1	\mathbf{r}^2
ρ_2	ρ_2	ρ_1	ρ_3	\mathbf{r}^2	1	\mathbf{r}^1
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\mathbf{r}^1	\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
ρ_3	ρ_3	ρ_2	ρ_1	\mathbf{r}^1	\mathbf{r}^2	$\mathbf{1}$

Need to check that with table:

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

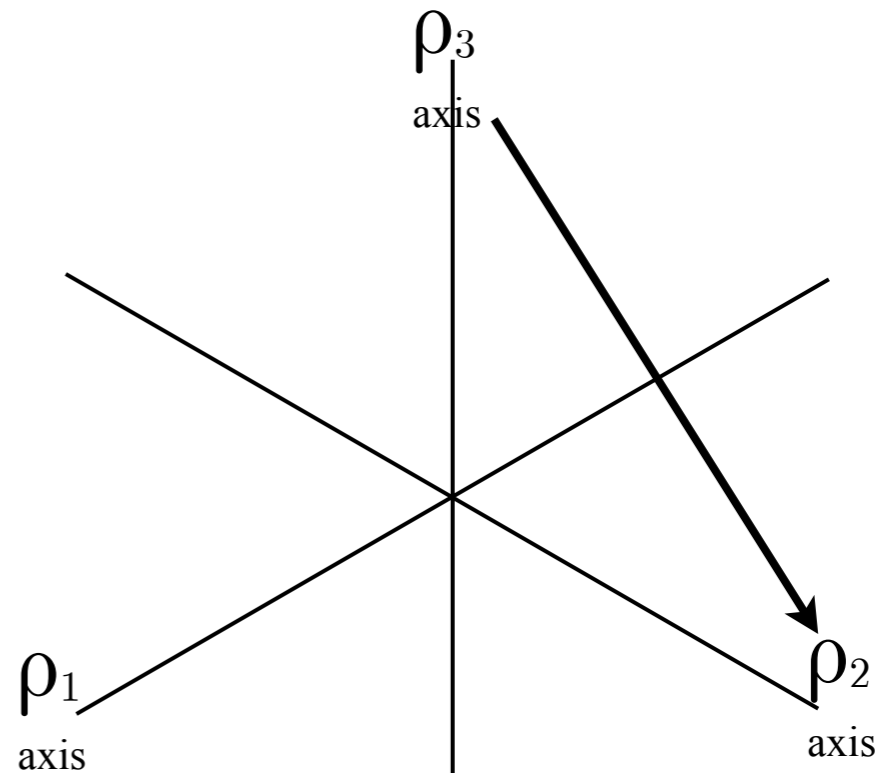
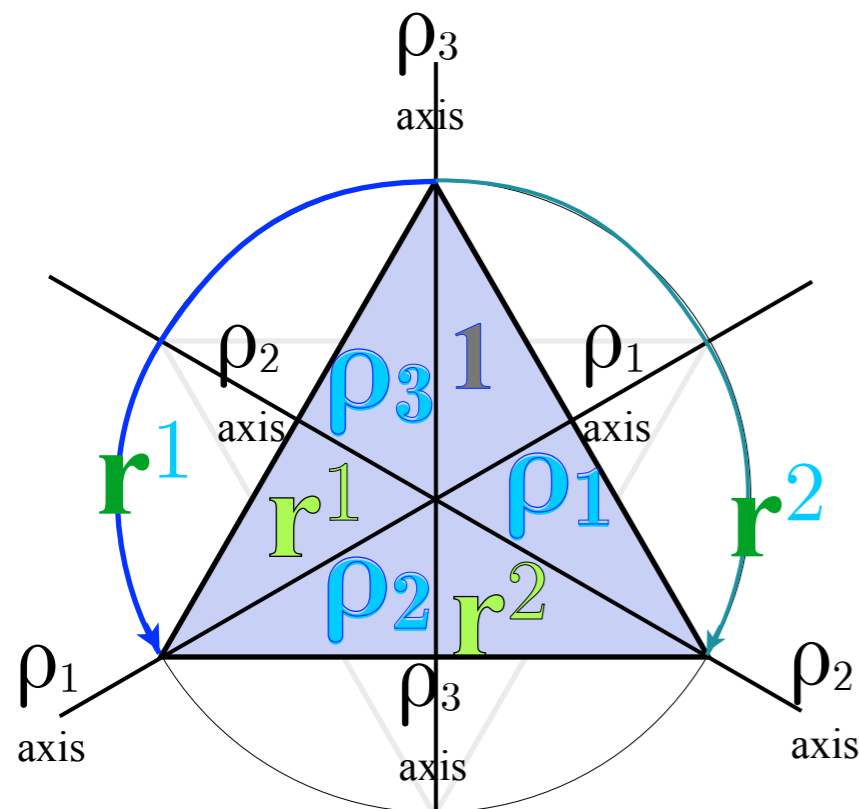
Checks out!

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\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
ρ_3	ρ_3	ρ_2	ρ_1	\mathbf{r}^1	\mathbf{r}^2	$\mathbf{1}$

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AMOP
reference links
on following page

2.21.18 class 12.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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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

Group theory and algebra of D_3 Center (Class algebra)

Self-symmetry (Normalizer).

Lagrange Coset Theorem for classes

1st-Stage spectral decomposition of “Group-table” Hamiltonian of D_3 symmetry

All-commuting operators \mathbf{K}_k

All-commuting projectors $\mathbf{P}^{(\alpha)}$

D_3 -invariant irep characters $\chi_k^{(\alpha)}$

Invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors

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3rd-Stage spectral decomposition of ALL of D_3

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GLOBAL vs LOCAL symmetry of states

...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$

Non-commutative symmetry expansion: Global-Local solution

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 ($r^p r^q = r^{p+q} = r^q r^p$).

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What we need to learn now:

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

While all H symmetry operations **COMMUTE** with H ($\mathbf{U} H = H \mathbf{U}$)

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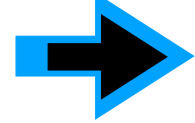
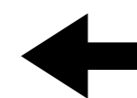
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Q: So how do we write H in terms of non-commutative \mathbf{U} ?

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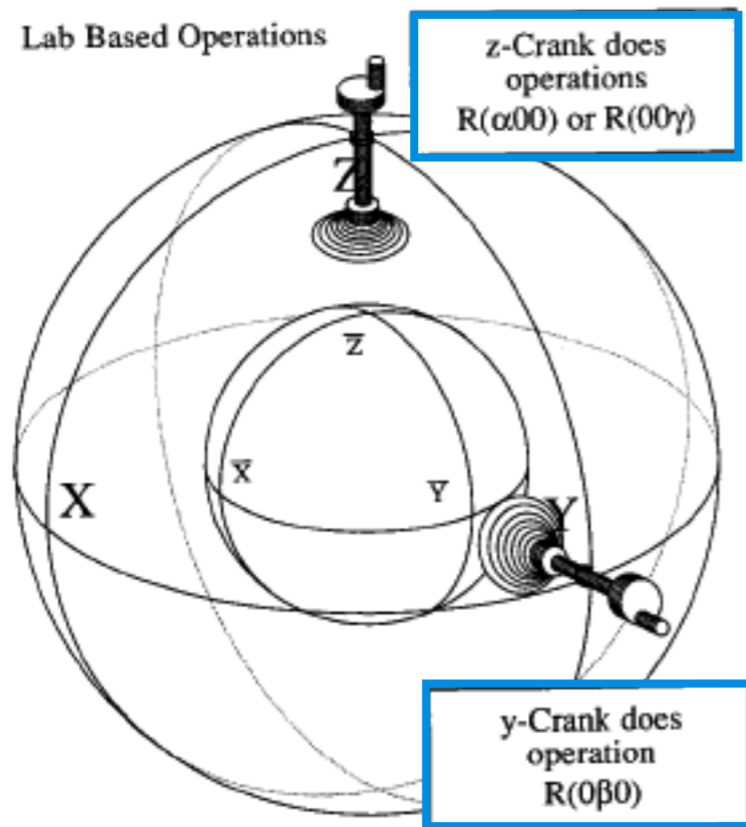
Global vs Local symmetry and Mock-Mach principle

*“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



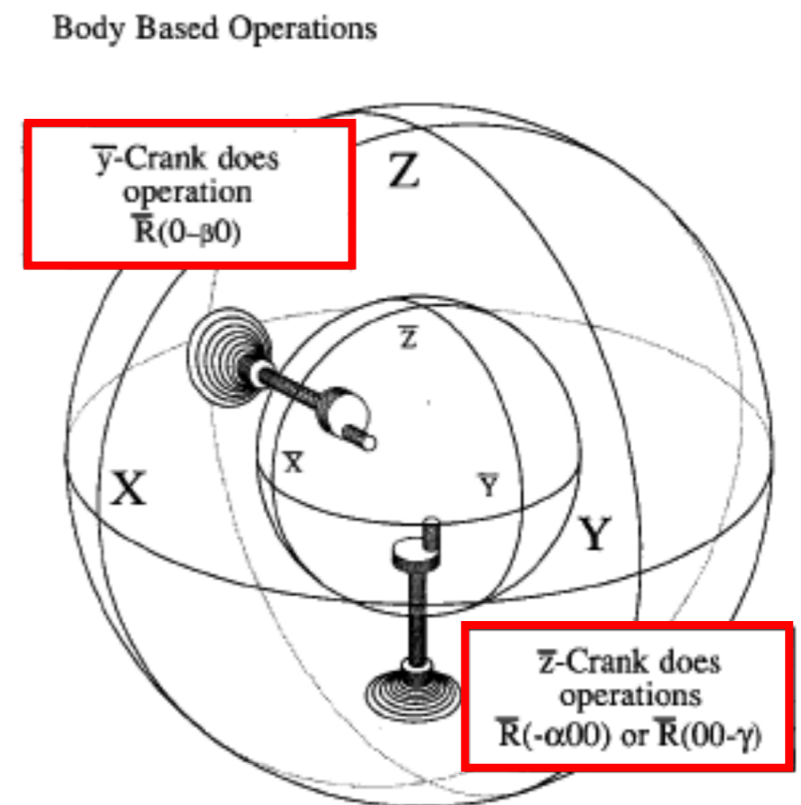
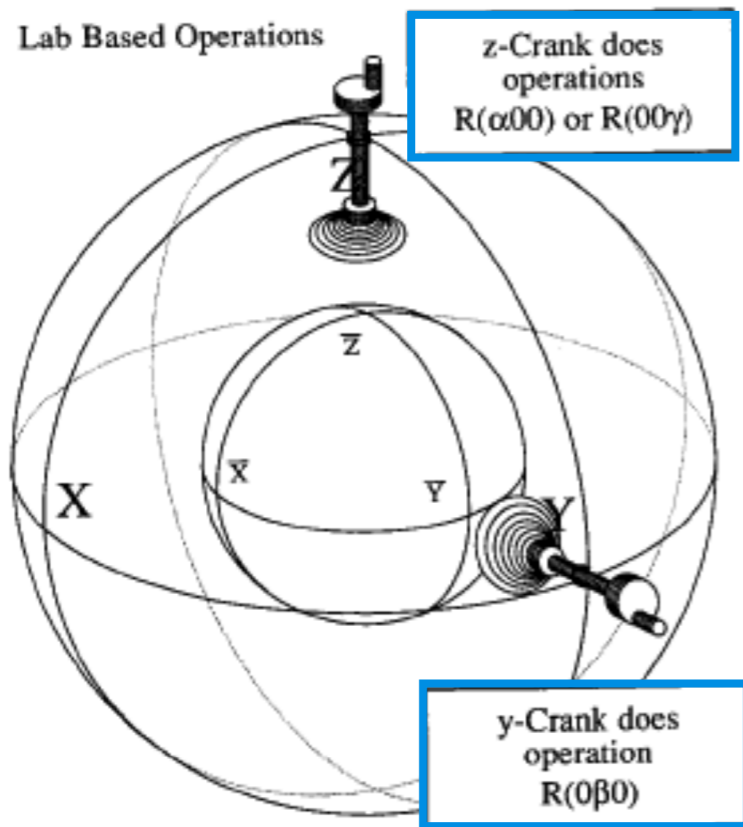
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Lab-fixed (Extrinsic-Global) \mathbf{R} vs. Body-fixed (Intrinsic-Local) $\bar{\mathbf{R}}$



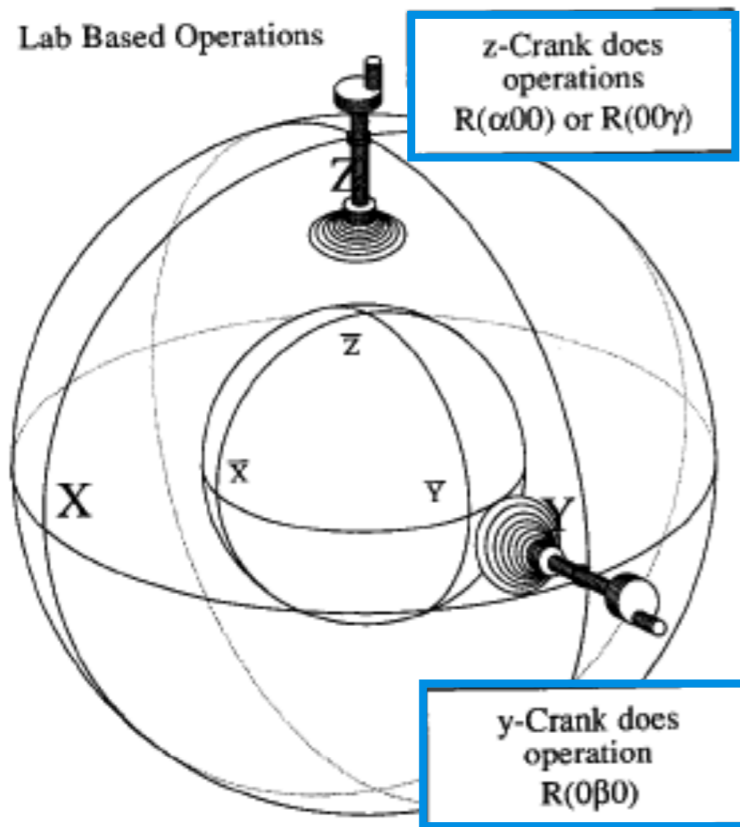
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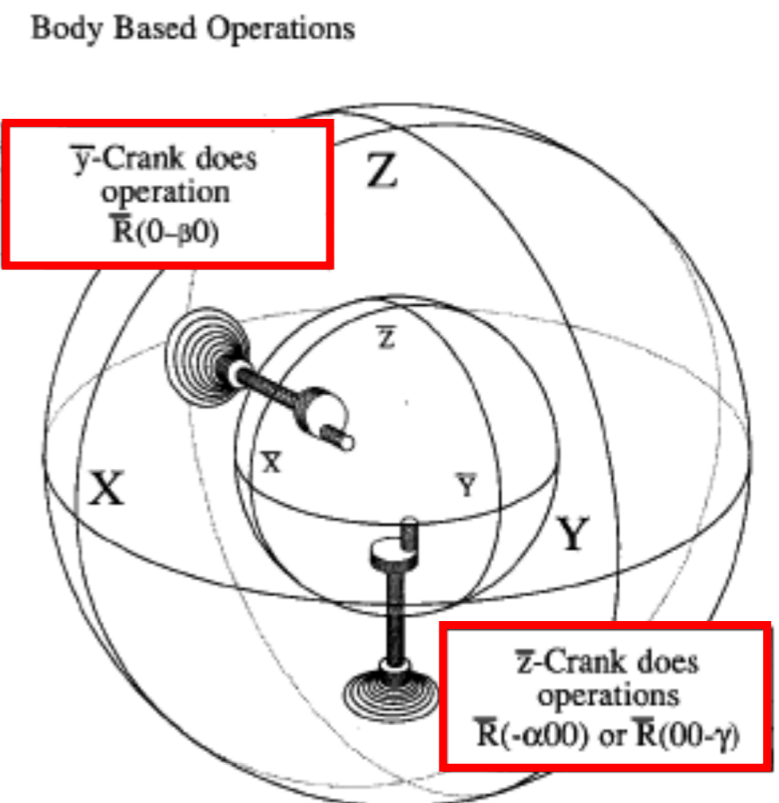
Lab-fixed (Extrinsic-Global) \mathbf{R} vs. Body-fixed (Intrinsic-Local) $\bar{\mathbf{R}}$



\mathbf{R} commutes

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

(because they're independent or “unentangled”)



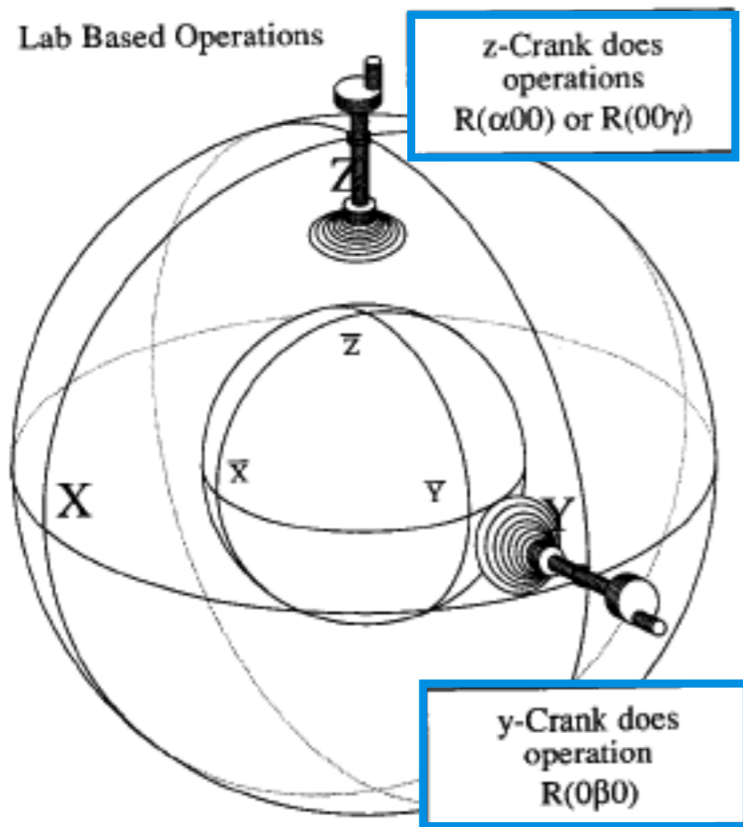
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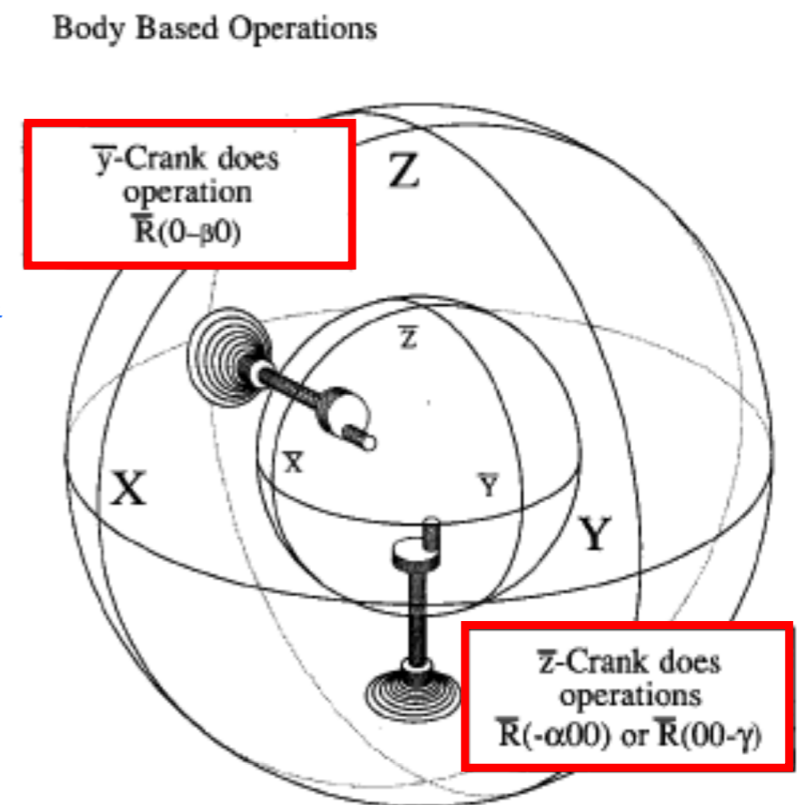


\mathbf{R} commutes
with *all* $\bar{\mathbf{R}}$
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*Mock-Mach
relativity principle*

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

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



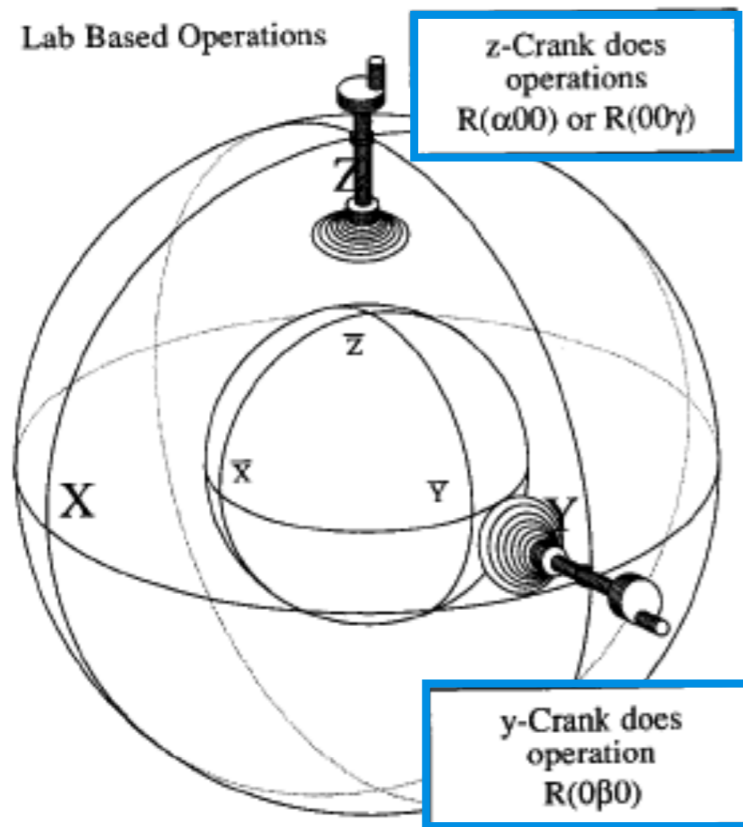
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Lab-fixed (Extrinsic-Global)**R** vs. Body-fixed (Intrinsic-Local) **\bar{R}**



R commutes

with *all* **\bar{R}**

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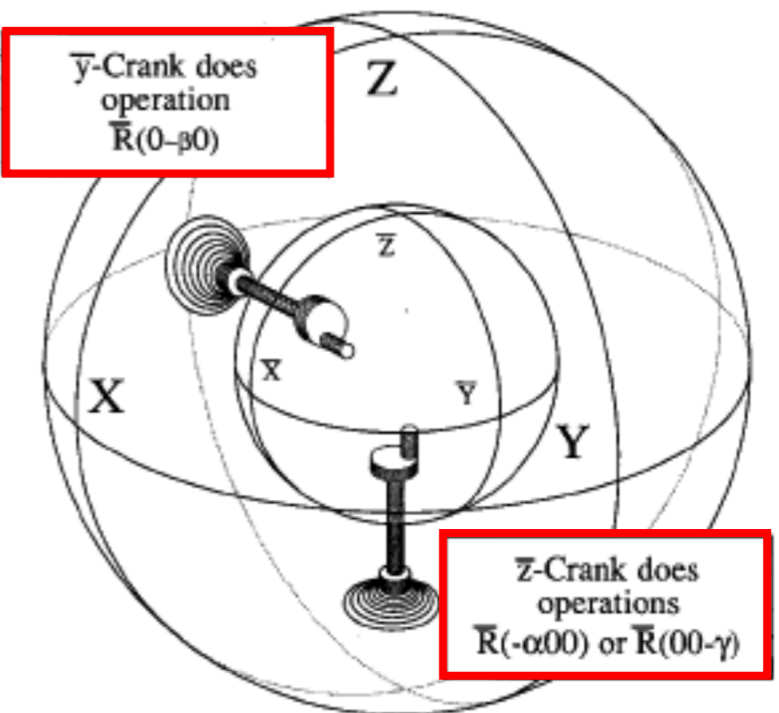
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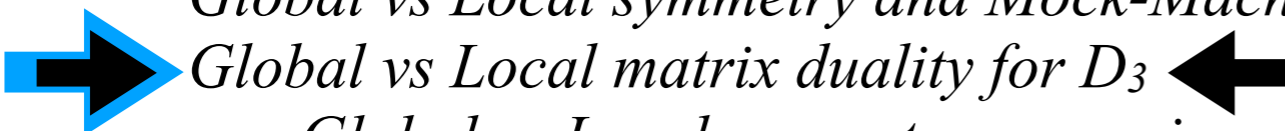
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Body Based Operations

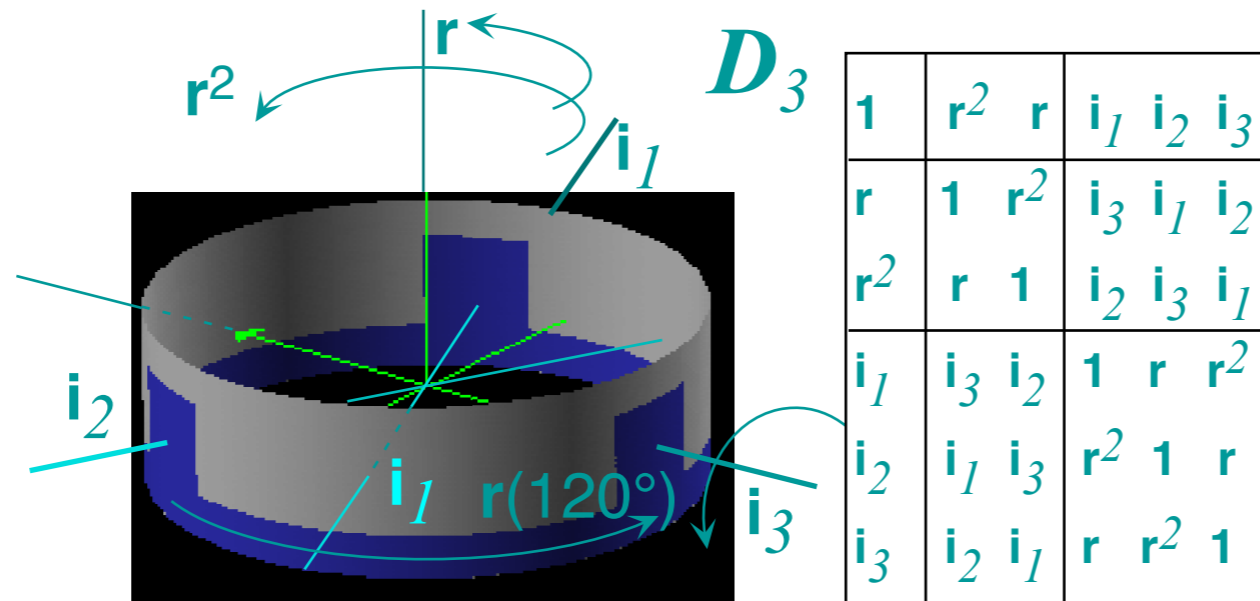
\bar{y} -Crank does operation $\bar{R}(0-\beta 0)$



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

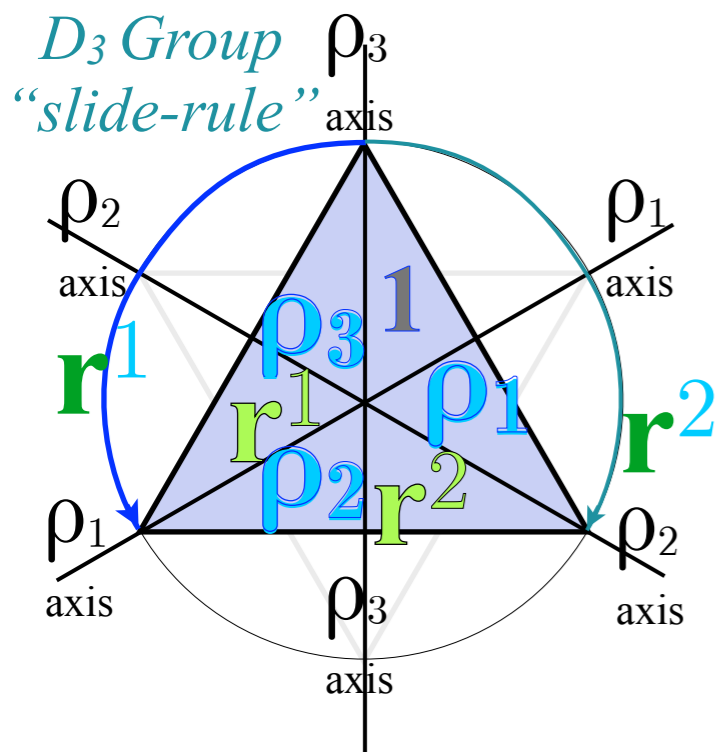
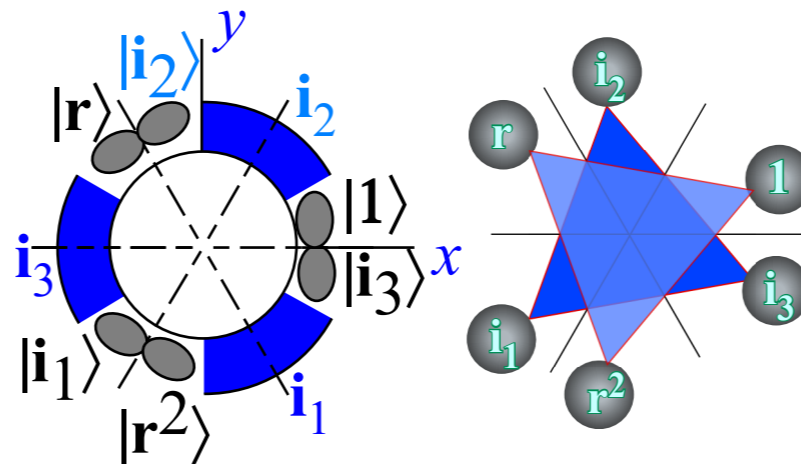
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Example of GLOBAL vs LOCAL symmetry algebra for $D_3 \sim C_{3v}$

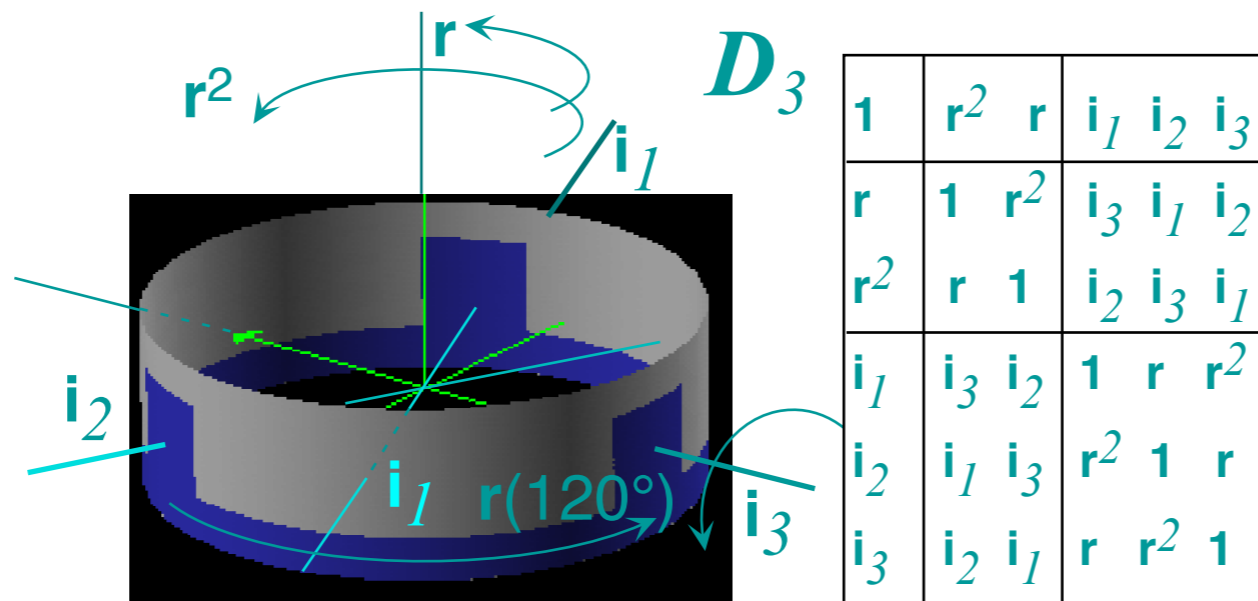


Here group operator notation $1, r, r^2, i_1, i_2, i_3$ matches $1, r^1, r^2, \rho_1, \rho_2, \rho_3$ used previously.

D_3 -defined local-wave bases

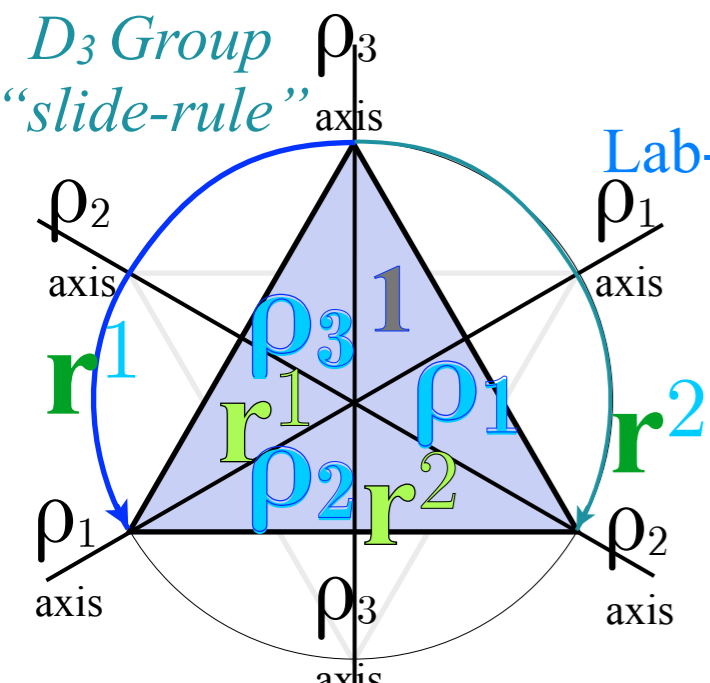
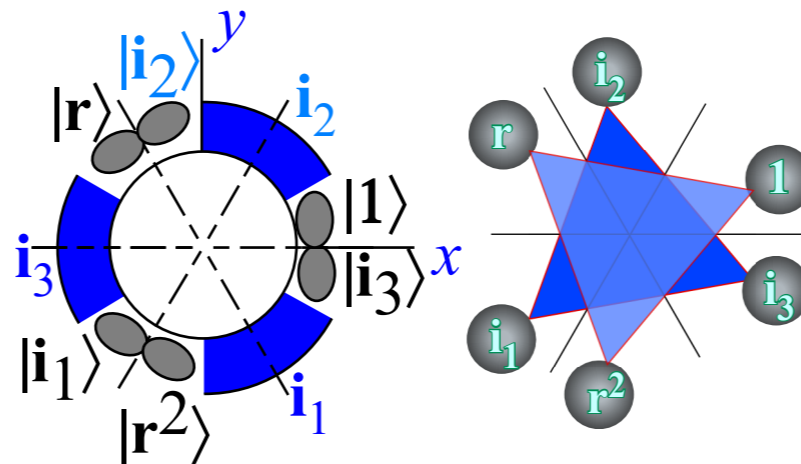


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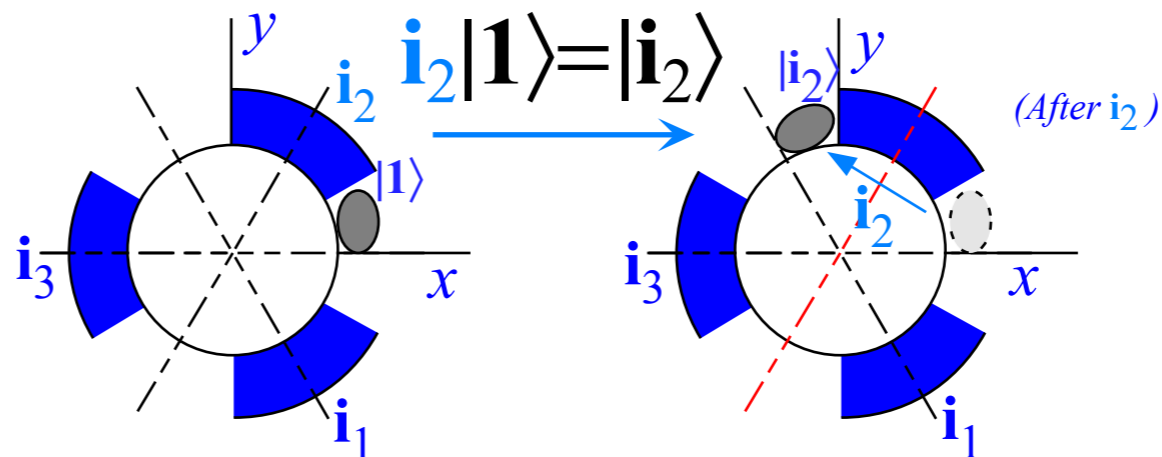


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D_3 -defined local-wave bases



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



Global vs Local symmetry matrix duality for D_3

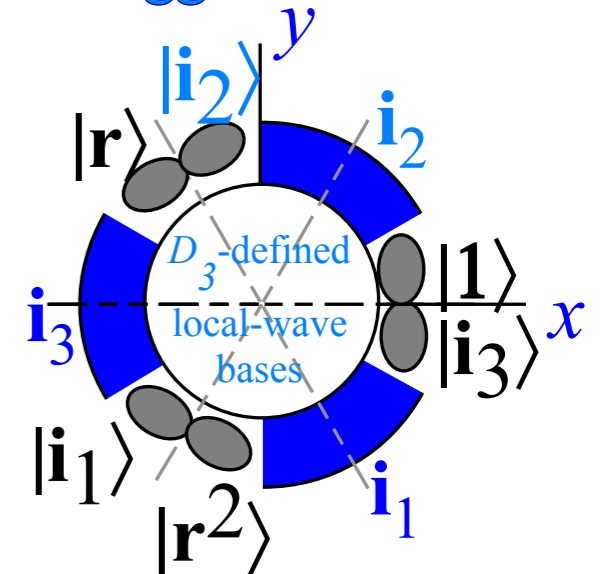
Example of RELATIVITY-DUALITY for $D_3 \sim C_{3v}$

To represent *external* $\{..T, U, V, \dots\}$ switch $g \leftrightarrow g^\dagger$ 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 & \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}
 \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



Global vs Local symmetry matrix duality for D_3

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

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

$\mathbf{1}$	\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 $g g^\dagger$ -table

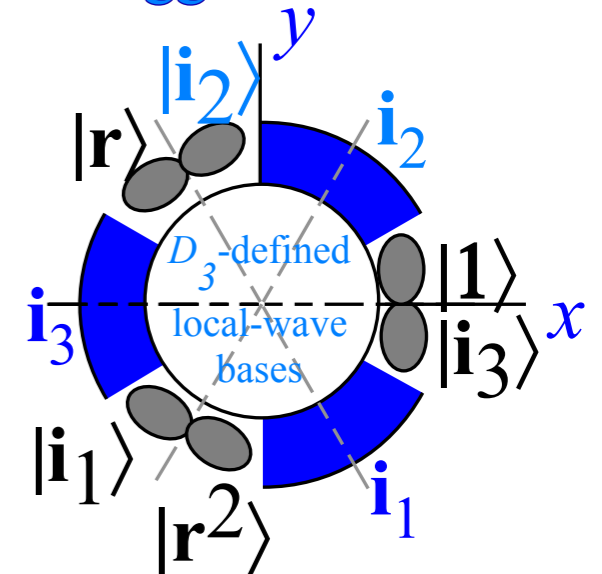
RESULT:

Any $R(\mathbf{T})$

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

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

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

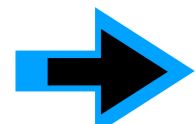
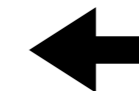


D_3 local $g^\dagger g$ -table

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

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

$\mathbf{1}$	\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	$\mathbf{1}$

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$* *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**Group theory and algebra of D_3 Center (Class algebra)**Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes**1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

Global vs Local symmetry expansion of D_3 Hamiltonian

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

RESULT:

Any $R(\mathbf{T})$

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

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

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

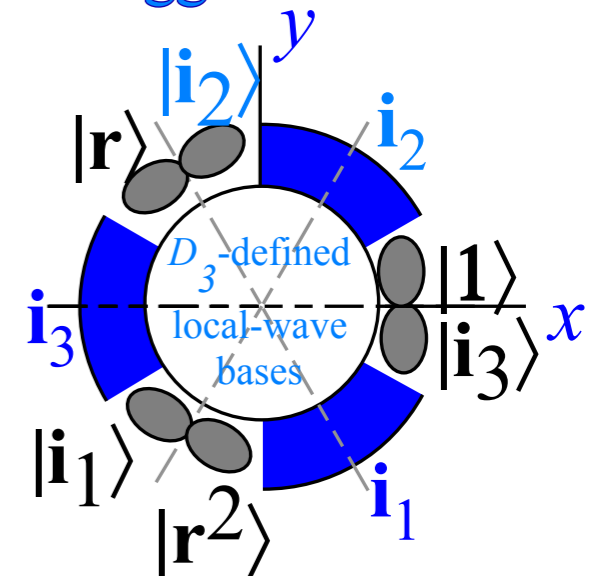
So an \mathbf{H} -matrix

having *Global* symmetry D_3

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

is made from

Local symmetry matrices



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

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

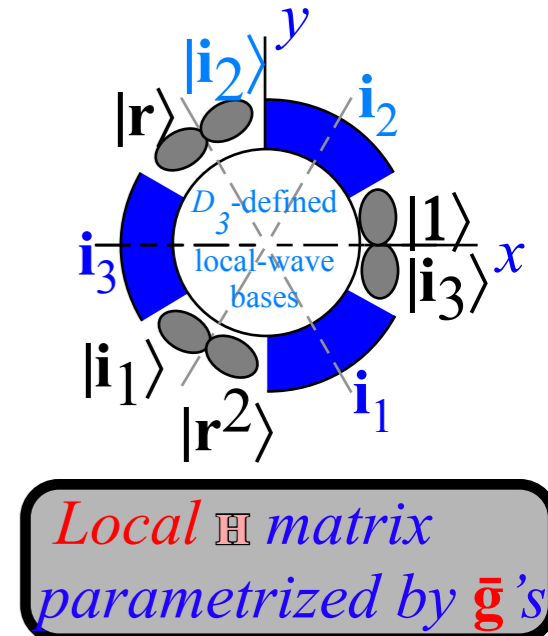
$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2	\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3
\mathbf{r}^2	$\mathbf{1}$	\mathbf{r}	\mathbf{i}_2	\mathbf{i}_3	\mathbf{i}_1
\mathbf{r}	\mathbf{r}^2	$\mathbf{1}$	\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2
\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3	$\mathbf{1}$	\mathbf{r}	\mathbf{r}^2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

Global vs Local symmetry expansion of D_3 Hamiltonian

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

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



RESULT:

Any $R(\mathbf{T})$

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

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

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

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

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

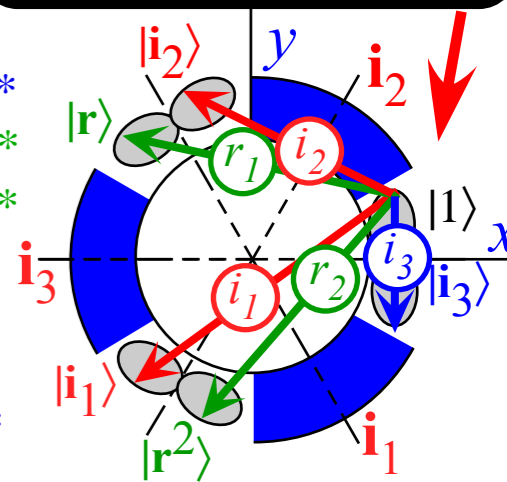
$$r_1 = \langle \mathbf{r} | \mathbb{H} | 1 \rangle = r_2^*$$

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

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

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

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



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

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

local D_3 defined
Hamiltonian matrix

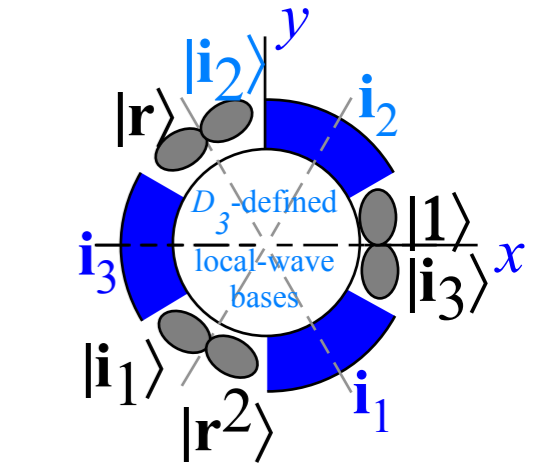
$$\mathbb{H} = \begin{matrix} & |1\rangle & |\mathbf{r}\rangle & |\mathbf{r}^2\rangle & |\mathbf{i}_1\rangle & |\mathbf{i}_2\rangle & |\mathbf{i}_3\rangle \\ \begin{matrix} \langle 1| \\ \langle \mathbf{r}| \\ \langle \mathbf{r}^2| \\ \langle \mathbf{i}_1| \\ \langle \mathbf{i}_2| \\ \langle \mathbf{i}_3|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

Global vs Local symmetry expansion of D_3 Hamiltonian

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

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



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

So an \mathbb{H} -matrix

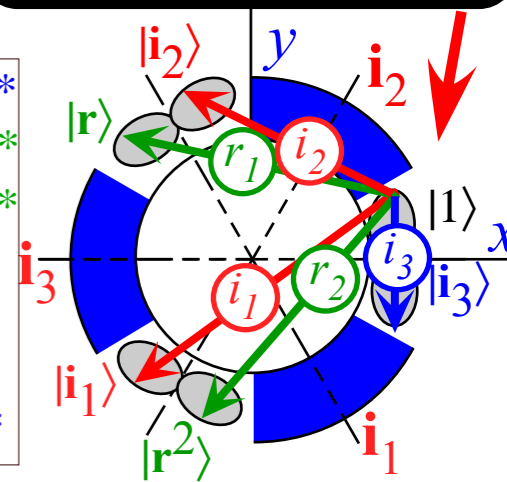
having *Global* symmetry D_3

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

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

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

local D_3 defined Hamiltonian matrix

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

Global vs Local symmetry expansion of D_3 Hamiltonian

Example of RELATIVITY-DUALITY for D

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

$$R^G(\mathbf{1}) = \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}, \quad R^G(\mathbf{r}) = \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},$$

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

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

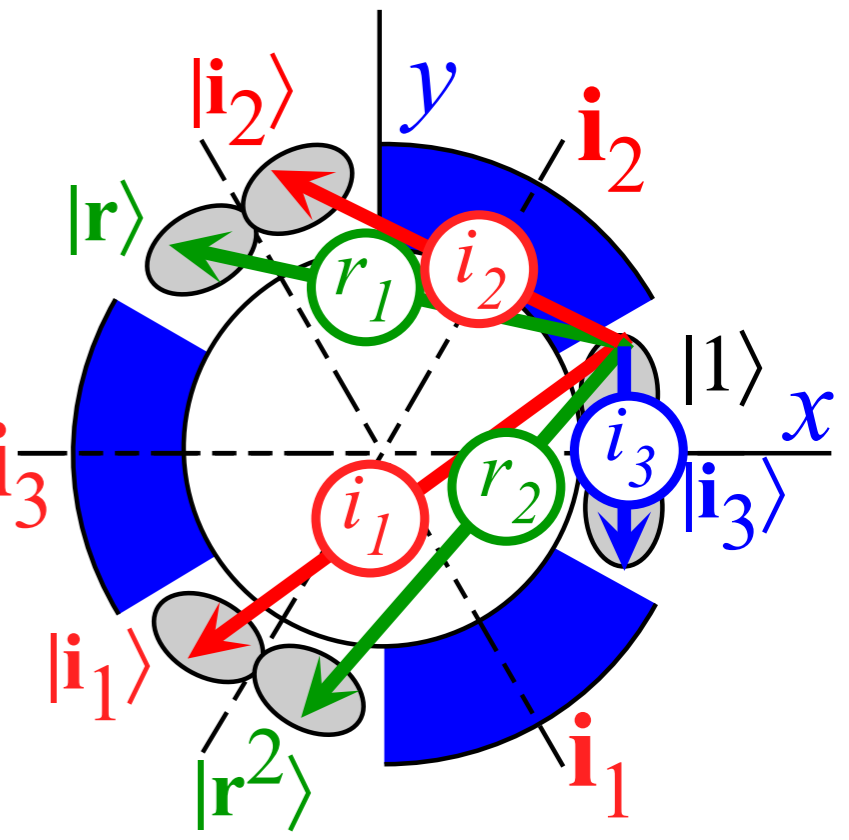
$$r_1 = \langle \mathbf{r} | \mathbf{H} | \mathbf{1} \rangle = r_2^*$$

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

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

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

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



RESULT:

Any $R(\mathbf{T})$ commute (Even if \mathbf{T} and \mathbf{U} do not...) with any $R(\mathbf{U})$...

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

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

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

is made from *Local* symmetry matrices

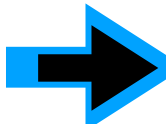
local- D_3 -defined Hamiltonian matrix

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

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

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

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

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$* *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* **Group theory and algebra of D_3 Center (Class algebra)***Self-symmetry (Normalizer).* *Lagrange Coset Theorem for classes**1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

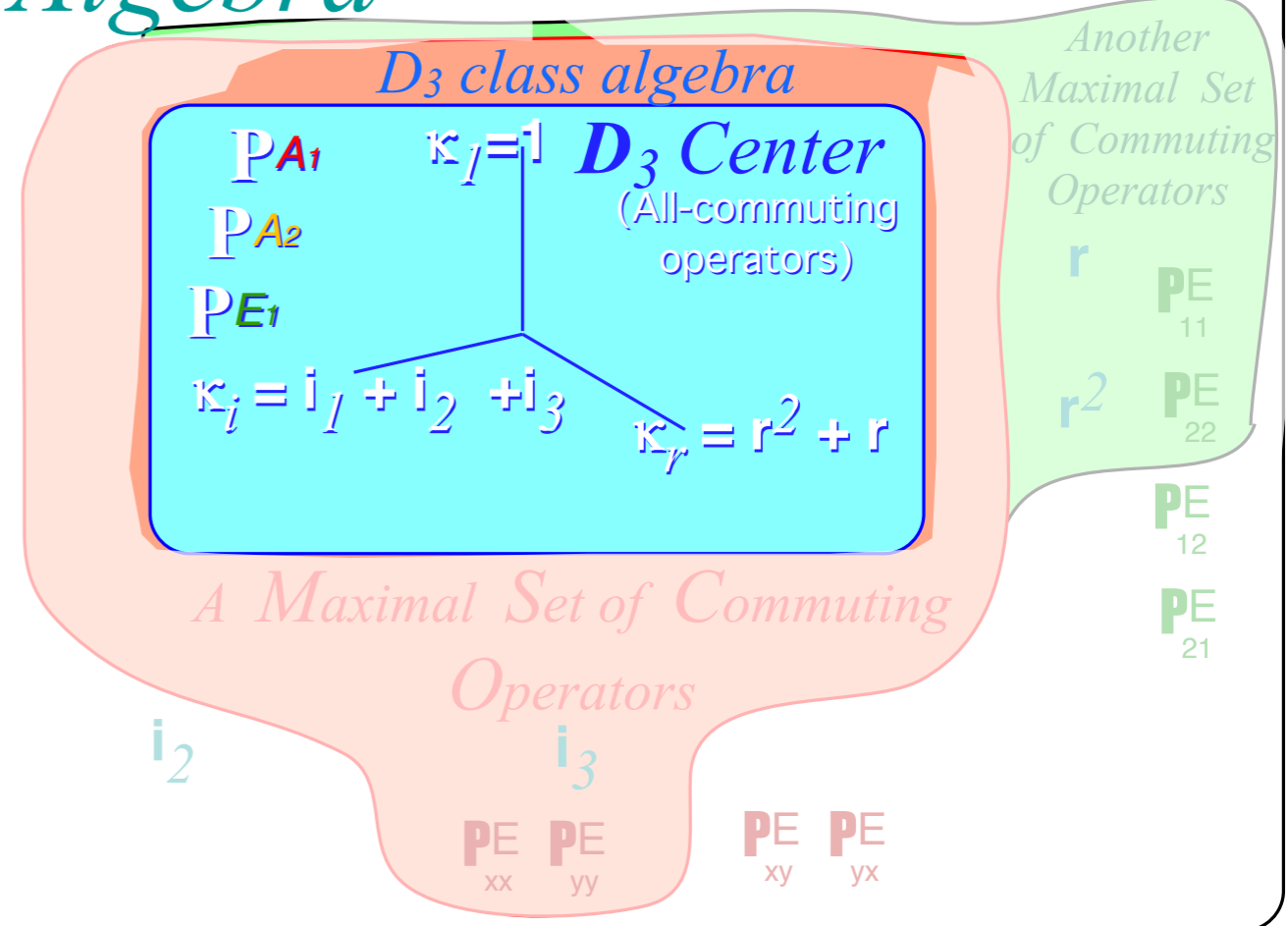
Class algebra $\{\kappa_1, \kappa_2, \kappa_3\}$ of D_3 Center

1	r ²	r	i ₁	i ₂	i ₃	→		$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
r	1	r ²	i ₃	i ₁	i ₂		κ_1	κ_1	κ_r	κ_i
r ²	r	1	i ₂	i ₃	i ₁		κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
i ₁	i ₃	i ₂	1	r	r ²		κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$
i ₂	i ₁	i ₃	r ²	1	r					
i ₃	i ₂	i ₁	r	r ²	1					

Class-sum κ_k commutes with all g_t

Class-sum κ_k invariance: $g_t \kappa_k = \kappa_k g_t$

D_3 Algebra



Review: Spectral resolution of D_3 Center (Class algebra)

1	r ²	r	i ₁	i ₂	i ₃
r	1	r ²	i ₃	i ₁	i ₂
r ²	r	1	i ₂	i ₃	i ₁
i ₁	i ₃	i ₂	1	r	r ²
i ₂	i ₁	i ₃	r ²	1	r
i ₃	i ₂	i ₁	r	r ²	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all g_t

Class-sum κ_k invariance:

$$g_t \kappa_k = \kappa_k g_t$$

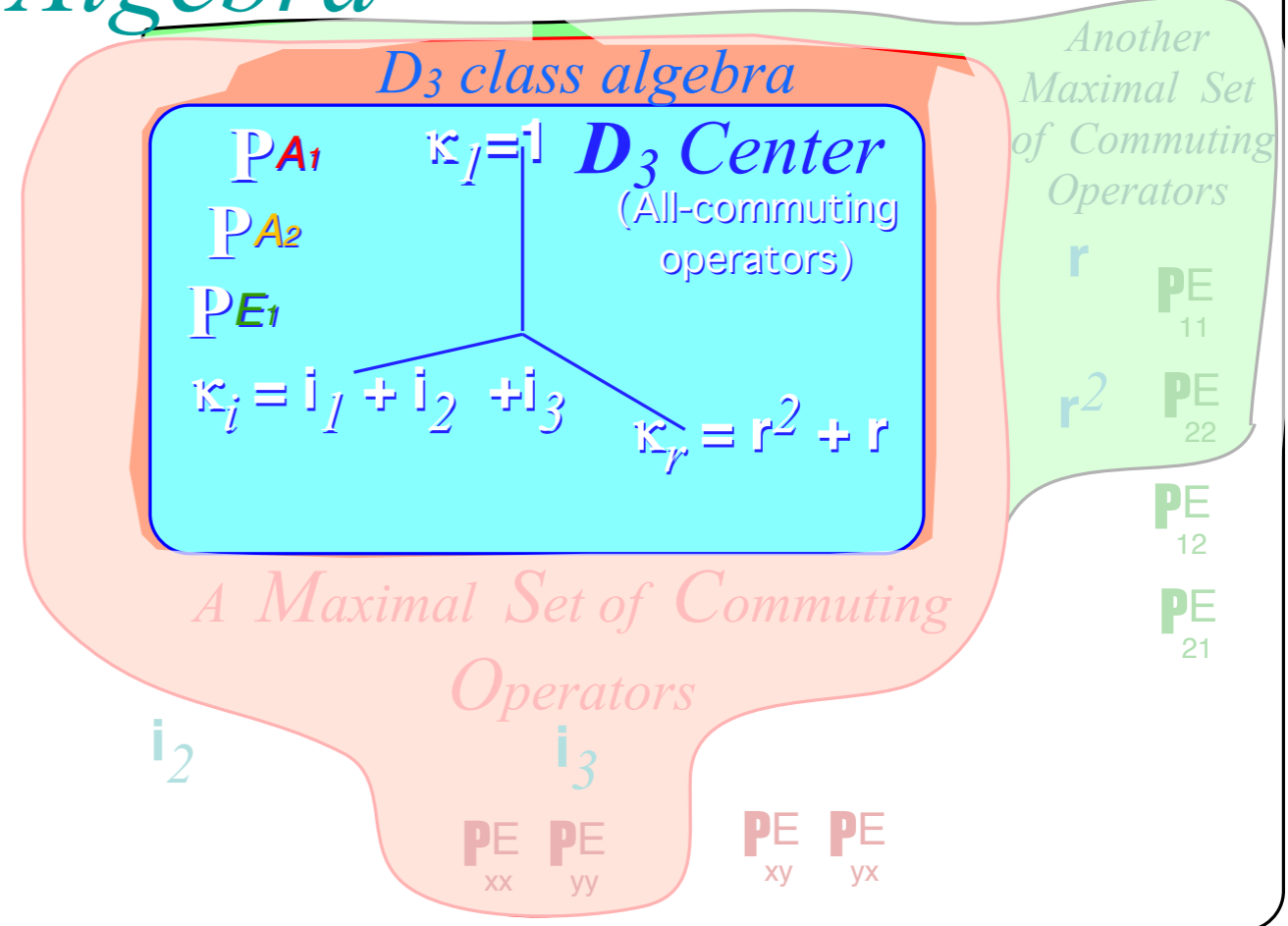
$\circ G$ = order of group:

$$(\circ D_3 = 6)$$

$\circ \kappa_k$ = order of class κ_k :

$$(\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3)$$

D_3 Algebra



Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all g_t

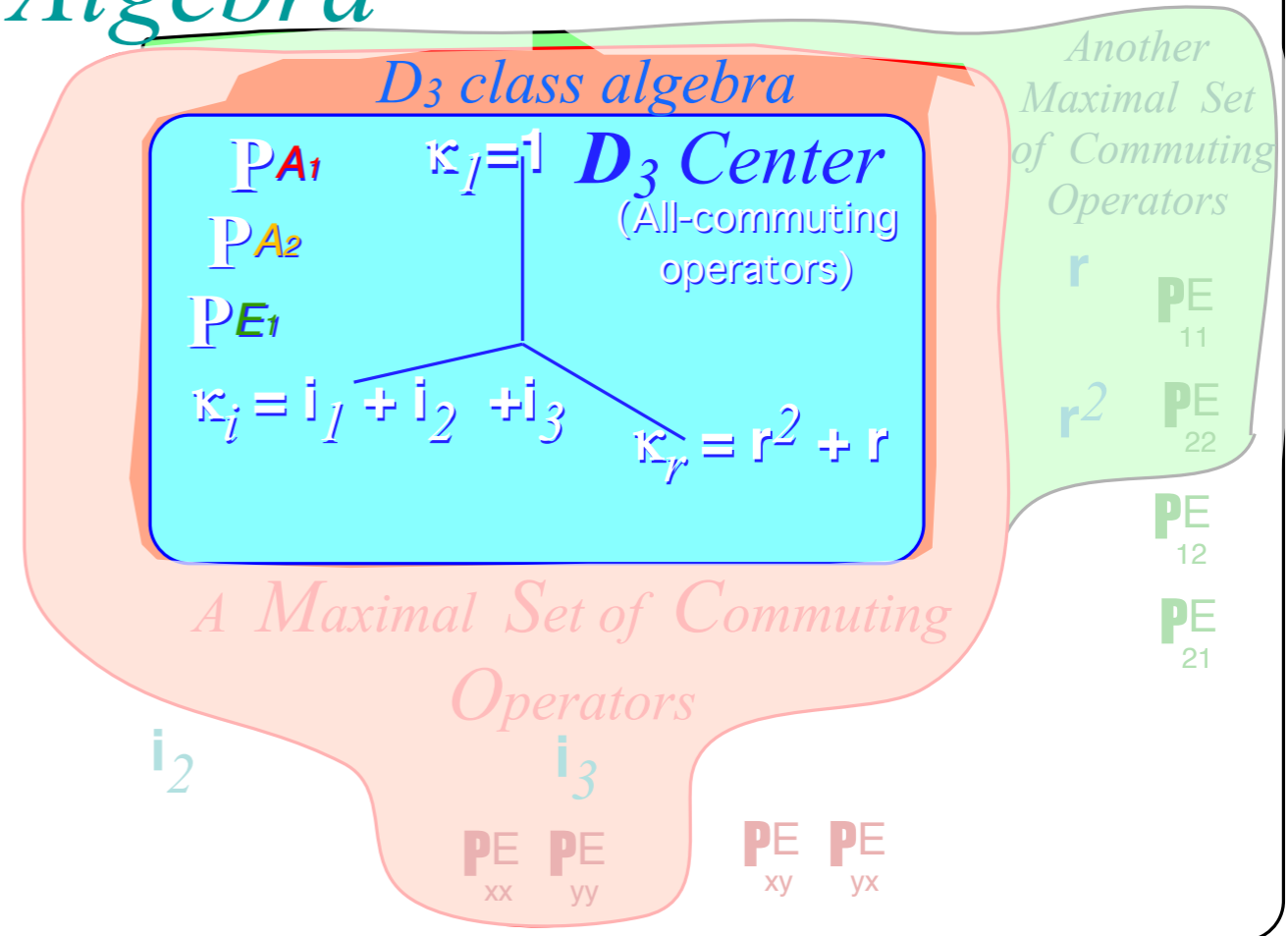
Class-sum κ_k invariance: $g_t \kappa_k g_t^{-1} = \kappa_k$ or: $g_t \kappa_k = \kappa_k g_t$

$\circ G =$ order of group: ($\circ D_3 = 6$)

$\circ \kappa_k =$ order of class κ_k : ($\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$)

$g_t \kappa_k g_t^{-1} = \kappa_k$ where: $\kappa_k = \sum_{j=1}^{j=\circ \kappa_k} g_j$

D_3 Algebra



AMOP
reference links
on following page

2.21.18 class 12.0: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics: D_3 and C_{3v} group products, classes, and irrep projection operators

32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups

Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3

Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators

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

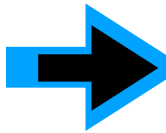
Deriving $D_3 \sim C_{3v}$ equivalence transformations and classes

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

 Group theory and algebra of D_3 Center (Class algebra)

Self-symmetry (Normalizer).  Lagrange Coset Theorem for classes

1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry

All-commuting operators \mathbf{K}_k

All-commuting projectors $\mathbf{P}^{(\alpha)}$

D_3 -invariant irep characters $\chi_k^{(\alpha)}$

Invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors

...and classes

3rd-Stage spectral decomposition of ALL of D_3

...and of Hamiltonian \mathbf{H}

GLOBAL vs LOCAL symmetry of states

...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$

Review: Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all g_t

Class-sum κ_k invariance:

$$g_t \kappa_k = \kappa_k g_t$$

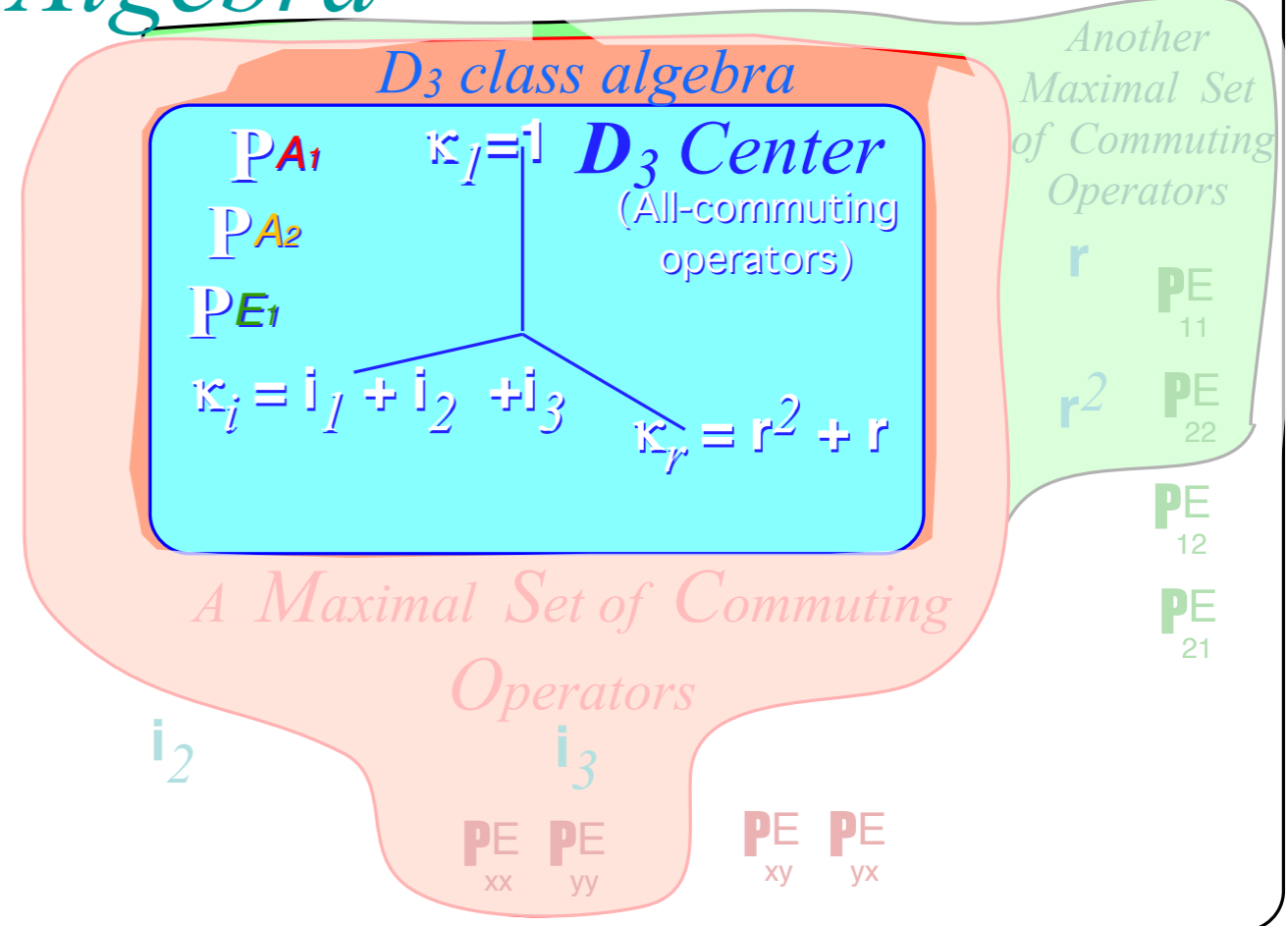
$\circ G$ = order of group: ($\circ D_3 = 6$)

$\circ \kappa_k$ = order of class κ_k : ($\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$)

$$g_t \kappa_k g_t^{-1} = \kappa_k \text{ where: } \kappa_k = \sum_{j=1}^{j=\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{t=\circ G} g_t g_k g_t^{-1}$$

$\circ s_k$ = order of g_k -self-symmetry: ($\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$)

D_3 Algebra



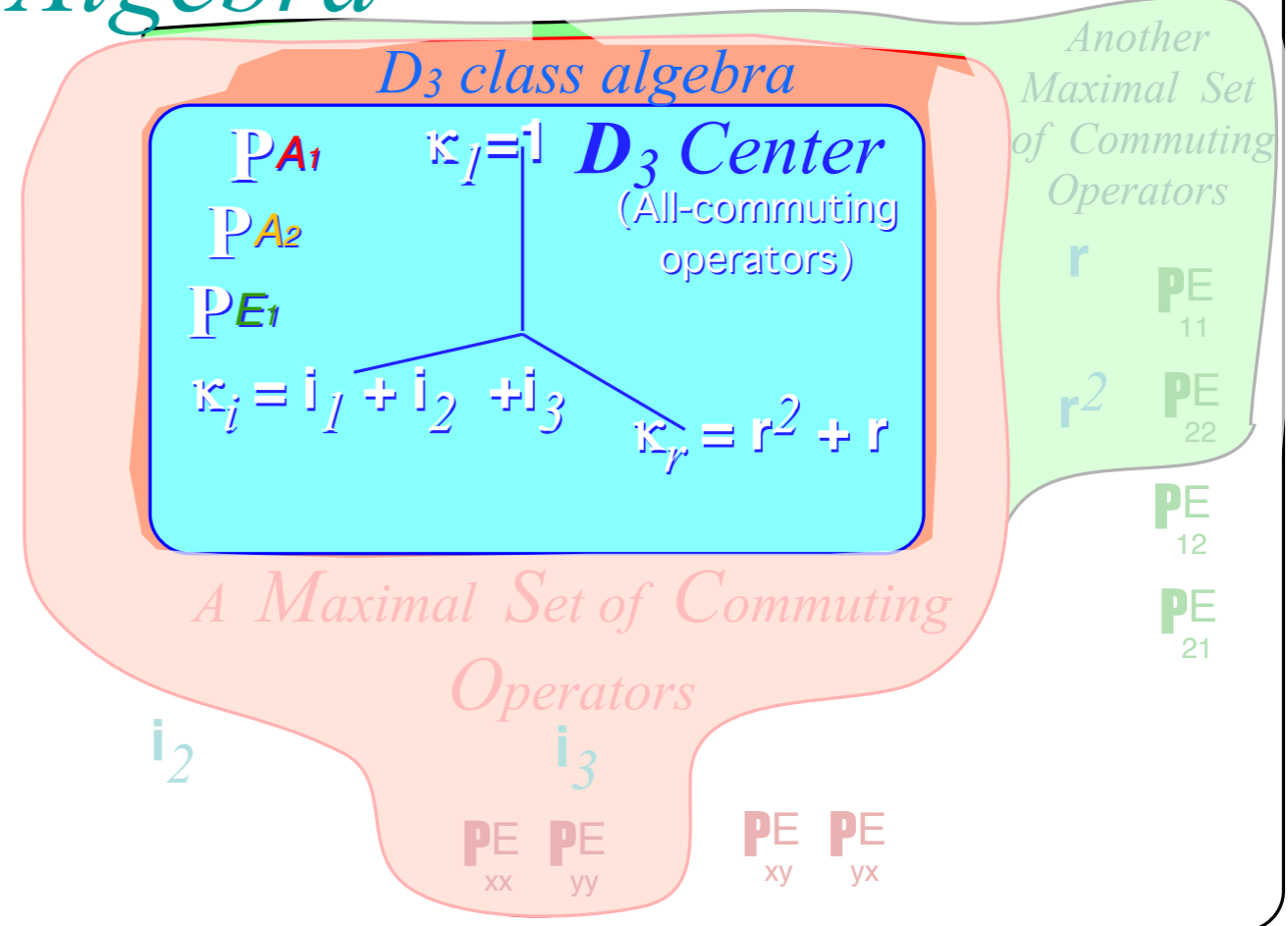
Group theory of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all g_t

D_3 Algebra



Another Maximal Set of Commuting Operators

- r PE₁₁
- r^2 PE₂₂
- PE₁₂
- PE₂₁

A Maximal Set of Commuting Operators

- i_1
- i_2
- i_3
- PE_{xx} PE_{yy}
- PE_{xy} PE_{yx}

Class-sum κ_k invariance:

$$g_t \kappa_k = \kappa_k g_t$$

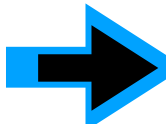
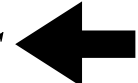
$\circ G$ = order of group: ($\circ D_3 = 6$)

$\circ \kappa_k$ = order of class κ_k : ($\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$)

$$g_t \kappa_k g_t^{-1} = \kappa_k \text{ where: } \kappa_k = \sum_{j=1}^{j=\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{t=\circ G} g_t g_k g_t^{-1}$$

$\circ s_k$ = order of g_k -self-symmetry: ($\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$)

$\circ s_k = \circ G / \circ \kappa_k$ $\circ s_k$ is an integer count of D_3 operators g_s that commute with g_k .

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$* *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* **Group theory and algebra of D_3 Center (Class algebra)***Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes* *1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

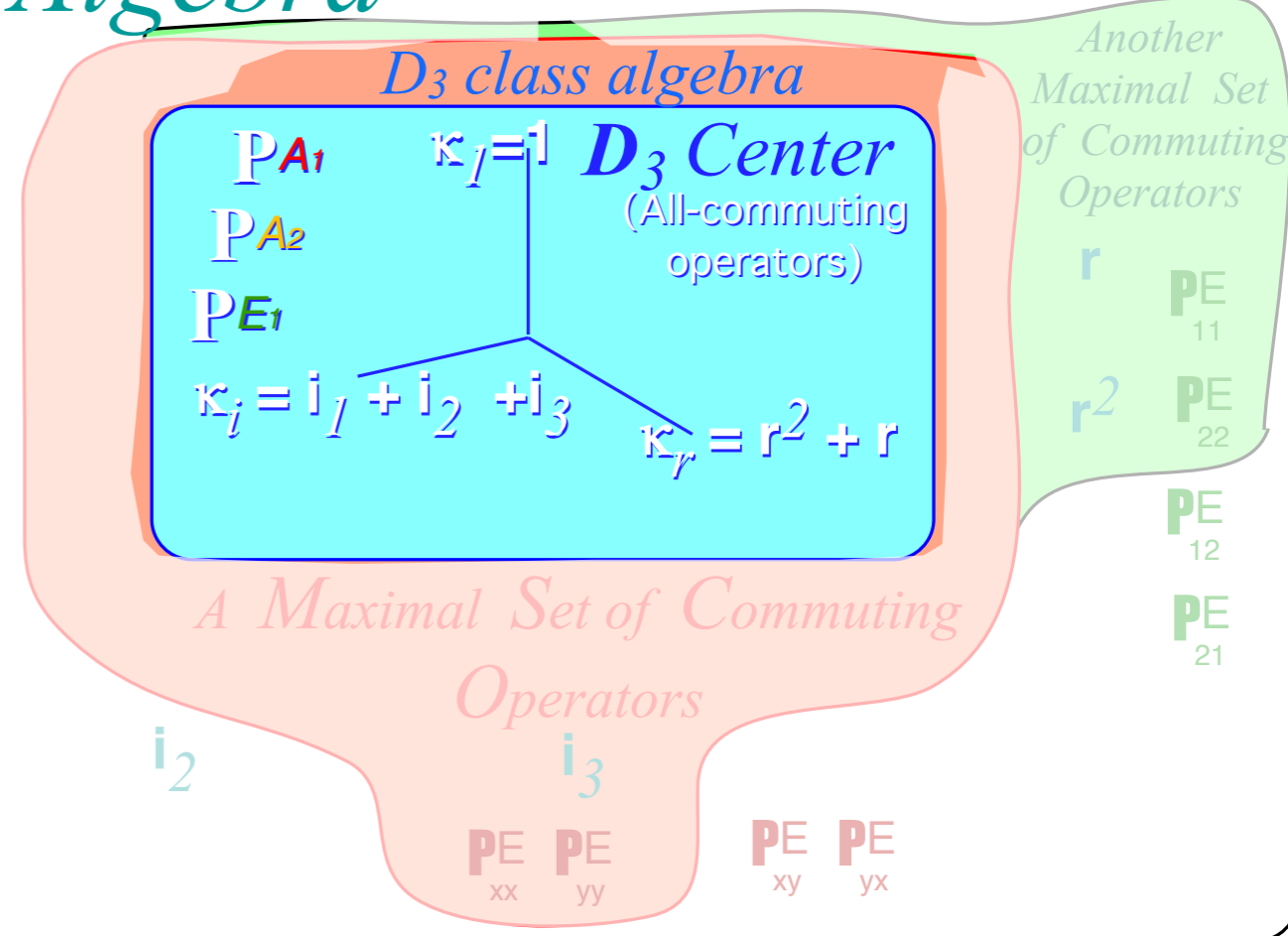
Review: Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all g_t

D_3 Algebra



- Class-sum κ_k invariance: $g_t \kappa_k = \kappa_k g_t$
- $\circ G$ = order of group: ($\circ D_3 = 6$)
- $\circ \kappa_k$ = order of class κ_k : ($\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$)
- $g_t \kappa_k g_t^{-1} = \kappa_k$ where: $\kappa_k = \sum_{j=1}^{\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{\circ G} g_t g_k g_t^{-1}$
- $\circ s_k$ = order of g_k -self-symmetry: ($\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$)

$\circ s_k = \circ G / \circ \kappa_k$ $\circ s_k$ is an integer count of D_3 operators g_s that commute with g_k .

...now a few pages to prove and apply this key integer ratio related to Lagrange's theorems.

Review: Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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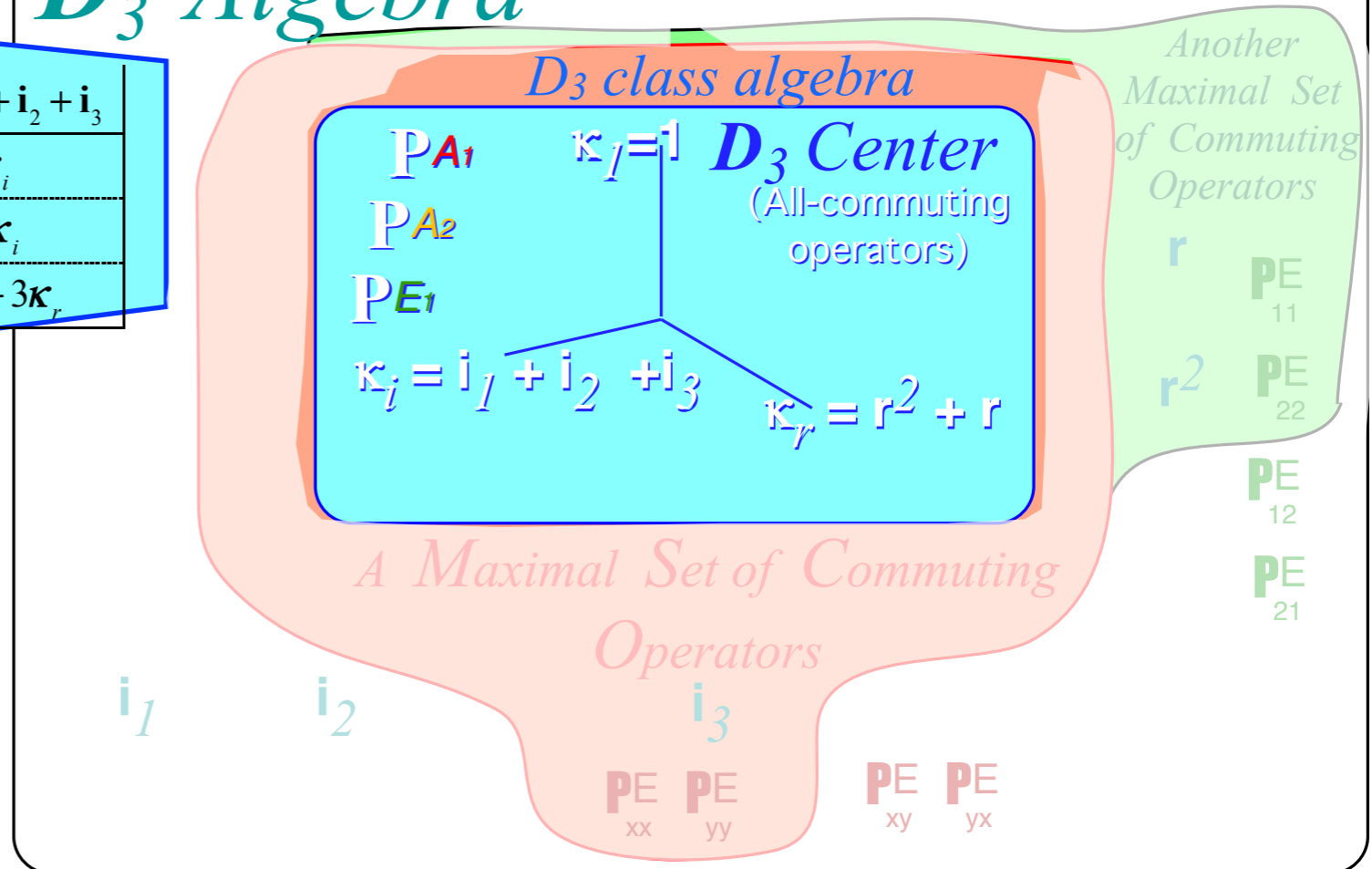
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$$\circ s_k = \circ G / \circ \kappa_k$$

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These operators g_s form the g_k -self-symmetry group s_k . Each g_s transforms g_k into itself: $g_s g_k g_s^{-1} = g_k$

D_3 Algebra



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r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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$$g_t \kappa_k g_t^{-1} = \kappa_k \text{ where: } \kappa_k = \sum_{j=1}^{j=\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{t=\circ G} g_t g_k g_t^{-1}$$

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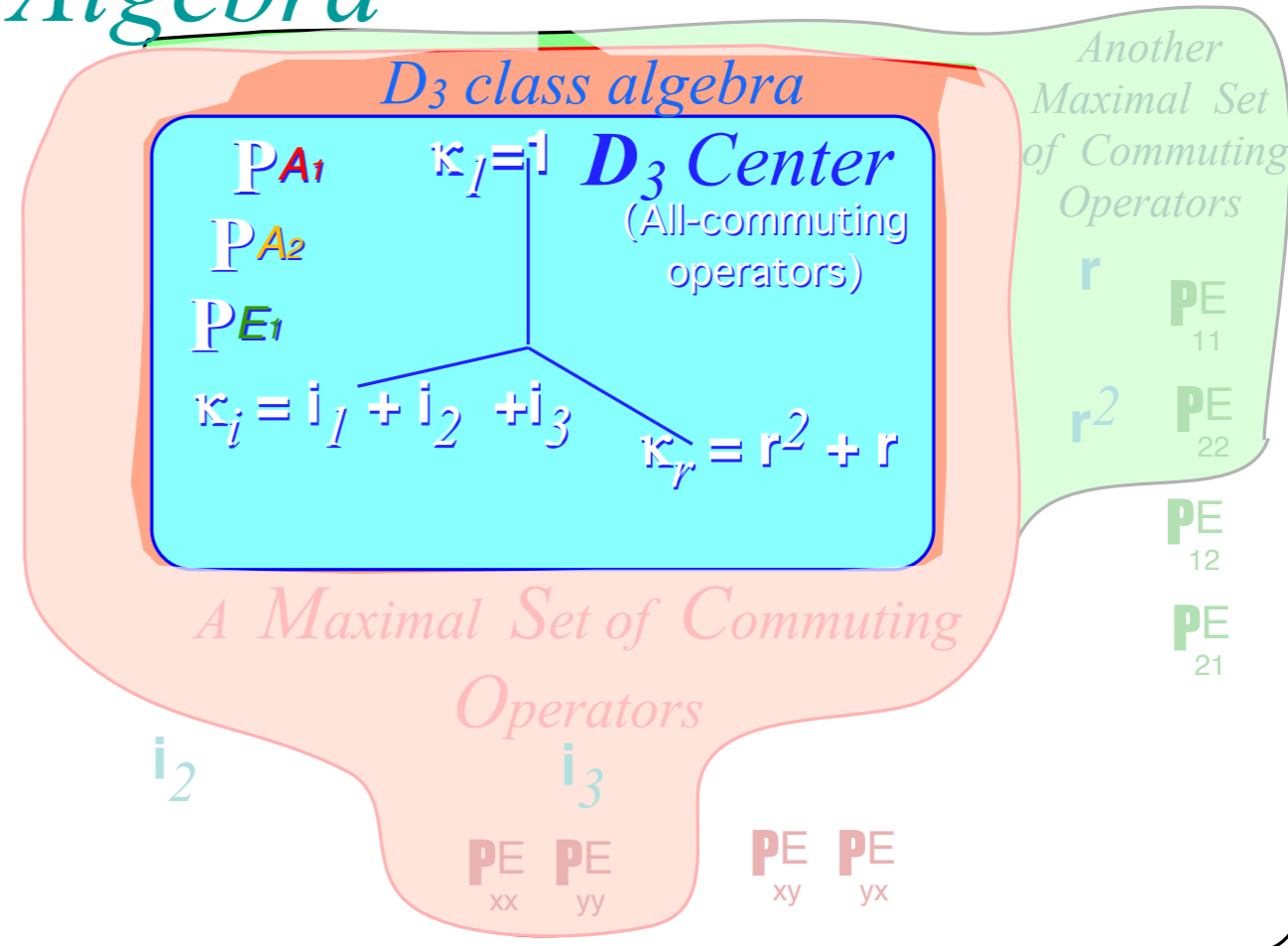
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⋮

D_3 Algebra



Review: Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
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	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
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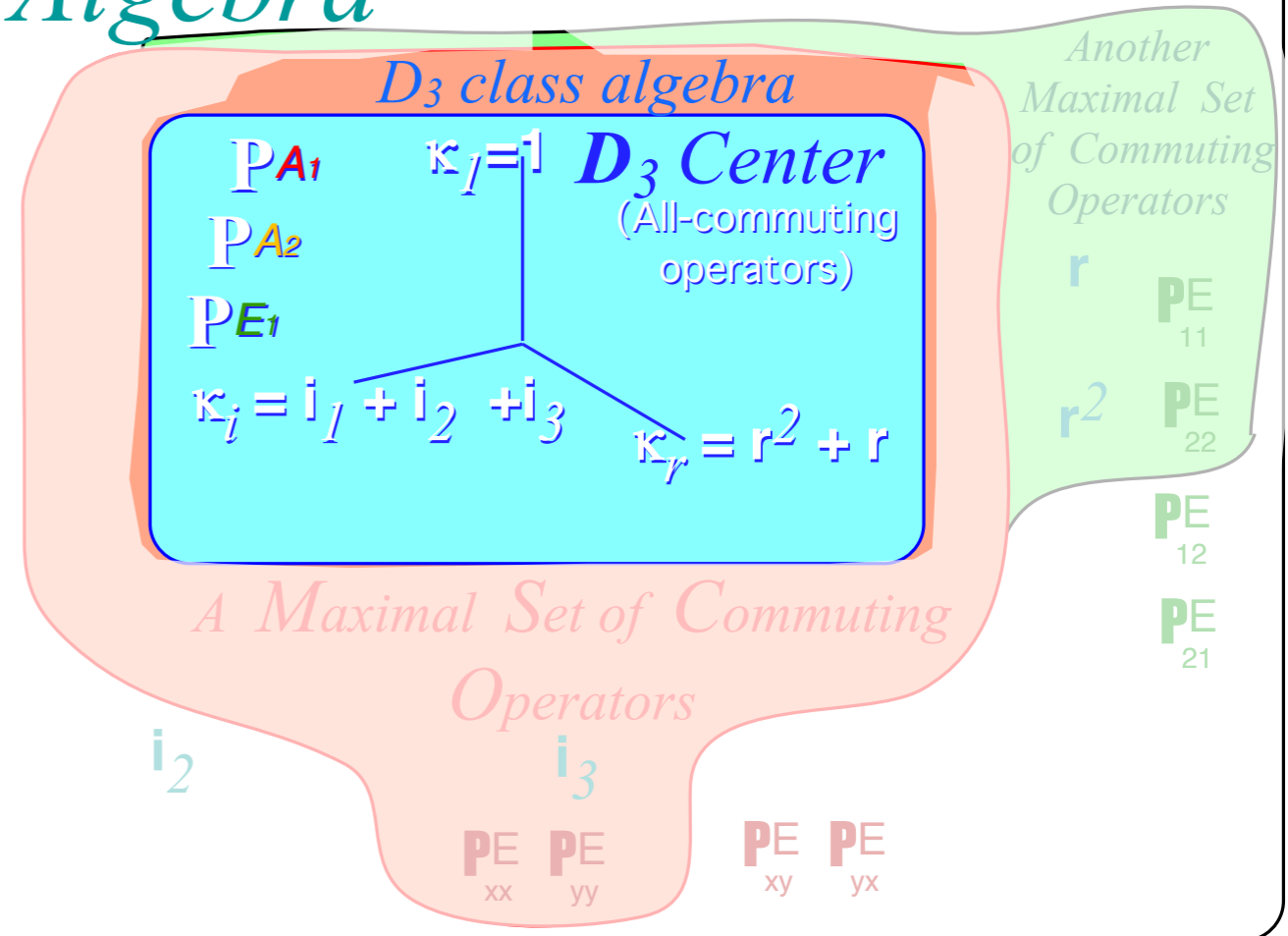
$$\text{that is: } g_t g_s g_k (g_t g_s)^{-1} = g_t g_s g_k g_s^{-1} g_t^{-1} = g_t g_k g_t^{-1} = g'_k,$$

Subgroup $s_k = \{g_0=1, g_1=g_k, g_2, \dots\}$ has $\ell = (\circ \kappa_k - 1)$ Left Cosets (one coset for each member of class κ_k).

$$g_l s_k = g_l \{g_0=1, g_1=g_k, g_2, \dots\},$$

⋮

D_3 Algebra



Review: Spectral resolution of D_3 Center (Class algebra)

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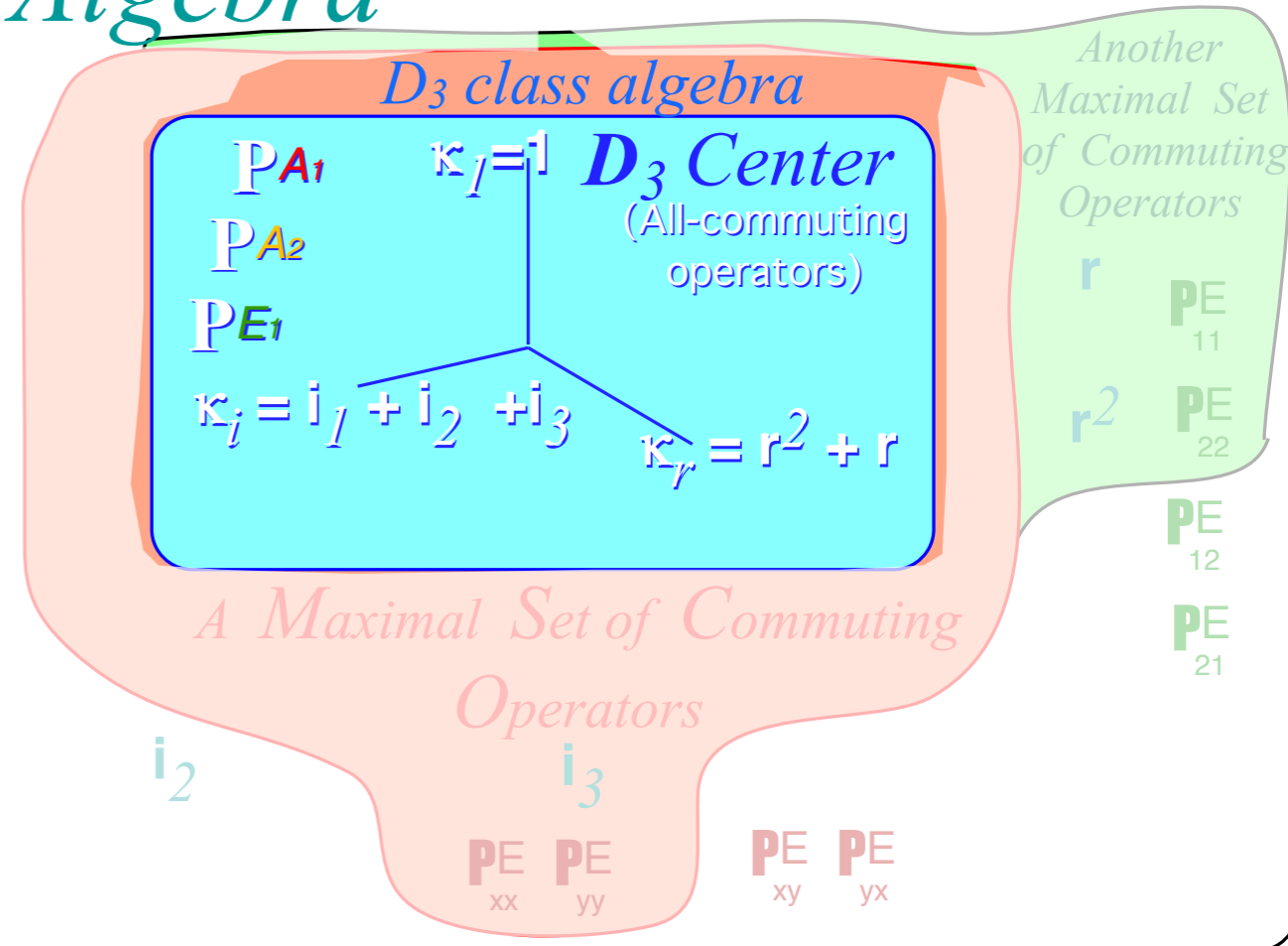
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that is: $g_t g_s g_k (g_t g_s)^{-1} = g_t g_s g_k g_s^{-1} g_t^{-1} = g_t g_k g_t^{-1} = g'_k$,

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$$\begin{aligned} g_1 s_k &= g_1 \{g_0=1, g_1=g_k, g_2, \dots\}, \\ g_2 s_k &= g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots \\ &\vdots \\ g_\ell s_k &= g_\ell \{g_0=1, g_1=g_k, g_2, \dots\} \end{aligned}$$

D_3 Algebra



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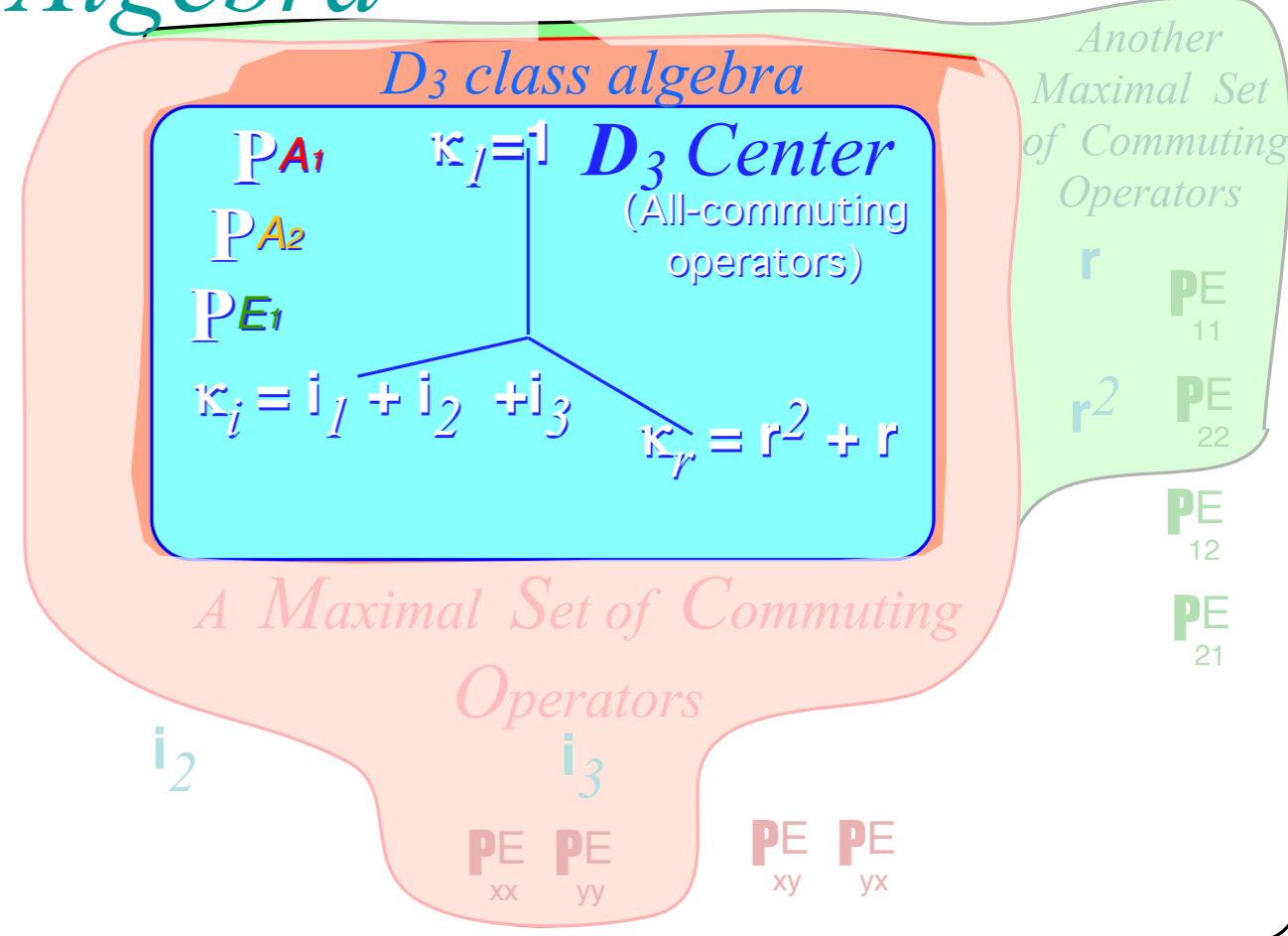
Subgroup $s_k = \{g_0=1, g_1=g_k, g_2, \dots\}$ has $\ell = (\circ \kappa_k - 1)$ Left Cosets (one coset for each member of class κ_k).

$$g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\},$$

$$g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots$$

They will divide the group of order $\circ D_3 = \circ \kappa_k \cdot \circ s_k$ evenly into $\circ \kappa_k$ subsets each of order $\circ s_k$.

D_3 Algebra



Review: Spectral resolution of D_3 Center (Class algebra)

1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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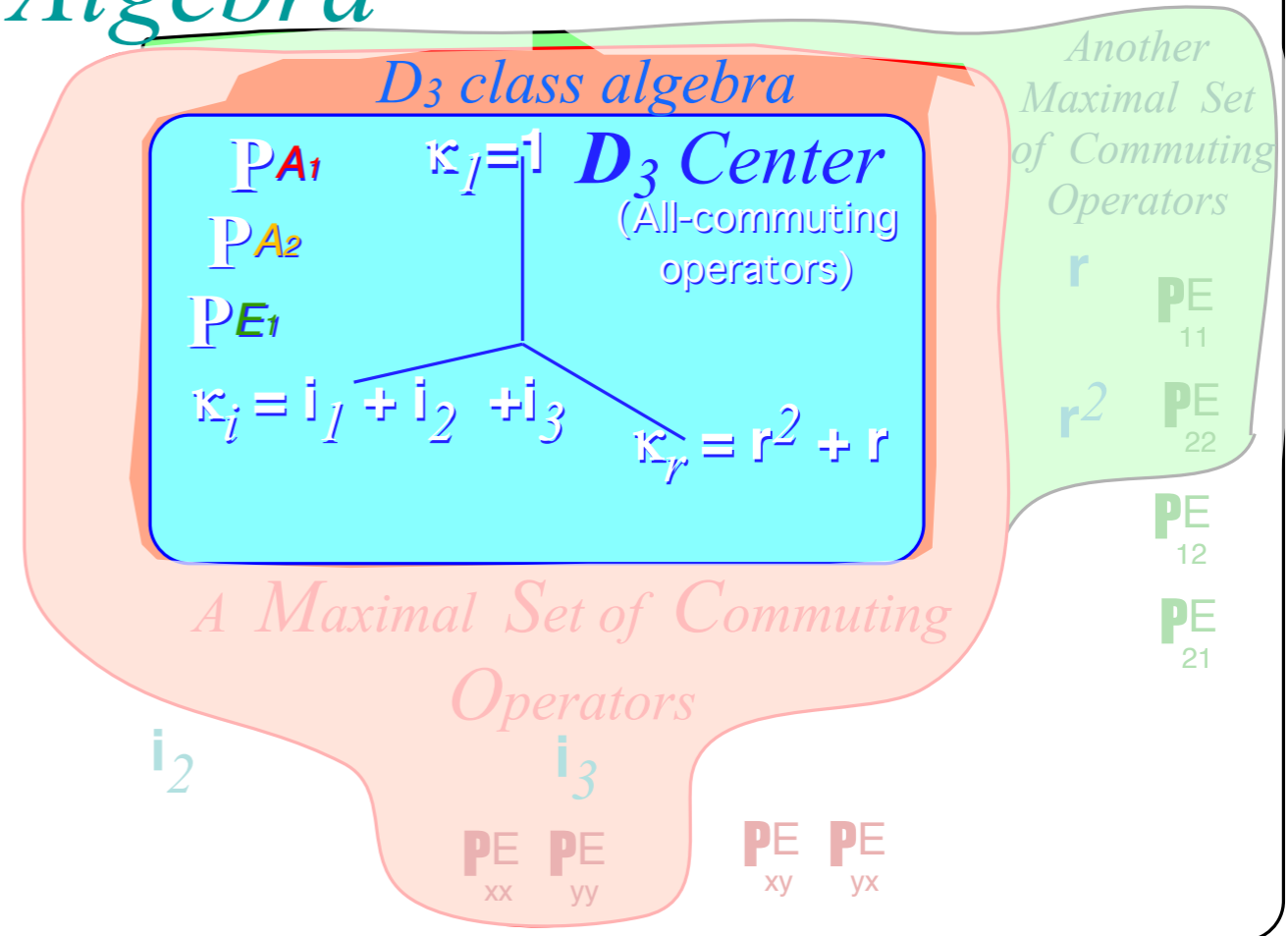
$$g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\},$$

$$g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots$$

These results are known as Lagrange's Coset Theorem(s)

They will divide the group of order $\circ D_3 = \circ \kappa_k \cdot \circ s_k$ evenly into $\circ \kappa_k$ subsets each of order $\circ s_k$.

D_3 Algebra



AMOP
reference links
on following page

2.21.18 class 12.0: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics: D_3 and C_{3v} group products, classes, and irrep projection operators

- 32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups
- Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3
 - Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators
 - Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$
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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
- Group theory and algebra of D_3 Center (Class algebra)
 - Self-symmetry (Normalizer). Lagrange Coset Theorem for classes
- ➔ 1st-Stage spectral decomposition of “Group-table” Hamiltonian of D_3 symmetry
 - All-commuting operators \mathbf{K}_k ← All-commuting projectors $\mathbf{P}^{(\alpha)}$
 - D_3 -invariant irep characters $\chi_k^{(\alpha)}$ Invariant numbers: Centrum, Rank, and Order
- 2nd-Stage spectral decompositions of global/local D_3
 - Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors ...and classes
- 3rd-Stage spectral decomposition of ALL of D_3 ...and of Hamiltonian \mathbf{H}
 - GLOBAL vs LOCAL symmetry of states ...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$

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

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

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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.

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

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

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

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	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

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

Note also:

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

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1	r¹	r²	i₁	i₂	i₃
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i₃	i₁	i₂	r¹	r²	1

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

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Class resolution into sum of eigenvalue · Projector

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

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

So: κ_r has an eigenvalue 2 and -1

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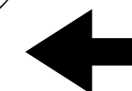
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\mathbf{r}^1	\mathbf{r}^2	1	\mathbf{i}_3	\mathbf{i}_1	\mathbf{i}_2
\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3	1	\mathbf{r}^1	\mathbf{r}^2
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Inverse resolution gives D_3 Character Table

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

$$\mathbf{P}^{A_1} = \frac{1}{18}(\kappa_3^2 + 3\kappa_3) = \frac{1}{18}(3\kappa_1 + 3\kappa_2 + 3\kappa_3)$$

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$$0 = (\kappa_3 + 3 \cdot \mathbf{1})\mathbf{P}^{A_2}$$

$$\kappa_3 \mathbf{P}^{A_2} = -3 \cdot \mathbf{P}^{A_2}$$

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

$$\kappa_3 \mathbf{P}^E = +0 \cdot \mathbf{P}^E$$

Class resolution into sum of eigenvalue · Projector

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

$$\kappa_2 = \kappa_r = 2 \cdot \mathbf{P}^{A_1} + 2 \cdot \mathbf{P}^{A_2} - 1 \cdot \mathbf{P}^E \quad \leftarrow \quad \kappa_r^2 = \kappa_r + 2 \cdot \mathbf{1} \Rightarrow (\kappa_r - 2 \cdot \mathbf{1})(\kappa_r + \mathbf{1}) = 0$$

$$\kappa_3 = \kappa_i = 3 \cdot \mathbf{P}^{A_1} - 3 \cdot \mathbf{P}^{A_2} + 0 \cdot \mathbf{P}^E \quad \text{So: } \kappa_r \text{ has an eigenvalue 2 and -1}$$

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

$$\mathbf{P}^{A_2} = \frac{(\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})}{(-3 - 3)(-3 - 0)}$$

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

Inverse resolution gives D_3 Character Table

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

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

$$\mathbf{P}^{A_1} = \frac{1}{18}(\kappa_3^2 + 3\kappa_3) = \frac{1}{18}(3\kappa_1 + 3\kappa_2 + 3\kappa_3)$$

$$\mathbf{P}^{A_2} = \frac{1}{18}(\kappa_3^2 - 3\kappa_3) = \frac{1}{18}(3\kappa_1 + 3\kappa_2 - 3\kappa_3)$$

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 κ_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 $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, \mathbf{P}^{A_2} , and \mathbf{P}^E

Note also:

$$\kappa_2^2 - \kappa_2 - 2 \cdot \mathbf{1} = 0 \quad 0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 + 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})$$

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

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

$$\kappa_3 \mathbf{P}^{A_1} = +3 \cdot \mathbf{P}^{A_1}$$

$$0 = (\kappa_3 + 3 \cdot \mathbf{1})\mathbf{P}^{A_2}$$

$$\kappa_3 \mathbf{P}^{A_2} = -3 \cdot \mathbf{P}^{A_2}$$

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

$$\kappa_3 \mathbf{P}^E = +0 \cdot \mathbf{P}^E$$

Class resolution into sum of eigenvalue · Projector

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

$$\kappa_2 = \kappa_r = 2 \cdot \mathbf{P}^{A_1} + 2 \cdot \mathbf{P}^{A_2} - 1 \cdot \mathbf{P}^E \quad \leftarrow \quad \kappa_r^2 = \kappa_r + 2 \cdot \mathbf{1} \Rightarrow (\kappa_r - 2 \cdot \mathbf{1})(\kappa_r + \mathbf{1}) = 0$$

$$\kappa_3 = \kappa_i = 3 \cdot \mathbf{P}^{A_1} - 3 \cdot \mathbf{P}^{A_2} + 0 \cdot \mathbf{P}^E \quad \text{So: } \kappa_r \text{ has an eigenvalue 2 and -1}$$

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

$$\mathbf{P}^{A_2} = \frac{(\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})}{(-3 - 3)(-3 - 0)}$$

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

Inverse resolution gives D_3 Character Table

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

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

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

$$\mathbf{P}^{A_1} = \frac{1}{18}(\kappa_3^2 + 3\kappa_3) = \frac{1}{18}(3\kappa_1 + 3\kappa_2 + 3\kappa_3)$$

$$\mathbf{P}^{A_2} = \frac{1}{18}(\kappa_3^2 - 3\kappa_3) = \frac{1}{18}(3\kappa_1 + 3\kappa_2 - 3\kappa_3)$$

$$\mathbf{P}^E = \frac{-1}{9}(\kappa_3^2 - 9 \cdot \mathbf{1}) = \frac{-1}{9}(3\kappa_1 + 3\kappa_2 - 9\kappa_1)$$

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$* *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**Group theory and algebra of D_3 Center (Class algebra)**Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes***➔** *1st-Stage spectral decomposition of “Group-table” Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irrep characters $\chi_k^{(\alpha)}$ ←**Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

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

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

1	r^1	r^2	i_1	i_2	i_3
r^2	1	r^1	i_2	i_3	i_1
r^1	r^2	1	i_3	i_1	i_2
i_1	i_2	i_3	1	r^1	r^2
i_2	i_3	i_1	r^2	1	r^1
i_3	i_1	i_2	r^1	r^2	1

Each class-sum κ_k commutes with all of D_3 .

$\kappa_1 = \mathbf{1}$	$\kappa_2 = r^1 + r^2$	$\kappa_3 = i_1 + i_2 + i_3$
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 $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, \mathbf{P}^{A_2} , and \mathbf{P}^E

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

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

$$\kappa_3 \mathbf{P}^{A_1} = +3 \cdot \mathbf{P}^{A_1}$$

$$0 = (\kappa_3 + 3 \cdot \mathbf{1}) \mathbf{P}^{A_2}$$

$$\kappa_3 \mathbf{P}^{A_2} = -3 \cdot \mathbf{P}^{A_2}$$

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

$$\kappa_3 \mathbf{P}^E = +0 \cdot \mathbf{P}^E$$

Class resolution into sum of eigenvalue · Projector

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

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

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

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

$$\mathbf{P}^{A_2} = \frac{(\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})}{(-3 - 3)(-3 - 0)}$$

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

Inverse resolution gives D_3 Character Table

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + r + r^2 + i_1 + i_2 + i_3)/6$$

$$\mathbf{P}^{A_2} = (\kappa_1 + \kappa_2 - \kappa_3)/6 = (\mathbf{1} + r + r^2 - i_1 - i_2 - i_3)/6$$

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

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

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

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

1	r^1	r^2	i_1	i_2	i_3
r^2	1	r^1	i_2	i_3	i_1
r^1	r^2	1	i_3	i_1	i_2
i_1	i_2	i_3	1	r^1	r^2
i_2	i_3	i_1	r^2	1	r^1
i_3	i_1	i_2	r^1	r^2	1

Each class-sum κ_k commutes with all of D_3 .

$\kappa_1 = \mathbf{1}$	$\kappa_2 = r^1 + r^2$	$\kappa_3 = i_1 + i_2 + i_3$
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 $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, \mathbf{P}^{A_2} , and \mathbf{P}^E

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

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

$$\kappa_3 \mathbf{P}^{A_1} = +3 \cdot \mathbf{P}^{A_1}$$

$$0 = (\kappa_3 + 3 \cdot \mathbf{1})\mathbf{P}^{A_2}$$

$$\kappa_3 \mathbf{P}^{A_2} = -3 \cdot \mathbf{P}^{A_2}$$

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

$$\kappa_3 \mathbf{P}^E = +0 \cdot \mathbf{P}^E$$

Class resolution into sum of eigenvalue · Projector

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

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

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

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

$$\mathbf{P}^{A_2} = \frac{(\kappa_3 - 3 \cdot \mathbf{1})(\kappa_3 - 0 \cdot \mathbf{1})}{(-3 - 3)(-3 - 0)}$$

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

Inverse resolution gives D_3 Character Table

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + r + r^2 + i_1 + i_2 + i_3)/6$$

$$\mathbf{P}^{A_2} = (\kappa_1 + \kappa_2 - \kappa_3)/6 = (\mathbf{1} + r + r^2 - i_1 - i_2 - i_3)/6$$

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

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

$$\chi_\kappa^{(\alpha)} = \text{Tr } D^{(\alpha)}(r_\kappa)$$

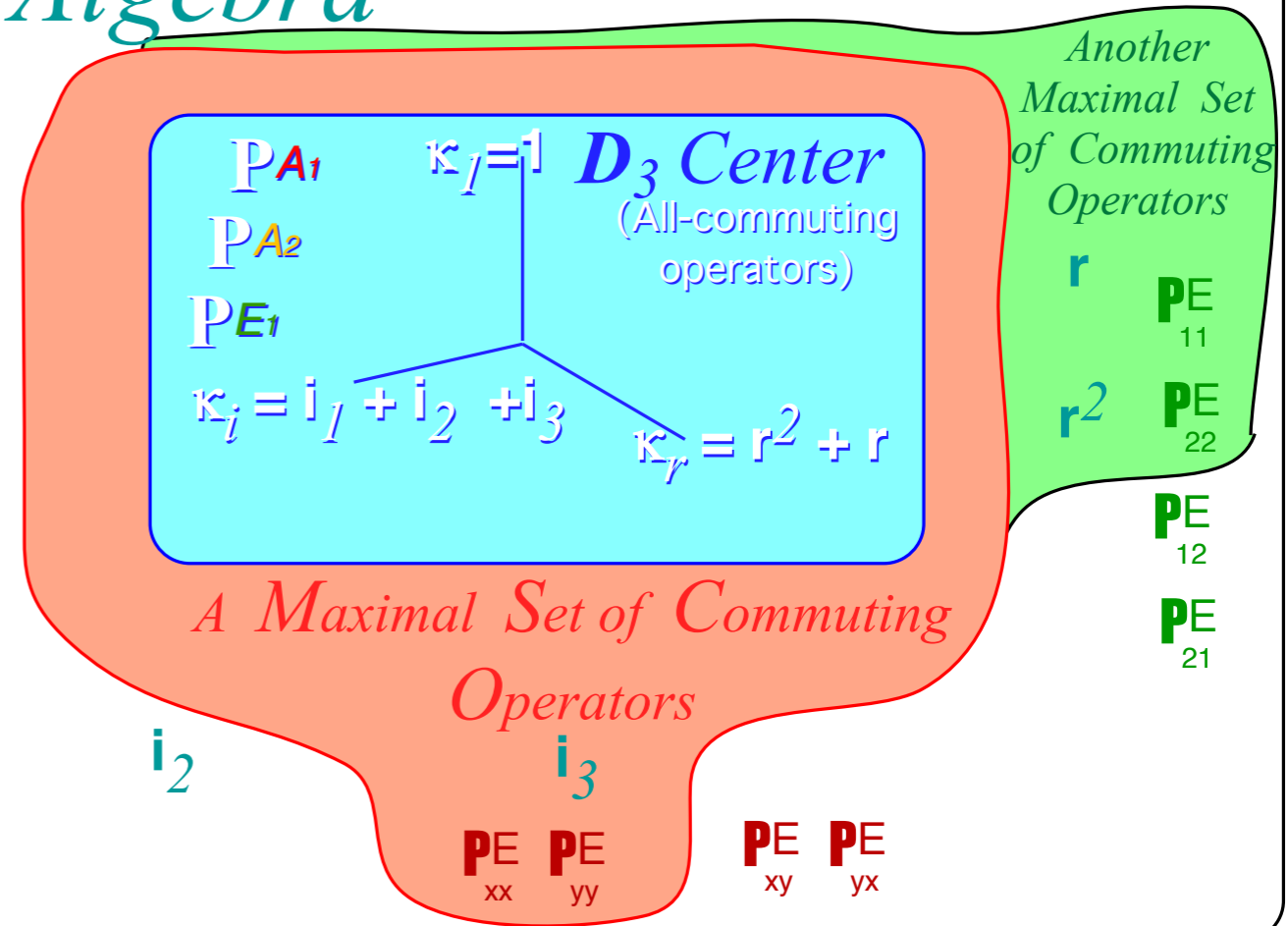
χ_κ^α	χ_1^α	χ_2^α	χ_3^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Review: 1st-Stage Spectral resolution of D_3 Center (All-commuting class projectors)

1	r²	r	i₁	i₂	i₃
r	1	r²	i₃	i₁	i₂
r²	r	1	i₂	i₃	i₁
i₁	i₃	i₂	1	r	r²
i₂	i₁	i₃	r²	1	r
i₃	i₂	i₁	r	r²	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

D_3 Algebra



Class-sum κ_k commutes with all g_t

Class-sum κ_k invariance:

$$g_t \kappa_k = \kappa_k g_t$$

$\circ G$ = order of group: ($\circ D_3 = 6$)

$\circ \kappa_k$ = order of class κ_k : ($\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$)

Class minimal equation

$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i$$

$$\kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot 1$$

$$0 = \kappa_i^3 - 9 \cdot \kappa_i = (\kappa_i - 3 \cdot 1)(\kappa_i + 3 \cdot 1)(\kappa_i - 0 \cdot 1)$$

Class ortho-complete $P\kappa$ relations

$$\kappa_1 = 1 \cdot P^{A_1} + 1 \cdot P^{A_2} + 1 \cdot P^E = 1 \quad (\text{Completeness})$$

$$\kappa_r = 2 \cdot P^{A_1} + 2 \cdot P^{A_2} - 1 \cdot P^E$$

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

$$\chi_k^{(\alpha)} = \text{Trace } D^{(\alpha)}(g_k)$$

$$\ell^{(\alpha)} = \text{Trace } D^{(\alpha)}(1)$$

$$\kappa_k = \sum_{(\alpha)} \frac{\circ \kappa_k \chi_k^{(\alpha)}}{\ell^{(\alpha)}} P^{(\alpha)}$$

irrep characters: $\chi_k^{(\alpha)}$
and dimensions: $\ell^{(\alpha)}$

$$P^{(\alpha)} = \frac{\ell^{(\alpha)}}{\circ G} \sum_k \chi_k^{(\alpha)*} \kappa_k$$

$$= \frac{\ell^{(\alpha)}}{\circ G} \sum_{g=1}^{\circ G} \chi_g^{(\alpha)*} g$$

χ_k^α	χ_1^α	χ_r^α	χ_i^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Find $\chi_1^{(\alpha)*} = \ell^{(\alpha)}$
using κ_1 coefficient

$$P^{(\alpha)} = \frac{(\ell^{(\alpha)})^2}{\circ G} \kappa_1 + \dots$$

$$P^{A_1} = (\kappa_1 + \kappa_r + \kappa_i)/6 = \frac{1}{6}(1 + r + r^2 + i_1 + i_2 + i_3)$$

$$P^{A_2} = (\kappa_1 + \kappa_r - \kappa_i)/6 = \frac{1}{6}(1 + r + r^2 - i_1 - i_2 - i_3)$$

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

AMOP 2.21.18 class 12.0: *Symmetry Principles for*
reference links *Advanced Atomic-Molecular-Optical-Physics*
on following page *William G. Harter - University of Arkansas*

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators**

32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups

Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3

Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators

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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

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Group theory and algebra of D_3 Center (Class algebra)

Self-symmetry (Normalizer).

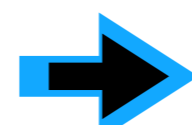
Lagrange Coset Theorem for classes

1st-Stage spectral decomposition of “Group-table” Hamiltonian of D_3 symmetry

All-commuting operators \mathbf{K}_k

All-commuting projectors $\mathbf{P}^{(\alpha)}$

D_3 -invariant irep characters $\chi_k^{(\alpha)}$



Invariant numbers: Centrum, Rank, and Order



2nd-Stage spectral decompositions of global/local D_3

Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors

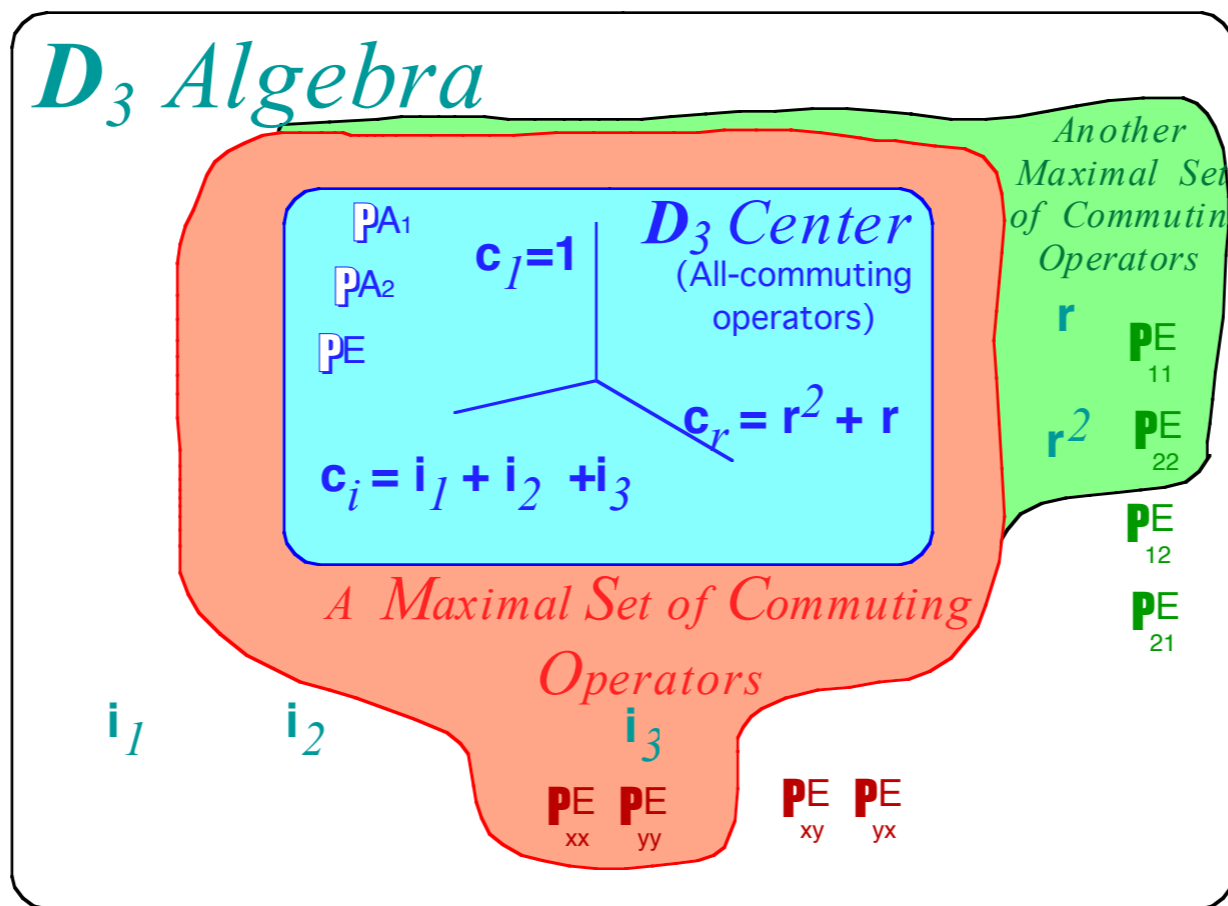
...and classes

3rd-Stage spectral decomposition of ALL of D_3

...and of Hamiltonian \mathbf{H}

GLOBAL vs LOCAL symmetry of states

...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$



(Fig. 15.2.1 QTCA)

Important invariant numbers or “characters”

$\ell^\alpha =$ 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

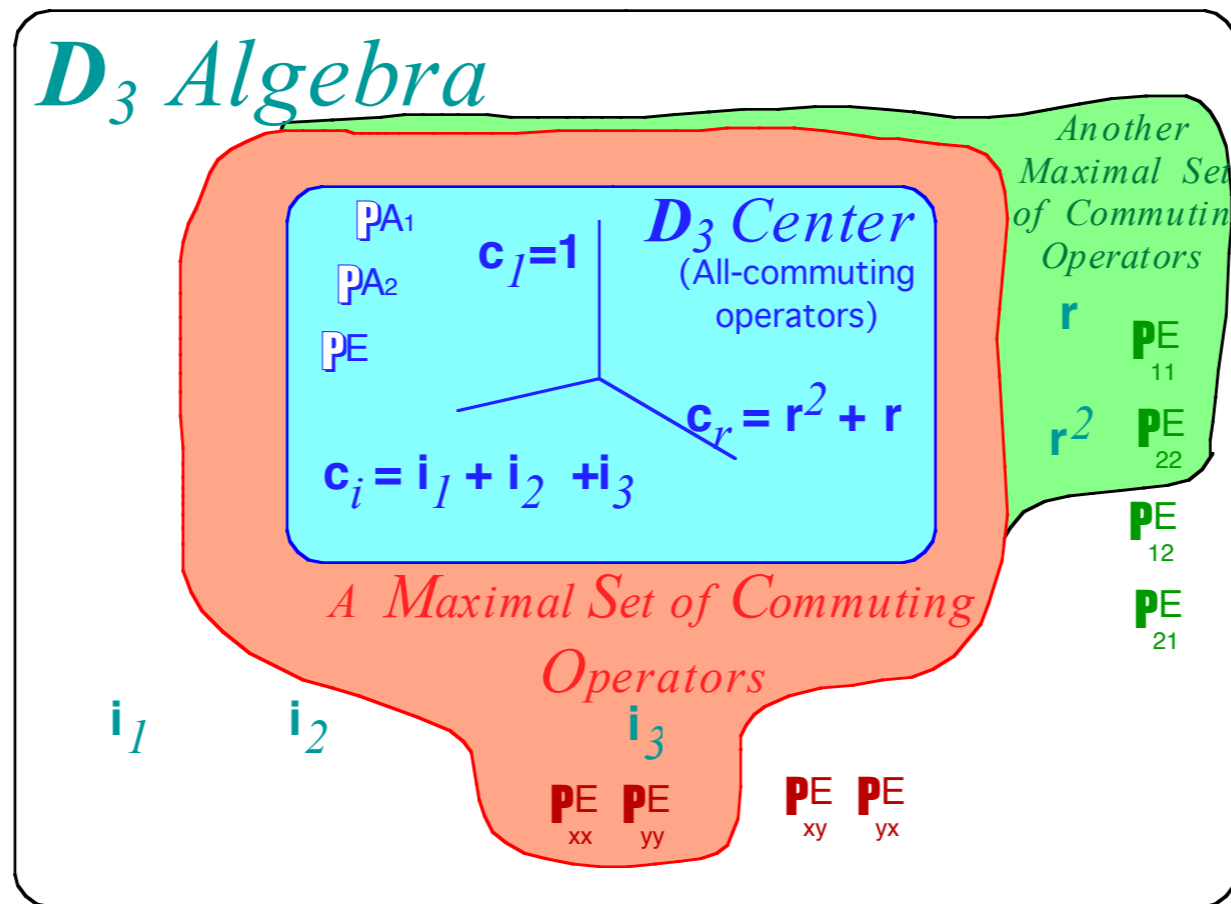
$$D_3 \quad \kappa = 1 \quad r^1 + r^2 \quad i_1 + i_2 + i_3$$

$$\mathbf{P}^{A_1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

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

D_3 Algebra



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

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

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

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

$$D_3 \quad \kappa = 1 \quad \mathbf{r}^1 + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

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

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

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

AMOP
reference links
on following page

2.21.18 class 12.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

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Self-symmetry (Normalizer).

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1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry

All-commuting operators \mathbf{K}_k

All-commuting projectors $\mathbf{P}^{(\alpha)}$

D_3 -invariant irrep characters $\chi_k^{(\alpha)}$

Invariant numbers: Centrum, Rank, and Order

 *2nd-Stage spectral decompositions of global/local D_3*

Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors  ...and classes

3rd-Stage spectral decomposition of ALL of D_3

...and of Hamiltonian \mathbf{H}

GLOBAL vs LOCAL symmetry of states

...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$

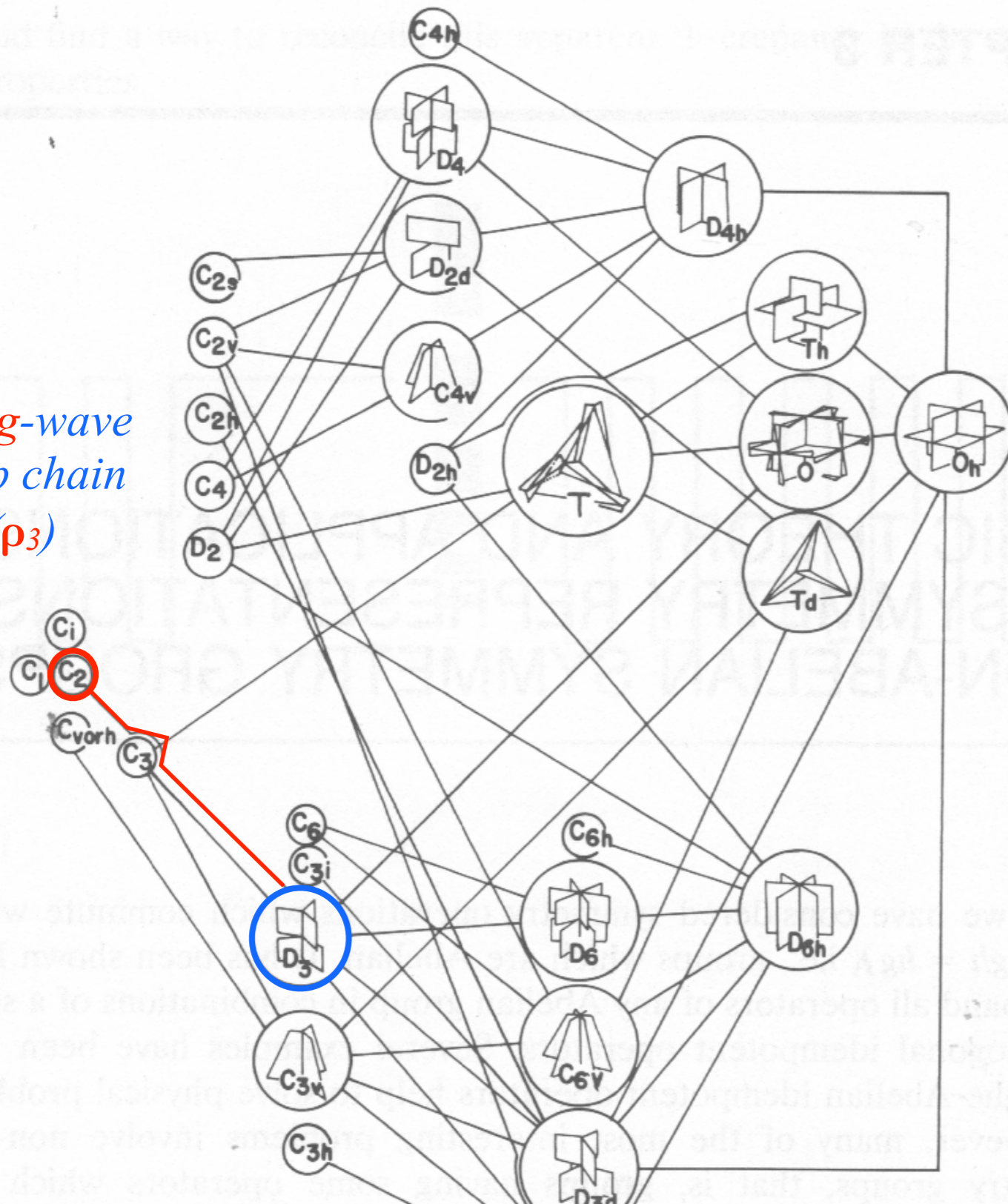
Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgroup(s) $C_2(\mathbf{i})$

Standing-wave
Subgroup chain
 $D_3 \supset C_2(\rho_3)$



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

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgroup(s) $C_2(\mathbf{i})$

$$D_3 \quad \kappa = \mathbf{1} \quad \mathbf{r}^1 + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

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$D_3 \supset C_2$ Correlation table

shows which products of

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**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$* *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**Group theory and algebra of D_3 Center (Class algebra)**Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes**1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irrep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order***→** *2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors ← ...and classes**3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

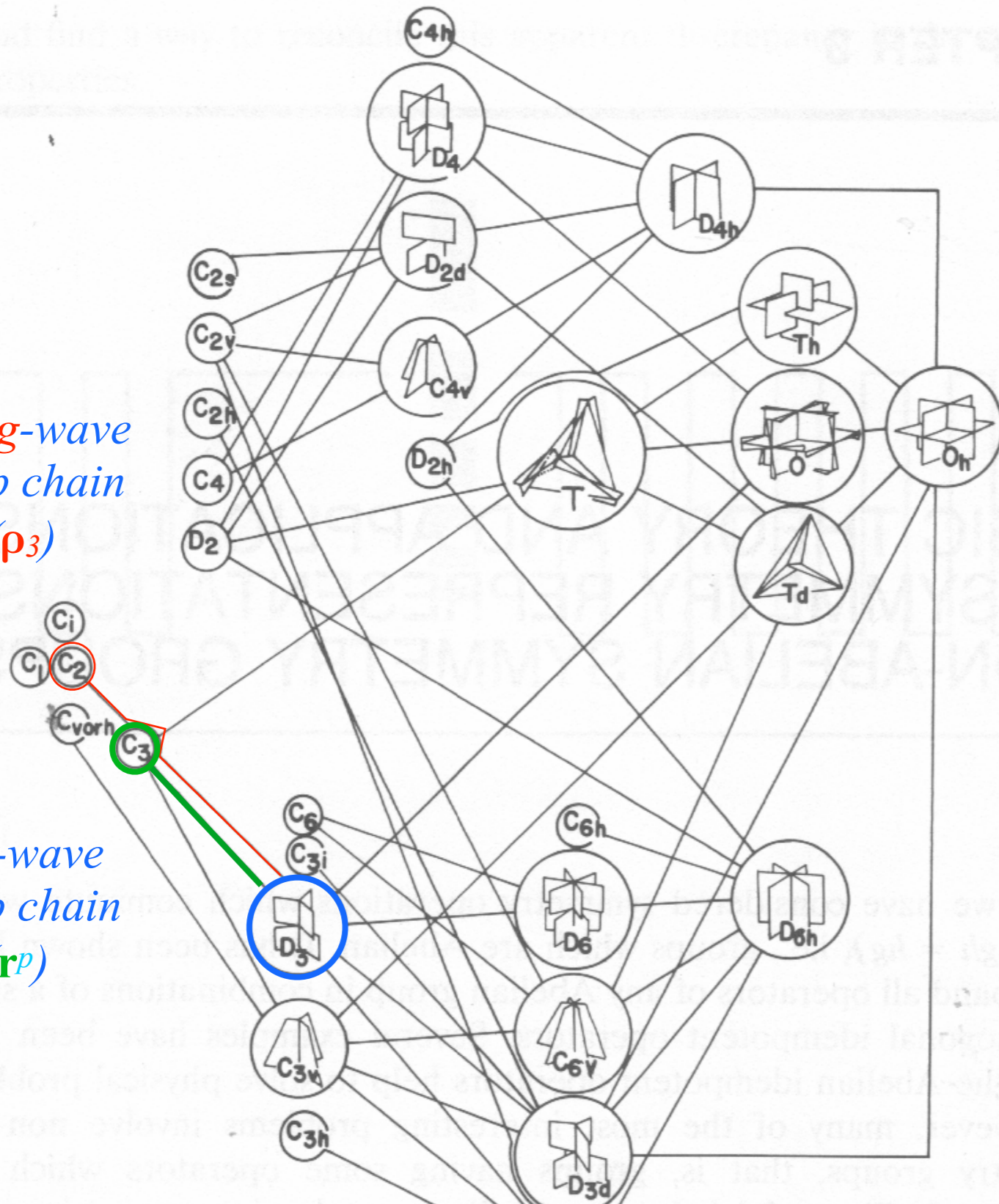
2nd-Stage

Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

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“ C_3 -friendly” irreducible projectors

$$\mathbf{P}^{(\alpha)} \mathbf{1} = \mathbf{P}^{(\alpha)} (p^{0_3} + p^{1_3} + p^{2_3})$$

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

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgroup(s) $C_2(\mathbf{i})$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)

$$D_3 \quad \kappa = \mathbf{1} \quad \mathbf{r}^l + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

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

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

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

$$C_2 \quad \kappa = \mathbf{1} \quad \mathbf{i}_3$$

$$p^{0_2} = \begin{bmatrix} 1 & 1 \end{bmatrix} / 2$$

$$p^{1_2} = \begin{bmatrix} 1 & -1 \end{bmatrix} / 2$$

Let:

$$\varepsilon = e^{-2\pi i/3}$$

$$C_3 \quad \kappa = \mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2$$

$$p^{0_3} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix} / 3$$

$$p^{1_3} = \begin{bmatrix} 1 & \varepsilon & \varepsilon^* \end{bmatrix} / 3$$

$$p^{2_3} = \begin{bmatrix} 1 & \varepsilon^* & \varepsilon \end{bmatrix} / 3$$

$D_3 \supset C_2$ Correlation table

shows which products of class projector $\mathbf{P}^{(\alpha)}$ with

C_2 -unit $1 = p^{0_2} + p^{1_2}$ will

make **IRREDUCIBLE** $\mathbf{P}_{n,n}^{(\alpha)}$

Rank $\rho(D_3)=4$ implies

there will be exactly 4

“ C_2 -friendly” irep projectors

$$\mathbf{P}^{(\alpha)} \mathbf{1} = \mathbf{P}^{(\alpha)} (p^{0_2} + p^{1_2})$$

$$= \mathbf{P}_{0_2 0_2}^{(\alpha)} + \mathbf{P}_{1_2 1_2}^{(\alpha)}$$



$$\mathbf{P}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (1 + \mathbf{i}_3) / 2 = (1 + \mathbf{r}^l + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

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

$$\mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (1 + \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^l - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) / 6$$

$$\mathbf{P}_{1_2 1_2}^E = \mathbf{P}^E p^{1_2} = \mathbf{P}^E (1 - \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^l - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3) / 6$$

$D_3 \supset C_2$ $0_2 \quad 1_2$

$$n^{A_1} = \begin{bmatrix} 1 & \cdot \end{bmatrix}$$

$$n^{A_2} = \begin{bmatrix} \cdot & 1 \end{bmatrix}$$

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$$1 = p^{0_2} + p^{1_2}$$

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$$\mathbf{P}^E = \begin{bmatrix} \mathbf{P}_{0_2 0_2}^E & \mathbf{P}_{1_2 1_2}^E \end{bmatrix}$$

Same for Correlation table: $D_3 \supset C_3$ $0_3 \quad 1_3 \quad 2_3$

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“ C_3 -friendly” irreducible projectors

$$\mathbf{P}^{(\alpha)} \mathbf{1} = \mathbf{P}^{(\alpha)} (p^{0_3} + p^{1_3} + p^{2_3})$$

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$$1 = p^{0_3} + p^{1_3} + p^{2_3}$$

$$\mathbf{P}^{A_1} = \begin{bmatrix} \mathbf{P}_{0_3 0_3}^{A_1} & \cdot & \cdot \end{bmatrix}$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} \mathbf{P}_{0_3 0_3}^{A_2} & \cdot & \cdot \end{bmatrix}$$

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$D_3 \supset C_2$ 0_2 1_2

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Same for Correlation table: $D_3 \supset C_3$ 0_3 1_3 2_3

$$n^{A_1} = \begin{bmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{bmatrix}$$

$$n^{A_2} = \begin{bmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \end{bmatrix}$$

$$n^E = \begin{bmatrix} \cdot & 1 & 1 \\ 1 & \cdot & \cdot \\ 1 & \cdot & \cdot \end{bmatrix}$$

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$$\mathbf{P}^{(\alpha)} \mathbf{1} = \mathbf{P}^{(\alpha)} (p^{0_3} + p^{1_3} + p^{2_3})$$

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$$\mathbf{P}_{0_3 0_3}^{A_1} = \mathbf{P}^{A_1} p^{0_3} = \mathbf{P}^{A_1} (1 + \mathbf{r}^l + \mathbf{r}^2) / 3 = (1 + \mathbf{r}^l + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

$$\mathbf{P}_{0_3 0_3}^{A_2} = \mathbf{P}^{A_2} p^{0_3} = \mathbf{P}^{A_2} (1 + \mathbf{r}^l + \mathbf{r}^2) / 3 = (1 + \mathbf{r}^l + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3) / 6$$

$$\mathbf{P}_{1_3 1_3}^E = \mathbf{P}^E p^{1_3} = \mathbf{P}^E (1 + \varepsilon \mathbf{r}^l + \varepsilon^* \mathbf{r}^2) / 3 = (1 + \varepsilon \mathbf{r}^l + \varepsilon^* \mathbf{r}^2) / 3$$

$$\mathbf{P}_{2_3 2_3}^E = \mathbf{P}^E p^{2_3} = \mathbf{P}^E (1 + \varepsilon^* \mathbf{r}^l + \varepsilon \mathbf{r}^2) / 3 = (1 + \varepsilon^* \mathbf{r}^l + \varepsilon \mathbf{r}^2) / 3$$

$$1 = p^{0_3} + p^{1_3} + p^{2_3}$$

$$\mathbf{P}^{A_1} = \begin{bmatrix} \mathbf{P}_{0_3 0_3}^{A_1} & \cdot & \cdot \\ \cdot & \mathbf{P}_{1_3 1_3}^{A_2} & \cdot \\ \cdot & \cdot & \mathbf{P}_{2_3 2_3}^{A_2} \end{bmatrix}$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} \mathbf{P}_{0_3 0_3}^{A_2} & \cdot & \cdot \\ \cdot & \mathbf{P}_{1_3 1_3}^{A_1} & \cdot \\ \cdot & \cdot & \mathbf{P}_{2_3 2_3}^{A_1} \end{bmatrix}$$

$$\mathbf{P}^E = \begin{bmatrix} \cdot & \mathbf{P}_{1_3 1_3}^E & \mathbf{P}_{2_3 2_3}^E \\ \mathbf{P}_{1_3 1_3}^E & \cdot & \cdot \\ \mathbf{P}_{2_3 2_3}^E & \cdot & \cdot \end{bmatrix}$$

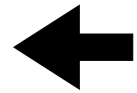
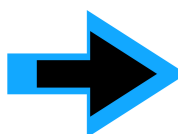
AMOP
reference links
on following page

2.21.18 class 12.0: Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics

William G. Harter - University of Arkansas

Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics: D_3 and C_{3v} group products, classes, and irrep projection operators

- 32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups
- Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3
 - Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators
 - Deriving $D_3 \sim C_{3v}$ products by group definition $|\mathbf{g}\rangle = \mathbf{g}|1\rangle$ of position ket $|\mathbf{g}\rangle$
 - 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
- Group theory and algebra of D_3 Center (Class algebra)
 - Self-symmetry (Normalizer). Lagrange Coset Theorem for classes
- 1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry
 - All-commuting operators \mathbf{K}_k All-commuting projectors $\mathbf{P}^{(\alpha)}$
 - D_3 -invariant irep characters $\chi_k^{(\alpha)}$ Invariant numbers: Centrum, Rank, and Order
- 2nd-Stage spectral decompositions of global/local D_3
 - Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors ...and classes
- 3rd-Stage spectral decomposition of ALL of D_3 ...and of Hamiltonian \mathbf{H}
 - GLOBAL vs LOCAL symmetry of states ...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$



2nd-Stage

2nd Step: (contd.) While some class projectors $\mathbf{P}^{(\alpha)}$ split in two, so ALSO DO some classes κ_k

Rank $\rho(D_3)=4$
idempotents

$\mathbf{P}^{(\alpha)}$

$$\begin{aligned} \mathbf{P}_{0_2 0_2}^{A_1} &= \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (1+i_3)/2 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6 \\ \mathbf{P}_{1_2 1_2}^{A_2} &= \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (1-i_3)/2 = (1 + r^1 + r^2 - i_1 - i_2 - i_3)/6 \\ \mathbf{P}_{0_2 0_2}^E &= \mathbf{P}^E p^{0_2} = \mathbf{P}^E (1+i_3)/2 = (21 - r^1 - r^2 - i_1 - i_2 + 2i_3)/6 \\ \mathbf{P}_{1_2 1_2}^E &= \mathbf{P}^E p^{1_2} = \mathbf{P}^E (1-i_3)/2 = (21 - r^1 - r^2 + i_1 + i_2 - 2i_3)/6 \end{aligned}$$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{0_2 0_2}^E + \mathbf{P}_{1_2 1_2}^E$
class κ_i splits into $\kappa_{i_{12}}$ and κ_{i_3}

Centrum $\kappa(D_3)=3$
idempotents
 $\mathbf{P}^{(\alpha)}$

4 different
idempotent

$\mathbf{P}_{n,n}^{(\alpha)}$

$$\begin{aligned} \mathbf{P}_{0_3 0_3}^{A_1} &= \mathbf{P}^{A_1} p^{0_3} = \mathbf{P}^{A_1} (1+r^1+r^2)/3 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6 \\ \mathbf{P}_{0_3 0_3}^{A_2} &= \mathbf{P}^{A_2} p^{0_3} = \mathbf{P}^{A_2} (1+r^1+r^2)/3 = (1 + r^1 + r^2 - i_1 - i_2 - i_3)/6 \\ \mathbf{P}_{1_3 1_3}^E &= \mathbf{P}^E p^{1_3} = \mathbf{P}^E (1+\varepsilon r^1 + \varepsilon^* r^2)/3 = (1 + \varepsilon r^1 + \varepsilon^* r^2)/3 \\ \mathbf{P}_{2_3 2_3}^E &= \mathbf{P}^E p^{2_3} = \mathbf{P}^E (1+\varepsilon^* r^1 + \varepsilon r^2)/3 = (1 + \varepsilon^* r^1 + \varepsilon r^2)/3 \end{aligned}$$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{1_3 1_3}^E + \mathbf{P}_{2_3 2_3}^E$
class κ_r splits into κ_{r_1} and κ_{r_2}

$$D_3 \quad \kappa = \begin{bmatrix} 1 & r^1+r^2 & i_1+i_2+i_3 \end{bmatrix}$$

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

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

$$\varepsilon = e^{-2\pi i/3}$$

2nd-Stage

2nd Step: (contd.) While some class projectors $\mathbf{P}^{(\alpha)}$ split in two, so ALSO DO some classes κ_k

Rank $\rho(D_3)=4$
idempotents

$\mathbf{P}^{(\alpha)}$

$$\mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (1+i_3)/2 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6$$

$$\mathbf{P}_{1_2 1_2}^{A_2} = \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (1-i_3)/2 = (1 + r^1 + r^2 - i_1 - i_2 - i_3)/6$$

$$\mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (1+i_3)/2 = (2 - r^1 - r^2 - i_1 - i_2 + 2i_3)/6$$

$$\mathbf{P}_{1_2 1_2}^E = \mathbf{P}^E p^{1_2} = \mathbf{P}^E (1-i_3)/2 = (2 - r^1 - r^2 + i_1 + i_2 - 2i_3)/6$$

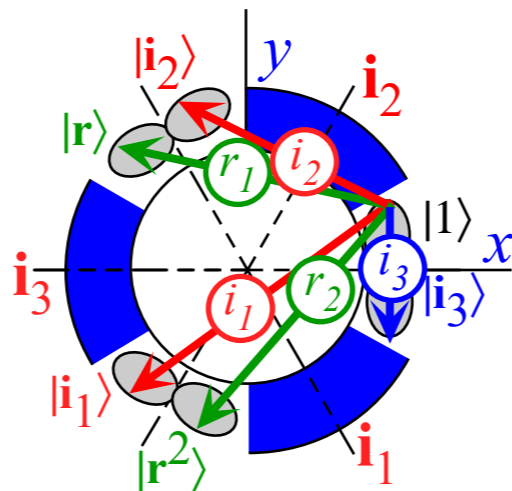
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class κ_i splits into $\kappa_{i_{12}}$ and κ_{i_3}

$r=r_2$ must equal r_1
 $i=i_2$ must equal i_1

For Local $D_3 \supset C_2(i_3)$ symmetry

i_3 is free parameter



Rank $\rho(D_3)=4$
parameters in either case

4 different idempotent

$\mathbf{P}_{n,n}^{(\alpha)}$

$$\mathbf{P}_{0_3 0_3}^{A_1} = \mathbf{P}^{A_1} p^{0_3} = \mathbf{P}^{A_1} (1+r^1+r^2)/3 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6$$

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$$\mathbf{P}_{1_3 1_3}^E = \mathbf{P}^E p^{1_3} = \mathbf{P}^E (1 + \epsilon r^1 + \epsilon^* r^2)/3 = (1 + \epsilon r^1 + \epsilon^* r^2)/3$$

$$\mathbf{P}_{2_3 2_3}^E = \mathbf{P}^E p^{2_3} = \mathbf{P}^E (1 + \epsilon^* r^1 + \epsilon r^2)/3 = (1 + \epsilon^* r^1 + \epsilon r^2)/3$$

$\epsilon = e^{-2\pi i/3}$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{1_3 1_3}^E + \mathbf{P}_{2_3 2_3}^E$

class κ_r splits into κ_{r_1} and κ_{r_2}

$i=i_1=i_2=i_3$

For Local $D_3 \supset C_3(r^p)$ symmetry

r_1 and r_2 are free

Centrum $\kappa(D_3)=3$
idempotents
 $\mathbf{P}^{(\alpha)}$

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Rank $\rho(D_3)=4$
 idempotents
 $\mathbf{P}_{n,n}^{(\alpha)}$

$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

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$$\mathbf{P}_{x,x}^E = \mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (\mathbf{1} + \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) / 6$$

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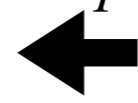
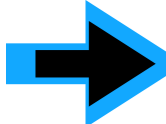
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 - Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors ...and classes
- 3rd-Stage spectral decomposition of ALL of D_3 ← ...and of Hamiltonian \mathbf{H}
 - GLOBAL vs LOCAL symmetry of states ...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$



Centrum $\kappa(D_3)=3$
idempotents
 $\mathbf{P}^{(\alpha)}$

$$D_3 \kappa = \mathbf{1} \quad \mathbf{r}^1 + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

$$\mathbf{P}^{A_1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} / 6$$

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Rank $\rho(D_3)=4$
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$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

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Spectral resolution of ALL 6 of D_3 :

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$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E) \cdot \mathbf{g} \cdot (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E)$$

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$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = \mathbf{P}_{x,x}^{A_1} \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^{A_1} + 0 + 0 + 0$$

$$+ 0 + \mathbf{P}_{y,y}^{A_2} \cdot \mathbf{g} \cdot \mathbf{P}_{y,y}^{A_2} + 0 + 0$$

$$+ 0 + 0 + \mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^E + \mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{y,y}^E$$

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$$\mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^E = D^{E_{x,x}}(\mathbf{g}) \mathbf{P}_{x,x}^E + 0 + 0 + \mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{x,y}^E$$

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Six D_3 projectors: 4 idempotents + 2 nilpotents (off-diag.)

	$\mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3$	
$\mathbf{P}_{x,x}^{A_1} =$	$(1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1) / 6$	
$\mathbf{P}_{y,y}^{A_2} =$	$(1 \quad 1 \quad 1 \quad -1 \quad -1 \quad -1) / 6$	
	$\mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3$	
$\mathbf{P}_{x,x}^E =$	$(2 \quad -1 \quad -1 \quad -1 \quad -1 \quad +2) / 6$	
$\mathbf{P}_{y,x}^E =$	$(0 \quad 1 \quad -1 \quad -1 \quad +1 \quad 0) / \sqrt{3/2}$	
	$\mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3$	
$\mathbf{P}_{x,y}^E =$	$(0 \quad -1 \quad 1 \quad -1 \quad +1 \quad 0) / \sqrt{3/2}$	
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idempotents
 $\mathbf{P}_{n,n}^{(\alpha)}$

$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

$$\mathbf{P}_{y,y}^{A_2} = \mathbf{P}_{1_2 1_2}^{A_2} = \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (\mathbf{1} - \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3) / 6$$

$$\mathbf{P}_{x,x}^E = \mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (\mathbf{1} + \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) / 6$$

$$\mathbf{P}_{y,y}^E = \mathbf{P}_{1_2 1_2}^E = \mathbf{P}^E p^{1_2} = \mathbf{P}^E (\mathbf{1} - \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3) / 6$$

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

The old 'g-equals-1-times-g-times-1' Trick

$$\mathbf{g} = \sum_m \sum_e \sum_b D_{eb}^{(m)}(\mathbf{g}) \mathbf{P}_{eb}^{(m)}$$

$$\mathbf{P}_{eb}^{(m)} = (\text{norm}) \sum_{\mathbf{g}} D_{eb}^{(m)*}(\mathbf{g}) \mathbf{g}$$

$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E) \cdot \mathbf{g} \cdot (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E)$$

$$\mathbf{g} = D^{A_1}(\mathbf{g}) \mathbf{P}_{x,x}^{A_1} + D^{A_2}(\mathbf{g}) \mathbf{P}_{y,y}^{A_2} + D^E(\mathbf{g}) \mathbf{P}_{x,x}^E + D^E(\mathbf{g}) \mathbf{P}_{y,y}^E + D^E(\mathbf{g}) \mathbf{P}_{x,y}^E + D^E(\mathbf{g}) \mathbf{P}_{y,x}^E$$

Six D_3 projectors: 4 idempotents + 2 nilpotents (off-diag.)

	$\mathbf{1}$	\mathbf{r}^1	\mathbf{r}^2	\mathbf{i}_1	\mathbf{i}_2	\mathbf{i}_3	
$\mathbf{P}_{x,x}^{A_1} =$	$(1$	1	1	1	1	$1)$	$/6$
$\mathbf{P}_{y,y}^{A_2} =$	$(1$	1	1	-1	-1	$-1)$	$/6$
$\mathbf{P}_{x,x}^E =$	$(2$	-1	-1	-1	-1	$+2)$	$/6$
$\mathbf{P}_{y,x}^E =$	$(0$	1	-1	-1	$+1$	$0)$	$/\sqrt{3}/2$
$\mathbf{P}_{x,y}^E =$	$(0$	-1	1	-1	$+1$	$0)$	$/\sqrt{3}/2$
$\mathbf{P}_{y,y}^E =$	$(2$	-1	-1	$+1$	$+1$	$-2)$	$/6$

Centrum $\kappa(D_3)=3$
idempotents
 $\mathbf{P}^{(\alpha)}$

$$D_3 \kappa = \mathbf{1} \quad \mathbf{r}^l + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

$$\mathbf{P}^{A_1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} / 6$$

$$\mathbf{P}^{A_2} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} / 6$$

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

Rank $\rho(D_3)=4$
idempotents
 $\mathbf{P}_{n,n}^{(\alpha)}$

$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^l + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

$$\mathbf{P}_{y,y}^{A_2} = \mathbf{P}_{1_2 1_2}^{A_2} = \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (\mathbf{1} - \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^l + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3) / 6$$

$$\mathbf{P}_{x,x}^E = \mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (\mathbf{1} + \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^l - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) / 6$$

$$\mathbf{P}_{y,y}^E = \mathbf{P}_{1_2 1_2}^E = \mathbf{P}^E p^{1_2} = \mathbf{P}^E (\mathbf{1} - \mathbf{i}_3) / 2 = (2\mathbf{1} - \mathbf{r}^l - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3) / 6$$

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

The old 'g-equals-1-times-g-times-1' Trick

$$\mathbf{g} = \sum_m \sum_e \sum_b D_{eb}^{(m)}(\mathbf{g}) \mathbf{P}_{eb}^{(m)}$$

$$\mathbf{P}_{eb}^{(m)} = (\text{norm}) \sum_{\mathbf{g}} D_{eb}^{(m)*}(\mathbf{g}) \mathbf{g}$$

$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E) \cdot \mathbf{g} \cdot (\mathbf{P}_{x,x}^{A_1} + \mathbf{P}_{y,y}^{A_2} + \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E)$$

$$\mathbf{g} = D^{A_1}(\mathbf{g}) \mathbf{P}_{x,x}^{A_1} + D^{A_2}(\mathbf{g}) \mathbf{P}_{y,y}^{A_2} + D^E(\mathbf{g}) \mathbf{P}_{x,x}^E + D^E(\mathbf{g}) \mathbf{P}_{y,y}^E + D^E(\mathbf{g}) \mathbf{P}_{x,y}^E + D^E(\mathbf{g}) \mathbf{P}_{y,x}^E$$

Six D_3 projectors: 4 idempotents + 2 nilpotents (off-diag.)

$$\mathbf{P}_{x,x}^{A_1} = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(1 \quad 1 \quad 1 \quad 1 \quad 1 \quad 1) / 6}$$

$$\mathbf{P}_{y,y}^{A_2} = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(1 \quad 1 \quad 1 \quad -1 \quad -1 \quad -1) / 6}$$

$$\mathbf{P}_{x,x}^E = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(2 \quad -1 \quad -1 \quad -1 \quad -1 \quad +2) / 6}$$

$$\mathbf{P}_{x,y}^E = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(0 \quad -1 \quad 1 \quad -1 \quad +1 \quad 0) / \sqrt{3/2}}$$

$$\mathbf{P}_{y,x}^E = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(0 \quad 1 \quad -1 \quad -1 \quad +1 \quad 0) / \sqrt{3/2}}$$

$$\mathbf{P}_{y,y}^E = \frac{\mathbf{1} \quad \mathbf{r}^l \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3}{(2 \quad -1 \quad -1 \quad +1 \quad +1 \quad -2) / 6}$$

where D_3 irreducible representations are:
 $D^{A_1}(\mathbf{g}) = +I, \quad D^{A_2}(\mathbf{g}) = \pm I,$

$$D^E(\mathbf{1}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, D^E(\mathbf{r}) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}, D^E(\mathbf{r}^2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & \frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & \frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

**Discrete symmetry subgroups of $O(3)$ and application to tunneling and vibrational dynamics:
 D_3 and C_{3v} group products, classes, and irrep projection operators***32 crystal point symmetries: 16 Abelian (commutative) and 16 non-Abelian groups**Smallest non-Abelian symmetry: 3- C_2 -axis D_3 vs. 3- C_v -plane C_{3v} isomorphic to permutation- S_3* *Relating C_2 -180° rotations \mathbf{R}_z , C_v -plane reflections σ_z , and inversion \mathbf{I} operators**Deriving $D_3 \sim C_{3v}$ products by group definition $|g\rangle = \mathbf{g}|1\rangle$ of position ket $|g\rangle$* *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**Group theory and algebra of D_3 Center (Class algebra)**Self-symmetry (Normalizer).**Lagrange Coset Theorem for classes**1st-Stage spectral decomposition of "Group-table" Hamiltonian of D_3 symmetry**All-commuting operators \mathbf{K}_k* *All-commuting projectors $\mathbf{P}^{(\alpha)}$* *D_3 -invariant irrep characters $\chi_k^{(\alpha)}$* *Invariant numbers: Centrum, Rank, and Order**2nd-Stage spectral decompositions of global/local D_3* *Subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$ split class projectors**...and classes***→** *3rd-Stage spectral decomposition of ALL of D_3* *...and of Hamiltonian \mathbf{H}* *GLOBAL vs LOCAL symmetry of states**...and group \mathbf{H} parameters $\{r, i_1, i_2, i_3\}$*

Global (LAB) symmetry

$$\mathbf{i}_3 |_{eb}^{(m)} \rangle = \mathbf{i}_3 \mathbf{P}_{eb}^{(m)} |1\rangle = (-1)^e |^{(m)} \rangle$$

$D_3 > C_2$ \mathbf{i}_3 projector states

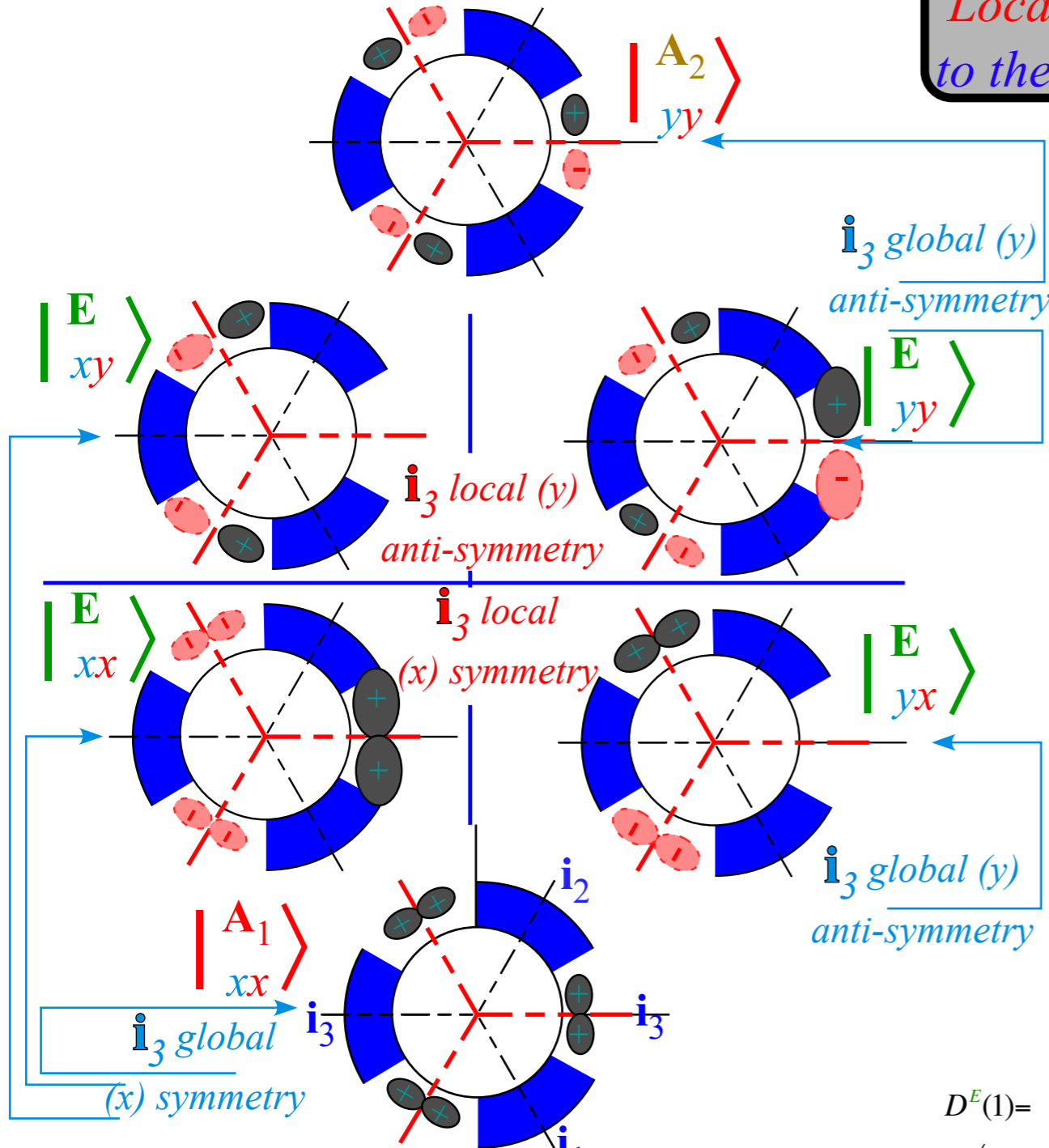
$$|_{eb}^{(m)} \rangle = \mathbf{P}_{eb}^{(m)} |1\rangle$$

Local (BOD) symmetry

$$\bar{\mathbf{i}}_3 |_{eb}^{(m)} \rangle = \bar{\mathbf{i}}_3 \mathbf{P}_{eb}^{(m)} |1\rangle = \mathbf{P}_{eb}^{(m)} \bar{\mathbf{i}}_3 |1\rangle = \mathbf{P}_{eb}^{(m)} \mathbf{i}_3^\dagger |1\rangle = (-1)^b |^{(m)} \rangle$$

Local $\bar{\mathbf{g}}$ commute through to the "inside" to be a \mathbf{g}^\dagger

Here the "Mock-Mach" is being applied!



$$\mathbf{P}_{y,y}^{A_2} = \frac{1 \ r^1 \ r^2 \ \mathbf{i}_1 \ \mathbf{i}_2 \ \mathbf{i}_3}{(1 \ 1 \ 1 \ -1 \ -1 \ -1)/6}$$

$$\mathbf{P}_{x,y}^E = \frac{(0 \ -1 \ 1 \ -1 \ +1 \ 0)/\sqrt{3/2}}{(2 \ -1 \ -1 \ +1 \ +1 \ -2)/6}$$

$$\mathbf{P}_{y,y}^E = \frac{(2 \ -1 \ -1 \ +1 \ +1 \ -2)/6}{(0 \ 1 \ -1 \ -1 \ +1 \ 0)/\sqrt{3/2}}$$

Ket norm factors detailed in Lect.17 p.23-30

$$\mathbf{P}_{x,x}^E = \frac{(2 \ -1 \ -1 \ -1 \ -1 \ +2)/6}{(0 \ 1 \ -1 \ -1 \ +1 \ 0)/\sqrt{3/2}}$$

$$\mathbf{P}_{y,x}^E = \frac{(0 \ 1 \ -1 \ -1 \ +1 \ 0)/\sqrt{3/2}}{(2 \ -1 \ -1 \ -1 \ -1 \ +2)/6}$$

$$\mathbf{P}_{x,x}^{A_1} = \frac{(1 \ 1 \ 1 \ 1 \ 1 \ 1)/6}{(1 \ 1 \ 1 \ 1 \ 1 \ 1)/6}$$

$$D^{A_1}(\mathbf{g}) = +I, \ D^{A_2}(\mathbf{r}^p) = +I, \ D^{A_2}(\mathbf{i}_q) = -I$$

$$D^E(\mathbf{l}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad D^E(\mathbf{r}) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix} \quad D^E(\mathbf{r}^2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix} \quad D^E(\mathbf{i}_1) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & \frac{1}{2} \end{pmatrix} \quad D^E(\mathbf{i}_2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & \frac{1}{2} \end{pmatrix} \quad D^E(\mathbf{i}_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$|{}^{(m)}_{eb}\rangle = \mathbf{P}_{eb}{}^{(m)}|\mathbf{1}\rangle$$

external LAB

internal BOD

symmetry label-e

symmetry label-b

GLOBAL

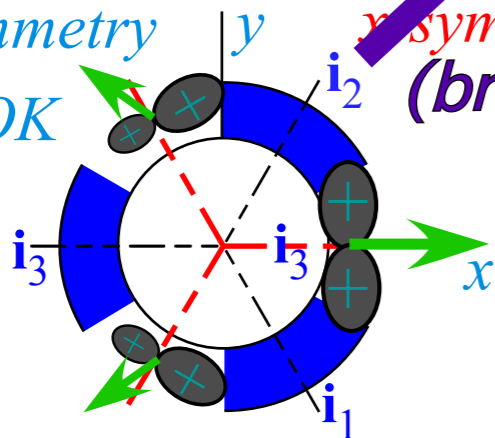
LOCAL

GLOBAL

$(i_3) = 0_2$

x-symmetry

\mathbf{i}_3 OK



~~LOCAL~~

~~$(i_3) = 0_2$~~

~~x-symmetry~~

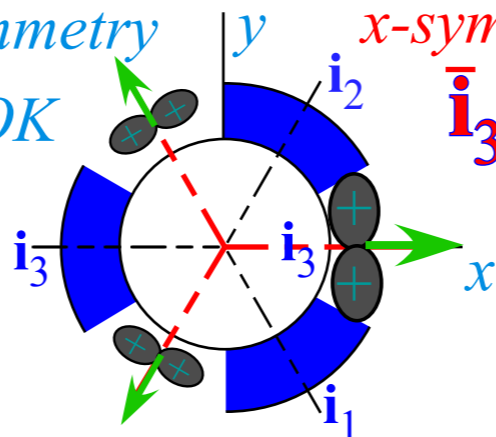
~~(broken $\bar{\mathbf{i}}_3$)~~

GLOBAL

$(i_3) = 0_2$

x-symmetry

\mathbf{i}_3 OK



LOCAL

$(i_3) = 0_2$

x-symmetry

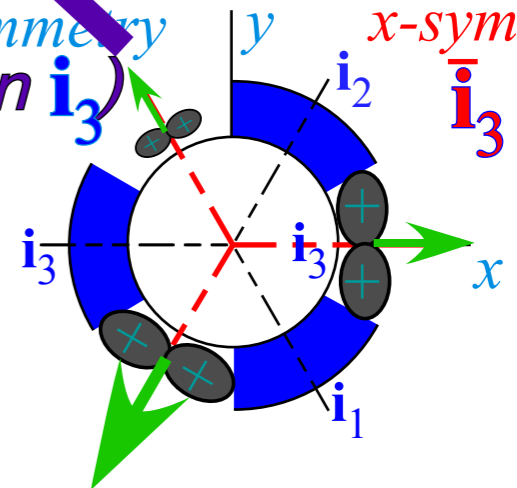
$\bar{\mathbf{i}}_3$ OK

~~GLOBAL~~

~~$(i_3) = 0_2$~~

~~x-symmetry~~

~~(broken \mathbf{i}_3)~~

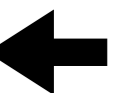


LOCAL

$(i_3) = 0_2$

x-symmetry

$\bar{\mathbf{i}}_3$ OK

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$$\mathbf{P}_{mn}^{(\mu)} = \frac{l^{(\mu)}}{G} \sum_{\mathbf{g}} D_{mn}^{(\mu)*}(\mathbf{g}) \mathbf{g}$$

Spectral Efficiency: Same $D(a)_{mn}$ projectors give a lot!

$$\begin{array}{c} \mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3 \\ \mathbf{P}_{x,x}^{A_1} = \frac{(1 \ 1 \ 1 \ 1 \ 1 \ 1)}{6} \\ \mathbf{P}_{y,y}^{A_2} = \frac{(1 \ 1 \ 1 \ -1 \ -1 \ -1)}{6} \end{array}$$

$$\begin{array}{c} \mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3 \\ \mathbf{P}_{x,x}^{E} = \frac{(2 \ -1 \ -1 \ -1 \ -1 \ +2)}{6} \\ \mathbf{P}_{y,x}^{E} = \frac{(0 \ 1 \ -1 \ -1 \ +1 \ 0)}{\sqrt{3}/2} \end{array}$$

$$\begin{array}{c} \mathbf{1} \quad \mathbf{r}^1 \quad \mathbf{r}^2 \quad \mathbf{i}_1 \quad \mathbf{i}_2 \quad \mathbf{i}_3 \\ \mathbf{P}_{x,y}^{E} = \frac{(0 \ -1 \ 1 \ -1 \ +1 \ 0)}{\sqrt{3}/2} \\ \mathbf{P}_{y,y}^{E} = \frac{(2 \ -1 \ -1 \ +1 \ +1 \ -2)}{6} \end{array}$$

- *Eigenstates (shown before)*
- *Complete Hamiltonian*

$$H^+ r_1^+ r_2^+ i_1^+ i_2^+ i_3$$

A₁-block

$$H^+ r_1^+ r_2^- i_1^- i_2^- i_3$$

A₂-block

$$\begin{array}{c} H^{-\frac{1}{2}r_1^{-\frac{1}{2}r_2^{-\frac{1}{2}i_1^{-\frac{1}{2}i_2^+ i_3}} \quad \frac{\sqrt{3}}{2}(-r_1^+ r_2^- i_1^+ i_2^-) \\ \frac{\sqrt{3}}{2}(+r_1^- r_2^- i_1^+ i_2^-) \quad H^{-\frac{1}{2}r_1^{-\frac{1}{2}r_2^+ \frac{1}{2}i_1^+ \frac{1}{2}i_2^- i_3} \end{array}$$

- *Local symmetry eigenvalue formulae* (Local Symmetry => off-diagonal=0)

$$\begin{array}{l} r_1 = r_2 = r_1^* = r, \quad i_1 = i_2 = i_1^* = i \\ \text{gives: } A_1\text{-level: } H + 2r + 2i + i_3 \\ A_2\text{-level: } H + 2r - 2i - i_3 \\ E_x\text{-level: } H - r - i + i_3 \\ E_y\text{-level: } H - r + i - i_3 \end{array}$$

Rigorous Global vs Local Calculus begins on p.90 of Lecture 17. Matrix forms on p. 125-129 and p. 130-146.

Global (LAB) symmetry

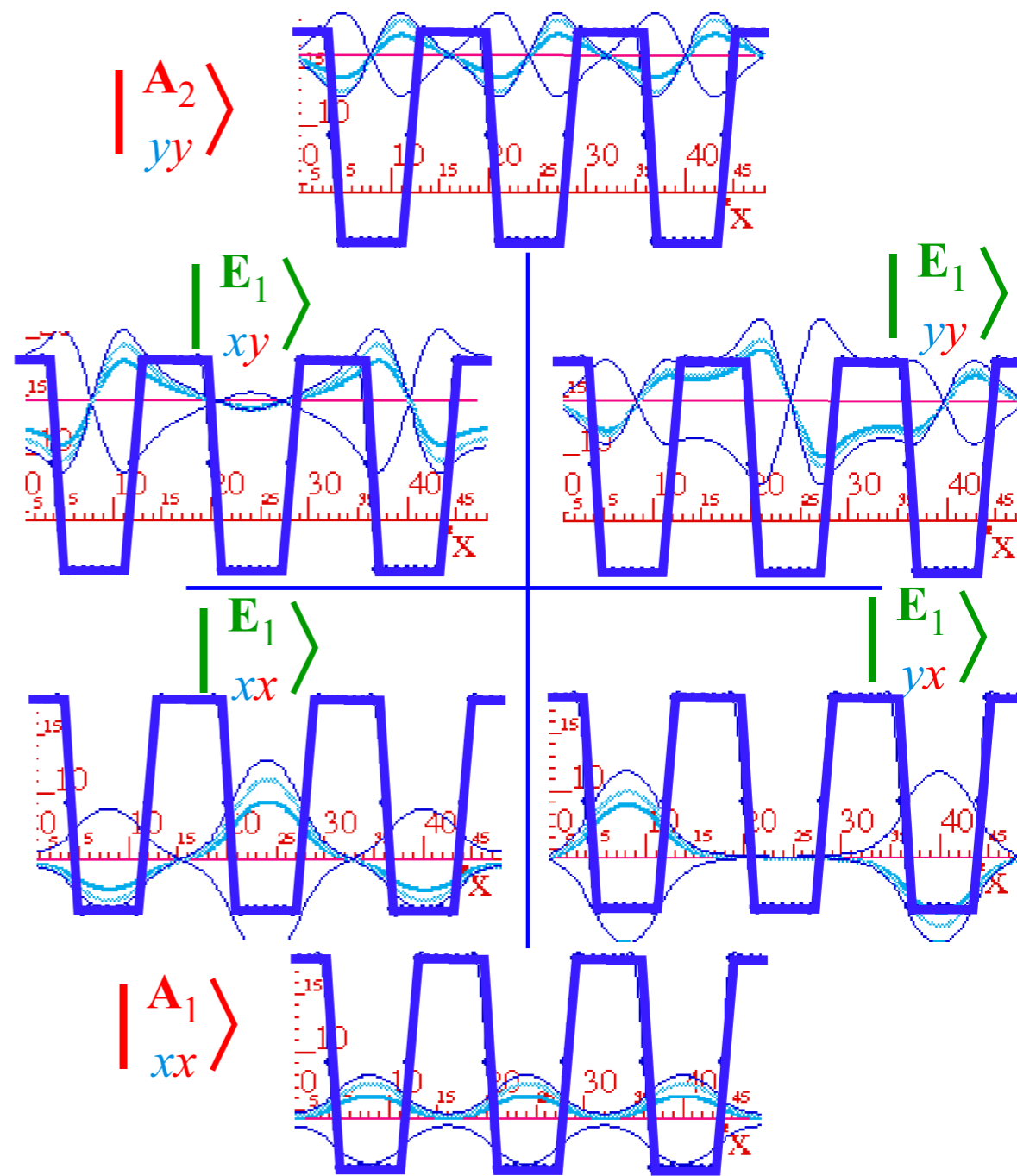
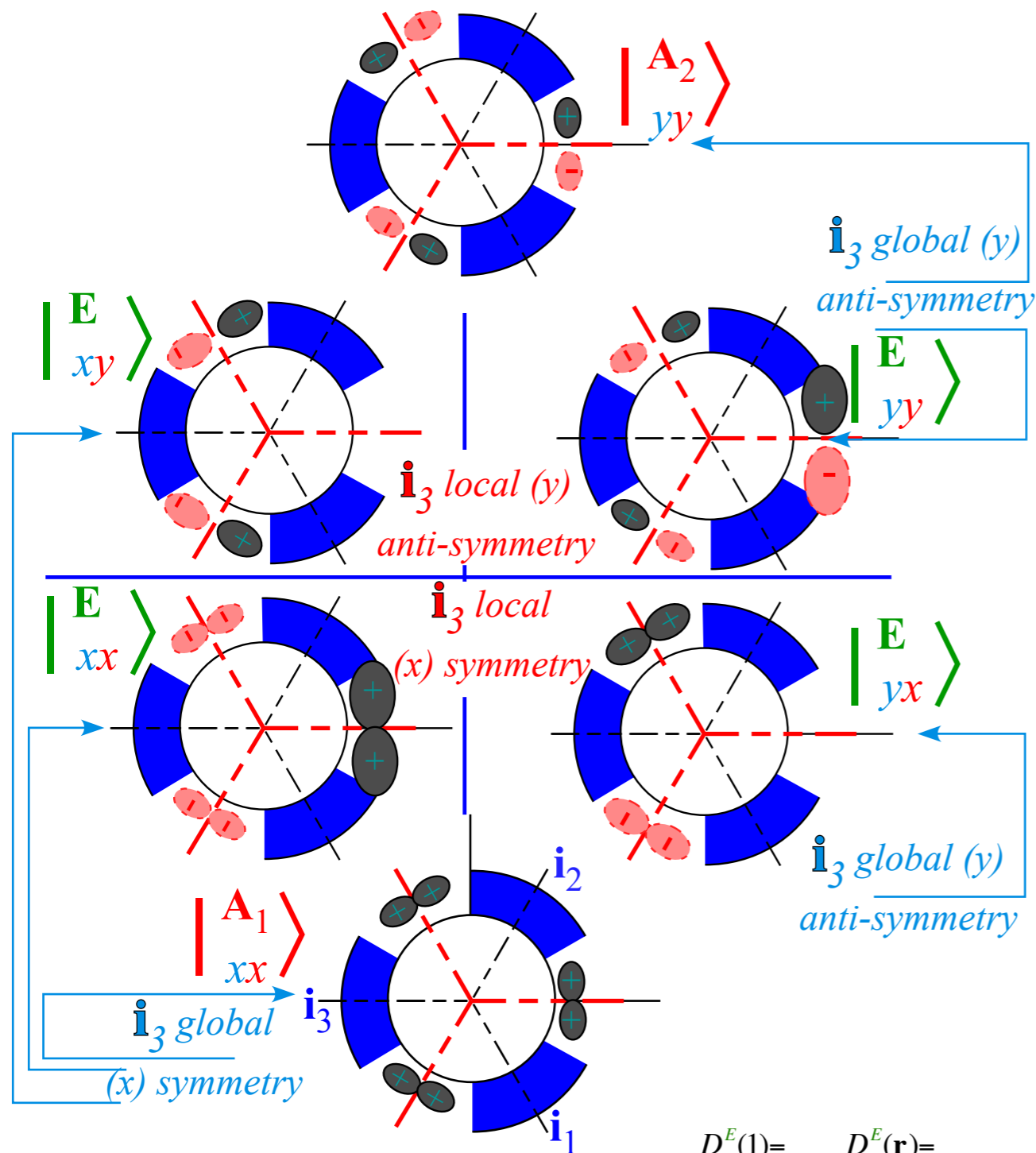
$D_3 \supset C_2$ i_3 projector states

Local (BOD) symmetry

$$\mathbf{i}_3 |_{eb}^{(m)} \rangle = \mathbf{i}_3 \mathbf{P}_{eb}^{(m)} |1\rangle = (-1)^e |^{(m)} \rangle$$

$$|_{eb}^{(m)} \rangle = \mathbf{P}_{eb}^{(m)} |1\rangle$$

$$\bar{\mathbf{i}}_3 |_{eb}^{(m)} \rangle = \bar{\mathbf{i}}_3 \mathbf{P}_{eb}^{(m)} |1\rangle = \mathbf{P}_{eb}^{(m)} \bar{\mathbf{i}}_3 |1\rangle = \mathbf{P}_{eb}^{(m)} \mathbf{i}_3^\dagger |1\rangle = (-1)^b |^{(m)} \rangle$$

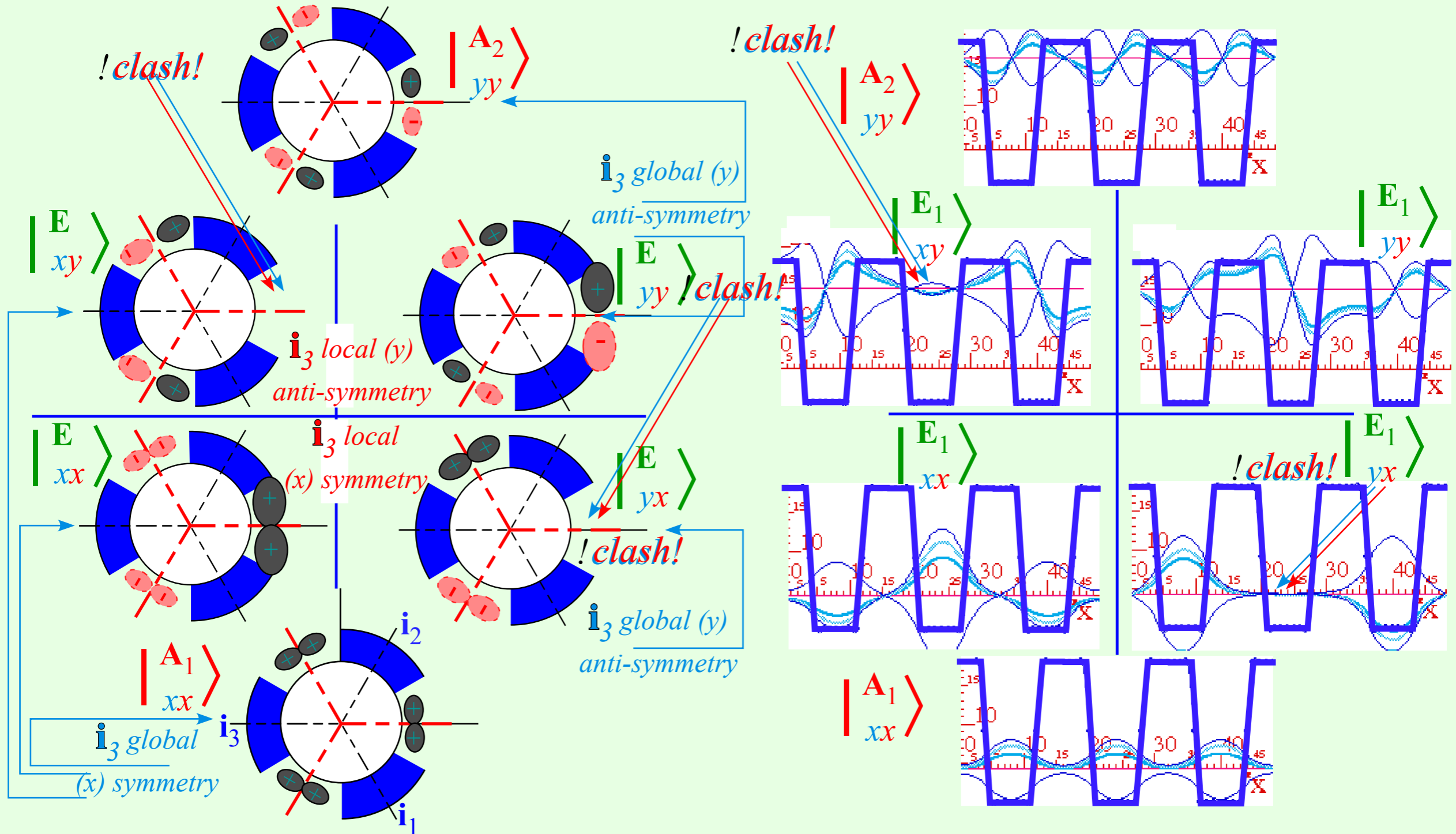


$$D^{A_1}(\mathbf{g}) = +I, D^{A_2}(\mathbf{r}^p) = +I, D^{A_2}(\mathbf{i}_q) = -I$$

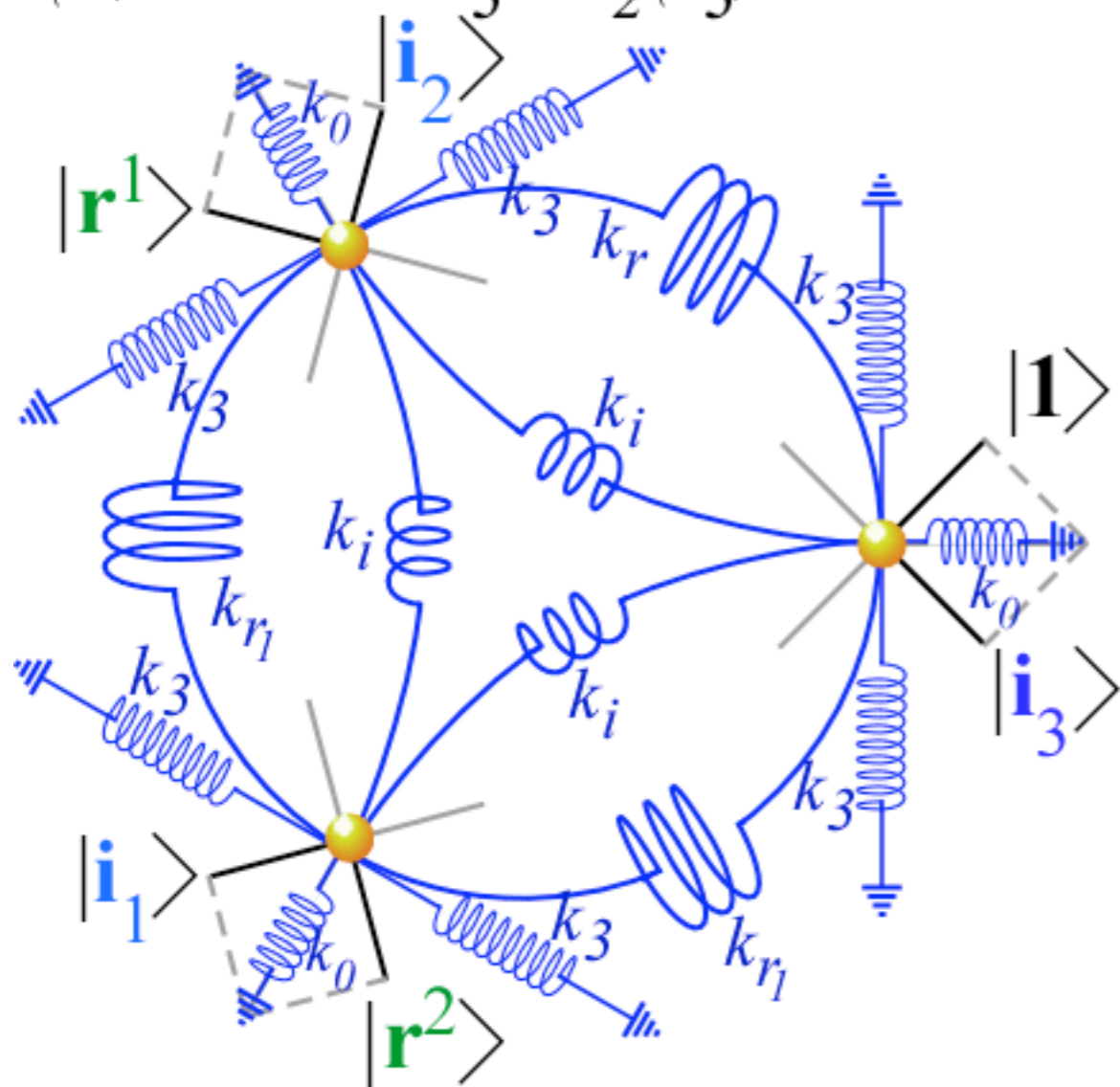
$$D^E(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, D^E(\mathbf{r}) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix}, D^E(\mathbf{r}^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_1) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{1}{2} \end{pmatrix}, D^E(\mathbf{i}_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

When there is no there, there...

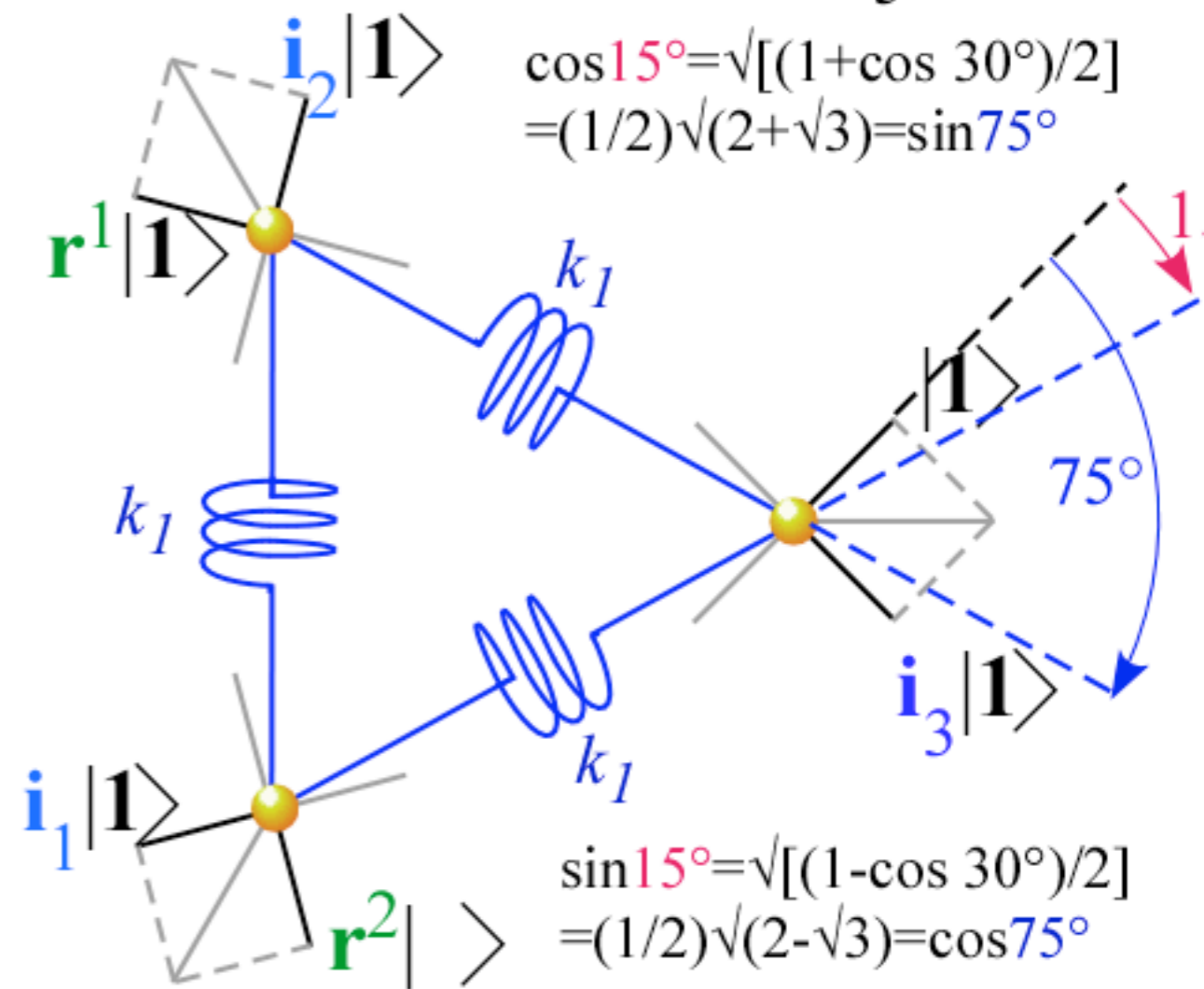
Nobody Home
where **LOCAL**
and **GLOBAL**



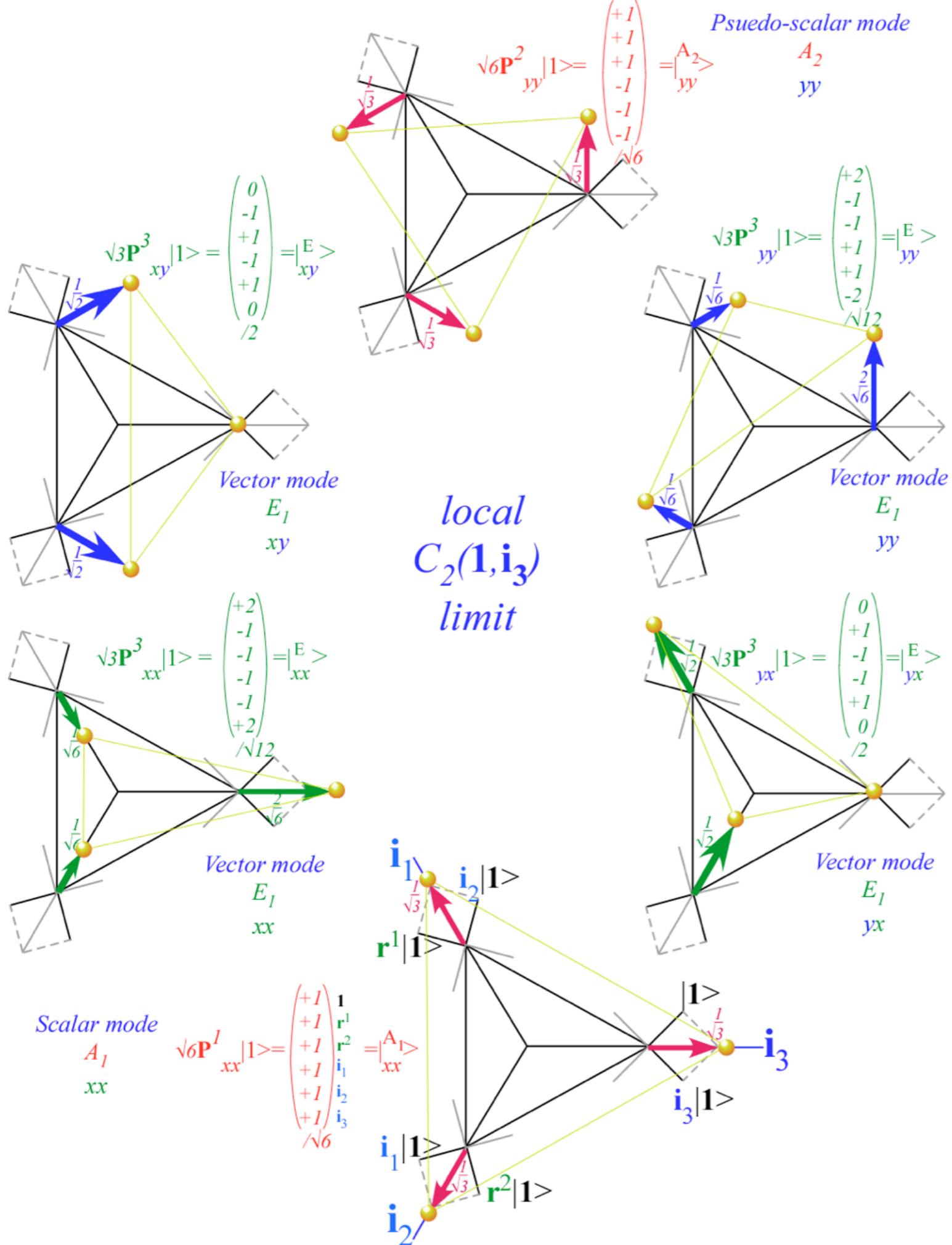
(a) Local $D_3 \supset C_2(i_3)$ model



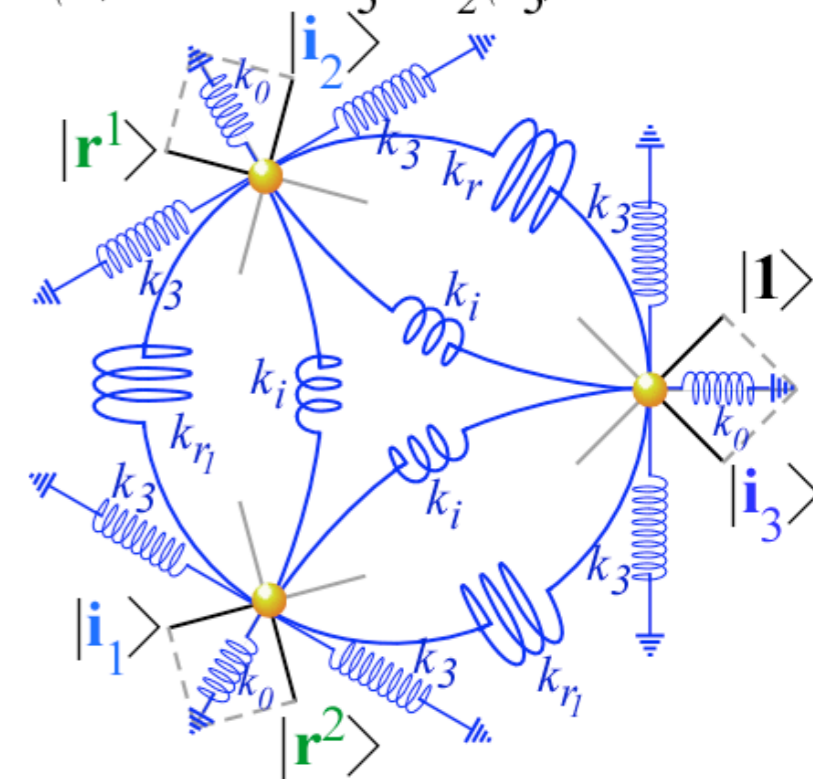
(b) Mixed local symmetry D_3 model



See p. 10-41 of
Lecture 18



(a) Local $D_3 \supset C_2(i_3)$ model



See p. 10-41 of
Lecture 18