Group Theory in Quantum Mechanics

Lecture 16 (3.28.13)

Local-symmetry eigensolutions and vibrational modes

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(PSDS - Ch. 4)

Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}{}_{jk}(g)$ and projector $\mathbf{P}^{\mu}{}_{jk}$ transformation

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

Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

Local symmetry limit

Global symmetry limit (free or "genuine" modes)

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

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

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

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Group operators $\mathbf{g}$, irreducible representations $D^{\mu}(\mathbf{g})$, and irreducible projectors $\mathbf{P}^{\mu}{}_{mn}$

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

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

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

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

Projector conjugation

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

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Application of irreducible projectors $\mathbf{P}^{\mu}{}_{mn}$

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

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

irep expressions:

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irep expressions: *Just †-conjugates* *†-irep expressions:*

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Bra-Ket normalization: $$\left\langle\begin{smallmatrix}\mu'\\ m'n'\end{smallmatrix}\middle|\begin{smallmatrix}\mu\\ mn\end{smallmatrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}}{norm.}\frac{\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm*.} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'n}|\mathbf{1}\rangle}{|norm.|^{2}} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$ *(if D is unitary)*

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Algebra and geometry of irreducible $D^{\mu}{}_{jk}(g)$ and projector $\mathbf{P}^{\mu}{}_{jk}$ transformation

(All-commuting $\mathbb{P}^{\mu}$)

$$\mathbf{P}^{\mu'}_{m'm'}\mathbf{g}\mathbf{P}^{\mu}_{nn} = \delta^{\mu'\mu} D^{\mu}_{m'n}(g)\mathbf{P}^{\mu}_{m'n}$$

$$\mathbf{P}^{\mu'}_{m'm'}\mathbf{g}\mathbf{P}^{\mu}_{nn} = \mathbf{P}^{\mu'}_{m'm'}\mathbb{P}^{\mu'}\mathbf{g}\,\mathbb{P}^{\mu}\,\mathbf{P}^{\mu}_{nn}$$

is zero unless

$\mu'=\mu$ *since*

$\mathbb{P}^{\mu'}\mathbf{g}\mathbb{P}^{\mu}=\mathbb{P}^{\mu'}\mathbb{P}^{\mu}\mathbf{g}$

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This gives a general $D^{\mu}_{jk}(g)$ transformation matrix formula

$$\left\langle \mathbf{P}^{\mu'}_{m'j'} \middle| \mathbf{g} \middle| \mathbf{P}^{\mu}_{nk} \right\rangle = \left\langle \mathbf{1} \middle| \mathbf{P}^{\mu'}_{j'm'}\mathbf{g}\mathbf{P}^{\mu}_{nk} \middle| \mathbf{1} \right\rangle / \, norm^{\mu'}_{j'}\, norm^{\mu}_{k}$$

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$$= \boxed{D^{\mu}_{m'n}(g)\delta^{\mu'\mu}}\left\langle \mathbf{1}\middle|\mathbf{P}^{\mu'}_{j'm'}\boxed{\mathbf{P}^{\mu'}_{m'n}}\mathbf{P}^{\mu}_{nk}\middle|\mathbf{1}\right\rangle / \, norm^{\mu'}_{j'}\, norm^{\mu}_{k}$$

Algebra and geometry of irreducible $D^{\mu}_{jk}(g)$ and projector $\mathbf{P}^{\mu}_{jk}$ transformation

(All-commuting $\mathbb{P}^{\mu}$)

$$\mathbf{P}^{\mu'}_{m'm'}\mathbf{g}\mathbf{P}^{\mu}_{nn} = \delta^{\mu'\mu} D^{\mu}_{m'n}(g)\mathbf{P}^{\mu}_{m'n}$$

$$\mathbf{P}^{\mu}_{mm}\mathbf{g}\mathbf{P}^{\mu}_{nn} = D^{\mu}_{mn}(g)\mathbf{P}^{\mu}_{mn}$$

$$\mathbf{P}^{\mu'}_{m'm'}\mathbf{g}\mathbf{P}^{\mu}_{nn} = \mathbf{P}^{\mu'}_{m'm'}\mathbb{P}^{\mu'}\mathbf{g}\,\mathbb{P}^{\mu}\,\mathbf{P}^{\mu}_{nn}$$

is zero unless $\mu'=\mu$ *since* $\mathbb{P}^{\mu'}\mathbf{g}\mathbb{P}^{\mu}=\mathbb{P}^{\mu'}\mathbb{P}^{\mu}\mathbf{g}$

This gives a general $D^{\mu}_{jk}(g)$ transformation matrix formula

$$\left\langle \mathbf{P}^{\mu'}_{m'j'}\middle|\mathbf{g}\middle|\mathbf{P}^{\mu}_{nk}\right\rangle = \left\langle \mathbf{1}\middle|\mathbf{P}^{\mu'}_{j'm'}\mathbf{g}\mathbf{P}^{\mu}_{nk}\middle|\mathbf{1}\right\rangle / \, norm^{\mu'}_{j'}\, norm^{\mu}_{k}$$

$$= \left\langle \mathbf{1}\middle|\mathbf{P}^{\mu'}_{j'm'}\boxed{\mathbf{P}^{\mu'}_{m'm'}\mathbf{g}\mathbf{P}^{\mu}_{nn}}\mathbf{P}^{\mu}_{nk}\middle|\mathbf{1}\right\rangle / \, norm^{\mu'}_{j'}\, norm^{\mu}_{k}$$

$$= \boxed{D^{\mu}_{m'n}(g)\delta^{\mu'\mu}}\left\langle \mathbf{1}\middle|\mathbf{P}^{\mu'}_{j'm'}\boxed{\mathbf{P}^{\mu'}_{m'n}}\mathbf{P}^{\mu}_{nk}\middle|\mathbf{1}\right\rangle / \, norm^{\mu'}_{j'}\, norm^{\mu}_{k}$$

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$$= D^{\mu}_{m'n}(g)\left\langle \mathbf{1}\middle|\mathbf{P}^{\mu}_{j'k}\middle|\mathbf{1}\right\rangle / \,norm^{\mu'}_{j'}\,norm^{\mu}_{k}$$

$$\left\langle \mathbf{P}^{\mu'}_{m'j'}\middle|\mathbf{g}\middle|\mathbf{P}^{\mu}_{nk}\right\rangle = D^{\mu}_{m'n}(g)\delta_{j'k} \qquad \left(norm^{\mu}_{k} = \sqrt{\frac{\ell^{\mu}}{{}^{\circ}G}} \right)$$

Review: *Projector formulae and subgroup splitting*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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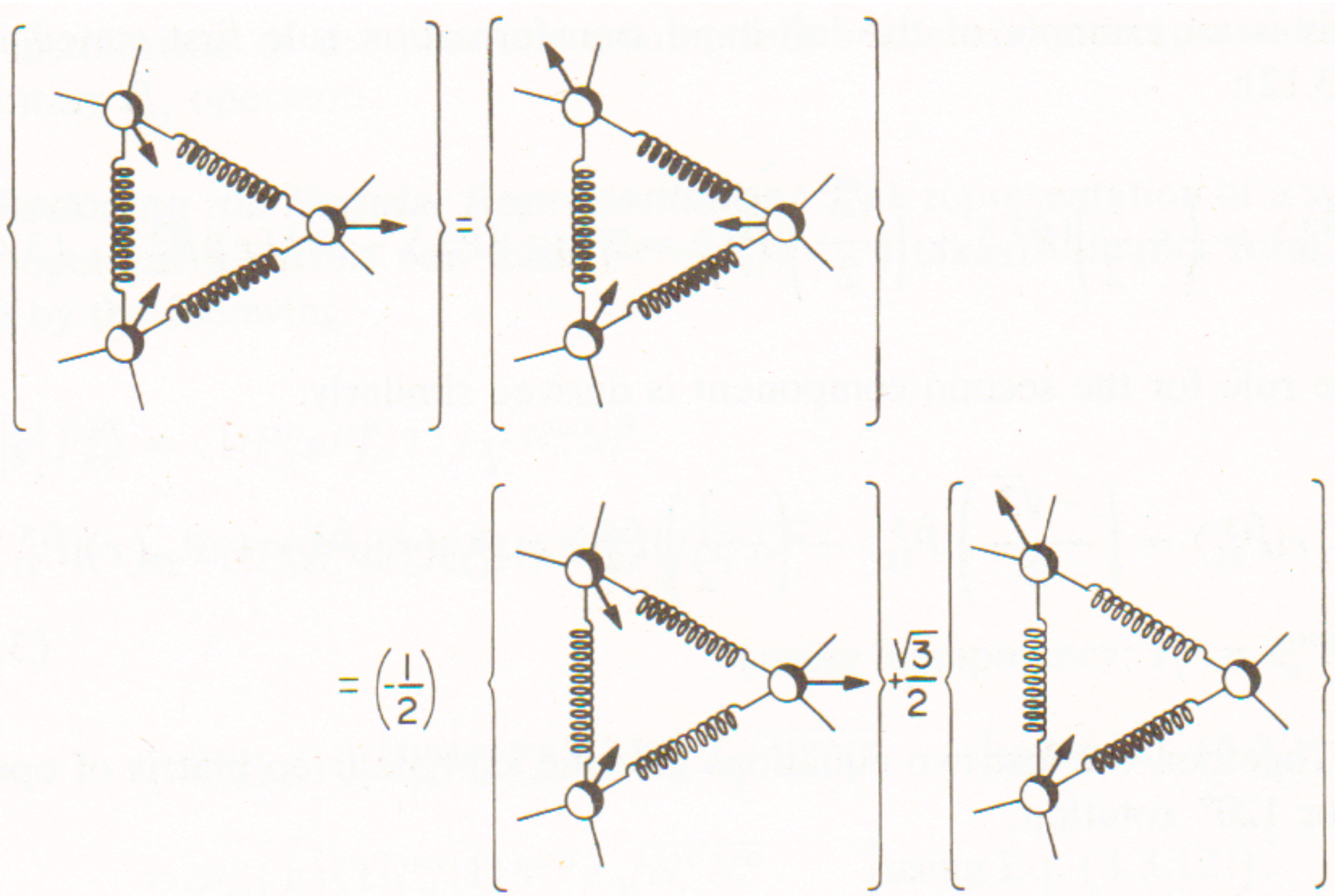
$-1/2 = D^{E_1}_{11}(r^1)$

$\mathbf{r}^1$



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

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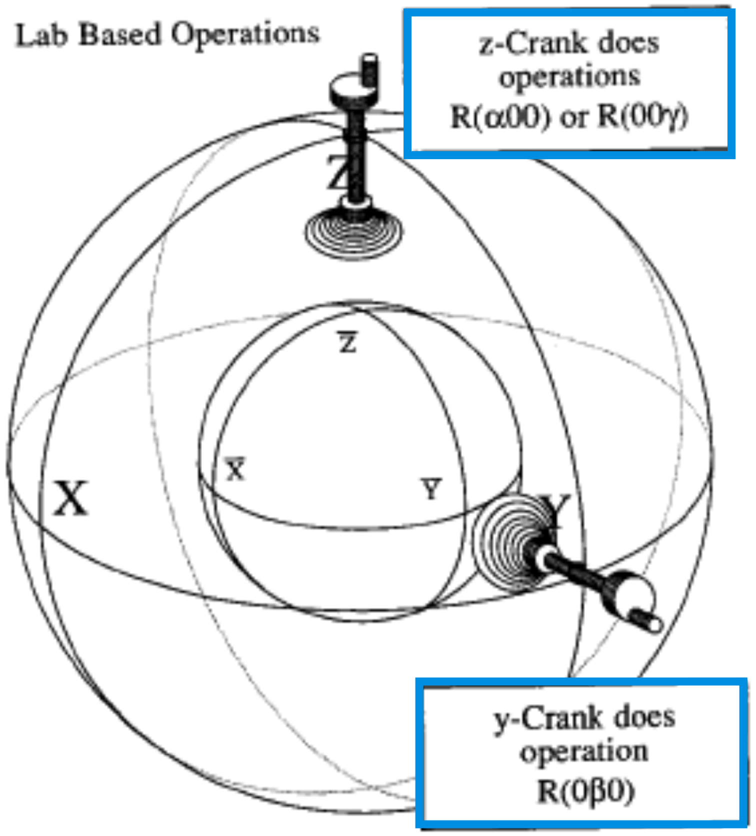
"Give me a place to stand...
and I will move the Earth"
Archimedes 287-212 B.C.E

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

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

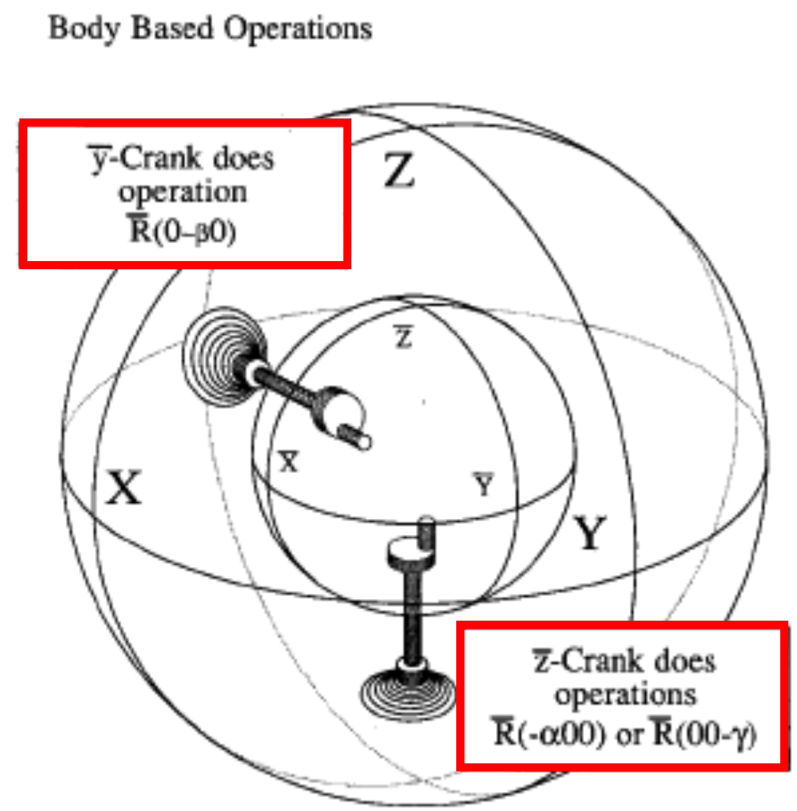


all **R**,**S**,..
commute with
all $\bar{\mathbf{R}}$,$\bar{\mathbf{S}}$,..

"Mock-Mach"
relativity principles

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

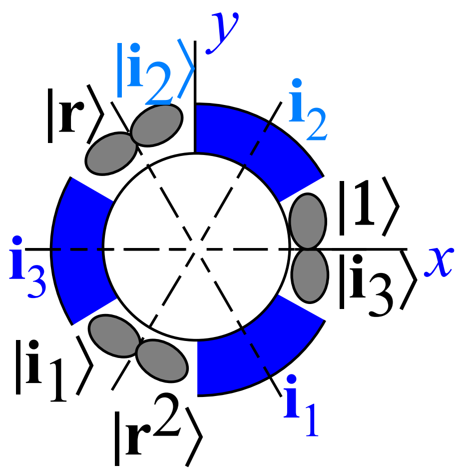
...for *one* state |1) *only!*

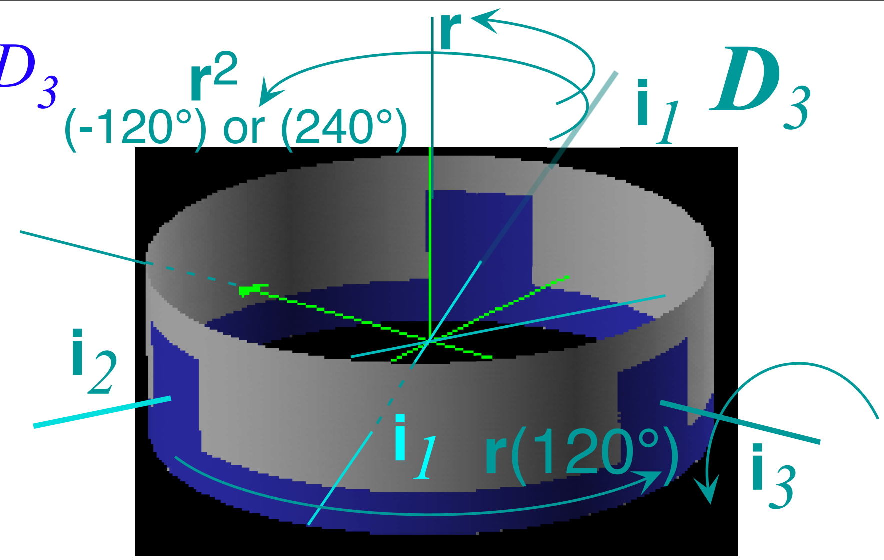


...But *how* do you actually *make* the **R** and $\bar{\mathbf{R}}$ operations?

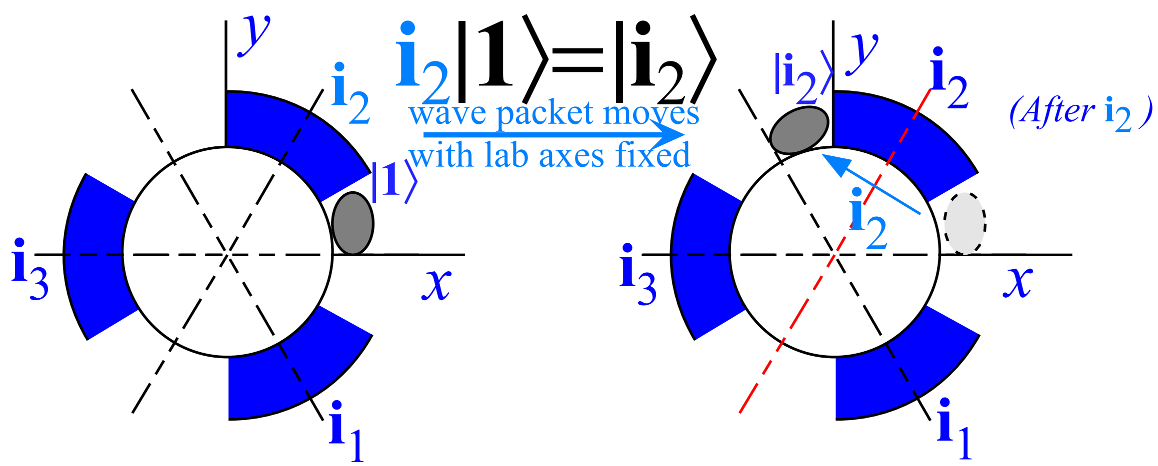
Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases





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



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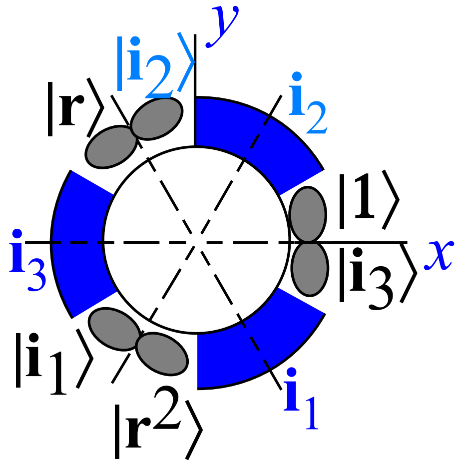
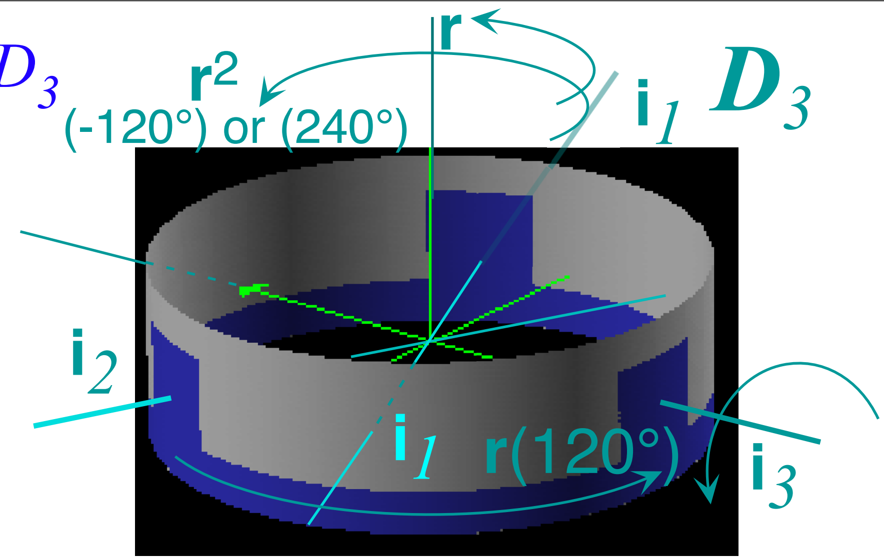
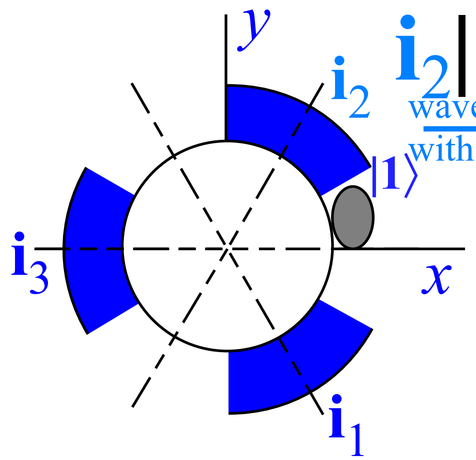


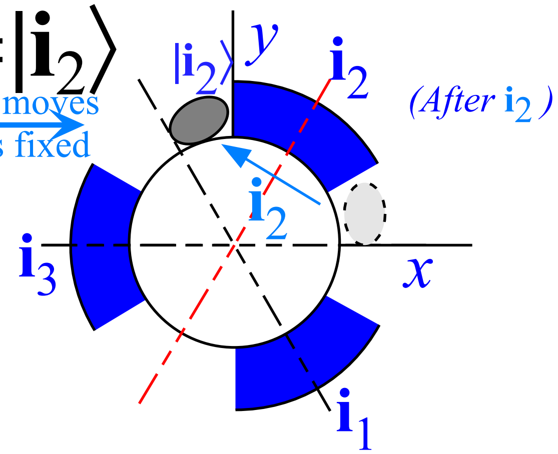


Lab-fixed (Extrinsic-Global) operations&axes fixed



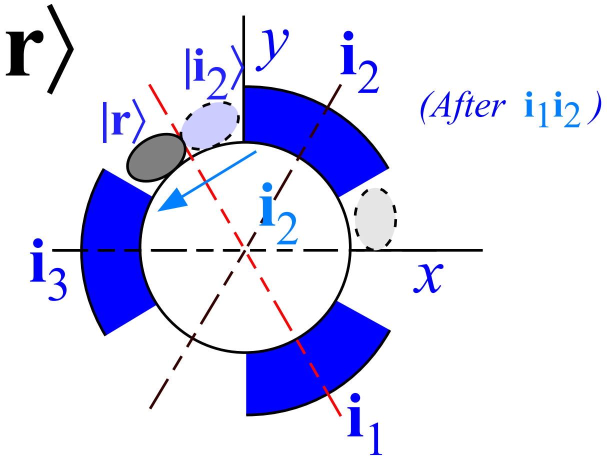
$\mathbf{i}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

wave packet moves with lab axes fixed



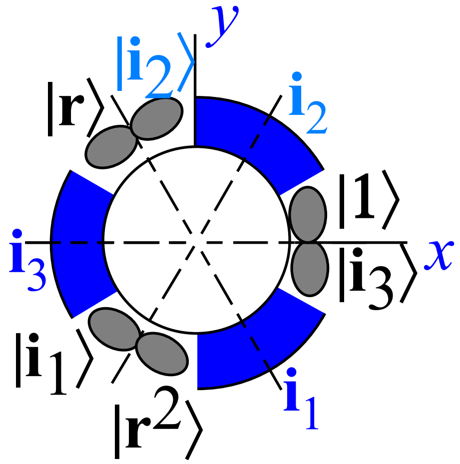
$\mathbf{i}_1\mathbf{i}_2|\mathbf{1}\rangle=\mathbf{r}|\mathbf{1}\rangle=|\mathbf{r}\rangle$

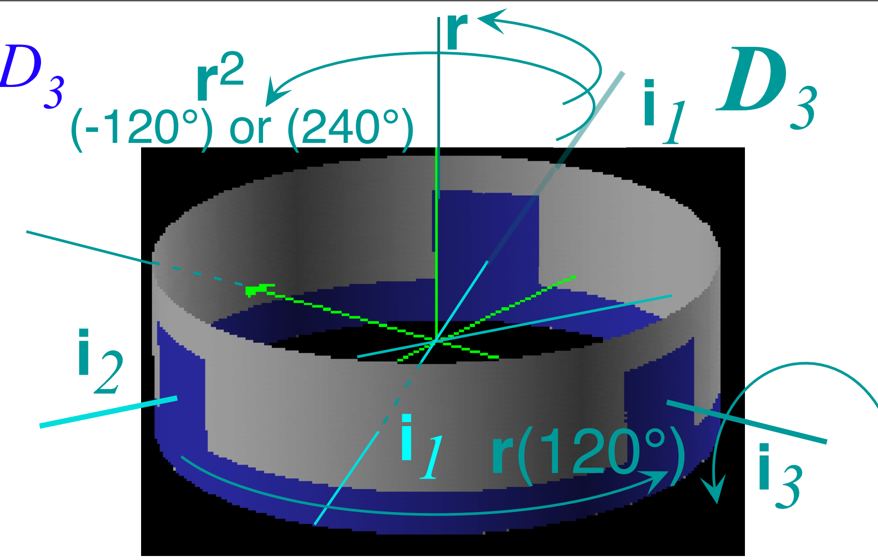
wave packet moves with lab axes fixed



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases





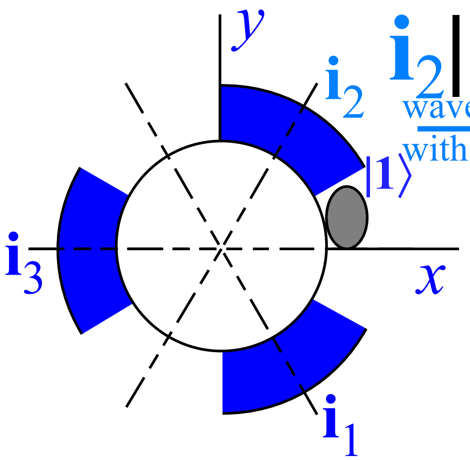
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

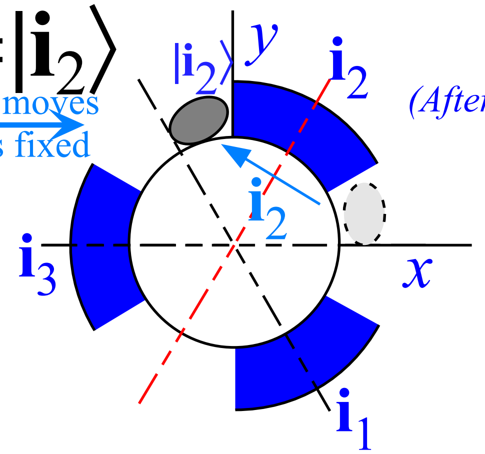
$\mathbf{i}_1\mathbf{i}_2 = \mathbf{r}$

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

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

wave packet moves with lab axes fixed

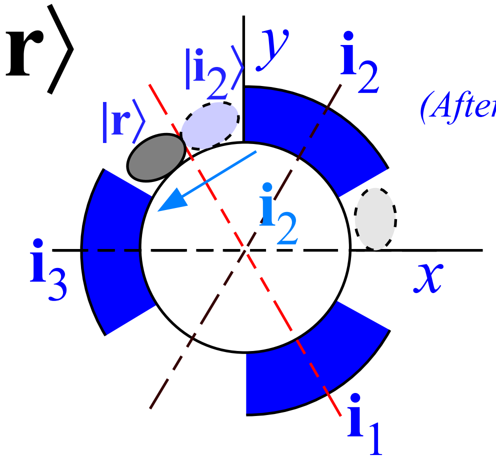




(After $\mathbf{i}_2$)

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

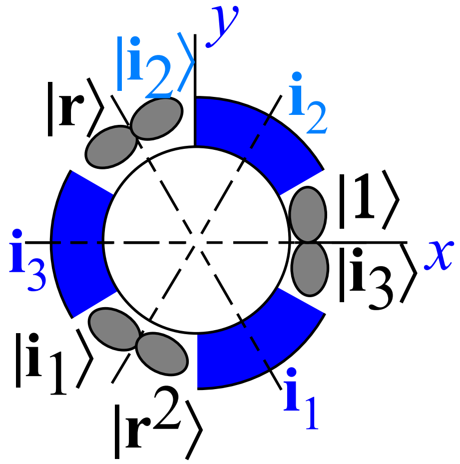
wave packet moves with lab axes fixed

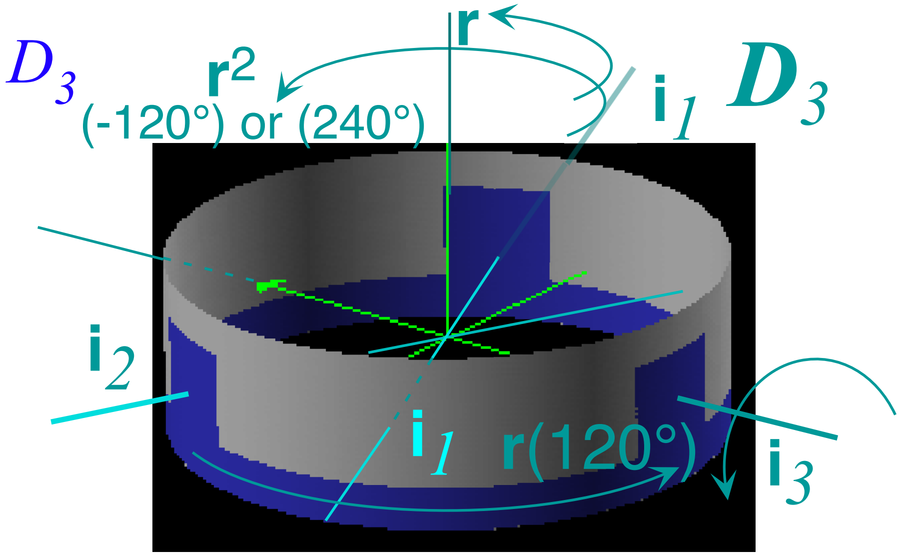


(After $\mathbf{i}_1\mathbf{i}_2$)

Details of RELATIVITY-DUALITY for D_3

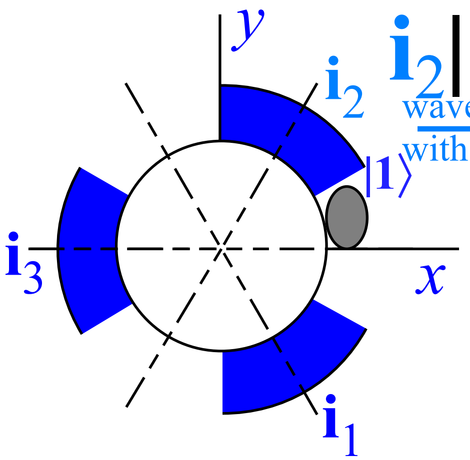
D_3-defined local-wave bases





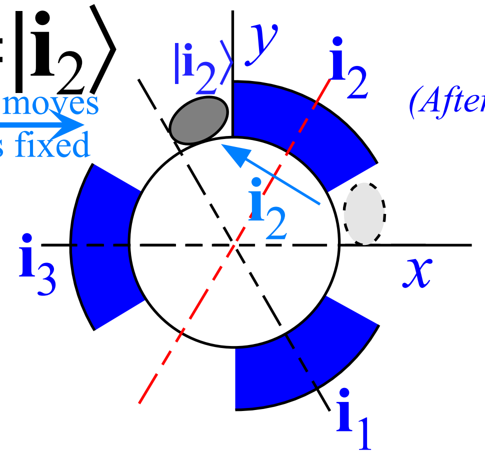
1	$\mathbf{r}^2$	**r**	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
r	**1**	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	**r**	**1**	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	**1**	**r**	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$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

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



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

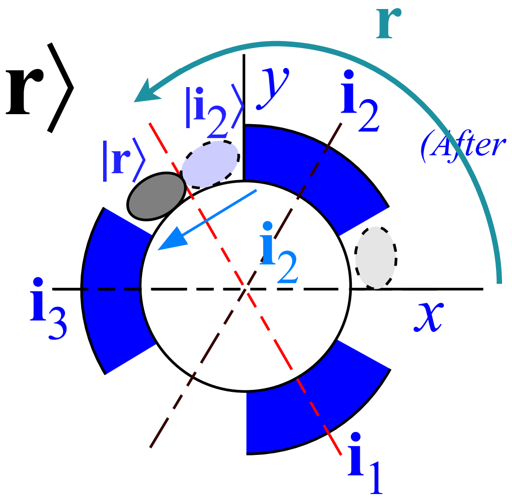
wave packet moves
with lab axes fixed



(After $\mathbf{i}_2$)

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

wave packet moves
with lab axes fixed

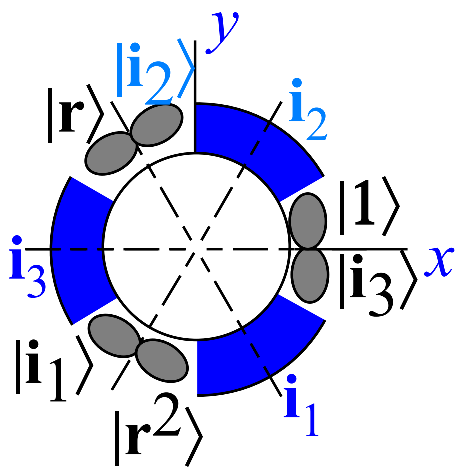


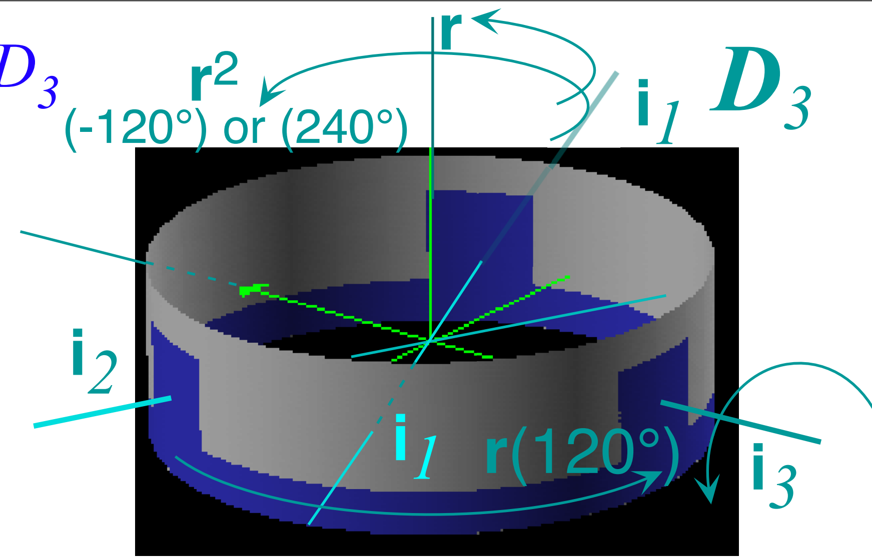
(After $\mathbf{i}_1\mathbf{i}_2$)

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

Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

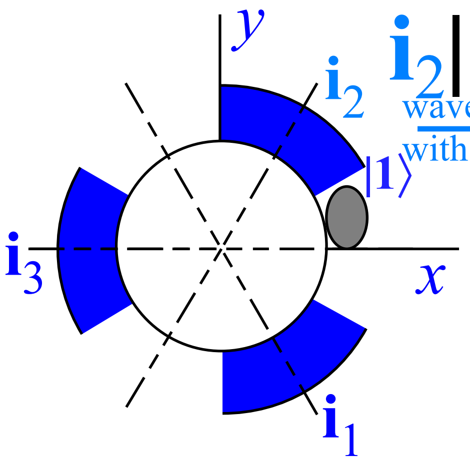




$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

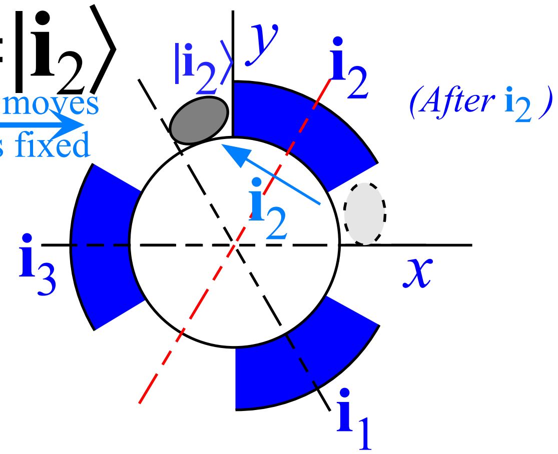
$\mathbf{i}_1\mathbf{i}_2=\mathbf{r}$

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



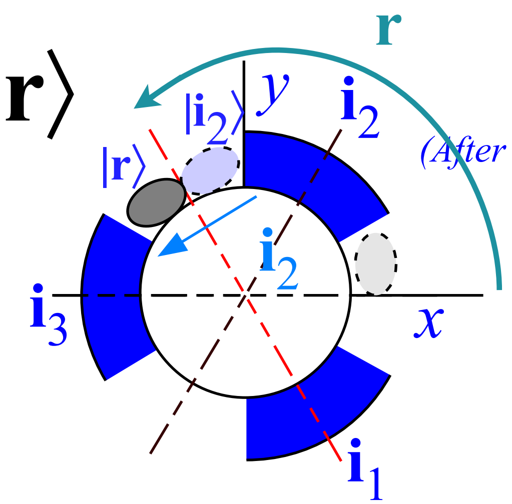
$\mathbf{i}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

wave packet moves with lab axes fixed



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

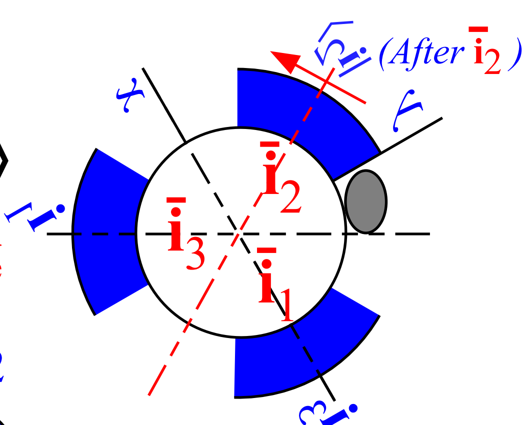
wave packet moves with lab axes fixed

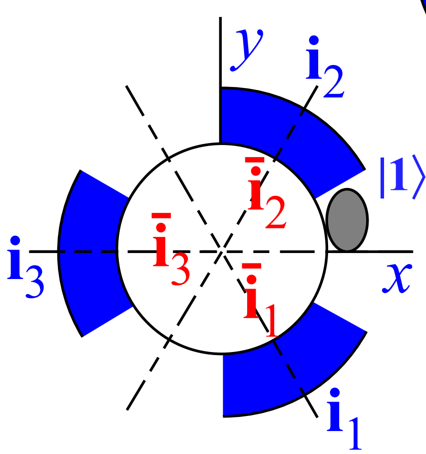


Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

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

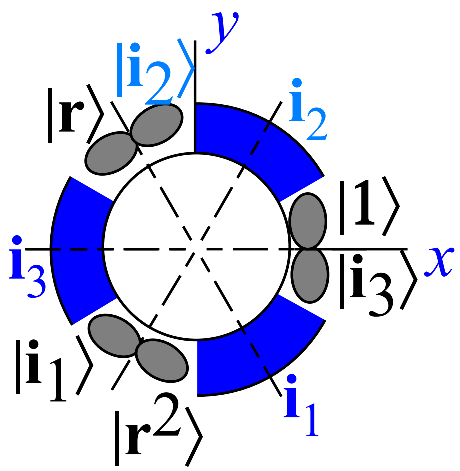
wave packet fixed while lab axes move

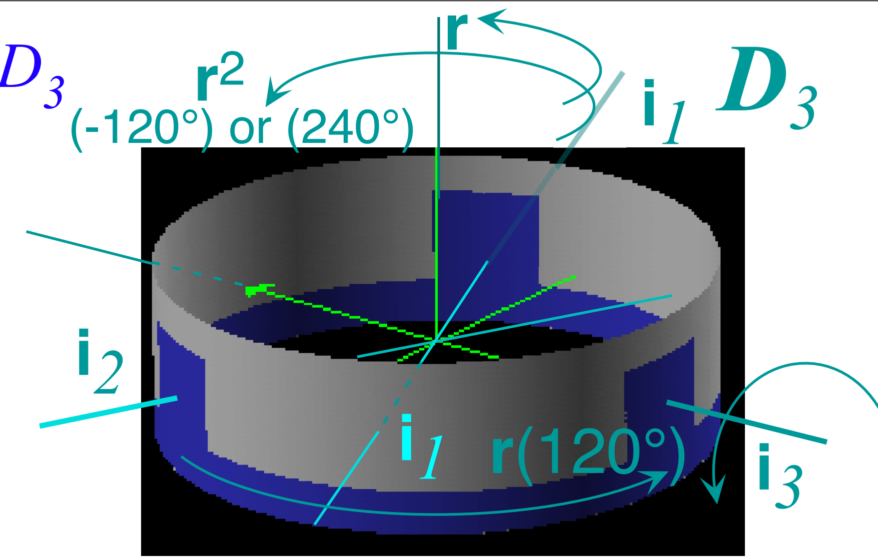




Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

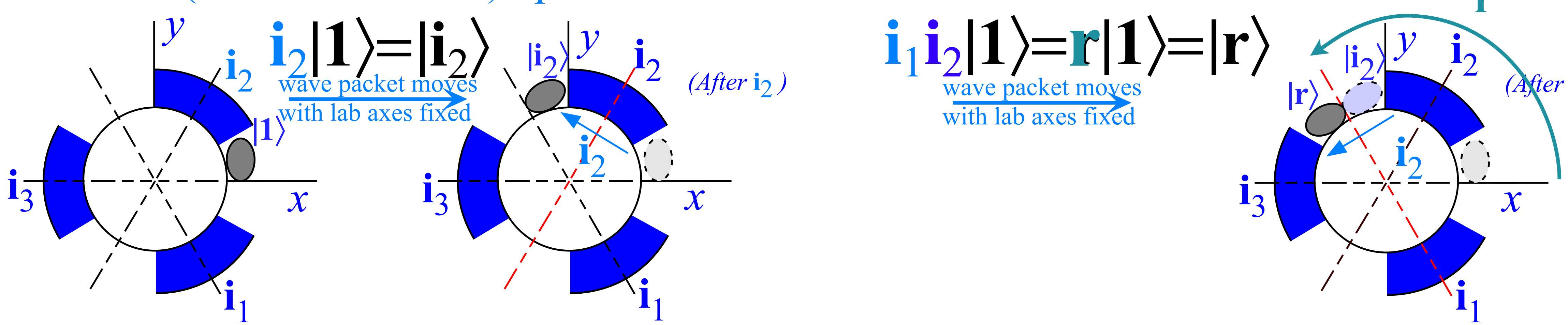




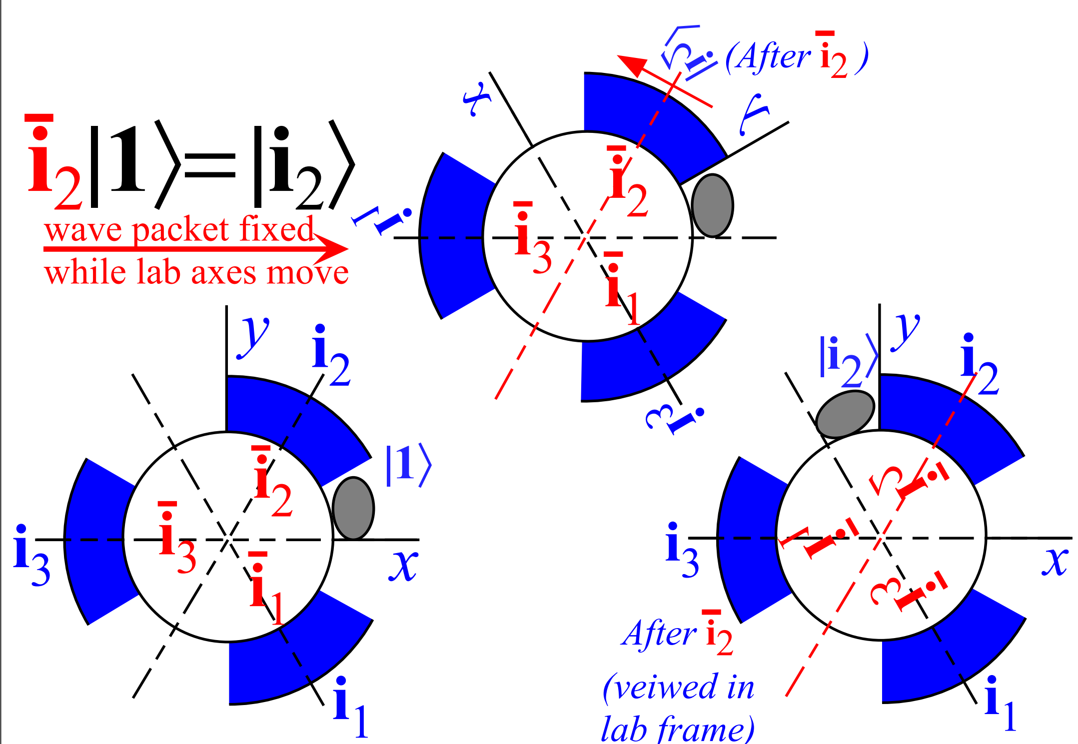
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

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

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

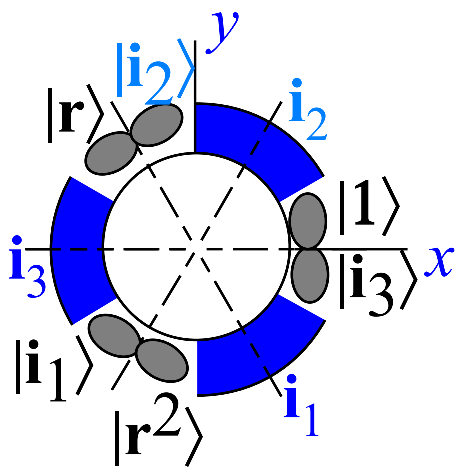


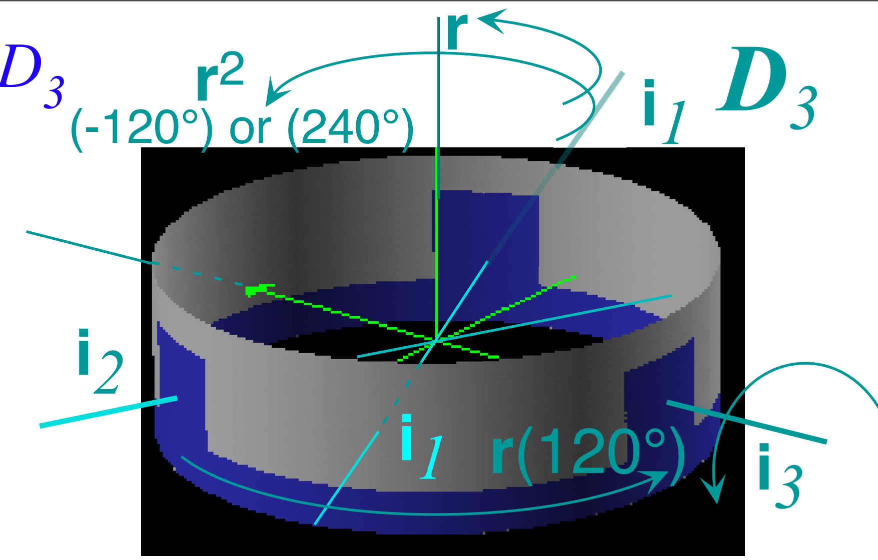
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases

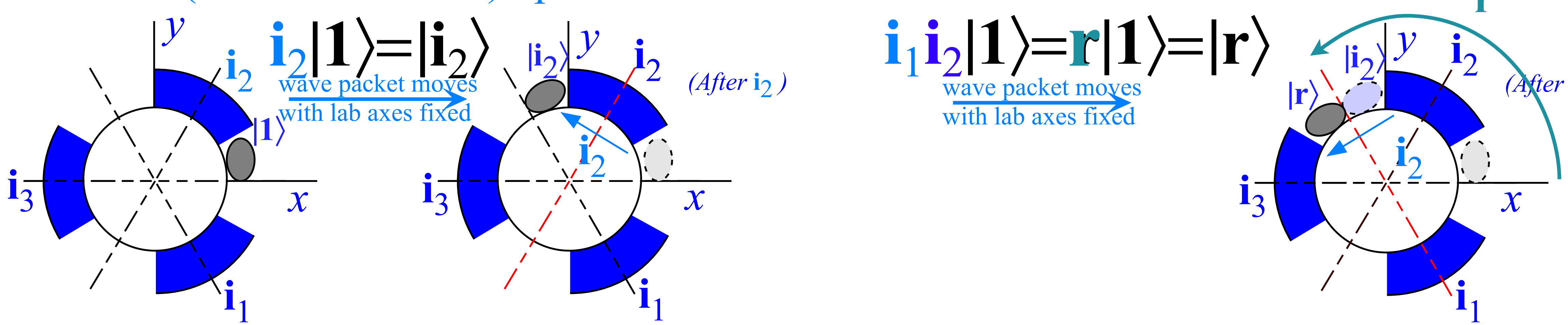




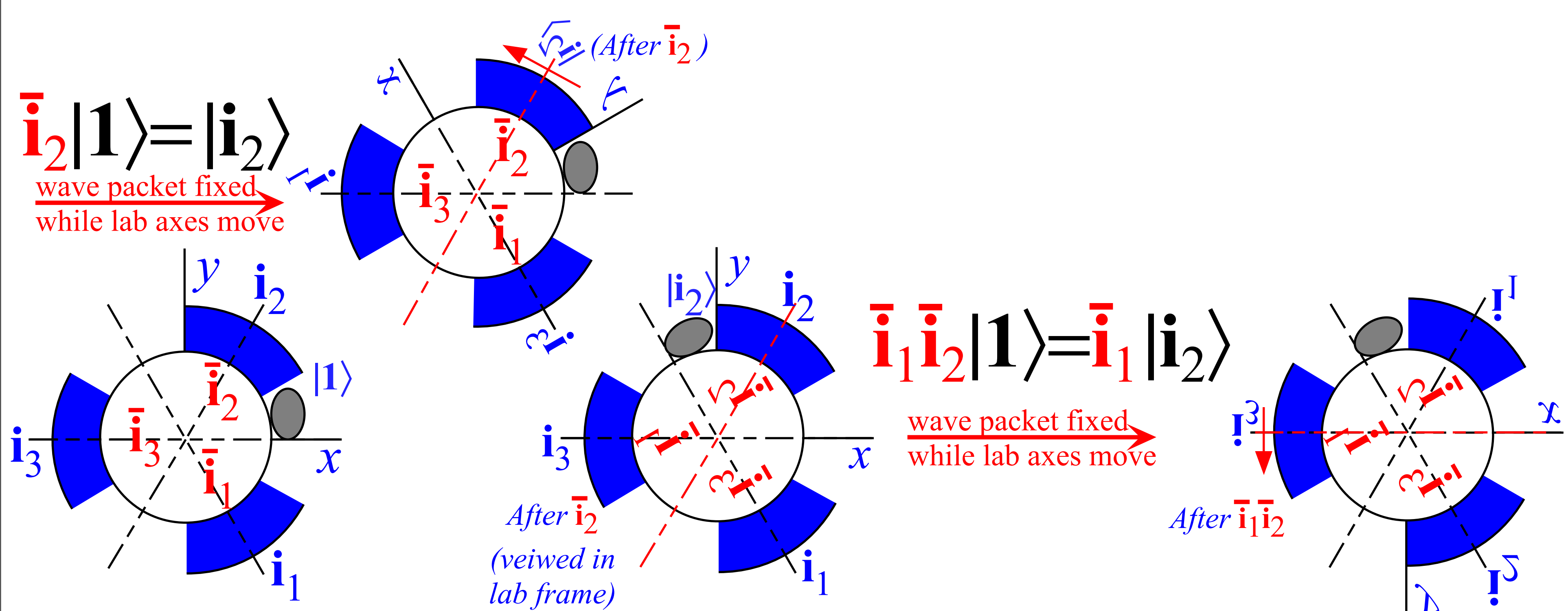
1	$\mathbf{r}^2$	**r**	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
r	**1**	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	**r**	**1**	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	**1**	**r**	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$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

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

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

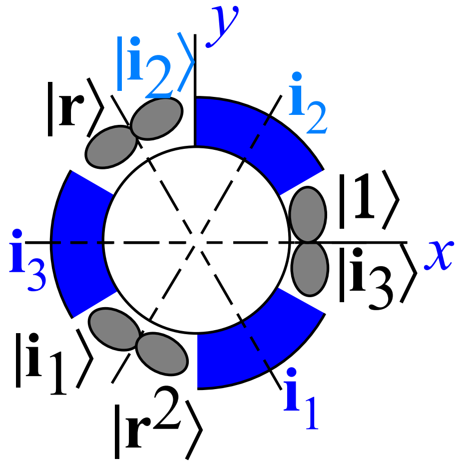


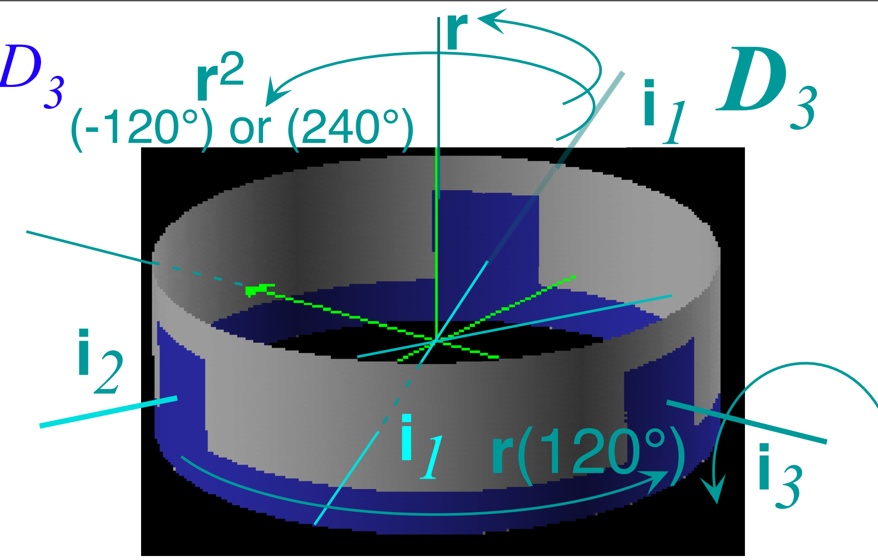
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)



Details of RELATIVITY-DUALITY for D_3

D_3-defined local-wave bases



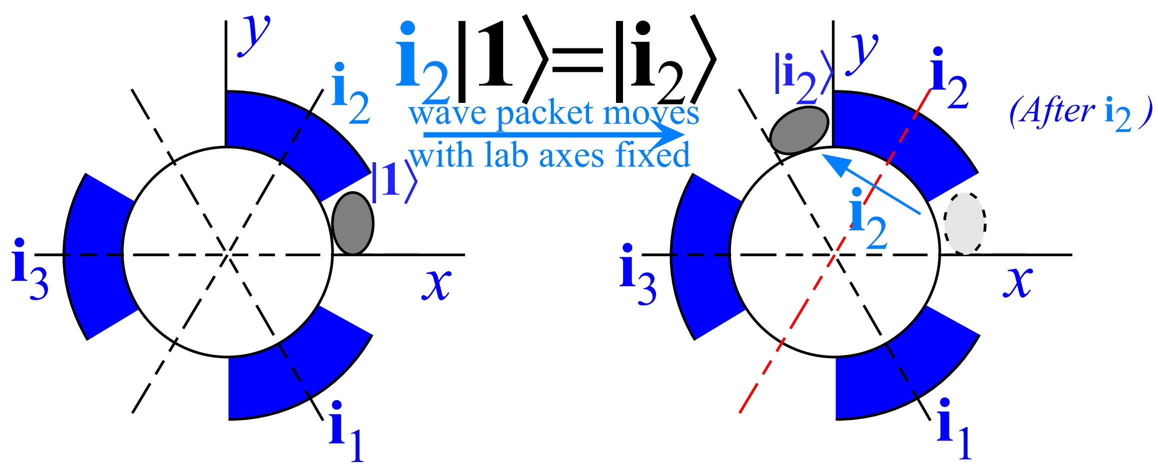


1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

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

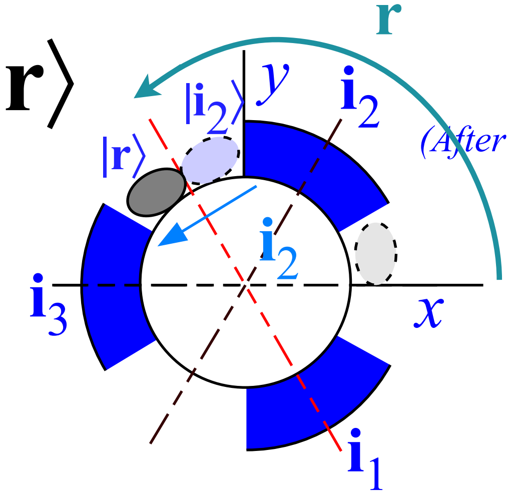
$i_2|1\rangle=|i_2\rangle$

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



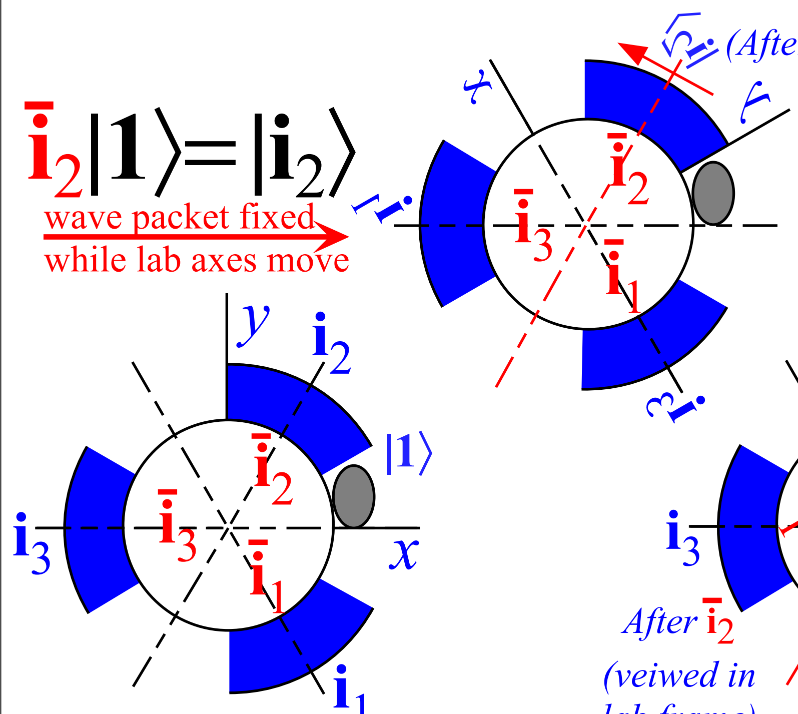
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

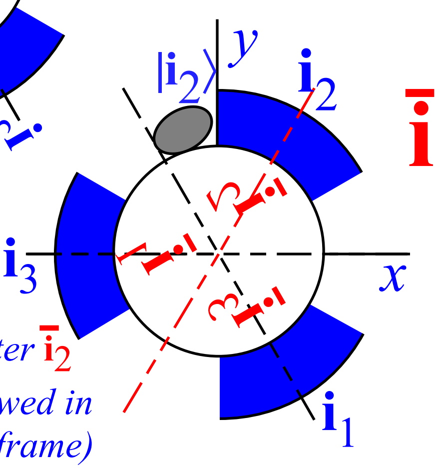
...but, THEY OBEY THE SAME GROUP TABLE.

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

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

wave packet fixed while lab axes move

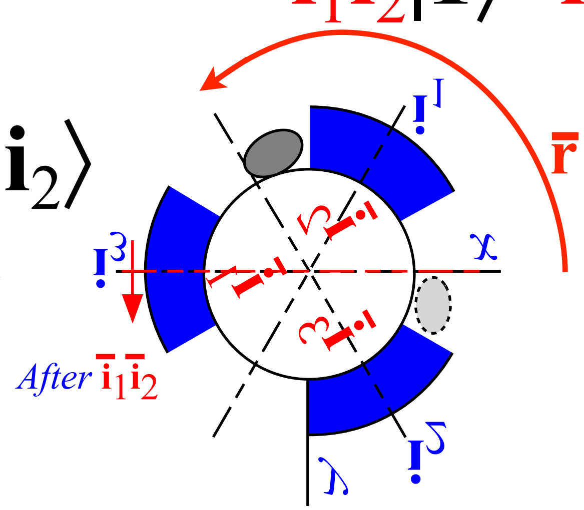




$\bar{i}_1\bar{i}_2|1\rangle=\bar{i}_1|i_2\rangle$

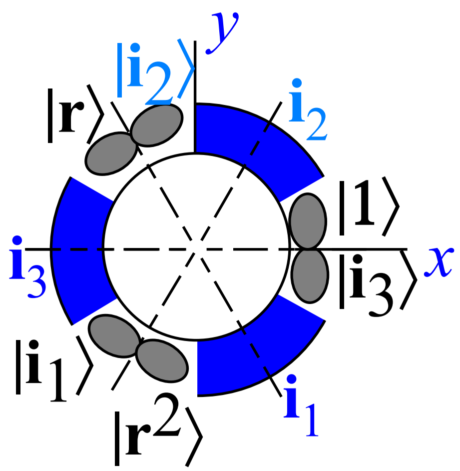
wave packet fixed while lab axes move

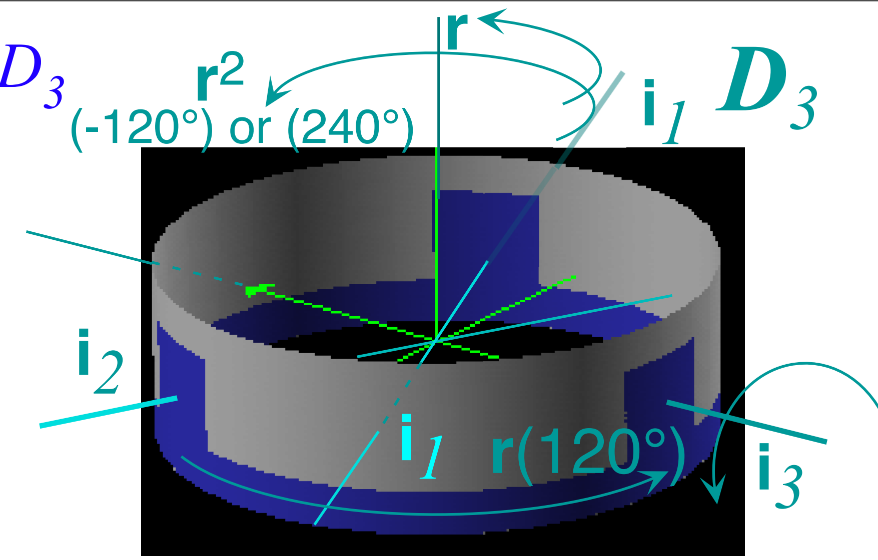
$\bar{i}_1\bar{i}_2|1\rangle=\bar{i}_1|i_2\rangle=\bar{r}|1\rangle$



Details of RELATIVITY-DUALITY for D_3

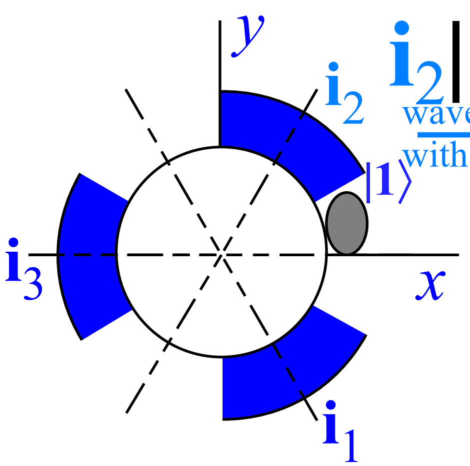
D_3-defined local-wave bases





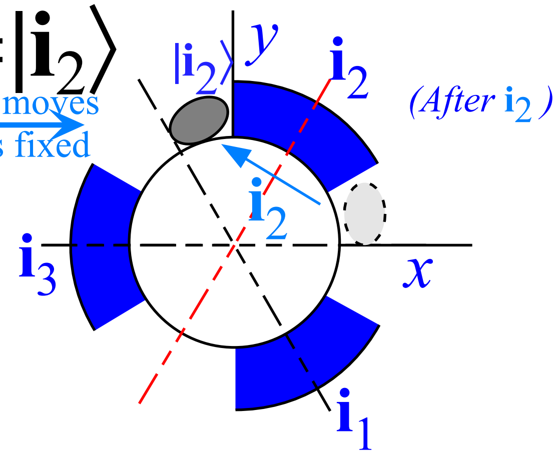
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

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



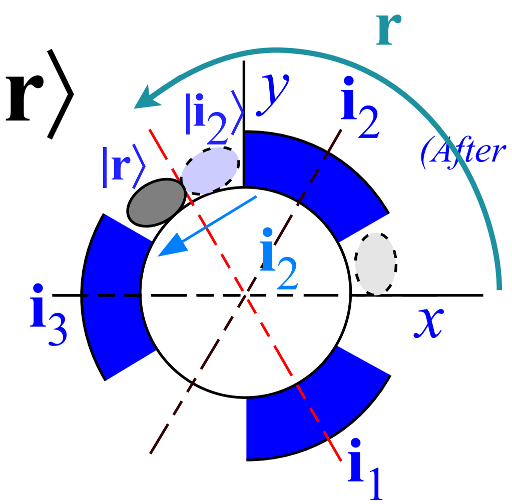
$\mathbf{i}_2|\mathbf{1}\rangle=|\mathbf{i}_2\rangle$

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)

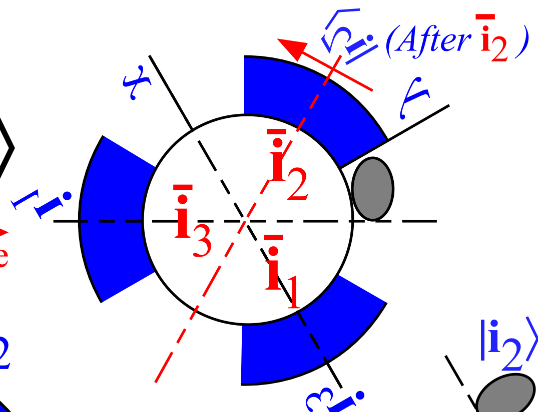
...but, THEY OBEY THE SAME GROUP TABLE.

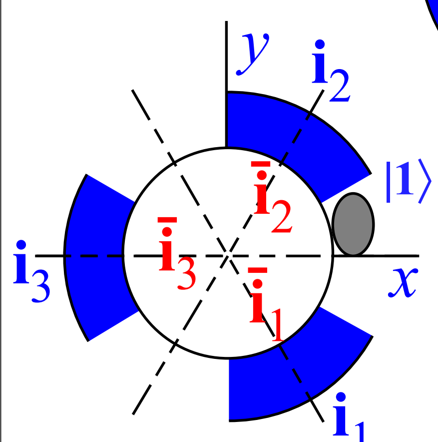
$\mathbf{i}_1\mathbf{i}_2=\mathbf{r}$ implies: $\bar{\mathbf{i}}_1\bar{\mathbf{i}}_2=\bar{\mathbf{r}}$

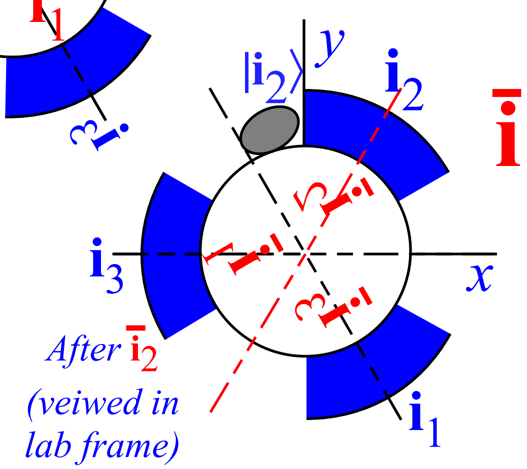
...and Mock-Mach principle $\bar{\mathbf{g}}|\mathbf{1}\rangle=\mathbf{g}^{-1}|\mathbf{1}\rangle$

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

wave packet fixed
while lab axes move



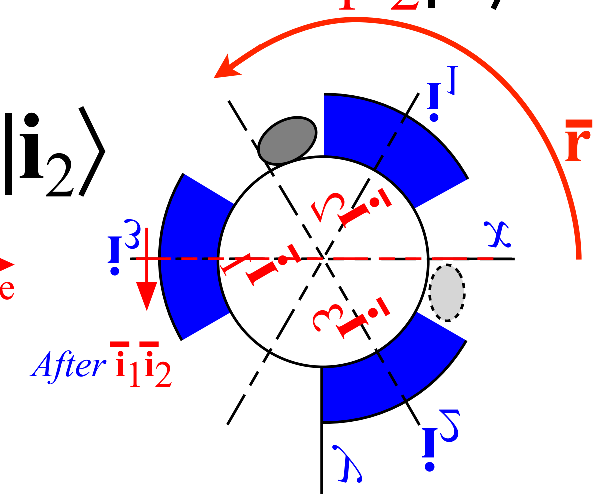


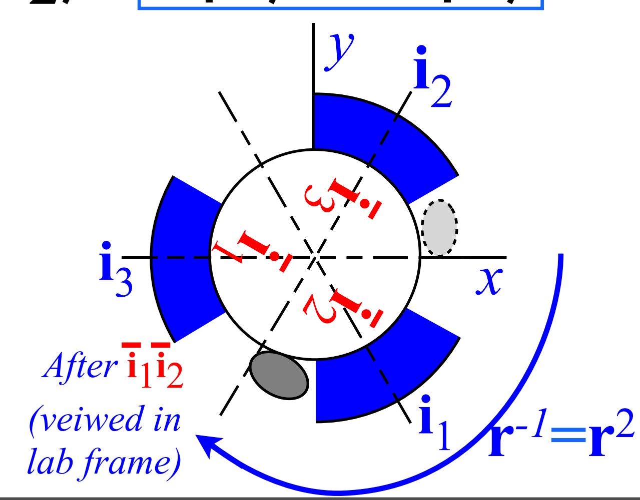


$\bar{\mathbf{i}}_1\bar{\mathbf{i}}_2|\mathbf{1}\rangle=\bar{\mathbf{i}}_1|\mathbf{i}_2\rangle=\boxed{\bar{\mathbf{r}}|\mathbf{1}\rangle=\mathbf{r}^2|\mathbf{1}\rangle}$

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

wave packet fixed
while lab axes move





Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}_{jk}(g)$ and projector $\mathbf{P}^{\mu}_{jk}$ transformation

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

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†

....and row-g with row-g†

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

D3 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

D3 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 $r^\dagger = r^2$. *(all others are self-conjugate)*

D3 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

D3 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 $D_3 \sim C_{3v}$

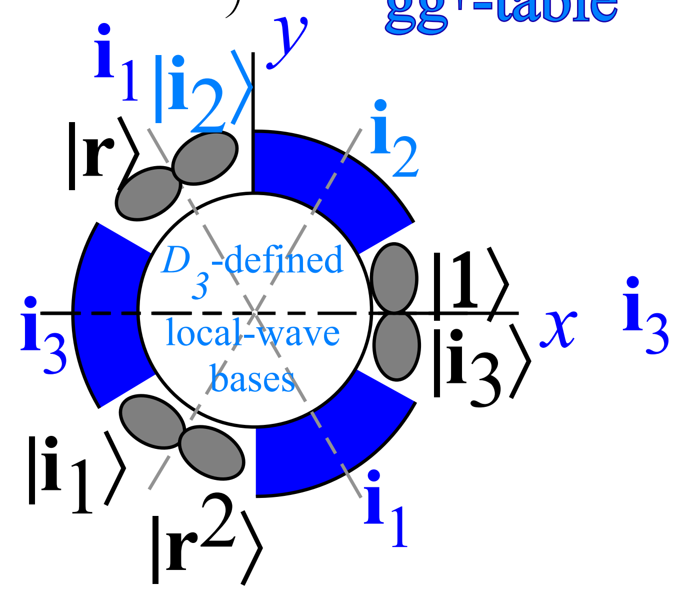
To represent *external* $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

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

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

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

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



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

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

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

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

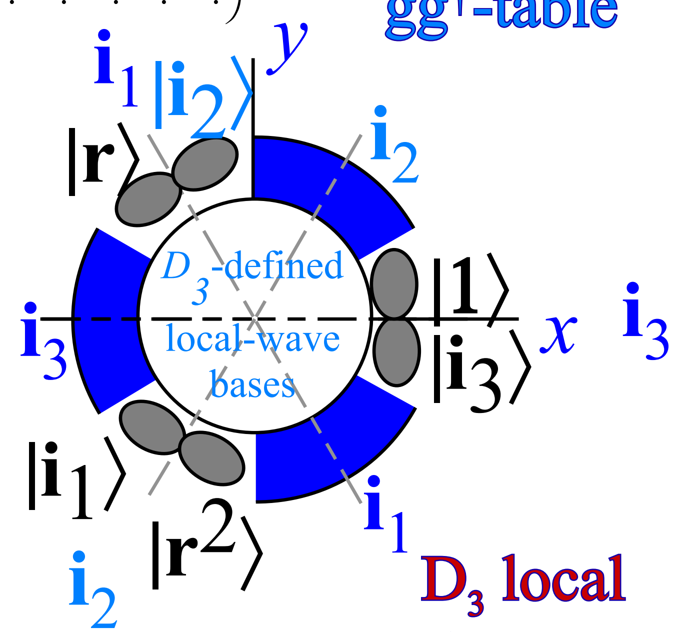
$$R^G(\mathbf{i}_1)=\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix},\quad R^G(\mathbf{i}_2)=\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\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

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

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

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

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



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

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

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

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

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

Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}{}_{jk}(g)$ *and projector* $\mathbf{P}^{\mu}{}_{jk}$ *transformation*

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*

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

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

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

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

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

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

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

$\overline{\mathbf{P}}^{(m)}_{ab}$ *...for LOCAL* $\overline{\mathbf{g}}$ *operators in* $\overline{D_3}$

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

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

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

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

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

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

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

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

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

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

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

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

Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}_{jk}(g)$ and projector $\mathbf{P}^{\mu}_{jk}$ transformation

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* ⬅

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.8-11 or p.33 Lect. 15)

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

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

For unitary $D^{(\mu)}$: (p.8-11)

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

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

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

For unitary $D^{(\mu)}$: (p.8-11)

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

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

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.8-11)

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

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

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

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.8-11)

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

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

subject to normalization:

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

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.8-11)

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

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

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

For unitary $D^{(\mu)}$: (p.8-11)

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

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

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

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

For unitary $D^{(\mu)}$: (p.8-11)

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

$$\left\langle\begin{matrix}\mu'\\ m'n'\end{matrix}\middle|\begin{matrix}\mu\\ mn\end{matrix}\right\rangle = \frac{\langle\mathbf{1}|\mathbf{P}^{\mu'}_{n'm'}\mathbf{P}^{\mu}_{mn}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\frac{\langle\mathbf{1}|\mathbf{P}^{\mu}_{n'n}|\mathbf{1}\rangle}{norm^2} = \delta^{\mu'\mu}\delta_{m'm}\delta_{n'n}$$ *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.11

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

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.8-11)

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

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

subject to normalization:

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

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

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.11

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

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

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

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

Use Mock-Mach commutation and

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

For unitary $D^{(\mu)}$: (p.8-11)

$|\mathbf{P}^{(\mu)}\rangle$*-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.11

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

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

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

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.8-11)

$|\mathbf{P}^{(\mu)}\rangle$-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.11

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

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

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

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

For unitary $D^{(\mu)}$: (p.8-11)

$|\mathbf{P}^{(\mu)}\rangle$-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.11

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

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

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

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

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

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.8-11)

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

subject to normalization:

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

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.11

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

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

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

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

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

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

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:

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

subject to normalization:

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

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

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.11

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

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

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

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

Use Mock-Mach commutation and inverse

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

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

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

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

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

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

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

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.11

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

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

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

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

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

Use Mock-Mach commutation and inverse

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

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

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.8-11)

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

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

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

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.11

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

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

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

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

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

Use Mock-Mach commutation and inverse

Global $\mathbf{g}$-matrix component

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

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

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

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*

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

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

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

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

Global **g***-matrix component*

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

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

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

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

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

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

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

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

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*

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

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

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

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*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}_{jk}(g)$ and projector $\mathbf{P}^{\mu}_{jk}$ transformation

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

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:*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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. 11):

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

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

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

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

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

Projector conjugation

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

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

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

subject to normalization (from p. 11):

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

(which will cancel out)

So, fuggettabout it!

D_3 Hamiltonian *local*- **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:

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

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

Mock-Mach commutation

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

(p.31)

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

subject to normalization (from p. 11):

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

(which will cancel out)

So, fuggettabout it!

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

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

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

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

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

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

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.18)

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

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

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

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

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

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

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

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

subject to normalization (from p. 11):

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

(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:

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

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

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

subject to normalization (from p. 11):

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:*

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

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

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

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

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

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

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

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

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

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:*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

D_3 Hamiltonian *local*- $\mathbf{H}$ 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:*

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

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

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

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

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

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

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

$C_2 = \{\mathbf{1}, \mathbf{i}_3\}$
Local symmetry determines all levels and eigenvectors with just 4 real parameters

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

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

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

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

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

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

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

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

$$\begin{pmatrix} \underbrace{\boxed{H+r_1+r_2+i_1+i_2+i_3}}_{A_1\text{-block}} & & & \\ & \underbrace{\boxed{H+r_1+r_2-i_1-i_2-i_3}}_{A_2\text{-block}} & & \\ & & H-\frac{1}{2}r_1-\frac{1}{2}r_2-\frac{1}{2}i_1-\frac{1}{2}i_2+i_3 & \frac{\sqrt{3}}{2}(-r_1+r_2-i_1+i_2) \\ & & \frac{\sqrt{3}}{2}(+r_1-r_2-i_1+i_2) & H-\frac{1}{2}r_1-\frac{1}{2}r_2+\frac{1}{2}i_1+\frac{1}{2}i_2-i_3 \end{pmatrix}$$

- *Local symmetery eigenvalue formulae* (L.S.=> off-diagonal zero.)

$C_2=\{\mathbf{1},\mathbf{i}_3\}$
Local symmetry determines all levels and eigenvectors with just 4 real parameters

$r_1=r_2=r_1{}^*=r,\qquad i_1=i_2=i_1{}^*=i$

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: $H-r+i-i_3$

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

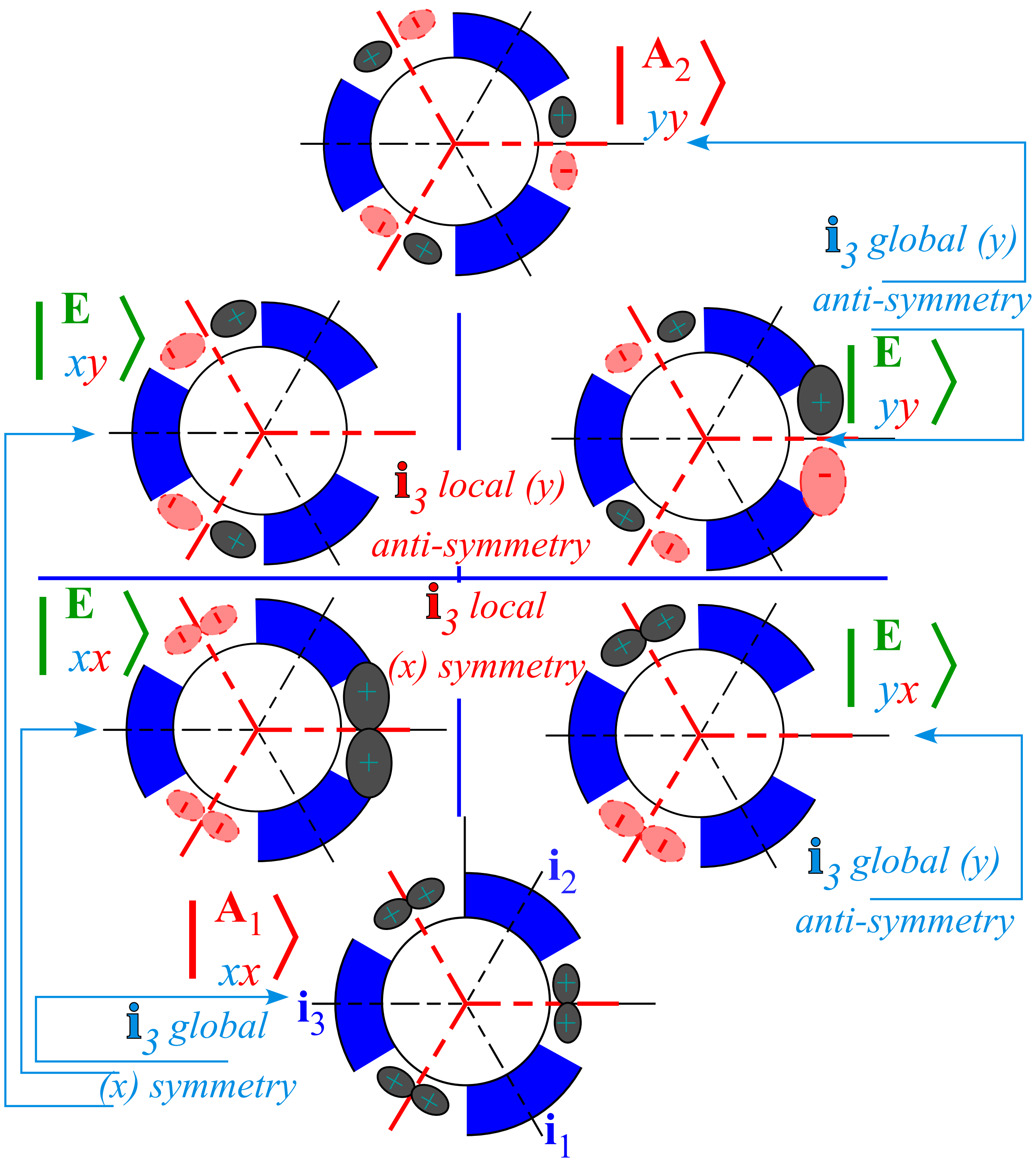
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

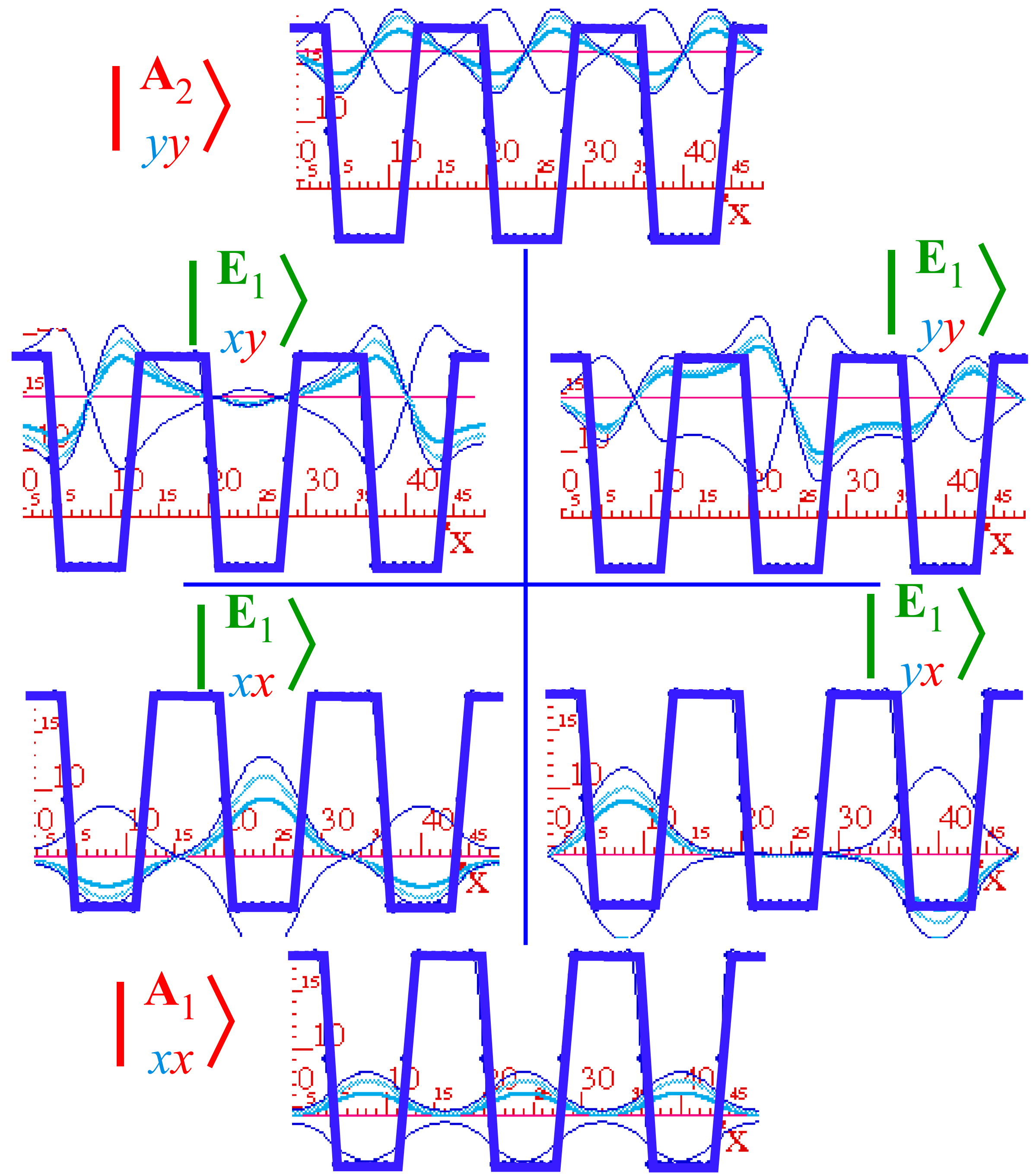
Global (LAB) symmetry

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

Local (BOD) symmetry

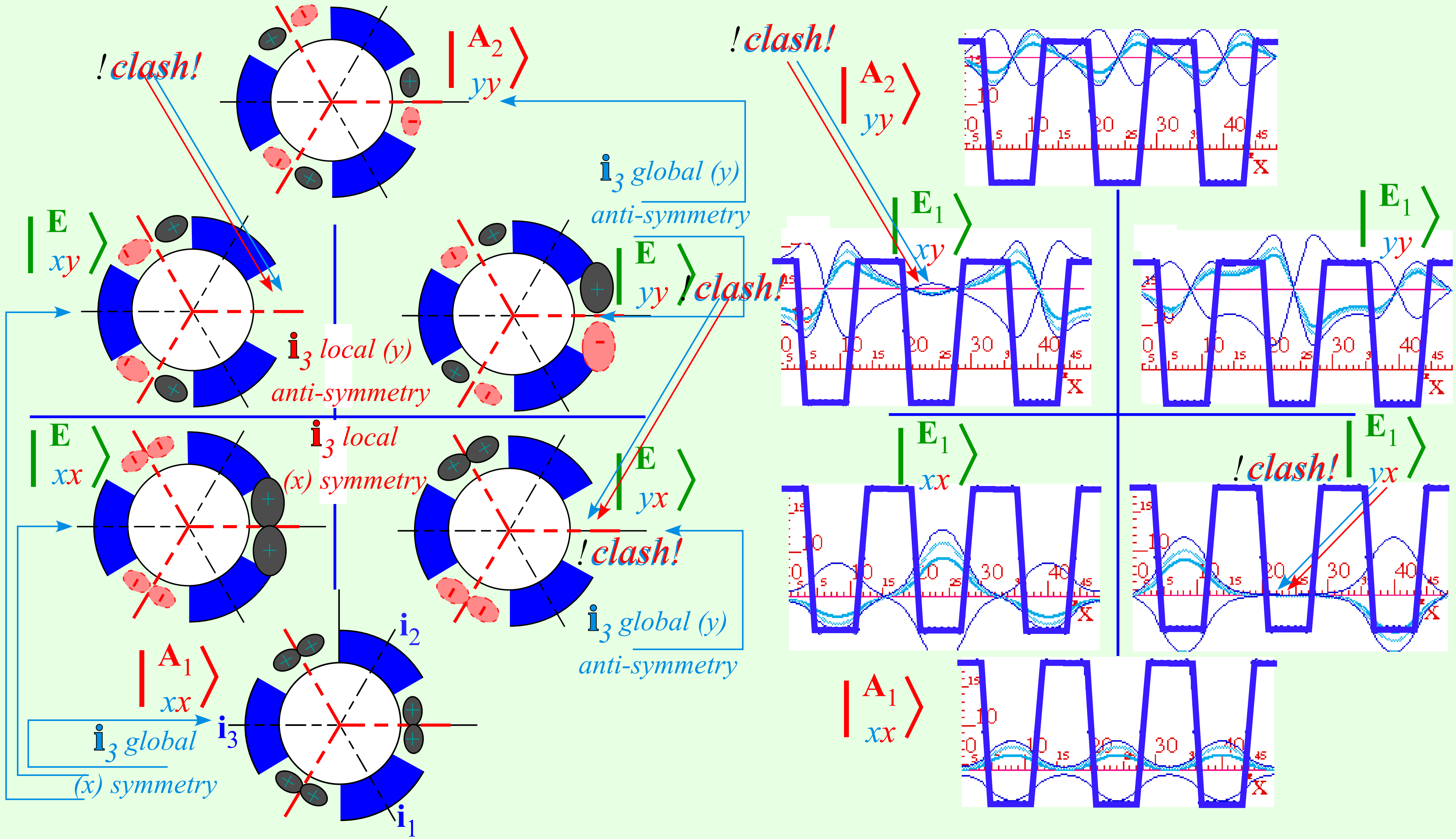
$$\bar{\mathbf{i}}_3\left|{}^{(m)}_{eb}\right\rangle = \bar{\mathbf{i}}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = \mathbf{P}^{(m)}_{eb}\bar{\mathbf{i}}_3\left|1\right\rangle = \mathbf{P}^{(m)}_{eb}\mathbf{i}_3^{\dagger}\left|1\right\rangle = (-1)^b\left|{}^{(m)}\right\rangle$$





When there is no there, there...

Nobody Home
where LOCAL
and GLOBAL



Review: Projector formulae and subgroup splitting

Algebra and geometry of irreducible $D^{\mu}{}_{jk}(g)$ and projector $\mathbf{P}^{\mu}{}_{jk}$ transformation

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

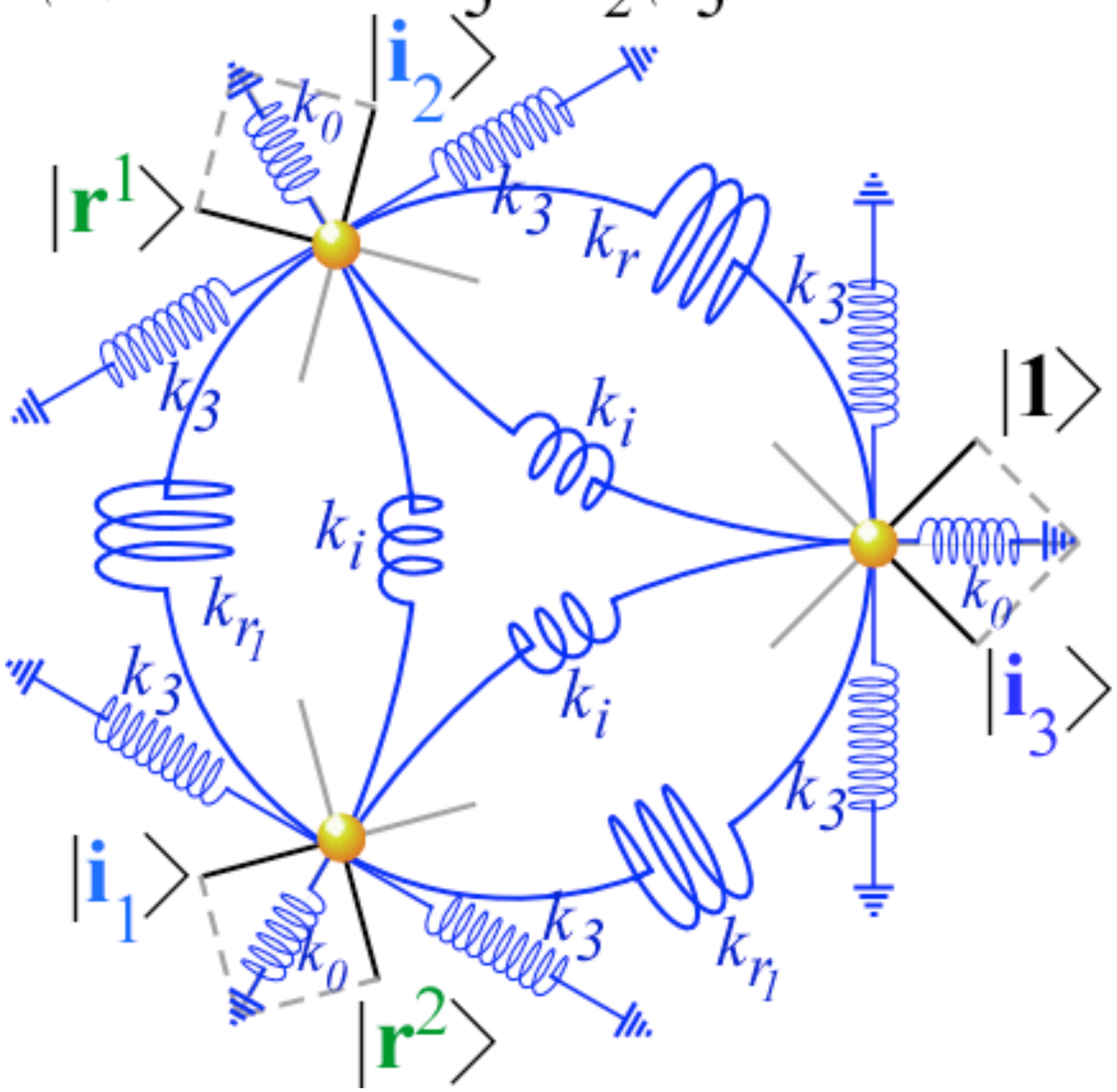
Hamiltonian local-symmetry eigensolution

Molecular vibrational mode eigensolution

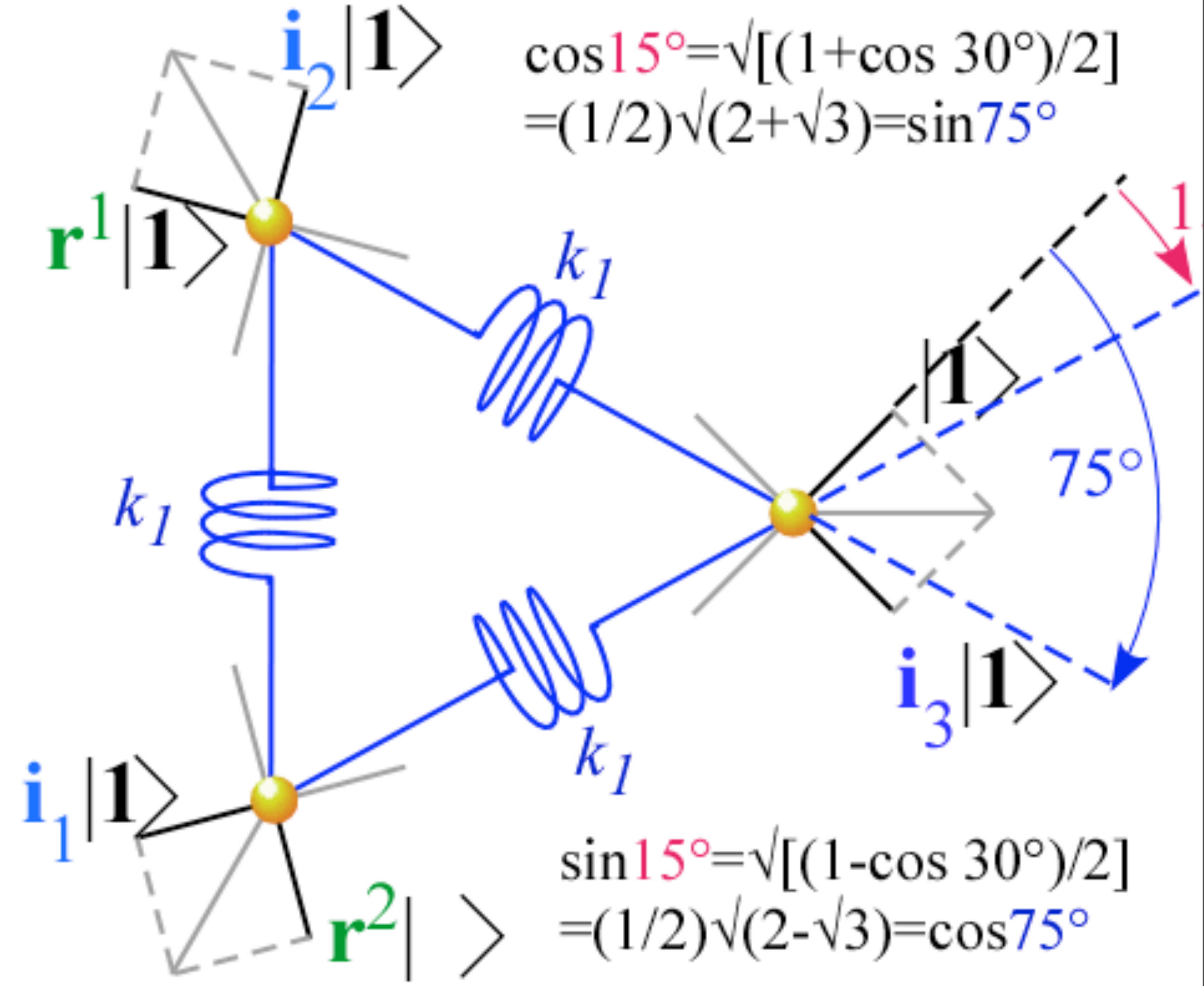
Local symmetry limit

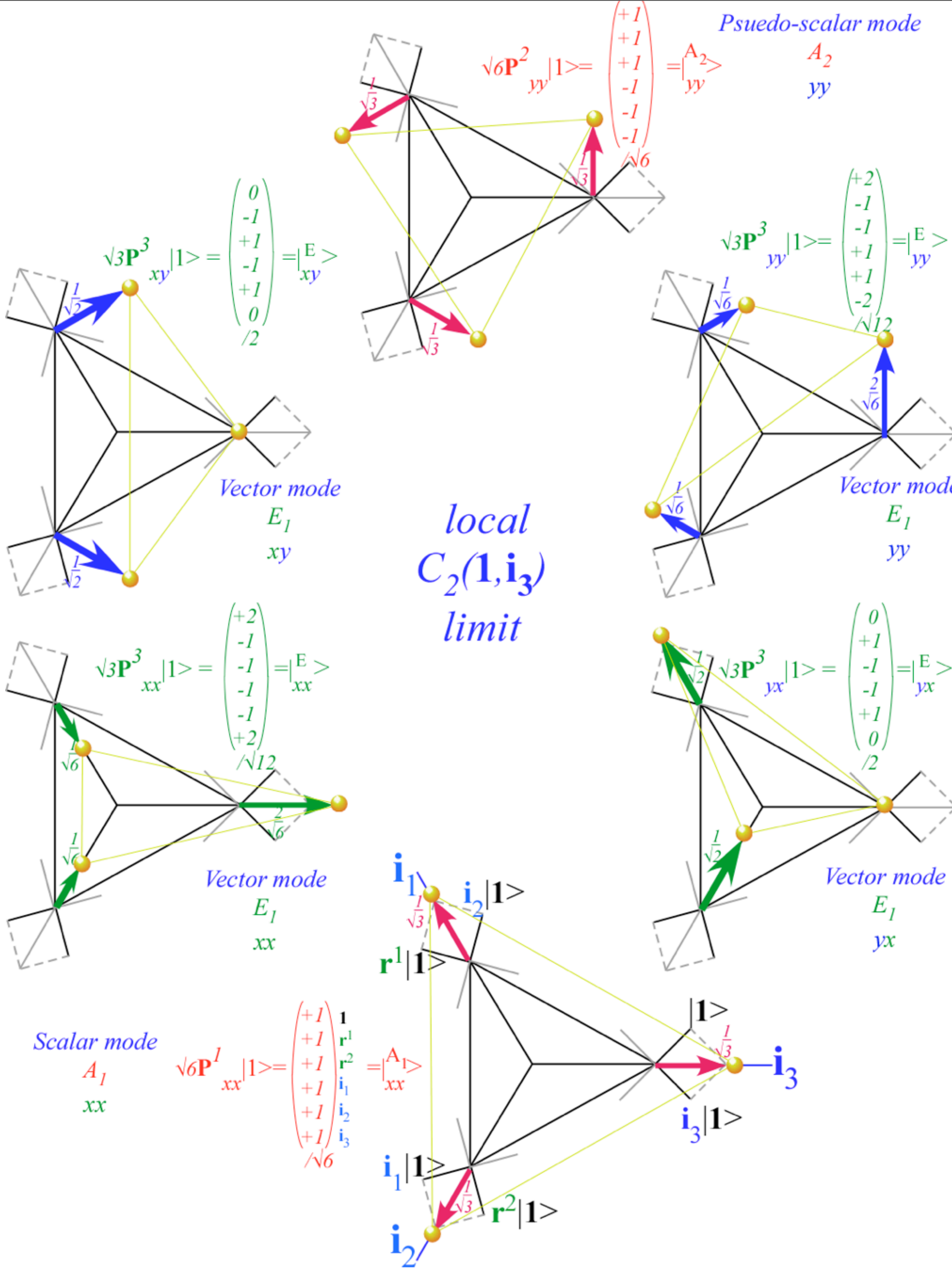
Global symmetry limit (free or "genuine" modes)

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

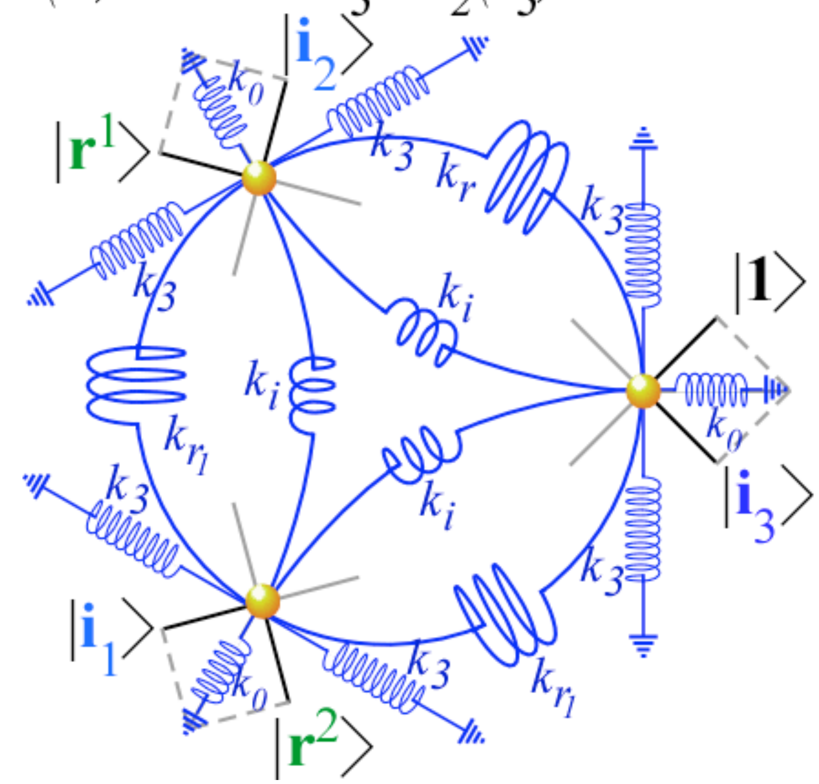


(b) Mixed local symmetry D_3 model

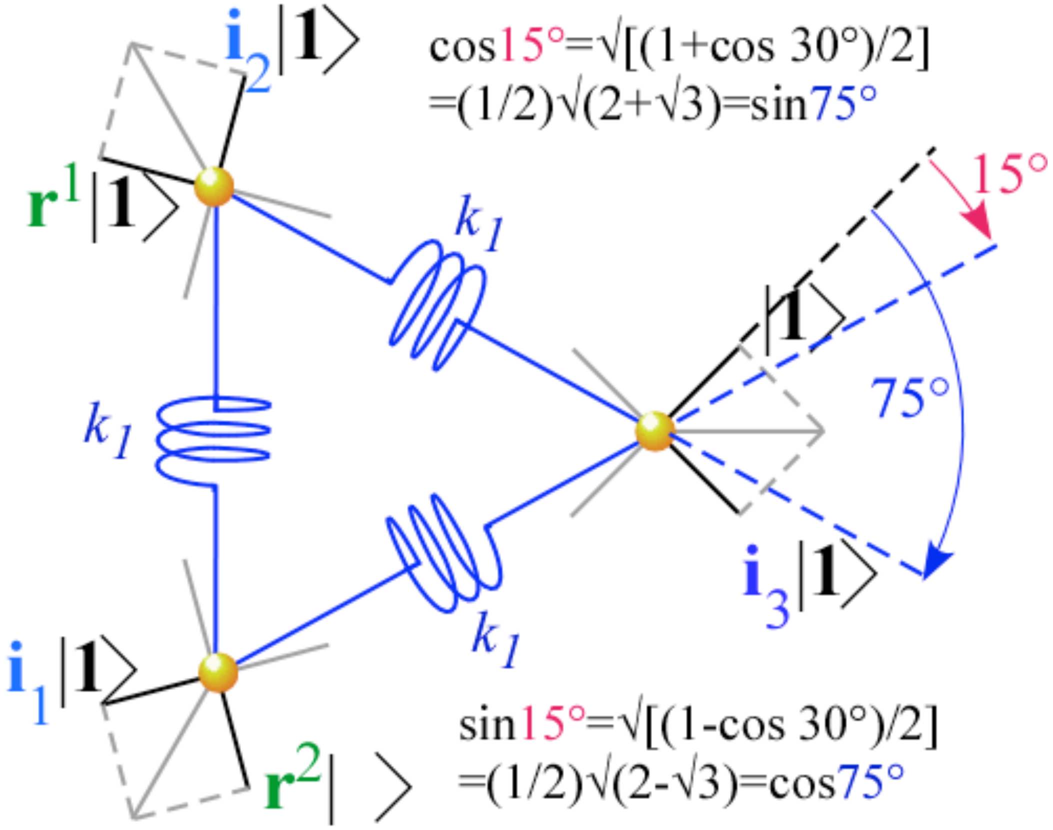




(a) Local $D_3 \supset C_2(i_3)$ model



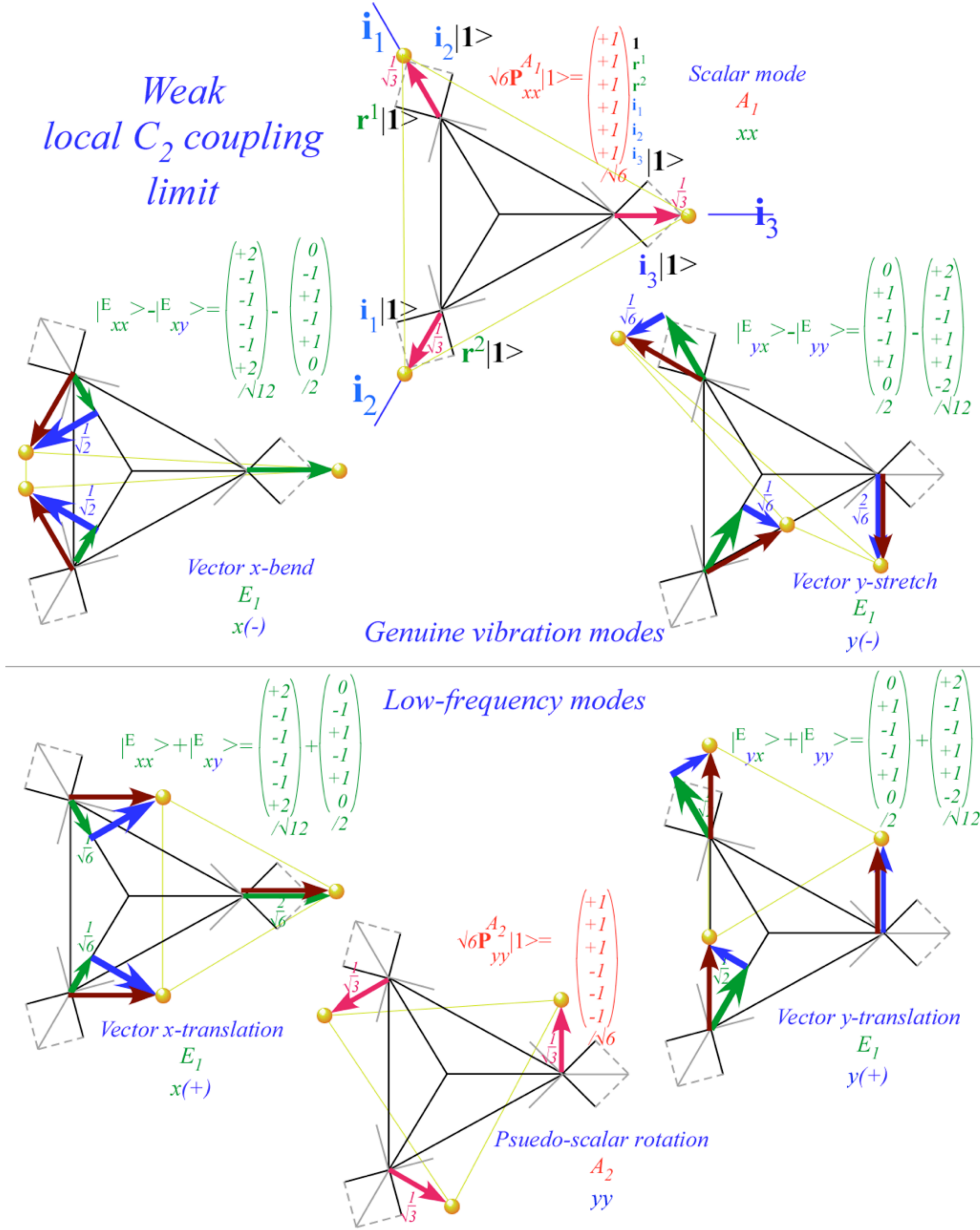
Mixed local symmetry D_3 model



$\cos 15° = \sqrt{[(1+\cos 30°)/2]}$
$= (1/2)\sqrt{(2+\sqrt{3})} = \sin 75°$

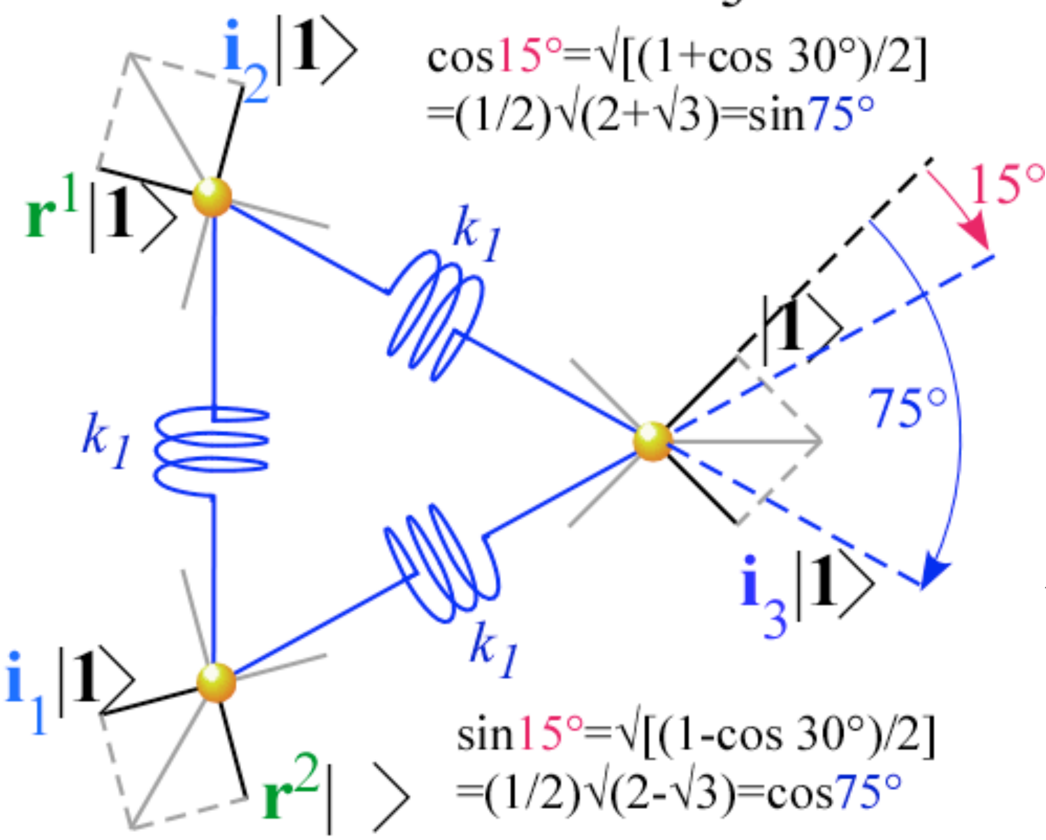
$\sin 15° = \sqrt{[(1-\cos 30°)/2]}$
$= (1/2)\sqrt{(2-\sqrt{3})} = \cos 75°$

Weak local C_2 coupling limit



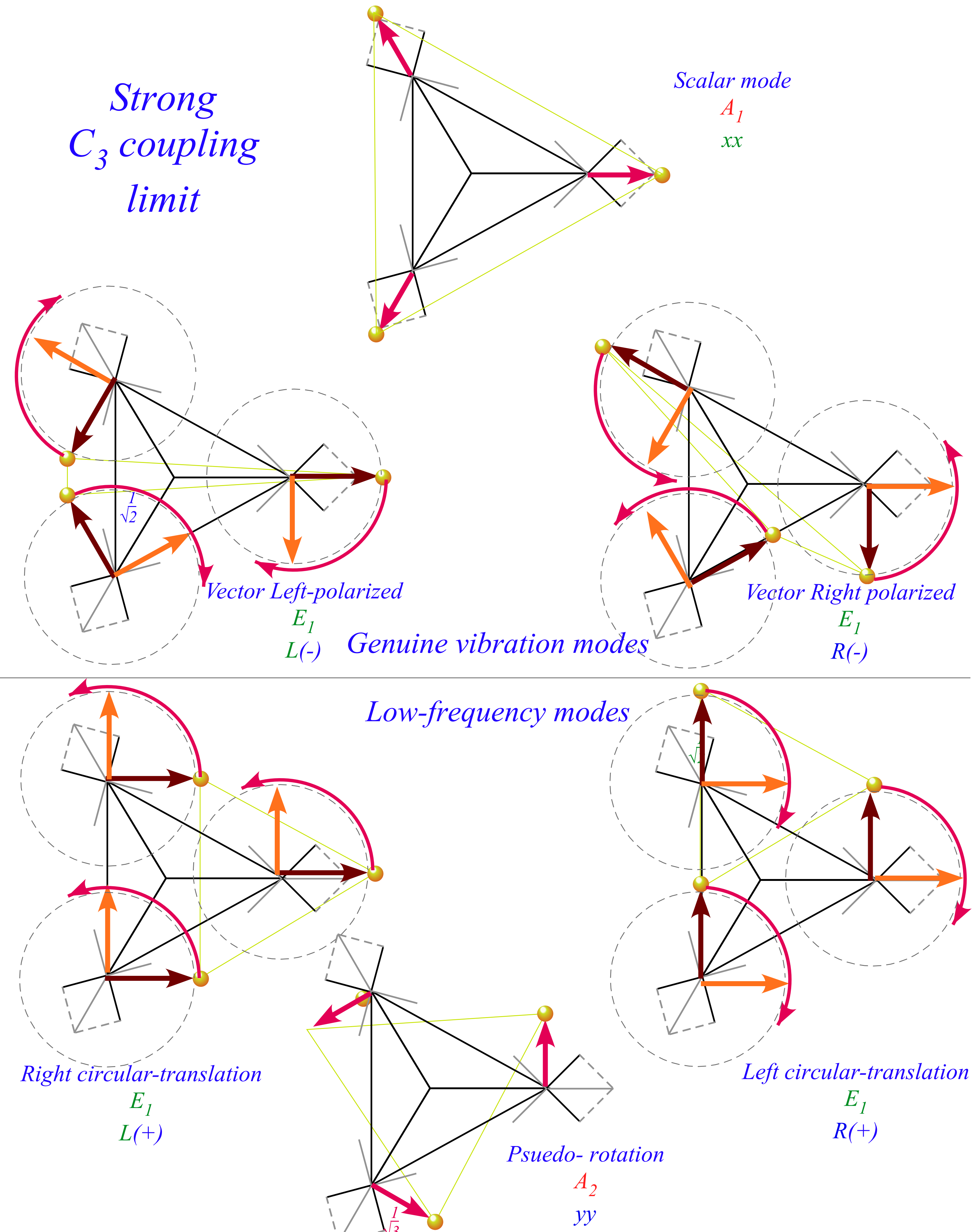
Strong C_3 coupling limit

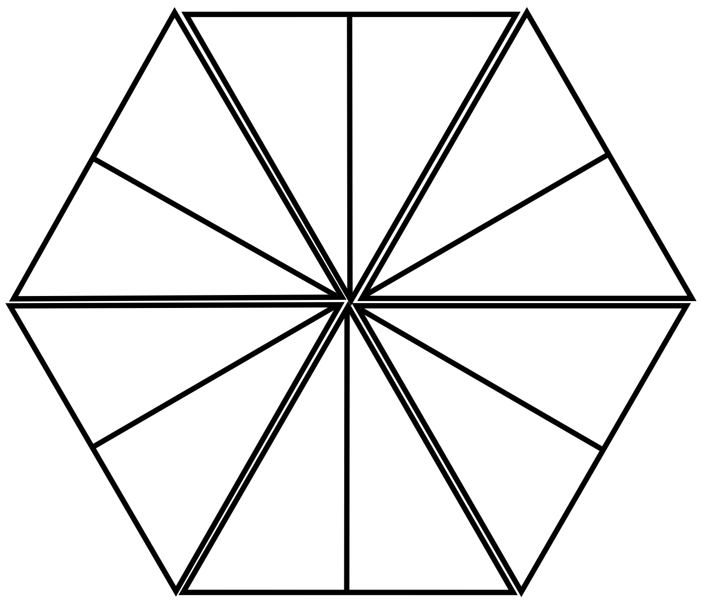
Mixed local symmetry D_3 model

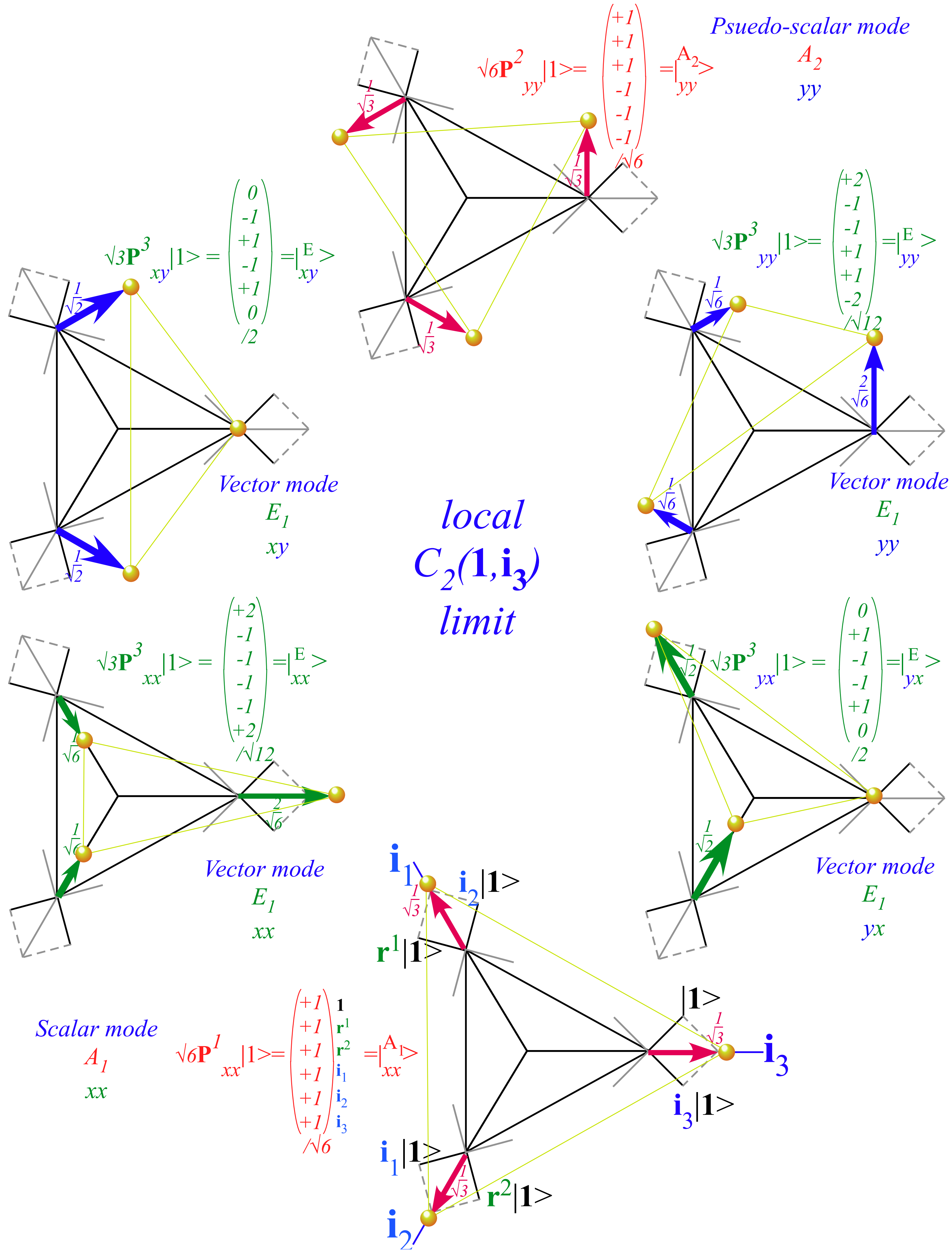


$\cos 15° = \sqrt{[(1+\cos 30°)/2]}$
$= (1/2)\sqrt{(2+\sqrt{3})} = \sin 75°$

$\sin 15° = \sqrt{[(1-\cos 30°)/2]}$
$= (1/2)\sqrt{(2-\sqrt{3})} = \cos 75°$






Psuedo-scalar mode
A2
yy
√6P²yy|1>=
=|A2 yy>
√3P³xy|1> =
=|E xy>
√3P³yy|1>=
=|E yy>
Vector mode
E1
xy
Vector mode
E1
yy
local
C2(1,i3)
limit
√3P³xx|1> =
=|E xx>
√3P³yx|1> =
=|E yx>
Vector mode
E1
xx
Vector mode
E1
yx
Scalar mode
A1
xx
√6P¹xx|1>=
=|A1 xx>
i1
i2|1>
r¹|1>
|1>
i3
i3|1>
i1|1>
i2
r²|1>