Group Theory in Quantum Mechanics

Lecture 16 (3.19.15)

Local-symmetry eigensolutions and wave modes

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 5 Ch. 15)
(PSDS - Ch. 4)

Review Stage 1: Group Center: Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$, characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

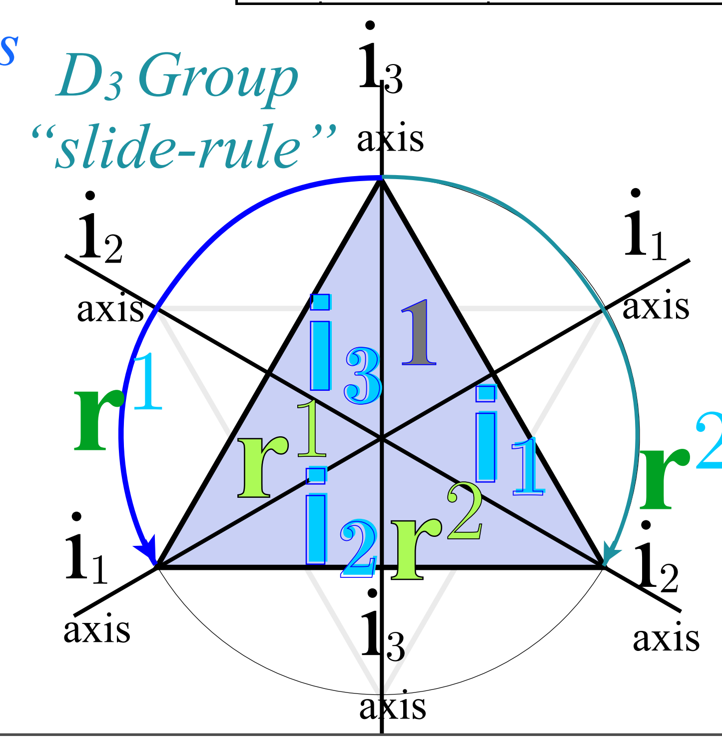
Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

- Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$
- $\mathbf{P}^{\mu}{}_{jk}$ transforms right-and-left
- $\mathbf{P}^{\mu}{}_{jk}$ -expansion in $\mathbf{g}$-operators
- Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^1)$

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

Details of Mock-Mach relativity-duality for D_3 groups and representations
- Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)
- Compare Global vs Local $|\mathbf{g}\rangle$-basis and Global vs Local $|\mathbf{P}^{(\mu)}\rangle$-basis



Hamiltonian and D_3 group matrices in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis
- Global vs. Local block rearrangement
- Hamiltonion eigen-matrix calculation
- Hamiltonian local-symmetry eigensolution
- (Vibrations treated in following Lecture 17)

Review Stage 1: Group Center:Class-sums κ_g ,characters $\chi^\mu(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^\mu$

*Review Stage 2: Group operators **g** and Mutually-Commuting projectors $\mathbf{P}^\mu_{kk}$*

*Review Stage 3: Weyl **g**-expansion in irreps $D^\mu_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^\mu_{jk}$*

Simple matrix algebra $\mathbf{P}^\mu_{ab}\mathbf{P}^\nu_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^\mu_{ad}$

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Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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$$\boldsymbol{\kappa}_{\mathbf{g}} = \sum_{\mu} \frac{{}^{\circ}\kappa_{g}\chi_{g}^{\mu}}{\ell^{\mu}} \mathbb{P}^{\mu}$$

$$\mathbb{P}^{\mu} = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G} \chi_{g}^{\mu *} \boldsymbol{\kappa}_{\mathbf{g}}$$

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Characters: $\chi_{g}^{\mu} \equiv TrD^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{h}\mathbf{g}\mathbf{h}^{-1})$

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See Lect.15 p. 20

$$\boldsymbol{\kappa}_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbb{P}^{E}$$

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

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

Use $\chi_{\mathbf{g}}^{A_1 *} = \ell^{A_1} = 1$

to find $\mathbf{P}^{A_1}$ *coefficients*

$\kappa_{\mathbf{g}} = {}^{\circ}\kappa_{g}\mathbf{P}^{A_1} + \ldots$

D_3 examples

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Use $\chi_{\mathbf{g}}^{A_1 *} = \ell^{A_1} = 1$

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$\kappa_{\mathbf{g}} = {}^{\circ}\kappa_g \mathbf{P}^{A_1} + \ldots$

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

See Lect.15 p. 23-24

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

Use $\chi_{\mathbf{1}}^{(\alpha)*} = \ell^{(\alpha)}$

to find $\kappa_{\mathbf{1}}$ *coefficients*

$\mathbf{P}^{(\alpha)} = \frac{(\ell^{(\alpha)})^2}{{}^{\circ}G} \kappa_{\mathbf{1}} + \ldots$

D_3 examples

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$\mathbb{P}^{\mu} = \mathbf{P}^{\mu}{}_{11} + \mathbf{P}^{\mu}{}_{22} + \ldots \mathbf{P}^{\mu}{}_{\ell^{\mu}\ell^{\mu}}$ *(Mutually-commuting Projectors* $\mathbf{P}^{\mu}{}_{mm}$*)*

$\mathbb{P}^{\mu}$ *splits into a number* ℓ^{μ} *of irreducible* $\mathbf{P}^{\mu}{}_{jj}$ *where* ℓ^{μ}*=dimension of irrep* D^{μ}

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$\mathbb{P}^{\mu}$ *splits into a number ℓ^{μ} of irreducible $\mathbf{P}^{\mu}{}_{jj}$ where ℓ^{μ}=dimension of irrep D^{μ}*

and sum of ℓ^{μ} is RANK of D_3

$\mathbb{P}^{\mu}$ *splitting* NOT *unique if $\ell^{\mu} > 1$ ....*

Example:

The splittable all-commuting projector in D_3

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

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$\mathbb{P}^{\mu}$ *splitting* NOT *unique if* $\ell^{\mu} > 1$*....* ...OR...

Splitting by $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ *(See Lect.15 p. 80)*

$$\mathbf{P}^{E}_{0_2,0_2} = \mathbf{P}^{E}_{x,x} = \mathbb{P}^{E}(\mathbf{1} + \mathbf{i}_3)/2$$

$$\mathbf{P}^{E}_{1_2,1_2} = \mathbf{P}^{E}_{y,y} = \mathbb{P}^{E}(\mathbf{1} - \mathbf{i}_3)/2$$

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Product algebra on group table:

$(\mathbf{1}$ ... $\pm\mathbf{i}_3)/2$

$\left(\frac{1}{3}\right)$ rows $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$; $\left(\frac{1}{6}\right)$

$2\mathbf{1}$	r^2	r	i_1	i_2	$\pm 2\mathbf{i}_3$
$-\mathbf{r}$	1	r^2	i_3	i_1	$\mp\mathbf{i}_2$
$-\mathbf{r}^2$	r	1	i_2	i_3	$\mp\mathbf{i}_1$
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

Example:

The splittable all-commuting projector in D_3

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Product algebra on group table:

$(\mathbf{1}$ $\pm\mathbf{i}_3)/2$

$\left(\frac{1}{3}\right)$ $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$

$2\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\pm 2\mathbf{i}_3$
$-\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mp\mathbf{i}_2$
$-\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mp\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}$
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$\left(\frac{1}{6}\right)$

Example:

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

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$$\mathbb{P}^{\mu} = \sum_{classes\,\kappa_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G}\chi^{\mu*}_{g}\kappa_{\mathbf{g}}$$

Review Stage 2: Group operators **g** *and Mutually-Commuting projectors* $\mathbf{P}^{\mu}_{kk}$

$$\mathbb{P}^{\mu} = \mathbf{P}^{\mu}_{11} + \mathbf{P}^{\mu}_{22} + \ldots \mathbf{P}^{\mu}_{\ell^{\mu}\ell^{\mu}}$$

(Mutually-commuting Projectors $\mathbf{P}^{\mu}_{mm}$*)*

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$\mathbb{P}^{\mu}$ *splitting* NOT *unique if* $\ell^{\mu} > 1$ ....

Splitting by $C_2=\{\mathbf{1},\mathbf{i}_3\}$ *(See Lect.15 p. 80)*

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...OR...

Splitting by $C_3=\{\mathbf{1},\mathbf{r}^1,\mathbf{r}^2\}$ *(See Lect.15 p. 84)*

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

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

Product algebra on group table:

$(\mathbf{1} \pm \mathbf{i}_3)/2$ applied to $\left(\frac{1}{3}\right)(2\mathbf{1}, -\mathbf{r}, -\mathbf{r}^2)$, table factor $\left(\frac{1}{6}\right)$:

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

$\left[(2-\varepsilon-\varepsilon^*)\mathbf{1} + (2\varepsilon^*-1-\varepsilon)\mathbf{r} + (2\varepsilon-\varepsilon^*-1)\mathbf{r}^2\right]/3\cdot3$

applied to $\left(\frac{1}{3}\right)(2\mathbf{1}, -\mathbf{r}, -\mathbf{r}^2)$, table factor $\left(\frac{1}{3\cdot3}\right)$:

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

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$$\mathbb{P}^{\mu} = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G}\chi^{\mu *}_{g}\boldsymbol{\kappa}_{\mathbf{g}}$$

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$$\mathbb{P}^{\mu} = \mathbf{P}^{\mu}{}_{11} + \mathbf{P}^{\mu}{}_{22} + \ldots \mathbf{P}^{\mu}{}_{\ell^{\mu}\ell^{\mu}}$$ *(Mutually-commuting Projectors $\mathbf{P}^{\mu}{}_{mm}$)*

$\mathbb{P}^{\mu}$ *splits into a number ℓ^{μ} of irreducible $\mathbf{P}^{\mu}{}_{jj}$ where ℓ^{μ}=dimension of irrep D^{μ}* *and sum of ℓ^{μ} is RANK of D_3*

$\mathbb{P}^{\mu}$ *splitting* NOT *unique if $\ell^{\mu} > 1$....* ...OR...

Splitting by $C_2=\{\mathbf{1},\mathbf{i}_3\}$ (*See Lect.15 p. 80*)

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

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

Splitting by $C_3=\{\mathbf{1},\mathbf{r}^1,\mathbf{r}^2\}$ (*See Lect.15 p. 84*)

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

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

Product algebra on group table:

$(\mathbf{1}$ ... $\pm\mathbf{i}_3)/2$, rows multiplied by $\left(\frac{1}{3}\right)$: $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$; overall factor $\left(\frac{1}{6}\right)$

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

$$\left[(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{1} + \varepsilon^*(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{r} + \varepsilon(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{r}^2\right]/3\cdot 3$$

$$\left[(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{1} + (2\varepsilon^*\text{-}1\text{-}\varepsilon)\mathbf{r} + (2\varepsilon\text{-}\varepsilon^*\text{-}1)\mathbf{r}^2\right]/3\cdot 3$$

Rows multiplied by $\left(\frac{1}{3}\right)$: $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$; overall factor $\left(\frac{1}{3\cdot 3}\right)$

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

Example:
The splittable all-commuting projector in D_3

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

Review Stage 1: Group Center: Class-sums κ_g, characters $\chi^\mu(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^\mu$

$$\boldsymbol{\kappa}_\mathbf{g} = \sum_\mu \frac{{}^\circ\kappa_g \chi^\mu_g}{\ell^\mu} \mathbb{P}^\mu$$

Characters: $\chi^\mu_g \equiv TrD^\mu(\mathbf{g}) = \chi^\mu(\mathbf{g}) = \chi^\mu(\mathbf{hgh}^{-1})$

$$\mathbb{P}^\mu = \sum_{classes\,\boldsymbol{\kappa}_\mathbf{g}} \frac{\ell^\mu}{{}^\circ G} \chi^{\mu *}_g \boldsymbol{\kappa}_\mathbf{g}$$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^\mu{}_{kk}$

$\mathbb{P}^\mu = \mathbf{P}^\mu{}_{11} + \mathbf{P}^\mu{}_{22} + \ldots\ \mathbf{P}^\mu{}_{\ell^\mu \ell^\mu}$ *(Mutually-commuting Projectors $\mathbf{P}^\mu{}_{mm}$)*

$\mathbb{P}^\mu$ *splits into a number ℓ^μ of irreducible $\mathbf{P}^\mu{}_{jj}$ where ℓ^μ=dimension of irrep D^μ and sum of ℓ^μ is RANK of D_3*

$\mathbb{P}^\mu$ *splitting* NOT *unique if $\ell^\mu > 1$....*

Splitting by $C_2=\{\mathbf{1},\mathbf{i}_3\}$ (*See Lect.15 p. 80*)

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

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

...OR...

Splitting by $C_3=\{\mathbf{1},\mathbf{r}^1,\mathbf{r}^2\}$ (*See Lect.15 p. 84*)

$$\mathbf{P}^E_{1_3,1_3} = \mathbf{P}^E_{+1_3,+1_3} = \mathbb{P}^E(\mathbf{1}+\varepsilon\,\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/3 = (\mathbf{1}+\varepsilon\,\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/3$$

$$\mathbf{P}^E_{2_3,2_3} = \mathbf{P}^E_{-1_3,-1_3} = \mathbb{P}^E(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\,\mathbf{r}^2)/3 = (\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\,\mathbf{r}^2)/3$$

$$\left[(3)\mathbf{1} + \varepsilon^*(3)\mathbf{r} + \varepsilon(3)\mathbf{r}^2\right]/3\cdot3$$

$$\left[(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{1} + \varepsilon^*(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{r} + \varepsilon(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{r}^2\right]/3\cdot3$$

$$\left[(2\text{-}\varepsilon\text{-}\varepsilon^*)\mathbf{1} + (2\varepsilon^*\text{-}1\text{-}\varepsilon)\mathbf{r} + (2\varepsilon\text{-}\varepsilon^*\text{-}1)\mathbf{r}^2\right]/3\cdot3$$

Product algebra on group table:

$(\mathbf{1} \quad \pm\mathbf{i}_3)/2$

Left row factors: $\left(\frac{1}{3}\right)$ $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$; right factor $\left(\frac{1}{6}\right)$

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

Left row factors: $\left(\frac{1}{3}\right)$ $2\mathbf{1}$, $-\mathbf{r}$, $-\mathbf{r}^2$; right factor $\left(\frac{1}{3\cdot3}\right)$

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

Example:
The splittable all-commuting projector in D_3

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

*Review Stage 2: Group operators **g** and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$*

*Review Stage 3: Weyl **g**-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$*

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

Review Stage 1: Group Center: Class-sums κ_g, characters $\chi^\mu(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^\mu$

$$\boldsymbol{\kappa}_{\mathbf{g}} = \sum_{\mu} \frac{{}^\circ\kappa_g \chi_g^\mu}{\ell^\mu} \mathbb{P}^\mu$$

Characters: $\chi_g^\mu \equiv TrD^\mu(\mathbf{g}) = \chi^\mu(\mathbf{g}) = \chi^\mu(\mathbf{hgh}^{-1})$

$$\mathbb{P}^\mu = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^\mu}{{}^\circ G} \chi_g^{\mu *} \boldsymbol{\kappa}_{\mathbf{g}}$$

*Review Stage 2: Group operators **g** and Mutually-Commuting projectors $\mathbf{P}^\mu{}_{kk}$*

$\mathbb{P}^\mu = \mathbf{P}^\mu{}_{11} + \mathbf{P}^\mu{}_{22} + \ldots\ \mathbf{P}^\mu{}_{\ell^\mu \ell^\mu}$ *(Mutually-commuting Projectors $\mathbf{P}^\mu{}_{mm}$)*

$\mathbb{P}^\mu$ *splits into a number ℓ^μ of irreducible $\mathbf{P}^\mu{}_{jj}$ where ℓ^μ=dimension of irrep D^μ*

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*Group **g**-expansion in Projectors $\mathbf{P}^\mu{}_{mn}$*

*Projector $\mathbf{P}^\mu{}_{mn}$ expansion in Group **g***

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$ *,characters* $\chi^{\mu}(\mathbf{g})$*, and All-Commuting Projectors* $\mathbb{P}^{\mu}$

$$\boldsymbol{\kappa}_{\mathbf{g}} = \sum_{\mu} \frac{{}^{\circ}\kappa_{g}\chi_{g}^{\mu}}{\ell^{\mu}} \mathbb{P}^{\mu}$$

Characters: $\chi_{g}^{\mu} \equiv TrD^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{h}\mathbf{g}\mathbf{h}^{-1})$

$$\mathbb{P}^{\mu} = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G}\chi_{g}^{\mu *}\boldsymbol{\kappa}_{\mathbf{g}}$$

Review Stage 2: Group operators $\mathbf{g}$ *and Mutually-Commuting projectors* $\mathbf{P}^{\mu}{}_{kk}$

$$\mathbb{P}^{\mu} = \mathbf{P}^{\mu}{}_{11} + \mathbf{P}^{\mu}{}_{22} + \ldots \mathbf{P}^{\mu}{}_{\ell^{\mu}\ell^{\mu}}$$ *(Mutually-commuting Projectors* $\mathbf{P}^{\mu}{}_{mm}$*)*

$\mathbb{P}^{\mu}$ *splits into a number* ℓ^{μ} *of irreducible* $\mathbf{P}^{\mu}{}_{jj}$ *where* ℓ^{μ}*=dimension of irrep* D^{μ}

Review Stage 3: Weyl $\mathbf{g}$*-expansion in irreps* $D^{\mu}{}_{jk}(g)$ *and Non-Commuting projectors* $\mathbf{P}^{\mu}{}_{jk}$

Group $\mathbf{g}$*-expansion in Projectors* $\mathbf{P}^{\mu}{}_{mn}$

Projector $\mathbf{P}^{\mu}{}_{mn}$ *expansion in Group* $\mathbf{g}$

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

The $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$ *development:*

(Lecture 15 p. 90-97)

Weyl development follows...

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

$$\begin{aligned}\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}=&\ \mathbf{P}_{x,x}^{A_1}\cdot\mathbf{g}\cdot\mathbf{P}_{x,x}^{A_1} + 0 + 0 + 0\\ &+ 0 + \mathbf{P}_{y,y}^{A_2}\cdot\mathbf{g}\cdot\mathbf{P}_{y,y}^{A_2} + 0 + 0\\ &+ 0 + 0 + \mathbf{P}_{x,x}^{E}\cdot\mathbf{g}\cdot\mathbf{P}_{x,x}^{E} + \mathbf{P}_{x,x}^{E}\cdot\mathbf{g}\cdot\mathbf{P}_{y,y}^{E}\\ &+ 0 + 0 + \mathbf{P}_{y,y}^{E}\cdot\mathbf{g}\cdot\mathbf{P}_{x,x}^{E} + \mathbf{P}_{y,y}^{E}\cdot\mathbf{g}\cdot\mathbf{P}_{y,y}^{E}\end{aligned}$$

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

$$\boldsymbol{\kappa}_{\mathbf{g}} = \sum_{\mu} \frac{{}^{\circ}\kappa_{g}\chi^{\mu}_{g}}{\ell^{\mu}} \mathbb{P}^{\mu}$$

Characters: $\chi^{\mu}_{g} \equiv TrD^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{g}) = \chi^{\mu}(\mathbf{hgh}^{-1})$

$$\mathbb{P}^{\mu} = \sum_{classes\,\boldsymbol{\kappa}_{\mathbf{g}}} \frac{\ell^{\mu}}{{}^{\circ}G}\chi^{\mu *}_{g}\boldsymbol{\kappa}_{\mathbf{g}}$$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

$\mathbb{P}^{\mu} = \mathbf{P}^{\mu}{}_{11} + \mathbf{P}^{\mu}{}_{22} + \ldots \mathbf{P}^{\mu}{}_{\ell^{\mu}\ell^{\mu}}$ *(Mutually-commuting Projectors $\mathbf{P}^{\mu}{}_{mm}$)*

$\mathbb{P}^{\mu}$ *splits into a number ℓ^{μ} of irreducible $\mathbf{P}^{\mu}{}_{jj}$ where ℓ^{μ}=dimension of irrep D^{μ}*

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Group $\mathbf{g}$-expansion in Projectors $\mathbf{P}^{\mu}{}_{mn}$

Projector $\mathbf{P}^{\mu}{}_{mn}$ expansion in Group $\mathbf{g}$

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

The $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$ development:

(Lecture 15 p. 90-97)

Weyl development follows...

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

$$\begin{aligned}
\mathbf{g} = \mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1} = {} & D^{A_1}(\mathbf{g})\mathbf{P}^{A_1}_{x,x} + 0 + 0 + 0 \\
& + 0 + D^{A_2}(\mathbf{g})\mathbf{P}^{A_2}_{y,y} + 0 + 0 \\
& + 0 + 0 + D^{E}_{x,x}(\mathbf{g})\mathbf{P}^{E}_{x,x} + D^{E}_{x,y}(\mathbf{g})\mathbf{P}^{E}_{x,y} \\
& + 0 + 0 + D^{E}_{y,x}(\mathbf{g})\mathbf{P}^{E}_{y,x} + D^{E}_{y,y}(\mathbf{g})\mathbf{P}^{E}_{y,y}
\end{aligned}$$

where:

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

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

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$ *,characters* $\chi^{\mu}(\mathbf{g})$*, and All-Commuting Projectors* $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ *and Mutually-Commuting projectors* $\mathbf{P}^{\mu}{}_{kk}$

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➡ *Simple matrix algebra* $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$ ⬅

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

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

Example of D_3 *transformation by matrix* $D^{E}{}_{jk}(\mathbf{r}^1)$

Details of Mock-Mach relativity-duality for D_3 *groups and representations*

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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

"g-equals-1·g·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* $\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}$

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

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*

where:

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

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

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

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

there arise two *nilpotent* projectors $\mathbf{P}^{E_1}_{yx}$, and $\mathbf{P}^{E_1}_{xy}$

Group product table boils down to simple projector matrix algebra

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

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

Generalizes to idempotent/nilpotent orthogonality known as Simple Matrix Algebra:

$$\mathbf{P}^{\mu}_{jk}\mathbf{P}^{\nu}_{mn}=\delta^{\mu\nu}\delta_{km}\mathbf{P}^{\mu}_{jn}$$

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

*Review Stage 2: Group operators **g** and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$*

*Review Stage 3: Weyl **g**-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$*

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^1)$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" 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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$$|\,norm.|^2 = \left\langle \mathbf{1} \right| \mathbf{P}^{\mu}_{nn} \left| \mathbf{1} \right\rangle$$

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A simple irep expression...

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

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A simple irep expression...

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

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

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ *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 $\mathbf{P}^{\mu}{}_{mn}$.

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

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

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

(Simple matrix algebra)

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

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

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 conjugate irep expression...

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

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

if D is unitary

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

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

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

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

$\mathbf{P}^{\mu}{}_{jk}$ *-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: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{°G} p^{\mu}_{mn}(g)\, \mathbf{g}$

$\mathbf{P}^{\mu}{}_{jk}$ *-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 $G = \{\mathbf{1}, \ldots, \mathbf{f}, \mathbf{g}, \mathbf{h}, \ldots\}$:

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

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

Regular representation of $D_3 \sim C_{3v}$ in the group-$|\mathbf{g}\rangle$ basis

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ -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: $\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\,\mathbf{g}$

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

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

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

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

Regular representation of $D_3 \sim C_{3v}$ in the group-$|\mathbf{g}\rangle$ basis

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

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

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

$\mathbf{P}^{\mu}{}_{jk}$ -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 **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**)*= $°G$

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

Regular representation of $D_3 \sim C_{3v}$ in the group-$|\mathbf{g}\rangle$ basis

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

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

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

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**)*= $^\circ G$

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

Regular representation of $D_3 \sim C_{3v}$ in the group-$|\mathbf{g}\rangle$ basis

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

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

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

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 **f** in group $G = \{\mathbf{1}, \ldots, \mathbf{f}, \mathbf{g}, \mathbf{h}, \ldots\}$:

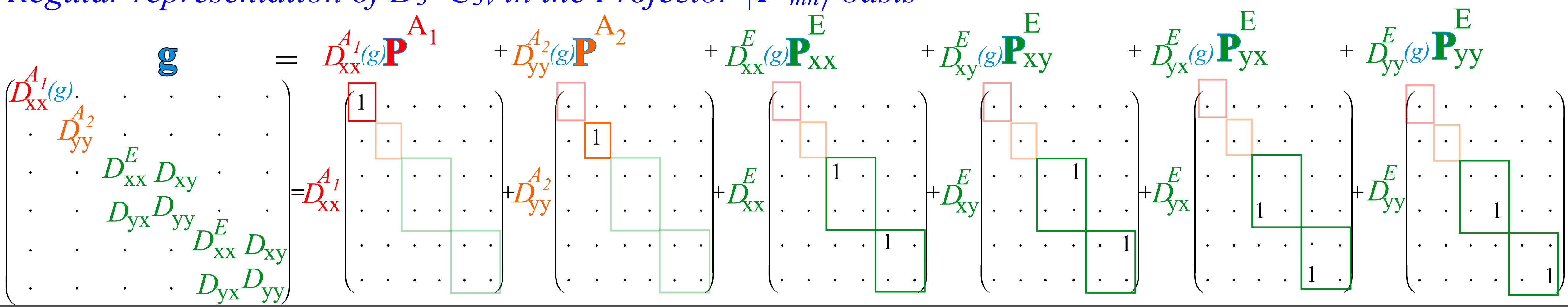
$$\mathbf{f}\cdot\mathbf{P}^{\mu}_{mn} = \sum_{\mathbf{g}}^{\circ G} p^{\mu}_{mn}(g)\, \mathbf{f}\cdot\mathbf{g} = \sum_{\mathbf{h}}^{\circ G} p^{\mu}_{mn}\left(\mathbf{f}^{-1}\mathbf{h}\right) \mathbf{h} \quad \text{, where: } \mathbf{h} = \mathbf{f}\cdot\mathbf{g}, \text{ or: } \mathbf{g} = \mathbf{f}^{-1}\mathbf{h},$$

Regular representation *TraceR(**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:

Regular representation of $D_3 \sim C_{3v}$ in the Projector-$|\mathbf{P}^{\mu}{}_{mn}\rangle$ basis



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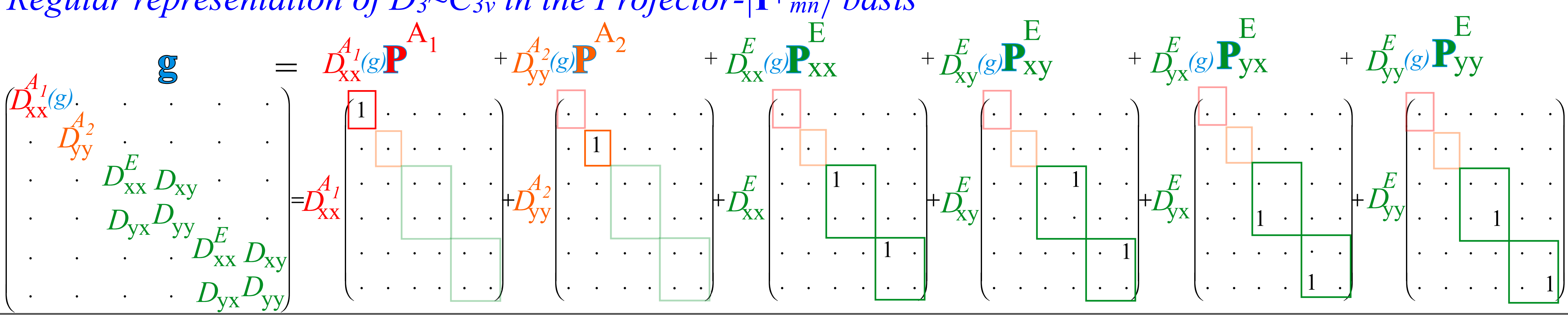
$$Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$$

Regular representation of $D_3 \sim C_{3v}$ in the Projector-$|\mathbf{P}^{\mu}{}_{mn}\rangle$ basis



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

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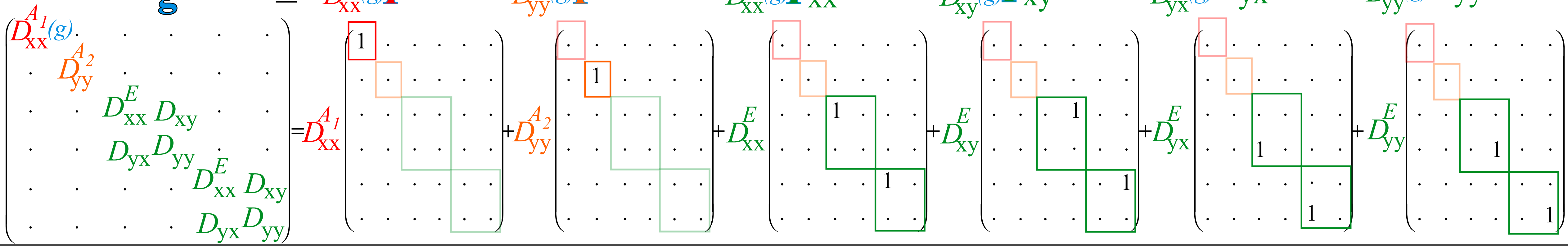
$$Trace\ R(\mathbf{P}^{\mu}_{mn}) = \delta_{mn}\ell^{(\mu)}$$

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

Regular representation of $D_3 \sim C_{3v}$ *in the Projector-*$|\mathbf{P}^{\mu}{}_{mn}\rangle$ *basis*

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



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

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

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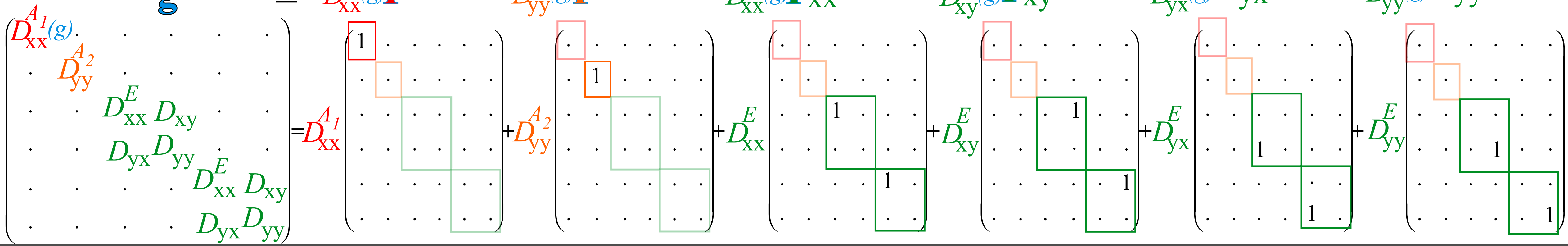
$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$



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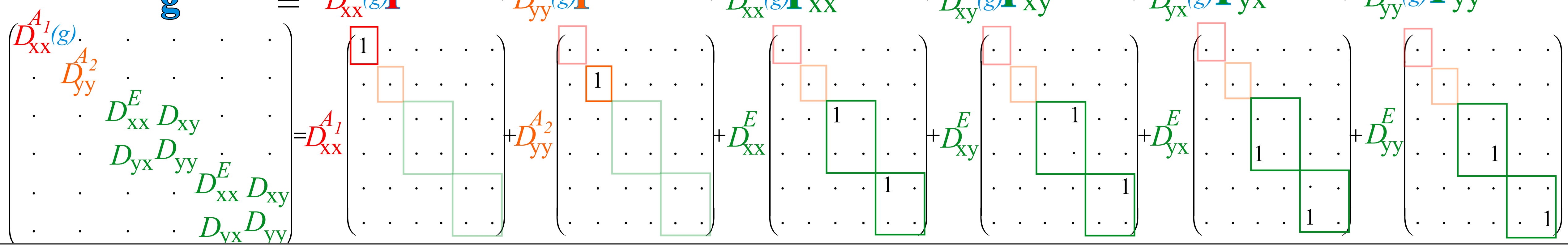
$$\mathbf{g} = D^{A_1}_{xx}(g)\mathbf{P}^{A_1} + D^{A_2}_{yy}(g)\mathbf{P}^{A_2} + D^{E}_{xx}(g)\mathbf{P}^{E}_{xx} + D^{E}_{xy}(g)\mathbf{P}^{E}_{xy} + D^{E}_{yx}(g)\mathbf{P}^{E}_{yx} + D^{E}_{yy}(g)\mathbf{P}^{E}_{yy}$$



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

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

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

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

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

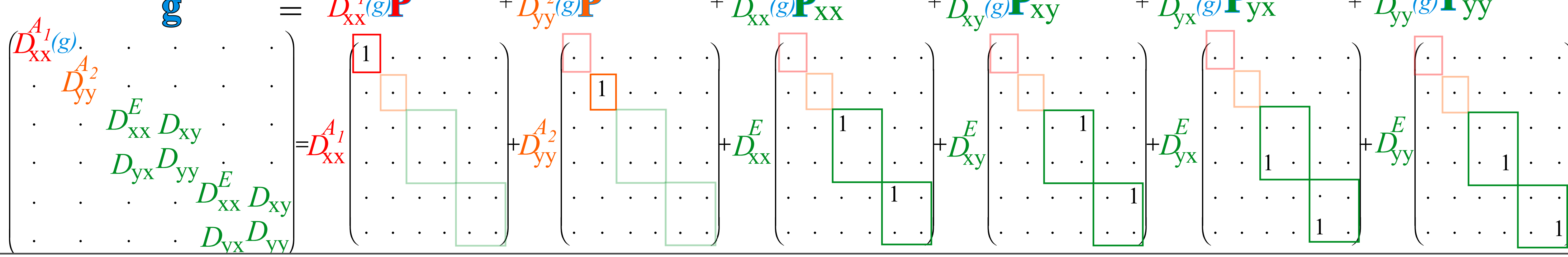
Solving for $p^{\mu}_{mn}(g)$: $\quad p^{\mu}_{mn}(\mathbf{f}) = \frac{1}{°G} Trace\, R\left(\mathbf{f}^{-1}\cdot\mathbf{P}^{\mu}_{mn}\right)$

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

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

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

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



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

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

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

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

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

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

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

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

$$\mathbf{P}^{\mu}_{mn} = \frac{\ell^{(\mu)}}{°G} \sum_{\mathbf{g}}^{°G} D^{\mu}_{nm}(g^{-1})\, \mathbf{g}$$

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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*($\mathbf{P}^{\mu}_{mn}$) is irep dimension $\ell^{(\mu)}$ for diagonal $\mathbf{P}^{\mu}_{mm}$ or *0* for off-diagonal $\mathbf{P}^{\mu}_{mn}$

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

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

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

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

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

Review Stage 1: Group Center:Class-sums $\boldsymbol{\kappa}_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

*Review Stage 2: Group operators **g** and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$*

*Review Stage 3: Weyl **g**-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$*

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

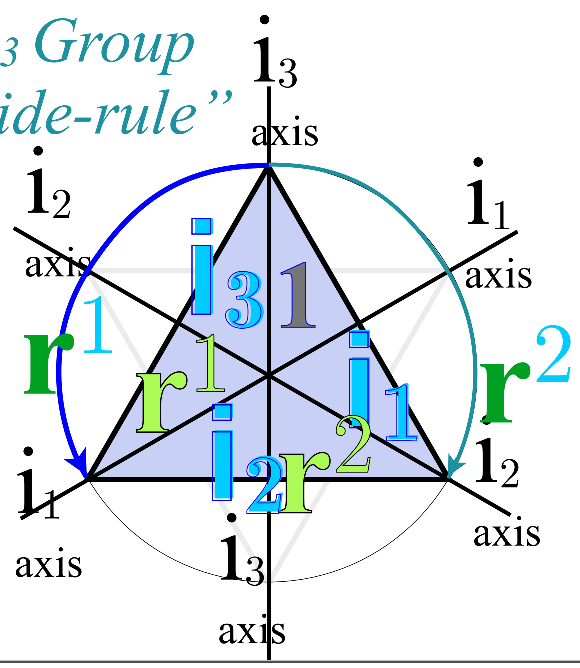
Local symmetry limit

Global symmetry limit (free or "genuine" modes)

Example of D_3 transformation by matrix $D^{E}_{jk}(\mathbf{r}^1)$

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1\left(\mathbf{1}-\tfrac{1}{2}\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{i}_2+\mathbf{i}_3\right)\left|\mathbf{1}\right\rangle/\sqrt{3}$$ given: $norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$

D_3 Group "slide-rule"



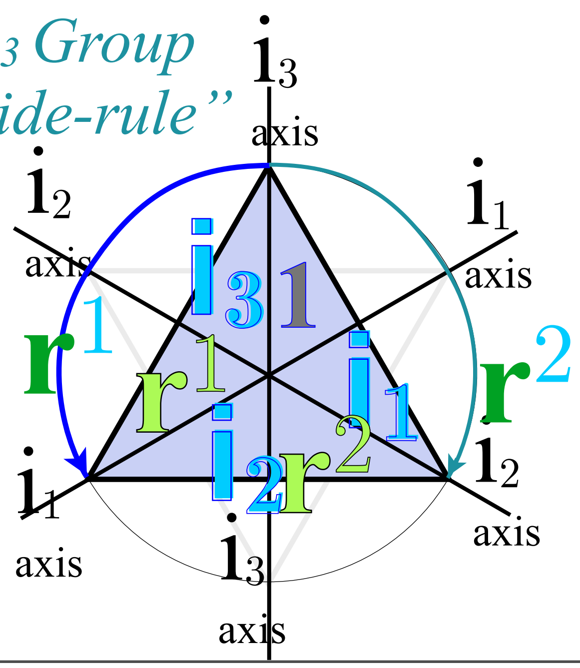
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

Example of D_3 transformation by matrix $D^E_{jk}(\mathbf{r}^1)$

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1(\mathbf{1}-\tfrac{1}{2}\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{i}_2+\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} \quad \text{given: } norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$$

$$= (\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{1}-\tfrac{1}{2}\mathbf{i}_3-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

D_3 Group "slide-rule"



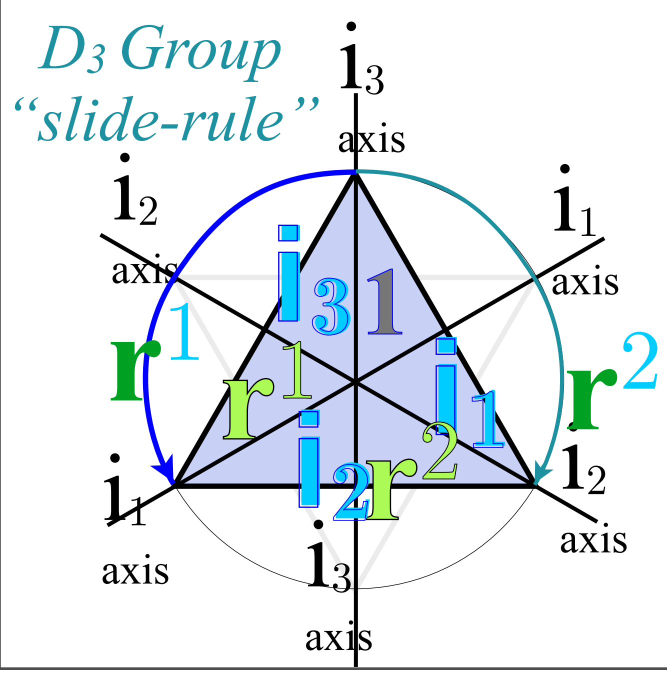
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

Example of D_3 transformation by matrix $D^E_{jk}(\mathbf{r}^1)$

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1(\mathbf{1}-\tfrac{1}{2}\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{i}_2+\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} \quad \text{given: } norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^{\circ}G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$$

$$= (\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{1}-\tfrac{1}{2}\mathbf{i}_3-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

$$= \mathbf{r}^1\begin{pmatrix}1\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\1\end{pmatrix}\frac{1}{\sqrt{3}} = (-\tfrac{1}{2}\mathbf{1}+\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2-\tfrac{1}{2}\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix}-\frac{1}{2}\\1\\-\frac{1}{2}\\-\frac{1}{2}\\1\\-\frac{1}{2}\end{pmatrix}\frac{1}{\sqrt{3}}$$



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

Example of D_3 transformation by matrix $D^{E}_{jk}(\mathbf{r}^1)$

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1\left(\mathbf{1} - \tfrac{1}{2}\mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{i}_1 - \tfrac{1}{2}\mathbf{i}_2 + \mathbf{i}_3\right)\left|\mathbf{1}\right\rangle/\sqrt{3} \quad \text{given: } norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$$

$$= \left(\mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{1} - \tfrac{1}{2}\mathbf{i}_3 - \tfrac{1}{2}\mathbf{i}_1 + \mathbf{i}_2\right)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

$$= \mathbf{r}^1\begin{pmatrix} 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 1 \end{pmatrix}\frac{1}{\sqrt{3}} = \left(-\tfrac{1}{2}\mathbf{1} + \mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{i}_1 + \mathbf{i}_2 - \tfrac{1}{2}\mathbf{i}_3\right)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix} -\frac{1}{2} \\ 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix}\frac{1}{\sqrt{3}}$$

$$\left|\mathbf{P}^{E_1}_{21}\right\rangle = \mathbf{P}^{E_1}_{21}\left|\mathbf{1}\right\rangle/\sqrt{3} = \left(0 + \tfrac{\sqrt{3}}{2}\mathbf{r}^1 - \tfrac{\sqrt{3}}{2}\mathbf{r}^2 - \tfrac{\sqrt{3}}{2}\mathbf{i}_1 + \tfrac{\sqrt{3}}{2}\mathbf{i}_2 + 0\right)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix} 0 \\ +\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ +\frac{1}{2} \\ 0 \end{pmatrix}$$

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

Example of D_3 transformation by matrix $D^{E}_{jk}(\mathbf{r}^1)$

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1\left(\mathbf{1} - \tfrac{1}{2}\mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{i}_1 - \tfrac{1}{2}\mathbf{i}_2 + \mathbf{i}_3\right)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

given: $norm^{E_1} = \sqrt{\dfrac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\dfrac{2}{6}} = \sqrt{\dfrac{1}{3}}$

$$= \left(\mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{1} - \tfrac{1}{2}\mathbf{i}_3 - \tfrac{1}{2}\mathbf{i}_1 + \mathbf{i}_2\right)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

$$= \mathbf{r}^1\begin{pmatrix} 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 1 \end{pmatrix}\frac{1}{\sqrt{3}} = \left(-\tfrac{1}{2}\mathbf{1} + \mathbf{r}^1 - \tfrac{1}{2}\mathbf{r}^2 - \tfrac{1}{2}\mathbf{i}_1 + \mathbf{i}_2 - \tfrac{1}{2}\mathbf{i}_3\right)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix} -\frac{1}{2} \\ 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 1 \\ -\frac{1}{2} \end{pmatrix}\frac{1}{\sqrt{3}}$$

- *product of this•that=* $\left\langle \mathbf{P}^{E_1}_{11}\right|\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \left(-\tfrac{1}{2} - \tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{4} - \tfrac{1}{2} - \tfrac{1}{2}\right)/\sqrt{3}\sqrt{3} = -\tfrac{3}{2}/3 = -1/2$

$$\left|\mathbf{P}^{E_1}_{21}\right\rangle = \mathbf{P}^{E_1}_{21}\left|\mathbf{1}\right\rangle/\sqrt{3} = \left(0 + \tfrac{\sqrt{3}}{2}\mathbf{r}^1 - \tfrac{\sqrt{3}}{2}\mathbf{r}^2 - \tfrac{\sqrt{3}}{2}\mathbf{i}_1 + \tfrac{\sqrt{3}}{2}\mathbf{i}_2 + 0\right)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix} 0 \\ +\frac{1}{2} \\ -\frac{1}{2} \\ -\frac{1}{2} \\ +\frac{1}{2} \\ 0 \end{pmatrix}$$

- *product of this•that=* $\left\langle \mathbf{P}^{E_1}_{21}\right|\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \left(0 + \tfrac{1}{2} + \tfrac{1}{4} + \tfrac{1}{4} + \tfrac{1}{2} + 0\right)/\sqrt{3} = \tfrac{3}{2}/\sqrt{3} = \sqrt{3}/2$

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

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1(\mathbf{1}-\tfrac{1}{2}\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{i}_2+\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} \quad norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$$

$$= (\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{1}-\tfrac{1}{2}\mathbf{i}_3-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

$$= \mathbf{r}^1\begin{pmatrix}1\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\1\end{pmatrix}\frac{1}{\sqrt{3}} = (-\tfrac{1}{2}\mathbf{1}+\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2-\tfrac{1}{2}\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix}-\frac{1}{2}\\1\\-\frac{1}{2}\\-\frac{1}{2}\\1\\-\frac{1}{2}\end{pmatrix}\frac{1}{\sqrt{3}} = -\frac{1}{2}\begin{pmatrix}1\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\1\end{pmatrix}\frac{1}{\sqrt{3}} + \frac{\sqrt{3}}{2}\begin{pmatrix}0\\+\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\+\frac{1}{2}\\0\end{pmatrix}$$

- *product of this•that*= $\left\langle\mathbf{P}^{E_1}_{11}\middle|\mathbf{r}^1\middle|\mathbf{P}^{E_1}_{11}\right\rangle = (-\tfrac{1}{2}-\tfrac{1}{2}+\tfrac{1}{4}+\tfrac{1}{4}-\tfrac{1}{2}-\tfrac{1}{2})/\sqrt{3}\sqrt{3} = -\tfrac{3}{2}/3 = -1/2 = D^{E_1}_{11}(r^1)$

$$\left|\mathbf{P}^{E_1}_{21}\right\rangle = \mathbf{P}^{E_1}_{21}\left|\mathbf{1}\right\rangle/\sqrt{3} = (0+\tfrac{\sqrt{3}}{2}\mathbf{r}^1-\tfrac{\sqrt{3}}{2}\mathbf{r}^2-\tfrac{\sqrt{3}}{2}\mathbf{i}_1+\tfrac{\sqrt{3}}{2}\mathbf{i}_2+0)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix}0\\+\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\+\frac{1}{2}\\0\end{pmatrix}$$

- *product of this•that*= $\left\langle\mathbf{P}^{E_1}_{21}\middle|\mathbf{r}^1\middle|\mathbf{P}^{E_1}_{11}\right\rangle = (0+\tfrac{1}{2}+\tfrac{1}{4}+\tfrac{1}{4}+\tfrac{1}{2}+0)/\sqrt{3} = \tfrac{3}{2}/\sqrt{3} = \sqrt{3}/2 = D^{E_1}_{21}(r^1)$

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

$$\mathbf{r}^1\left|\mathbf{P}^{E_1}_{11}\right\rangle = \mathbf{r}^1\mathbf{P}^{E_1}_{11}\left|\mathbf{1}\right\rangle/\sqrt{3} = \mathbf{r}^1(\mathbf{1}-\tfrac{1}{2}\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1-\tfrac{1}{2}\mathbf{i}_2+\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} \qquad norm^{E_1} = \sqrt{\frac{\ell^{E_1}}{{}^\circ G}} = \sqrt{\frac{2}{6}} = \sqrt{\frac{1}{3}}$$

$$= (\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{1}-\tfrac{1}{2}\mathbf{i}_3-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2)\left|\mathbf{1}\right\rangle/\sqrt{3}$$

$$= \mathbf{r}^1\begin{pmatrix}1\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\1\end{pmatrix}\frac{1}{\sqrt{3}} = (-\tfrac{1}{2}\mathbf{1}+\mathbf{r}^1-\tfrac{1}{2}\mathbf{r}^2-\tfrac{1}{2}\mathbf{i}_1+\mathbf{i}_2-\tfrac{1}{2}\mathbf{i}_3)\left|\mathbf{1}\right\rangle/\sqrt{3} = \begin{pmatrix}-\frac{1}{2}\\1\\-\frac{1}{2}\\-\frac{1}{2}\\1\\-\frac{1}{2}\end{pmatrix}\frac{1}{\sqrt{3}} = -\frac{1}{2}\begin{pmatrix}1\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\1\end{pmatrix}\frac{1}{\sqrt{3}} + \frac{\sqrt{3}}{2}\begin{pmatrix}0\\+\frac{1}{2}\\-\frac{1}{2}\\-\frac{1}{2}\\+\frac{1}{2}\\0\end{pmatrix}$$

$-1/2 = D^{E_1}_{11}(r^1)$

$\mathbf{r}^1$

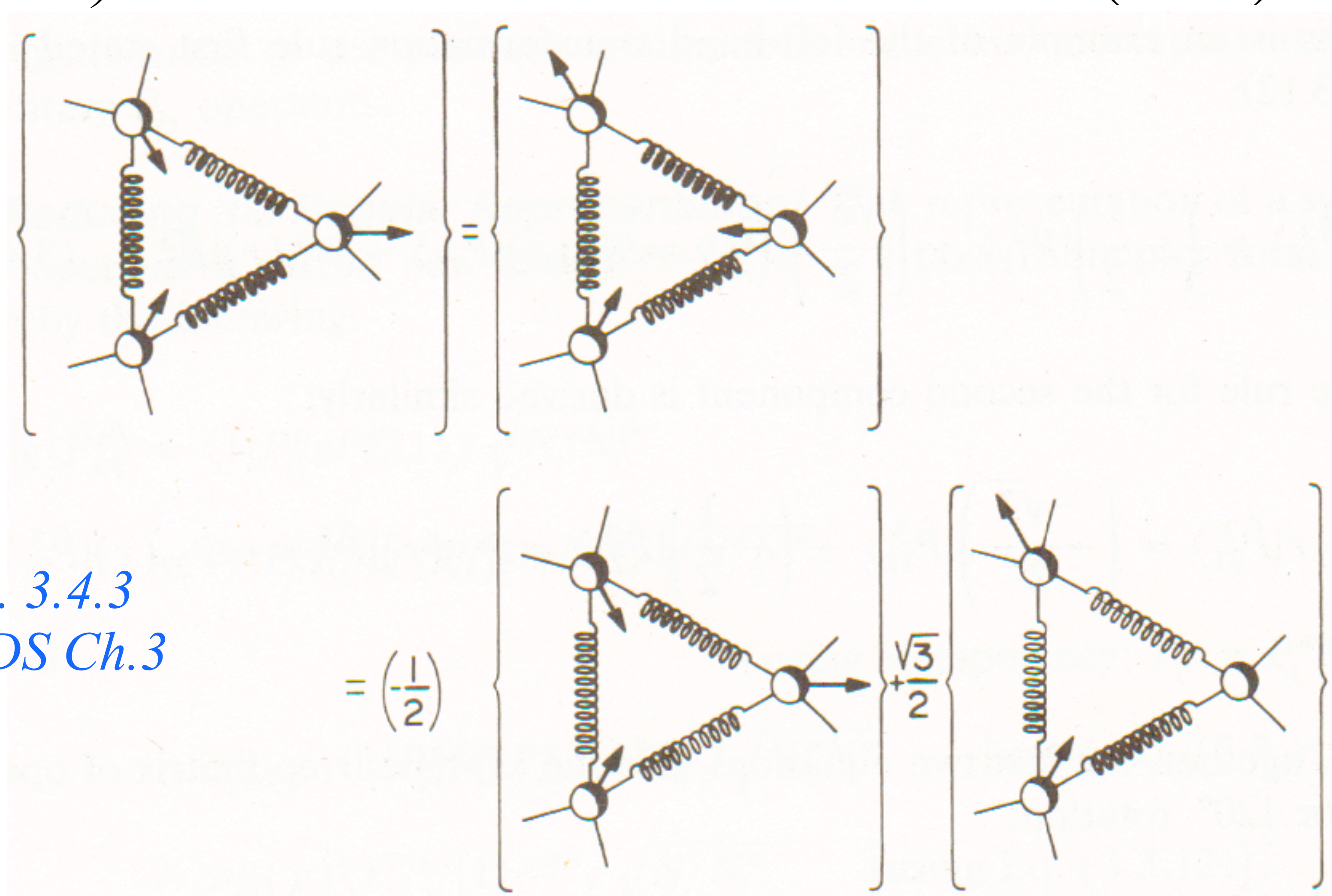


Fig. 3.4.3
PSDS Ch.3

$\sqrt{3}/2 = D^{E_1}_{21}(r^1)$

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

Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

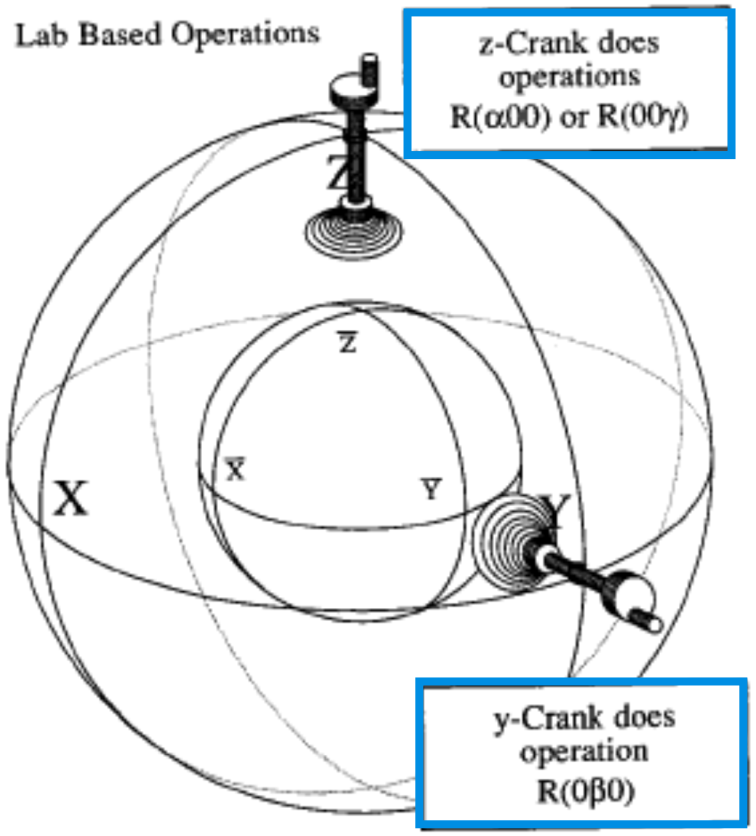
Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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

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

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

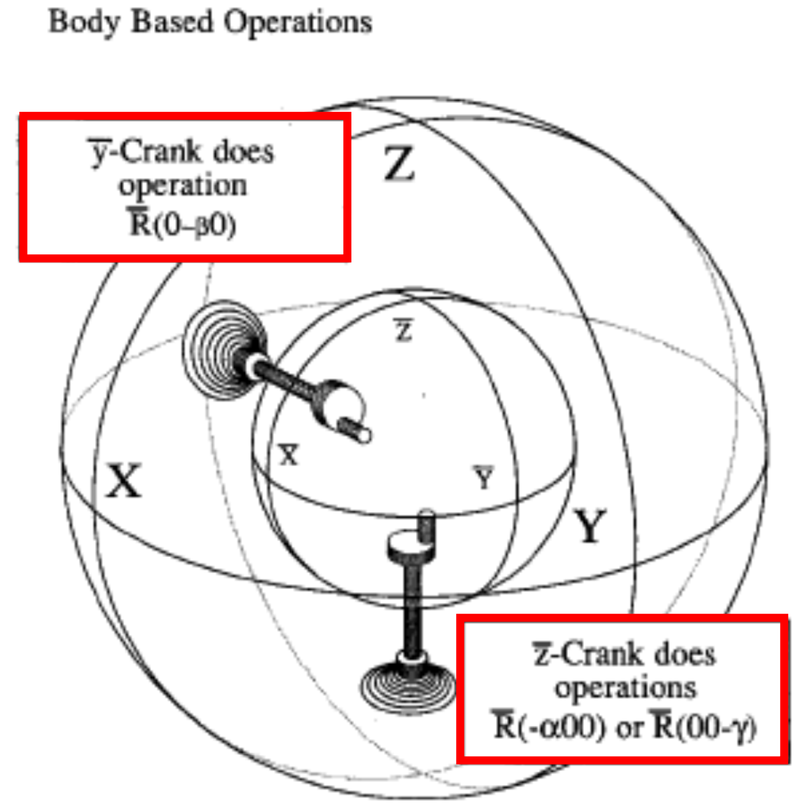


all **R**,**S**,..
commute with
all $\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..

"Mock-Mach"
relativity principles

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

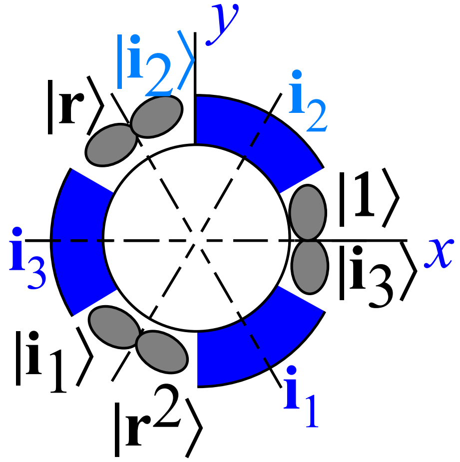
...for *one* state |1) *only!*

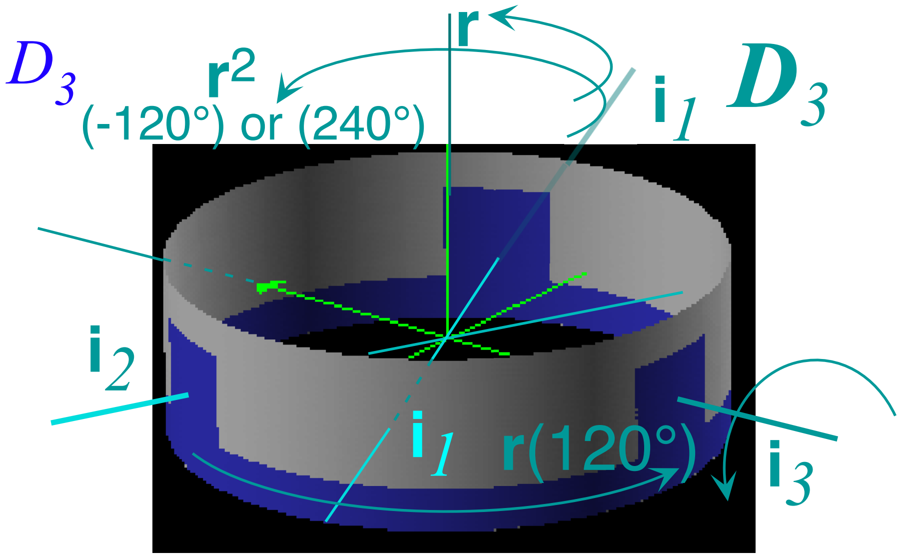


...But *how* do you actually *make* the **R** and $\bar{\mathbf{R}}$ operations?

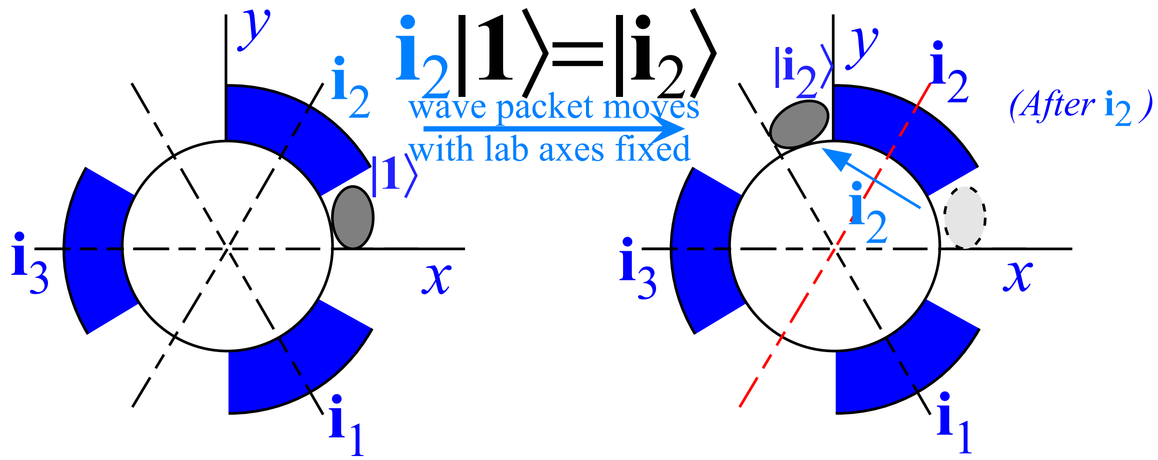
Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases



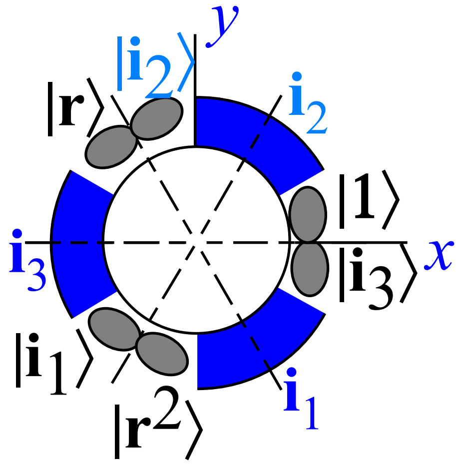


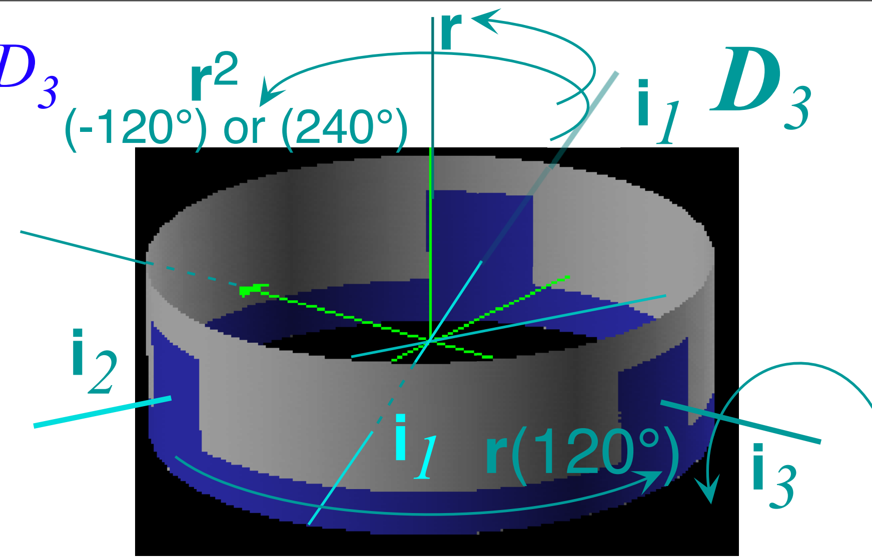
Lab-fixed (Extrinsic-Global) operations&axes fixed



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

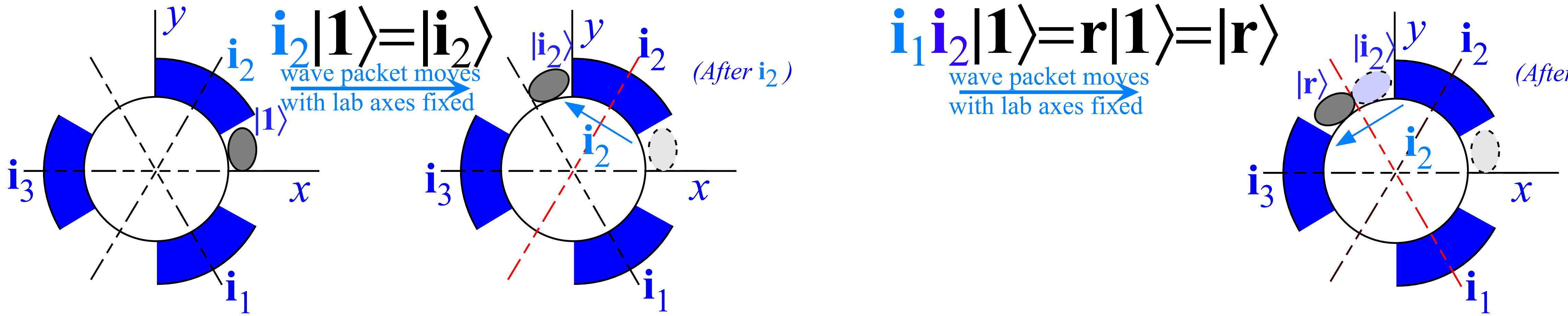




Lab-fixed (Extrinsic-Global) operations&axes fixed

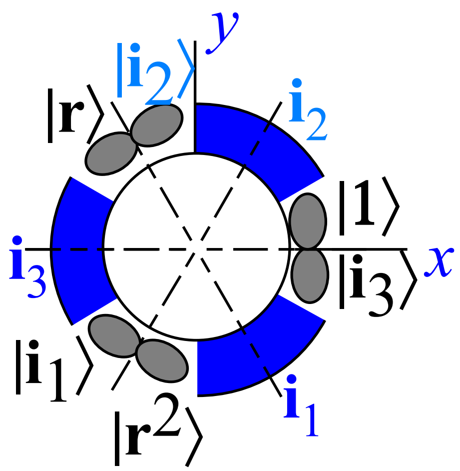
$\mathbf{i}_2|\mathbf{1}\rangle = |\mathbf{i}_2\rangle$

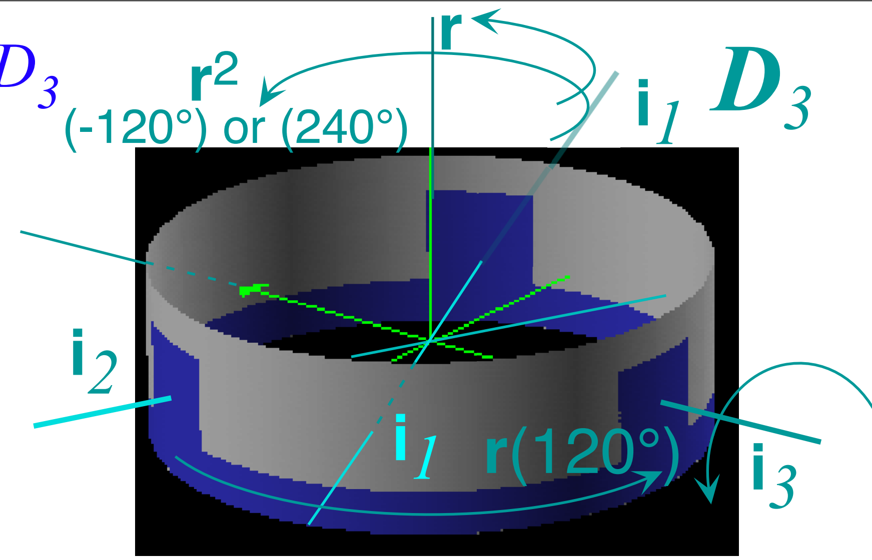
$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle = \mathbf{r}|\mathbf{1}\rangle = |\mathbf{r}\rangle$



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

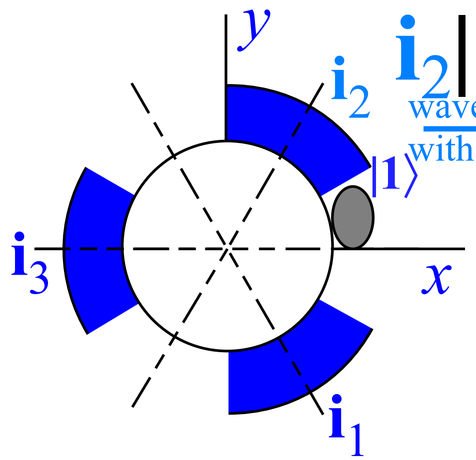




1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

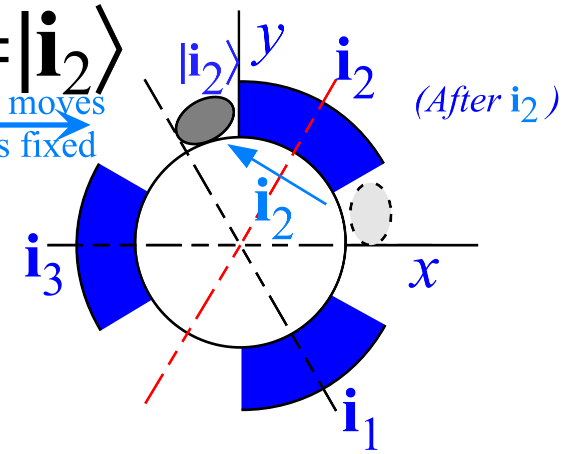
$i_1 i_2 = r$

Lab-fixed (Extrinsic-Global) operations&axes fixed



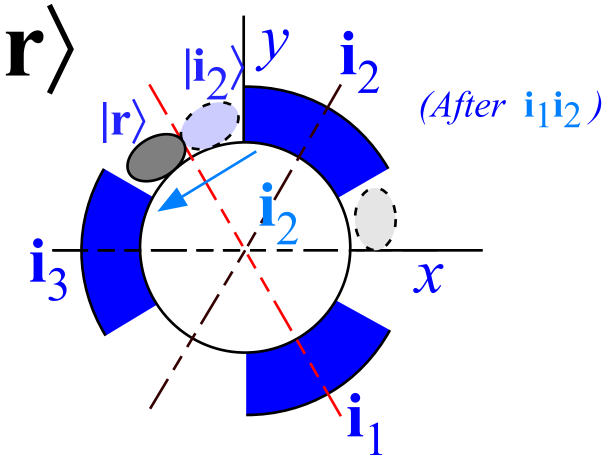
$$\mathbf{i}_2|\mathbf{1}\rangle = |\mathbf{i}_2\rangle$$

wave packet moves with lab axes fixed



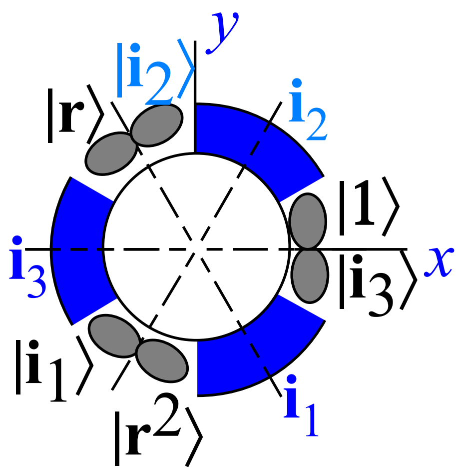
$$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle = \mathbf{r}|\mathbf{1}\rangle = |\mathbf{r}\rangle$$

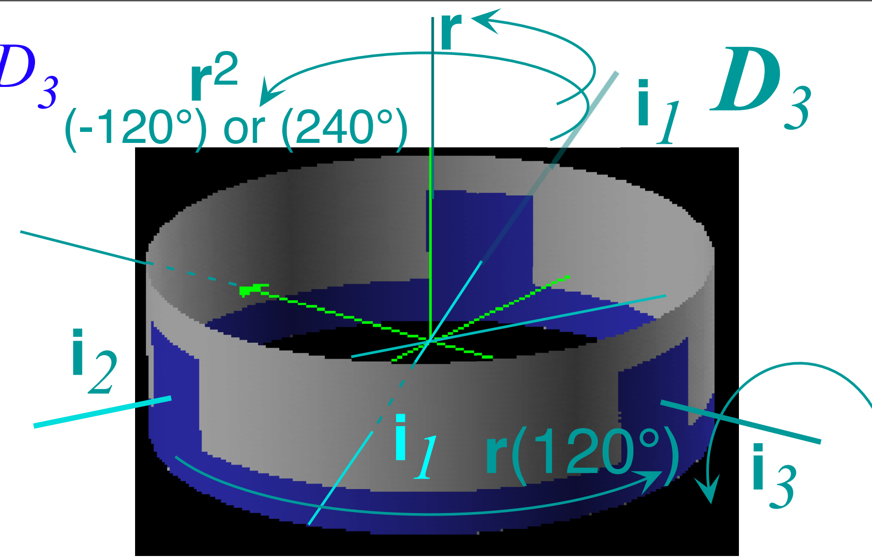
wave packet moves with lab axes fixed



Details of RELATIVITY-DUALITY for D_3

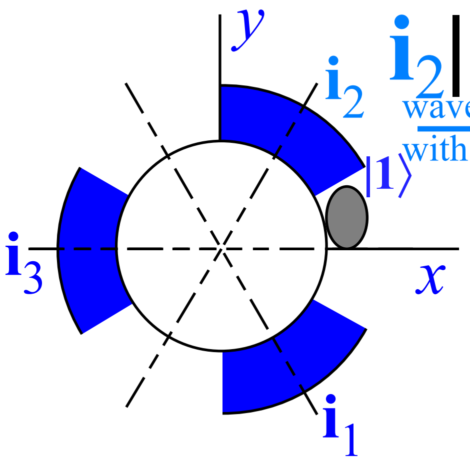
D_3-defined local-wave bases





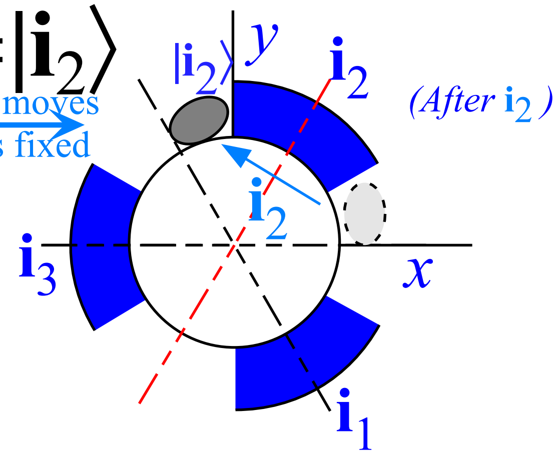
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

Lab-fixed (Extrinsic-Global) operations&axes fixed



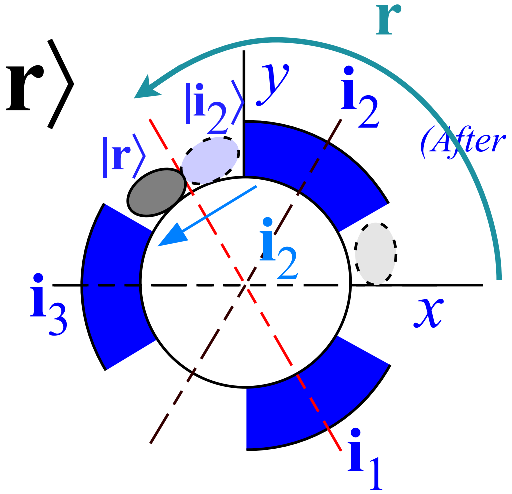
$\mathbf{i}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

wave packet moves with lab axes fixed



$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle=\mathbf{r}|\mathbf{1}\rangle=|\mathbf{r}\rangle$

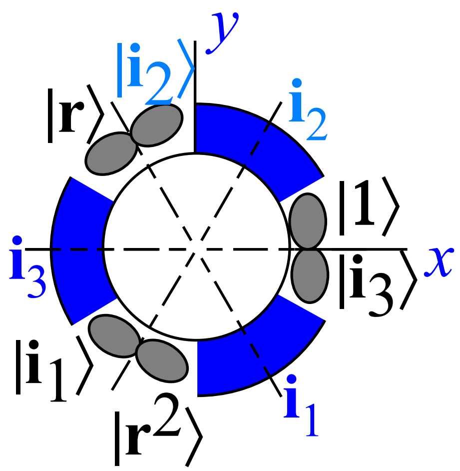
wave packet moves with lab axes fixed

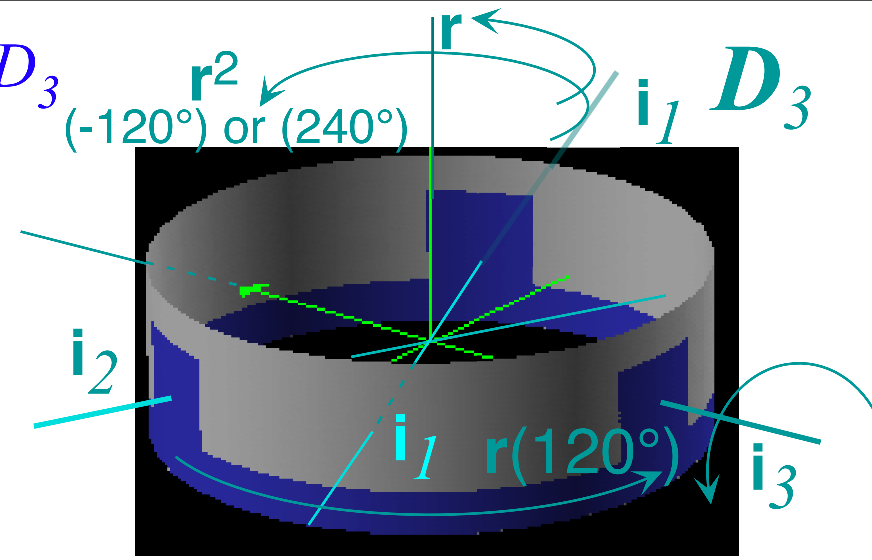


$\mathbf{i}_1\mathbf{i}_2 = \mathbf{r}$

Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

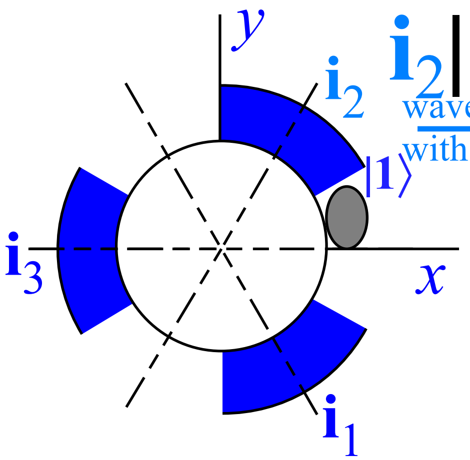




$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

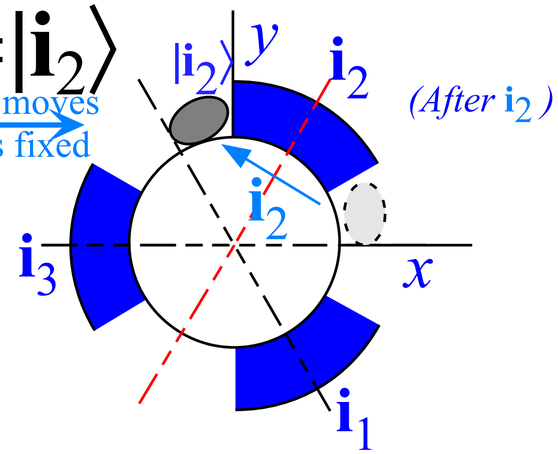
$\mathbf{i}_1\mathbf{i}_2 = \mathbf{r}$

Lab-fixed (Extrinsic-Global) operations&axes fixed



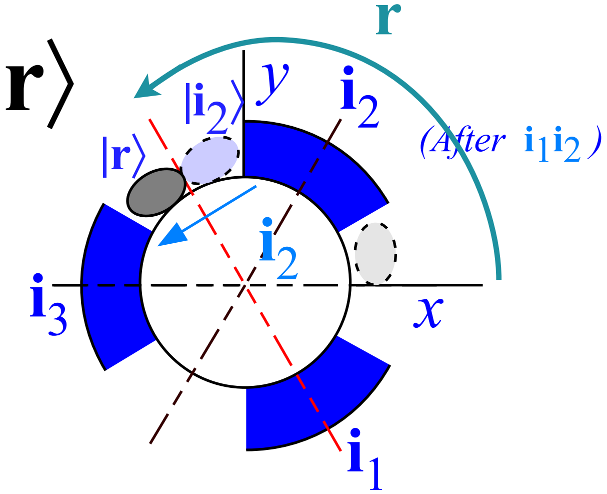
$\mathbf{i}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

wave packet moves with lab axes fixed



$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle=\mathbf{r}|\mathbf{1}\rangle=|\mathbf{r}\rangle$

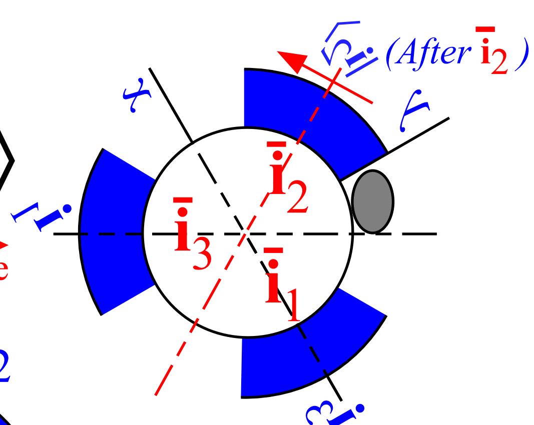
wave packet moves with lab axes fixed

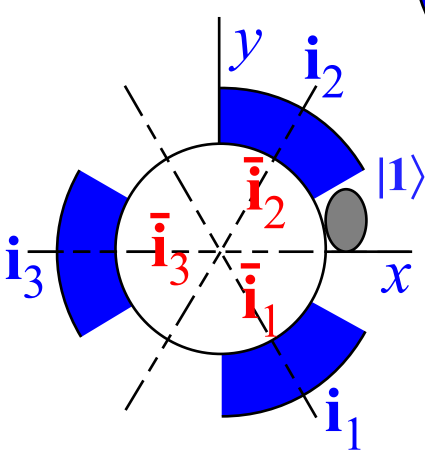


Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

$\bar{\mathbf{i}}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

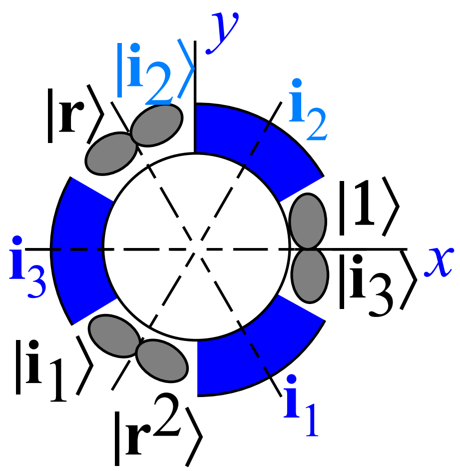
wave packet fixed while lab axes move

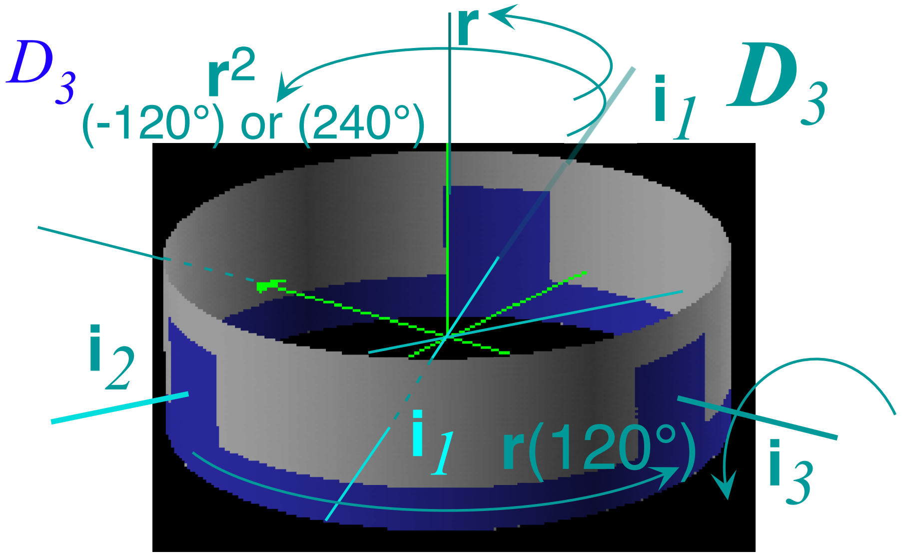




Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

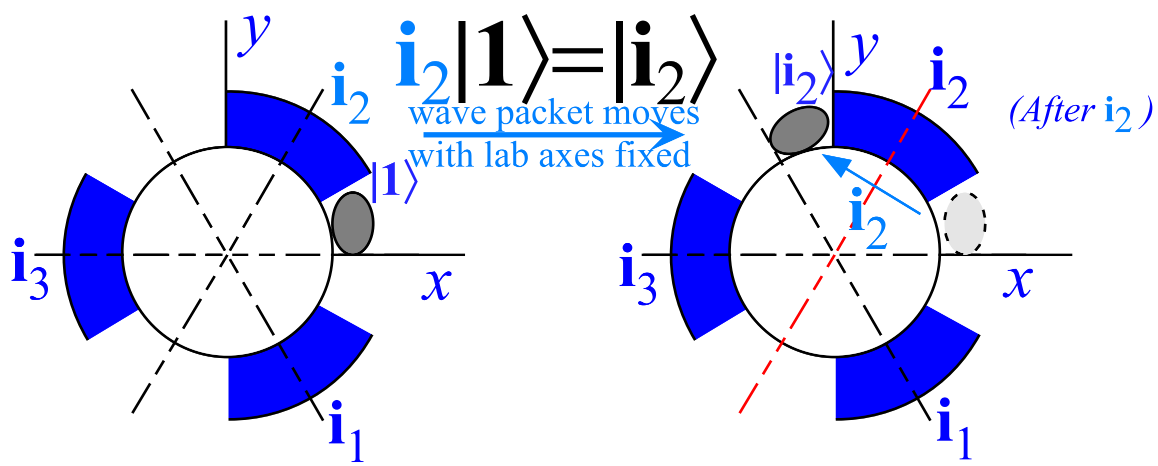


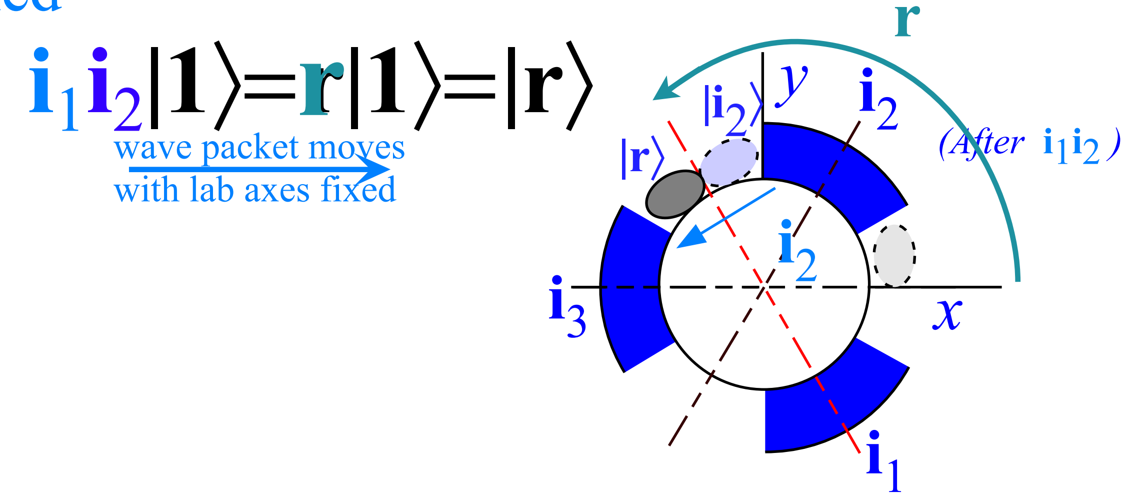


1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

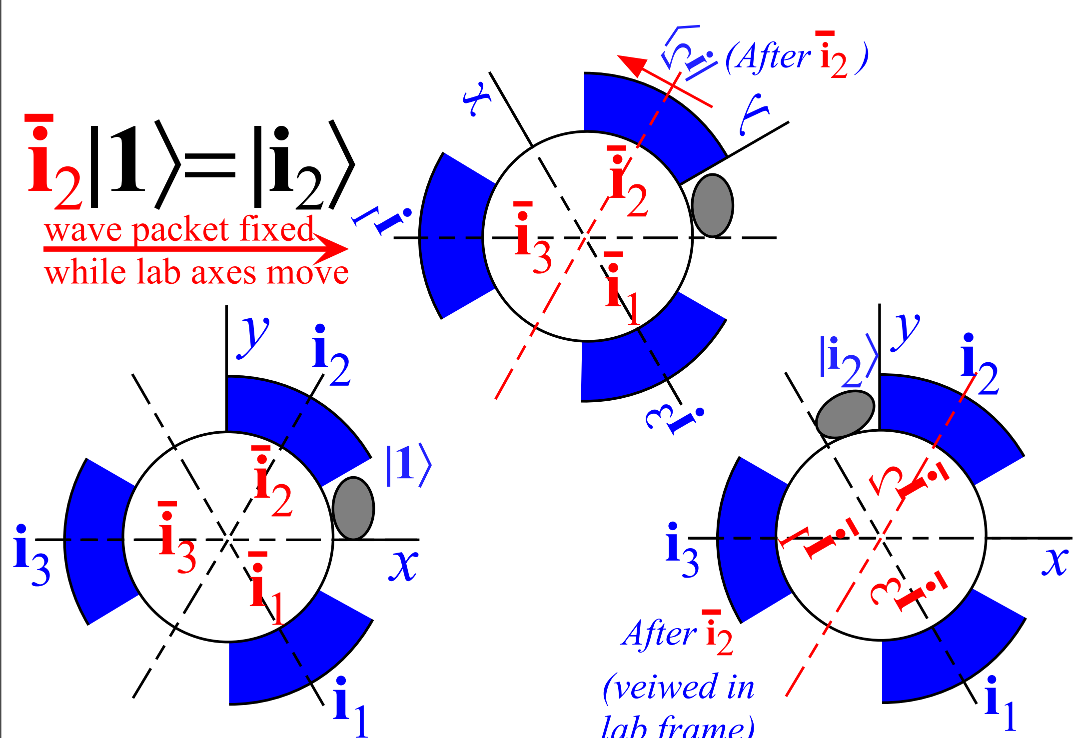
$i_1 i_2 = r$

Lab-fixed (Extrinsic-Global) operations&axes fixed



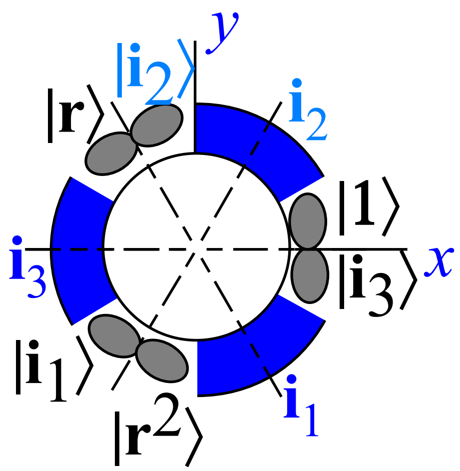


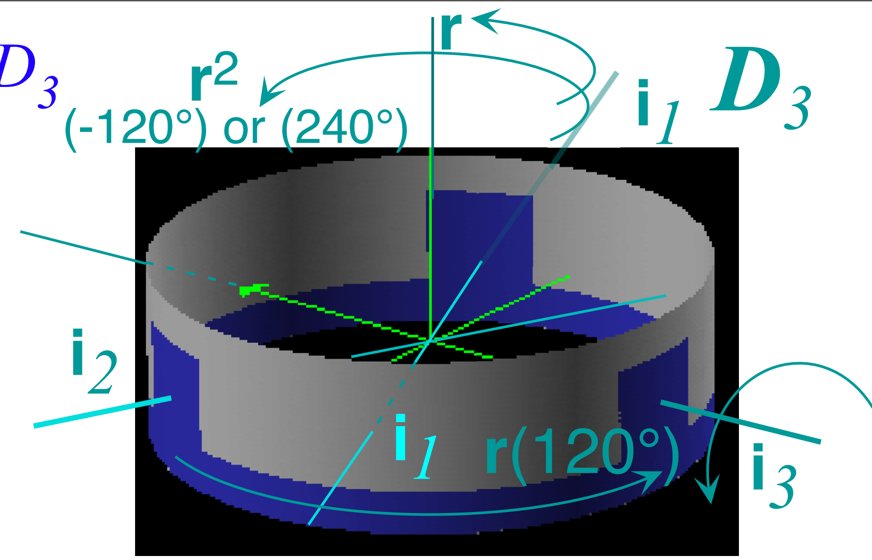
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

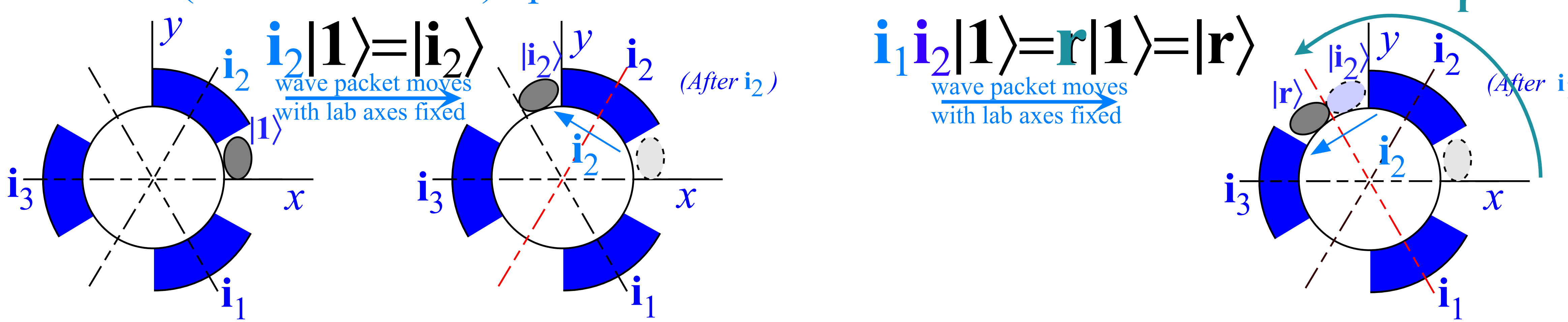




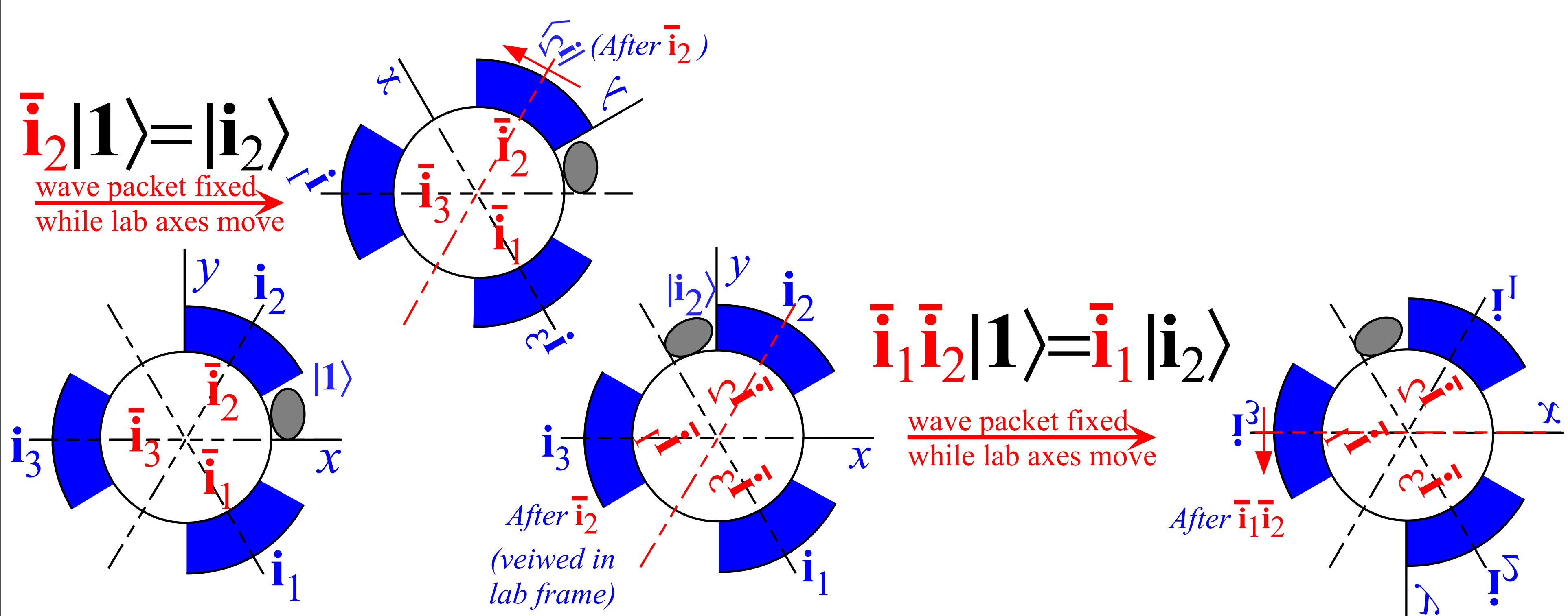
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

$i_1 i_2 = r$

Lab-fixed (Extrinsic-Global) operations&axes fixed

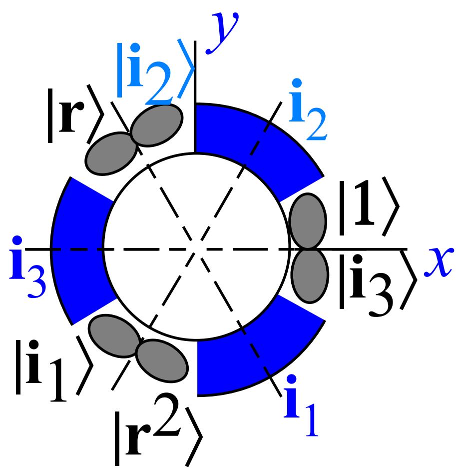


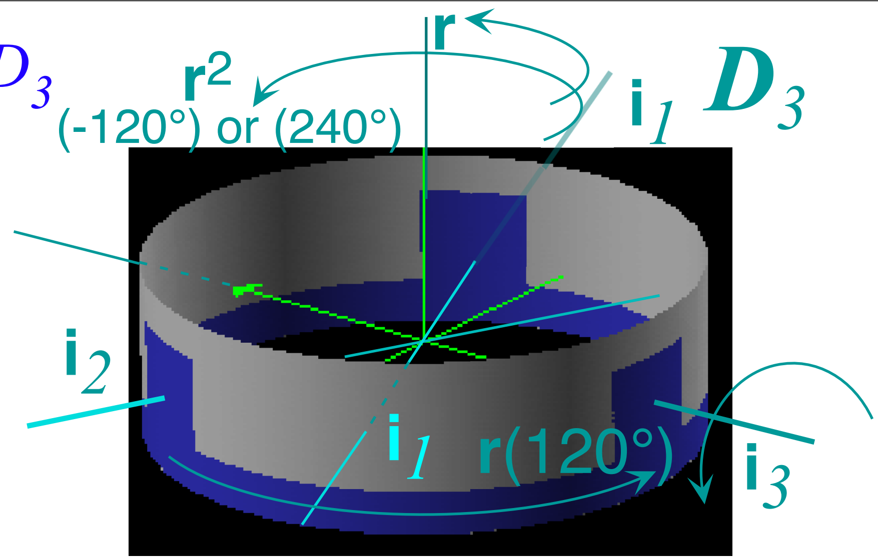
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases



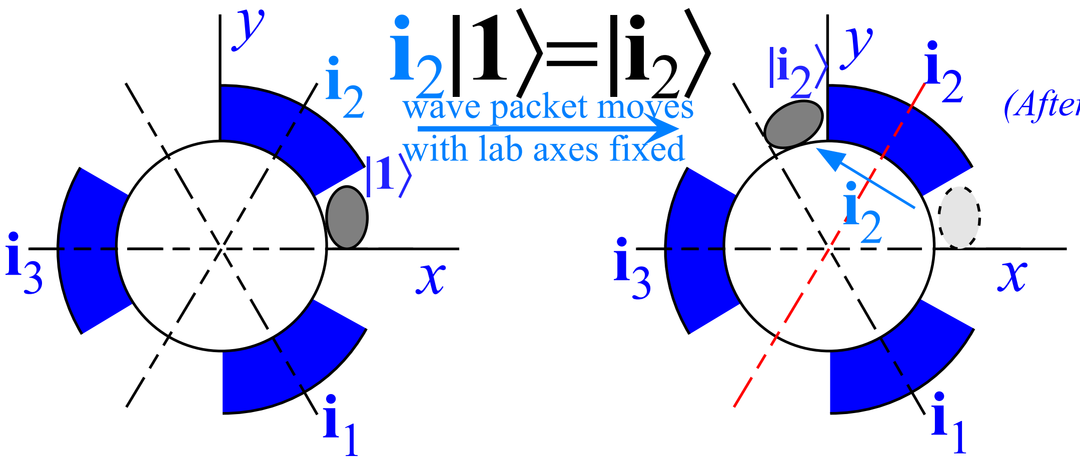


1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

Lab-fixed (Extrinsic-Global) operations&axes fixed

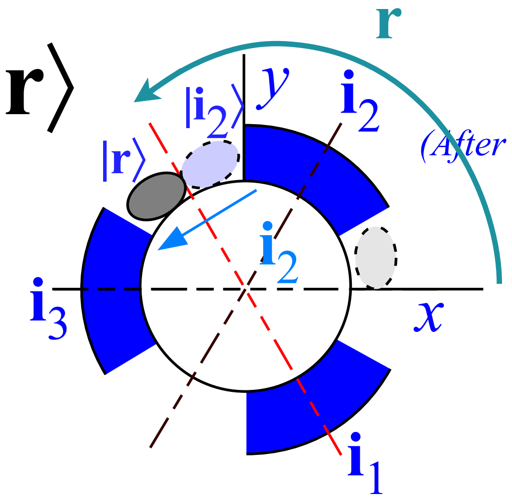
$\mathbf{i}_2|\mathbf{1}\rangle = |\mathbf{i}_2\rangle$

wave packet moves with lab axes fixed



$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle = \mathbf{r}|\mathbf{1}\rangle = |\mathbf{r}\rangle$

wave packet moves with lab axes fixed



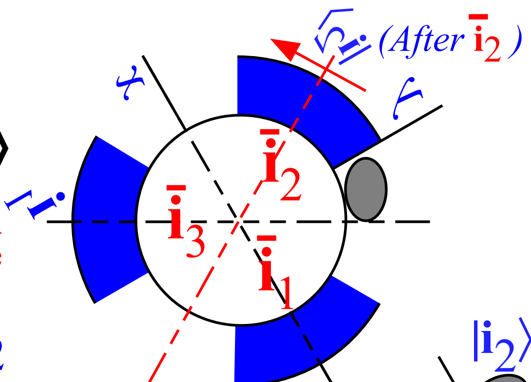
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

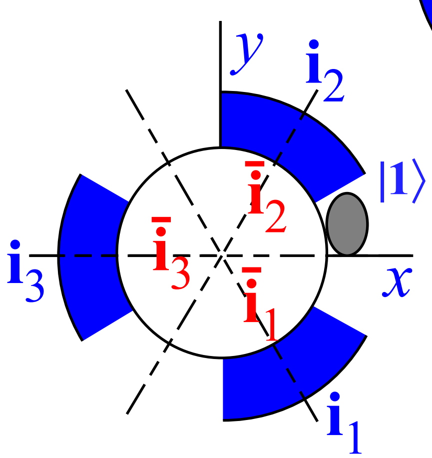
...but, THEY OBEY THE SAME GROUP TABLE.

$\mathbf{i}_1\mathbf{i}_2 = \mathbf{r}$ implies: $\bar{\mathbf{i}}_1\bar{\mathbf{i}}_2 = \bar{\mathbf{r}}$

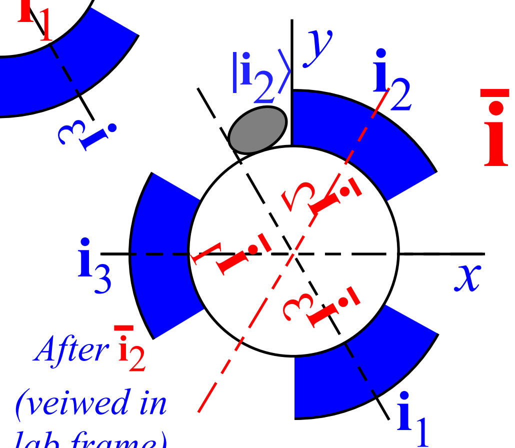
$\bar{\mathbf{i}}_2|\mathbf{1}\rangle = |\mathbf{i}_2\rangle$

wave packet fixed while lab axes move



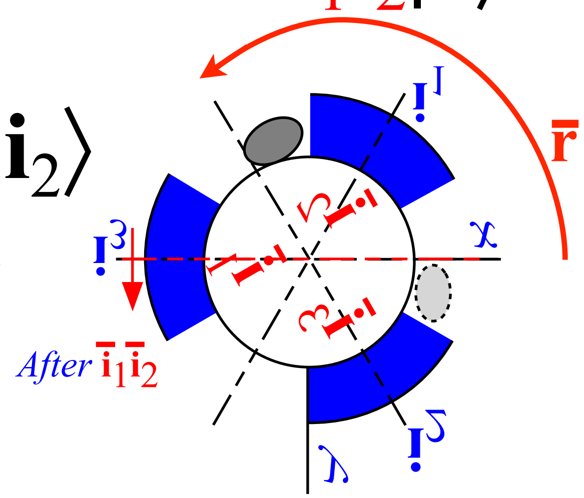


$\bar{\mathbf{i}}_1\bar{\mathbf{i}}_2|\mathbf{1}\rangle = \bar{\mathbf{i}}_1|\mathbf{i}_2\rangle$



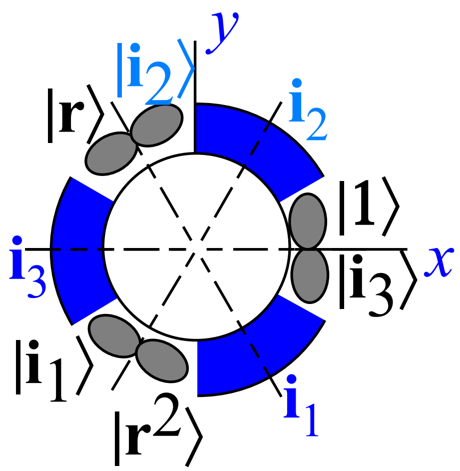
wave packet fixed while lab axes move

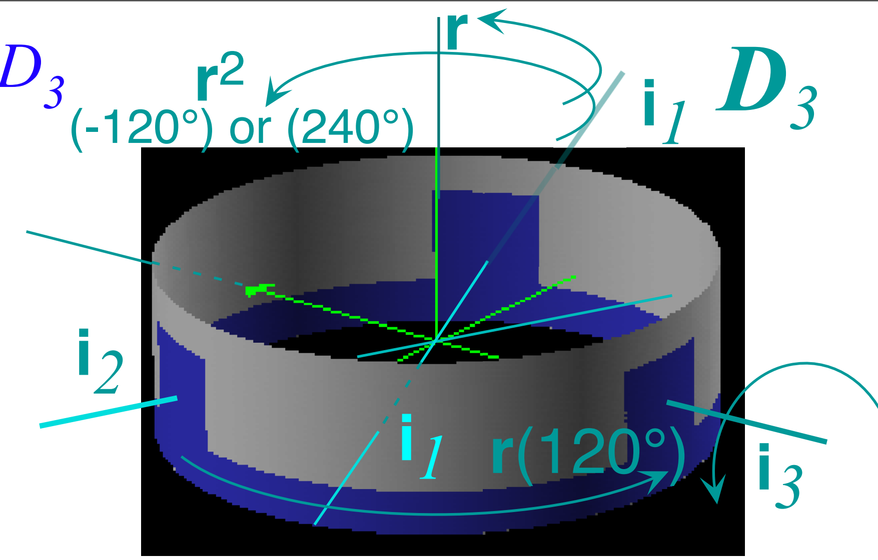
$\bar{\mathbf{i}}_1\bar{\mathbf{i}}_2|\mathbf{1}\rangle = \bar{\mathbf{i}}_1|\mathbf{i}_2\rangle = \bar{\mathbf{r}}|\mathbf{1}\rangle$



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases



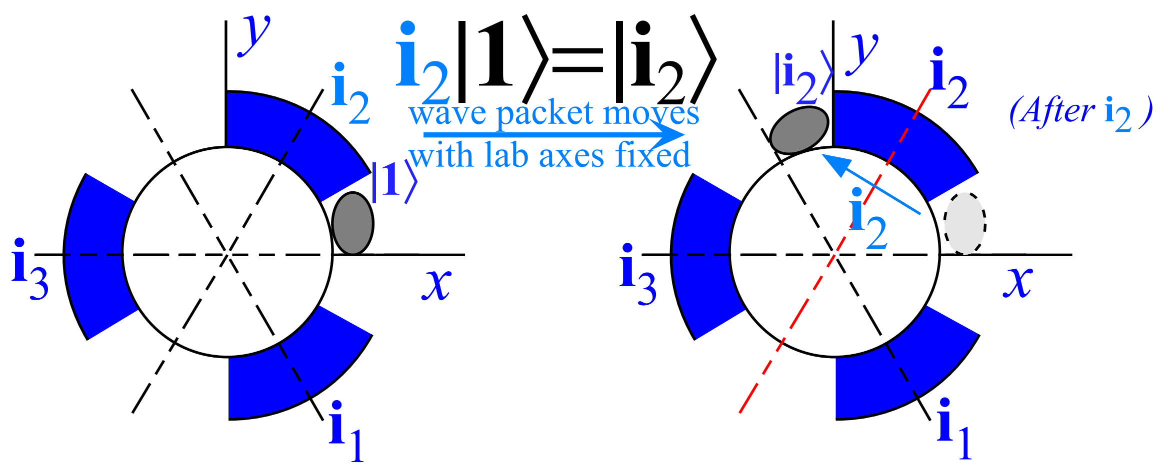


1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

Lab-fixed (Extrinsic-Global) operations&axes fixed

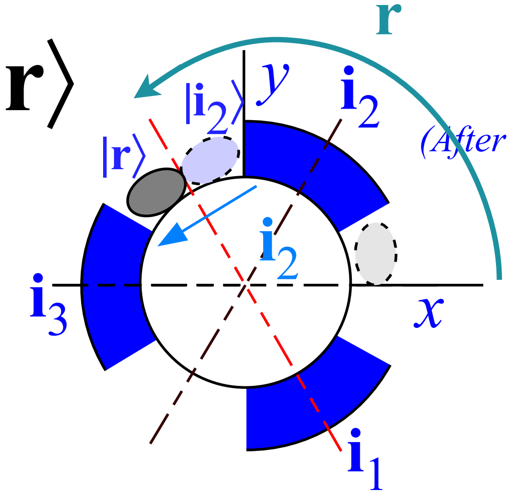
$i_2|1\rangle=|i_2\rangle$

wave packet moves with lab axes fixed



$i_1 i_2|1\rangle=r|1\rangle=|r\rangle$

wave packet moves with lab axes fixed



Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

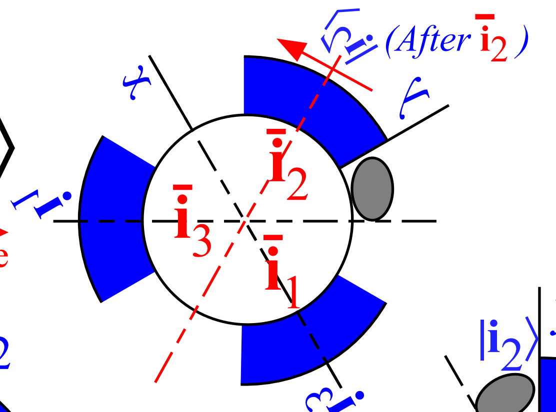
...but, THEY OBEY THE SAME GROUP TABLE.

$i_1 i_2 = r$ implies: $\bar{i}_1\bar{i}_2=\bar{r}$

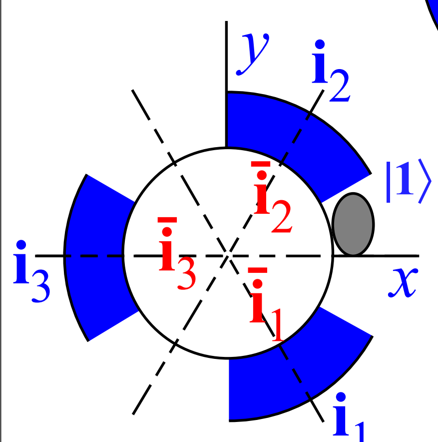
...and Mock-Mach principle $\bar{g}|1\rangle=g^{-1}|1\rangle$

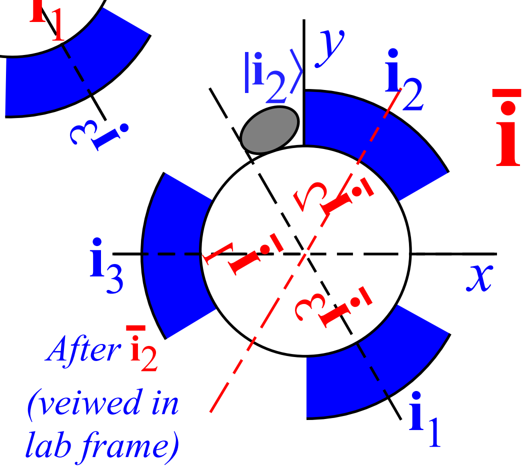
$\bar{i}_2|1\rangle=|i_2\rangle$

wave packet fixed while lab axes move



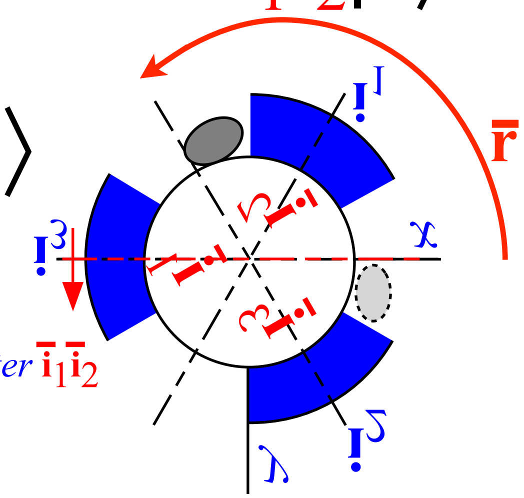
$\bar{i}_1\bar{i}_2|1\rangle=\bar{i}_1\,|i_2\rangle=\bar{r}\,|1\rangle=r^2\,|1\rangle$

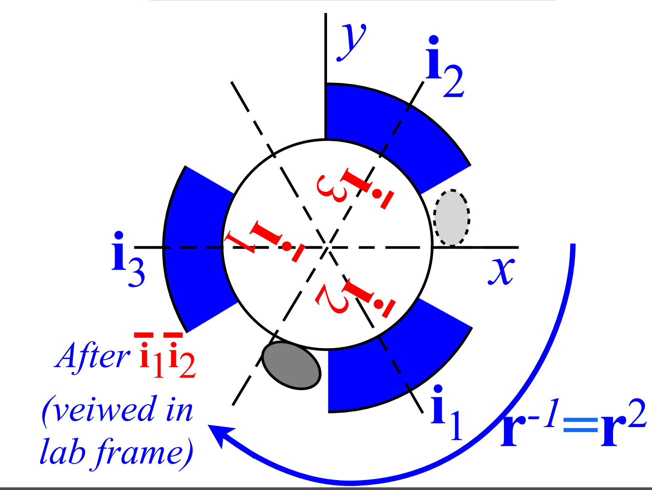




$\bar{i}_1\bar{i}_2|1\rangle=\bar{i}_1\,|i_2\rangle$

wave packet fixed while lab axes move





Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" 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_2	r^2	1	r
i_3	i_1	i_2	r	r^2	1

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

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

Just switch r with $\mathbf{r}^\dagger = \mathbf{r}^2$.

(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_2	r^2	1	r
i_3	i_1	i_2	r	r^2	1

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

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

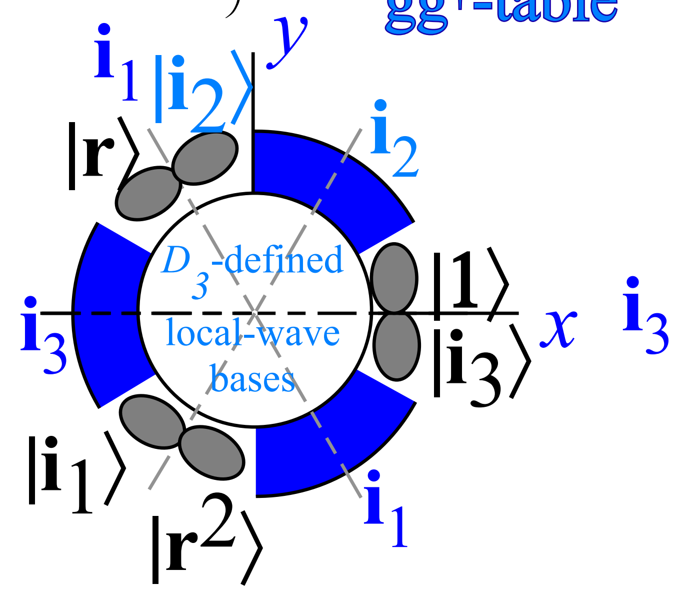
To represent *external* {..**T**,**U**,**V**,... }switch **g** ⇄ **g**† on top of group table

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

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

1	$\mathbf{r}^2$	**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**

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



Compare Global vs Local |g⟩-basis

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

To represent *external* {..**T**,**U**,**V**,... }switch **g** ⇄ **g**† on top of group table

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

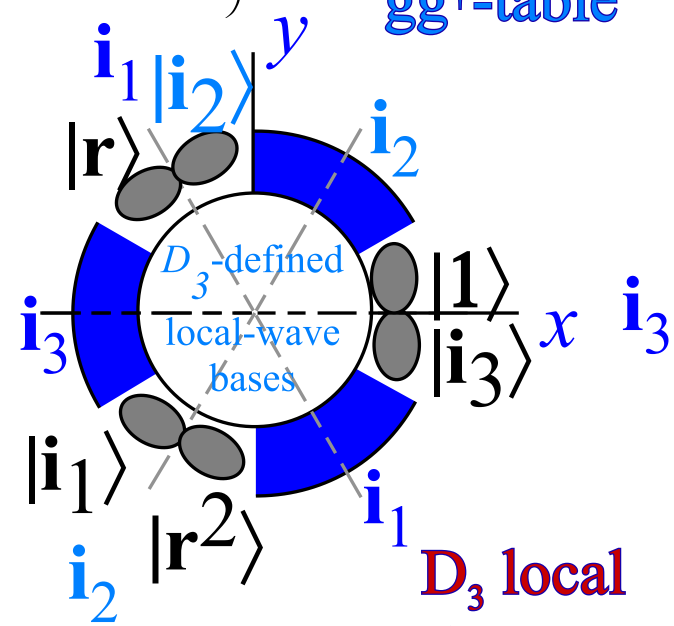
$R^G(\mathbf{i}_1) = \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot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

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†-table

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

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



D_3 local
g†g-table

To represent *internal* {..$\bar{\mathbf{T}}$,$\bar{\mathbf{U}}$,$\bar{\mathbf{V}}$,... } switch **g** ⇄ **g**† 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_2	r^2	1	r
i_3	i_1	i_2	r	r^2	1

Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$ *,characters* $\chi^{\mu}(\mathbf{g})$*, and All-Commuting Projectors* $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ *and Mutually-Commuting projectors* $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$*-expansion in irreps* $D^{\mu}{}_{jk}(g)$ *and Non-Commuting projectors* $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\,\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 *transformation by matrix* $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 *groups and representations*

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonian local-symmetry eigensolution

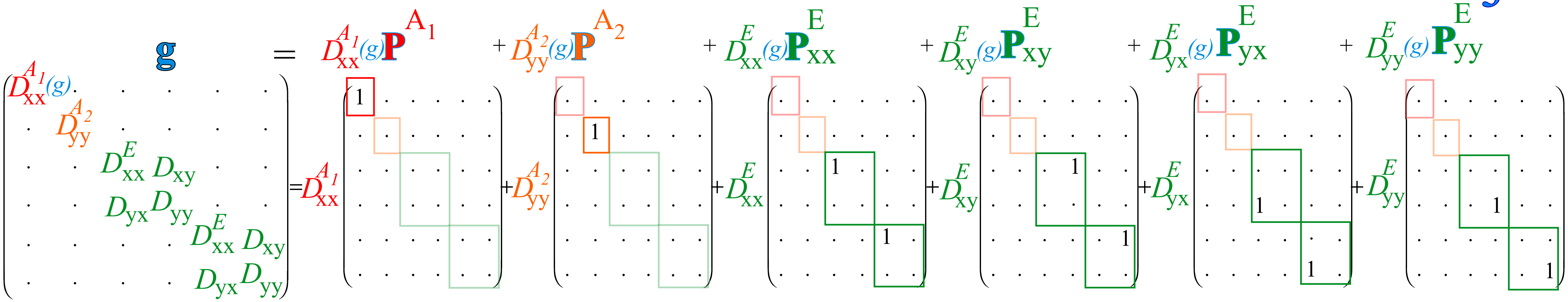
Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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



Global

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

Product table entry $\mathbf{P}^{E}_{ab}$ shows location of a 1 in the regular representation $R(\mathbf{P}^{E}_{ab})$ of that GLOBAL projection operator.

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

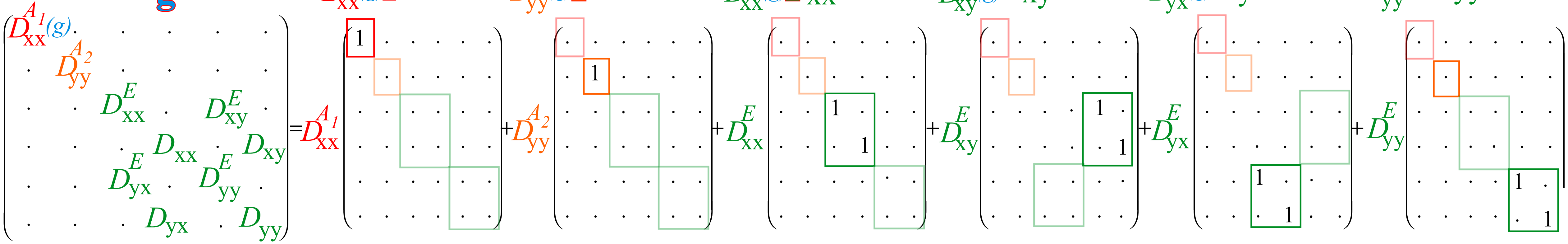
Local

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

Product table entry $\mathbf{P}^E_{ab}$ shows location of a 1 in the regular representation $R(\mathbf{P}^E_{ab})$ of that LOCAL projection operator.

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

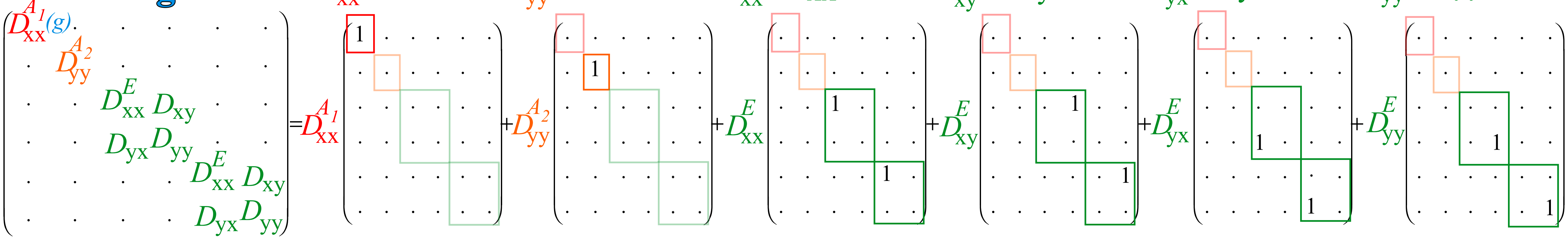
$$\bar{\mathbf{g}} = D^{A_1}_{xx}(g)\bar{\mathbf{P}}^{A_1} + D^{A_2}_{yy}(g)\bar{\mathbf{P}}^{A_2} + D^{E}_{xx}(g)\bar{\mathbf{P}}^{E}_{xx} + D^{E}_{xy}(g)\bar{\mathbf{P}}^{E}_{xy} + D^{E}_{yx}(g)\bar{\mathbf{P}}^{E}_{yx} + D^{E}_{yy}(g)\bar{\mathbf{P}}^{E}_{yy}$$



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

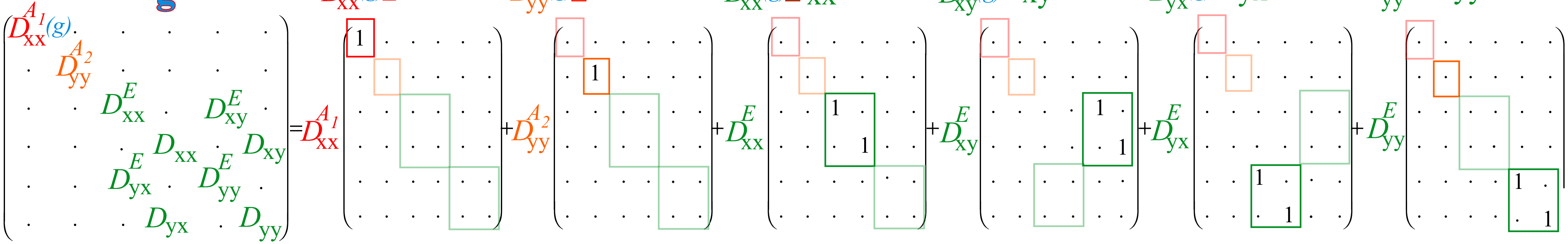
Matrix "Placeholders" $\mathbf{P}^{(m)}_{ab}$ *for GLOBAL* $\mathbf{g}$ *operators in* D_3

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



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

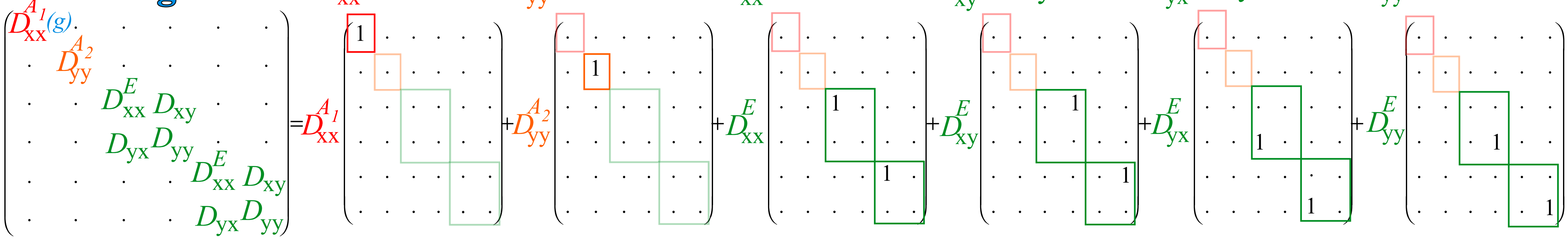
$$\bar{\mathbf{g}} = D^{A_1}_{xx}(g)\bar{\mathbf{P}}^{A_1} + D^{A_2}_{yy}(g)\bar{\mathbf{P}}^{A_2} + D^{E}_{xx}(g)\bar{\mathbf{P}}^{E}_{xx} + D^{E}_{xy}(g)\bar{\mathbf{P}}^{E}_{xy} + D^{E}_{yx}(g)\bar{\mathbf{P}}^{E}_{yx} + D^{E}_{yy}(g)\bar{\mathbf{P}}^{E}_{yy}$$



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

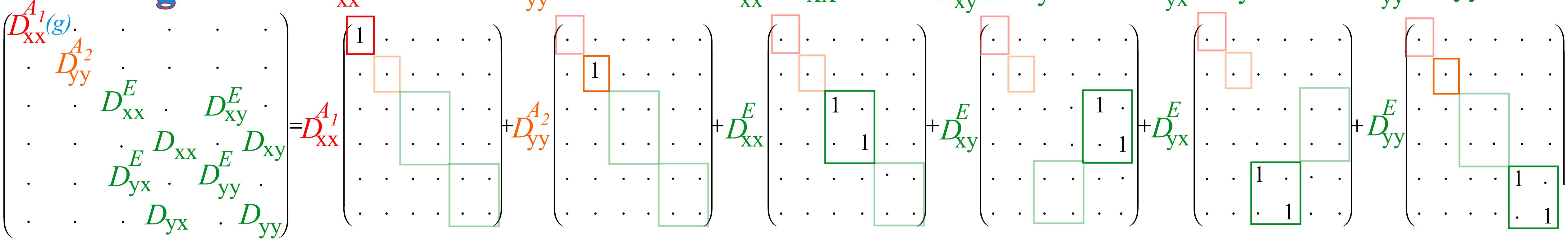
Matrix "Placeholders" $\mathbf{P}^{(m)}_{ab}$ *for GLOBAL* $\mathbf{g}$ *operators in* D_3

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



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

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



Note how any global g-matrix commutes with any local g-matrix

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

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

For example:

$$\begin{bmatrix} \cdot & b \\ \cdot & \cdot \end{bmatrix}\begin{bmatrix} A & \cdot \\ \cdot & A \end{bmatrix} = \begin{bmatrix} A & \cdot \\ \cdot & A \end{bmatrix}\begin{bmatrix} \cdot & b \\ \cdot & \cdot \end{bmatrix}$$

$$= \begin{bmatrix} \cdot & bA \\ \cdot & \cdot \end{bmatrix} = \begin{bmatrix} \cdot & Ab \\ \cdot & \cdot \end{bmatrix}$$

It's an example of old-fashioned Schur's Lemma

Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonion eigen-matrix calculation

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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.51)

$|\mathbf{P}^{(\mu)}\rangle$-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

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

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

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

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

For unitary $D^{(\mu)}$*: (p.51)*

$|\mathbf{P}^{(\mu)}\rangle$*-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* $|\mathbf{1}\rangle$ *to give:*

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

subject to normalization:

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

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.51)

$|\mathbf{P}^{(\mu)}\rangle$*-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* $|\mathbf{1}\rangle$ *to give:*

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

subject to normalization:

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

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.51)

$|\mathbf{P}^{(\mu)}\rangle$-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 $|\mathbf{1}\rangle$ to give:

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

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

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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 $\left|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle$

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

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

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subject to normalization:

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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.27

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

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

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

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.27

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

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

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:

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

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.27

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

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

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

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

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

Use Mock-Mach commutation and inverse

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.51)

$|\mathbf{P}^{(\mu)}\rangle$-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 $|\mathbf{1}\rangle$ to give:*

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

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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.27

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

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

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$$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$ 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.27

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

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

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

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

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

Use Mock-Mach commutation and inverse

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

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

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 $\left|{}^{\mu}_{mn}\right\rangle$

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

Matrix is same as given on p.27

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

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

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

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

Use Mock-Mach commutation and inverse

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

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

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

$$\mathbf{P}^{\mu}_{mn}\mathbf{g}^{-1} = \sum_{m'=1}^{\ell^{\mu}}\sum_{n'=1}^{\ell^{\mu}} \mathbf{P}^{\mu}_{mn}\mathbf{P}^{\mu}_{m'n'}D^{\mu}_{m'n'}(g^{-1})$$
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Hamiltonian and D_3 global-$\mathbf{g}$ and local-$\bar{\mathbf{g}}$ group matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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

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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.27

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

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

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

← Use Mock-Mach commutation and inverse

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

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

$$= \sum_{n'=1}^{\ell^\mu} D^{\mu}_{nn'}(g^{-1})\left|\begin{smallmatrix}\mu\\ mn'\end{smallmatrix}\right\rangle$$

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

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

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

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subject to normalization:

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

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.27

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

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

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

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

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

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

Use Mock-Mach commutation and inverse

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

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

$$= \sum_{n'=1}^{\ell^{\mu}} D^{\mu}_{nn'}(g^{-1})\left|\begin{smallmatrix}\mu\\ mn'\end{smallmatrix}\right\rangle$$

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

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

If D is unitary

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 $|\mathbf{1}\rangle$ to give:

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

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.27

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

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

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

Use Mock-Mach commutation and inverse

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

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

Global $\mathbf{g}$-matrix component

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

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

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

If D is unitary

Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

➡ *Global vs. Local block rearrangement* ⬅

Hamiltonion eigen-matrix calculation

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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

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

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

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

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

Global **g***-matrix component*

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

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

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

If D is unitary

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

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

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

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

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

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

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

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

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

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

Global $\mathbf{g}$-matrix component

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

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

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

If D is unitary

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

If D is unitary

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

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

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

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

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

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

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

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

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

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

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

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

Global g-matrix component

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

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

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

If D is unitary

Review Stage 1: *Group Center:Class-sums* $\kappa_{\mathbf{g}}$ *,characters* $\chi^{\mu}(\mathbf{g})$*, and All-Commuting Projectors* $\mathbb{P}^{\mu}$

Review Stage 2: *Group operators* $\mathbf{g}$ *and Mutually-Commuting projectors* $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: *Weyl* $\mathbf{g}$*-expansion in irreps* $D^{\mu}{}_{jk}(g)$ *and Non-Commuting projectors* $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 *transformation by matrix* $D^{E}{}_{jk}(\mathbf{r}^1)$

Details of Mock-Mach relativity-duality for D_3 *groups and representations*

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

➡ *Hamiltonion eigen-matrix calculation* ⬅

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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:*

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:

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$, $|\mathbf{P}^{A_2}_{yy}\rangle$, $|\mathbf{P}^{E_1}_{xx}\rangle$, $|\mathbf{P}^{E_1}_{xy}\rangle$, $|\mathbf{P}^{E_1}_{yx}\rangle$, $|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle$$

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:

$$\begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ (\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle$$

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. 86-96):

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

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$ $|\mathbf{P}^{A_2}_{yy}\rangle$ $|\mathbf{P}^{E_1}_{xx}\rangle|\mathbf{P}^{E_1}_{xy}\rangle$ $|\mathbf{P}^{E_1}_{yx}\rangle|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G\bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle \Big/ (norm)^2$$

Projector conjugation

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

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

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

subject to normalization (from p. 86-96):

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

(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:*

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

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

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

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2}$$

Mock-Mach commutation

$$\mathbf{r}\,\bar{\mathbf{r}} = \bar{\mathbf{r}}\,\mathbf{r}$$

(p.61)

subject to normalization (from p. 86-96):

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

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

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

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

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$, $|\mathbf{P}^{A_2}_{yy}\rangle$, $|\mathbf{P}^{E_1}_{xx}\rangle$, $|\mathbf{P}^{E_1}_{xy}\rangle$, $|\mathbf{P}^{E_1}_{yx}\rangle$, $|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G\bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^oG}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha*}_{ab}(g)$$

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.21)

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:*

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

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\mu^*}_{ab}(g)$$

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

subject to normalization (from p. 86-96):

$$norm = \sqrt{\langle \mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{^\circ G}}$$ *(which will cancel out)*

So, fuggettabout it!

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:

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

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

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$, $|\mathbf{P}^{A_2}_{yy}\rangle$, $|\mathbf{P}^{E_1}_{xx}\rangle|\mathbf{P}^{E_1}_{xy}\rangle$, $|\mathbf{P}^{E_1}_{yx}\rangle|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\mu^*}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\mu^*}_{ab}(g)$$

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

subject to normalization (from p. 86-96):

$$norm = \sqrt{\langle \mathbf{1}|\mathbf{P}^{\mu}_{nn}|\mathbf{1}\rangle} = \sqrt{\frac{\ell^{(\mu)}}{^\circ G}}$$ (which will cancel out)

So, fuggettabout it!

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:*

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

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

Basis: $|\mathbf{P}^{A_1}_{xx}\rangle$ $|\mathbf{P}^{A_2}_{yy}\rangle$ $|\mathbf{P}^{E_1}_{xx}\rangle|\mathbf{P}^{E_1}_{xy}\rangle$ $|\mathbf{P}^{E_1}_{yx}\rangle|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \overline{T}(\mathbf{H})_G\overline{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

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- 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:*

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$, $|\mathbf{P}^{A_2}_{yy}\rangle$, $|\mathbf{P}^{E_1}_{xx}\rangle|\mathbf{P}^{E_1}_{xy}\rangle$, $|\mathbf{P}^{E_1}_{yx}\rangle|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\delta_{mn} \langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^{\mu}_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

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:*

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

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

$$|\mathbf{P}^{A_1}_{xx}\rangle \quad |\mathbf{P}^{A_2}_{yy}\rangle \quad |\mathbf{P}^{E_1}_{xx}\rangle |\mathbf{P}^{E_1}_{xy}\rangle \quad |\mathbf{P}^{E_1}_{yx}\rangle |\mathbf{P}^{E_1}_{yy}\rangle$$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab} = \langle \mathbf{P}^{\mu}_{ma} | \mathbf{H} | \mathbf{P}^{\mu}_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^{\mu}_{am} \mathbf{H} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^{\mu}_{am} \mathbf{P}^{\mu}_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H} \, \mathbf{P}^{\mu}_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) \;= r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E *}_{xx}(1) + r_1 D^{E *}_{xx}(r^1) + r_1^* D^{E *}_{xx}(r^2) + i_1 D^{E *}_{xx}(i_1) + i_2 D^{E *}_{xx}(i_2) + i_3 D^{E *}_{xx}(i_3) \;= (2 r_0 - r_1 - r_1^* - i_1 - i_2 + 2 i_3)/2$$

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

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

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

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

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{array}{c} \begin{array}{cccccc} |\mathbf{P}^{A_1}_{xx}\rangle & |\mathbf{P}^{A_2}_{yy}\rangle & |\mathbf{P}^{E_1}_{xx}\rangle & |\mathbf{P}^{E_1}_{xy}\rangle & |\mathbf{P}^{E_1}_{yx}\rangle & |\mathbf{P}^{E_1}_{yy}\rangle \end{array} \\ \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right) \end{array}$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma} | \mathbf{H} | \mathbf{P}^\mu_{nb} \rangle = \frac{\langle \mathbf{1} | \mathbf{P}^\mu_{am} \mathbf{H} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2} = \frac{\langle \mathbf{1} | \mathbf{H} \mathbf{P}^\mu_{am} \mathbf{P}^\mu_{nb} | \mathbf{1} \rangle}{(norm)^2} = \delta_{mn} \frac{\langle \mathbf{1} | \mathbf{H}\, \mathbf{P}^\mu_{ab} | \mathbf{1} \rangle}{(norm)^2} = \sum_{g=1}^{{}^\circ G} \langle \mathbf{1} | \mathbf{H} | \mathbf{g} \rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{{}^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) \; = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) \; = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) \; = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx}$$

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:*

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

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

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

$$(\mathbf{H})_P=\bar{T}(\mathbf{H})_G\bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^{\alpha}_{ab}=\langle \mathbf{P}^{\mu}_{ma}|\mathbf{H}|\mathbf{P}^{\mu}_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^{\mu}_{am}\mathbf{H}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^{\mu}_{am}\mathbf{P}^{\mu}_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\delta_{mn}\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^{\mu}_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle\mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1}=r_0D^{A_1 *}(1)+r_1D^{A_1 *}(r^1)+r_1^*D^{A_1 *}(r^2)+i_1D^{A_1 *}(i_1)+i_2D^{A_1 *}(i_2)+i_3D^{A_1 *}(i_3) \;=r_0+r_1+r_1^*+i_1+i_2+i_3$$

$$H^{A_2}=r_0D^{A_2 *}(1)+r_1D^{A_2 *}(r^1)+r_1^*D^{A_2 *}(r^2)+i_1D^{A_2 *}(i_1)+i_2D^{A_2 *}(i_2)+i_3D^{A_2 *}(i_3) =r_0+r_1+r_1^*-i_1-i_2-i_3$$

$$H^{E_1}_{xx}=r_0D^{E *}_{xx}(1)+r_1D^{E *}_{xx}(r^1)+r_1^*D^{E *}_{xx}(r^2)+i_1D^{E *}_{xx}(i_1)+i_2D^{E *}_{xx}(i_2)+i_3D^{E *}_{xx}(i_3) \;=(2r_0-r_1-r_1^*-i_1-i_2+2i_3)/2$$

$$H^{E_1}_{xy}=r_0D^{E *}_{xy}(1)+r_1D^{E *}_{xy}(r^1)+r_1^*D^{E *}_{xy}(r^2)+i_1D^{E *}_{xy}(i_1)+i_2D^{E *}_{xy}(i_2)+i_3D^{E *}_{xy}(i_3) \;=\sqrt{3}(-r_1+r_1^*-i_1+i_2)/2 =H^{E *}_{yx}$$

$$H^{E_1}_{yy}=r_0D^{E *}_{yy}(1)+r_1D^{E *}_{yy}(r^1)+r_1^*D^{E *}_{yy}(r^2)+i_1D^{E *}_{yy}(i_1)+i_2D^{E *}_{yy}(i_2)+i_3D^{E *}_{yy}(i_3) \;=(2r_0-r_1-r_1^*+i_1+i_2-2i_3)/2$$

Coefficients $D^{\mu}_{mn}(g)$ *are irreducible representations (ireps) of* **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- **H** matrices in $|\mathbf{P}^{(\mu)}\rangle$-basis

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

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

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

Columns: $|\mathbf{P}^{A_1}_{xx}\rangle$, $|\mathbf{P}^{A_2}_{yy}\rangle$, $|\mathbf{P}^{E_1}_{xx}\rangle|\mathbf{P}^{E_1}_{xy}\rangle$, $|\mathbf{P}^{E_1}_{yx}\rangle|\mathbf{P}^{E_1}_{yy}\rangle$

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G\bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma}|\mathbf{H}|\mathbf{P}^\mu_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^\mu_{am}\mathbf{H}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^\mu_{am}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^\mu_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle\mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx}$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2$$

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators $\mathbf{g}$ and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$

Review Stage 3: Weyl $\mathbf{g}$-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^1)$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonion eigen-matrix calculation

➡ *Hamiltonian local-symmetry eigensolution* ⬅

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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

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

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

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

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

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G \bar{T}^\dagger = \begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma}|\mathbf{H}|\mathbf{P}^\mu_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^\mu_{am}\mathbf{H}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^\mu_{am}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^\mu_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1*}(1) + r_1 D^{A_1*}(r^1) + r_1^* D^{A_1*}(r^2) + i_1 D^{A_1*}(i_1) + i_2 D^{A_1*}(i_2) + i_3 D^{A_1*}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 \qquad = r_0 + 2r_1 + 2i_{12} + i_3$$

$$H^{A_2} = r_0 D^{A_2*}(1) + r_1 D^{A_2*}(r^1) + r_1^* D^{A_2*}(r^2) + i_1 D^{A_2*}(i_1) + i_2 D^{A_2*}(i_2) + i_3 D^{A_2*}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 \qquad = r_0 + 2r_1 - 2i_{12} - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2 \qquad = r_0 - r_1 - i_{12} + i_3$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx} \qquad = 0$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2 \qquad = r_0 - r_1 + i_{12} - i_3$$

$$\begin{pmatrix} H^{E_1}_{xx} & H^{E_1}_{xy} \\ H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$= \begin{pmatrix} r_0 - r_1 - i_{12} + i_3 & 0 \\ 0 & r_0 - r_1 - i_{12} - i_3 \end{pmatrix}_{For:\, r_1 = r_1^* \, and:\, i_1 = i_2}$$

Choosing local $C_2 = \{\mathbf{1}, \mathbf{i}_3\}$ *symmetry with local constraints* $r_1 = r_1^* = r_2$ *and* $i_1 = i_2 = i_{12}$

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

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

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

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

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

$$(\mathbf{H})_P = \bar{T}(\mathbf{H})_G\bar{T}^\dagger = \left(\begin{array}{c|c|cc|cc} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{array}\right)$$

$$H^\alpha_{ab} = \langle \mathbf{P}^\mu_{ma}|\mathbf{H}|\mathbf{P}^\mu_{nb}\rangle = \frac{\langle \mathbf{1}|\mathbf{P}^\mu_{am}\mathbf{H}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \frac{\langle \mathbf{1}|\mathbf{H}\mathbf{P}^\mu_{am}\mathbf{P}^\mu_{nb}|\mathbf{1}\rangle}{(norm)^2} = \delta_{mn}\frac{\langle \mathbf{1}|\mathbf{H}\,\mathbf{P}^\mu_{ab}|\mathbf{1}\rangle}{(norm)^2} = \sum_{g=1}^{^\circ G}\langle \mathbf{1}|\mathbf{H}|\mathbf{g}\rangle D^{\alpha *}_{ab}(g) = \sum_{g=1}^{^\circ G} r_g D^{\alpha *}_{ab}(g)$$

$$H^{A_1} = r_0 D^{A_1 *}(1) + r_1 D^{A_1 *}(r^1) + r_1^* D^{A_1 *}(r^2) + i_1 D^{A_1 *}(i_1) + i_2 D^{A_1 *}(i_2) + i_3 D^{A_1 *}(i_3) = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 \quad = r_0 + 2r_1 + 2i_{12} + i_3$$

$$H^{A_2} = r_0 D^{A_2 *}(1) + r_1 D^{A_2 *}(r^1) + r_1^* D^{A_2 *}(r^2) + i_1 D^{A_2 *}(i_1) + i_2 D^{A_2 *}(i_2) + i_3 D^{A_2 *}(i_3) = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 \quad = r_0 + 2r_1 - 2i_{12} - i_3$$

$$H^{E_1}_{xx} = r_0 D^{E*}_{xx}(1) + r_1 D^{E*}_{xx}(r^1) + r_1^* D^{E*}_{xx}(r^2) + i_1 D^{E*}_{xx}(i_1) + i_2 D^{E*}_{xx}(i_2) + i_3 D^{E*}_{xx}(i_3) = (2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3)/2 \quad = r_0 - r_1 - i_{12} + i_3$$

$$H^{E_1}_{xy} = r_0 D^{E*}_{xy}(1) + r_1 D^{E*}_{xy}(r^1) + r_1^* D^{E*}_{xy}(r^2) + i_1 D^{E*}_{xy}(i_1) + i_2 D^{E*}_{xy}(i_2) + i_3 D^{E*}_{xy}(i_3) = \sqrt{3}(-r_1 + r_1^* - i_1 + i_2)/2 = H^{E*}_{yx} \quad = 0$$

$$H^{E_1}_{yy} = r_0 D^{E*}_{yy}(1) + r_1 D^{E*}_{yy}(r^1) + r_1^* D^{E*}_{yy}(r^2) + i_1 D^{E*}_{yy}(i_1) + i_2 D^{E*}_{yy}(i_2) + i_3 D^{E*}_{yy}(i_3) = (2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3)/2 \quad = r_0 - r_1 + i_{12} - i_3$$

$C_2 = \{\mathbf{1}, \mathbf{i_3}\}$
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 $i_1 = i_2 = i_{12}$

$$\mathbf{P}^{(\mu)}_{mn} = \frac{\ell^{(\mu)}}{°G}\sum_{\mathbf{g}} D^{(\mu)*}_{mn}(g)\,\mathbf{g}$$

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

	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

	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

	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

•Eigenstates (shown before)

•Complete Hamiltonian

$$\begin{pmatrix} H+r_1+r_2+i_1+i_2+i_3 & & & \\ & H+r_1+r_2-i_1-i_2-i_3 & & \\ & & H-\frac{1}{2}r_1-\frac{1}{2}r_2-\frac{1}{2}i_1-\frac{1}{2}i_2+i_3 & \frac{\sqrt{3}}{2}(-r_1+r_2-i_1+i_2) \\ & & \frac{\sqrt{3}}{2}(+r_1-r_2-i_1+i_2) & H-\frac{1}{2}r_1-\frac{1}{2}r_2+\frac{1}{2}i_1+\frac{1}{2}i_2-i_3 \end{pmatrix}$$

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: $H - r + i - i_3$

$C_2=\{\mathbf{1},\mathbf{i}_3\}$

Local symmetry determines all levels and eigenvectors with just 4 real parameters

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

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

Global (LAB) symmetry

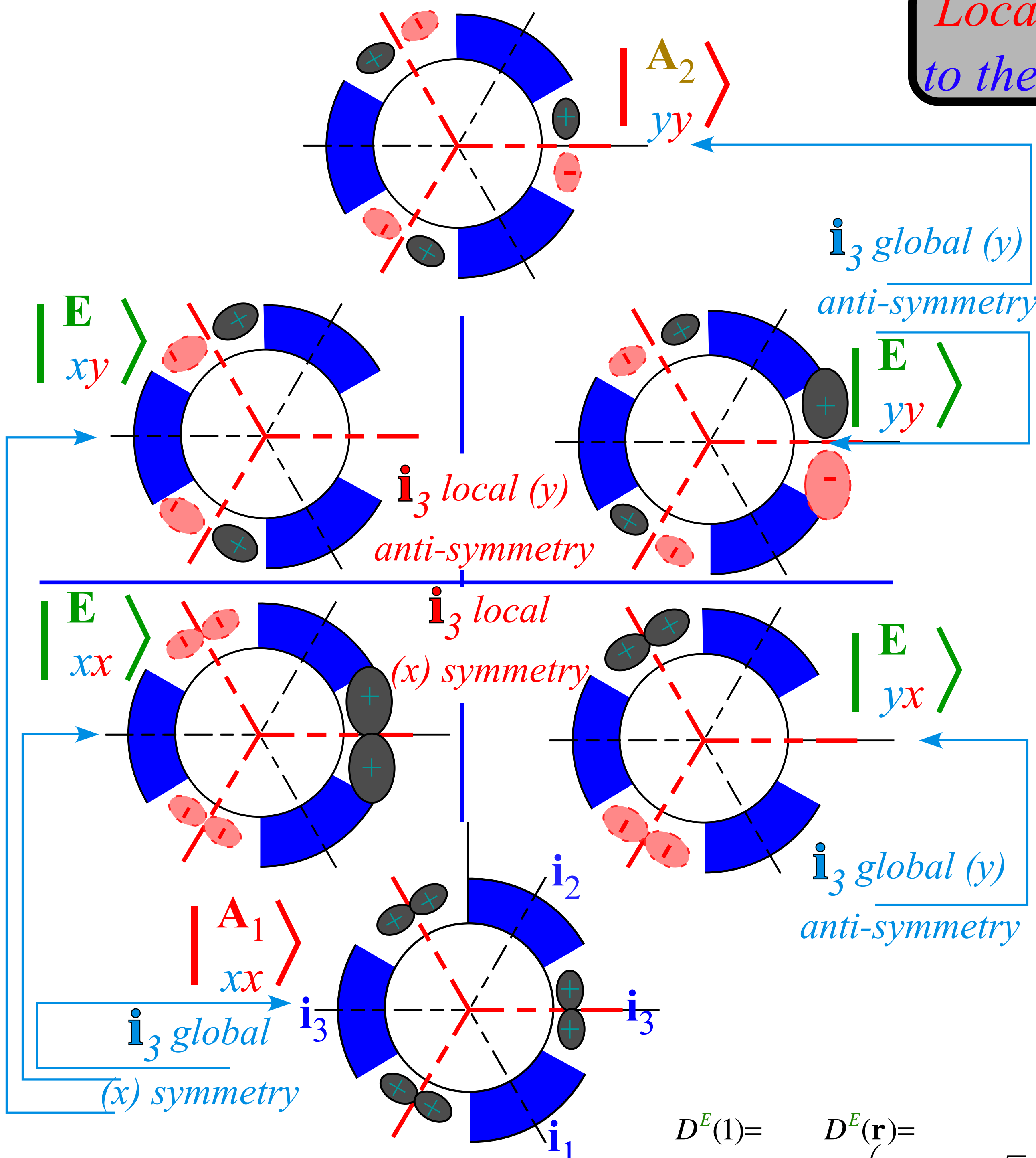
$$\mathbf{i}_3\left|{}^{(m)}_{eb}\right\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = (-1)^e\left|{}^{(m)}\right\rangle$$

Local (BOD) symmetry

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

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

Here the "Mock-Mach" is being applied!



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

$$D^{A_1}(\mathbf{g}) = +1,\quad D^{A_2}(\mathbf{r}^p) = +1,\quad D^{A_2}(\mathbf{i}_q) = -1$$

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

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

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

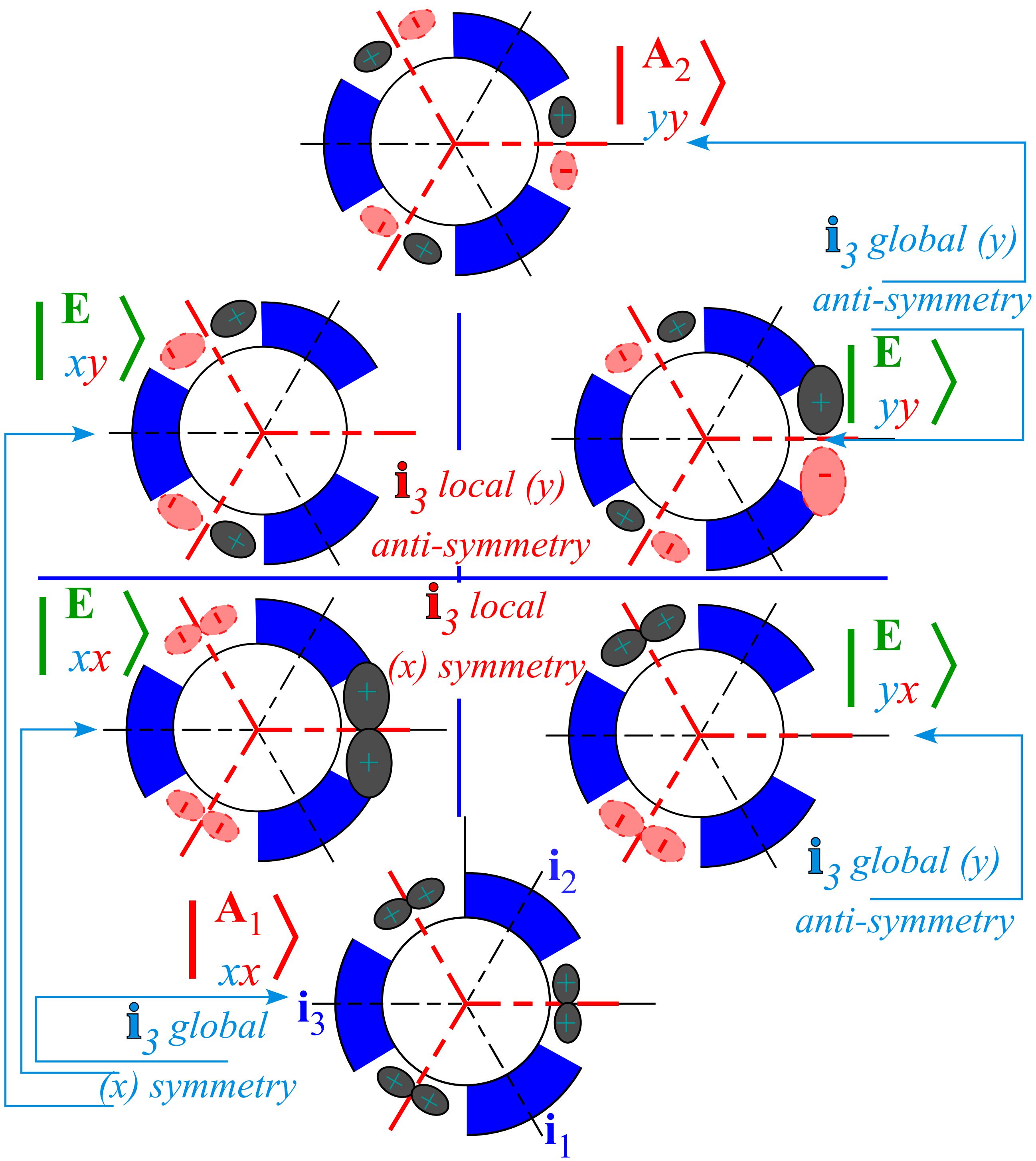
$$|^{(m)}_{eb}\rangle = \mathbf{P}^{(m)}_{eb}|1\rangle$$

Global (LAB) symmetry

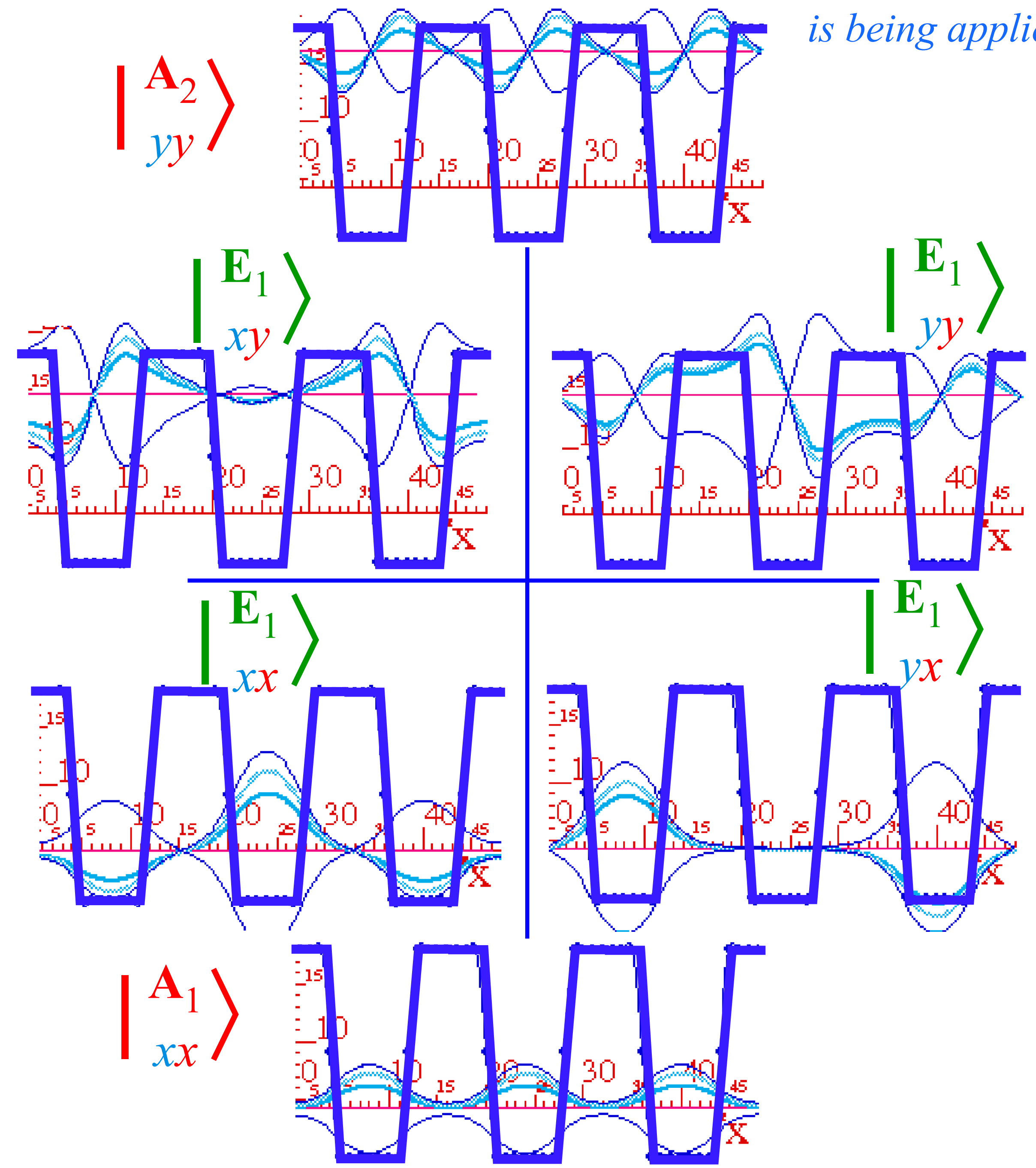
$$\mathbf{i}_3|^{(m)}_{eb}\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}|1\rangle = (-1)^e\,|^{(m)}\rangle$$

Local (BOD) symmetry

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

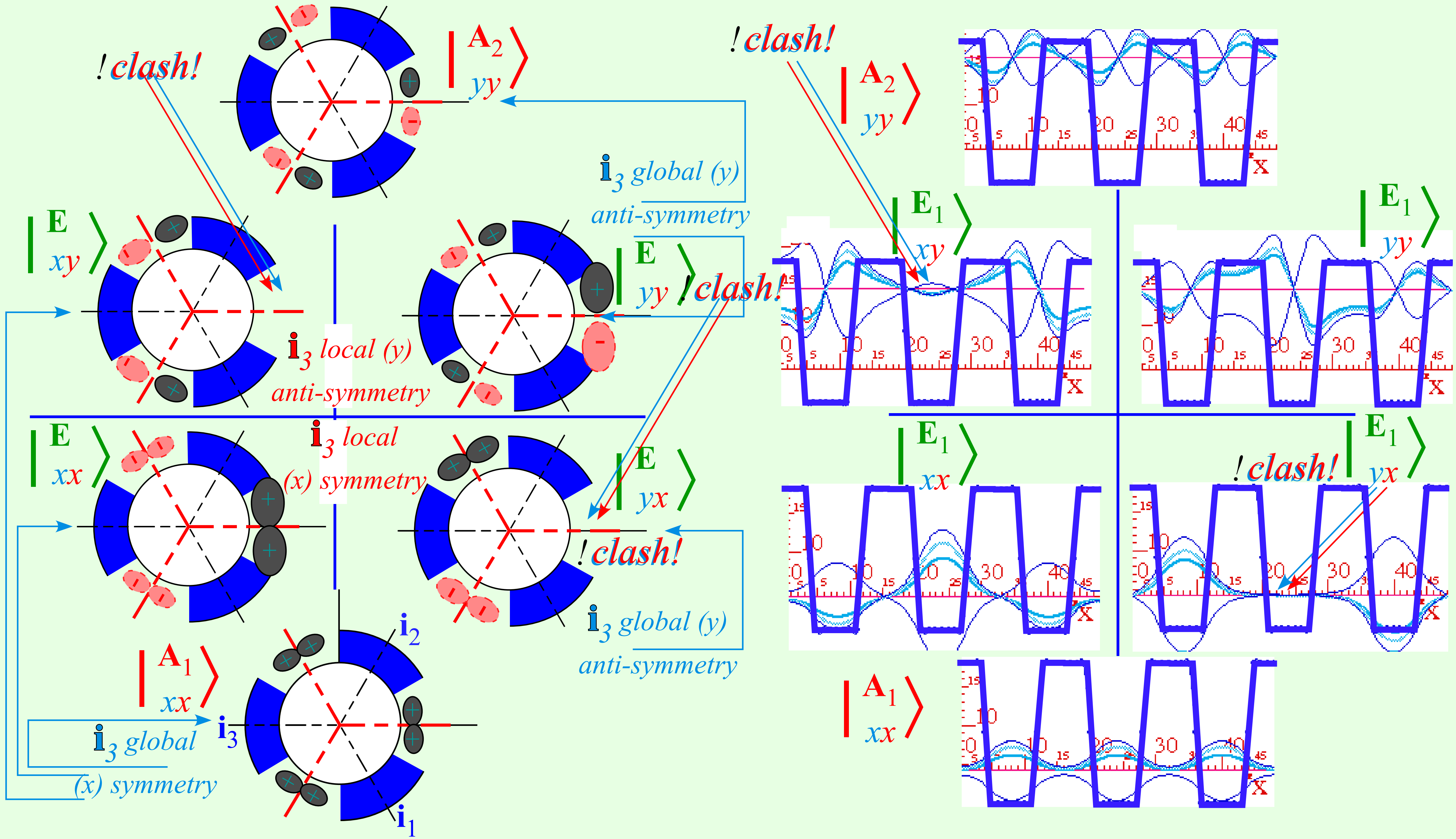


Here the "Mock-Mach" is being applied!



When there is no there, there...

Nobody Home
where LOCAL
and GLOBAL



Review Stage 1: Group Center:Class-sums $\kappa_{\mathbf{g}}$,characters $\chi^{\mu}(\mathbf{g})$, and All-Commuting Projectors $\mathbb{P}^{\mu}$

Review Stage 2: Group operators **g** *and Mutually-Commuting projectors $\mathbf{P}^{\mu}{}_{kk}$*

Review Stage 3: Weyl **g***-expansion in irreps $D^{\mu}{}_{jk}(g)$ and Non-Commuting projectors $\mathbf{P}^{\mu}{}_{jk}$*

Simple matrix algebra $\mathbf{P}^{\mu}{}_{ab}\mathbf{P}^{\nu}{}_{cd} = \delta^{\mu\nu}\delta_{bc}\mathbf{P}^{\mu}{}_{ad}$

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

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

Example of D_3 transformation by matrix $D^{E}{}_{jk}(\mathbf{r}^{1})$

Details of Mock-Mach relativity-duality for D_3 groups and representations

Lab-fixed(Extrinsic-Global) vs. Body-fixed (Intrinsic-Local)

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

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

Global vs. Local block rearrangement

Hamiltonion eigen-matrix calculation

Hamiltonian local-symmetry eigensolution

➔ *Molecular vibrational mode eigensolution* ⬅

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

Video Lecture 16 Ended here. Vibrations treated in Lecture 17