Group Theory in Quantum Mechanics

Lecture 18 (3.16.17)

Vibrational modes and symmetry reciprocity: Induced reps

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

(PSDS - Ch. 4)

Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

Molecular vibrational modes vs. Hamiltonian eigenmodes

- Molecular K-matrix construction
- $D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions
- D_3-direct-connection K-matrix eigensolutions
- $D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Applied symmetry reduction and splitting

- Subduced irep $D^\alpha(D_3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation
- Subduced irep $D^\alpha(D_3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ correlation

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

- Induced rep $d^a(C_2)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus ..$ correlation
- Induced rep $d^a(C_3)\uparrow D_3 = D^\alpha \oplus D^\beta \oplus ..$ correlation

D_6 symmetry and Hexagonal Bands

- Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps
- Induced rep $d^a(C_2)\uparrow D_6 = D^\alpha \oplus D^\beta \oplus ..$ correlation
- Induced rep $d^a(C_6)\uparrow D_6 = D^\alpha \oplus D^\beta \oplus ..$ correlation

Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

Molecular vibrational modes vs. Hamiltonian eigenmodes

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Applied symmetry reduction and splitting

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

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Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

Induced rep $d^{a}(C_2)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

Induced rep $d^{a}(C_3)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

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

Review excerpts of Lecture 17

D_3 global group product table

1	r^2	r	i$_1$	i$_2$	i$_3$
r	1	r^2	i$_3$	i$_1$	i$_2$
r^2	r	1	i$_2$	i$_3$	i$_1$
i$_1$	i$_3$	i$_2$	1	r	r^2
i$_2$	i$_1$	i$_3$	r^2	1	r
i$_3$	i$_2$	i$_1$	r	r^2	1

D_3 global projector product table

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

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

Change Global to Local by switching

...column-P with column-P†

....and row-P with row-P†

Just switch r with r†=r^2. *(all others are self-conjugate)*

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

D_3 local group table

1	r	r^2	i$_1$	i$_2$	i$_3$
r^2	1	r	i$_2$	i$_3$	i$_1$
r	r^2	1	i$_3$	i$_1$	i$_2$
i$_1$	i$_2$	i$_3$	1	r	r^2
i$_2$	i$_3$	i$_2$	r^2	1	r
i$_3$	i$_1$	i$_2$	r	r^2	1

D_3 local projector product table

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

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

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

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

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

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

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

Global $\mathbf{g}$-matrix component

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

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

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

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

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

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

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

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

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

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

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

Review excerpts of Lecture 17

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:*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

A_1-block: $H + r_1 + r_2 + i_1 + i_2 + i_3$

A_2-block: $H + r_1 + r_2 - i_1 - i_2 - i_3$

E-block:

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

$\mathbf{P}^{\mu}_{mn}$ **g**-*expansion in Lect.17 p. 35-51*

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

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

$r_1=r_2=r_1^*=r,\quad i_1=i_2=i_1^*=i$

gives:
- A_1-level: $H+2r+2i+i_3$
- A_2-level: $H+2r-2i-i_3$
- E_x-level: $H-r-i+i_3$
- E_y-level: $H-r+i-i_3$

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

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

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

Global (LAB) symmetry

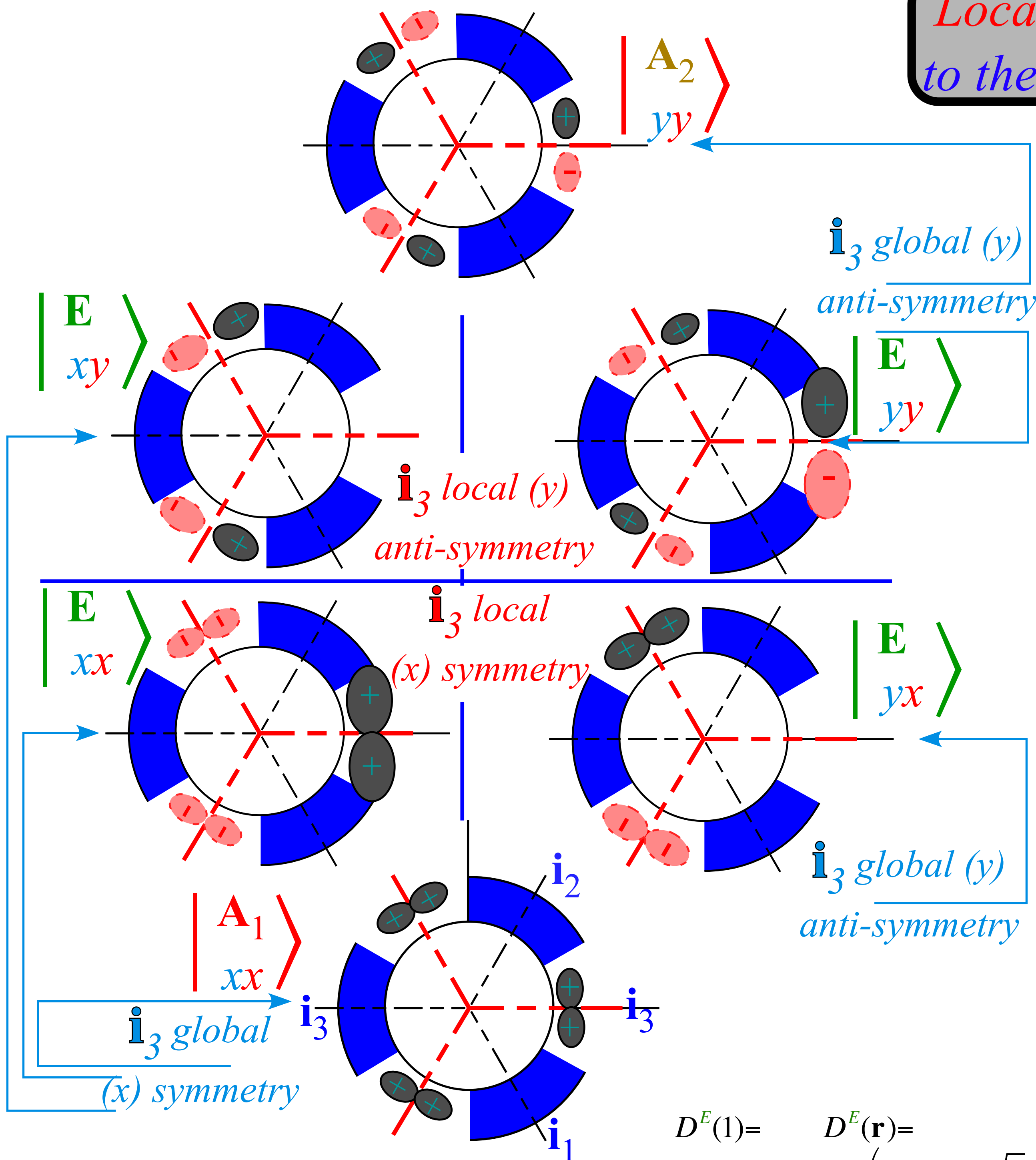
$$\mathbf{i}_3|^{(m)}_{eb}\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}|1\rangle = (-1)^e\,|^{(m)}\rangle$$

Local (BOD) symmetry

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

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

Here the "Mock-Mach" is being applied!



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

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

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

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

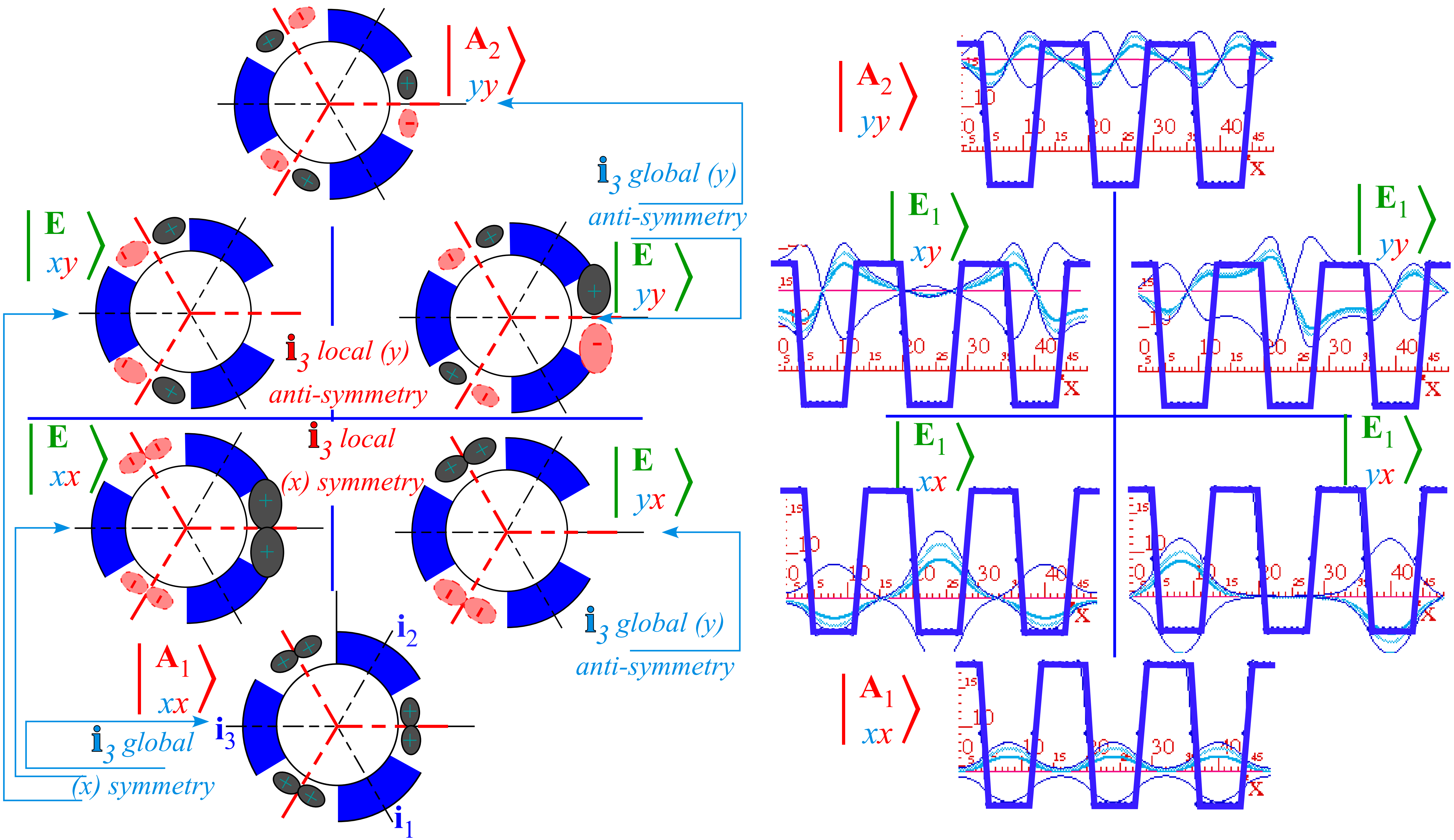
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

Global (LAB) symmetry

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

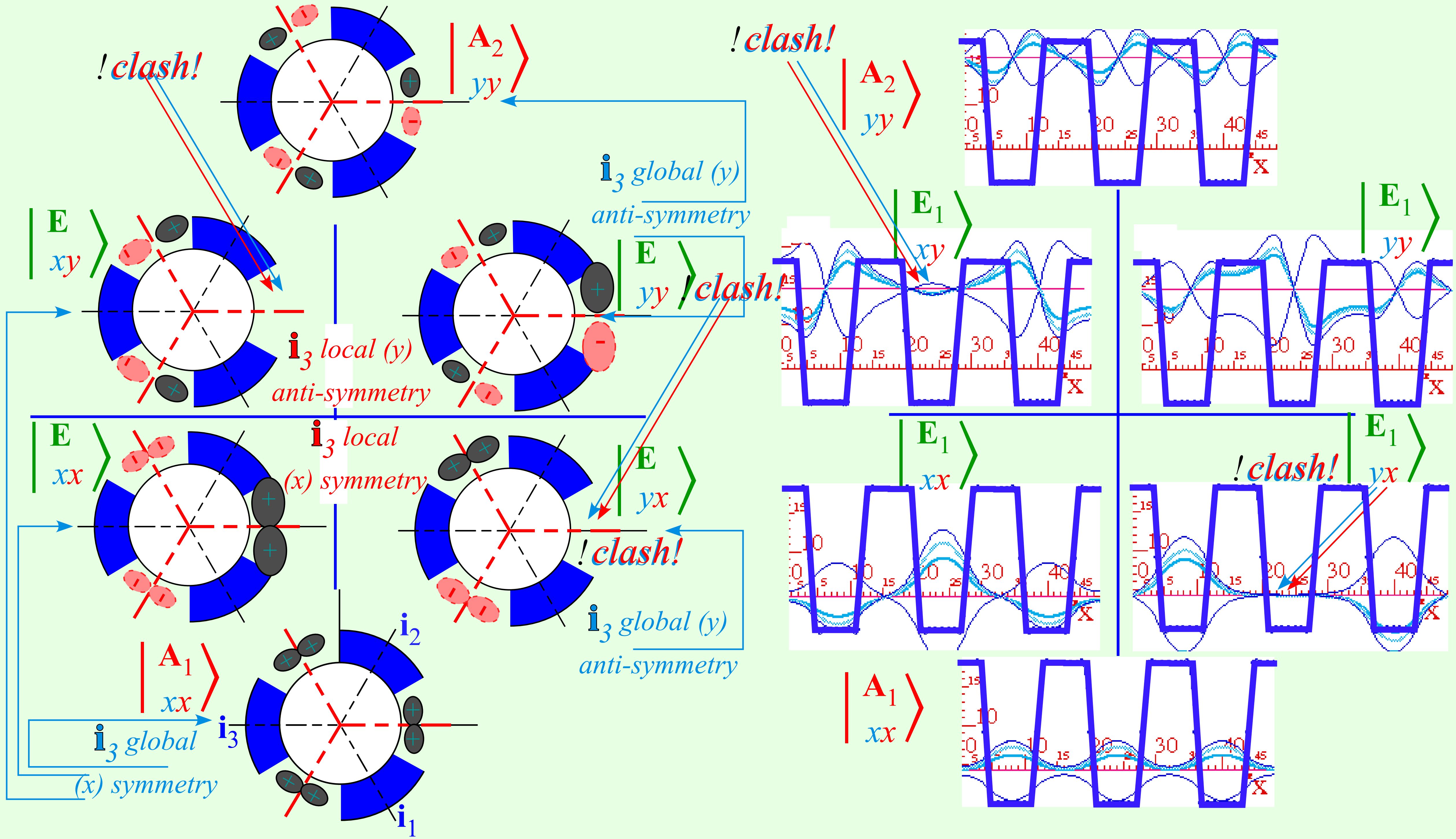
Local (BOD) symmetry

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



When there is no there, there...

Nobody Home
where LOCAL
and GLOBAL



Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

Molecular vibrational modes vs. Hamiltonian eigenmodes

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ *local-symmetry K-matrix eigensolutions*

D_3*-direct-connection K-matrix eigensolutions*

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ *local symmetry K-matrix eigensolutions*

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Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ *correlation*

Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ *correlation*

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

Induced rep $d^{a}(C_2)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ *correlation*

Induced rep $d^{a}(C_3)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ *correlation*

D_6 *symmetry and Hexagonal Bands*

Cross product of the C_2 *and* D_3 *characters gives all* $D_6 = D_3 \times C_2$ *characters and ireps*

Molecular vibrational modes vs. Hamiltonian eigenmodes

Classical equations of coupled harmonic motion are Newtonian **F**=**M**·**a** relations of n-dimensional force vector **F**, acceleration vector **a**, and mass operator **M**=M·**1** for D_3-symmetry. Force **F** is a (-)derivative of potential $V(x)$ that becomes a **F**=-**K**·**x** matrix expression.

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Apart from normalization, eigen*vectors* of $\mathbf{H}$ and $\mathbf{K}$ are the same.

And, each eigen*value* set corresponds to its respective energy spectrum.

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Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

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$D_3 \supset C_2(i_3)$ *local-symmetry K-matrix eigensolutions*

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Classical modes are eigenvectors of force-field matrix K or operator $\mathbf{K}$.

Harmonic potential $V(\mathbf{x})$ is a quadratic K-form of coordinates x_a based on six D_3-labeled axes $\hat{\mathbf{x}}^a$ or $|a\rangle$.

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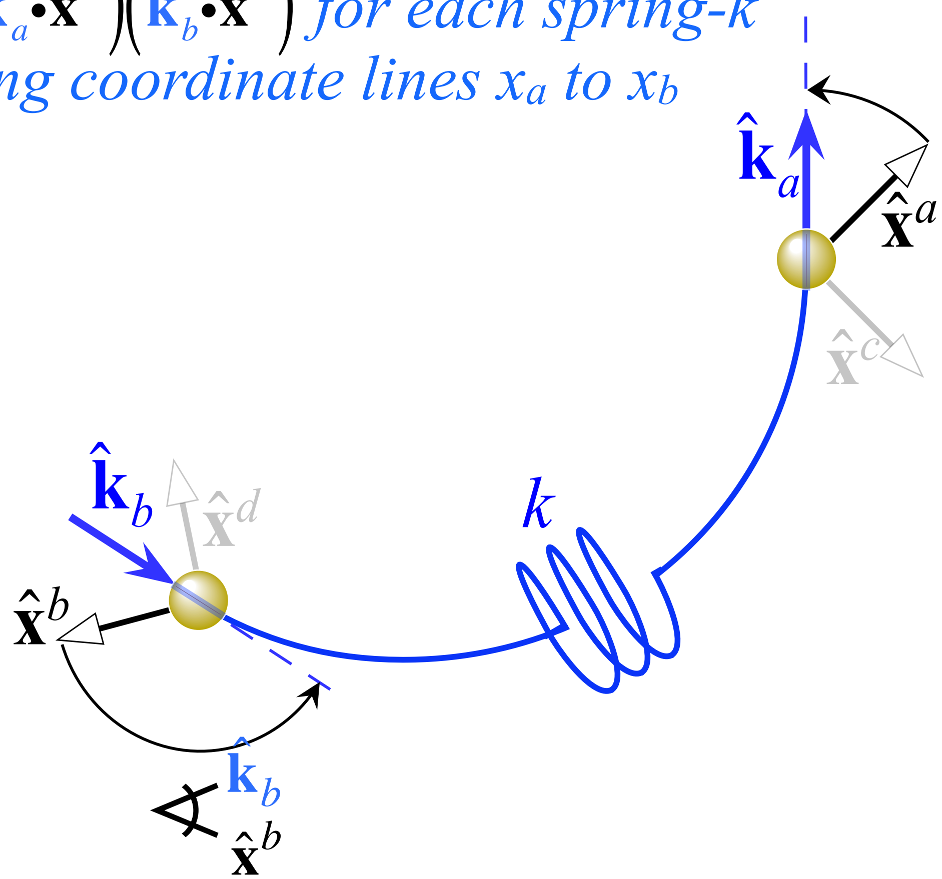
Coupling $K_{ab}{=}\langle a|\mathbf{K}|b\rangle$
Sum $k\cdot\left(\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a\right)\left(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b\right)$ *for each spring-k*
connecting coordinate lines x_a *to* x_b



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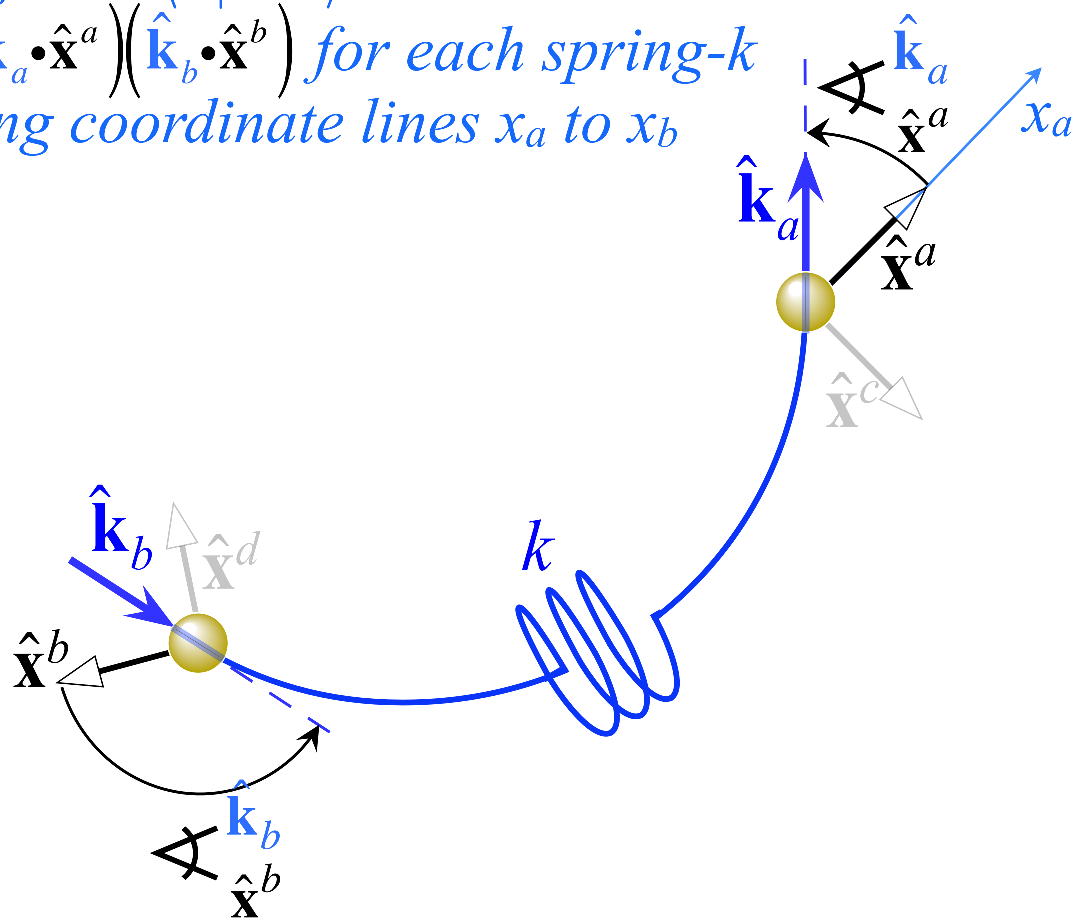
Diagonal $K_{aa}{=}\langle a|\mathbf{K}|a\rangle$
Sum $-\frac{1}{2}k\cdot\left(\hat{\mathbf{k}}_a\bullet\hat{\mathbf{x}}^a\right)^2$ *for each spring-k*
connected to coordinate line x_a



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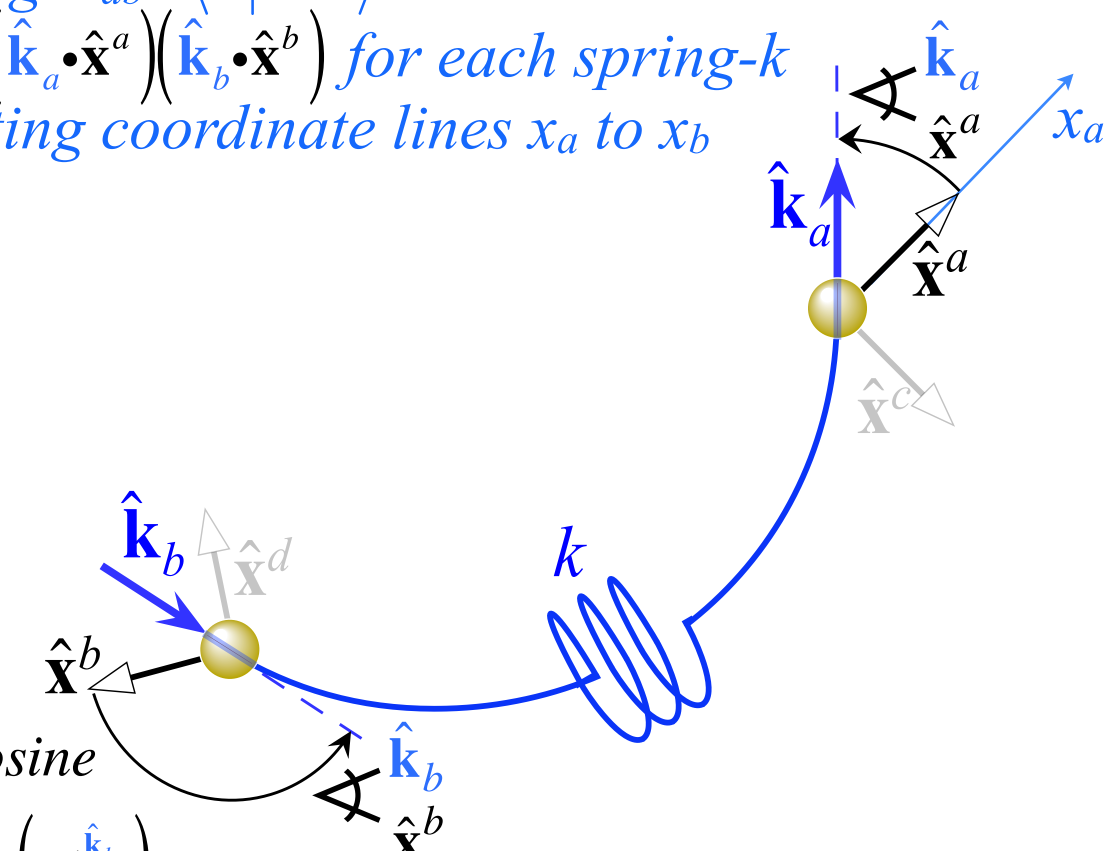

Direction cosine
$(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b) = \cos\left(\measuredangle^{\hat{\mathbf{k}}_b}_{\hat{\mathbf{x}}^b}\right)$
at b-end of k - spring

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$$\begin{aligned} V(x) &= \sum_{(k)} \frac{k}{2}(\Delta\ell_k)^2 = \sum_{(k)} \frac{k}{2} \sum_{a,b} (\hat{\mathbf{k}}_a \bullet \mathbf{x}^a - \hat{\mathbf{k}}_b \bullet \mathbf{x}^b)^2 \\ &= \sum_{(k)} \frac{k}{2} \sum_a (\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a)^2 x_a^2 - \sum_{(k)} k \sum_{a\neq b} (\hat{\mathbf{k}}_a \bullet \hat{\mathbf{x}}^a)(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b) x_a x_b \end{aligned}$$

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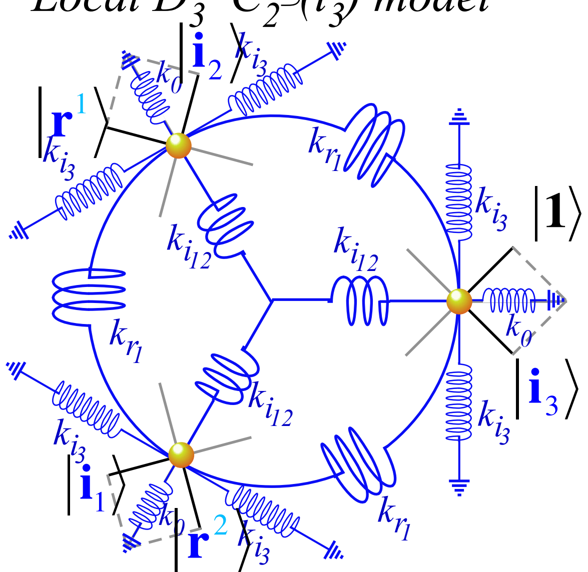
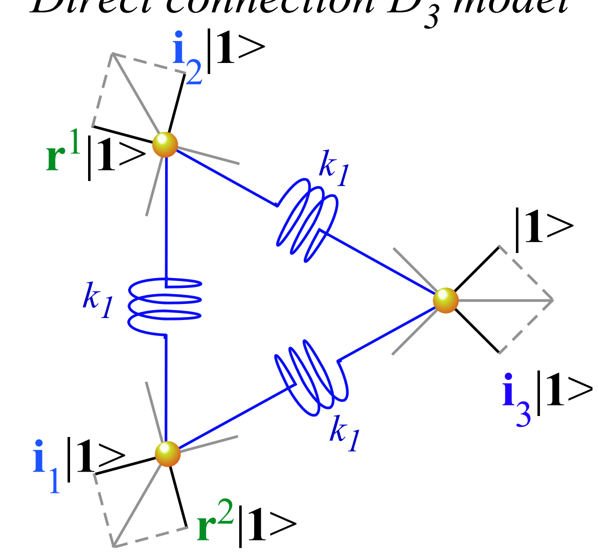
Local $D_3 \supset C_2(i_3)$ model



Direct connection D_3 model



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Applied symmetry reduction and splitting

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

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D_6 symmetry and Hexagonal Bands

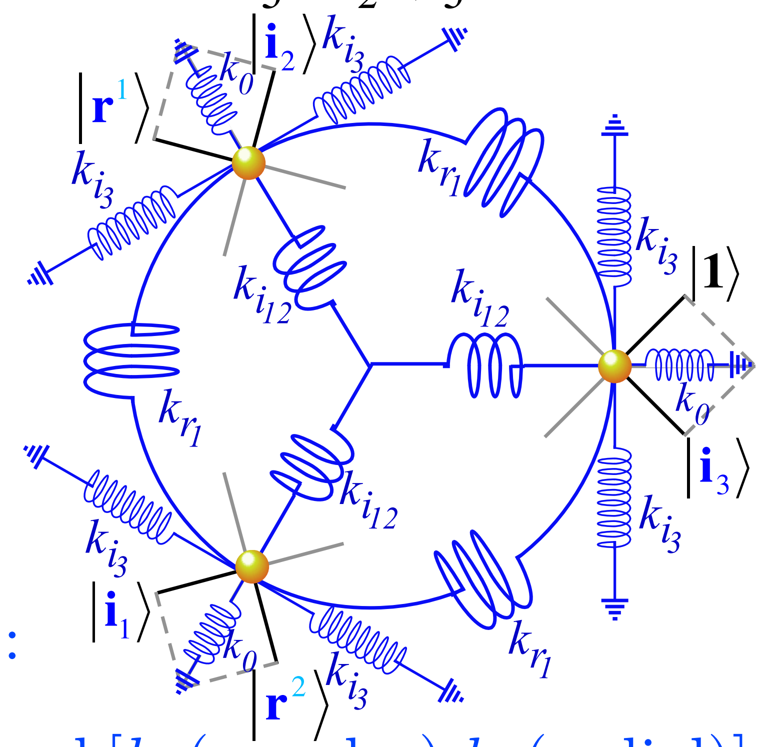
Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigensolutions

*Generic **K**-matrix (Top row)*

$$\langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Local D_3 $C_2 \supset (i_3)$ model



$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix

1^{st}-row parameters $g_b = \langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = K_{1b}$ of the force matrix K_{ab}:

$D_3 \supset C_2(i_3)$ model has internal [k_r(angular),k_i(radial)] and external [k_3(angular),k_0(radial)] constants between masses and lab frame.

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigensolutions

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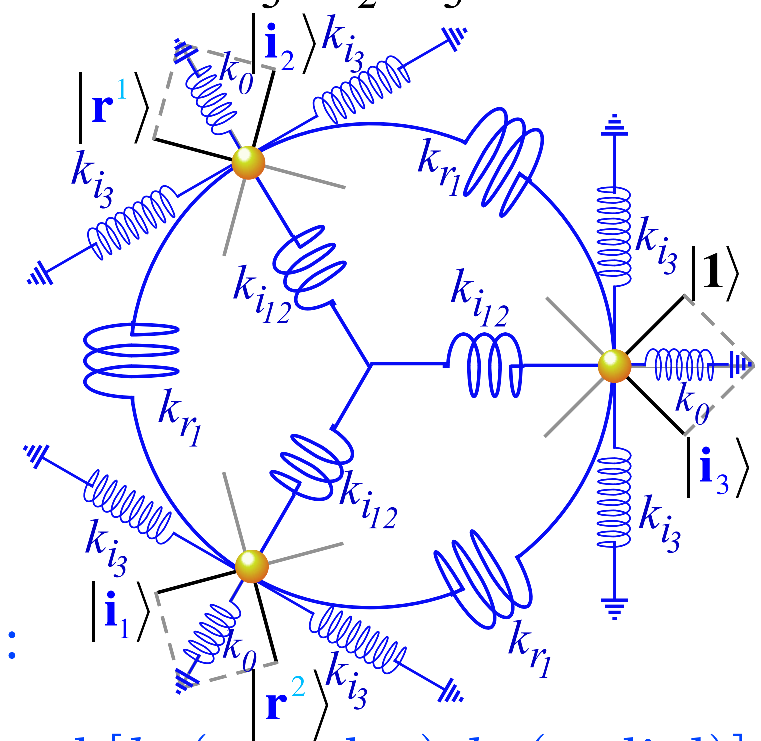

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \left[\begin{array}{cccccc} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{array}\right]$$

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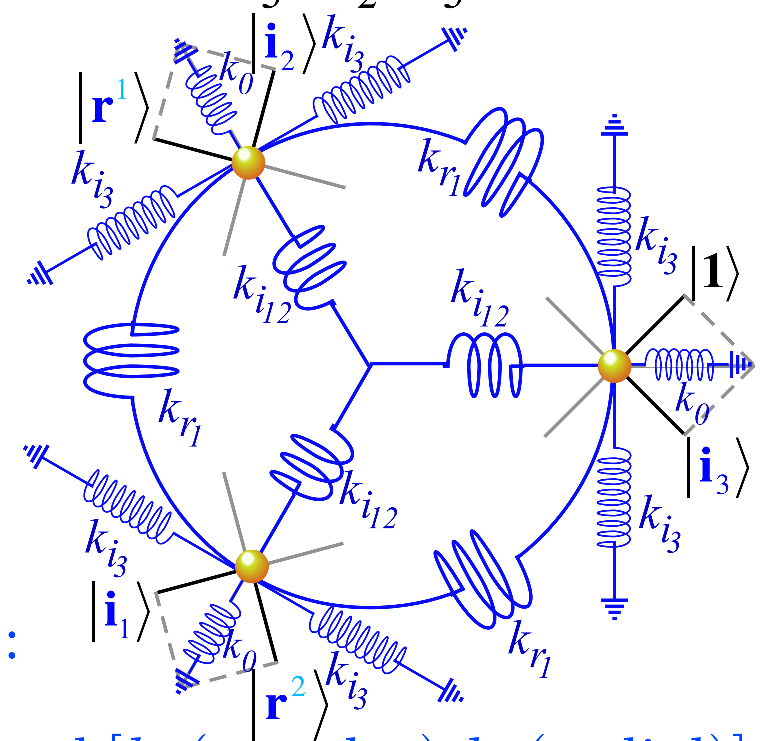
$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle \mathbf{1}\| \mathbf{K} \|g_b\rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r$ $-k_3$ $+k_0/2$

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigensolutions

Generic **K***-matrix (Top row)*

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Local D_3 $C_2 \supset (i_3)$ model



$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix

1^{st}-row parameters $g_b = \langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = K_{1b}$ of the force matrix K_{ab}:

$D_3 \supset C_2(i_3)$ model has internal [k_r(angular),k_i(radial)] and external [k_3(angular),k_0(radial)] constants between masses and lab frame.

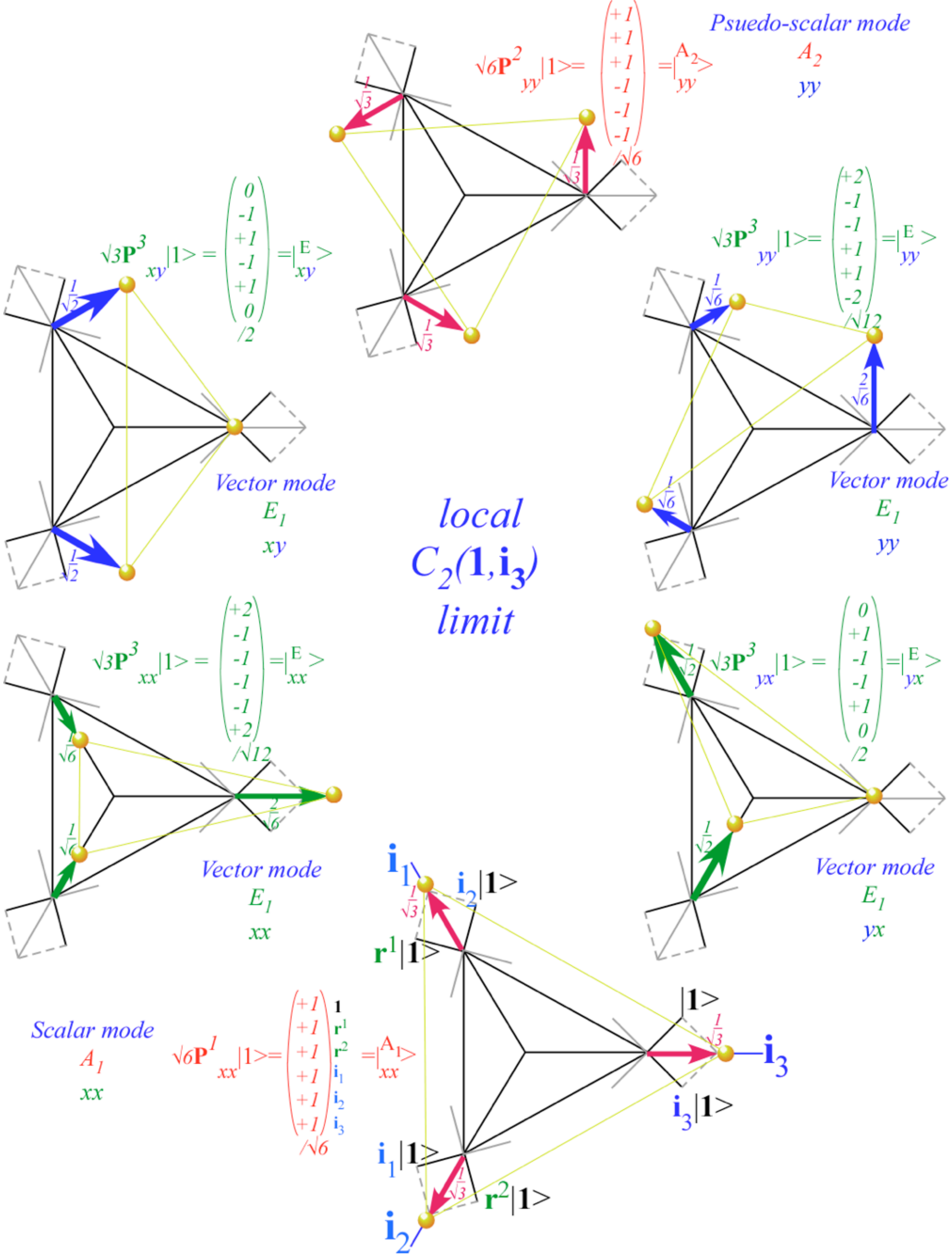
$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle \mathbf{1}\| \mathbf{K} \|g_b\rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r$ $-k_3$ $+k_0/2$

$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

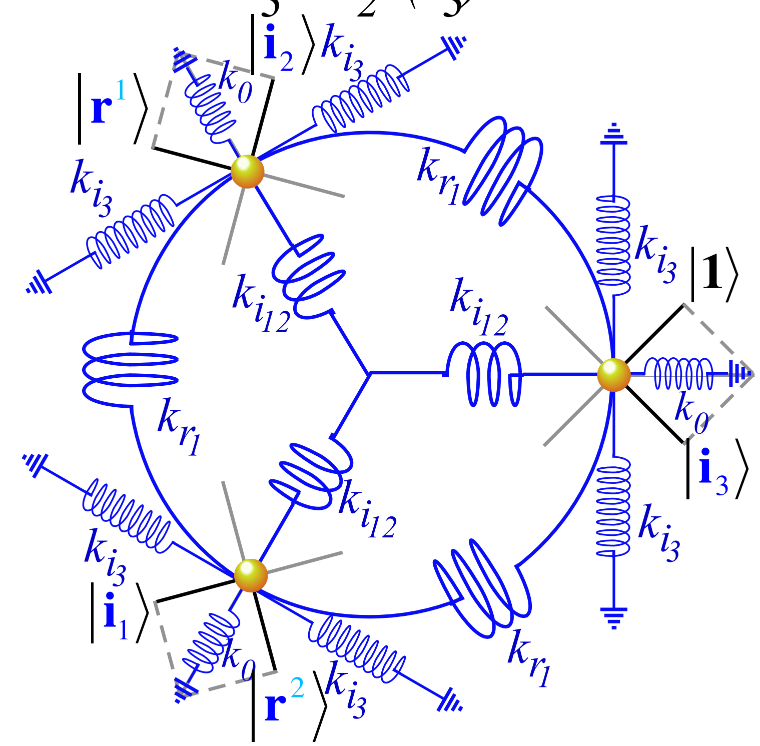
$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = k_0 + 3k_i$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = 3k_3$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix} = \begin{pmatrix} k_0 & 0 \\ 0 & k_3 + 2k_r \end{pmatrix}$$



Local $D_3 \supset C_2(i_3)$ model



Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

Molecular vibrational modes vs. Hamiltonian eigenmodes

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Applied symmetry reduction and splitting

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ correlation

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

Induced rep $d^a(C_2)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

Induced rep $d^a(C_3)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation

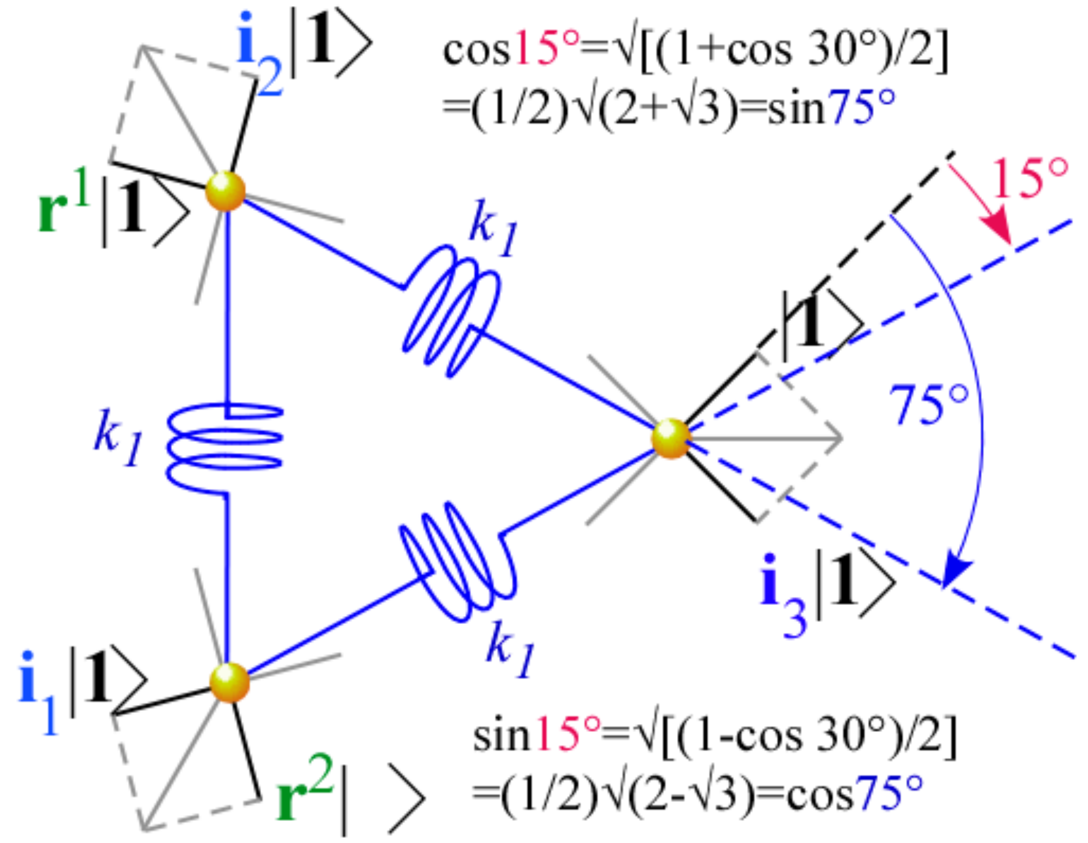
D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

D_3-direct-connection K-matrix eigensolutions

Generic **K***-matrix (Top row)*

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



D_3-direct-connection vibrational K-matrix

D_3-direct-connection K-matrix eigensolutions

*Generic **K**-matrix (Top row)*

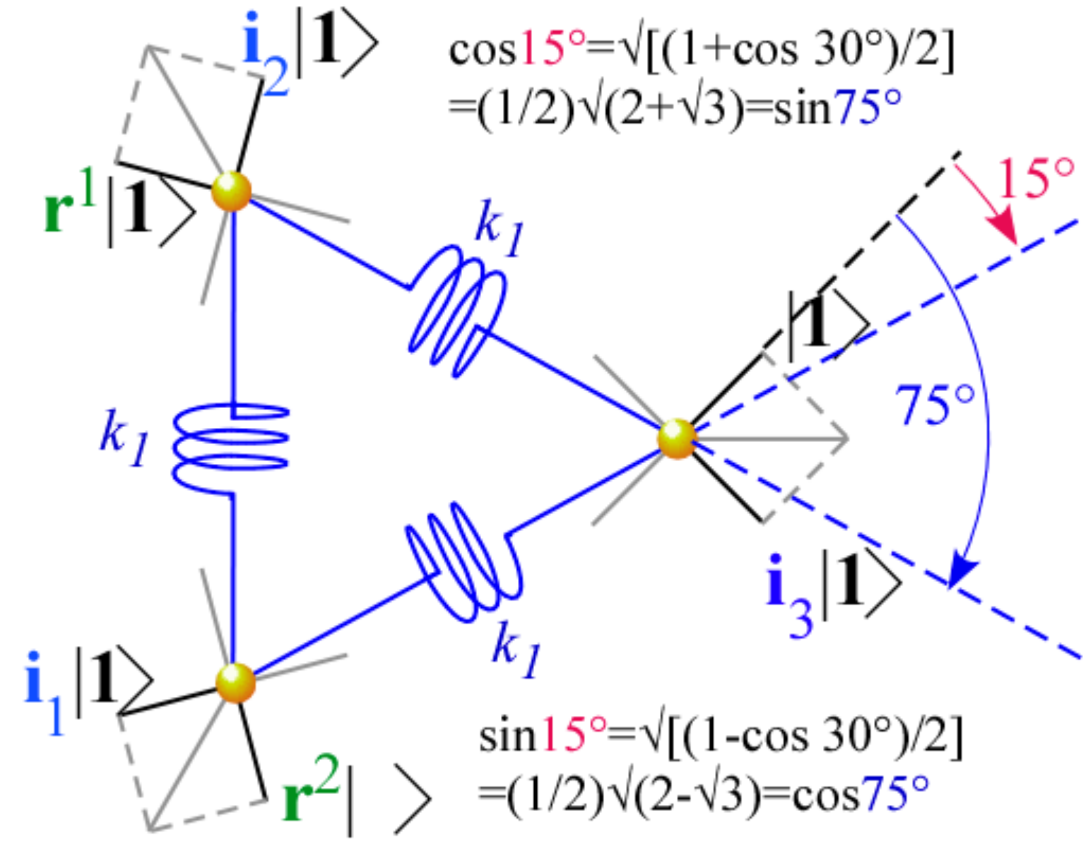
$$\langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

*Generic **K**-matrix D_3 projections*

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

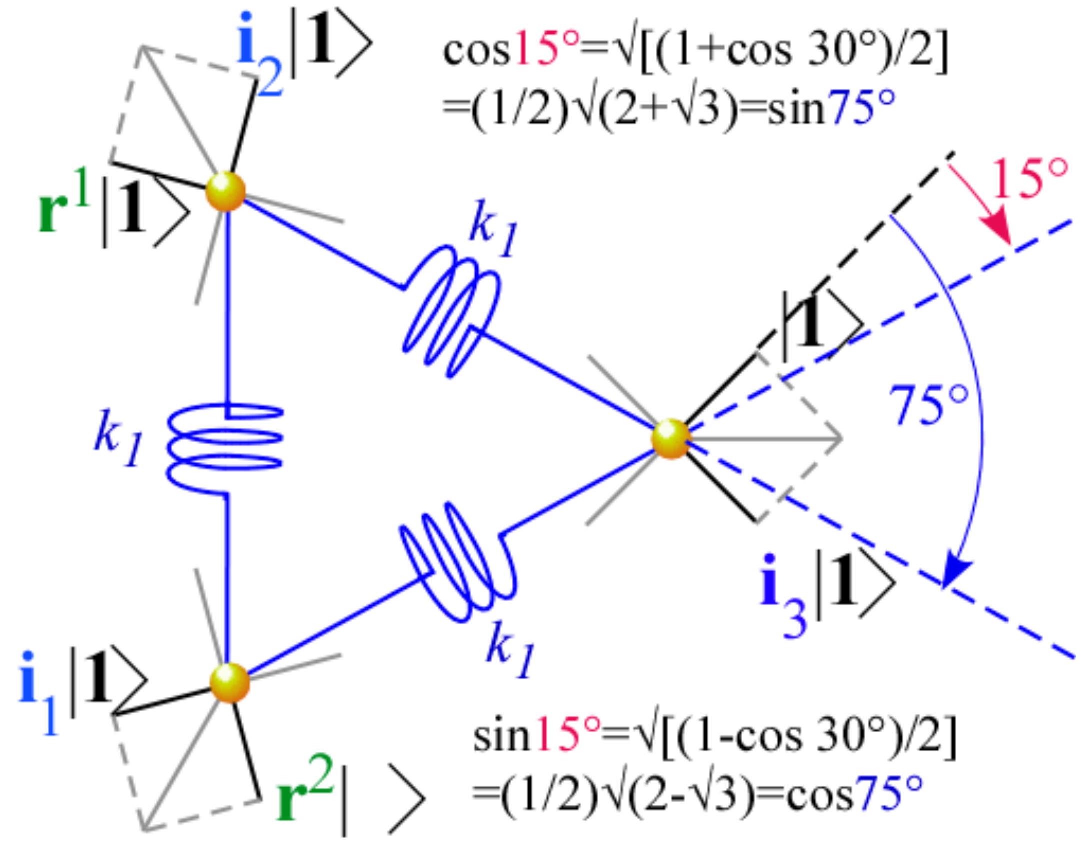
$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$



D_3-direct-connection K-matrix eigensolutions

Generic **K**-*matrix (Top row)*

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



Generic **K**-*matrix D_3 projections*

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

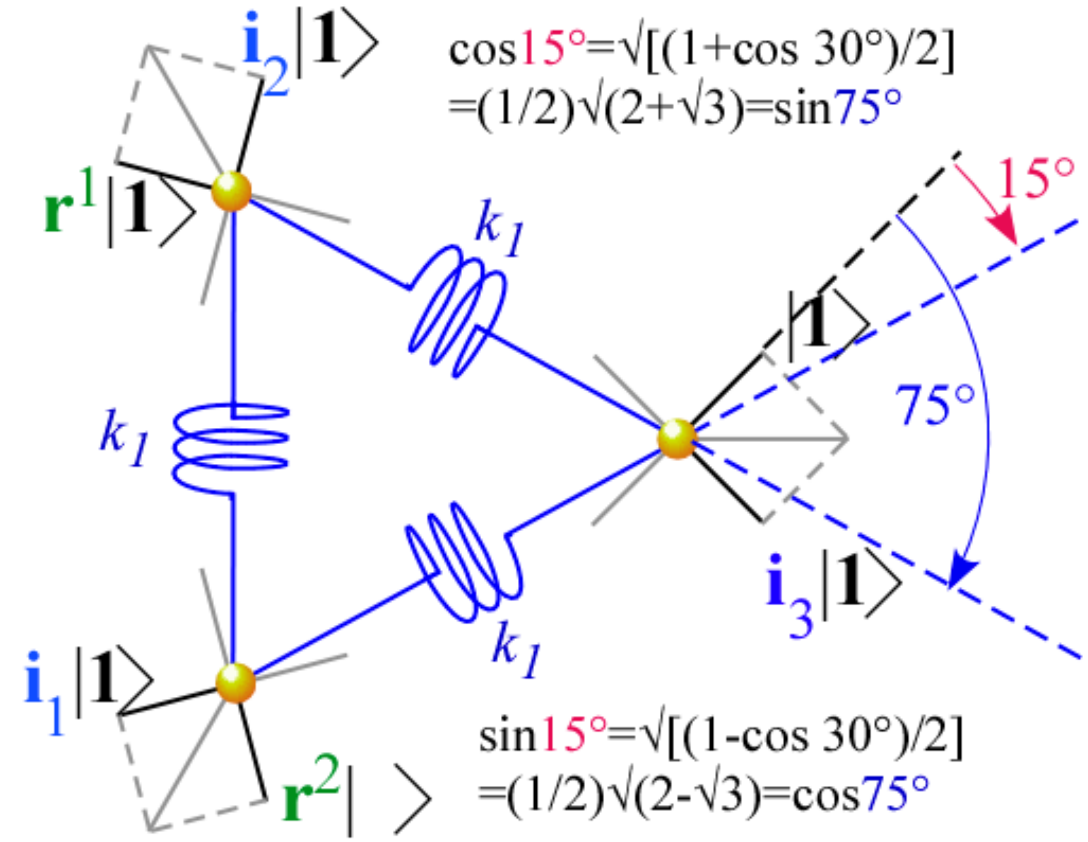
$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

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

D_3-direct-connection vibrational K-*matrix*

$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle\mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_1(\cos^2 75^\circ + \cos^2 15^\circ) = k_1$	$k_1 \cos 75^\circ \cdot \cos 15^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 75^\circ = \frac{k_1}{4}$	$k_1 \cos 15^\circ \cdot \cos 15^\circ = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75^\circ \cdot \cos 75^\circ = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75^\circ - \cos^2 15^\circ) = \frac{k_1}{2}$

D_3-direct-connection K-matrix eigensolutions



cos15°=√[(1+cos 30°)/2]
=(1/2)√(2+√3)=sin75°

sin15°=√[(1-cos 30°)/2]
=(1/2)√(2-√3)=cos75°

Generic K-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

Generic K-matrix D_3 projections

$$K^{A_1}_{xx} = r_0+r_1+r_1^*+i_1+i_2+i_3$$
$$K^{A_2}_{yy} = r_0+r_1+r_1^*-i_1-i_2-i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0-r_1-r_1^*-i_1-i_2+2i_3 & \sqrt{3}(-r_1+r_1^*-i_1+i_2) \\ \sqrt{3}(-r_1^*+r_1-i_1+i_2) & 2r_0-r_1-r_1^*+i_1+i_2-2i_3 \end{pmatrix}$$

D_3-direct-connection vibrational K-matrix

$\vert g_b\rangle$	$\vert\mathbf{1}\rangle$	$\vert\mathbf{r}^1\rangle$	$\vert\mathbf{r}^2\rangle$	$\vert\mathbf{i}_1\rangle$	$\vert\mathbf{i}_2\rangle$	$\vert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\vert\,\mathbf{K}\,\vert g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

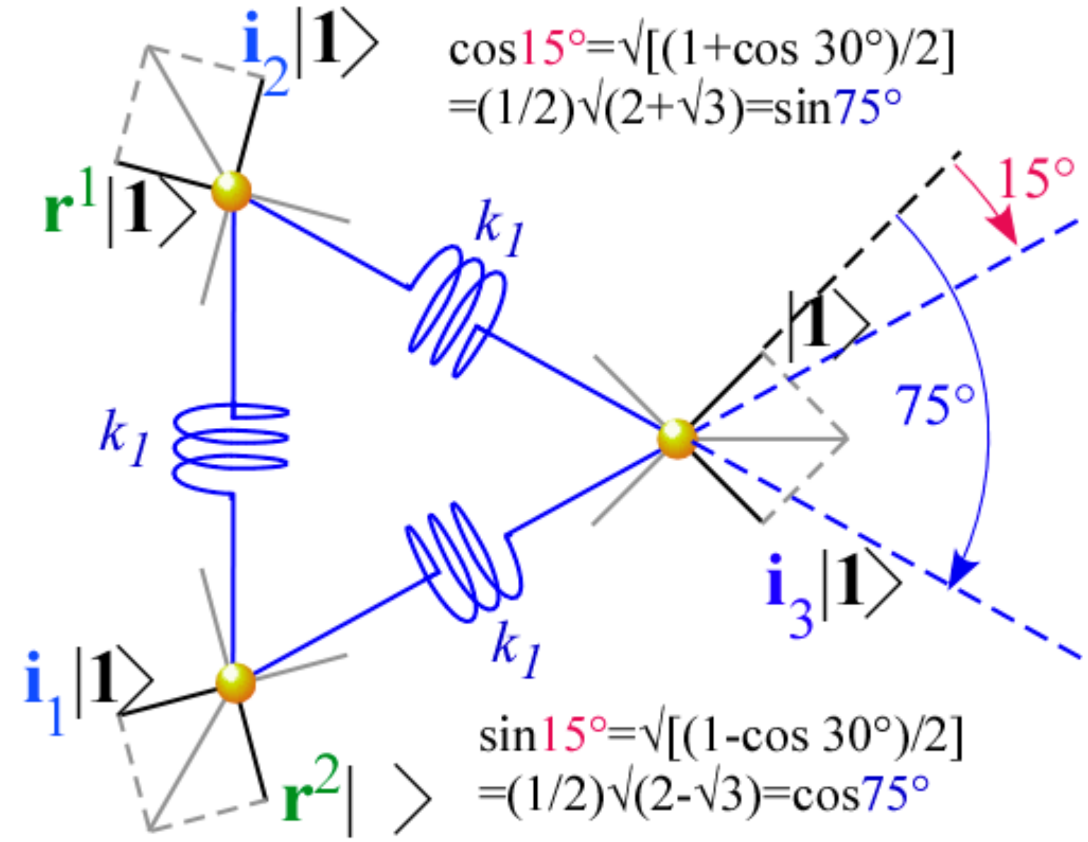
$$= k_1+\frac{k_1}{4}+\frac{k_1}{4}+\frac{k_1}{2}+\frac{k_1}{2}+\frac{k_1}{2} = \frac{3k_1}{2}+\frac{3k_1}{2} = 3k_1$$
$$= k_1+\frac{k_1}{4}+\frac{k_1}{4}-\frac{k_1}{2}-\frac{k_1}{2}-\frac{k_1}{2} = \frac{3k_1}{2}-\frac{3k_1}{2} = 0$$

$$K^{A_1}_{xx} = r_0+r_1+r_1^*+i_1+i_2+i_3$$
$$K^{A_2}_{yy} = r_0+r_1+r_1^*-i_1-i_2-i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0-r_1-r_1^*-i_1-i_2+2i_3 & \sqrt{3}(-r_1+r_1^*-i_1+i_2) \\ \sqrt{3}(-r_1^*+r_1-i_1+i_2) & 2r_0-r_1-r_1^*+i_1+i_2-2i_3 \end{pmatrix}$$

D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



Generic **K**-matrix D_3 projections

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$
$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

D_3-direct-connection vibrational K-matrix

$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle\mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

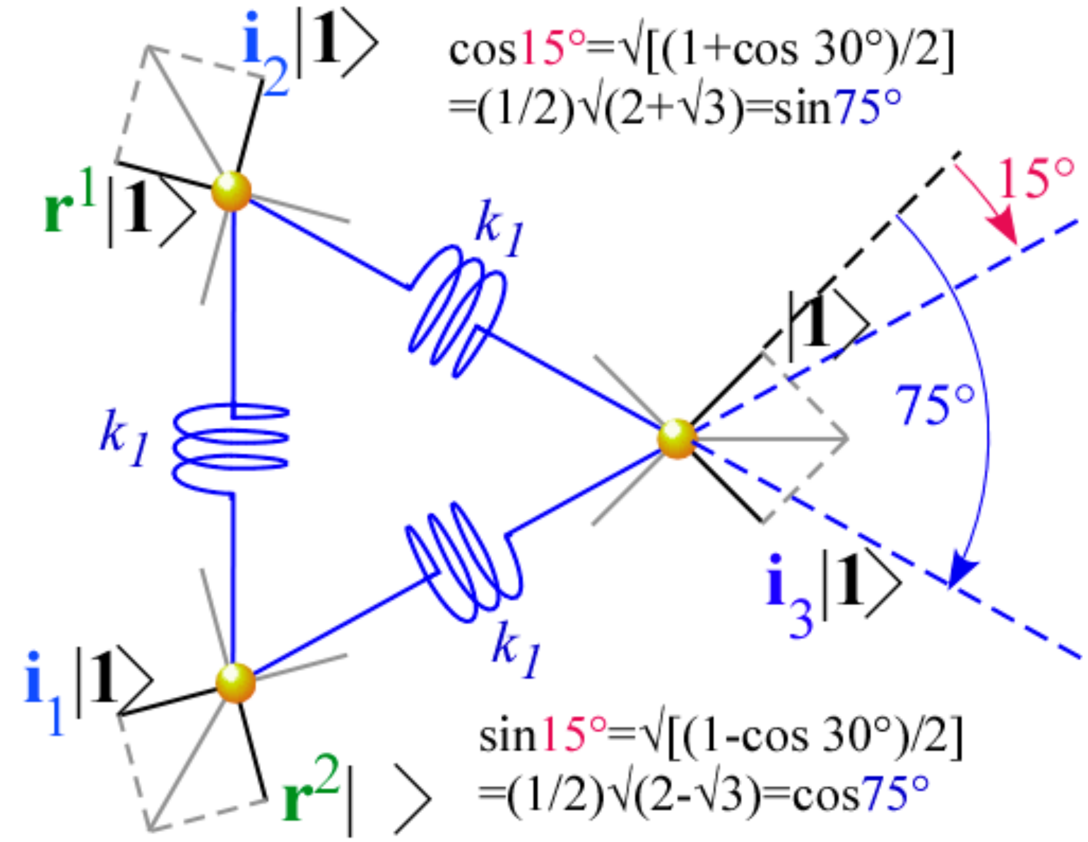
$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = k_1 + \frac{k_1}{4} + \frac{k_1}{4} + \frac{k_1}{2} + \frac{k_1}{2} + \frac{k_1}{2} = \frac{3k_1}{2} + \frac{3k_1}{2} = 3k_1$$
$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = k_1 + \frac{k_1}{4} + \frac{k_1}{4} - \frac{k_1}{2} - \frac{k_1}{2} - \frac{k_1}{2} = \frac{3k_1}{2} - \frac{3k_1}{2} = 0$$
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{2}\left(2k_1 - \frac{k_1}{4} - \frac{k_1}{4} - \frac{k_1}{2} - \frac{k_1}{2} + 2\frac{k_1}{2}\right) = \frac{1}{2}\left(2k_1 - \frac{k_1}{2} - k_1 + k_1\right) = \frac{3k_1}{4} & \\ \frac{\sqrt{3}}{2}\left(-\frac{k_1}{4} + \frac{k_1}{4} + \frac{k_1\sqrt{3}}{4} + \frac{k_1\sqrt{3}}{4}\right) = \frac{k_1 3}{4} & \frac{1}{2}\left(2k_1 - \frac{k_1}{4} - \frac{k_1}{4} + \frac{k_1}{2} + \frac{k_1}{2} - 2\frac{k_1}{2}\right) = \frac{3k_1}{4} \end{pmatrix}$$

D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



Generic **K**-matrix D_3 projections

$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

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

D_3-direct-connection vibrational K-matrix

$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle \mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

D_3-direct-connection vibrational K-matrix eigenvalues $K_m/M=\omega_m^2$

$$K_{xx}^{A_1} = 3k_1$$

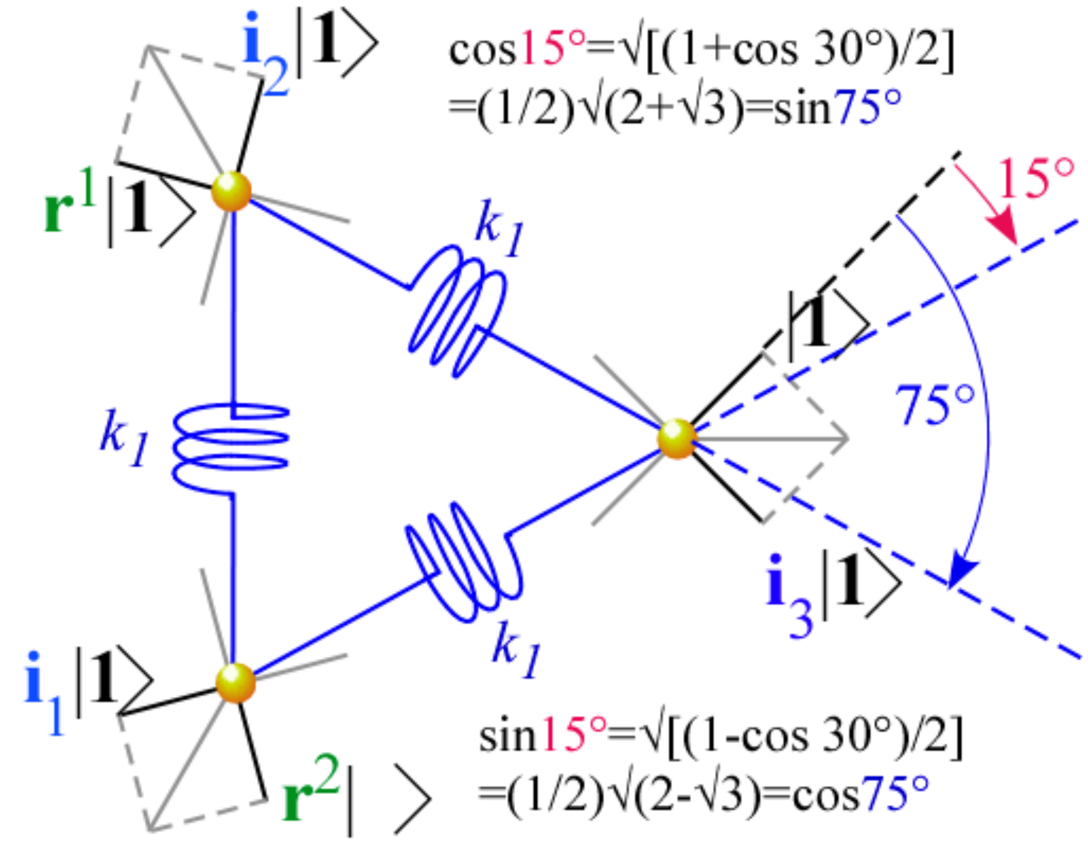
$$K_{yy}^{A_2} = 0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

D_3-direct-connection K-matrix eigensolutions

Generic **K**-matrix (Top row)

$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$



Generic **K**-matrix D_3 projections

$$K^{A_1}_{xx} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3$$

$$K^{A_2}_{yy} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3$$

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

D_3-direct-connection vibrational K-matrix

$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle\mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 75° = \frac{k_1}{4}$	$k_1 \cos 15° \cdot \cos 15° = \frac{k_1(2-\sqrt{3})}{4}$	$k_1 \cos 75° \cdot \cos 75° = \frac{k_1(2+\sqrt{3})}{4}$	$k_1(\cos^2 75° - \cos^2 15°) = \frac{k_1}{2}$

D_3-direct-connection vibrational K-matrix eigenvalues $K_m/M=\omega_m^2$

$$K^{A_1}_{xx} = 3k_1$$

$$K^{A_2}_{yy} = 0$$

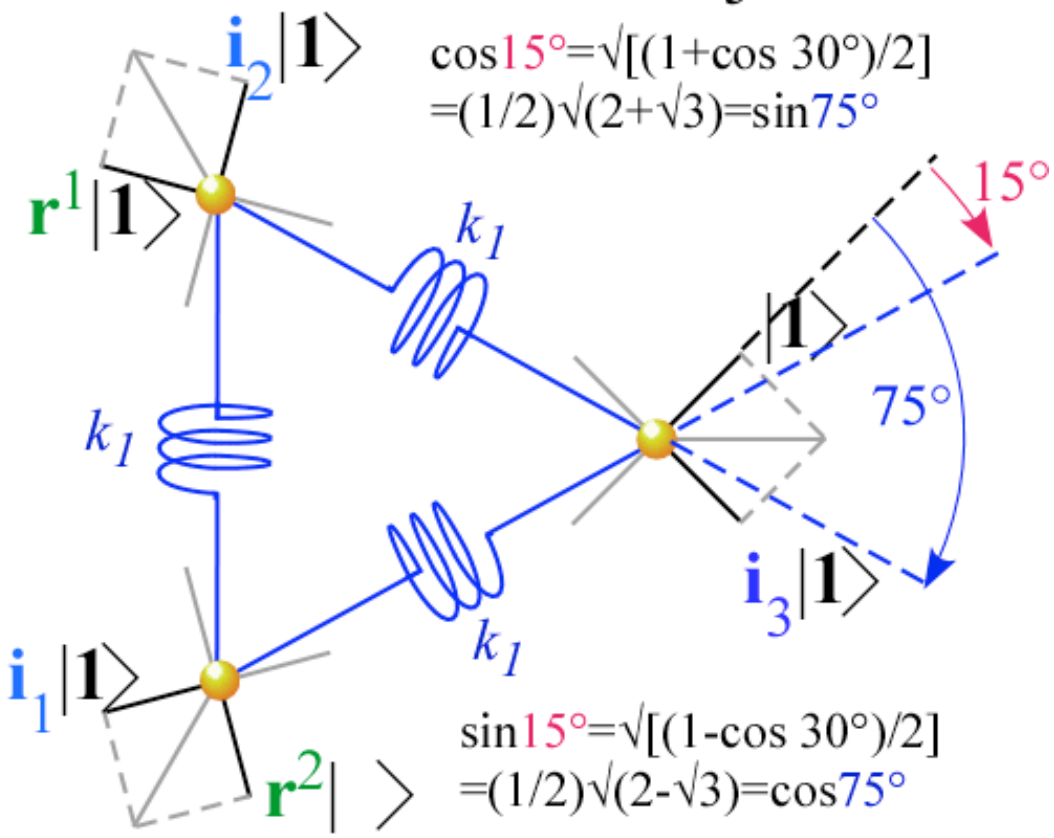
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(+) \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + \left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = \frac{3k_1}{2}\left|\begin{matrix} E_1 \\ g(+) \end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(-) \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle - \left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = 0\left|\begin{matrix} E_1 \\ g(-) \end{matrix}\right\rangle, \quad g = (x \text{ or } y).$$

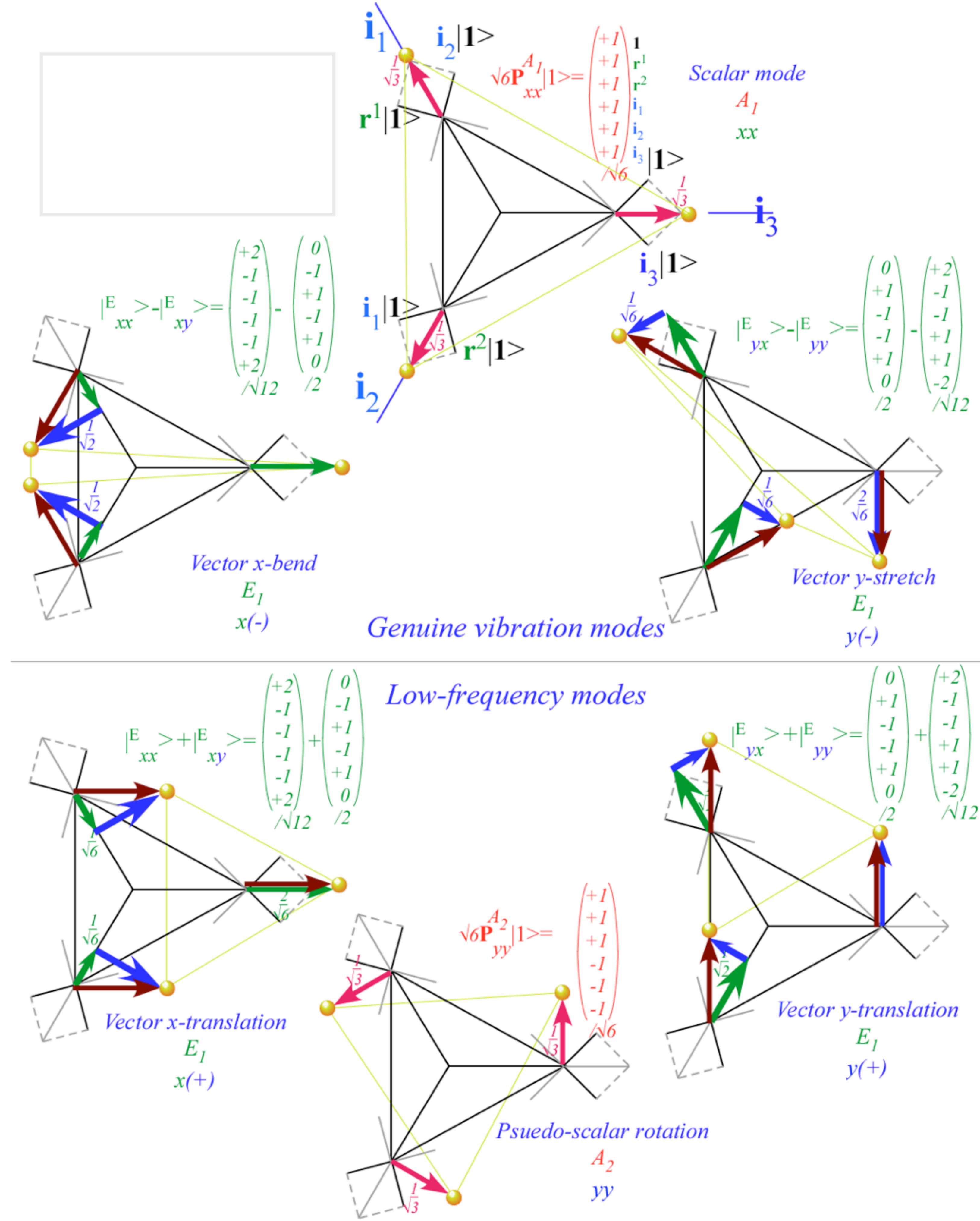
Mixed local symmetry D_3 model



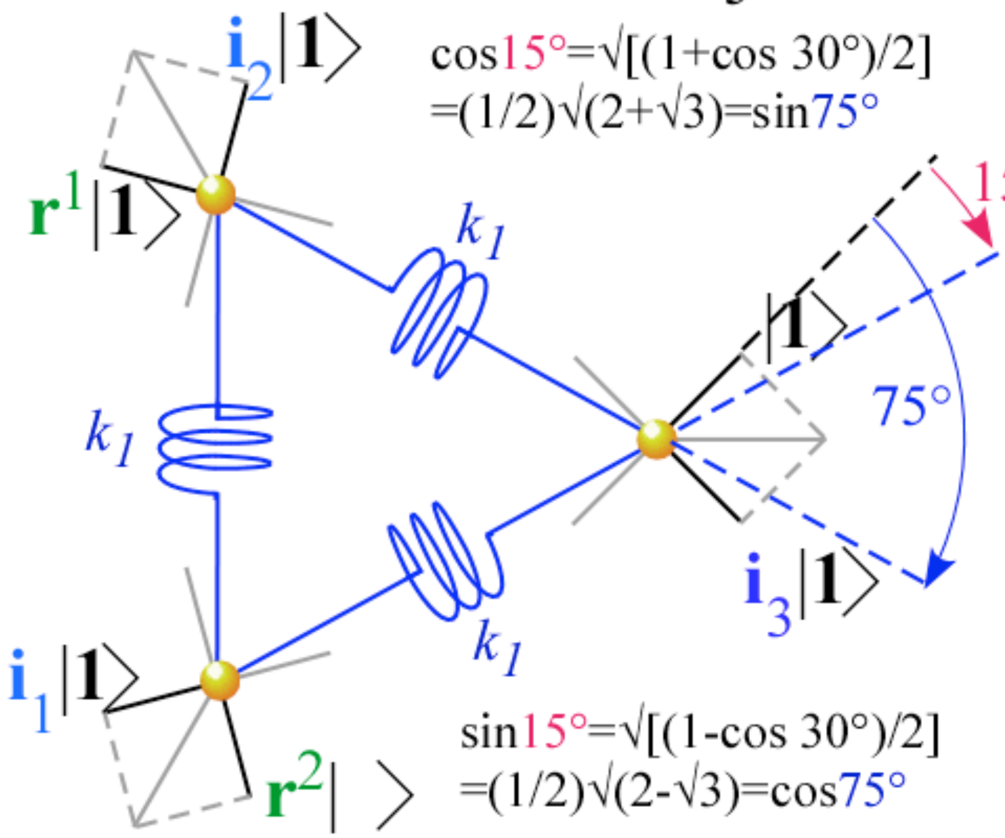
$$K_{xx}^{A_1} = 3k_1$$

$$K_{yy}^{A_2} = 0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$



Mixed local symmetry D_3 model



$$K^{A_1}_{xx} = 3k_1$$

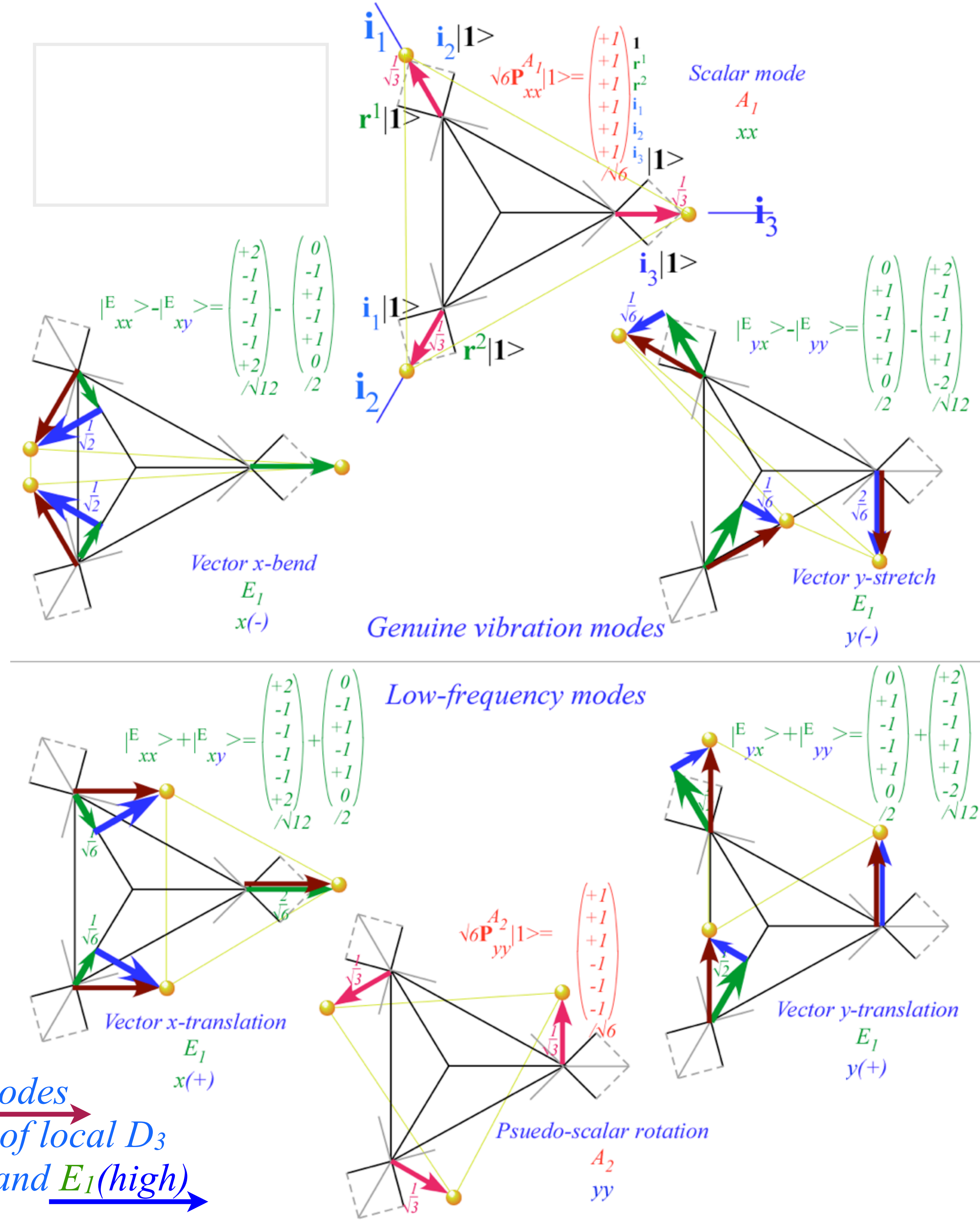
$$K^{A_2}_{yy} = 0$$

$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

E_1 Eigenvalues: $\frac{3k_1}{2}$ $\quad 0$

E_1 Eigenvectors: $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$ $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$

Mixed modes
in terms of local D_3
E_1(low) and E_1(high)



Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$-basis

Molecular vibrational modes vs. Hamiltonian eigenmodes

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ local-symmetry K-matrix eigensolutions

D_3-direct-connection K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Applied symmetry reduction and splitting

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

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Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

Induced rep $d^a(C_2)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus$.. correlation

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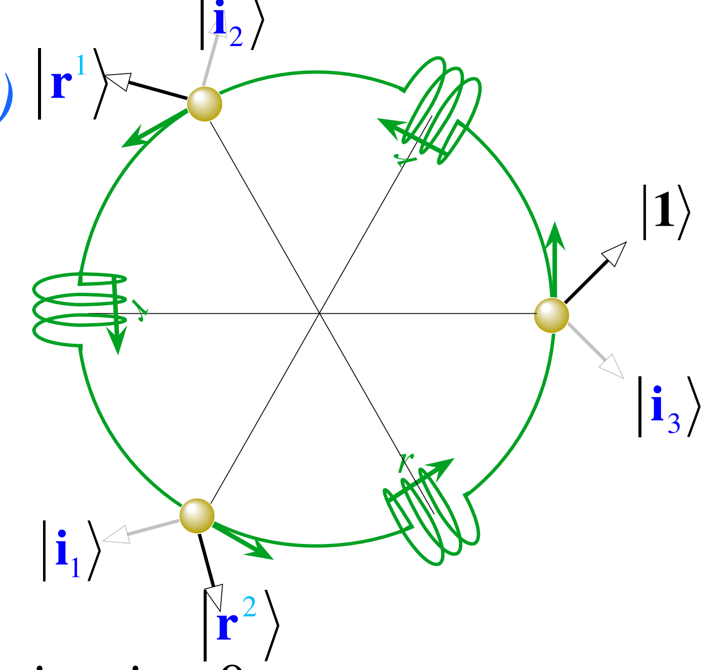
D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

Generic $\mathbf{K}$-matrix (Top row)

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

$$\langle \mathbf{1}|\mathbf{K}_{C_3}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & ir & -ir & 0 & 0 & 0 \end{bmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix

Set: $r_1 = r = -r_2^*$, and: $i_1 = i_2 = i_3 = 0$

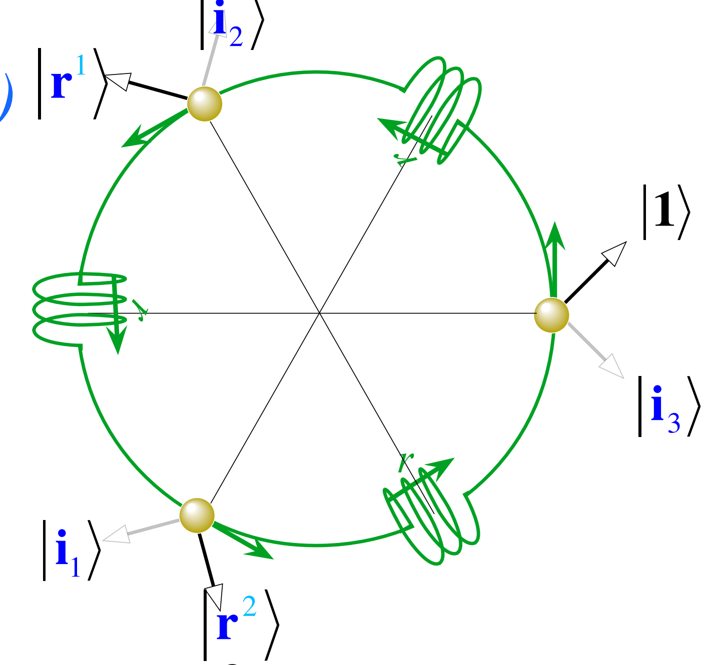
$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = r_0$$

$$K_{yy}^{A_2} = r_0 + r_1 + r_1^* - i_1 - i_2 - i_3 = r_0$$

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}_{\substack{r_1 = r = -r_2^* \\ i_1 = i_2 = i_3 = 0}} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix}$$

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



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$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

$$K_{xx}^{A_1} = r_0$$

$$K_{yy}^{A_2} = r_0$$

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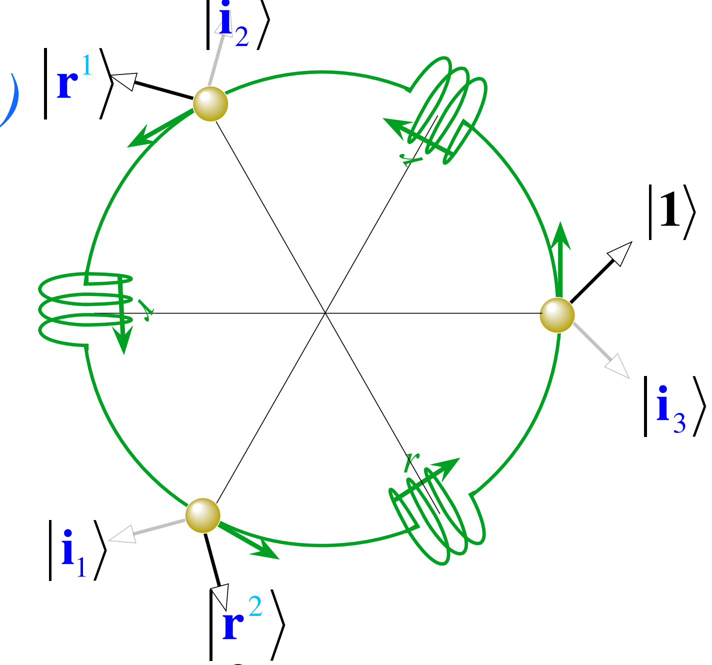

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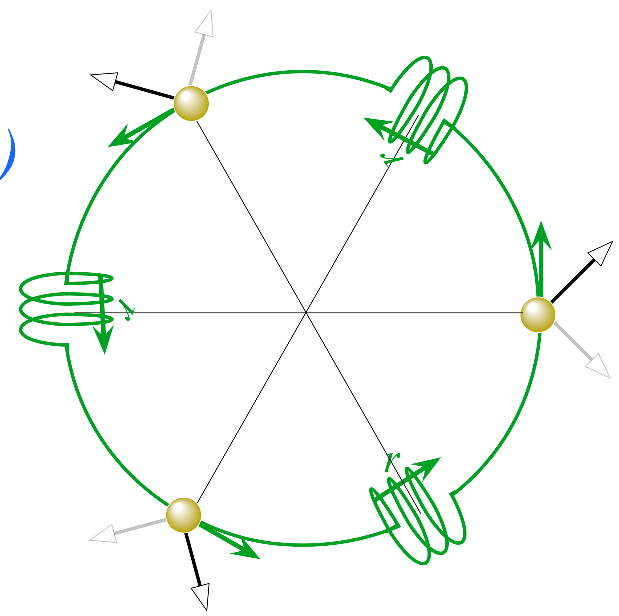
E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = +r\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle - i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = -r\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle.$$

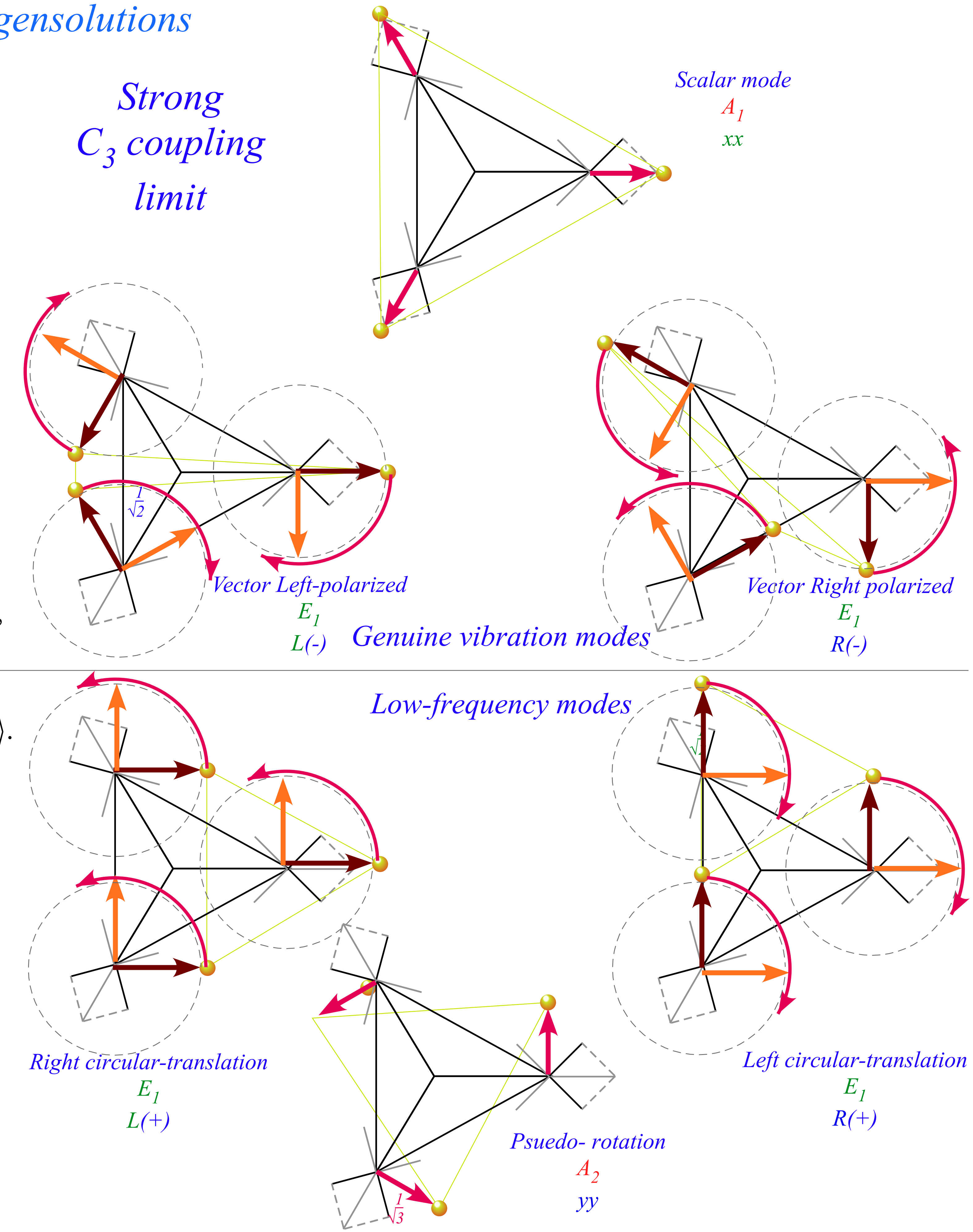
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry K-matrix eigensolutions

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = +r\,\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle,$$

$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle - i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = -r\,\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(2)_3 \end{matrix}\right\rangle.$$



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Applied symmetry reduction and splitting

Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

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D_6 symmetry and Hexagonal Bands

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ *correlation*

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
	$= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus$.. correlation

$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
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	$= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

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$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ *relabel/split*	D^{α} *relabel/reduce*	ω^{α} *relabel/split*
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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \rightarrow \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$
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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \to \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \to \omega^{0_2}$
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A_1	1	·
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E_1	1	1

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ correlation

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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{0_3} = \mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \to \omega^{0_3}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{1_3} + \mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \to \omega^{1_3}$
	$= \mathbf{P}^{E_1}_{1_3 1_3} + \mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3} \oplus d^{2_3}$	$\searrow \omega^{2_3}$

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$D_3 \supset C_2$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \to \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$	$\Rightarrow \omega^{E_1} \to \omega^{0_2}$
	$= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$d^{0_2} \oplus d^{1_2}$	$\searrow \omega^{1_2}$

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A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{0_3} = \mathbf{P}^{A_2}_{0_3 0_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2} \to \omega^{0_3}$
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A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

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A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_2}=\mathbf{P}^{A_1}_{0_20_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1}\to\omega^{0_2}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{1_2}=\mathbf{P}^{A_2}_{1_21_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2}\to\omega^{1_2}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $=\mathbf{P}^{E_1}_{0_20_2}+\mathbf{P}^{E_1}_{1_21_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2}\oplus d^{1_2}$	$\Rightarrow \omega^{E_1}\to\omega^{0_2}$ $\searrow\omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D^{A_1}(D_3)\downarrow C_2 \sim d^{0_2}$

$D^{A_2}(D_3)\downarrow C_2 \sim d^{1_2}$

$D^{E_1}(D_3)\downarrow C_2 \sim d^{0_2}\oplus d^{1_2}$

$d^{0_2}(C_2)\Uparrow D_3 \sim D^{A_1}\oplus D^{E_1}$

$d^{1_2}(C_2)\Uparrow D_3 \sim D^{A_2}\oplus D^{E_1}$

Spontaneous symmetry breaking and clustering: Induced rep $d^{a}(C_2)\uparrow D^3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

Applied symmetry reduction and splitting: Subduced irep $D^{\alpha}(D^3)\downarrow C_3 = d^{0_3}\oplus d^{1_3}\oplus$.. correlation

$D_3 \supset C_3$	$\mathbf{P}^{\alpha}$ relabel/split	D^{α} relabel/reduce	ω^{α} relabel/split
A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_30_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1}\to\omega^{0_3}$
A_2	$\mathbf{P}^{A_2}=\mathbf{P}^{A_2}\mathbf{P}^{0_3}=\mathbf{P}^{A_2}_{0_30_3}$	$\Rightarrow D^{A_2}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_2}\to\omega^{0_3}$
E_1	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$ $=\mathbf{P}^{E_1}_{1_31_3}+\mathbf{P}^{E_1}_{2_32_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$ $d^{1_3}\oplus d^{2_3}$	$\Rightarrow \omega^{E_1}\to\omega^{1_3}$ $\searrow\omega^{2_3}$

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

$D^{A_1}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{A_2}(D_3)\downarrow C_3 \sim d^{0_3}$

$D^{E_1}(D_3)\downarrow C_3 \sim d^{1_3}\oplus d^{2_3}$

$d^{0_3}(C_3)\Uparrow D_3 \sim D^{A_1}\oplus D^{A_2}$

$d^{1_3}(C_3)\Uparrow D_3 \sim D^{E_1}$

$d^{2_3}(C_3)\Uparrow D_3 \sim D^{E_1}$

Spontaneous symmetry breaking and clustering: Induced rep $d^{a}(C_3)\uparrow D^3 = D^{\alpha}\oplus D^{\beta}\oplus$.. correlation

Frobenius Reciprocity Theorem

$$\text{Number of } D^{\alpha} \text{ in } d^{k}(K) \uparrow G = \text{ Number of } d^{k} \text{ in } D^{\alpha}(G) \downarrow K$$

Frobenius Reciprocity Theorem

$$\text{Number of } D^{\alpha} \text{ in } d^{k}(K)\uparrow G = \text{ Number of } d^{k} \text{ in } D^{\alpha}(G)\downarrow K$$

..and regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

Frobenius Reciprocity Theorem

$$\text{Number of } D^\alpha \text{ in } d^k(K)\uparrow G = \text{ Number of } d^k \text{ in } D^\alpha(G)\downarrow K$$

..and regular representation

$D_3 \supset C_1$	$0_1 = 1_1$
A_1	1
A_2	1
E_1	2

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
A_2	·	1
E_1	1	1

$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

Review: Hamiltonian local-symmetry eigensolution in global and local $|\mathbf{P}^{(\mu)}\rangle$*-basis*

Molecular vibrational modes vs. Hamiltonian eigenmodes

Molecular K-matrix construction

$D_3 \supset C_2(i_3)$ *local-symmetry K-matrix eigensolutions*

D_3*-direct-connection K-matrix eigensolutions*

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ *local symmetry K-matrix eigensolutions*

Applied symmetry reduction and splitting

Subduced irep $D^\alpha(D^3)\downarrow C_2 = d^{0_2} \oplus d^{1_2} \oplus ..$ *correlation*

Subduced irep $D^\alpha(D^3)\downarrow C_3 = d^{0_3} \oplus d^{1_3} \oplus ..$ *correlation*

Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

Induced rep $d^a(C_2)\uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ *correlation*

Induced rep $d^a(C_3)\uparrow D^3 = D^\alpha \oplus D^\beta \oplus ..$ *correlation*

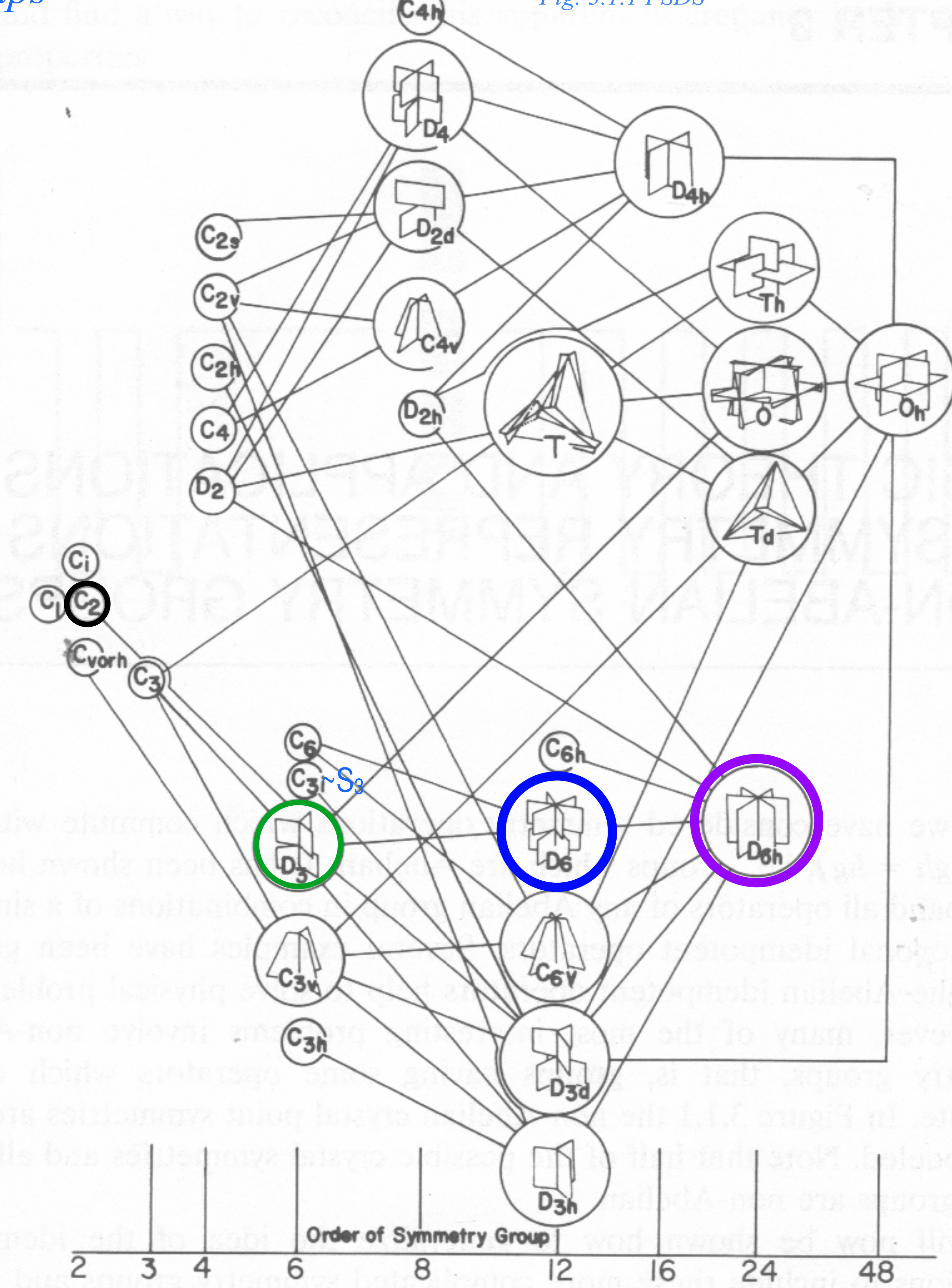
D_6 *symmetry and Hexagonal Bands*

Cross product of the C_2 *and* D_3 *characters gives all* $D_6 = D_3 \times C_2$ *characters and ireps*

Hexagonal D-family-1: $D_{6h} \supset D_6 \supset D_3 \supset C_2$

of the 32 crystal point groups

Fig. 3.1.1 PSDS



D_6 symmetry and Hexagonal Bands

D_6 is the *outer product* (×) *product* $D_3 \times C_2$ of D_3 and C_2. (Requires C_2 to commute with all of D_3.)

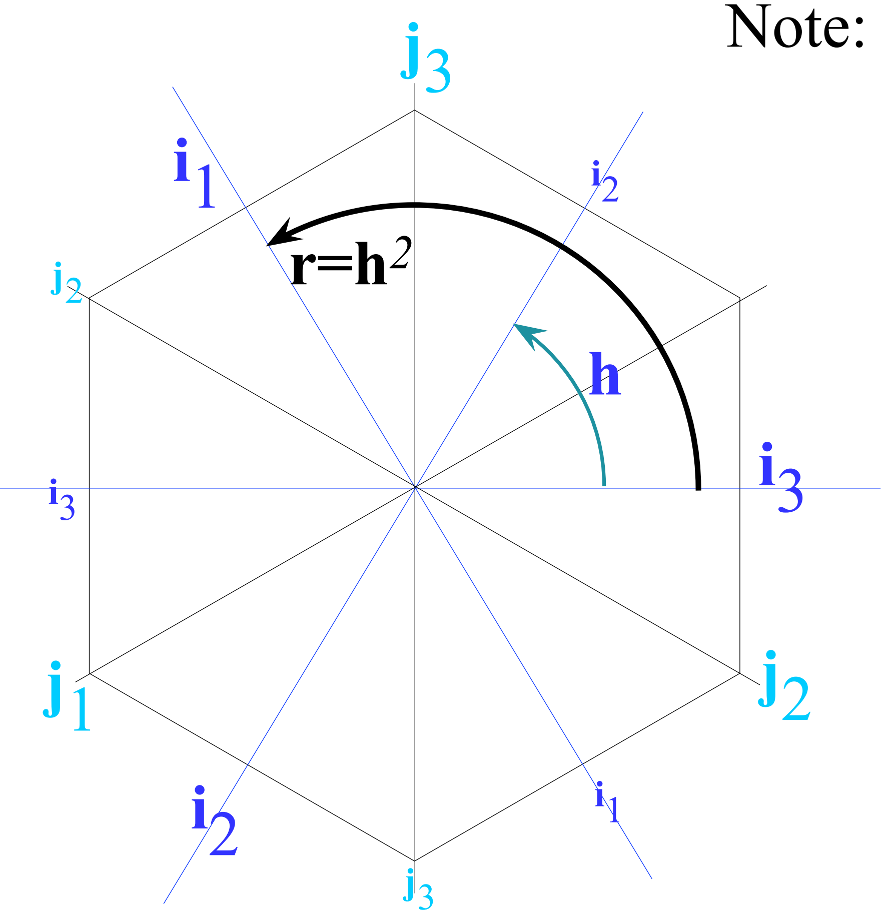
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$$

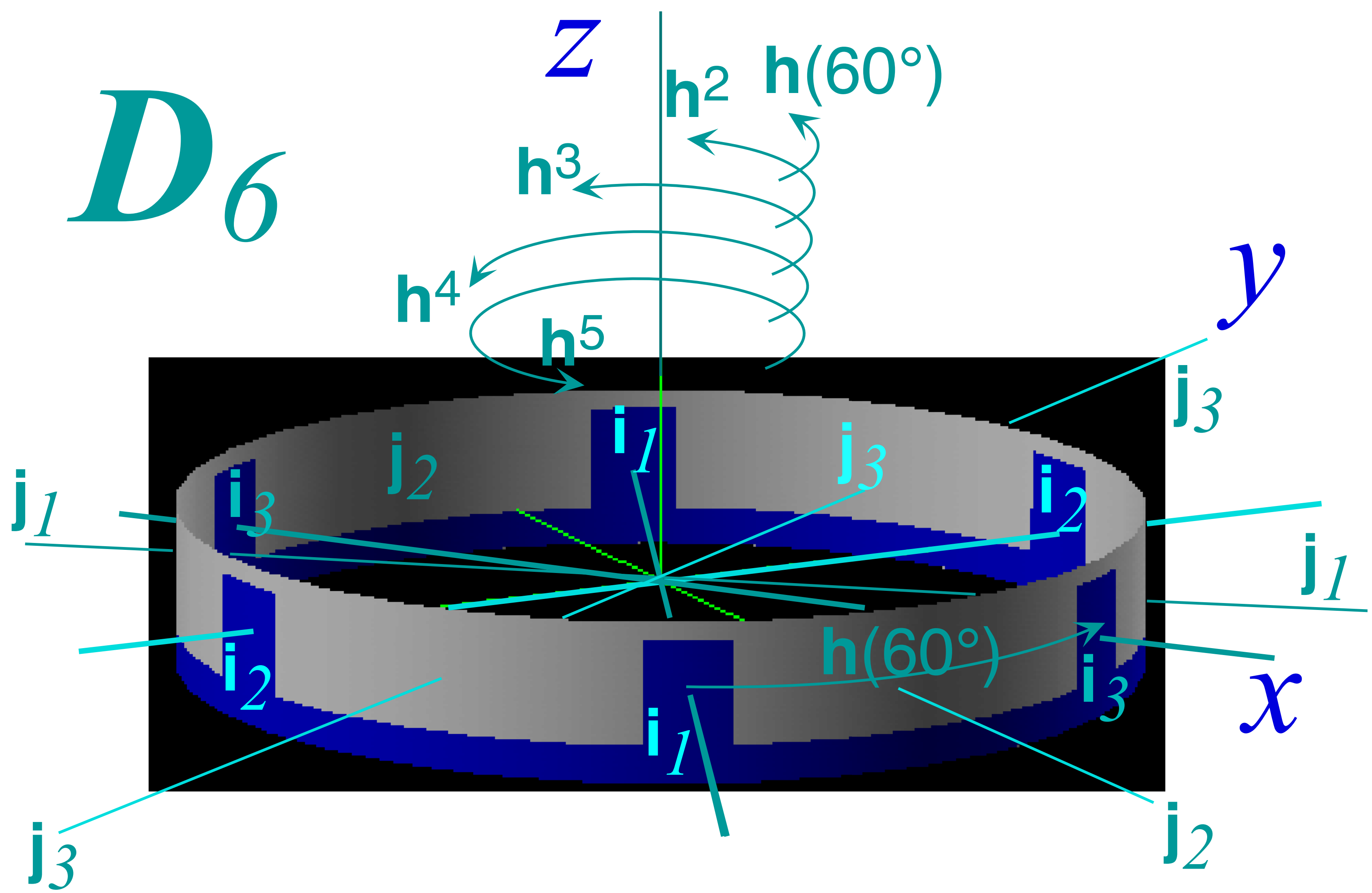
× product and D_6 operators. Define *hexagonal generator* **h** of subgroup $C_6 = \{\mathbf{1}, \mathbf{h}, \mathbf{h}^2, \mathbf{h}^3, \mathbf{h}^4\ \mathbf{h}^5\}$

$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{1}\cdot\mathbf{R}_z, \mathbf{r}\cdot\mathbf{R}_z, \mathbf{r}^2\cdot\mathbf{R}^z, \mathbf{i}_1\cdot\mathbf{R}_z, \mathbf{i}_2\cdot\mathbf{R}_z, \mathbf{i}_3\cdot\mathbf{R}_z\}$$

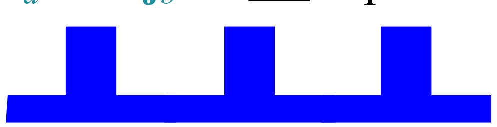
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$$

Note: $\mathbf{h}^2 = \mathbf{r}$ and $\mathbf{h}^3 = \mathbf{R}_z$ and $\mathbf{h}^4 = \mathbf{r}^2$ and $\mathbf{h}^5 = \mathbf{r}\cdot\mathbf{R}_z$





NOTE:
The $\mathbf{i}_a$ and $\mathbf{j}_b$ do <u>not</u> flip over the potential plot.



Electrostatic potential $V(\phi)$ doesn't care which way is "up." Wells remain wells, and barriers remain barriers under all *D6* operations.

Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters.

D_3	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})$	1	1	1
$\chi^{A_2}(\mathbf{g})$	1	1	−1
$\chi^{E_1}(\mathbf{g})$	2	−1	0

×

C_2^z	$\mathbf{1}$	$\mathbf{R}_z$
(A)	1	1
(B)	1	−1

=

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{r},\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{1}\cdot\mathbf{R}_z$	$\{\mathbf{r},\mathbf{r}^2\}\cdot\mathbf{R}_z$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}\cdot\mathbf{R}_z$
$A_1\cdot(A)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$A_2\cdot(A)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$1\cdot1$	$-1\cdot1$
$E_2\cdot(A)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot1$	$-1\cdot1$	$0\cdot1$
$A_1\cdot(B)$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$1\cdot(-1)$
$A_2\cdot(B)$	$1\cdot1$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$	$-1\cdot(-1)$
$E_1\cdot(B)$	$2\cdot1$	$-1\cdot1$	$0\cdot1$	$2\cdot(-1)$	$-1\cdot(-1)$	$0\cdot(-1)$

$\chi_g^\mu(D_6) =$

$D_3 \times C_2^z$	$\mathbf{1}$	$\{\mathbf{h}^2,\mathbf{h}^4\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$	$\mathbf{h}^3$	$\{\mathbf{h},\mathbf{h}^5\}$	$\{\mathbf{j}_1,\mathbf{j}_2,\mathbf{j}_3\}$
A_1	1	1	1	1	1	1
A_2	1	1	-1	1	1	-1
E_2	2	-1	0	2	-1	0
B_2	1	1	1	-1	-1	-1
B_1	1	1	-1	-1	-1	1
E_1	2	-1	0	−2	1	0

(Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups)

Unit translation
or
60° *hex rotation* **h**
determines
A_p vs B_p
(+1) vs (-1)

Odd vs Even

Y-rotation
or
180° *flip* $\mathbf{j}_3$
determines
X_1 vs X_2
(+1) vs (-1)

"Always-the-same vs Back-and-forth"

Cross product of the C_2 and D_3 ireps gives all $D_6 = D_3 \times C_2$ ireps.

g =	**1**	$\mathbf{r}=\mathbf{h}^2$	$\mathbf{r}^2=\mathbf{h}^4$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{h}^3$	$\mathbf{h}^3\mathbf{r}=\mathbf{h}^5$	$\mathbf{h}^3\mathbf{r}^2=\mathbf{h}^1$	$\mathbf{h}^3\mathbf{i}_1=\mathbf{j}_1$	$\mathbf{h}^3\mathbf{i}_2=\mathbf{j}_2$	$\mathbf{h}^3\mathbf{i}_3=\mathbf{j}_3$
$D^{A_1}(g)=$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g)=$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_2}(g)=$	1	1	1	1	1	1	-1	-1	-1	- 1	-1	-1
$D^{B_1}(g)=$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

Unit translation
or
60° *hex rotation* **h**
determines
A_p vs B_p
(+1) vs (-1)

Y-rotation
or
180° *flip* $\mathbf{j}_3$
determines
X_1 vs X_2
(+1) vs (-1)

"Always-the-same vs Back-and-forth"

Odd vs Even

Cross product of the C_2 and D_3 ireps gives all $D_6 = D_3 \times C_2$ ireps.

$\mathbf{g} =$	$\mathbf{1}$	$\mathbf{r}=\mathbf{h}^2$	$\mathbf{r}^2=\mathbf{h}^4$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{h}^3$	$\mathbf{h}^3\mathbf{r}=\mathbf{h}^5$	$\mathbf{h}^3\mathbf{r}^2=\mathbf{h}^1$	$\mathbf{h}^3\mathbf{i}_1=\mathbf{j}_1$	$\mathbf{h}^3\mathbf{i}_2=\mathbf{j}_2$	$\mathbf{h}^3\mathbf{i}_3=\mathbf{j}_3$
$D^{A_1}(g) =$	1	1	1	1	1	1	1	1	1	1	1	1
$D^{A_2}(g) =$	1	1	1	-1	-1	-1	1	1	1	-1	-1	-1
$D^{E_2}(g) =$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
$D^{B_2}(g) =$	1	1	1	1	1	1	-1	-1	-1	- 1	-1	-1
$D^{B_1}(g) =$	1	1	1	-1	-1	-1	-1	-1	-1	1	1	1
$D^{E_1}(g) =$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} \frac{1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

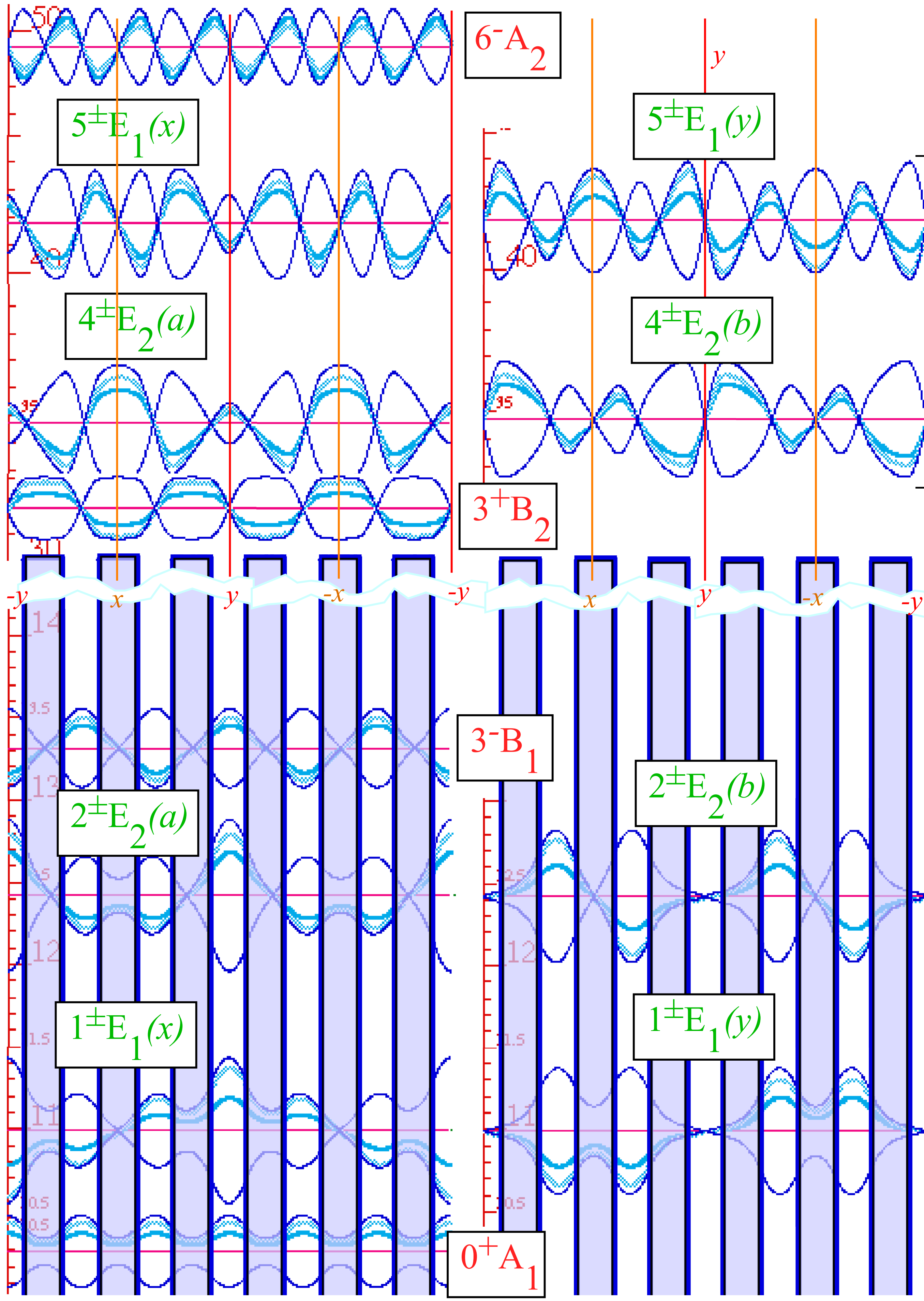
Unit translation
or
60° *hex rotation* **h**
determines
A_p vs B_p
(+1) vs (-1)

Y-rotation
or
180° *flip* $\mathbf{j}_3$
determines
X_1 vs X_2
(+1) vs (-1)

$D_6 \supset C_2(j_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_2	·	1
B_1	1	·
E_1	1	1

$D_6 \supset C_3(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

D_6 Band structure and related induced representations



$D_6 \supset C_3(h)$	0_6	1_6	2_6	3_6	4_6	5_6
A_1	1	·	·	·	·	·
A_2	1	·	·	·	·	·
E_2	·	·	1	·	1	·
B_2	·	·	·	1	·	·
B_1	·	·	·	1	·	·
E_1	·	1	·	·	·	1

$1_2 \uparrow D_3 \sim A_2 \oplus E_2 \oplus E_1 \oplus B_2$

Odd Band or Cluster

$0_2 \uparrow D_3 \sim A_1 \oplus E_1 \oplus E_2 \oplus B_1$

Even Band or Cluster

$D_3 \supset C_2(j_3)$	0_2	1_2
A_1	1	·
A_2	·	1
E_2	1	1
B_2	·	1
B_1	1	·
E_1	1	1