AMOP reference links on following page

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

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General formulae for spectral decomposition (D_3 examples)

*Weyl **g**-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

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Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

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.*

AMOP reference links on page 2

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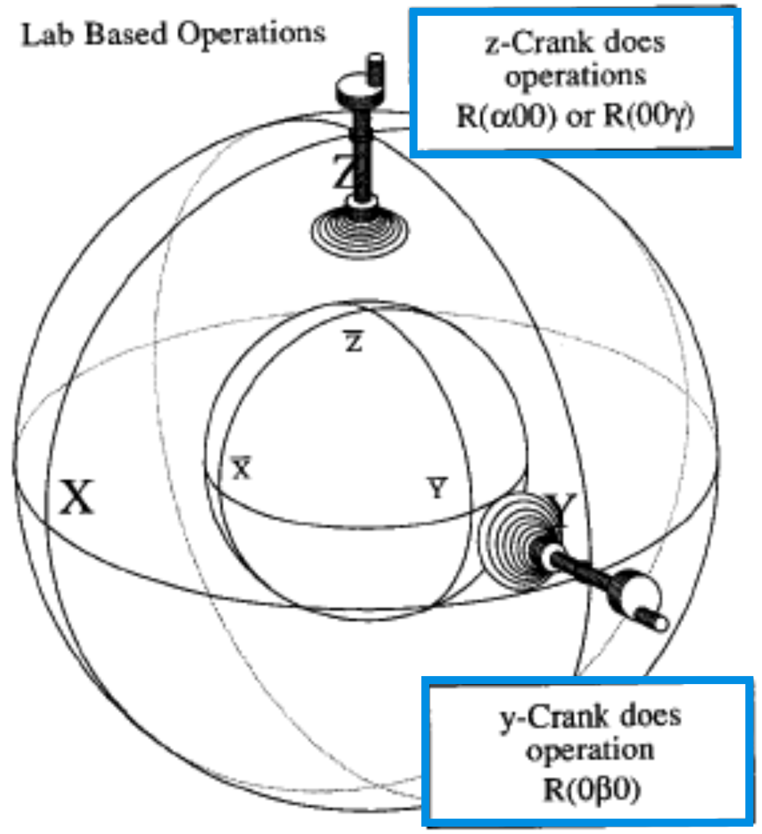
Review 1. *Global vs Local symmetry and Mock-Mach principle*

"Give me a place to stand...
and I will move the Earth"
Archimedes 287-212 B.C.E

Recall AMO12 p.41

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

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



R *commutes*

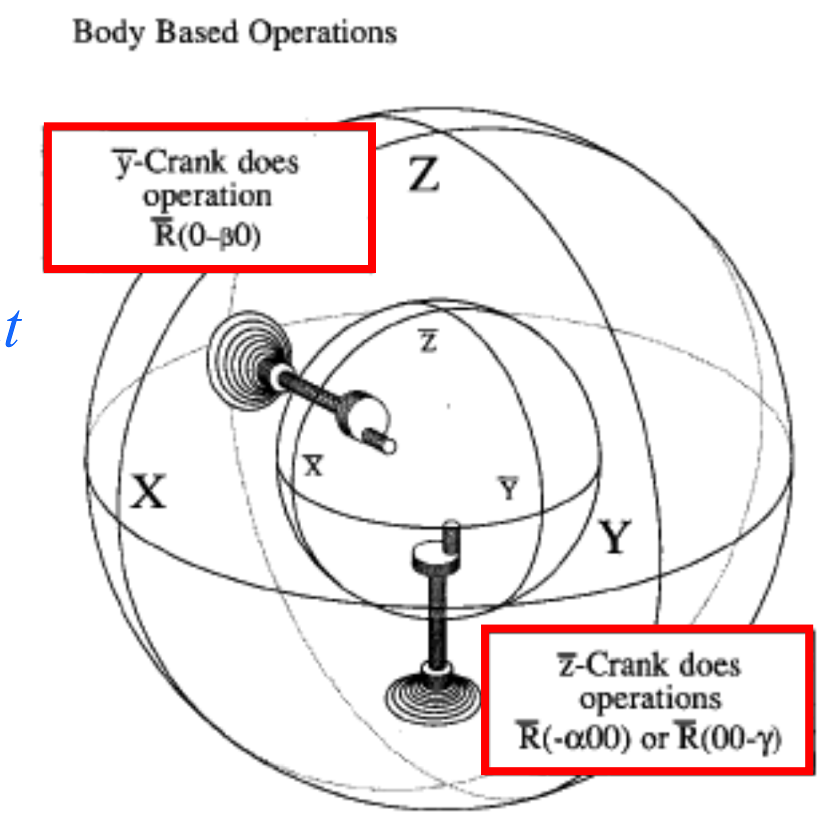
with *all* $\bar{\mathbf{R}}$

(because they're independent or "unentangled")

Mock-Mach relativity principle

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

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



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

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Review 2. *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,... }switch $g \leftrightarrows g^\dagger$ on top of group table

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

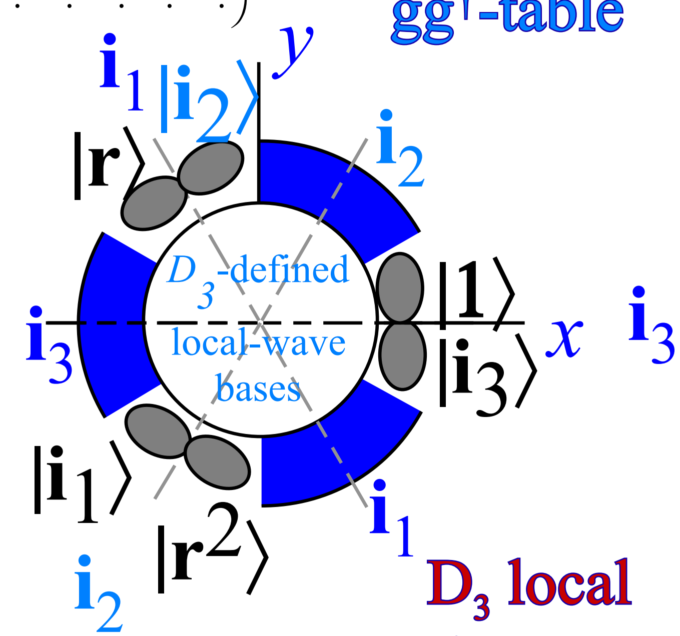
$$R^G(\mathbf{i}_1)=\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix}, R^G(\mathbf{i}_2)=\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\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

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

D_3 global $gg^\dagger$-table

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

...and **T U**=**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 $g \leftrightarrows g^\dagger$ on side of group table

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

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

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

Recall AMO12 p.50

AMOP reference links on page 2

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Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian* *Recall AMO12 p.58*

Example of RELATIVITY-DUALITY for D

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

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

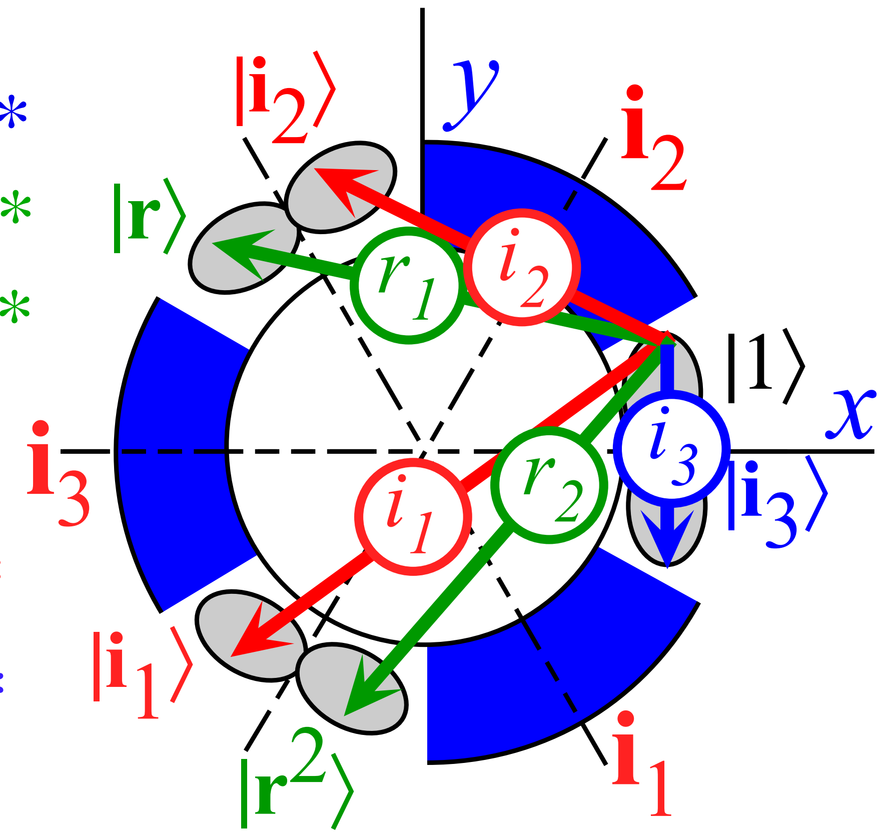
RESULT:
Any $R(\mathbf{T})$
commute (Even if **T** and **U** do not...)
with any $R(\bar{\mathbf{U}})$...

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

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

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

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



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

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

is made from ***Local*** *symmetry matrices*

This is a <u>complete</u> set of D_3 *coupling* or *"tunneling"* parameters!

local-D_3-defined Hamiltonian matrix

$\mathbb{H}=$

	$\lvert\mathbf{1})$	$\lvert\mathbf{r})$	$\lvert\mathbf{r}^2)$	$\lvert\mathbf{i}_1)$	$\lvert\mathbf{i}_2)$	$\lvert\mathbf{i}_3)$
$(\mathbf{1}\lvert$	H	r_1	r_2	i_1	i_2	i_3
$(\mathbf{r}\lvert$	r_2	H	r_1	i_2	i_3	i_1
$(\mathbf{r}^2\lvert$	r_1	r_2	H	i_3	i_1	i_2
$(\mathbf{i}_1\lvert$	i_1	i_2	i_3	H	r_1	r_2
$(\mathbf{i}_2\lvert$	i_2	i_3	i_1	r_2	H	r_1
$(\mathbf{i}_3\lvert$	i_3	i_1	i_2	r_1	r_2	H

AMOP reference links on page 2

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Review 4. *Spectral resolution of* $\mathbf{D_3}$ *Center (Class algebra)*

Recall AMO12 p.93

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

$\rightarrow$

	$\kappa_1=\mathbf{1}$	$\kappa_r=\mathbf{r}+\mathbf{r}^2$	$\kappa_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$

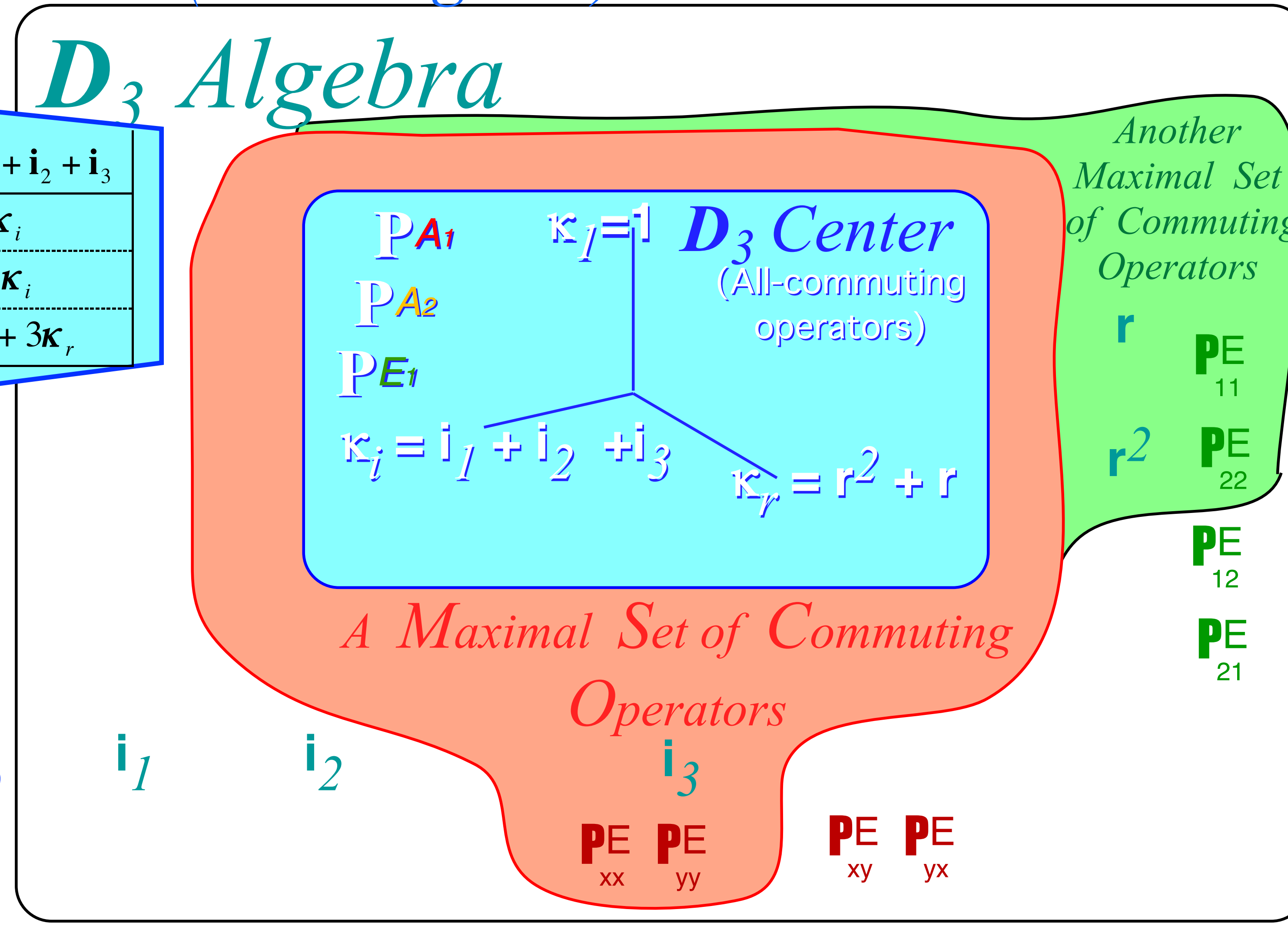
Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k=\boldsymbol{\kappa}_k\mathbf{g}_t$

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

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

$$\boldsymbol{\kappa}_1=1\cdot\mathbf{P}^{A_1}+1\cdot\mathbf{P}^{A_2}+1\cdot\mathbf{P}^{E}=\mathbf{1}\quad\textit{(Class completeness)}$$
$$\boldsymbol{\kappa}_r=2\cdot\mathbf{P}^{A_1}+2\cdot\mathbf{P}^{A_2}-1\cdot\mathbf{P}^{E}$$
$$\boldsymbol{\kappa}_i=3\cdot\mathbf{P}^{A_1}-3\cdot\mathbf{P}^{A_2}+0\cdot\mathbf{P}^{E}$$



D_3 Class projectors:

$$\mathbf{P}^{A_1}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r+\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$
$$\mathbf{P}^{A_2}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r-\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$
$$\mathbf{P}^{E}=(2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_r+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

D_3 Class characters:

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

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of* D_3 *Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g**-*expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ *and ireps* D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 *examples)*

Weyl **g**-*expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms right-and-left*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g**-*operators: Inverse of Weyl form*

D_3 *Hamiltonian and* D_3 *group matrices in global and local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis* D_3 *global-***g** *matrix structure versus* D_3 *local-*$\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 *tunneling band theory*

Ortho-complete D_3 *parameter analysis of eigensolutions*

Classical analog for bands of vibration modes

Review 5. Spectral resolution of D_3 Center (Class algebra) and its C_2 subgroup splitting

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

$\rightarrow$

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

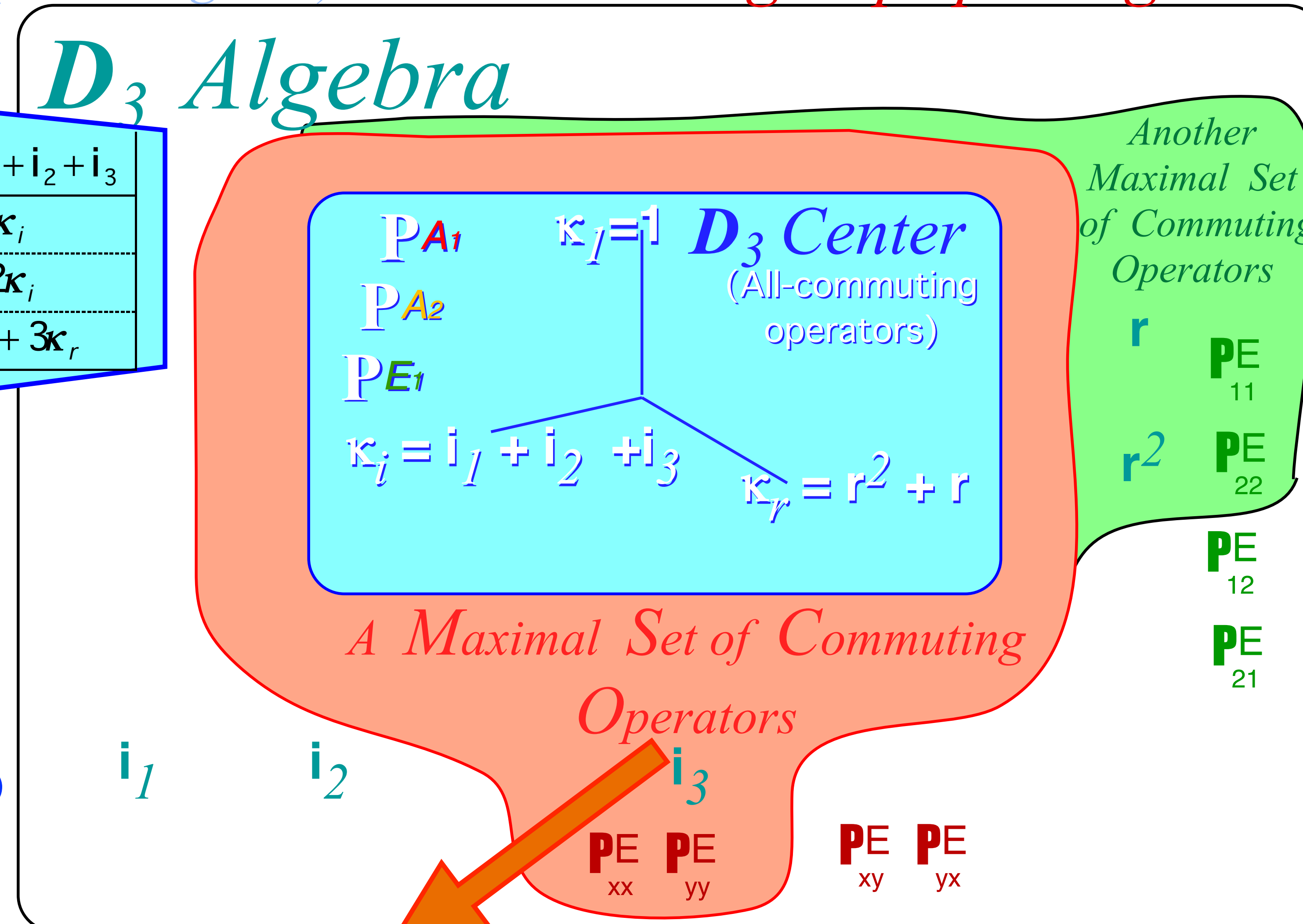
Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k=\boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3=6)$

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

$$\boldsymbol{\kappa}_1=1\cdot\mathbf{P}^{A_1}+1\cdot\mathbf{P}^{A_2}+1\cdot\mathbf{P}^{E}=\mathbf{1}\quad \textit{(Class completeness)}$$
$$\boldsymbol{\kappa}_r=2\cdot\mathbf{P}^{A_1}+2\cdot\mathbf{P}^{A_2}-1\cdot\mathbf{P}^{E}$$
$$\boldsymbol{\kappa}_i=3\cdot\mathbf{P}^{A_1}-3\cdot\mathbf{P}^{A_2}+0\cdot\mathbf{P}^{E}$$



Subgroup $C_2=\{\mathbf{1},\mathbf{i}_3\}$ relabels irreducible class projectors:

D_3 Class projectors:

$$\mathbf{P}^{A_1}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r+\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \rightarrow \mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_20_2}$$
$$\mathbf{P}^{A_2}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r-\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6 \rightarrow \mathbf{P}^{A_2}=\mathbf{P}^{A_2}_{1_21_2}$$
$$\mathbf{P}^{E}=(2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_r+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

...and splits reducible projector $\mathbf{P}^{E_1}=\mathbf{P}^{E_1}_{0_20_2}+\mathbf{P}^{E_1}_{1_21_2}$

$$\mathbf{P}^{E}_{0_20_2}=\mathbf{P}^{E}\mathbf{p}^{0_2}=\mathbf{P}^{E}\tfrac{1}{2}(\mathbf{1}+\mathbf{i}_3)=\tfrac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$$
$$+\mathbf{P}^{E}_{1_21_2}=\mathbf{P}^{E}\mathbf{p}^{1_2}=\mathbf{P}^{E}\tfrac{1}{2}(\mathbf{1}-\mathbf{i}_3)=\tfrac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$$
$$=\tfrac{1}{3}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2)$$

D_3 Class characters:

χ^α_k	χ^α_1	χ^α_r	χ^α_i
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	-1
$\alpha=E$	2	-1	0

C_2	$\mathbf{1}$	$\mathbf{i}_3$
0_2	1	1
1_2	1	-1

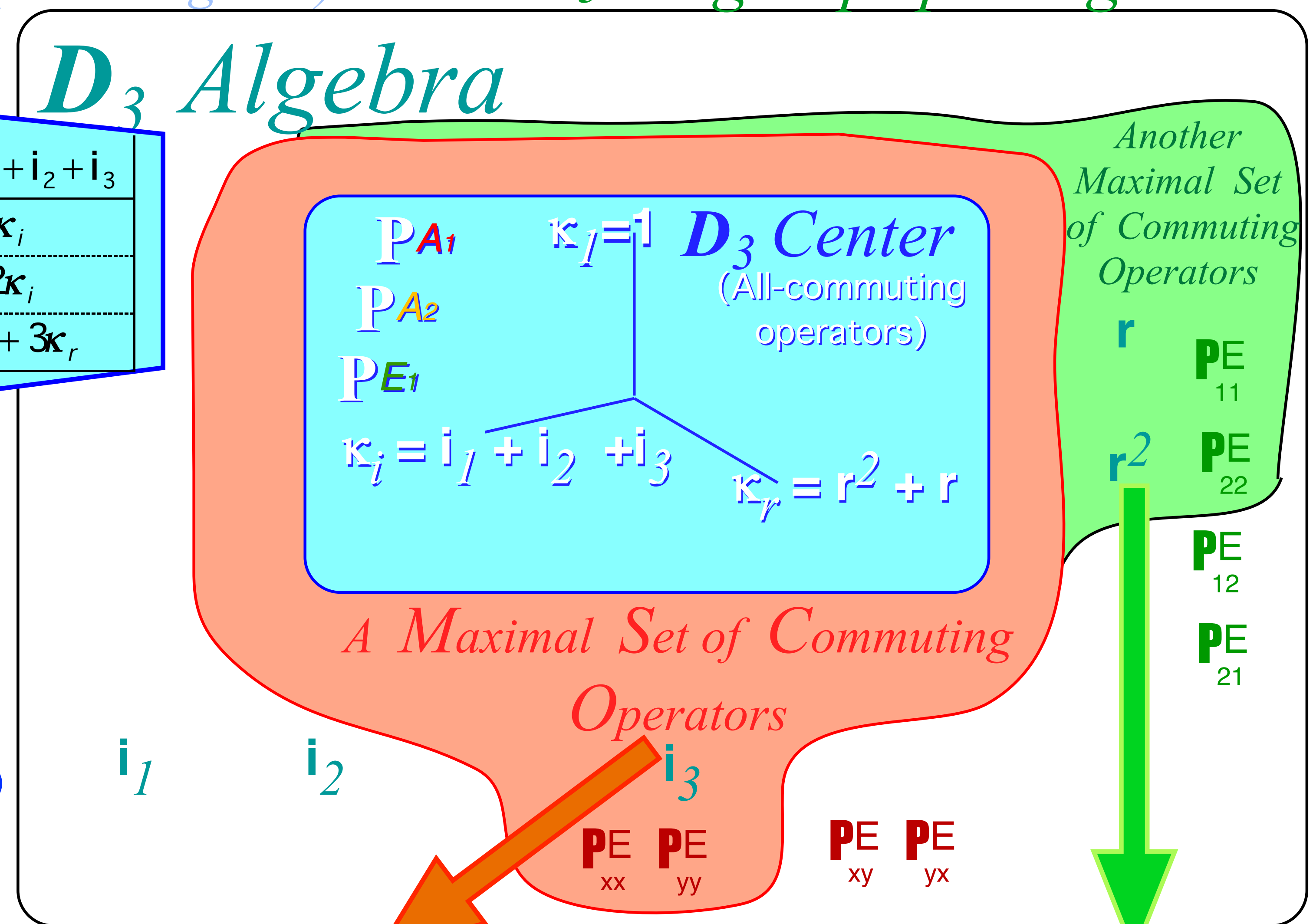
Review 5. Spectral resolution of D_3 Center (Class algebra) or its C_3 subgroup splitting

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

$\rightarrow$

	$\kappa_1=1$	$\kappa_r=r+r^2$	$\kappa_i=i_1+i_2+i_3$
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 $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$



Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

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$$\boldsymbol{\kappa}_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E} = \mathbf{1} \quad \textit{(Class completeness)}$$

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

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

Subgroup $C_2=\{\mathbf{1},\mathbf{i}_3\}$ relabels irreducible class projectors:

Subgroup $C_3=\{\mathbf{1},\mathbf{r}^1,\mathbf{r}^2\}$ does similarly:

D_3 Class projectors:

$$\mathbf{P}^{A_1} = (\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r+\boldsymbol{\kappa}_i)/6 = (\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \rightarrow \mathbf{P}^{A_1}=\mathbf{P}^{A_1}_{0_20_2}$$

$$\mathbf{P}^{A_2} = (\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r-\boldsymbol{\kappa}_i)/6 = (\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6 \rightarrow \mathbf{P}^{A_2}=\mathbf{P}^{A_2}_{1_21_2}$$

$$\mathbf{P}^{E} = (2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_r+0)/3 = (2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

C_3: $\mathbf{P}^{A_1}=\mathbf{P}^{A_1}$, $\mathbf{P}^{A_2}=\mathbf{P}^{A_2}$

...and splits reducible projector $\mathbf{P}^E=\mathbf{P}^E_{0_20_2}+\mathbf{P}^E_{1_21_2}$

$$\mathbf{P}^{E}_{0_20_2} = \mathbf{P}^E\mathbf{p}^{0_2} = \mathbf{P}^E\tfrac{1}{2}(\mathbf{1}+\mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$$

$$+\mathbf{P}^{E}_{1_21_2} = \mathbf{P}^E\mathbf{p}^{1_2} = \mathbf{P}^E\tfrac{1}{2}(\mathbf{1}+\mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$$

$$= \tfrac{1}{3}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2)$$

$$\mathbf{P}^{E}_{1_31_3} = \mathbf{P}^E\mathbf{p}^{1_3} = \mathbf{P}^E\tfrac{1}{3}(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2) = \tfrac{1}{3}(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)$$

$$+\mathbf{P}^{E}_{2_32_3} = \mathbf{P}^E\mathbf{p}^{2_3} = \mathbf{P}^E\tfrac{1}{3}(\mathbf{1}+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2) = \tfrac{1}{3}(\mathbf{1}+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)$$

$$= \tfrac{1}{3}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2)$$

...and splits differently

$\mathbf{P}^E=\mathbf{P}^{E_1}_{1_31_3}+\mathbf{P}^{E_1}_{2_32_3}$

D_3 Class characters:

χ^α_k	χ^α_1	χ^α_r	χ^α_i
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	-1
$\alpha=E$	2	-1	0

C_3	1	r^1	r^2
0_3	1	1	1
1_3	1	ε	ε^*
2_3	1	ε^*	ε

AMOP reference links on page 2

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William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

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*Weyl **g**-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms right-and-left

*$\mathbf{P}^\mu_{jk}$ -expansion in **g**-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

*$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-**g** matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Review 6.

3rd-Stage: **g**=**1**·**g**·**1** *trick gives nilpotent projectors* $\mathbf{P}^{E}_{12}=(\mathbf{P}^{E}_{21})^{\dagger}$ *and Weyl* **g**-*expansion:* $\mathbf{g}=\Sigma D^{\alpha}_{ij}(\mathbf{g})\mathbf{P}^{\alpha}_{ij}$

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

D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

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

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

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D3 :

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

$$\mathbf{g}=\Sigma_m\Sigma_e\Sigma_b D^{(m)}_{eb}(\mathbf{g})\,\mathbf{P}^{(m)}_{eb}$$

$$\mathbf{P}^{(m)}_{eb}=(norm)\Sigma_{\mathbf{g}} D^{(m)*}_{eb}(\mathbf{g})\,\mathbf{g}$$

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

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

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

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

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

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

Review 6.

3rd-Stage: $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^{E}{}_{12}=(\mathbf{P}^{E}{}_{21})^{\dagger}$ *and Weyl* $\mathbf{g}$*-expansion:* $\mathbf{g}=\Sigma D^{\alpha}{}_{ij}(\mathbf{g})\mathbf{P}^{\alpha}{}_{i}$

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

$$\mathbf{g}=\Sigma_m\Sigma_e\Sigma_b D^{(m)}_{eb}(g)\,\mathbf{P}^{(m)}_{eb}$$

$$\mathbf{P}^{(m)}_{eb}= {}_{(norm)}\Sigma_{\mathbf{g}} D^{(m)*}_{eb}(g)\,\mathbf{g}$$

The old ‘g-equals-1-times-g-times-1’ Trick

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

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

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

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

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

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

where D_3 *irreducible representations* are: $D^{A_1}(\mathbf{g})=+1$, $D^{A_2}(\mathbf{g})=\pm 1$,

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

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$\mathbf{P}^\mu{}_{jk}$ *transforms right-and-left*

$\mathbf{P}^\mu{}_{jk}$ *-expansion in* **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-* **g** *matrix structure versus D_3 local-* $\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ *and ireps* D_{ab}^{E}

$D^{E}_{0_2 0_2}(r^1)\mathbf{P}^{E}_{0_2 0_2}\mathbf{r}^1\mathbf{P}^{E}_{0_2 0_2} = \mathbf{P}^{E}_{0_2 0_2}$ with $\mathbf{P}^{E}_{0_2 0_2} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$ is represented by

Redefining 2-index $\mathbf{P}_{ab}^{E}$ *and* D_{ab}^{E}

$$\left\langle {}^{E}_{0_2 0_2} \middle| \mathbf{r}^1 \middle| {}^{E}_{0_2 0_2} \right\rangle = \tfrac{1}{\sqrt{12}} \begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix} \left(\begin{array}{ccc|ccc} & & 1 & & & \\ 1 & & & & & \\ & 1 & & & & \\ \hline & & & & 1 & \\ & & & & & 1 \\ & & & 1 & & \end{array}\right) \begin{pmatrix} 2 \\ -1 \\ -1 \\ -1 \\ -1 \\ 2 \end{pmatrix} \tfrac{1}{\sqrt{12}}$$

This gives *on*-diagonal irep component: $D^{E}_{0_2 0_2}(r^1)$

$$D^{E}_{0_2 0_2}(r^1) = \tfrac{1}{12} \begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} -1 \\ 2 \\ -1 \\ -1 \\ 2 \\ -1 \end{pmatrix} = \tfrac{1}{12}\left(-2-2+1+1-2-2\right) = \tfrac{-6}{12} = \tfrac{-1}{2}$$

2-index $\mathbf{P}_{ab}^{E}$ *projectors were split from class (all-commuting)* $\mathbf{P}^{E}$

$$\begin{array}{l} \mathbf{P}^{E}_{0_2} = \mathbf{P}^{E}\mathbf{p}^{0_2} = \mathbf{P}^{E}\,\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3) = \mathbf{P}^{E}_{0_2 0_2} \\ +\mathbf{P}^{E}_{1_2} = \mathbf{P}^{E}\mathbf{p}^{1_2} = \mathbf{P}^{E}\,\tfrac{1}{2}(\mathbf{1} + \mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3) = \mathbf{P}^{E}_{1_2 1_2} \\ \hline \qquad\qquad \mathbf{P}^{E} = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2) \end{array}$$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

$\mathbf{P}^E_{0_2 0_2}\mathbf{r}^1\mathbf{P}^E_{1_2 1_2} = D^E_{0_2 1_2}(r^1)\mathbf{P}^E_{0_2 1_2}$ with $\mathbf{P}^E_{1_2 1_2} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$ is represented by

$$\left\langle {}^{E}_{0_2 0_2} \middle| \mathbf{r}^1 \middle| {}^{E}_{1_2 1_2} \right\rangle = \tfrac{1}{\sqrt{12}}\begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix}\left(\begin{array}{ccc|ccc} & & 1 & & & \\ 1 & & & & & \\ & 1 & & & & \\ \hline & & & & 1 & \\ & & & & & 1 \\ & & & 1 & & \end{array}\right)\begin{pmatrix} 2 \\ -1 \\ -1 \\ +1 \\ +1 \\ -2 \end{pmatrix}\tfrac{1}{\sqrt{12}}$$

...but this fails to give *off*-diagonal irep $D^E_{0_2 1_2}(r^1)$

$$D^E_{0_2 1_2}(r^1) = \tfrac{1}{12}\begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix}\begin{pmatrix} -1 \\ 2 \\ -1 \\ +1 \\ -2 \\ +1 \end{pmatrix} = \tfrac{1}{12}\left(-2-2+1-1+2+2\right) = 0$$

Zero!!?
...gr-rr!

2-index $\mathbf{P}_{ab}^E$ projectors were split from class (all-commuting) $\mathbf{P}^E$

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

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

$$\mathbf{P}^E = \tfrac{1}{3}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2)$$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with:* $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ *and ireps* D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 examples)

Weyl **g***-expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms right-and-left*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-*$\mathbf{g}$ *matrix structure versus D_3 local-*$\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

Deriving $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$ given: $\mathbf{P}^E_{0_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$ and: $\mathbf{P}^E_{1_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$

so: $\mathbf{r}^1\mathbf{P}^E_{1_2}=\frac{1}{6}(2\mathbf{r}^1-\mathbf{r}^2-\mathbf{1}+\mathbf{i}_3+\mathbf{i}_1-2\mathbf{i}_2)$

D_3 $\mathbf{gg}^\dagger$ *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$=\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$

Definition of $\mathbf{P}^E_{0_2 0_2}$:

$$D^E_{0_2 0_2}(\mathbf{r}^1)\mathbf{P}^E_{0_2 0_2}=\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{0_2}$$

Definition of $\mathbf{P}^E_{0_2 1_2}$:

$$D^E_{0_2 1_2}(\mathbf{r}^1)\mathbf{P}^E_{0_2 1_2}=\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ *and ireps* D_{ab}^E

Deriving $\mathbf{P}_{0_2}^E \mathbf{r}^1 \mathbf{P}_{1_2}^E$ given: $\mathbf{P}_{0_2}^E = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$ and: $\mathbf{P}_{1_2}^E = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$

so: $\mathbf{r}^1 \mathbf{P}_{1_2}^E = \frac{1}{6}(2\mathbf{r}^1 - \mathbf{r}^2 - \mathbf{1} + \mathbf{i}_3 + \mathbf{i}_1 - 2\mathbf{i}_2)$

D_3 $\mathbf{gg}^\dagger$ *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$= \mathbf{P}_{0_2}^E \mathbf{r}^1 \mathbf{P}_{1_2}^E = \frac{1}{36}(0\mathbf{1} + 9\mathbf{r}^1 - 9\mathbf{r}^2 + 9\mathbf{i}_1 - 9\mathbf{i}_2 + 0\mathbf{i}_3)$

Definition of $\mathbf{P}_{0_2 0_2}^E$:

$D_{0_2 0_2}^E(\mathbf{r}^1)\mathbf{P}_{0_2 0_2}^E = \mathbf{P}_{0_2}^E \mathbf{r}^1 \mathbf{P}_{0_2}^E$

Definition of $\mathbf{P}_{0_2 1_2}^E$:

$D_{0_2 1_2}^E(\mathbf{r}^1)\mathbf{P}_{0_2 1_2}^E = \mathbf{P}_{0_2}^E \mathbf{r}^1 \mathbf{P}_{1_2}^E$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ *and ireps* D_{ab}^{E}

Deriving $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$ given: $\mathbf{P}^E_{0_2} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$ and: $\mathbf{P}^E_{1_2} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$

so: $\mathbf{r}^1\mathbf{P}^E_{1_2} = \frac{1}{6}(2\mathbf{r}^1 - \mathbf{r}^2 - \mathbf{1} + \mathbf{i}_3 + \mathbf{i}_1 - 2\mathbf{i}_2)$

D_3 gg† *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$= \mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2} = \frac{1}{36}(0\mathbf{1} + 9\mathbf{r}^1 - 9\mathbf{r}^2 + 9\mathbf{i}_1 - 9\mathbf{i}_2 + 0\mathbf{i}_3)$

So: $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2} = \frac{1}{4}(\mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$ has transpose: $\mathbf{P}^E_{1_2}\mathbf{r}^2\mathbf{P}^E_{0_2} = \frac{1}{4}(-\mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$

Definition of $\mathbf{P}^E_{0_2 0_2}$:

$D^E_{0_2 0_2}(\mathbf{r}^1)\mathbf{P}^E_{0_2 0_2} = \mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{0_2}$

Definition of $\mathbf{P}^E_{0_2 1_2}$:

$D^E_{0_2 1_2}(\mathbf{r}^1)\mathbf{P}^E_{0_2 1_2} = \mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

Deriving $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$ given: $\mathbf{P}^E_{0_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$ and: $\mathbf{P}^E_{1_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$

so: $\mathbf{r}^1\mathbf{P}^E_{1_2}=\frac{1}{6}(2\mathbf{r}^1-\mathbf{r}^2-\mathbf{1}+\mathbf{i}_3+\mathbf{i}_1-2\mathbf{i}_2)$

D_3 $\mathbf{gg}^\dagger$ *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$$=\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}=\frac{1}{36}(0\mathbf{1}+9\mathbf{r}^1-9\mathbf{r}^2+9\mathbf{i}_1-9\mathbf{i}_2+0\mathbf{i}_3)$$

So: $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}=\frac{1}{4}(\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1-\mathbf{i}_2)$ has transpose: $\mathbf{P}^E_{1_2}\mathbf{r}^2\mathbf{P}^E_{0_2}=\frac{1}{4}(-\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1-\mathbf{i}_2)$

Product: $\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$ $\mathbf{P}^E_{1_2}\mathbf{r}^2\mathbf{P}^E_{0_2}$

Definition of $\mathbf{P}^E_{0_21_2}$:

$$D^E_{0_21_2}(\mathbf{r}^1)\mathbf{P}^E_{0_21_2}=\mathbf{P}^E_{0_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$$

Definition of $\mathbf{P}^E_{1_20_2}$:

$$D^E_{1_20_2}(\mathbf{r}^1)\mathbf{P}^E_{1_20_2}=\mathbf{P}^E_{1_2}\mathbf{r}^1\mathbf{P}^E_{0_2}$$

Definition of $\mathbf{P}^E_{1_21_2}$:

$$D^E_{1_21_2}(\mathbf{r}^1)\mathbf{P}^E_{1_21_2}=\mathbf{P}^E_{1_2}\mathbf{r}^1\mathbf{P}^E_{1_2}$$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ *and ireps* D_{ab}^{E}

Deriving $\mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E}$ given: $\mathbf{P}_{0_2}^{E} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$ and: $\mathbf{P}_{1_2}^{E} = \frac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3)$

so: $\mathbf{r}^1\mathbf{P}_{1_2}^{E} = \frac{1}{6}(2\mathbf{r}^1 - \mathbf{r}^2 - \mathbf{1} + \mathbf{i}_3 + \mathbf{i}_1 - 2\mathbf{i}_2)$

D_3 $\mathbf{gg}^\dagger$ *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$= \mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E} = \frac{1}{36}(0\mathbf{1} + 9\mathbf{r}^1 - 9\mathbf{r}^2 + 9\mathbf{i}_1 - 9\mathbf{i}_2 + 0\mathbf{i}_3)$

So: $\mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E} = \frac{1}{4}(\mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$ has transpose: $\mathbf{P}_{1_2}^{E}\mathbf{r}^2\mathbf{P}_{0_2}^{E} = \frac{1}{4}(-\mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$

Product: $\mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E}\,\mathbf{P}_{1_2}^{E}\mathbf{r}^2\mathbf{P}_{0_2}^{E} = \mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{r}^2\mathbf{P}_{0_2}^{E} = \mathbf{P}_{0_2}^{E}\mathbf{1}\mathbf{P}_{0_2}^{E} = \mathbf{P}_{0_2}^{E}$

Definition of $\mathbf{P}_{0_2 1_2}^{E}$:

$D_{0_2 1_2}^{E}(\mathbf{r}^1)\mathbf{P}_{0_2 1_2}^{E} = \mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E}$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ and ireps D_{ab}^{E}

Deriving $\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}$ given: $\mathbf{P}^{E}_{0_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)$ and: $\mathbf{P}^{E}_{1_2}=\frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)$

so: $\mathbf{r}^1\mathbf{P}^{E}_{1_2}=\frac{1}{6}(2\mathbf{r}^1-\mathbf{r}^2-\mathbf{1}+\mathbf{i}_3+\mathbf{i}_1-2\mathbf{i}_2)$

D_3 $\mathbf{gg}^\dagger$ *form*	$-\mathbf{1}$	$-\mathbf{r}^2$	$2\mathbf{r}^1$	$+\mathbf{i}_1$	$-2\mathbf{i}_2$	$+\mathbf{i}_3$
$2\mathbf{1}$	$-2\mathbf{1}$	$-2\mathbf{r}^2$	$4\mathbf{r}^1$	$2\mathbf{i}_1$	$-4\mathbf{i}_2$	$2\mathbf{i}_3$
$-\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$-2\mathbf{r}^2$	$-\mathbf{i}_3$	$2\mathbf{i}_1$	$-\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$-2\mathbf{1}$	$-\mathbf{i}_2$	$2\mathbf{i}_3$	$-\mathbf{i}_1$
$-\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$-2\mathbf{i}_2$	$-\mathbf{1}$	$2\mathbf{r}^1$	$-\mathbf{r}^2$
$-\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$-2\mathbf{i}_3$	$-\mathbf{r}^2$	$2\mathbf{1}$	$-\mathbf{r}^1$
$2\mathbf{i}_3$	$-2\mathbf{i}_3$	$-2\mathbf{i}_2$	$4\mathbf{i}_1$	$2\mathbf{r}^1$	$-4\mathbf{r}^2$	$2\mathbf{1}$

$$=\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}=\frac{1}{36}(0\mathbf{1}+9\mathbf{r}^1-9\mathbf{r}^2+9\mathbf{i}_1-9\mathbf{i}_2+0\mathbf{i}_3)$$

So: $\boxed{\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}=\frac{1}{4}(\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1-\mathbf{i}_2)}$ has transpose: $\boxed{\mathbf{P}^{E}_{1_2}\mathbf{r}^2\mathbf{P}^{E}_{0_2}=\frac{1}{4}(-\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1-\mathbf{i}_2)}$

Product: $\boxed{\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}}\boxed{\mathbf{P}^{E}_{1_2}\mathbf{r}^2\mathbf{P}^{E}_{0_2}}=\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{r}^2\mathbf{P}^{E}_{0_2}=\mathbf{P}^{E}_{0_2}\mathbf{1}\mathbf{P}^{E}_{0_2}=\mathbf{P}^{E}_{0_2}$

Definition of $\mathbf{P}^{E}_{0_2 1_2}$:

$$D^{E}_{0_2 1_2}(\mathbf{r}^1)\mathbf{P}^{E}_{0_2 1_2}=\mathbf{P}^{E}_{0_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}$$

Definition of $\mathbf{P}^{E}_{1_2 0_2}$:

$$D^{E}_{1_2 0_2}(\mathbf{r}^1)\mathbf{P}^{E}_{1_2 0_2}=\mathbf{P}^{E}_{1_2}\mathbf{r}^1\mathbf{P}^{E}_{0_2}$$

Definition of $\mathbf{P}^{E}_{1_2 1_2}$:

$$D^{E}_{1_2 1_2}(\mathbf{r}^1)\mathbf{P}^{E}_{1_2 1_2}=\mathbf{P}^{E}_{1_2}\mathbf{r}^1\mathbf{P}^{E}_{1_2}$$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ and ireps D_{ab}^{E}

D_3 $\mathbf{gg}^\dagger$ *form*	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}^1$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}^1$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}^1$	$\mathbf{r}^1$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}^1$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}^1$
$\mathbf{i}_3$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{1}$

Find product of : $\mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E} = \frac{1}{4}(\mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$

and transpose: $\mathbf{P}_{1_2}^{E}\mathbf{r}^2\mathbf{P}_{0_2}^{E} = \frac{1}{4}(-\mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)$

$$\frac{1}{16}\begin{array}{c|cccc}
 & \mathbf{r}^2 & -\mathbf{r}^1 & \mathbf{i}_1 & -\mathbf{i}_2 \\ \hline
\mathbf{r}^1 & \mathbf{1} & -\mathbf{r}^2 & \mathbf{i}_3 & -\mathbf{i}_1 \\
-\mathbf{r}^2 & -\mathbf{r}^1 & \mathbf{1} & -\mathbf{i}_2 & \mathbf{i}_3 \\
\mathbf{i}_1 & \mathbf{i}_3 & -\mathbf{i}_2 & \mathbf{1} & -\mathbf{r}^1 \\
-\mathbf{i}_2 & -\mathbf{i}_1 & \mathbf{i}_3 & -\mathbf{r}^2 & \mathbf{1}
\end{array}$$

$$\mathbf{P}_{0_2}^{E}\mathbf{r}^1\mathbf{P}_{1_2}^{E}\mathbf{P}_{1_2}^{E}\mathbf{r}^2\mathbf{P}_{0_2}^{E} = \frac{1}{8}\left(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3\right) \qquad = \frac{1}{16}\left(4\mathbf{1} - 2\mathbf{r}^1 - 2\mathbf{r}^2 - 2\mathbf{i}_1 - 2\mathbf{i}_1 + 4\mathbf{i}_3\right)$$

$$= D_{0_2 1_2}^{E}(\mathbf{r}^1)\mathbf{P}_{0_2 1_2}^{E} D_{1_2 0_2}^{E}(\mathbf{r}^2)\mathbf{P}_{1_2 0_2}^{E} = \left|D_{0_2 1_2}^{E}(\mathbf{r}^1)\right|^2 \mathbf{P}_{0_2 0_2}^{E}$$

Compare to original projector: $\mathbf{P}_{0_2}^{E} = \frac{1}{6}(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3) = \mathbf{P}_{0_2 0_2}^{E}$ Solve for: $\left|D_{0_2 1_2}^{E}(\mathbf{r}^1)\right|^2 = \frac{\frac{1}{8}}{\frac{1}{6}} = \frac{3}{4}$

$$D_{0_2 1_2}^{E}(\mathbf{r}^1) = \pm\frac{\sqrt{3}}{2}$$

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^{E}$ and ireps D_{ab}^{E}

Defining $D^{E}_{1_2 0_2}(r^1)\mathbf{P}^{E}_{1_2}\mathbf{r}^1\mathbf{P}^{E}_{0_2} = \mathbf{P}^{E}_{1_2 0_2}$ for off-diagonal $D^{E}_{1_2 0_2}(r^1)$ projector $\mathbf{P}^{E}_{1_2 0_2}$ is represented by

$$\left\langle {}^{E}_{0_2 0_2} \middle| \mathbf{r}^1 \middle| {}^{E}_{1_2 0_2} \right\rangle = \tfrac{1}{\sqrt{12}}\begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix} \left(\begin{array}{ccc|ccc} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{array}\right) \begin{pmatrix} 0 \\ -1 \\ +1 \\ +1 \\ -1 \\ 0 \end{pmatrix} \tfrac{1}{2}$$

$$D^{E}_{0_2 0_2}(r^1) = \tfrac{1}{\sqrt{12}}\begin{pmatrix} 2 & -1 & -1 & -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ -1 \\ -1 \\ 0 \\ 1 \end{pmatrix} \tfrac{1}{2} = \tfrac{1}{4\sqrt{3}}\left(2-0+1+1-0+2\right) = \tfrac{6}{4\sqrt{3}} = \tfrac{\sqrt{3}}{2}$$

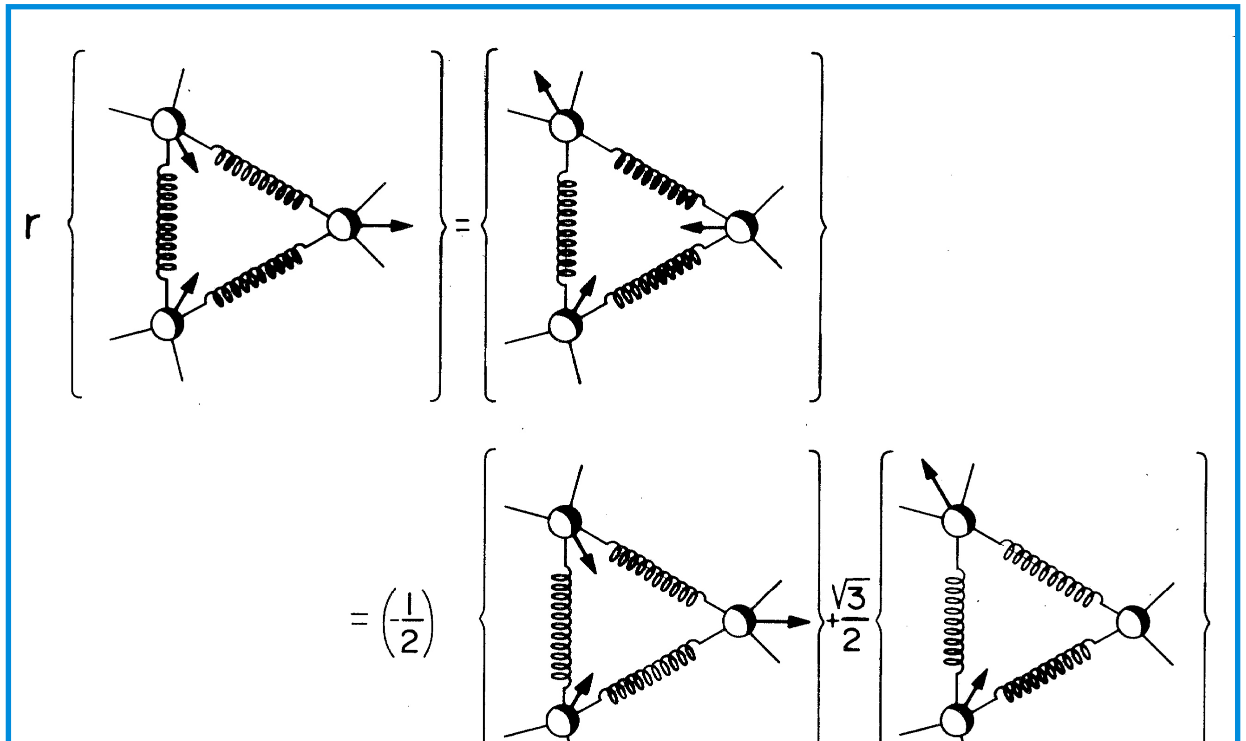
Using normalized: $\left|\mathbf{P}^{E}_{0_2 1_2}\right\rangle = \tfrac{1}{2}(\mathbf{r}^1 - \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)\left|\mathbf{1}\right\rangle$

or transpose: $\left\langle \mathbf{P}^{E}_{1_2 0_2}\right| = \left\langle \mathbf{1}\right|(-\mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 - \mathbf{i}_2)\tfrac{1}{2}$

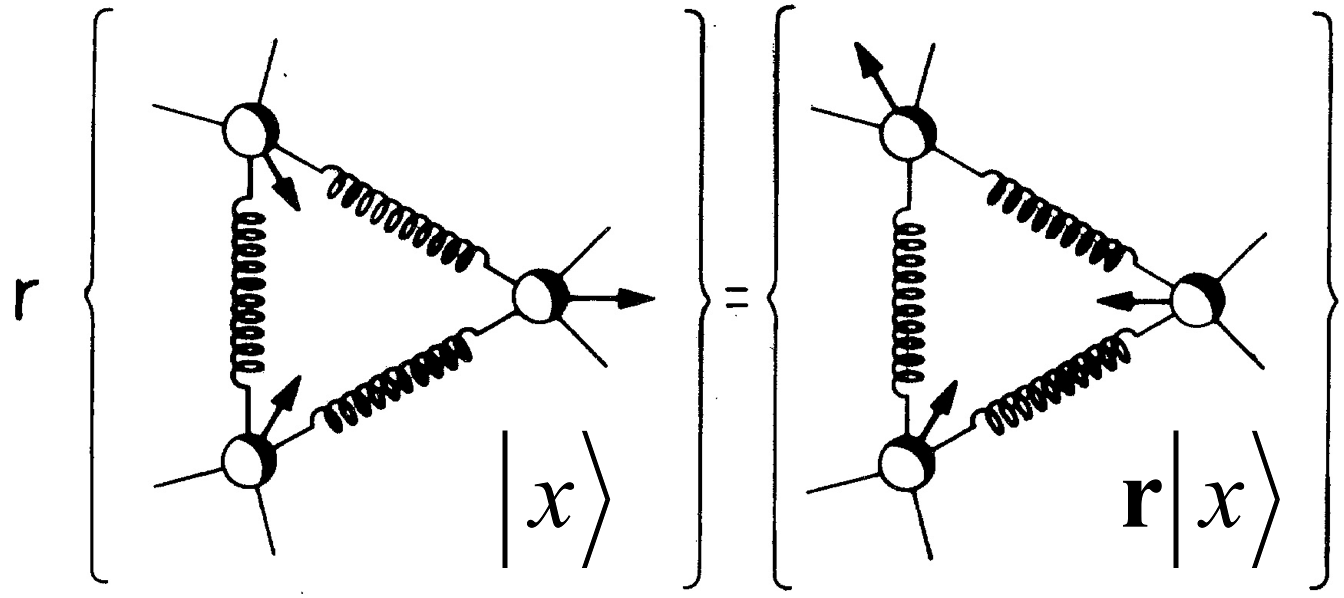
$$\mathbf{P}^{E}_{0_2} = \mathbf{P}^{E}\mathbf{p}^{0_2} = \mathbf{P}^{E}\tfrac{1}{2}(\mathbf{1}+\mathbf{i}_3) = \tfrac{1}{6}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3)$$

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

$$= \tfrac{1}{3}(2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2)$$

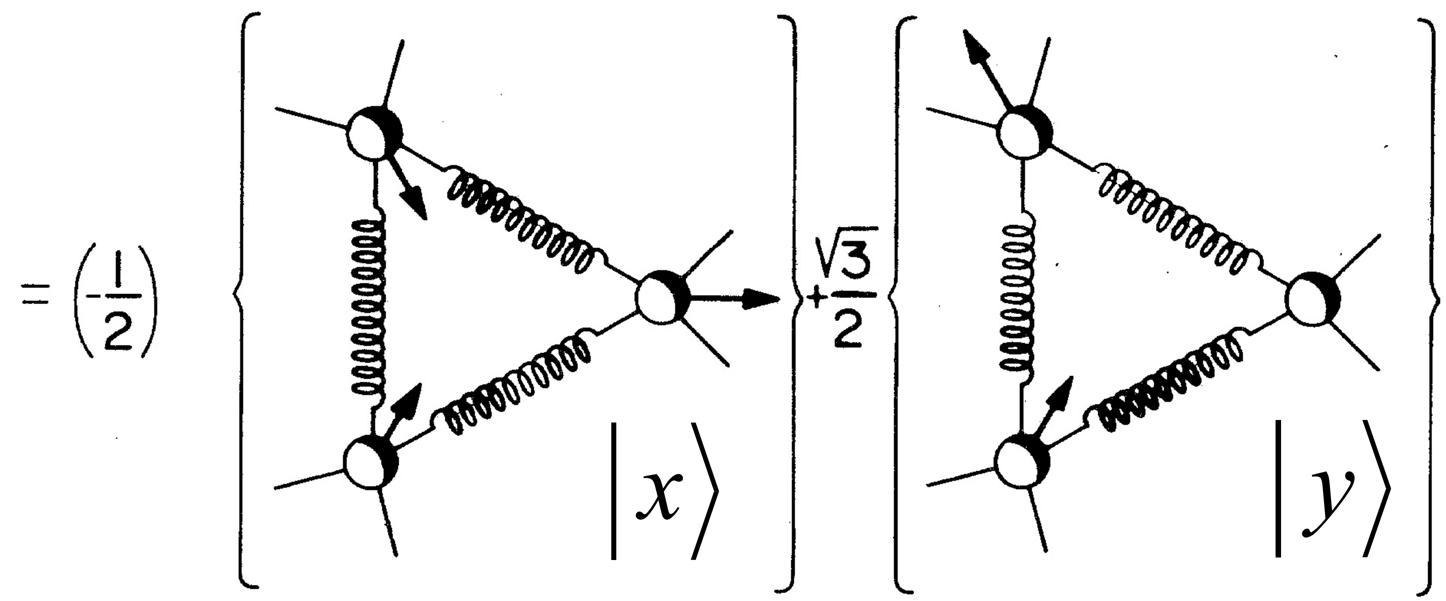


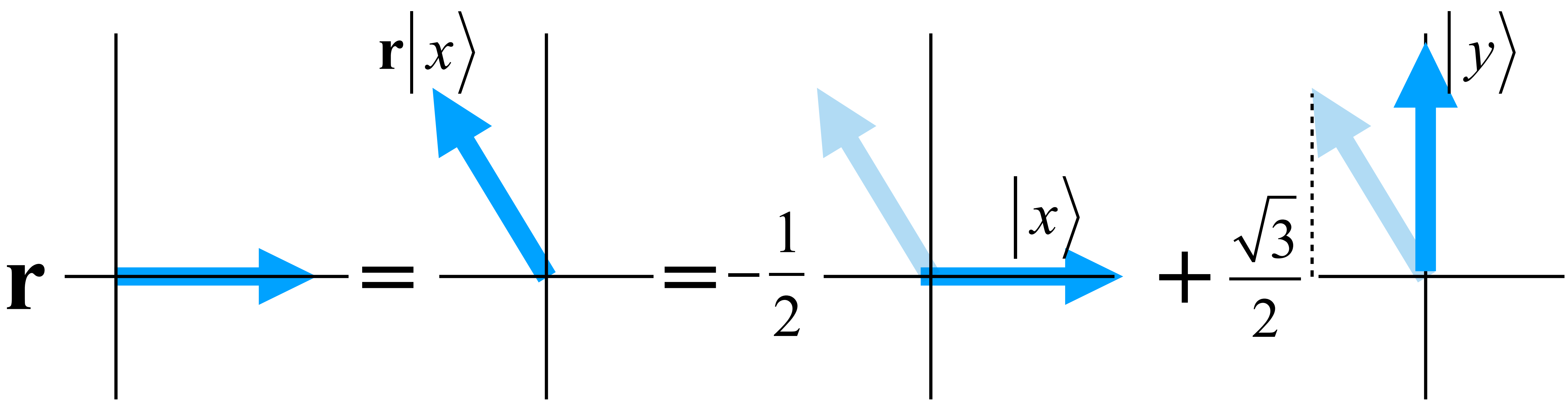
PSDS*Fig.3.4.3*



PSDS*Fig.3.4.3*

The simplest way to compute (and visualize) D_3 irep $D^E(\mathbf{r})$





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2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

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Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ *and ireps* D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 examples)

Weyl **g***-expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms right-and-left*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-***g** *matrix structure versus D_3 local-*$\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Compare Global vs Local $|\mathbf{g}\rangle$-basis vs. Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

D_3 global group product table

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

Change Global to Local by switching

...column-g with column-$g^\dagger$

....and row-g with row-$g^\dagger$

Just switch r with $r^\dagger = r^2$.

(all others are self-conjugate)

D_3 local group table

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

Compare Global vs Local $|\mathbf{g}\rangle$*-basis*

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

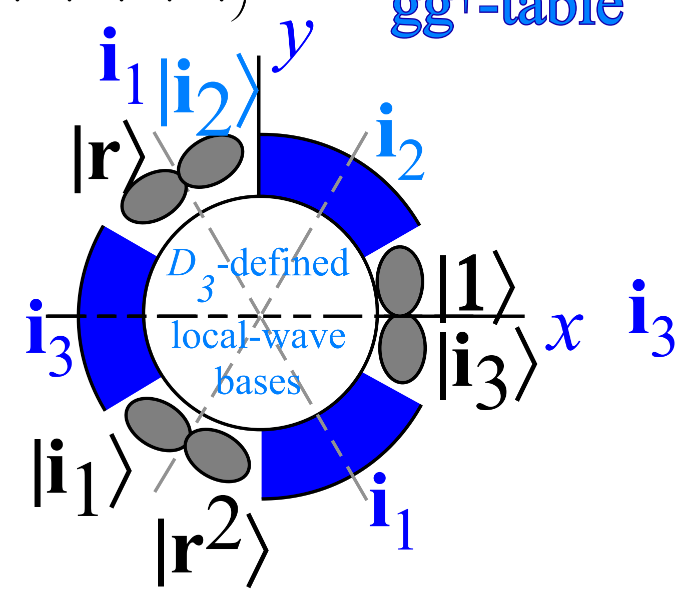
To represent *external* $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

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

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

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

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



Compare Global vs Local $|\mathbf{g}\rangle$-basis

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

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

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

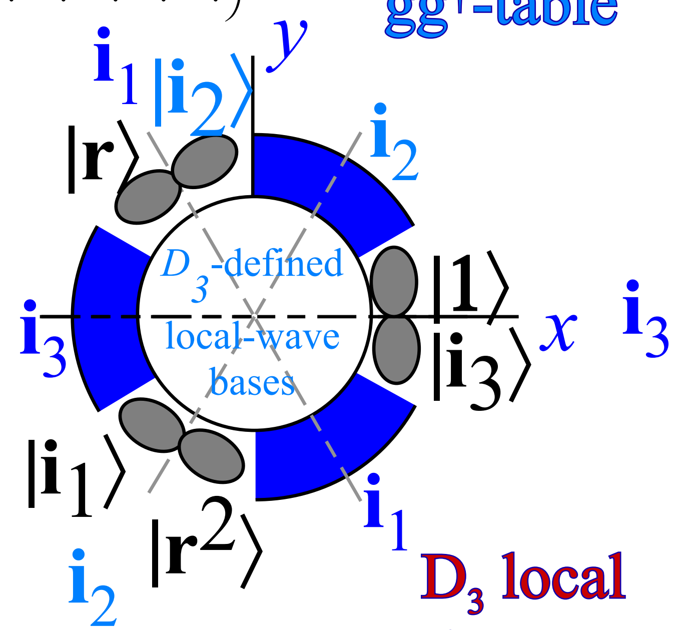
$$R^G(\mathbf{i}_1)=\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix},\quad R^G(\mathbf{i}_2)=\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\c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

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**

D_3 global $gg^\dagger$-table

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

...and **T U**=**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 $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on side of group table

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

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

1	**r**	**r**^{2}	**i**$_1$	**i**$_2$	**i**$_3$
r^2	**1**	**r**	**i**$_2$	**i**$_3$	**i**$_1$
r	**r**^{2}	**1**	**i**$_3$	**i**$_1$	**i**$_2$
i$_1$	**i**$_2$	**i**$_3$	**1**	**r**	**r**^{2}
i$_2$	**i**$_3$	**i**$_1$	**r**^{2}	**1**	**r**
i$_3$	**i**$_1$	**i**$_2$	**r**	**r**^{2}	**1**

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$|\mathbf{P}^{(\mu)}\rangle$*-basis* D_3 *global-*$\mathbf{g}$ *matrix structure versus* D_3 *local-*$\bar{\mathbf{g}}$ *matrix structure*

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D_3 global group product table

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

D_3 global projector product table

D_3	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E}_{xx}$	·	·	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	·	·
$\mathbf{P}^{E}_{yx}$	·	·	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$	·	·
$\mathbf{P}^{E}_{xy}$	·	·	·	·	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{y}$	·	·	·	·	$\mathbf{P}^{E}_{y}$	$\mathbf{P}^{E}_{y}$

$$\mathbf{P}^{(m)}_{ab}\mathbf{P}^{(n)}_{cd} = \delta^{mn}\delta_{bc}\,\mathbf{P}^{(m)}_{ad}$$

Change Global to Local by switching

...column-P with column-P†

....and row-P with row-P†

Just switch r with $r^\dagger = r^2$.

(all others are self-conjugate)

D_3 local group table

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

(Just switch $\mathbf{P}^{E}_{yx}$ with $\mathbf{P}^{E\dagger}_{yx} = \mathbf{P}^{E}_{xy}$.)

D_3 local projector product table

	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E}_{xx}$	·	·	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$	0
$\mathbf{P}^{E}_{xy}$	·	·	0	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{yx}$	·	·	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$	0
$\mathbf{P}^{E}_{yy}$	·	·	0	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$

$$\overline{\mathbf{P}}^{(m)}_{ab}\overline{\mathbf{P}}^{(n)}_{cd} = \delta^{mn}\delta_{bc}\,\overline{\mathbf{P}}^{(m)}_{ad}$$

Compare Global $|\mathbf{P}^{(\mu)}\rangle$-basis vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

Matrix "Placeholders" $\mathbf{P}^{(m)}_{ab}$ for GLOBAL $\mathbf{g}$ operators in D_3

$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & D_{xy} & \cdot & \cdot \\ \cdot & \cdot & D_{yx} & D_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D^{E}_{xx} & D_{xy} \\ \cdot & \cdot & \cdot & \cdot & D_{yx} & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} \boxed{1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \boxed{1} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + D^{E}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

D_3	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\mathbf{P}^{A_2}_{yy}$	$\cdot$	$\mathbf{P}^{A_2}_{yy}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\mathbf{P}^{E}_{xx}$	$\cdot$	$\cdot$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	$\cdot$	$\cdot$
$\mathbf{P}^{E}_{yx}$	$\cdot$	$\cdot$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$	$\cdot$	$\cdot$
$\mathbf{P}^{E}_{xy}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{y}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\mathbf{P}^{E}_{y}$	$\mathbf{P}^{E}_{y}$

Compare Global $|\mathbf{P}^{(\mu)}\rangle$-basis vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

Matrix "Placeholders" $\mathbf{P}^{(m)}_{ab}$ *for GLOBAL* $\mathbf{g}$ *operators in D_3*

$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & D_{xy} & \cdot & \cdot \\ \cdot & \cdot & D_{yx} & D_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D^{E}_{xx} & D_{xy} \\ \cdot & \cdot & \cdot & \cdot & D_{yx} & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + D^{E}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

$\overline{\mathbf{P}}^{(m)}_{ab}$ *...for LOCAL* $\overline{\mathbf{g}}$ *operators in $\overline{D}_3$*

$$\overline{\mathbf{g}} = D^{A_1}_{xx}(g)\overline{\mathbf{P}}^{A_1} + D^{A_2}_{yy}(g)\overline{\mathbf{P}}^{A_2} + D^{E}_{xx}(g)\overline{\mathbf{P}}^{E}_{xx} + D^{E}_{xy}(g)\overline{\mathbf{P}}^{E}_{xy} + D^{E}_{yx}(g)\overline{\mathbf{P}}^{E}_{yx} + D^{E}_{yy}(g)\overline{\mathbf{P}}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & \cdot & D^{E}_{xy} & \cdot \\ \cdot & \cdot & \cdot & D_{xx} & \cdot & D_{xy} \\ \cdot & \cdot & D^{E}_{yx} & \cdot & D^{E}_{yy} & \cdot \\ \cdot & \cdot & \cdot & D_{yx} & \cdot & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\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 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + D^{E}_{yy}\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 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E}_{xx}$	·	·	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$	0
$\mathbf{P}^{E}_{xy}$	·	·	0	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{yx}$	·	·	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$	0
$\mathbf{P}^{E}_{yy}$	·	·	0	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$

Compare Global $|\mathbf{P}^{(\mu)}\rangle$*-basis vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

Matrix "Placeholders" $\mathbf{P}_{ab}^{(m)}$ *for GLOBAL* $\mathbf{g}$ *operators in* D_3

$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & D_{xy} & \cdot & \cdot \\ \cdot & \cdot & D_{yx} & D_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D^{E}_{xx} & D_{xy} \\ \cdot & \cdot & \cdot & \cdot & D_{yx} & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + D^{E}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

$\bar{\mathbf{P}}_{ab}^{(m)}$ *...for LOCAL* $\bar{\mathbf{g}}$ *operators in* $\bar{D}_3$

$$\bar{\mathbf{g}} = D^{A_1}_{xx}(g)\bar{\mathbf{P}}^{A_1} + D^{A_2}_{yy}(g)\bar{\mathbf{P}}^{A_2} + D^{E}_{xx}(g)\bar{\mathbf{P}}^{E}_{xx} + D^{E}_{xy}(g)\bar{\mathbf{P}}^{E}_{xy} + D^{E}_{yx}(g)\bar{\mathbf{P}}^{E}_{yx} + D^{E}_{yy}(g)\bar{\mathbf{P}}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & \cdot & D^{E}_{xy} & \cdot \\ \cdot & \cdot & \cdot & D_{xx} & \cdot & D_{xy} \\ \cdot & \cdot & D^{E}_{yx} & \cdot & D^{E}_{yy} & \cdot \\ \cdot & \cdot & \cdot & D_{yx} & \cdot & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\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 & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + D^{E}_{yy}\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 & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

D_3	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E}_{xx}$	·	·	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$	·	·
$\mathbf{P}^{E}_{yx}$	·	·	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{yy}$	·	·
$\mathbf{P}^{E}_{xy}$	·	·	·	·	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{y}$	·	·	·	·	$\mathbf{P}^{E}_{y}$	$\mathbf{P}^{E}_{y}$

GLOBAL **P***-matrix commutes LOCAL* **P***-matrix*

$$\left(\begin{array}{cc|cc} a & b & \cdot & \cdot \\ c & d & \cdot & \cdot \\ \hline \cdot & \cdot & a & b \\ \cdot & \cdot & c & d \end{array}\right) \cdot \left(\begin{array}{cc|cc} A & \cdot & B & \cdot \\ \cdot & A & \cdot & B \\ \hline C & \cdot & D & \cdot \\ \cdot & C & \cdot & D \end{array}\right) = \left(\begin{array}{cc|cc} A & \cdot & B & \cdot \\ \cdot & A & \cdot & B \\ \hline C & \cdot & D & \cdot \\ \cdot & C & \cdot & D \end{array}\right) \cdot \left(\begin{array}{cc|cc} a & b & \cdot & \cdot \\ c & d & \cdot & \cdot \\ \hline \cdot & \cdot & a & b \\ \cdot & \cdot & c & d \end{array}\right)$$

$$\left(\begin{array}{cc|cc} aA & bA & aB & bB \\ cA & dA & cB & dB \\ \hline aC & bC & aD & bD \\ cC & dC & cD & dD \end{array}\right) = \left(\begin{array}{cc|cc} Aa & Ab & Ba & Bb \\ Ac & Ad & Bc & Bd \\ \hline Ca & Cb & Da & Db \\ Cc & Cd & Dc & Dd \end{array}\right)$$

	$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_2}_{yy}$	$\mathbf{P}^{E}_{xx}$	$\mathbf{P}^{E}_{yx}$	$\mathbf{P}^{E}_{xy}$	$\mathbf{P}^{E}_{yy}$
$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E}_{xx}$	·	·	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$	0
$\mathbf{P}^{E}_{xy}$	·	·	0	$\mathbf{P}^{E}_{xx}$	0	$\mathbf{P}^{E}_{xy}$
$\mathbf{P}^{E}_{yx}$	·	·	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$	0
$\mathbf{P}^{E}_{yy}$	·	·	0	$\mathbf{P}^{E}_{yx}$	0	$\mathbf{P}^{E}_{yy}$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ *and ireps* D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 examples)

Weyl **g***-expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms right-and-left*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-*$\mathbf{g}$ *matrix structure versus D_3 local-*$\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Weyl expansion of $\mathbf{g}$ *in irep* $D^{\mu}{}_{jk}(g)\mathbf{P}^{\mu}{}_{jk}$

"$\mathbf{g}$-equals-$\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$-trick"

Irreducible idempotent completeness $\mathbf{1} = \mathbf{P}^{A_1} + \mathbf{P}^{A_2} + \mathbf{P}^{E_1}_{xx} + \mathbf{P}^{E_1}_{yy}$ *completely expands group by* $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$

$$\mathbf{g} = \mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1} = \sum_{\mu}\sum_{m}\sum_{n} D^{\mu}_{mn}(g)\,\mathbf{P}^{\mu}_{mn} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E_1}_{xx}(g)\mathbf{P}^{E_1}_{xx} + D^{E_1}_{xy}(g)\mathbf{P}^{E_1}_{xy}$$

$$+ D^{E_1}_{yx}(g)\mathbf{P}^{E_1}_{yx} + D^{E_1}_{yy}(g)\mathbf{P}^{E_1}_{yy}$$

For irreducible class idempotents sub-indices $_{xx}$ *or* $_{yy}$ *are* <u>*optional*</u>

Previous notation:

$\mathbf{P}^{A_1}_{0_2 0_2} = \mathbf{P}^{A_1}_{xx}$

$\mathbf{P}^{A_2}_{1_2 1_2} = \mathbf{P}^{A_2}_{yy}$

$\mathbf{P}^{E_1}_{0_2 0_2} = \mathbf{P}^{E_1}_{xx}$ $\quad$ $\mathbf{P}^{E_1}_{0_2 1_2} = \mathbf{P}^{E_1}_{xy}$

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Weyl expansion of g in irep $D^{\mu}{}_{jk}(g)\mathbf{P}^{\mu}{}_{jk}$

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Weyl expansion of **g** *in irep* $D^{\mu}{}_{jk}(g)\mathbf{P}^{\mu}{}_{jk}$

*"***g***-equals-***1**·**g**·**1***-trick"*

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For split idempotents sub-indices $_{xx}$ *or* $_{yy}$ *are essential*

$$\mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{yy} = D^{E_1}_{yy}(g)\mathbf{P}^{E_1}_{yy}$$

Besides four *idempotent* projectors $\mathbf{P}^{A_1}, \mathbf{P}^{A_2}, \mathbf{P}^{E_1}_{xx}$, and $\mathbf{P}^{E_1}_{yy}$

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$$+ D^{E_1}_{yx}(g)\mathbf{P}^{E_1}_{yx} + D^{E_1}_{yy}(g)\mathbf{P}^{E_1}_{yy}$$

Previous notation:
$\mathbf{P}^{E_1}_{0_20_2} = \mathbf{P}^{E_1}_{xx}$ $\mathbf{P}^{E_1}_{0_21_2} = \mathbf{P}^{E_1}_{xy}$
$\mathbf{P}^{E_1}_{1_20_2} = \mathbf{P}^{E_1}_{yx}$ $\mathbf{P}^{E_1}_{1_21_2} = \mathbf{P}^{E_1}_{yy}$

For irreducible class idempotents sub-indices $_{xx}$ *or* $_{yy}$ *are* *optional*

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For split idempotents sub-indices $_{xx}$ *or* $_{yy}$ *are* *essential*

$$,\quad \mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{xx} = D^{E_1}_{yx}(g)\boxed{\mathbf{P}^{E_1}_{yx}},\quad \mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{yy} = D^{E_1}_{yy}(g)\mathbf{P}^{E_1}_{yy}$$

Besides four *idempotent* projectors $\mathbf{P}^{A_1}, \mathbf{P}^{A_2}, \mathbf{P}^{E_1}_{xx}$, and $\mathbf{P}^{E_1}_{yy}$

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where:

$$\mathbf{P}^{A_1}_{xx}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}_{xx} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1}_{xx},\quad \mathbf{P}^{A_2}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}_{yy} = D^{A_2}_{yy}(g)\mathbf{P}^{A_2}_{yy},\quad \mathbf{P}^{E_1}_{xx}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{xx} = D^{E_1}_{xx}(g)\mathbf{P}^{E_1}_{xx},\quad \mathbf{P}^{E_1}_{xx}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{yy} = D^{E_1}_{xy}(g)\boxed{\mathbf{P}^{E_1}_{xy}}$$

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Generalizes...

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For split idempotents
sub-indices $_{xx}$ *or* $_{yy}$ *are essential*

, $\mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{xx} = D^{E_1}_{yx}(g)\mathbf{P}^{E_1}_{yx}$, $\mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{yy} = D^{E_1}_{yy}(g)\mathbf{P}^{E_1}_{yy}$

Besides four *idempotent* projectors $\mathbf{P}^{A_1}, \mathbf{P}^{A_2}, \mathbf{P}^{E_1}_{xx}$, and $\mathbf{P}^{E_1}_{yy}$

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Idempotent projector orthogonality... $\boxed{\mathbf{P}_i\,\mathbf{P}_j = \delta_{ij}\,\mathbf{P}_i = \mathbf{P}_j\,\mathbf{P}_i}$

Generalizes to idempotent/nilpotent orthogonality
known as Simple Matrix Algebra: $\boxed{\mathbf{P}^{\mu}_{jk}\mathbf{P}^{\nu}_{mn} = \delta^{\mu\nu}\delta_{km}\mathbf{P}^{\mu}_{jn}}$

Weyl expansion of **g** *in irep* $D^{\mu}{}_{jk}(g)\mathbf{P}^{\mu}{}_{jk}$

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Previous notation:
$\mathbf{P}^{E_1}_{0202}=\mathbf{P}^{E_1}_{xx}$ $\mathbf{P}^{E_1}_{0212}=\mathbf{P}^{E_1}_{xy}$
$\mathbf{P}^{E_1}_{1202}=\mathbf{P}^{E_1}_{yx}$ $\mathbf{P}^{E_1}_{1212}=\mathbf{P}^{E_1}_{yy}$

For irreducible class idempotents sub-indices $_{xx}$ *or* $_{yy}$ *are* *optional*

where:

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Group product table boils down to simple projector matrix algebra

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$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	·	·	·	·	·
$\mathbf{P}^{A_2}_{yy}$	·	$\mathbf{P}^{A_2}_{yy}$	·	·	·	·
$\mathbf{P}^{E_1}_{xx}$	·	·	$\mathbf{P}^{E_1}_{xx}$	$\mathbf{P}^{E_1}_{xy}$	·	·
$\mathbf{P}^{E_1}_{yx}$	·	·	$\mathbf{P}^{E_1}_{yx}$	$\mathbf{P}^{E_1}_{yy}$	·	·
$\mathbf{P}^{E_1}_{xy}$	·	·	·	·	$\mathbf{P}^{E_1}_{xx}$	$\mathbf{P}^{E_1}_{xy}$
$\mathbf{P}^{E_1}_{yy}$	·	·	·	·	$\mathbf{P}^{E_1}_{yx}$	$\mathbf{P}^{E_1}_{yy}$

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$$,\quad \mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{xx} = D^{E_1}_{yx}(g)\,\mathbf{P}^{E_1}_{yx},\quad \mathbf{P}^{E_1}_{yy}\cdot\mathbf{g}\cdot\mathbf{P}^{E_1}_{yy} = D^{E_1}_{yy}(g)\,\mathbf{P}^{E_1}_{yy}$$

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$\mathbf{P}^{A_1}_{xx}$	$\mathbf{P}^{A_1}_{xx}$	.	.	.	.	.
$\mathbf{P}^{A_2}_{yy}$	.	$\mathbf{P}^{A_2}_{yy}$	.	.	.	.
$\mathbf{P}^{E_1}_{xx}$	.	.	$\mathbf{P}^{E_1}_{xx}$	$\mathbf{P}^{E_1}_{xy}$	.	.
$\mathbf{P}^{E_1}_{yx}$	.	.	$\mathbf{P}^{E_1}_{yx}$	$\mathbf{P}^{E_1}_{yy}$	.	.
$\mathbf{P}^{E_1}_{xy}$	.	.	.	.	$\mathbf{P}^{E_1}_{xx}$	$\mathbf{P}^{E_1}_{xy}$
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$$\boxed{\mathbf{P}^{\mu}_{jk}\mathbf{P}^{\nu}_{mn} = \delta^{\mu\nu}\delta_{km}\mathbf{P}^{\mu}_{jn}}$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

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Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}{}^E$ *and ireps* $D_{ab}{}^E$

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 examples)

Weyl **g**-*expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms left and right*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g**-*operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-* **g** *matrix structure versus D_3 local-* $\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

$$\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$$

Spectral decomposition defines *left and right irep transformation* due to spectrally decomposed **g** acting on left and right side of projector $\mathbf{P}^{\mu}{}_{mn}$.

$$\mathbf{g}\mathbf{P}^{\mu}_{mn} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right) \mathbf{P}^{\mu}_{mn}$$

Use $\mathbf{P}^{\mu}_{mn}$-orthonormality

$$\mathbf{P}^{\mu'}_{m'n'}\mathbf{P}^{\mu}_{mn} = \delta^{\mu'\mu}\delta_{n'm}\mathbf{P}^{\mu}_{m'n}$$

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Left-action transforms irep-ket $\mathbf{g}\left| {}^{\mu}_{mn} \right\rangle = \frac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

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A simple irep expression...

$$\left\langle {\mu \atop m'n} \right| \mathbf{g} \left| {\mu \atop mn} \right\rangle = D^{\mu}_{m'm}(g)$$

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

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$$\left\langle \begin{matrix} \mu \\ m'n \end{matrix} \right| \mathbf{g} \left| \begin{matrix} \mu \\ mn \end{matrix} \right\rangle = D^{\mu}_{m'm}(g)$$

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$$= \delta^{\mu'\mu} \delta_{m'm} \frac{\langle \mathbf{1} | \mathbf{P}^{\mu'}_{n'n} | \mathbf{1} \rangle}{|\,norm.|^2}$$

$$= \delta^{\mu'\mu} \delta_{m'm} \delta_{n'n}$$

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

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Classical analog for bands of vibration modes

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

$$\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$$

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Use $\mathbf{P}^{\mu}_{mn}$-orthonormality

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$$= \sum_{n'}^{\ell^\mu} D^{\mu}_{nn'}(g)\, \mathbf{P}^{\mu}_{mn'}$$

Left-action transforms irep-ket $\mathbf{g}\left|\begin{smallmatrix}\mu \\ mn\end{smallmatrix}\right\rangle = \frac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

$$\mathbf{g}\left|\begin{matrix}\mu \\ mn\end{matrix}\right\rangle = \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g) \left|\begin{matrix}\mu \\ m'n\end{matrix}\right\rangle$$

A simple irep expression...

$$\left\langle\begin{matrix}\mu \\ m'n\end{matrix}\right| \mathbf{g} \left|\begin{matrix}\mu \\ mn\end{matrix}\right\rangle = D^{\mu}_{m'm}(g)$$

...requires proper normalization: $\left\langle\begin{matrix}\mu' \\ m'n'\end{matrix}\middle|\begin{matrix}\mu \\ mn\end{matrix}\right\rangle = \frac{\left\langle \mathbf{1}\right| \mathbf{P}^{\mu'}_{n'm'}}{norm.} \frac{\mathbf{P}^{\mu}_{mn}\left|\mathbf{1}\right\rangle}{norm^*.}$

$$= \delta^{\mu'\mu} \delta_{m'm} \frac{\left\langle \mathbf{1}\right| \mathbf{P}^{\mu'}_{n'n} \left|\mathbf{1}\right\rangle}{|norm.|^2}$$

$$|norm.|^2 = \left\langle \mathbf{1}\right| \mathbf{P}^{\mu}_{nn} \left|\mathbf{1}\right\rangle \qquad = \delta^{\mu'\mu} \delta_{m'm} \delta_{n'n}$$

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

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Use $\mathbf{P}^{\mu}_{mn}$-orthonormality

$$\mathbf{P}^{\mu'}_{m'n'} \mathbf{P}^{\mu}_{mn} = \delta^{\mu'\mu} \delta_{n'm} \mathbf{P}^{\mu}_{m'n}$$

Projector conjugation

$$\left(|m\rangle\langle n| \right)^{\dagger} = |n\rangle\langle m|$$

$$\left(\mathbf{P}^{\mu}_{mn} \right)^{\dagger} = \mathbf{P}^{\mu}_{nm}$$

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Left-action transforms irep-ket $\mathbf{g}\left| {}^{\mu}_{mn} \right\rangle = \frac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

Right-action transforms irep-bra $\left\langle {}^{\mu}_{mn} \right| \mathbf{g}^{\dagger} = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{nm}\mathbf{g}^{\dagger}}{norm^{*}}$

$$\mathbf{g}\left| {}^{\mu}_{mn} \right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g) \left| {}^{\mu}_{m'n} \right\rangle$$

A simple irep expression...

$$\left\langle {}^{\mu}_{m'n} \right| \mathbf{g} \left| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{m'm}(g)$$

...requires proper normalization: $\left\langle {}^{\mu'}_{m'n'} \middle| {}^{\mu}_{mn} \right\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}}{norm.} \frac{\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^{*}.}$

$$= \delta^{\mu'\mu} \delta_{m'm} \frac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'n}|\mathbf{1}\rangle}{|norm.|^{2}}$$

$$|norm.|^{2} = \langle \mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle$$

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$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

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Left-action transforms irep-ket $\mathbf{g}\left| {}^{\mu}_{mn} \right\rangle = \dfrac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

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Right-action transforms irep-bra $\left\langle {}^{\mu}_{mn} \right| \mathbf{g}^\dagger = \dfrac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{nm}\mathbf{g}^\dagger}{norm^*}$

$$\left\langle {}^{\mu}_{mn} \right| \mathbf{g}^\dagger = \left\langle {}^{\mu}_{m'n} \right| \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(\mathbf{g}^\dagger)$$

A simple irep expression...

$$\left\langle {}^{\mu}_{m'n} \right| \mathbf{g} \left| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{m'm}(g)$$

...requires proper normalization: $\left\langle {}^{\mu'}_{m'n'} \middle| {}^{\mu}_{mn} \right\rangle = \dfrac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}}{norm.} \dfrac{\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^*.}$

$$= \delta^{\mu'\mu} \delta_{m'm} \frac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'n}|\mathbf{1}\rangle}{|norm.|^2}$$

$$|norm.|^2 = \langle \mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle \qquad = \delta^{\mu'\mu} \delta_{m'm} \delta_{n'n}$$

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

$$\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\,\mathbf{P}^{\mu'}_{m'n'} \right)$$

Spectral decomposition defines *left and right irep transformation* due to spectrally decomposed $\mathbf{g}$ acting on left and right side of projector $\mathbf{P}^{\mu}{}_{mn}$.

$$\mathbf{g}\mathbf{P}^{\mu}_{mn} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\,\mathbf{P}^{\mu'}_{m'n'} \right)\mathbf{P}^{\mu}_{mn}$$

$$= \sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\,\delta^{\mu'\mu}\delta_{n'm}\mathbf{P}^{\mu}_{m'n}$$

$$= \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g)\,\mathbf{P}^{\mu}_{m'n}$$

Use $\mathbf{P}^{\mu}_{mn}$-orthonormality

$$\mathbf{P}^{\mu'}_{m'n'}\mathbf{P}^{\mu}_{mn} = \delta^{\mu'\mu}\delta_{n'm}\mathbf{P}^{\mu}_{m'n}$$

Projector conjugation

$$\left(|m\rangle\langle n|\right)^\dagger = |n\rangle\langle m|$$

$$\left(\mathbf{P}^{\mu}_{mn}\right)^\dagger = \mathbf{P}^{\mu}_{nm}$$

$$\mathbf{P}^{\mu}_{mn}\mathbf{g} = \mathbf{P}^{\mu}_{mn}\left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\,\mathbf{P}^{\mu'}_{m'n'} \right)$$

$$= \sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\,\delta^{\mu'\mu}\delta_{nm'}\mathbf{P}^{\mu}_{mn'}$$

$$= \sum_{n'}^{\ell^\mu} D^{\mu}_{nn'}(g)\,\mathbf{P}^{\mu}_{mn'}$$

Left-action transforms irep-ket $\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

A simple irep expression...

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right|\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Right-action transforms irep-bra $\left\langle\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right|\mathbf{g}^\dagger = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nm}\mathbf{g}^\dagger}{norm^*}$

$$\left\langle\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right|\mathbf{g}^\dagger = \left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right|\sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(\mathbf{g}^\dagger)$$

A less-simple irep expression...

$$\left\langle\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right|\mathbf{g}^\dagger\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g^\dagger)$$

...requires proper normalization: $\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}}{norm.}\frac{\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm*.}$

$$= \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'n}|\mathbf{1}\rangle}{|norm.|^2}$$

$$|norm.|^2 = \langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle$$

$$= \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

$\mathbf{P}^{\mu}{}_{jk}$ *transforms right-and-left*

$$\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$$

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$$= \sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \delta^{\mu'\mu} \delta_{n'm} \mathbf{P}^{\mu}_{m'n}$$

$$= \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\, \mathbf{P}^{\mu}_{m'n}$$

Use $\mathbf{P}^{\mu}_{mn}$-orthonormality

$$\mathbf{P}^{\mu'}_{m'n'} \mathbf{P}^{\mu}_{mn} = \delta^{\mu'\mu} \delta_{n'm} \mathbf{P}^{\mu}_{m'n}$$

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$$= \sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \delta^{\mu'\mu} \delta_{nm'} \mathbf{P}^{\mu}_{mn'}$$

$$= \sum_{n'}^{\ell^{\mu}} D^{\mu}_{nn'}(g)\, \mathbf{P}^{\mu}_{mn'}$$

Left-action transforms irep-ket $\mathbf{g}\left| {\mu \atop mn} \right\rangle = \dfrac{\mathbf{g}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm.}$

$$\mathbf{g}\left| {\mu \atop mn} \right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g) \left| {\mu \atop m'n} \right\rangle$$

A simple irep expression...

$$\left\langle {\mu \atop m'n} \right| \mathbf{g} \left| {\mu \atop mn} \right\rangle = D^{\mu}_{m'm}(g)$$

Right-action transforms irep-bra $\left\langle {\mu \atop mn} \right| \mathbf{g}^{\dagger} = \dfrac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{nm}\mathbf{g}^{\dagger}}{norm^{*}}$

$$\left\langle {\mu \atop mn} \right| \mathbf{g}^{\dagger} = \left\langle {\mu \atop m'n} \right| \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(\mathbf{g}^{\dagger})$$

A less-simple irep expression...

$$\left\langle {\mu \atop mn} \right| \mathbf{g}^{\dagger} \left| {\mu \atop m'n} \right\rangle = D^{\mu}_{m'm}(g^{\dagger})$$

$$= D^{\mu *}_{mm'}(g)$$

if D is unitary

...requires proper normalization: $\left\langle {\mu' \atop m'n'} \middle| {\mu \atop mn} \right\rangle = \dfrac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}}{norm.} \dfrac{\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm*.}$

$$= \delta^{\mu'\mu} \delta_{m'm} \frac{\langle \mathbf{1}|\mathbf{P}^{\mu'}_{n'n}|\mathbf{1}\rangle}{|norm.|^{2}}$$

$$|norm.|^{2} = \langle \mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle$$

$$= \delta^{\mu'\mu} \delta_{m'm} \delta_{n'n}$$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g**-*expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}{}^E$ and ireps $D_{ab}{}^E$

Comparison: Global vs Local $|\mathbf{g}\rangle$-basis versus Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

General formulae for spectral decomposition (D_3 examples)

Weyl **g**-*expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms left and right

$\mathbf{P}^\mu_{jk}$ -expansion in **g**-*operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-$\mathbf{g}$ matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* $\mathbf{g}$*-operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

Derive coefficients $p^{\mu}_{mn}(g)$ of inverse Weyl expansion: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\,\mathbf{g}$

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* $\mathbf{g}$*-operators*

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Left action by operator $\mathbf{f}$ in group $G = \{\mathbf{1},\ldots,\mathbf{f},\mathbf{g},\mathbf{h},\ldots\}$:

$$\mathbf{f} \cdot \mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\, \mathbf{f} \cdot \mathbf{g}$$

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* $\mathbf{g}$*-operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

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$$\mathbf{f} \cdot \mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{{}^\circ G} p^{\mu}_{mn}(g)\, \mathbf{f} \cdot \mathbf{g} = \sum_{\mathbf{h}}^{{}^\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) \mathbf{h} \quad \text{, where: } \mathbf{h} = \mathbf{f} \cdot \mathbf{g}, \text{ or: } \mathbf{g} = \mathbf{f}^{-1}\mathbf{h},$$

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Regular representation *TraceR(*$\mathbf{h}$*)* is zero except for *TraceR(*$\mathbf{1}$*)*= $\circ G$

Regular representation of $D_3 \sim C_{3v}$

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* **g**-*operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

Derive coefficients $p^{\mu}_{mn}(g)$ of inverse Weyl expansion: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{°G} p^{\mu}_{mn}(g)\,\mathbf{g}$

Left action by operator $\mathbf{f}$ in group $G = \{\mathbf{1}, \ldots, \mathbf{f}, \mathbf{g}, \mathbf{h}, \ldots\}$:

$$\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{°G} p^{\mu}_{mn}(g)\,\mathbf{f}\cdot\mathbf{g} = \sum_{\mathbf{h}}^{°G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right)\mathbf{h} \quad \text{, where: } \mathbf{h} = \mathbf{f}\cdot\mathbf{g}, \text{ or: } \mathbf{g} = \mathbf{f}^{-1}\mathbf{h},$$

Regular representation *TraceR*(**h**) is zero except for *TraceR*(**1**)= $°G$

$$Trace\ R\left(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}\right) = \sum_{\mathbf{h}}^{°G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) TraceR\left(\mathbf{h}\right)$$

Regular representation of $D_3 \sim C_{3v}$

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* **g***-operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

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Regular representation *TraceR(***h***)* is zero except for *TraceR(***1***)*= $\circ G$

$$Trace\ R(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}) = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}(\mathbf{f}^{-1}\mathbf{h})\,TraceR(\mathbf{h}) = p^{\mu}_{mn}(\mathbf{f}^{-1}\mathbf{1})\,TraceR(\mathbf{1})$$

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

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

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

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$$\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\, \mathbf{f}\cdot\mathbf{g} = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}(\mathbf{f}^{-1}\mathbf{h})\,\mathbf{h} \quad \text{, where: } \mathbf{h} = \mathbf{f}\cdot\mathbf{g}, \text{ or: } \mathbf{g} = \mathbf{f}^{-1}\mathbf{h},$$

Regular representation *TraceR*($\mathbf{h}$) is zero except for *TraceR*($\mathbf{1}$)$= {}^{\circ}G$

$$Trace\ R\left(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}\right) = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) TraceR(\mathbf{h}) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{1}\right) TraceR(\mathbf{1}) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\right) {}^{\circ}G$$

Regular representation of $D_3 \sim C_{3v}$

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* **g***-operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^\mu} \sum_{n'}^{\ell^\mu} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

Derive coefficients $p^{\mu}_{mn}(g)$ of inverse Weyl expansion: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\,\mathbf{g}$

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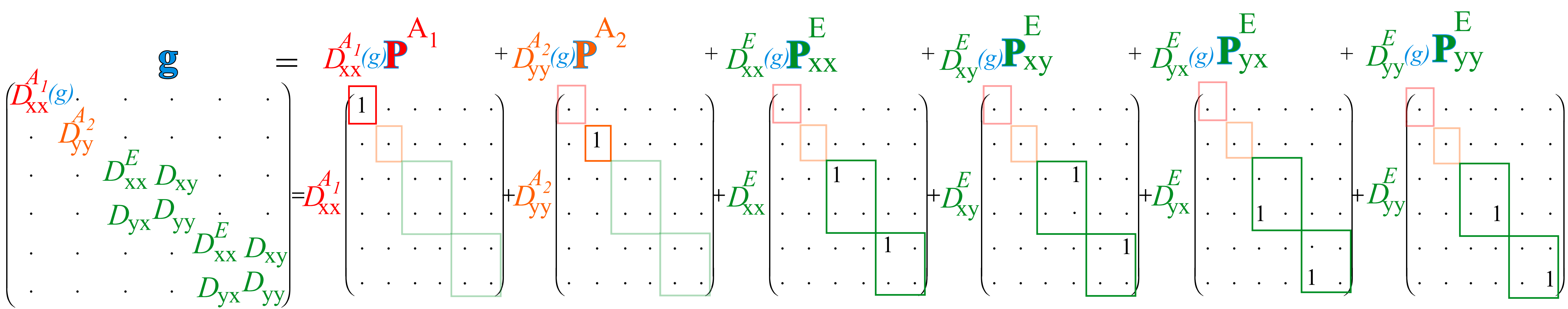
Regular representation *TraceR(***h***)* is zero except for *TraceR(***1***)*= $\circ G$

$$Trace\ R\left(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}\right) = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) TraceR\left(\mathbf{h}\right) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{1}\right) TraceR\left(\mathbf{1}\right) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\right)\circ G$$

Regular representation *TraceR(*$\mathbf{P}^{\mu}_{mn}$*)* is irep dimension $\ell^{(\mu)}$ for diagonal $\mathbf{P}^{\mu}_{mm}$ or zero otherwise:



$\mathbf{P}^{\mu}{}_{jk}$ -expansion in $\mathbf{g}$-operators

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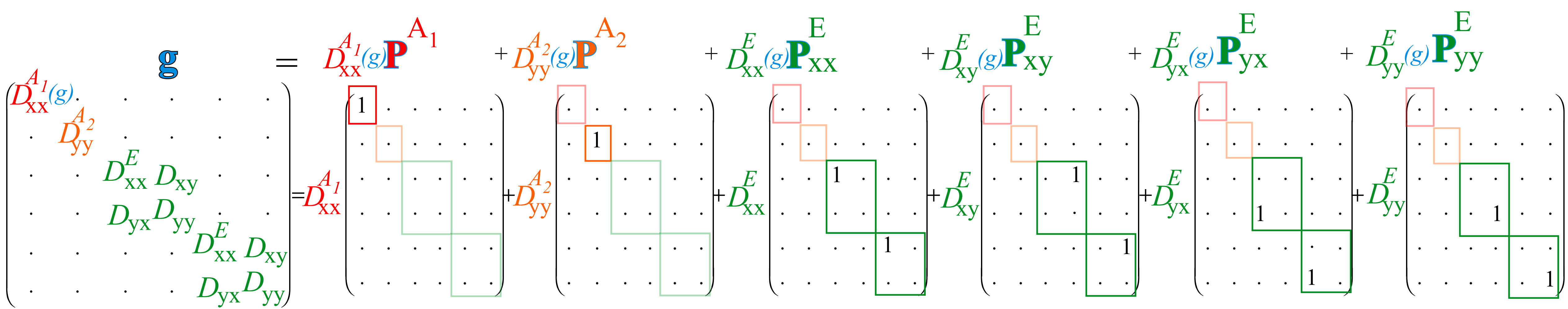
$$Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn} \ell^{(\mu)}$$



$\mathbf{P}^{\mu}{}_{jk}$ -*expansion in* **g**-*operators*

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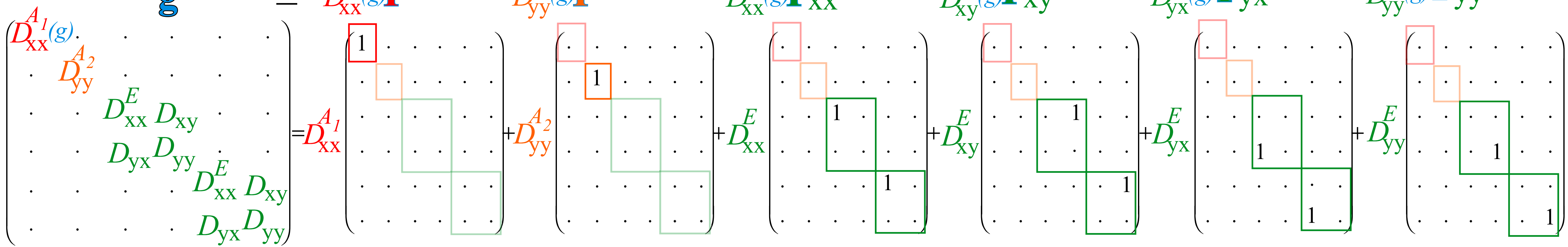
$$\mathit{Trace}\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$$

Solving for $p^{\mu}_{mn}(g)$: $p^{\mu}_{mn}(\mathbf{f}) = \frac{1}{{}^\circ G}\mathit{Trace}\ R\left(\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn}\right)$

$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$



$\mathbf{P}^{\mu}{}_{jk}$ -expansion in g-operators

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

Derive coefficients $p^{\mu}_{mn}(g)$ of inverse Weyl expansion: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{{}^\circ G} p^{\mu}_{mn}(g)\, \mathbf{g}$

Left action by operator $\mathbf{f}$ in group $G = \{\mathbf{1}, \ldots, \mathbf{f}, \mathbf{g}, \mathbf{h}, \ldots\}$:

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Regular representation *TraceR(h)* is zero except for *TraceR(1)*= $^\circ G$

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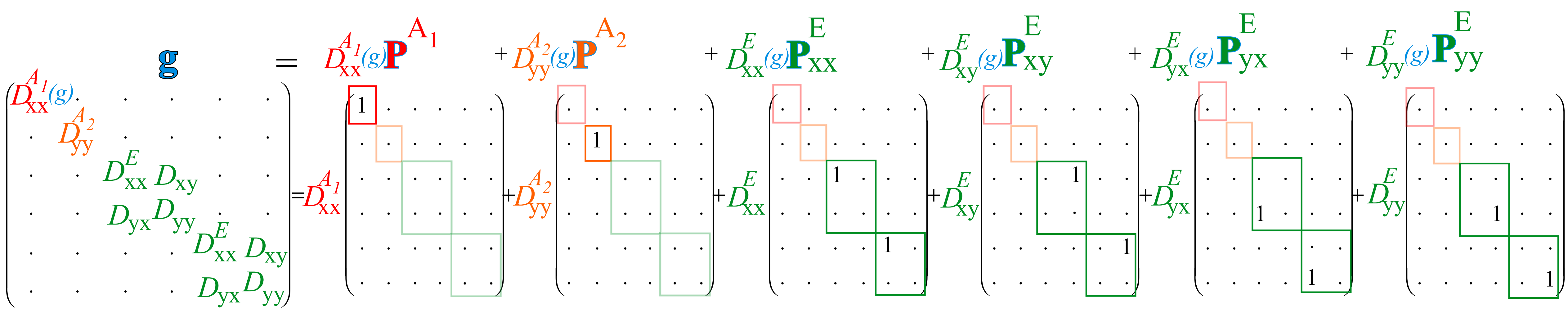
Solving for $p^{\mu}_{mn}(g)$: $p^{\mu}_{mn}(\mathbf{f}) = \frac{1}{{}^\circ G} Trace\ R\left(\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn}\right)$

Use left-action: $\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right) \mathbf{P}^{\mu}_{m'n}$



$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* $\mathbf{g}$*-operators*

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

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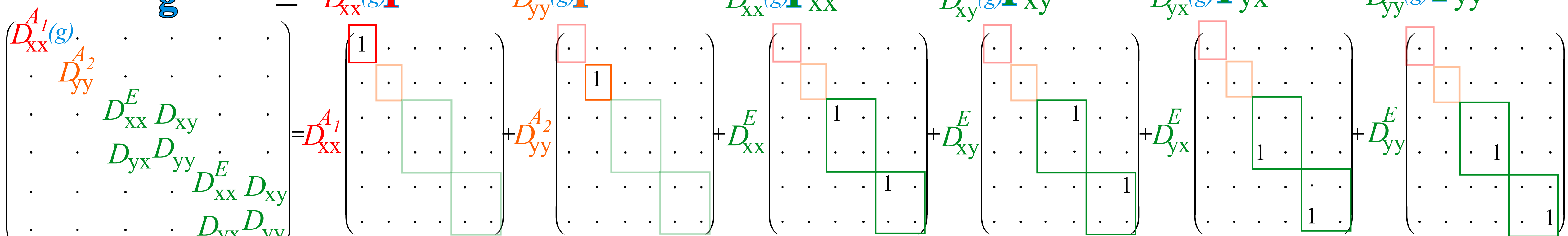

$\mathbf{P}^{\mu}{}_{jk}$ *-expansion in* **g***-operators*

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$$= \frac{1}{{}^\circ G}\sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right) Trace\ R\left(\mathbf{P}^{\mu}_{m'n}\right)$$

Use: $Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$

$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$

$$\begin{pmatrix} D^{A_1}_{xx}(g) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D^{A_2}_{yy} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D^{E}_{xx} & D_{xy} & \cdot & \cdot \\ \cdot & \cdot & D_{yx} & D_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D^{E}_{xx} & D_{xy} \\ \cdot & \cdot & \cdot & \cdot & D_{yx} & D_{yy} \end{pmatrix} = D^{A_1}_{xx}\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{A_2}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{xy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D^{E}_{yx}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + D^{E}_{yy}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

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Use: $Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$

$$= \frac{\ell^{(\mu)}}{\circ G} D^{\mu}_{nm}\left(\mathbf{f}^{-1}\right)$$

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Regular representation *TraceR*(**h**) is zero except for *TraceR*(**1**)= $\circ G$

$$Trace\,R\left(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}\right) = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) TraceR\left(\mathbf{h}\right) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{1}\right) TraceR\left(\mathbf{1}\right) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\right)\circ G$$

Regular representation *TraceR*($\mathbf{P}^{\mu}_{mn}$) is irep dimension $\ell^{(\mu)}$ for diagonal $\mathbf{P}^{\mu}_{mm}$ or zero otherwise:

$$Trace\,R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$$

Solving for $p^{\mu}_{mn}(g)$: $p^{\mu}_{mn}(\mathbf{f}) = \dfrac{1}{\circ G} Trace\,R\left(\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn}\right)$ Use left-action: $\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right)\mathbf{P}^{\mu}_{m'n}$

$$= \frac{1}{\circ G} \sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right) Trace\,R\left(\mathbf{P}^{\mu}_{m'n}\right)$$

Use: $Trace\,R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$

$$= \frac{\ell^{(\mu)}}{\circ G} D^{\mu}_{nm}\left(\mathbf{f}^{-1}\right)$$

$$\boxed{\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{\circ G} \sum_{\mathbf{g}}^{\circ G} D^{\mu}_{nm}\left(g^{-1}\right)\mathbf{g}}$$

$\mathbf{P}^{\mu}{}_{jk}$ -expansion in $\mathbf{g}$-operators

Need inverse of Weyl form: $\mathbf{g} = \left(\sum_{\mu'} \sum_{m'}^{\ell^{\mu}} \sum_{n'}^{\ell^{\mu}} D^{\mu'}_{m'n'}(g)\, \mathbf{P}^{\mu'}_{m'n'} \right)$

Derive coefficients $p^{\mu}_{mn}(g)$ of inverse Weyl expansion: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{^\circ G} p^{\mu}_{mn}(g)\,\mathbf{g}$

Left action by operator $\mathbf{f}$ in group $G = \{\mathbf{1},\ldots,\mathbf{f},\mathbf{g},\mathbf{h},\ldots\}$:

$$\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{^\circ G} p^{\mu}_{mn}(g)\,\mathbf{f}\cdot\mathbf{g} = \sum_{\mathbf{h}}^{^\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right)\mathbf{h} \quad \text{, where: } \mathbf{h} = \mathbf{f}\cdot\mathbf{g}, \text{ or: } \mathbf{g} = \mathbf{f}^{-1}\mathbf{h},$$

Regular representation $TraceR(\mathbf{h})$ is zero except for $TraceR(\mathbf{1}) = {^\circ G}$

$$Trace\ R\left(\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn}\right) = \sum_{\mathbf{h}}^{^\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) TraceR(\mathbf{h}) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{1}\right) TraceR(\mathbf{1}) = p^{\mu}_{mn}\left(\mathbf{f}^{-1}\right){^\circ G}$$

Regular representation $TraceR(\mathbf{P}^{\mu}_{mn})$ is irep dimension $\ell^{(\mu)}$ for diagonal $\mathbf{P}^{\mu}_{mm}$ or zero otherwise:

$$Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$$

Solving for $p^{\mu}_{mn}(g)$: $p^{\mu}_{mn}(\mathbf{f}) = \frac{1}{^\circ G} Trace\ R\left(\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn}\right)$ Use left-action: $\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right)\mathbf{P}^{\mu}_{m'n}$

$$= \frac{1}{^\circ G}\sum_{m'}^{\ell^{(\mu)}} D^{\mu}_{m'm}\left(\mathbf{f}^{-1}\right) Trace\ R\left(\mathbf{P}^{\mu}_{m'n}\right)$$

Use: $Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$

$$= \frac{\ell^{(\mu)}}{^\circ G} D^{\mu}_{nm}\left(\mathbf{f}^{-1}\right) \qquad \left(= \frac{\ell^{(\mu)}}{^\circ G} D^{\mu *}_{mn}(\mathbf{f}) \quad \text{for unitary } D^{\mu}_{nm} \right)$$

$$\boxed{\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{^\circ G}\sum_{\mathbf{g}}^{^\circ G} D^{\mu}_{nm}\left(g^{-1}\right)\mathbf{g} \qquad \left(\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{^\circ G}\sum_{\mathbf{g}}^{^\circ G} D^{\mu *}_{mn}(g)\,\mathbf{g} \quad \text{for unitary } D^{\mu}_{nm} \right)}$$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$-basis versus Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

General formulae for spectral decomposition (D_3 examples)

Weyl **g***-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms left and right

$\mathbf{P}^\mu_{jk}$ -expansion in **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-$\mathbf{g}$ matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\overline{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

$|\mathbf{P}^{(\mu)}\rangle$-basis are projected by $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^\circ G} \sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ *acting on original ket $|\mathbf{1}\rangle$*

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

$|\mathbf{P}^{(\mu)}\rangle$*-basis are projected by* $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^\circ G}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ *acting on original ket* $|\mathbf{1}\rangle$

$$\left|{\mu \atop mn}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle \frac{1}{norm}$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

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$$\left|\begin{smallmatrix}\mu \\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^{\circ}G\cdot norm}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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$$\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^{\circ}G\cdot norm}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$ *subject to normalization:*

$$\left\langle\begin{matrix}\mu'\\ m'n'\end{matrix}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2}$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

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subject to normalization:

$$\left\langle {}^{\mu'}_{m'n'} \middle| {}^{\mu}_{mn} \right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2}$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\overline{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}\left|\mathbf{1}\right\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)\left|\mathbf{g}\right\rangle$$ *subject to normalization:*

$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\left\langle\mathbf{1}\middle|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}\middle|\mathbf{1}\right\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\left\langle\mathbf{1}\middle|\mathbf{P}^{\mu}_{n'n}\middle|\mathbf{1}\right\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$ *where:* $norm = \sqrt{\left\langle\mathbf{1}\middle|\mathbf{P}^{\mu}_{nn}\middle|\mathbf{1}\right\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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Left-action of global $\mathbf{g}$ *on irep-ket* $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\middle|\mathbf{g}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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$|\mathbf{P}^{(\mu)}\rangle$-basis are projected by $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^{\circ}G}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ acting on original ket $|\mathbf{1}\rangle$

$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^{\circ}G\cdot norm}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

where: $norm = \sqrt{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^{\circ}G}}$

Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right|\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$ is quite different

$$\bar{\mathbf{g}}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^{\circ}G}{\ell^{(\mu)}}}$$

$$= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^{\circ}G}{\ell^{(\mu)}}}$$

Use Mock-Mach commutation and

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

$|\mathbf{P}^{(\mu)}\rangle$-basis are projected by $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^\circ G} \sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ *acting on original ket* $|\mathbf{1}\rangle$

$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

where: $norm = \sqrt{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$

Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\middle|\mathbf{g}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$ *is quite different*

$$\bar{\mathbf{g}}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

$$= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

Use Mock-Mach commutation and inverse

$$= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

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$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$ *subject to normalization:*

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Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\middle|\mathbf{g}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$ *is quite different*

$$\bar{\mathbf{g}}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

$$= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

Use Mock-Mach commutation and inverse

$$= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

compute $\mathbf{g}^{-1}$ right action

$$\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} = \sum_{m'=1}^{\ell^{\mu}}\sum_{n'=1}^{\ell^{\mu}}\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

$|\mathbf{P}^{(\mu)}\rangle$-basis are projected by $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^{\circ}G} \sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ acting on original ket $|\mathbf{1}\rangle$

$$\left|\begin{matrix}\mu\\mn\end{matrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^{\circ}G\cdot norm}\sum_{\mathbf{g}}^{{}^{\circ}G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{matrix}\mu'\\m'n'\end{matrix}\middle|\begin{matrix}\mu\\mn\end{matrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

where: $norm = \sqrt{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^{\circ}G}}$

Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{matrix}\mu\\mn\end{matrix}\right\rangle$

$$\mathbf{g}\left|\begin{matrix}\mu\\mn\end{matrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{matrix}\mu\\m'n\end{matrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{matrix}\mu\\m'n\end{matrix}\middle|\mathbf{g}\middle|\begin{matrix}\mu\\mn\end{matrix}\right\rangle = D^{\mu}_{m'm}(g)$$

compute $\mathbf{g}^{-1}$ right action

$$\boxed{\begin{aligned}\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} &= \sum_{m'=1}^{\ell^{\mu}}\sum_{n'=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})\\ &= \sum_{n'=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mn'}\, D^{\mu}_{nn'}(g^{-1})\end{aligned}}$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{matrix}\mu\\mn\end{matrix}\right\rangle$ is quite different

$$\bar{\mathbf{g}}\left|\begin{matrix}\mu\\mn\end{matrix}\right\rangle = \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^{\circ}G}{\ell^{(\mu)}}}$$

$$= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^{\circ}G}{\ell^{(\mu)}}}$$

Use Mock-Mach commutation and inverse

$$= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^{\circ}G}{\ell^{(\mu)}}}$$

Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\overline{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

For unitary $D^{(\mu)}$: (p.33)

$|\mathbf{P}^{(\mu)}\rangle$-basis are projected by $\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{{}^\circ G} \sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)\,\mathbf{g} = \mathbf{P}^{\mu\dagger}_{nm}$ *acting on original ket* $|\mathbf{1}\rangle$

$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

where: $norm = \sqrt{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$

Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^{\mu}} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\middle|\mathbf{g}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

Left-action of local $\overline{\mathbf{g}}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$ is quite different

$$\overline{\mathbf{g}}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \overline{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

$$= \mathbf{P}^{\mu}_{mn}\overline{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

Use Mock-Mach commutation and inverse

$$= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

$$= \sum_{n'=1}^{\ell^{\mu}} D^{\mu}_{nn'}(g^{-1})\mathbf{P}^{\mu}_{mn'}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}$$

compute $\mathbf{g}^{-1}$ right action

$$\boxed{\begin{aligned}\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} &= \sum_{m'=1}^{\ell^{\mu}}\sum_{n'=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})\\ &= \sum_{n'=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mn'}\,D^{\mu}_{nn'}(g^{-1})\end{aligned}}$$

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$$\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

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Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

$$\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g)\left|\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{smallmatrix}\mu\\ m'n\end{smallmatrix}\right|\mathbf{g}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = D^{\mu}_{m'm}(g)$$

compute $\mathbf{g}^{-1}$ right action

$$\boxed{\begin{aligned}\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} &= \sum_{m'=1}^{\ell^\mu}\sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})\\ &= \sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn'}\;D^{\mu}_{nn'}(g^{-1})\end{aligned}}$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$ *is quite different*

$$\begin{aligned}\bar{\mathbf{g}}\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle &= \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\mathbf{P}^{\mu}_{mn'}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\left|\begin{smallmatrix}\mu\\ mn'\end{smallmatrix}\right\rangle\end{aligned}$$

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$$\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{matrix}\mu'\\ m'n'\end{matrix}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

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Matrix is same as given on p.23-28

$$\left\langle\begin{matrix}\mu\\ m'n\end{matrix}\middle|\mathbf{g}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = D^{\mu}_{m'm}(g)$$

compute $\mathbf{g}^{-1}$ right action

$$\boxed{\begin{aligned}\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} &= \sum_{m'=1}^{\ell^\mu}\sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})\\ &= \sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn'}\,D^{\mu}_{nn'}(g^{-1})\end{aligned}}$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle$ is quite different

$$\begin{aligned}\bar{\mathbf{g}}\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle &= \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\mathbf{P}^{\mu}_{mn'}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\left|\begin{matrix}\mu\\ mn'\end{matrix}\right\rangle\end{aligned}$$

Use Mock-Mach commutation and inverse

Local $\bar{\mathbf{g}}$-matrix component

$$\boxed{\left\langle\begin{matrix}\mu\\ mn'\end{matrix}\middle|\bar{\mathbf{g}}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu^*}_{n'n}(g)}$$

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$$\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G\cdot norm}\sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization:

$$\left\langle\begin{matrix}\mu'\\ m'n'\end{matrix}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$

where: $norm = \sqrt{\langle\mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$

Left-action of global $\mathbf{g}$ on irep-ket $\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle$

$$\mathbf{g}\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \sum_{m'}^{\ell^\mu} D^{\mu}_{m'm}(g)\left|\begin{matrix}\mu\\ m'n\end{matrix}\right\rangle$$

Matrix is same as given on p.23-28

$$\left\langle\begin{matrix}\mu\\ m'n\end{matrix}\middle|\mathbf{g}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = D^{\mu}_{m'm}(g)$$

compute $\mathbf{g}^{-1}$ right action

$$\boxed{\begin{aligned}\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} &= \sum_{m'=1}^{\ell^\mu}\sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})\\ &= \sum_{n'=1}^{\ell^\mu}\mathbf{P}^{\mu}_{mn'}\;D^{\mu}_{nn'}(g^{-1})\end{aligned}}$$

Left-action of local $\bar{\mathbf{g}}$ on irep-ket $\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle$ *is quite different*

$$\begin{aligned}\bar{\mathbf{g}}\left|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle &= \bar{\mathbf{g}}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\bar{\mathbf{g}}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\mathbf{P}^{\mu}_{mn'}|\mathbf{1}\rangle\sqrt{\frac{{}^\circ G}{\ell^{(\mu)}}}\\ &= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\left|\begin{matrix}\mu\\ mn'\end{matrix}\right\rangle\end{aligned}$$

Use Mock-Mach commutation and inverse

***Global** $\mathbf{g}$-matrix component*

$$\boxed{\left\langle\begin{matrix}\mu\\ m'n\end{matrix}\middle|\mathbf{g}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = D^{\mu}_{m'm}(g)}$$

***Local** $\bar{\mathbf{g}}$-matrix component*

$$\boxed{\left\langle\begin{matrix}\mu\\ mn'\end{matrix}\middle|\bar{\mathbf{g}}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu^*}_{n'n}(g)}$$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with:* $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{ij}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}{}^E$ *and ireps* $D_{ab}{}^E$

Comparison: Global vs Local $|\mathbf{g}\rangle$*-basis versus Global vs Local* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

General formulae for spectral decomposition (D_3 examples)

Weyl **g***-expansion in irep* $D^\mu_{jk}(g)$ *and projectors* $\mathbf{P}^\mu_{jk}$

$\mathbf{P}^\mu_{jk}$ *transforms left and right*

$\mathbf{P}^\mu_{jk}$ *-expansion in* **g***-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$|\mathbf{P}^{(\mu)}\rangle$*-basis D_3 global-***g** *matrix structure versus D_3 local-*$\bar{\mathbf{g}}$ *matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

$|\mathbf{P}^{(\mu)}\rangle$-*basis* D_3 *global*-$\mathbf{g}$ *matrix structure versus* D_3 *local*-$\bar{\mathbf{g}}$ *matrix structure*

$$R^P(\mathbf{g}) = TR^G(\mathbf{g})T^\dagger =$$

$$\begin{array}{cccccc}
|\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle
\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\
\hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\
\hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} & \cdot & \cdot \\
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy} & \cdot & \cdot \\
\hline
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} \\
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy}
\end{array}\right)$$

$|\mathbf{P}^{(\mu)}\rangle$-*base ordering to concentrate global*-$\mathbf{g}$ *D-matrices*

Global $\mathbf{g}$-*matrix component*

$$\boxed{\left\langle {}^{\mu}_{m'n} \middle| \mathbf{g} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{m'm}(g)}$$

Local $\bar{\mathbf{g}}$-*matrix component*

$$\boxed{\left\langle {}^{\mu}_{mn'} \middle| \bar{\mathbf{g}} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu *}_{n'n}(g)}$$

$|\mathbf{P}^{(\mu)}\rangle$-*basis* D_3 *global*-$\mathbf{g}$ *matrix structure versus* D_3 *local*-$\bar{\mathbf{g}}$ *matrix structure*

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\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy}(\mathbf{g}) & \cdot & \cdot \\
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy}(\mathbf{g}) & \cdot & \cdot \\ \hline
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy}(\mathbf{g}) \\
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy}(\mathbf{g})
\end{array}\right)$$

$|\mathbf{P}^{(\mu)}\rangle$-*base ordering to concentrate global*-$\mathbf{g}$ *D-matrices*

$$R^P(\bar{\mathbf{g}}) = TR^G(\bar{\mathbf{g}})T^\dagger =$$

$$\begin{array}{cccccc}
|\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle
\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1 *}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2 *}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1 *}_{xx}(\mathbf{g}) & \cdot & D^{E_1 *}_{xy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1 *}_{xx}(\mathbf{g}) & \cdot & D^{E_1 *}_{xy}(\mathbf{g}) \\ \hline
\cdot & \cdot & D^{E_1 *}_{yx}(\mathbf{g}) & \cdot & D^{E_1 *}_{yy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1 *}_{yx}(\mathbf{g}) & \cdot & D^{E_1 *}_{yy}(\mathbf{g})
\end{array}\right)$$

here
Local $\bar{\mathbf{g}}$-*matrix*
is not concentrated

Global $\mathbf{g}$-*matrix component*

$$\boxed{\left\langle {}^{\mu}_{m'n} \middle| \mathbf{g} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{m'm}(g)}$$

Local $\bar{\mathbf{g}}$-*matrix component*

$$\boxed{\left\langle {}^{\mu}_{mn'} \middle| \bar{\mathbf{g}} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu *}_{n'n}(g)}$$

$|\mathbf{P}^{(\mu)}\rangle$*-basis* D_3 *global-*$\mathbf{g}$ *matrix structure versus* D_3 *local-*$\bar{\mathbf{g}}$ *matrix structure*

$$R^P(\mathbf{g}) = TR^G(\mathbf{g})T^\dagger =$$

$$\begin{array}{c}
\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\
\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} & \cdot & \cdot \\
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy} & \cdot & \cdot \\ \hline
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} \\
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy}
\end{array}\right)
\end{array}$$

$|\mathbf{P}^{(\mu)}\rangle$*-base ordering to concentrate global-*$\mathbf{g}$ *D-matrices*

$$R^P(\bar{\mathbf{g}}) = TR^G(\bar{\mathbf{g}})T^\dagger =$$

$$\begin{array}{c}
\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\
\left(\begin{array}{c|c|cc|cc}
D^{A_1 *}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2 *}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1 *}_{xx}(\mathbf{g}) & \cdot & D^{E_1 *}_{xy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1 *}_{xx}(\mathbf{g}) & \cdot & D^{E_1 *}_{xy}(\mathbf{g}) \\ \hline
\cdot & \cdot & D^{E_1 *}_{yx}(\mathbf{g}) & \cdot & D^{E_1 *}_{yy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1 *}_{yx}(\mathbf{g}) & \cdot & D^{E_1 *}_{yy}(\mathbf{g})
\end{array}\right)
\end{array}$$

here
Local $\bar{\mathbf{g}}$*-matrix*
is not concentrated

$$\bar{R}^P(\mathbf{g}) = \bar{T}R^G(\mathbf{g})\bar{T}^\dagger =$$

$$\begin{array}{c}
\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\
\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & \cdot & D^{E_1}_{xy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1}_{xx} & \cdot & D^{E_1}_{xy} \\ \hline
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & \cdot & D^{E_1}_{yy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1}_{yx} & \cdot & D^{E_1}_{yy}
\end{array}\right)
\end{array}$$

here
global $\mathbf{g}$*-matrix*
is not concentrated

Global $\mathbf{g}$*-matrix component*

$$\boxed{\left\langle {}^{\mu}_{m'n} \middle| \mathbf{g} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{m'm}(g)}$$

Local $\bar{\mathbf{g}}$*-matrix component*

$$\boxed{\left\langle {}^{\mu}_{mn'} \middle| \bar{\mathbf{g}} \middle| {}^{\mu}_{mn} \right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu *}_{n'n}(g)}$$

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\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} & \cdot & \cdot \\
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy} & \cdot & \cdot \\ \hline
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & D^{E_1}_{xy} \\
\cdot & \cdot & \cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & D^{E_1}_{yy}
\end{array}\right)$$

$$R^P(\bar{\mathbf{g}}) = TR^G(\bar{\mathbf{g}})T^\dagger =$$

$$\begin{array}{cccccc}
|\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle
\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1*}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2*}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1*}_{xx}(\mathbf{g}) & \cdot & D^{E_1*}_{xy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1*}_{xx}(\mathbf{g}) & \cdot & D^{E_1*}_{xy}(\mathbf{g}) \\ \hline
\cdot & \cdot & D^{E_1*}_{yx}(\mathbf{g}) & \cdot & D^{E_1*}_{yy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1*}_{yx}(\mathbf{g}) & \cdot & D^{E_1*}_{yy}(\mathbf{g})
\end{array}\right)$$

$|\mathbf{P}^{(\mu)}\rangle$-base ordering to concentrate global-$\mathbf{g}$ D-matrices

$$\bar{R}^P(\mathbf{g}) = \bar{T}R^G(\mathbf{g})\bar{T}^\dagger =$$

$$\begin{array}{cccccc}
|\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle
\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1}_{xx}(\mathbf{g}) & \cdot & D^{E_1}_{xy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1}_{xx} & \cdot & D^{E_1}_{xy} \\ \hline
\cdot & \cdot & D^{E_1}_{yx}(\mathbf{g}) & \cdot & D^{E_1}_{yy}(\mathbf{g}) & \cdot \\
\cdot & \cdot & \cdot & D^{E_1}_{yx} & \cdot & D^{E_1}_{yy}
\end{array}\right)$$

$$\bar{R}^P(\bar{\mathbf{g}}) = \bar{T}R^G(\bar{\mathbf{g}})\bar{T}^\dagger =$$

$$\begin{array}{cccccc}
|\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle
\end{array}$$

$$\left(\begin{array}{c|c|cc|cc}
D^{A_1*}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & D^{A_2*}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot \\ \hline
\cdot & \cdot & D^{E_1*}_{xx}(\mathbf{g}) & D^{E_1*}_{xy}(\mathbf{g}) & \cdot & \cdot \\
\cdot & \cdot & D^{E_1*}_{yx}(\mathbf{g}) & D^{E_1*}_{yy}(\mathbf{g}) & \cdot & \cdot \\ \hline
\cdot & \cdot & \cdot & \cdot & D^{E_1*}_{xx}(\mathbf{g}) & D^{E_1*}_{xy}(\mathbf{g}) \\
\cdot & \cdot & \cdot & \cdot & D^{E_1*}_{yx}(\mathbf{g}) & D^{E_1*}_{yy}(\mathbf{g})
\end{array}\right)$$

$|\mathbf{P}^{(\mu)}\rangle$-base ordering to concentrate local-$\bar{\mathbf{g}}$ D-matrices and $\mathbf{H}$-matrices

Global $\mathbf{g}$*-matrix component*

$$\boxed{\left\langle {\mu \atop m'n} \middle| \mathbf{g} \middle| {\mu \atop mn} \right\rangle = D^{\mu}_{m'm}(g)}$$

Local $\bar{\mathbf{g}}$*-matrix component*

$$\boxed{\left\langle {\mu \atop mn'} \middle| \bar{\mathbf{g}} \middle| {\mu \atop mn} \right\rangle = D^{\mu}_{nn'}(g^{-1}) = D^{\mu*}_{n'n}(g)}$$

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

AMOP reference links on page 2

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$-basis versus Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

General formulae for spectral decomposition (D_3 examples)

*Weyl **g**-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms left and right

*$\mathbf{P}^\mu_{jk}$ -expansion in **g**-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

*$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-**g** matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

D_3 Hamiltonian *local-* $\mathbf{H}$ *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{o_G} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

D_3 Hamiltonian *local-* **H** *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{o_G} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ (\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathsf{P}^{\mu}_{ma} | \mathsf{H} | \mathsf{P}^{\mu}_{nb} \rangle$$

D_3 Hamiltonian *local-* $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ (\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle$$

Let: $\left|\begin{smallmatrix}\mu \\ mn\end{smallmatrix}\right\rangle \equiv \left|\mathbf{P}^{\mu}_{mn}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle \frac{1}{norm}$

$$\left|\begin{smallmatrix}\mu \\ mn\end{smallmatrix}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle \frac{1}{norm} = \frac{\ell^{(\mu)}}{^\circ G \cdot norm} \sum_{\mathbf{g}}^{^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization (from p. 116-122):

$$norm = \sqrt{\langle \mathbf{1} | \mathbf{P}^{\mu}_{nn} | \mathbf{1} \rangle} = \sqrt{\frac{\ell^{(\mu)}}{^\circ G}}$$ *(which will cancel out)*

So, fuggettabout it!

D_3 Hamiltonian *local*- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array}$$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2}$$

Projector conjugation p.31

$$\left(|m\rangle\langle n|\right)^\dagger = |n\rangle\langle m|$$

$$\left(\mathbf{P}^{\mu}_{mn}\right)^\dagger = \mathbf{P}^{\mu}_{nm}$$

$$\left|{\mu \atop mn}\right\rangle = \mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle \frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G \cdot norm} \sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g)|\mathbf{g}\rangle$$

subject to normalization (from p. 116-122):

$$norm = \sqrt{\langle \mathbf{1} | \mathbf{P}^{\mu}_{nn} | \mathbf{1} \rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$$ *(which will cancel out)*

So, fuggettabout it!

D_3 Hamiltonian *local-* $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{c} \quad |\mathbf{P}^{A_1}_{xx}\rangle \; |\mathbf{P}^{A_2}_{yy}\rangle \; |\mathbf{P}^{E_1}_{xx}\rangle |\mathbf{P}^{E_1}_{xy}\rangle \; |\mathbf{P}^{E_1}_{yx}\rangle |\mathbf{P}^{E_1}_{yy}\rangle \end{array}$$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma} | \mathbf{H} | \mathbf{P}^\mu_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^\mu_{am} \mathbf{H} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^\mu_{am} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2}$$

Mock-Mach commutation

$$\mathbf{r}\,\bar{\mathbf{r}} = \bar{\mathbf{r}}\,\mathbf{r}$$

(p.89)

$$\left| \begin{smallmatrix} \mu \\ mn \end{smallmatrix} \right\rangle = \mathbf{P}^\mu_{mn} |\mathbf{1}\rangle \frac{1}{norm} = \frac{\ell^{(\mu)}}{{}^\circ G \cdot norm} \sum_{\mathbf{g}}^{{}^\circ G} D^{\mu^*}_{mn}(g) |\mathbf{g}\rangle$$

subject to normalization *(from p. 116-122)*:

$$norm = \sqrt{\langle \mathbf{1} | \mathbf{P}^\mu_{nn} | \mathbf{1} \rangle} = \sqrt{\frac{\ell^{(\mu)}}{{}^\circ G}}$$ *(which will cancel out)*

So, fuggettabout it!

D_3 Hamiltonian *local*- $\mathbf{H}$ *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array}$$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma} | \mathbf{H} | \mathbf{P}^\mu_{nb} \rangle = \underbrace{\langle \mathbf{1} | \mathbf{P}^\mu_{am} \mathbf{H} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}_{(norm)^2} = \underbrace{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^\mu_{am} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}_{(norm)^2} = \delta_{mn} \underbrace{\langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^\mu_{ab} | \mathbf{1} \rangle}_{(norm)^2} = \sum_{g=1}^{{}^oG} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\mu *}_{ab}(g)$$

Use $\mathbf{P}^\mu_{mn}$-orthonormality

$$\mathbf{P}^{\mu'}_{m'n'} \mathbf{P}^{\mu}_{mn} = \delta^{\mu'\mu} \delta_{n'm} \mathbf{P}^\mu_{m'n}$$

(p.18)

D_3 *Hamiltonian local-* $\mathbf{H}$ *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{c} \begin{array}{cccccc} \left|\mathbf{P}^{A_1}_{xx}\right\rangle & \left|\mathbf{P}^{A_2}_{yy}\right\rangle & \left|\mathbf{P}^{E_1}_{xx}\right\rangle & \left|\mathbf{P}^{E_1}_{xy}\right\rangle & \left|\mathbf{P}^{E_1}_{yx}\right\rangle & \left|\mathbf{P}^{E_1}_{yy}\right\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \left\langle \mathbf{P}^{\mu}_{ma} \middle| \mathbf{H} \middle| \mathbf{P}^{\mu}_{nb} \right\rangle = \underset{(norm)^2}{\underline{\langle \mathbf{1}|}} \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} |\mathbf{1}\rangle = \langle \mathbf{1}| \mathbf{H} \mathbf{P}^{\mu}_{am} \underset{(norm)^2}{\underline{\mathbf{P}^{\mu}_{nb} |\mathbf{1}\rangle}} = \delta_{mn} \langle \mathbf{1}| \mathbf{H} \underset{(norm)^2}{\underline{\mathbf{P}^{\mu}_{ab} |\mathbf{1}\rangle}} = \sum_{g=1}^{{}^\circ G} \langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\mu^*}_{ab}(g)$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_3 Hamiltonian local- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

$\mathbf{H}$ matrix in $|\mathbf{g}\rangle$-basis:

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ matrix in $|\mathbf{P}^{(\mu)}\rangle$-basis:

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G\bar{T}^\dagger = \begin{array}{c} \begin{matrix} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{matrix} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{{}^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\mu^*}_{ab}(g) = \sum_{g=1}^{{}^\circ G} r_g D^{\mu^*}_{ab}(g)$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of **D_3 Center** (All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with:* $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g***-expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}{}^E$ and ireps $D_{ab}{}^E$

Comparison: Global vs Local $|\mathbf{g}\rangle$-basis versus Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

General formulae for spectral decomposition (D_3 examples)

*Weyl **g**-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms left and right

*$\mathbf{P}^\mu_{jk}$ -expansion in **g**-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

*$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-**g** matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

D_3 Hamiltonian *local*- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{c} \\ (\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \end{array}
\begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\
\left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^{\mu}_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* **g**

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_3 Hamiltonian *local*- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G=\sum_{g=1}^{{}^oG} r_g\,\mathbf{g}=\begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3\\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2\\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1\\ i_i & i_3 & i_2 & r_0 & r_1 & r_2\\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1\\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P=\bar{T}(\mathbf{H})_G\bar{T}^\dagger=\begin{array}{c}
\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array}\\
\left(\begin{array}{c|c|cc|cc}
H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot\\ \hline
\cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot\\ \hline
\cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot\\
\cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot\\ \hline
\cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy}\\
\cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy}
\end{array}\right)\end{array}$$

$$H^{\alpha}_{ab}=\langle\mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle=\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2}=\frac{\langle\mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2}=\delta_{mn}\frac{\langle\mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2}=\sum_{g=1}^{{}^\circ G}\langle\mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g)=\sum_{g=1}^{{}^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1}=r_0D^{A_1*}(1)+r_1D^{A_1*}(r^1)+r_1^*D^{A_1*}(r^2)+i_1D^{A_1*}(i_1)+i_2D^{A_1*}(i_2)+i_3D^{A_1*}(i_3)\;=r_0+r_1+r_1^*+i_1+i_2+i_3$$

$$H^{A_2}=r_0D^{A_2*}(1)+r_1D^{A_2*}(r^1)+r_1^*D^{A_2*}(r^2)+i_1D^{A_2*}(i_1)+i_2D^{A_2*}(i_2)+i_3D^{A_2*}(i_3)\;=r_0+r_1+r_1^*-i_1-i_2-i_3$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* **g**

$\mathbf{g}=$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g})=$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g})=$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g})=$	$\begin{pmatrix}1&\cdot\\ \cdot&1\end{pmatrix}$	$\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\ \frac{\sqrt3}{2}&-\frac12\end{pmatrix}$	$\begin{pmatrix}-\frac12&\frac{\sqrt3}{2}\\ -\frac{\sqrt3}{2}&-\frac12\end{pmatrix}$	$\begin{pmatrix}-\frac12&-\frac{\sqrt3}{2}\\ -\frac{\sqrt3}{2}&\frac12\end{pmatrix}$	$\begin{pmatrix}-\frac12&\frac{\sqrt3}{2}\\ \frac{\sqrt3}{2}&\frac12\end{pmatrix}$	$\begin{pmatrix}1&0\\ 0&-1\end{pmatrix}$

D_3 Hamiltonian *local*- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) \;= r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E *}_{xx}(1) + r_1 D^{E *}_{xx}(r^1) + r_1^* D^{E *}_{xx}(r^2) + i_1 D^{E *}_{xx}(i_1) + i_2 D^{E *}_{xx}(i_2) + i_3 D^{E *}_{xx}(i_3) \;= (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_3 Hamiltonian *local-* $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G=\sum_{g=1}^{^oG} r_g \bar{\mathbf{g}}=\begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P=\bar{T}(\mathbf{H})_G\bar{T}^\dagger=\begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab}=\langle\mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle=\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2}=\frac{\langle\mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2}=\delta_{mn}\frac{\langle\mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2}=\sum_{g=1}^{^\circ G}\langle\mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g)=\sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1}=r_0D^{A_1*}(1)+r_1D^{A_1*}(r^1)+r_1^*D^{A_1*}(r^2)+i_1D^{A_1*}(i_1)+i_2D^{A_1*}(i_2)+i_3D^{A_1*}(i_3)\ =r_0+r_1+r_1^*+i_1+i_2+i_3$$

$$H^{A_2}=r_0D^{A_2*}(1)+r_1D^{A_2*}(r^1)+r_1^*D^{A_2*}(r^2)+i_1D^{A_2*}(i_1)+i_2D^{A_2*}(i_2)+i_3D^{A_2*}(i_3)\ =r_0+r_1+r_1^*-i_1-i_2-i_3$$

$$H^{E_1}_{xx}=r_0D^{E*}_{xx}(1)+r_1D^{E*}_{xx}(r^1)+r_1^*D^{E*}_{xx}(r^2)+i_1D^{E*}_{xx}(i_1)+i_2D^{E*}_{xx}(i_2)+i_3D^{E*}_{xx}(i_3)\ =(2r_0-r_1-r_1^*-i_1-i_2+2i_3)/2$$

$$H^{E_1}_{xy}=r_0D^{E*}_{xy}(1)+r_1D^{E*}_{xy}(r^1)+r_1^*D^{E*}_{xy}(r^2)+i_1D^{E*}_{xy}(i_1)+i_2D^{E*}_{xy}(i_2)+i_3D^{E*}_{xy}(i_3)\ =\sqrt{3}(-r_1+r_1^*-i_1+i_2)/2=H^{E*}_{yx}$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g}=$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g})=$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g})=$	1	1	1	−1	−1	−1
$D^{E_1}_{x,y}(\mathbf{g})=$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_3 Hamiltonian *local*- $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

$\mathbf{H}$ *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

$\mathbf{H}$ *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array}$$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^{\mu}_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) \;\; = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) \;\; = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) \;\; = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx}$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) \;\; = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* $\mathbf{g}$

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$D^{A_1}(\mathbf{g}) =$	1	1	1	1	1	1
$D^{A_2}(\mathbf{g}) =$	1	1	1	-1	-1	-1
$D^{E_1}_{x,y}(\mathbf{g}) =$	$\begin{pmatrix} 1 & \cdot \\ \cdot & 1 \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

D_3 Hamiltonian *local-* $\mathbf{H}$ *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{^oG} r_g \bar{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma} | \mathbf{H} | \mathbf{P}^\mu_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^\mu_{am} \mathbf{H} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^\mu_{am} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^\mu_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx}$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2$$

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

D_3 Hamiltonian *local-* $\mathbf{H}$ matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \overline{\mathbf{g}} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$\begin{array}{c} \\ (\mathbf{H})_P = \overline{T}(\mathbf{H})_G \overline{T}^\dagger = \end{array} \begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma}|\mathbf{H}|\mathbf{P}^\mu_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^\mu_{am}\mathbf{H}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^\mu_{am}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^\mu_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{{}^\circ G} \langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{{}^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 \qquad = r_0 + 2r_1 + 2i_{12} + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 \qquad = r_0 + 2r_1 - 2i_{12} - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2 \qquad = r_0 - r_1 - i_{12} + i_3$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx} \qquad = 0$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2 \qquad = r_0 - r_1 + i_{12} - i_3$$

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$= \begin{pmatrix} r_0 - r_1 - i_{12} + i_3 & 0 \\ 0 & r_0 - r_1 - i_{12} - i_3 \end{pmatrix}_{For:\, r_1 = r_1^* \, and:\, i_1 = i_2}$$

Choosing local $C_2 = \{\mathbf{1}, \mathbf{i_3}\}$ *symmetry with local constraints* $r_1 = r_1^* = r_2$ *and* $i_1 = i_2$

D_3 Hamiltonian *local-* **H** *matrices in* $|\mathbf{P}^{(\mu)}\rangle$*-basis*

H *matrix in* $|\mathbf{g}\rangle$*-basis:*

$$(\mathbf{H})_G = \sum_{g=1}^{{}^oG} r_g \mathbf{g} = \begin{pmatrix} r_0 & r_2 & r_1 & i_1 & i_2 & i_3 \\ r_1 & r_0 & r_1 & i_3 & i_1 & i_2 \\ r_2 & r_1 & r_0 & i_2 & i_3 & i_1 \\ i_i & i_3 & i_2 & r_0 & r_1 & r_2 \\ i_2 & i_1 & i_3 & r_2 & r_0 & r_1 \\ i_3 & i_2 & i_1 & r_1 & r_2 & r_0 \end{pmatrix}$$

H *matrix in* $|\mathbf{P}^{(\mu)}\rangle$*-basis:*

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array}$$

$$\left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{{}^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{{}^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 \qquad = r_0 + 2r_1 + 2i_{12} + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 \qquad = r_0 + 2r_1 - 2i_{12} - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E *}_{xx}(1) + r_1 D^{E *}_{xx}(r^1) + r_1^* D^{E *}_{xx}(r^2) + i_1 D^{E *}_{xx}(i_1) + i_2 D^{E *}_{xx}(i_2) + i_3 D^{E *}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2 \qquad = r_0 - r_1 - i_{12} + i_3$$

$$H^{E_1}_{xy} = r_0 D^{E *}_{xy}(1) + r_1 D^{E *}_{xy}(r^1) + r_1^* D^{E *}_{xy}(r^2) + i_1 D^{E *}_{xy}(i_1) + i_2 D^{E *}_{xy}(i_2) + i_3 D^{E *}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E *}_{yx} \qquad = 0$$

$$H^{E_1}_{yy} = r_0 D^{E *}_{yy}(1) + r_1 D^{E *}_{yy}(r^1) + r_1^* D^{E *}_{yy}(r^2) + i_1 D^{E *}_{yy}(i_1) + i_2 D^{E *}_{yy}(i_2) + i_3 D^{E *}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2 \qquad = r_0 - r_1 + i_{12} - i_3$$

$C_2 = \{\mathbf{1}, \mathbf{i}_3\}$
Local symmetry determines all levels and eigenvectors with just 4 real parameters

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$= \begin{pmatrix} r_0 - r_1 - i_{12} + i_3 & 0 \\ 0 & r_0 - r_1 - i_{12} - i_3 \end{pmatrix}_{For:\ r_1 = r_1^* \ and:\ i_1 = i_2}$$

Choosing local $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ *symmetry with local constraints* $r_1 = r_1^* = r_2$ *and* $i_1 = i_2$

$$\mathbf{P}^{(\mu)}_{mn} = \frac{\ell^{(\mu)}}{°G}\sum_{\mathbf{g}} D^{(\mu)*}_{mn}(\mathbf{g})\,\mathbf{g}$$

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

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

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

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

•Eigenstates (shown before)

•Complete Hamiltonian

$$\begin{pmatrix} \boxed{H+r_1+r_2+i_1+i_2+i_3} & & & \\ & \boxed{H+r_1+r_2-i_1-i_2-i_3} & & \\ & & H-\frac{1}{2}r_1-\frac{1}{2}r_2-\frac{1}{2}i_1-\frac{1}{2}i_2+i_3 & \frac{\sqrt{3}}{2}(-r_1+r_2-i_1+i_2) \\ & & \frac{\sqrt{3}}{2}(+r_1-r_2-i_1+i_2) & H-\frac{1}{2}r_1-\frac{1}{2}r_2+\frac{1}{2}i_1+\frac{1}{2}i_2-i_3 \end{pmatrix}$$

A_1-block

A_2-block

•Local symmetery eigenvalue formulae *(L.S.=> off-diagonal zero.)*

$r_1 = r_2 = r_1{}^* = r, \quad i_1 = i_2 = i_1{}^* = i$

gives:

A_1-level: $H + 2r + 2i + i_3$

A_1-level: $H + 2r - 2i - i_3$

E_x-level: $H - r - i + i_3$

E_y-level: $H - r + i - i_3$

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

Global (LAB) symmetry

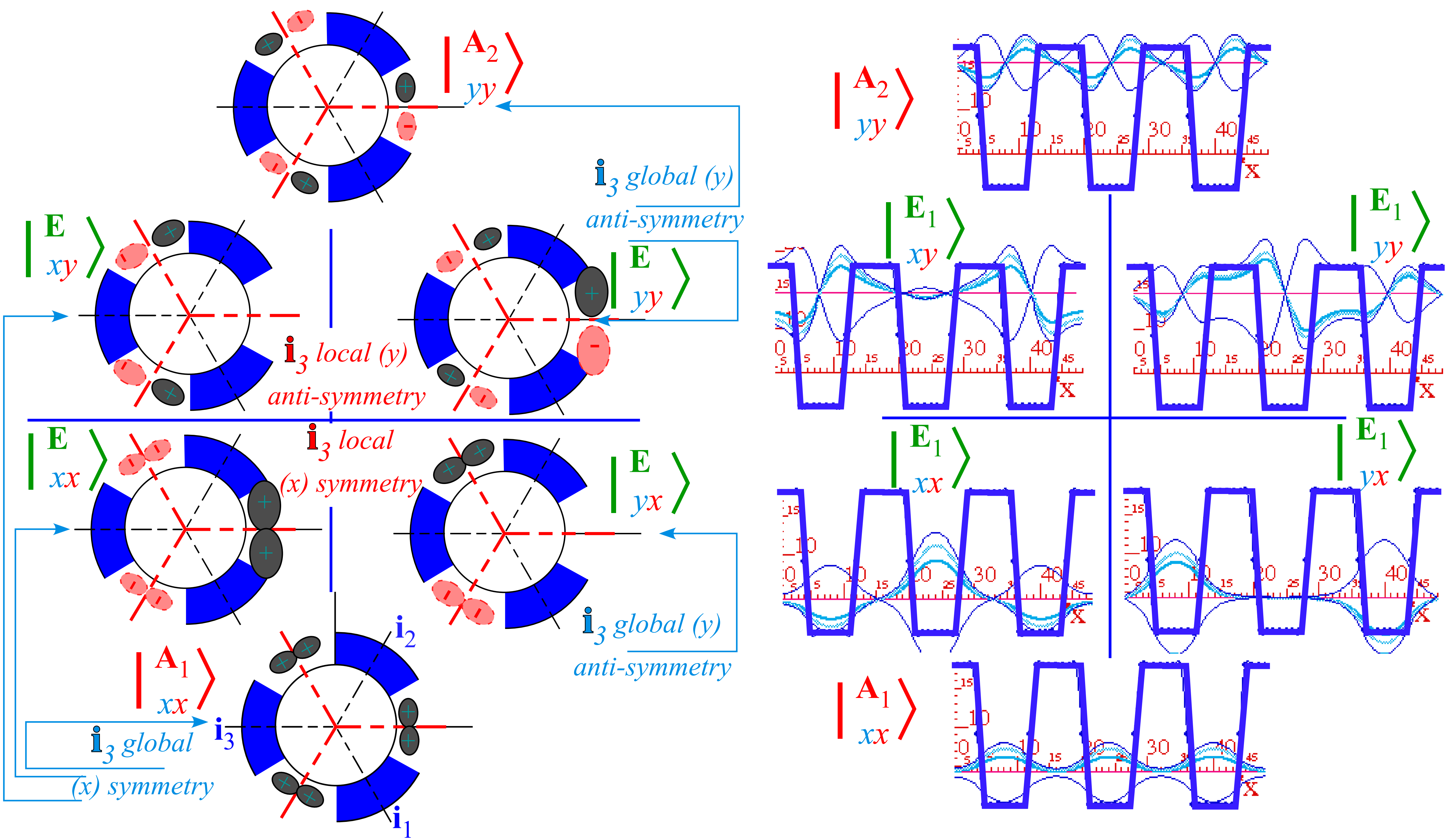
$$\mathbf{i}_3|{}^{(m)}_{eb}\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}|1\rangle = (-1)^e\,|{}^{(m)}\rangle$$

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

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

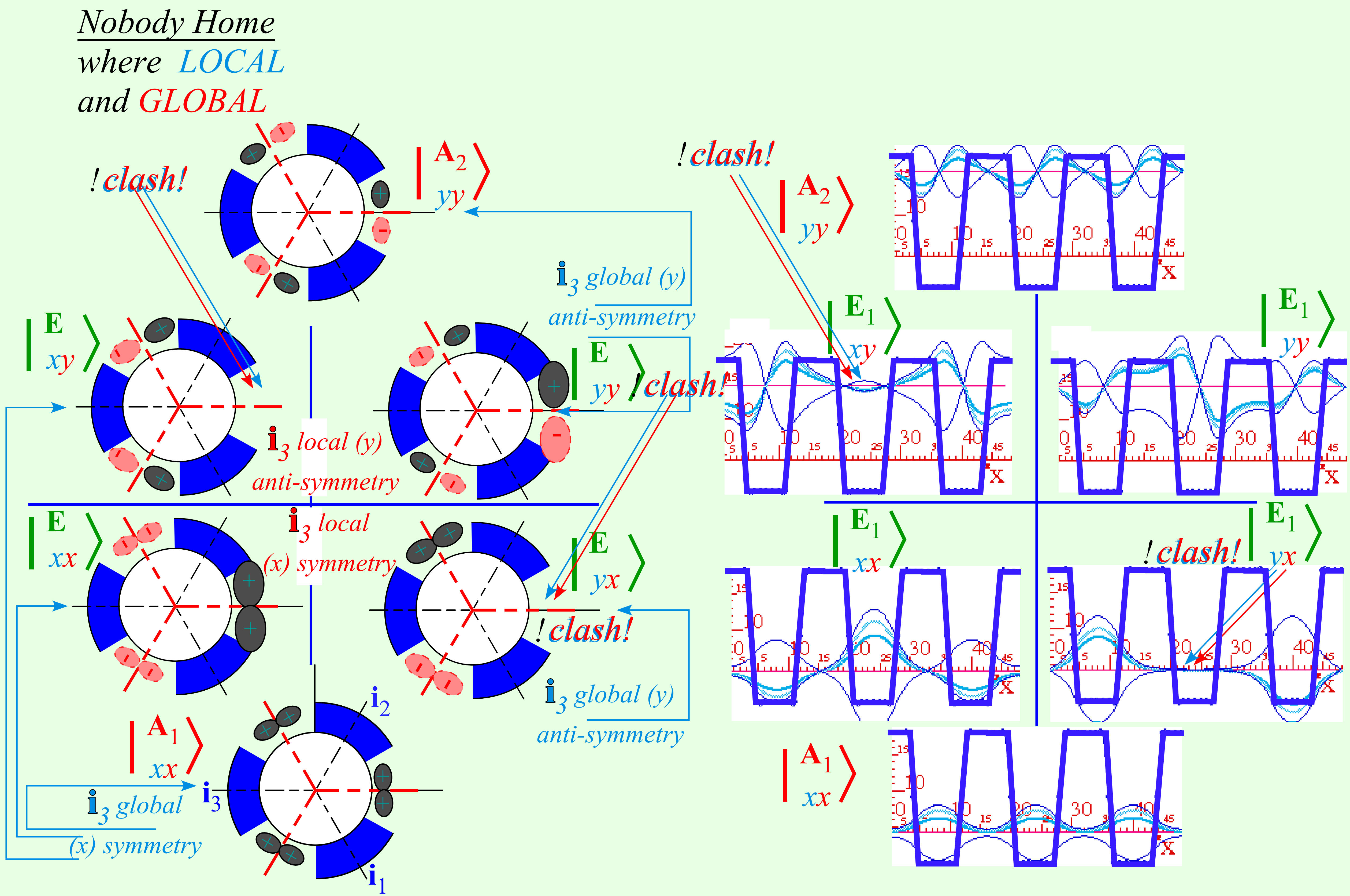
Local (BOD) symmetry

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



Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

When there is no there, there...



AMOP reference links on page 2

2.26.18 class 13.0: *Symmetry Principles for Advanced Atomic-Molecular-Optical-Physics*

William G. Harter - University of Arkansas

Discrete symmetry subgroups of O(3) using Mock-Mach principle: $D_3 \sim C_{3v}$ LAB vs BOD group and projection operator formulation of ortho-complete eigensolutions

Review 1. *Global vs Local symmetry and Mock-Mach principle*

Review 2. *LAB-BOD (Global -Local) mutually commuting representations of* $D_3 \sim C_{3v}$

Review 3. *Global vs Local symmetry expansion of D_3 Hamiltonian*

Review 4. 1st-Stage: *Spectral resolution of **D_3 Center** (All-commuting class projectors and characters)*

Review 5. 2nd-Stage: $D_3 \supset C_2$ *or* $D_3 \supset C_3$ *sub-group-chain projectors split class projectors* $\mathbf{P}^E = \mathbf{P}^E_{11} + \mathbf{P}^E_{22}$ *with*: $\mathbf{1} = \Sigma \mathbf{P}^\alpha_{jj}$

Review 6. 3rd-Stage: $\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1}$ *trick gives nilpotent projectors* $\mathbf{P}^E_{12} = (\mathbf{P}^E_{21})^\dagger$ *and Weyl* **g**-*expansion:* $\mathbf{g} = \Sigma D^\alpha_{ij}(\mathbf{g}) \mathbf{P}^\alpha_{ij}$.

Deriving diagonal and off-diagonal projectors $\mathbf{P}_{ab}^E$ and ireps D_{ab}^E

Comparison: Global vs Local $|\mathbf{g}\rangle$-basis versus Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis

General formulae for spectral decomposition (D_3 examples)

*Weyl **g**-expansion in irep $D^\mu_{jk}(g)$ and projectors $\mathbf{P}^\mu_{jk}$*

$\mathbf{P}^\mu_{jk}$ transforms left and right

*$\mathbf{P}^\mu_{jk}$ -expansion in **g**-operators: Inverse of Weyl form*

D_3 Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

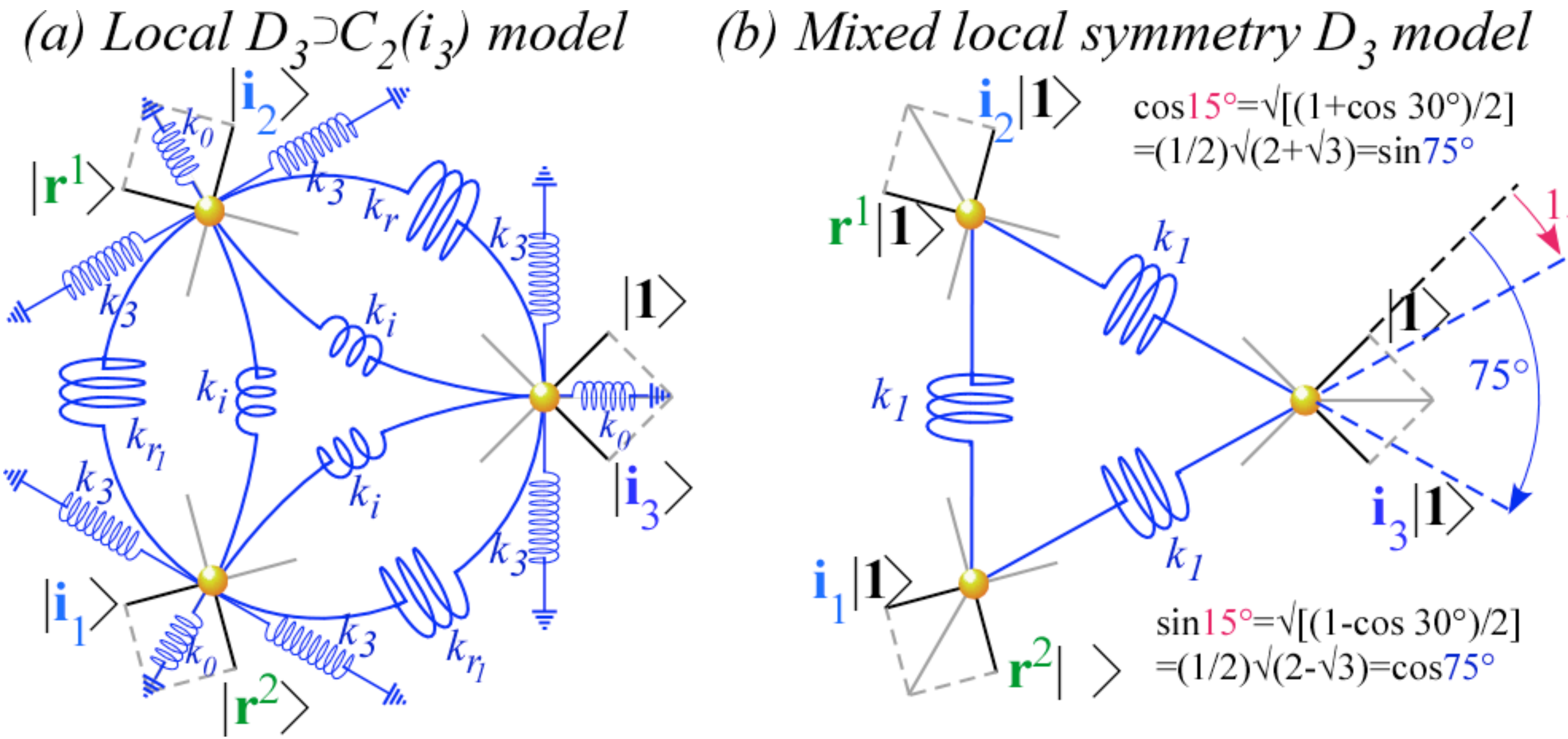
*$|\mathbf{P}^{(\mu)}\rangle$-basis D_3 global-**g** matrix structure versus D_3 local-$\bar{\mathbf{g}}$ matrix structure*

Local vs global x-symmetry and y-antisymmetry D_3 tunneling band theory

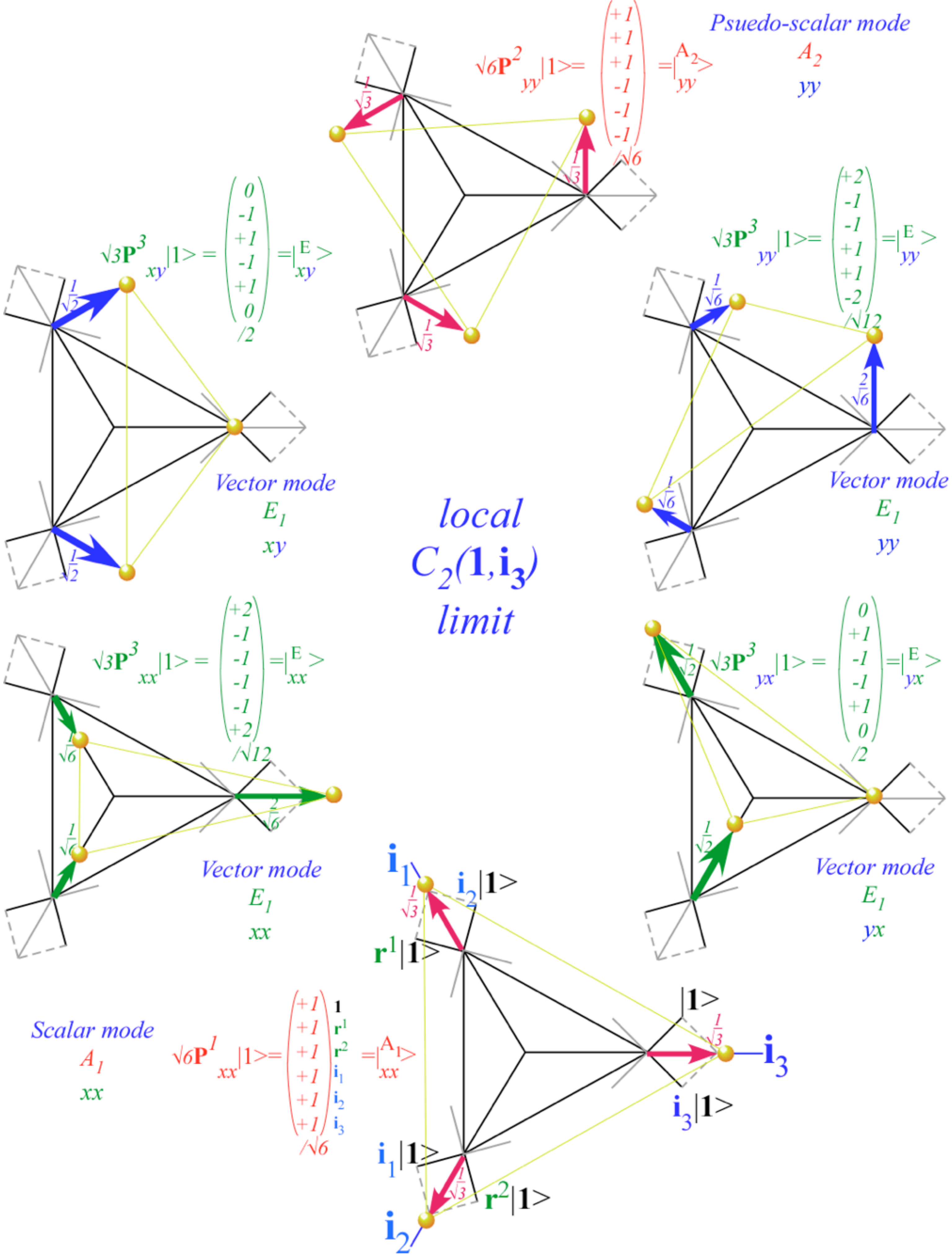
Ortho-complete D_3 parameter analysis of eigensolutions

Classical analog for bands of vibration modes

Classical analog for bands of vibration modes



Classical analog for vibration modes



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