Group Theory in Quantum Mechanics

Lecture 17 (3.20.15)

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*
- *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*

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

Review excerpts of Lecture 16

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

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

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

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

D_3 local projector product table

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

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

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

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

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 ←

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

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

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

$|\mathbf{P}^{(\mu)}\rangle$-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 **g**-*matrix component*

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

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

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

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

Review excerpts of Lecture 16

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:*

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

$$\begin{pmatrix} H^{A_1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & H^{A_2} & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} & \cdot & \cdot \\ \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{xx} & H^{E_1}_{xy} \\ \cdot & \cdot & \cdot & \cdot & H^{E_1}_{yx} & H^{E_1}_{yy} \end{pmatrix}$$

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

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

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

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

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

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

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

Review excerpts of Lecture 16

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

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

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

A_1-block A_2-block

- •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

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

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

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

Global (LAB) symmetry

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

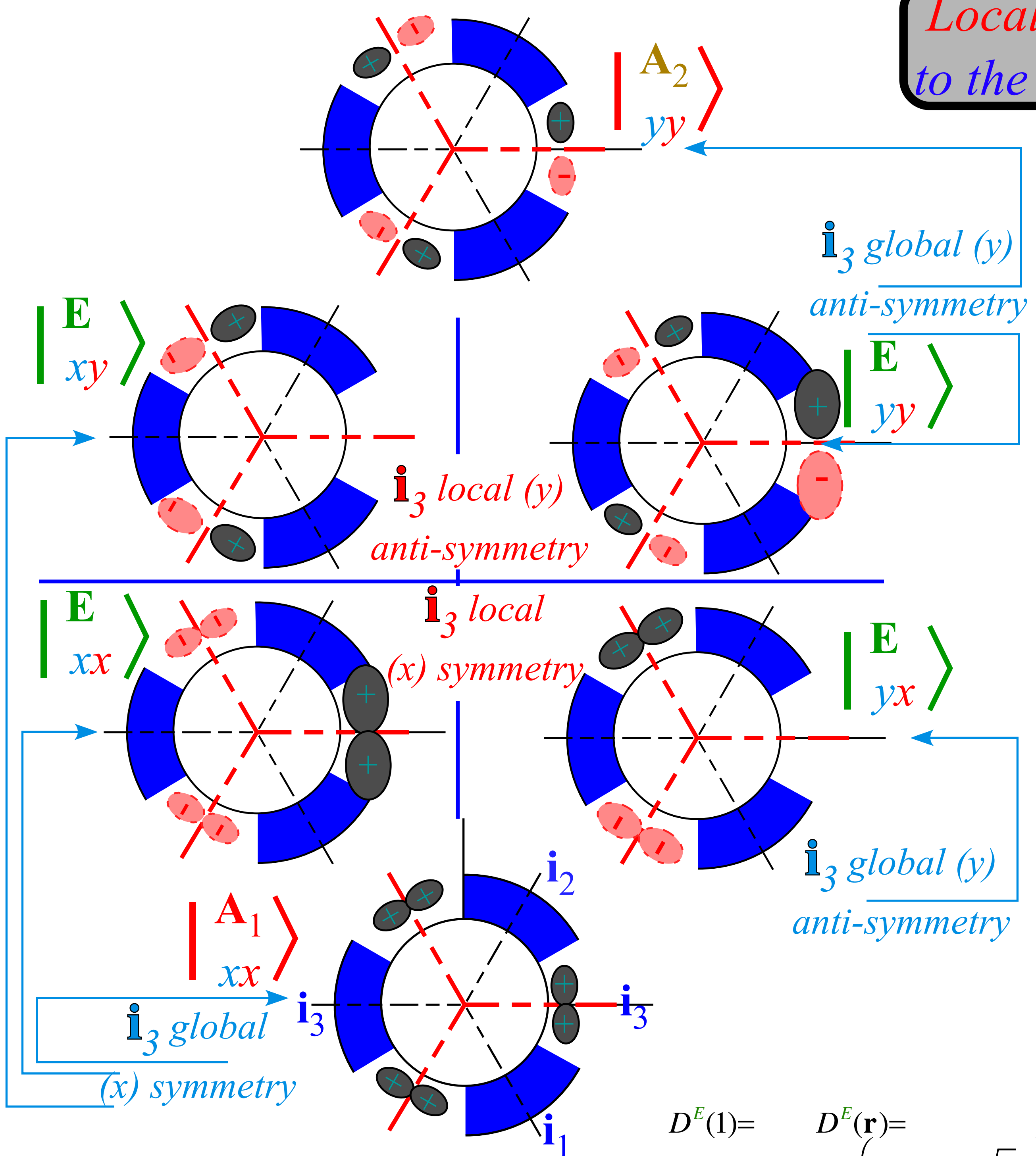
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

Local (BOD) symmetry

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

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

Here the "Mock-Mach" is being applied!



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

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

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

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

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

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

Global (LAB) symmetry

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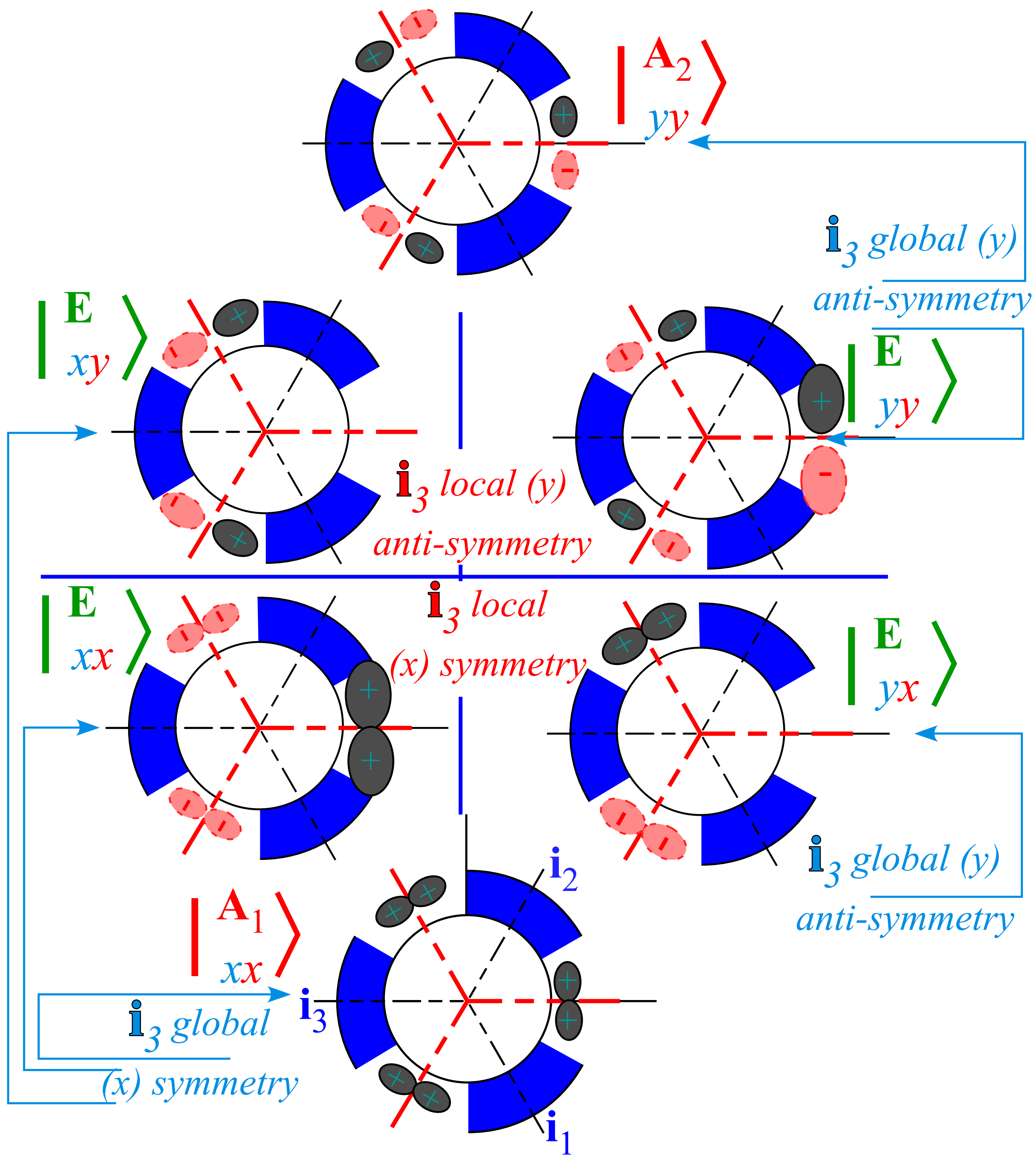
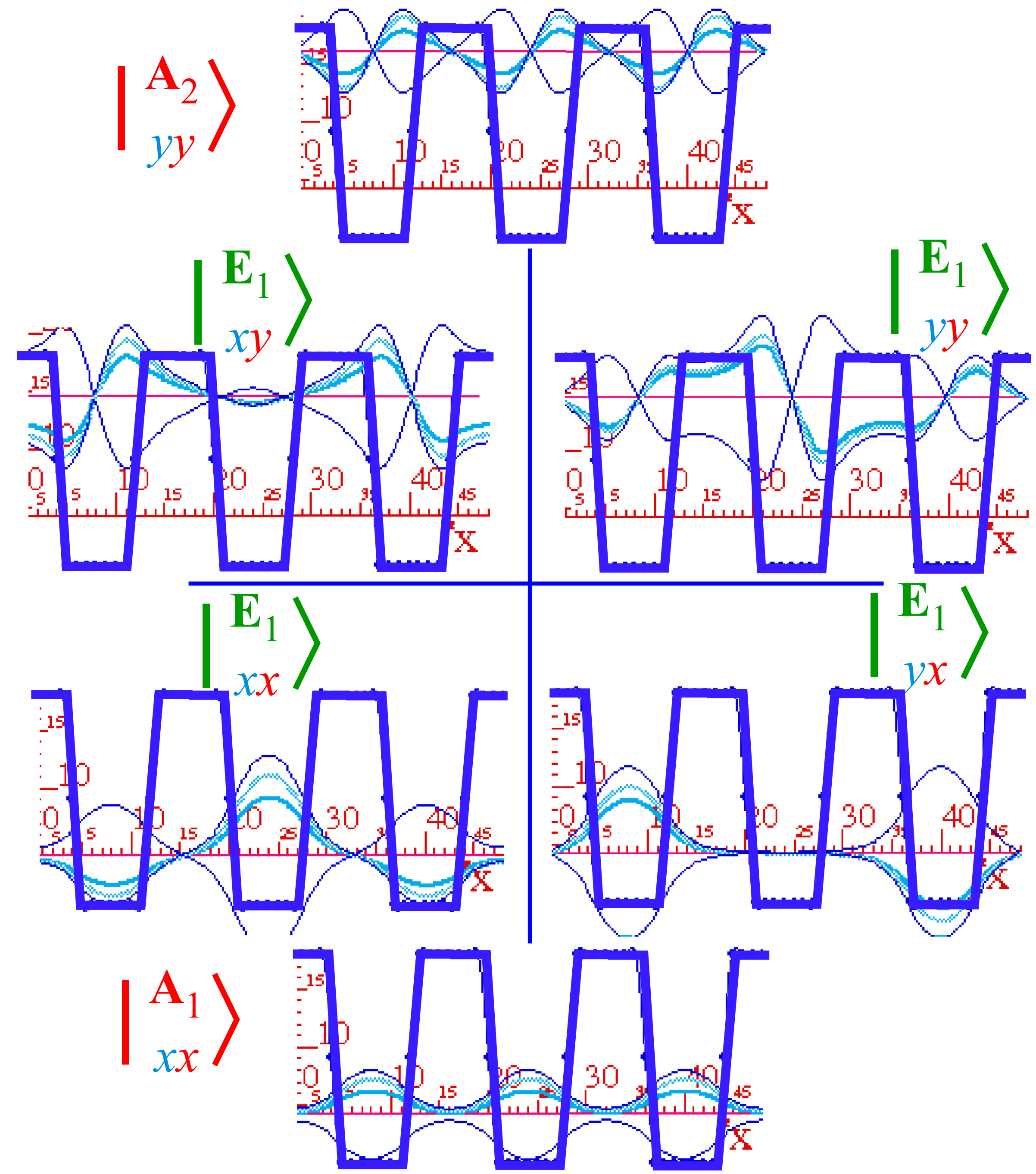
Local (BOD) symmetry

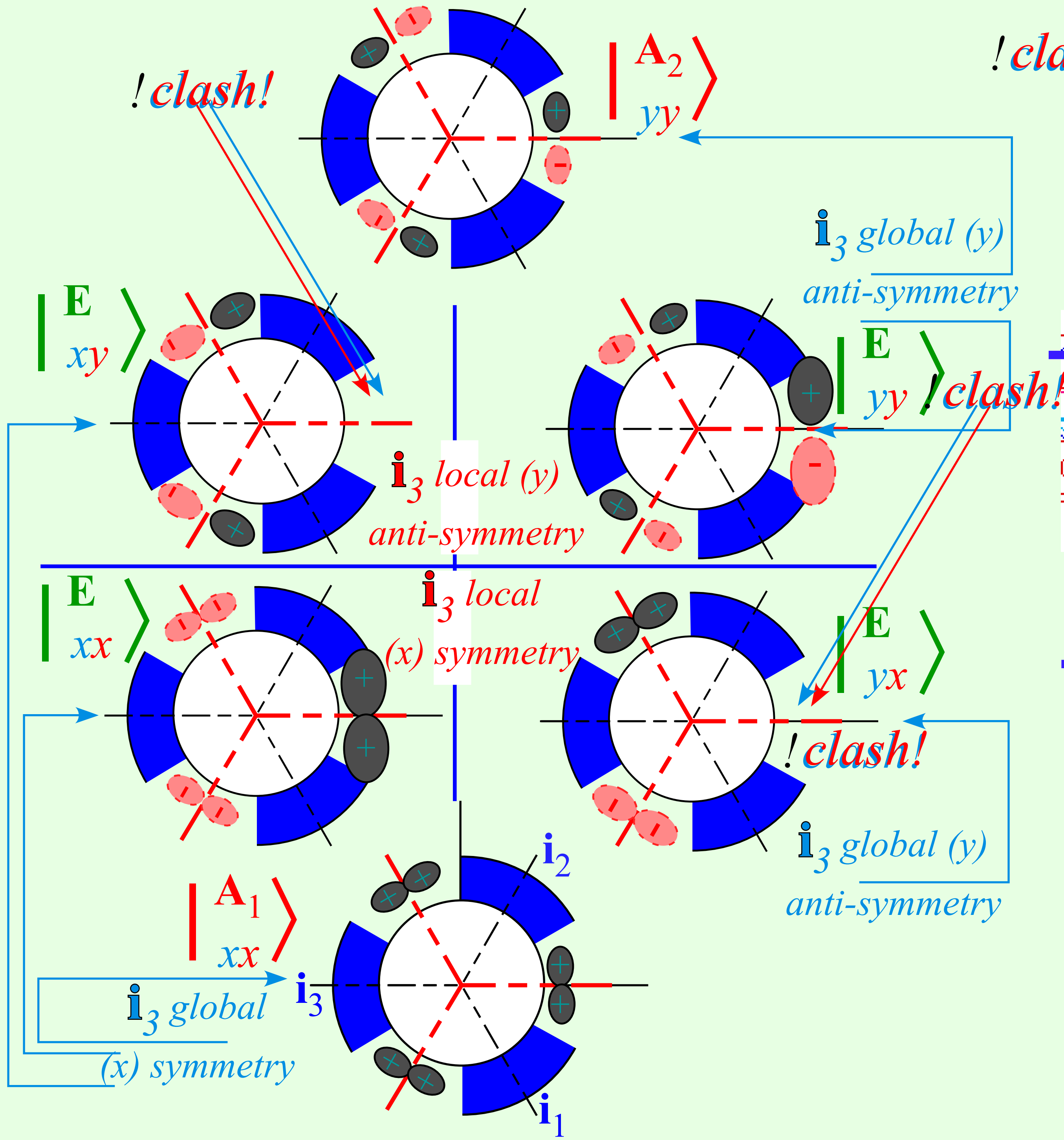
$$\bar{\mathbf{i}}_3\left|{}^{(m)}_{eb}\right\rangle = \bar{\mathbf{i}}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = \mathbf{P}^{(m)}_{eb}\bar{\mathbf{i}}_3\left|1\right\rangle = \mathbf{P}^{(m)}_{eb}\mathbf{i}_3^{\dagger}\left|1\right\rangle = (-1)^b \left|{}^{(m)}\right\rangle$$

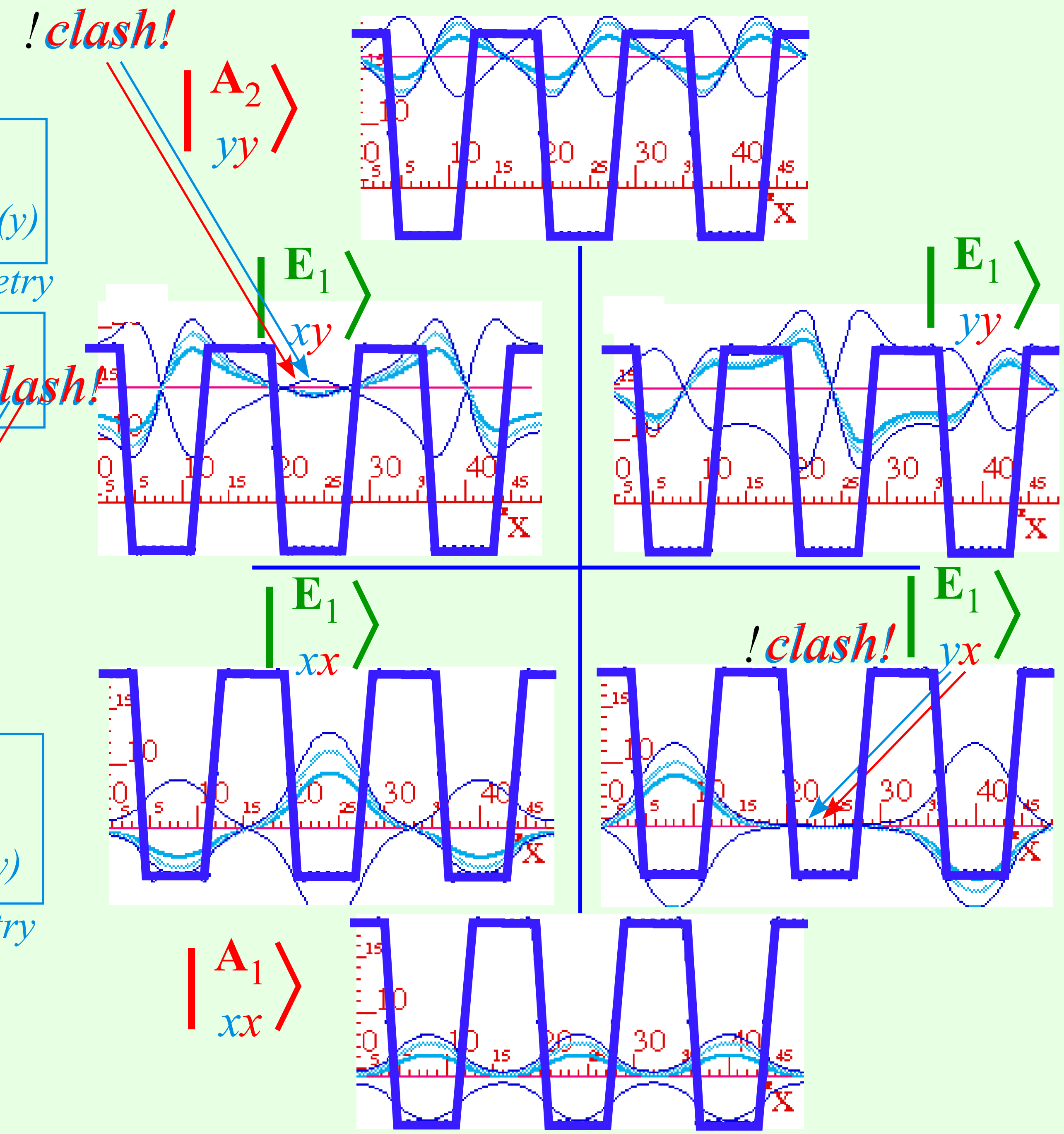




When there is no there, there...

<u>Nobody Home</u>
where LOCAL
and GLOBAL





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

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

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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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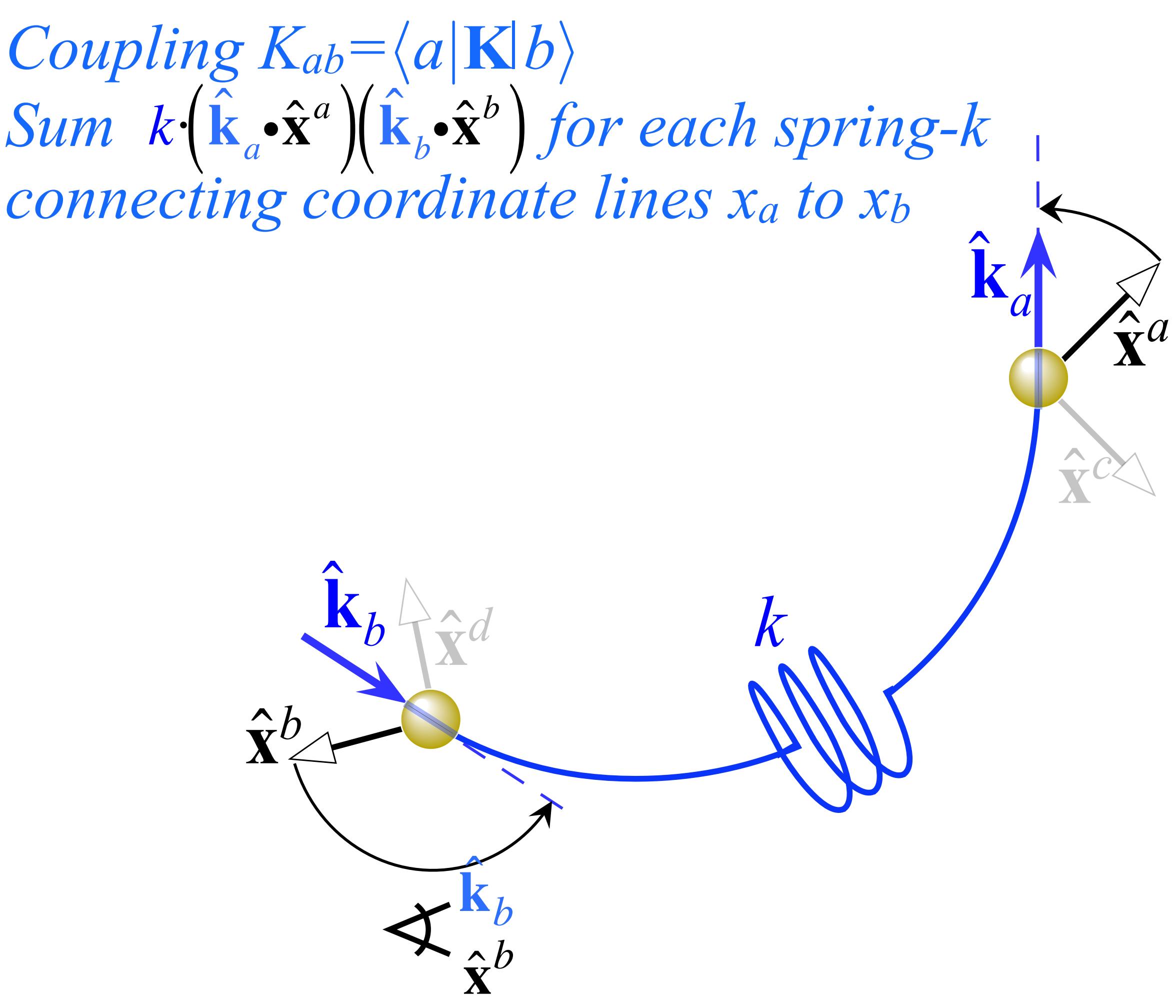

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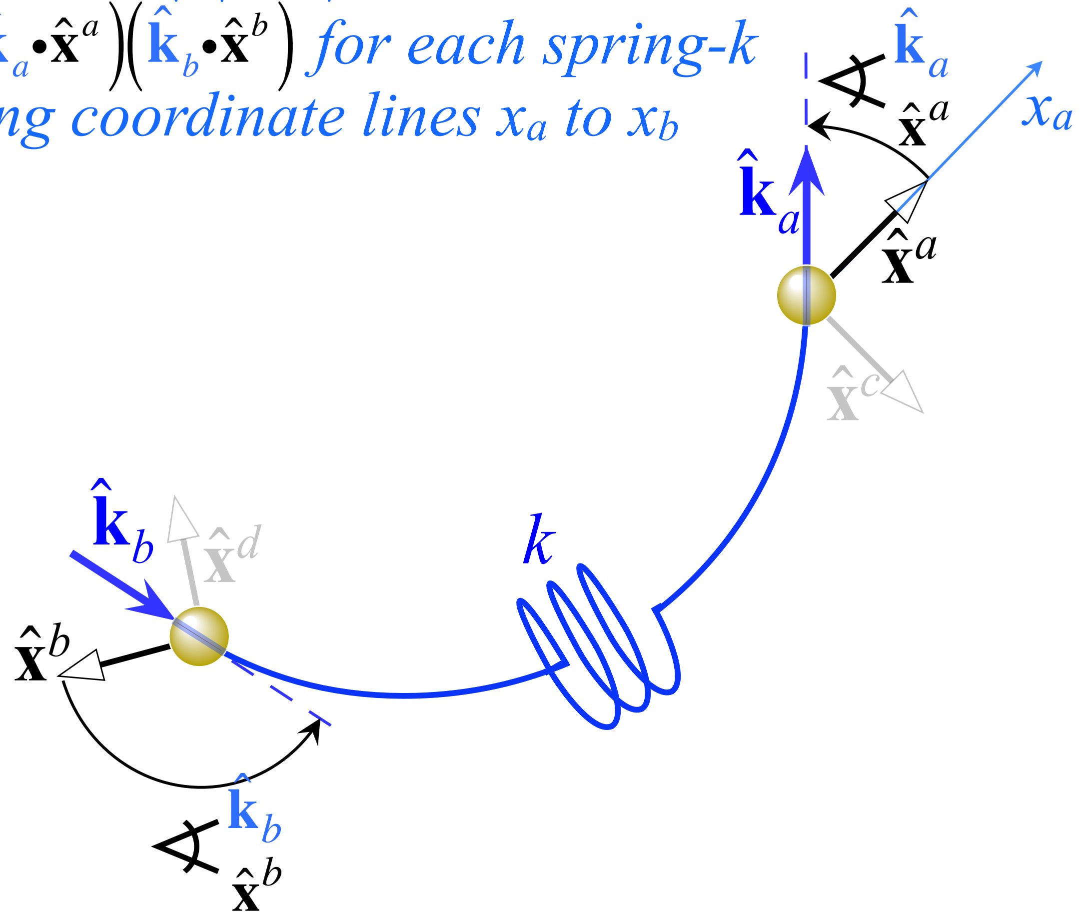
Coupling $K_{ab}=\langle a|\mathbf{K}|b\rangle$
Sum $k\cdot(\hat{\mathbf{k}}_a\bullet\hat{\mathbf{x}}^a)(\hat{\mathbf{k}}_b\bullet\hat{\mathbf{x}}^b)$ *for each spring-k connecting coordinate lines* x_a *to* x_b

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



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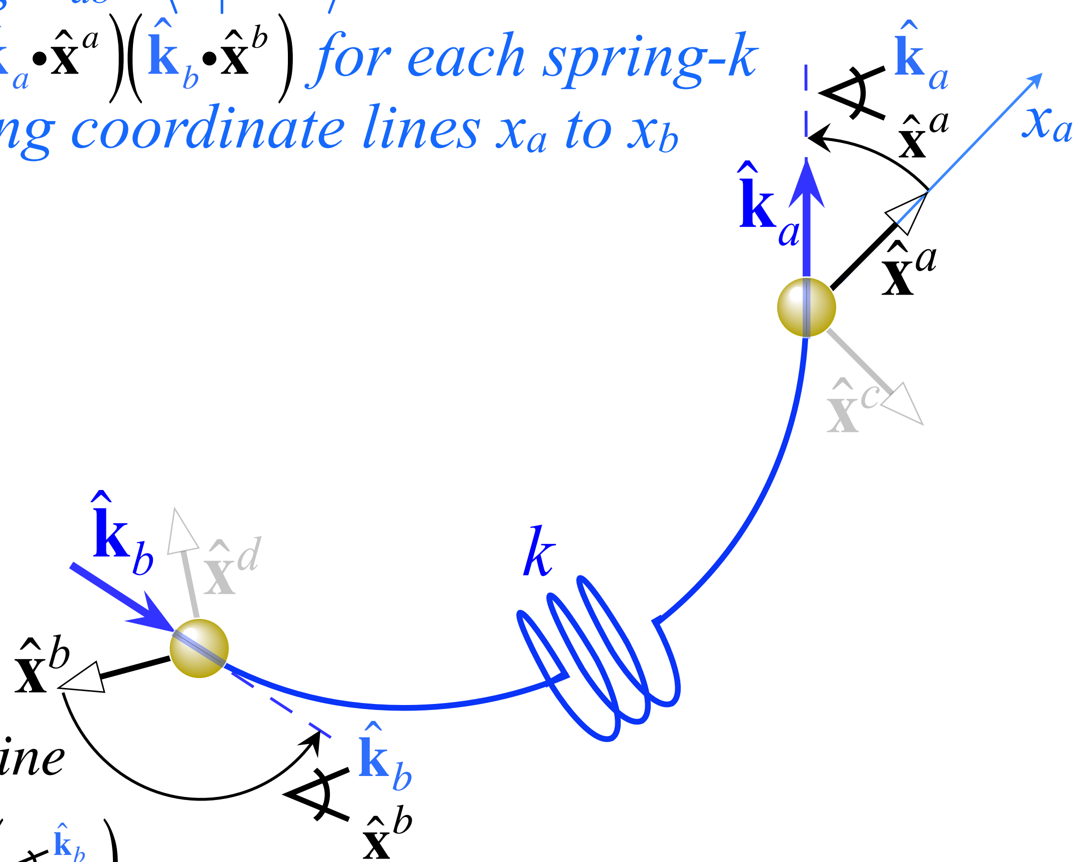

Direction cosine

$(\hat{\mathbf{k}}_b \bullet \hat{\mathbf{x}}^b) = \cos(\sphericalangle^{\hat{\mathbf{k}}_b}_{\hat{\mathbf{x}}^b})$

at b-end of k - spring

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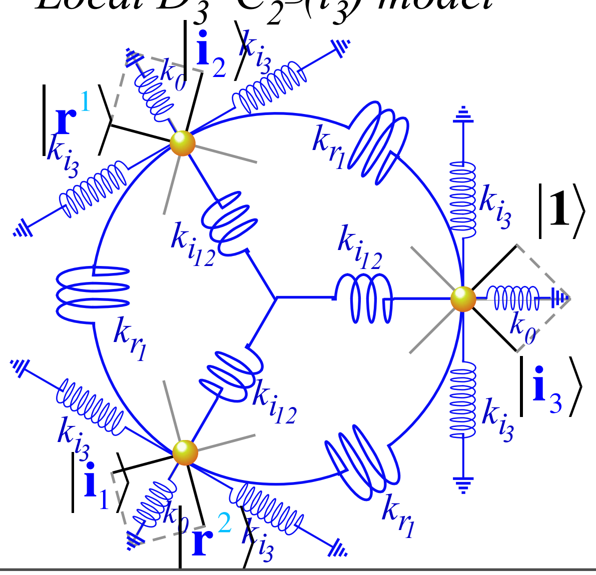
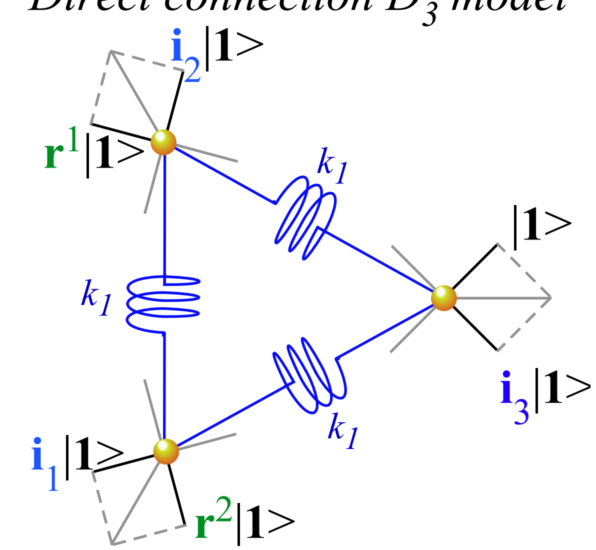
Local D_3 $C_2 \supset (i_3)$ model



Direct connection D_3 model



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

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

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

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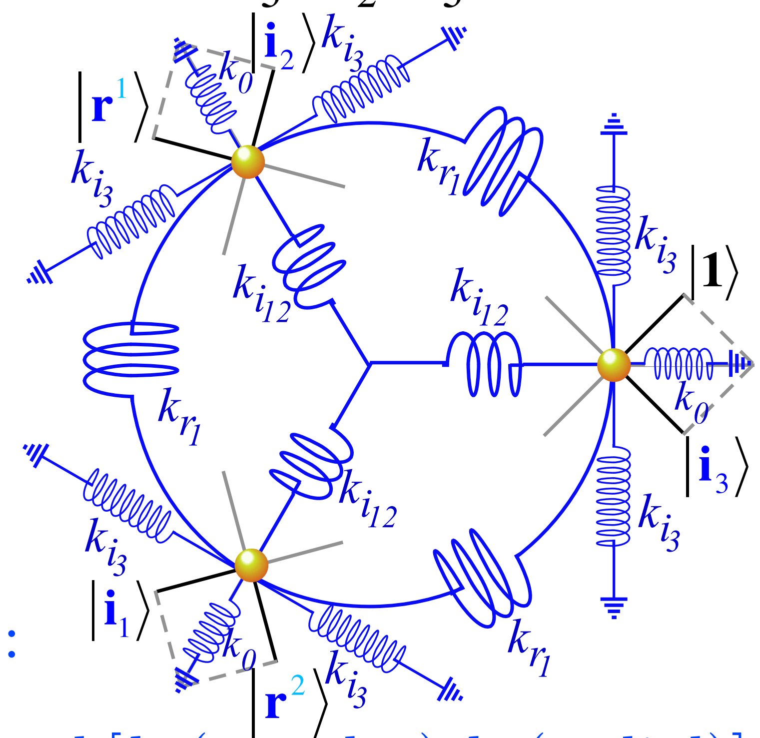

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1^{st}-row parameters $g_b = \langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = K_{1b}$ of the force matrix K_{ab}:

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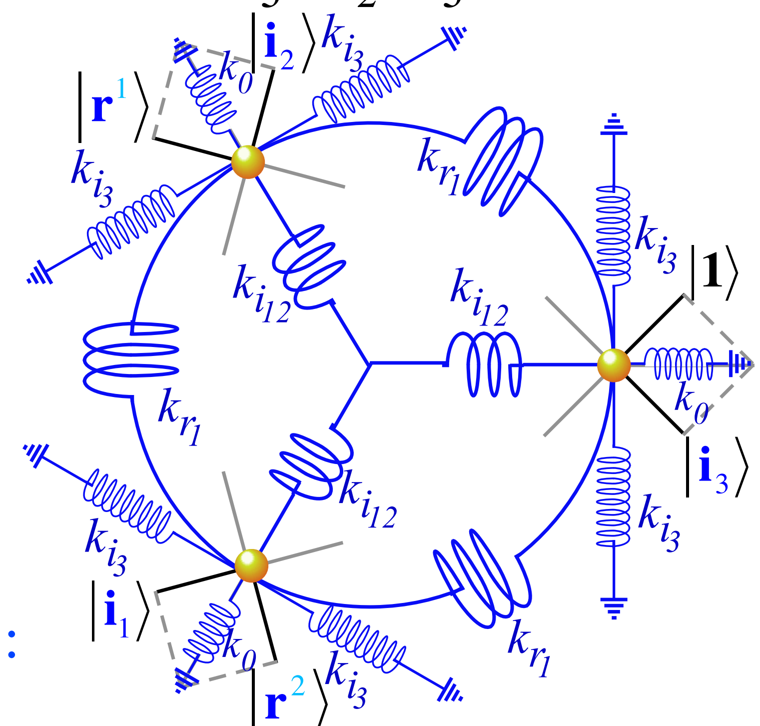

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$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle \mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$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

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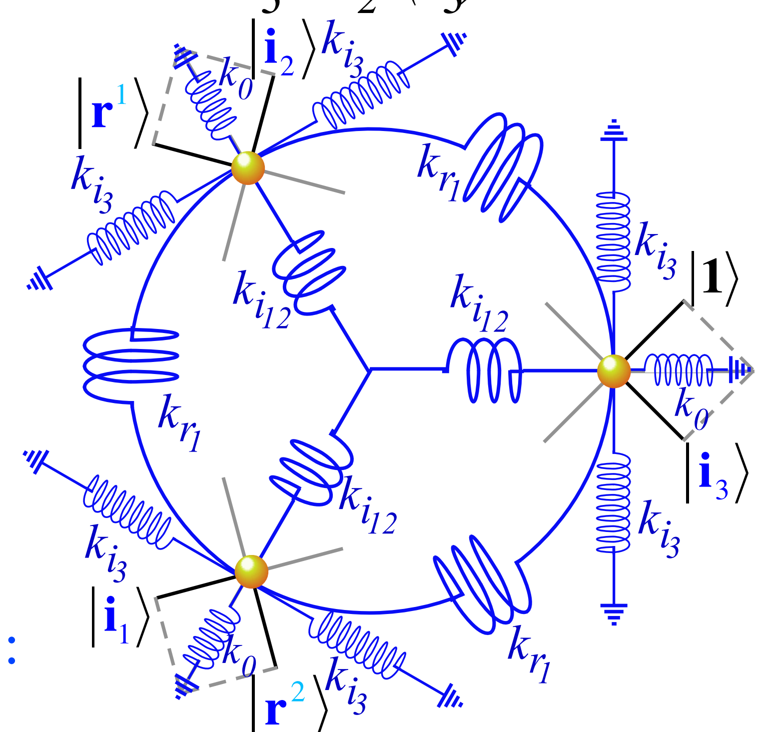


$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix

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.

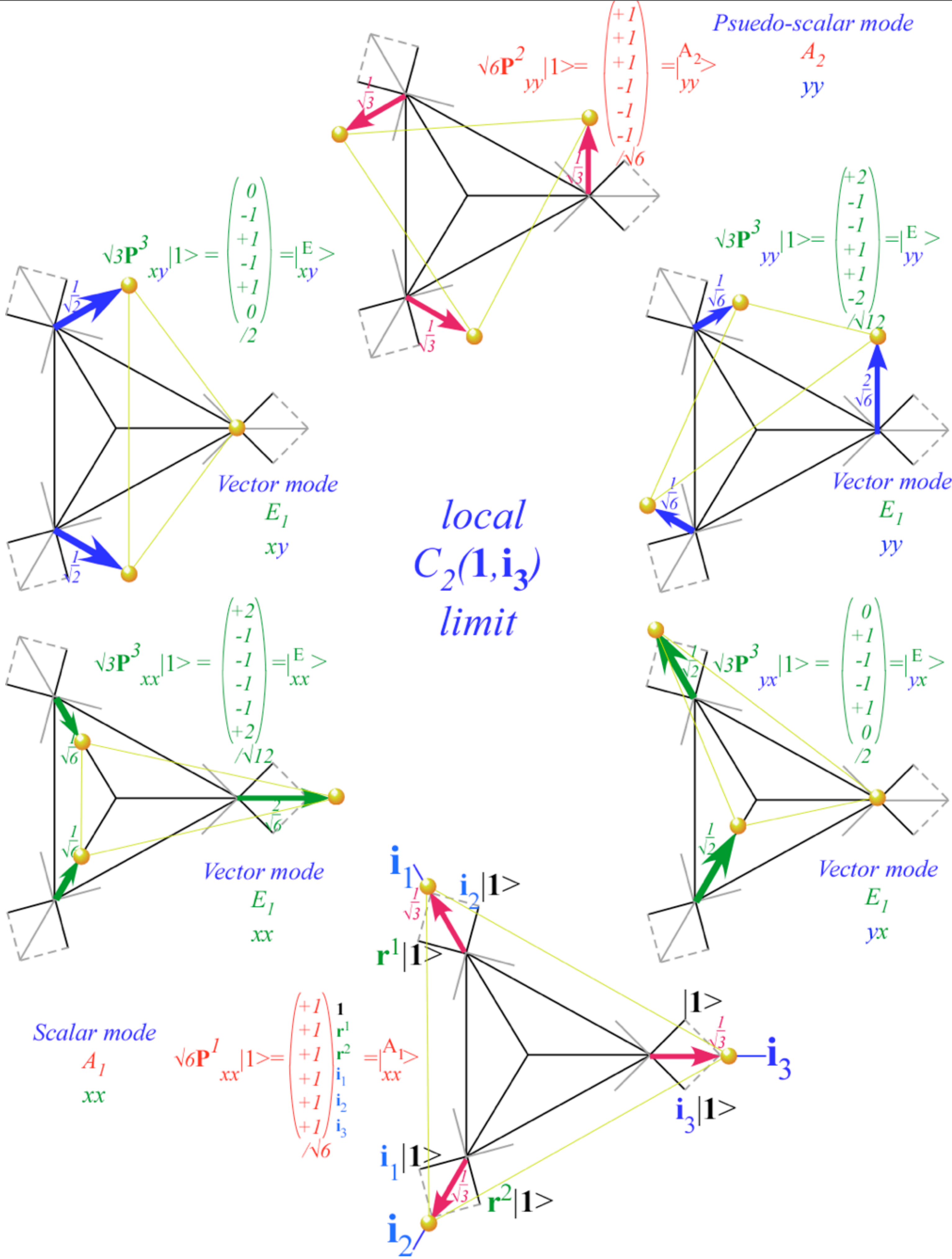
$\|g_b\rangle$	$\|\mathbf{1}\rangle$	$\|\mathbf{r}^1\rangle$	$\|\mathbf{r}^2\rangle$	$\|\mathbf{i}_1\rangle$	$\|\mathbf{i}_2\rangle$	$\|\mathbf{i}_3\rangle$
$\langle \mathbf{1}\|\mathbf{K}\|g_b\rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $-k_r/2$ $+0$ $+0$	$k_i/2$ $+k_r/2$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

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

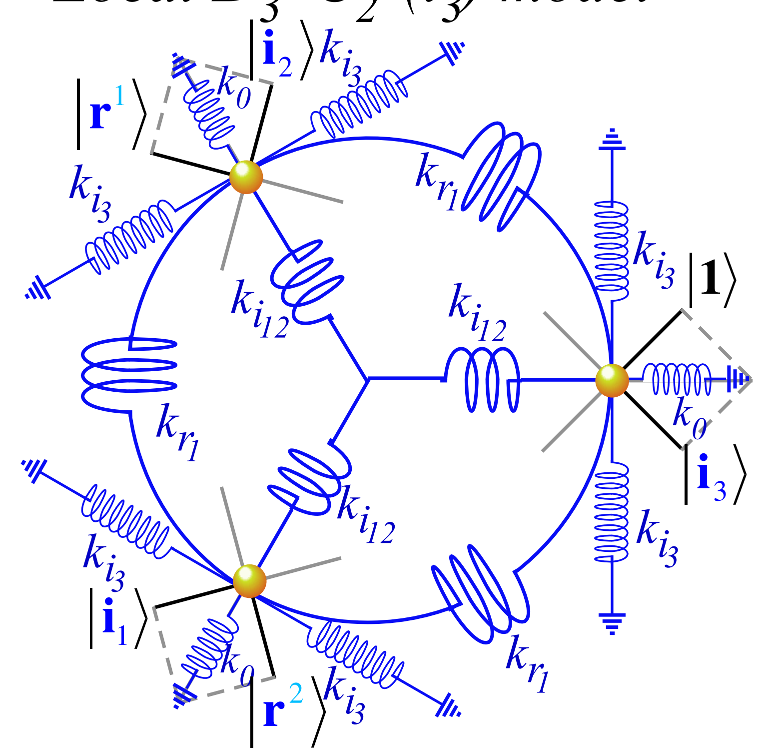
$$K_{xx}^{A_1} = r_0 + r_1 + r_1^* + i_1 + i_2 + i_3 = k_0 + 3k_i$$

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

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



Local $D_3 \; C_2 \supset (i_3)$ 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*

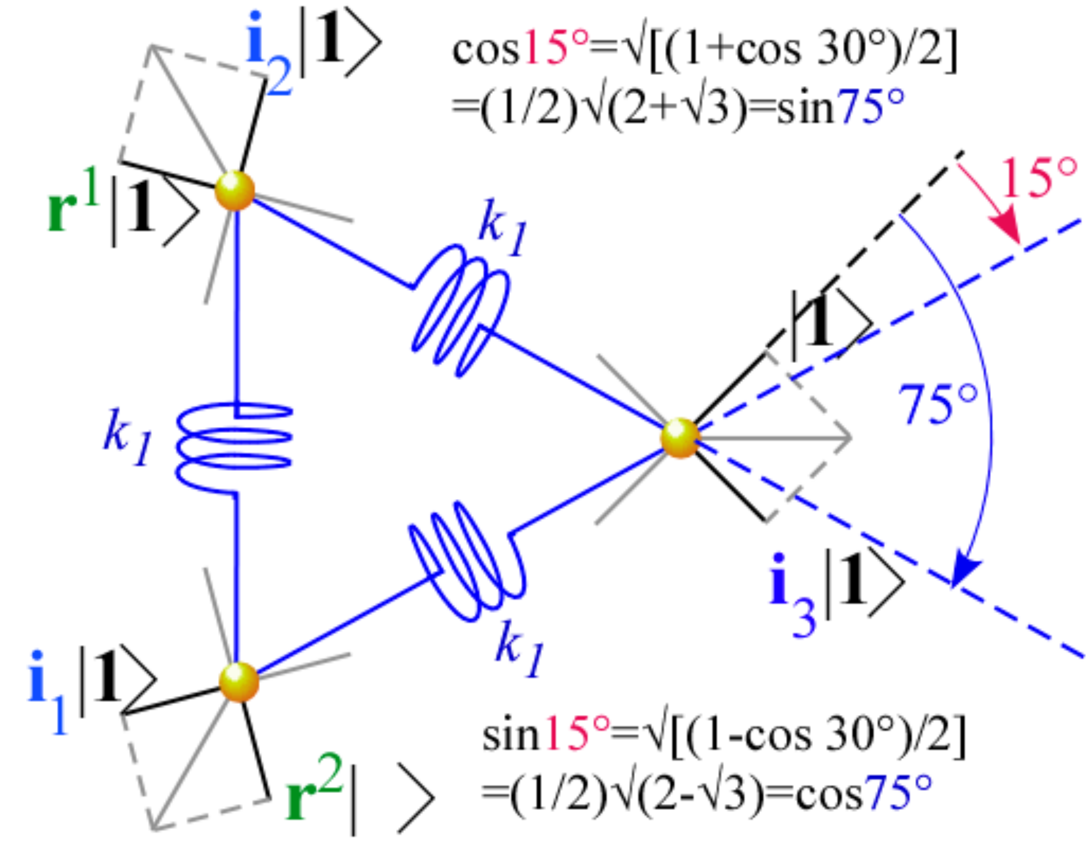
Cross product of the C_2 *and* D_3 *characters gives all* $D_6 = D_3 \times C_2$ *characters and ireps*

D₃-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



D3-direct-connection K-matrix eigensolutions

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

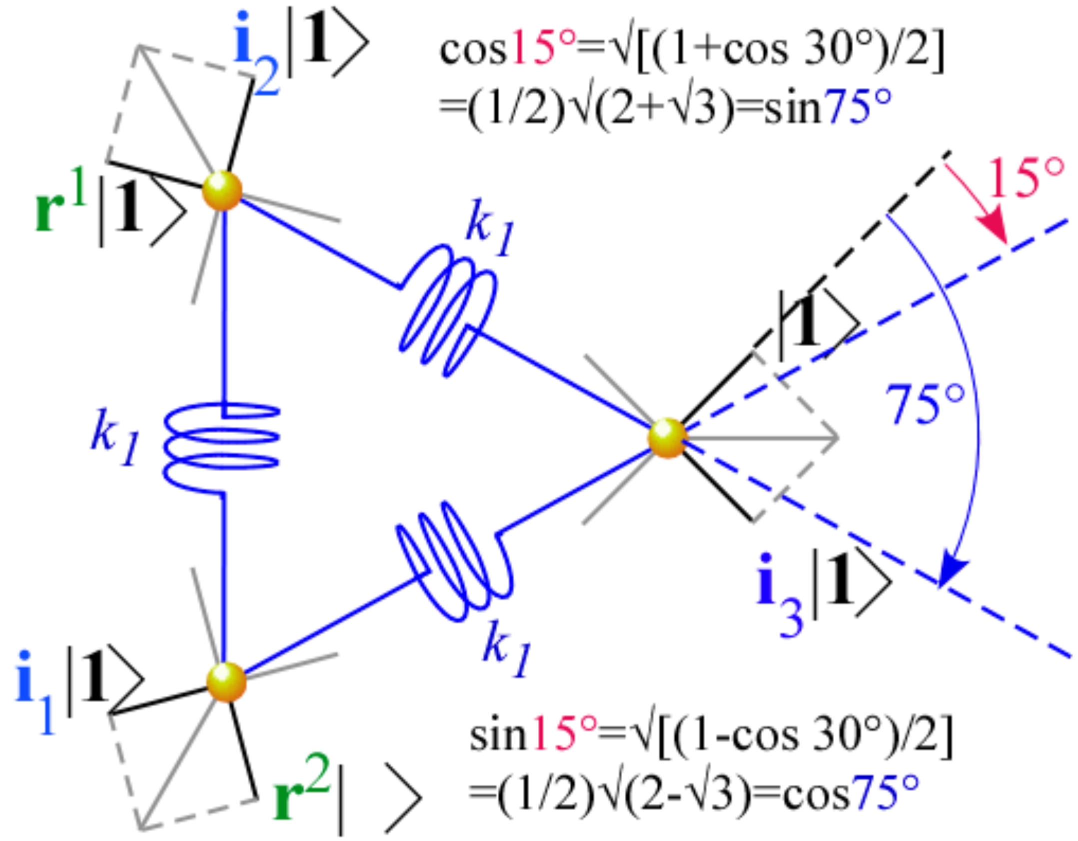
$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

*Generic **K**-matrix D3 projections*

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

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

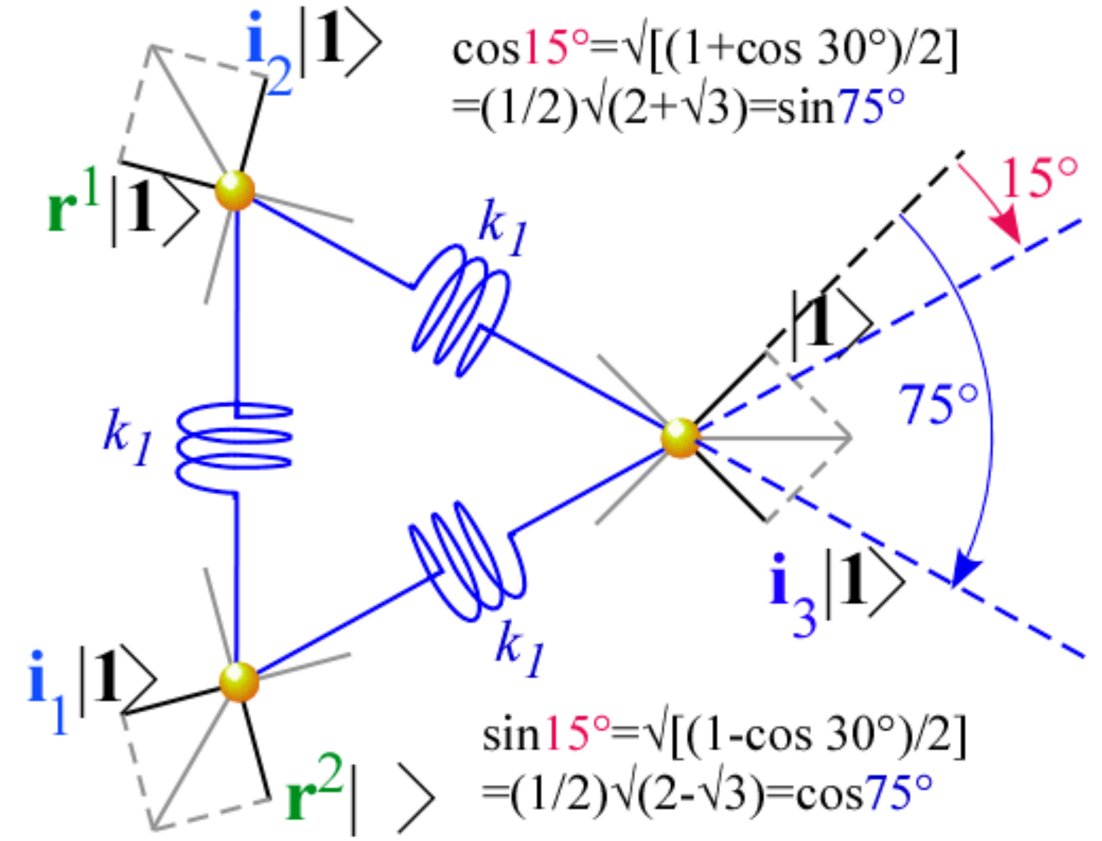
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$



D_3-direct-connection 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

$$K^{A_1}_{xx} = r_0+r_1+r_1^*+i_1+i_2+i_3$$
$$K^{A_2}_{yy} = r_0+r_1+r_1^*-i_1-i_2-i_3$$

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

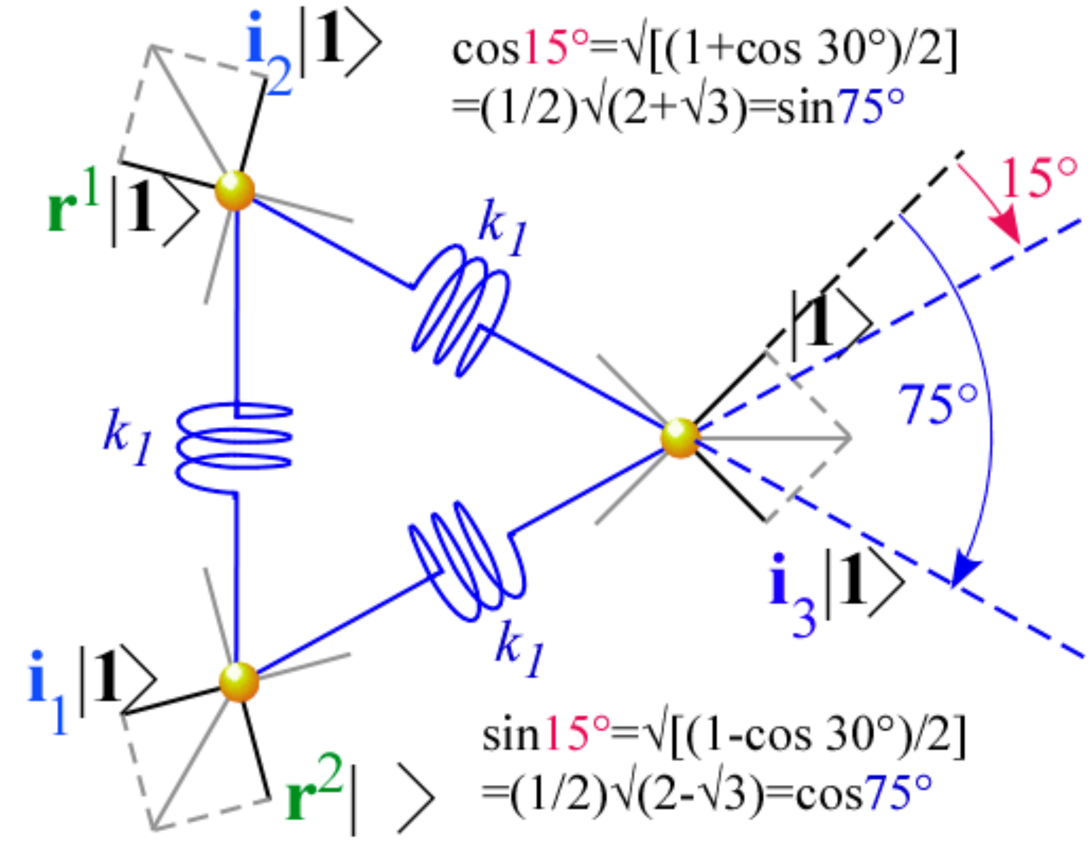
D_3-direct-connection vibrational K-matrix

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

D_3-direct-connection 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 $K_m/M=\omega_m^2$

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

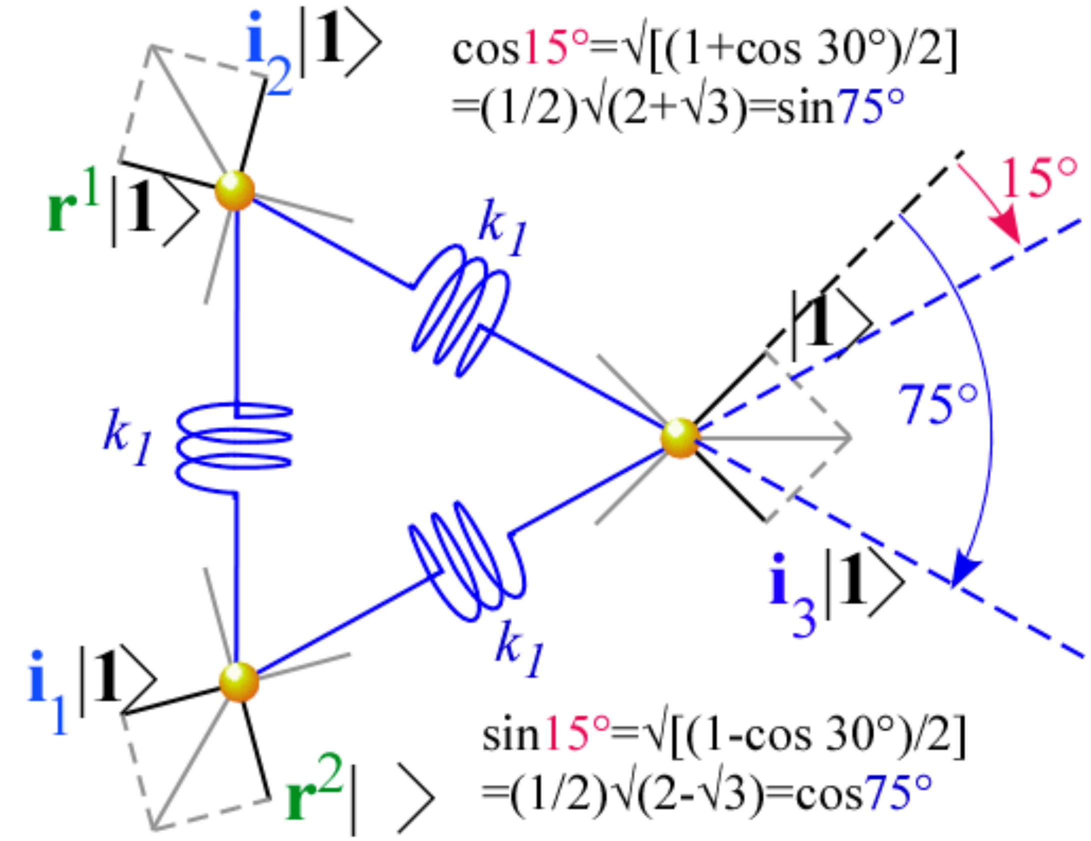
$$K^{A_2}_{yy} = 0$$

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

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

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

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

D_3-direct-connection vibrational K-matrix

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

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

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

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

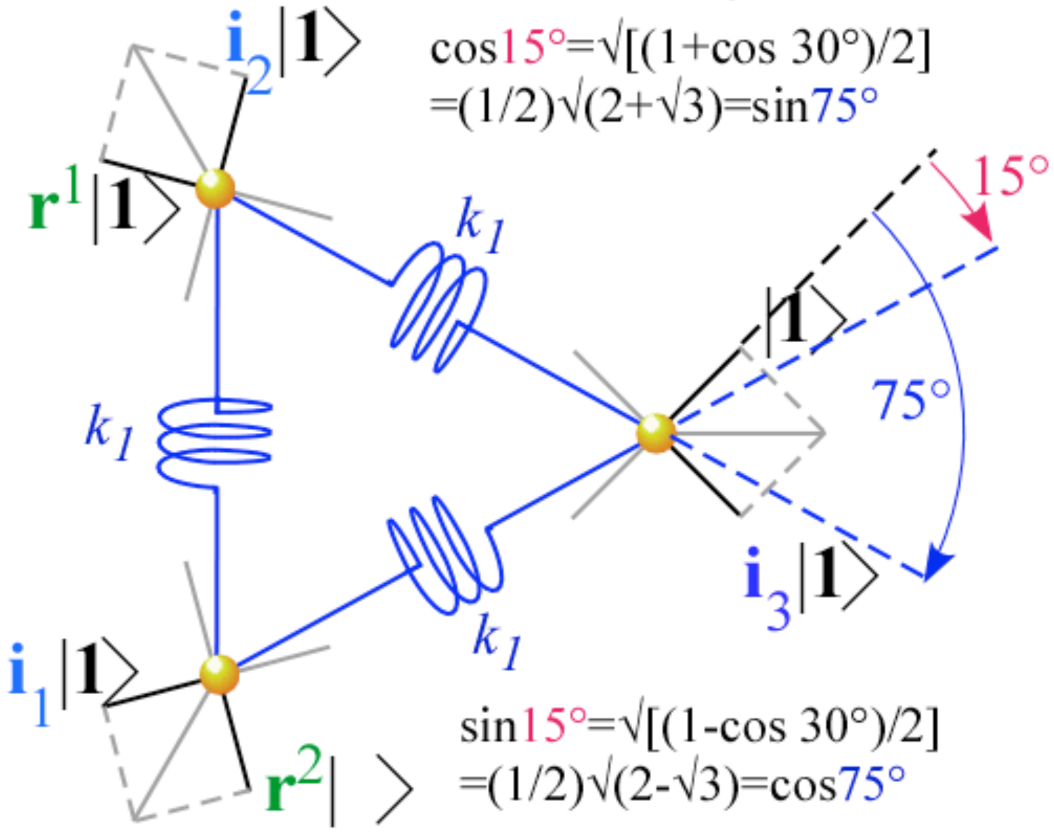
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

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



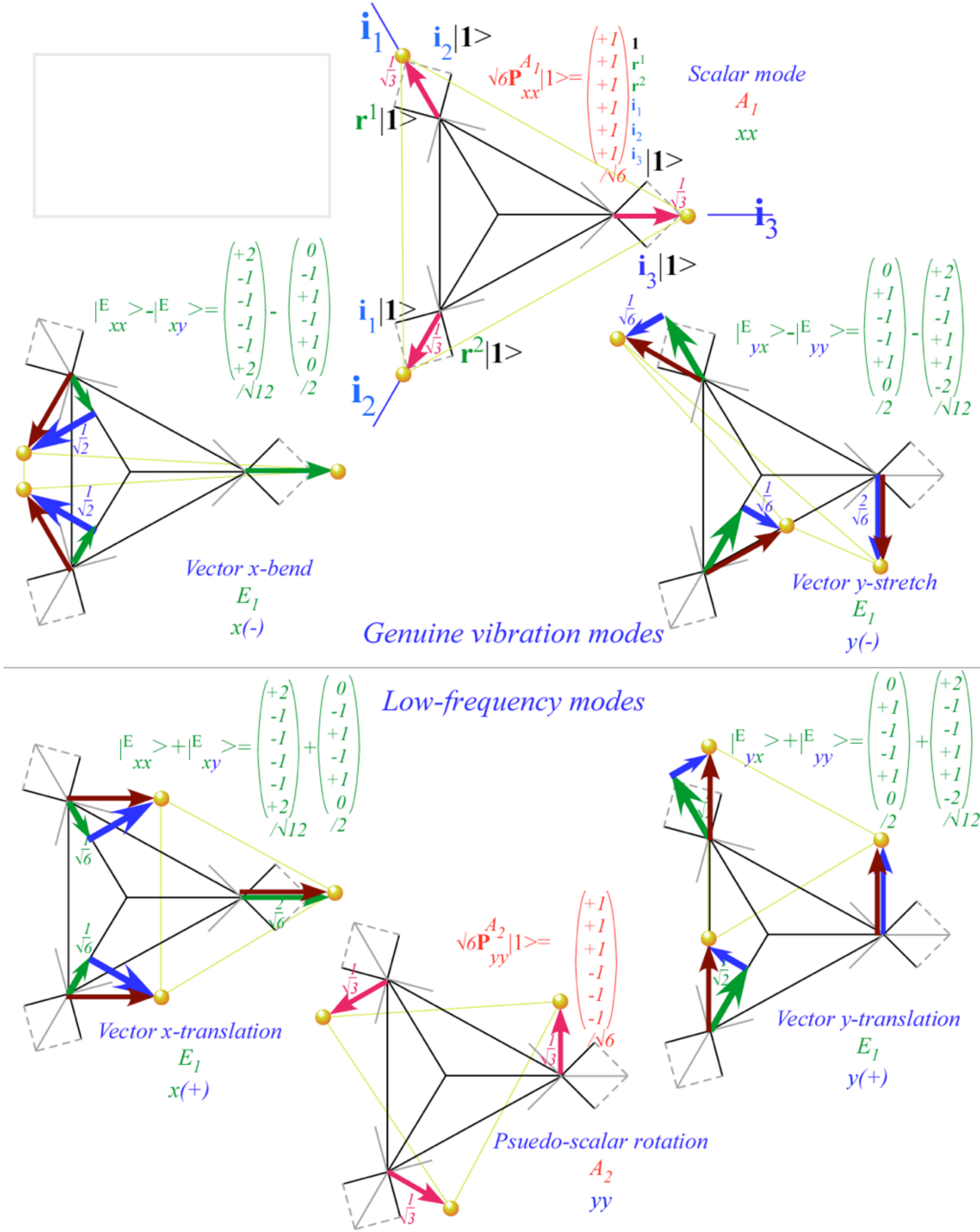
cos15°=√[(1+cos 30°)/2]
=(1/2)√(2+√3)=sin75°

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

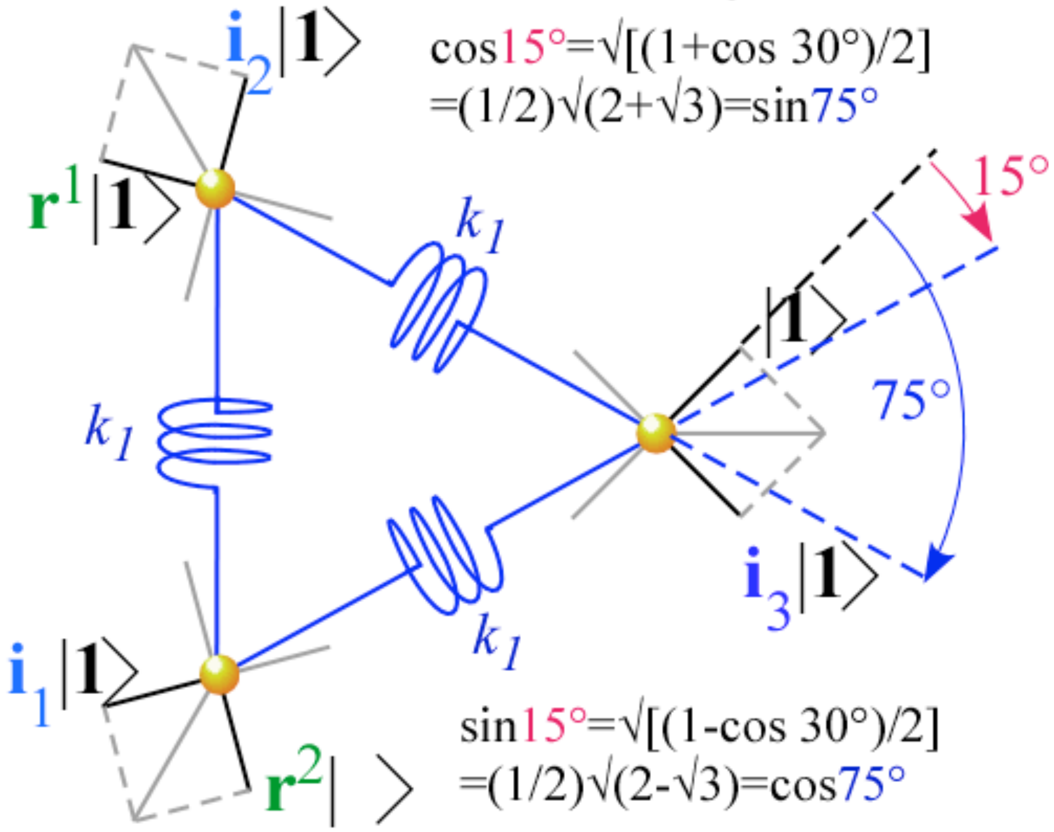
$$K^{A_1}_{xx} = 3k_1$$

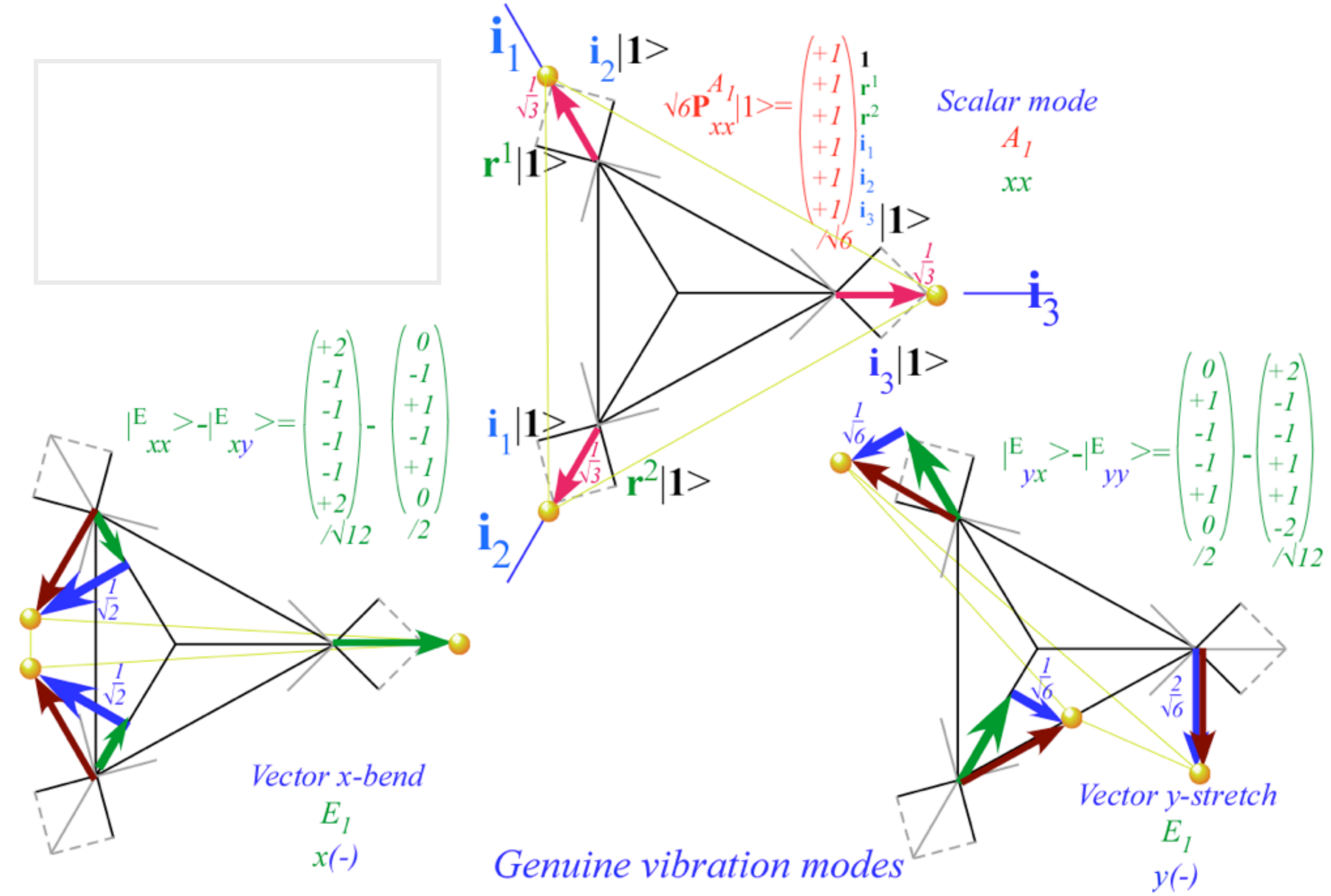
$$K^{A_2}_{yy} = 0$$

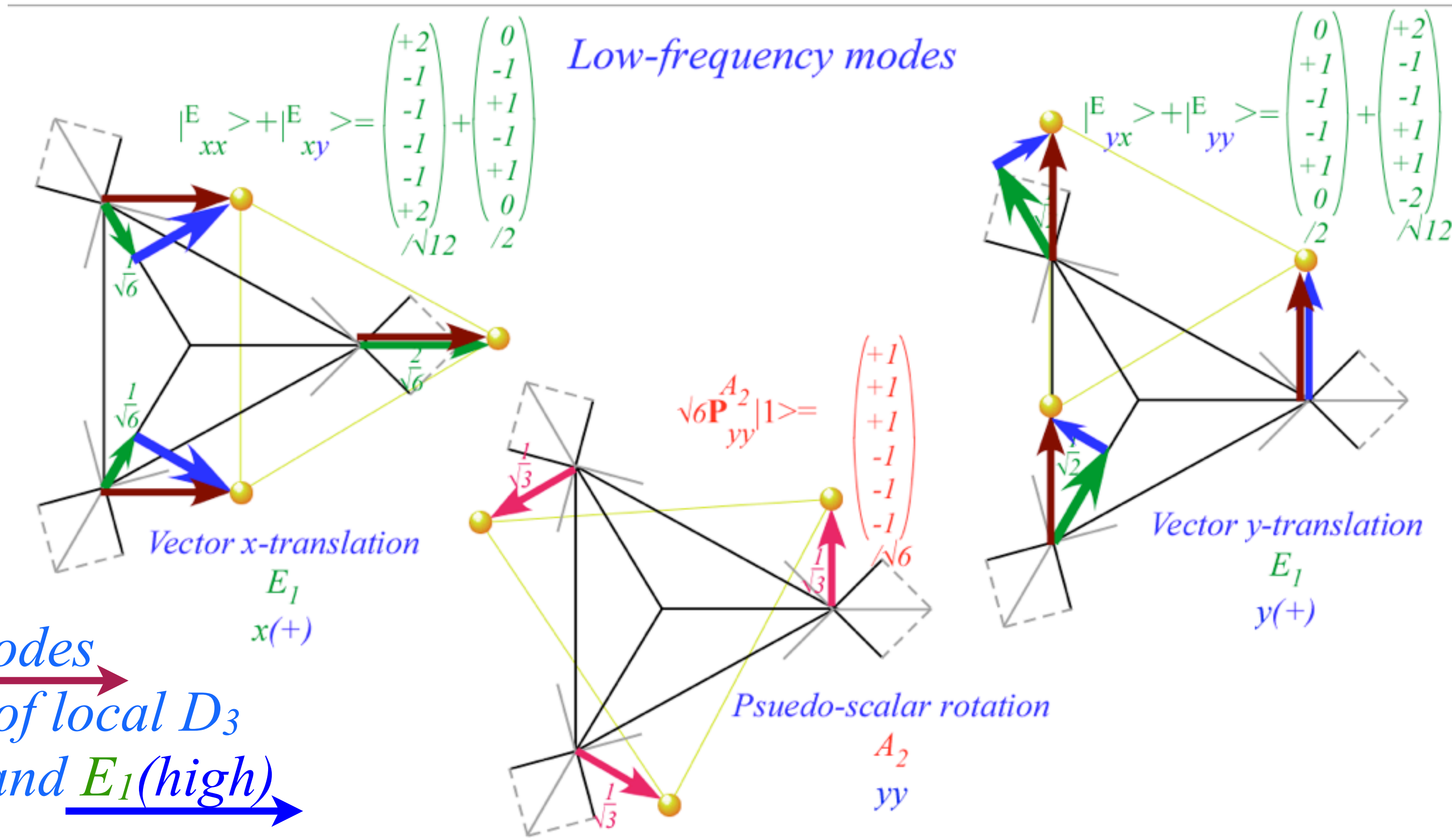
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$



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

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

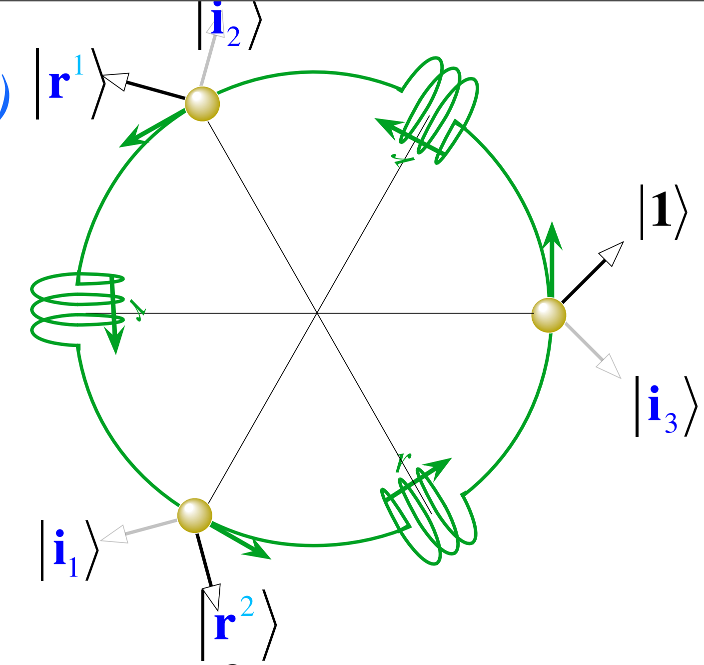
Cross product of the C_2 and D_3 characters gives all $D_6 = D_3 \times C_2$ characters and ireps

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

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

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

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



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

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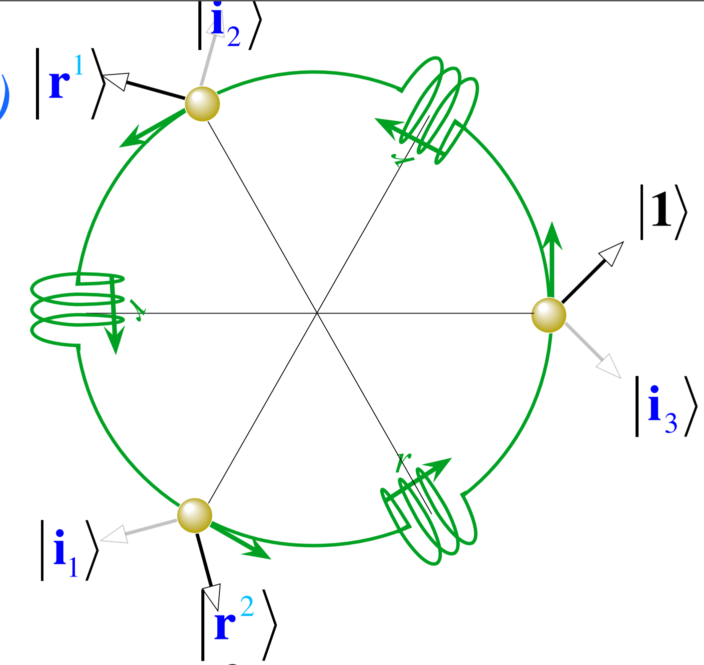
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



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

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

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

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

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

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

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

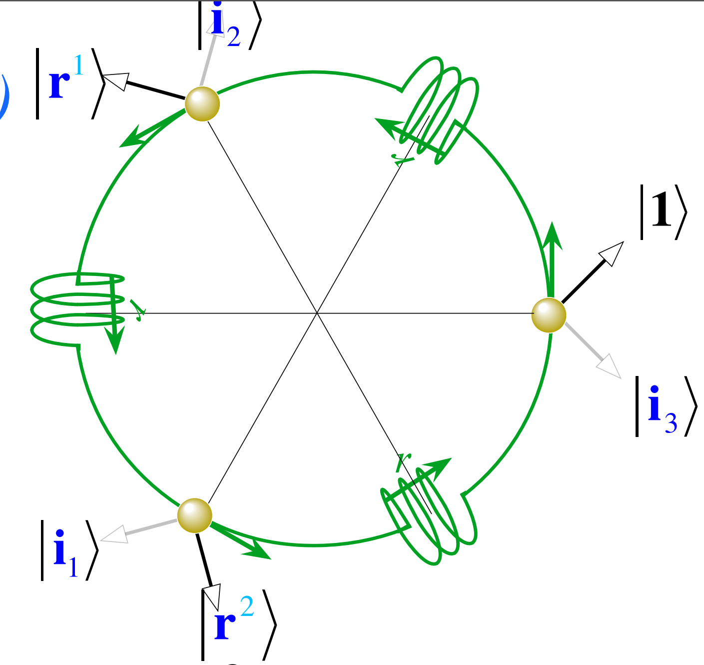
$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix} \Rightarrow \begin{pmatrix} r_0 + r\frac{\sqrt{3}}{2} & 0 \\ 0 & r_0 - r\frac{\sqrt{3}}{2} \end{pmatrix}$$

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

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

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

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



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

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

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

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

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

$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} r_0 & -ir\frac{\sqrt{3}}{2} \\ +ir\frac{\sqrt{3}}{2} & r_0 \end{pmatrix} \Rightarrow \begin{pmatrix} r_0 + r\frac{\sqrt{3}}{2} & 0 \\ 0 & r_0 - r\frac{\sqrt{3}}{2} \end{pmatrix}$$

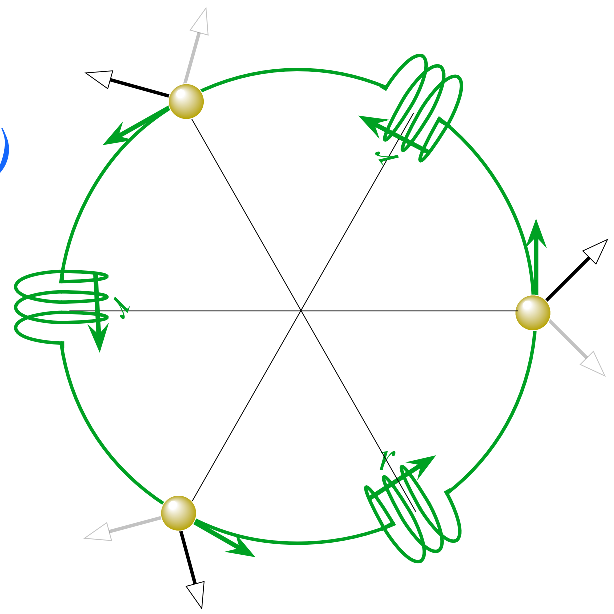
E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

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

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

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

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



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

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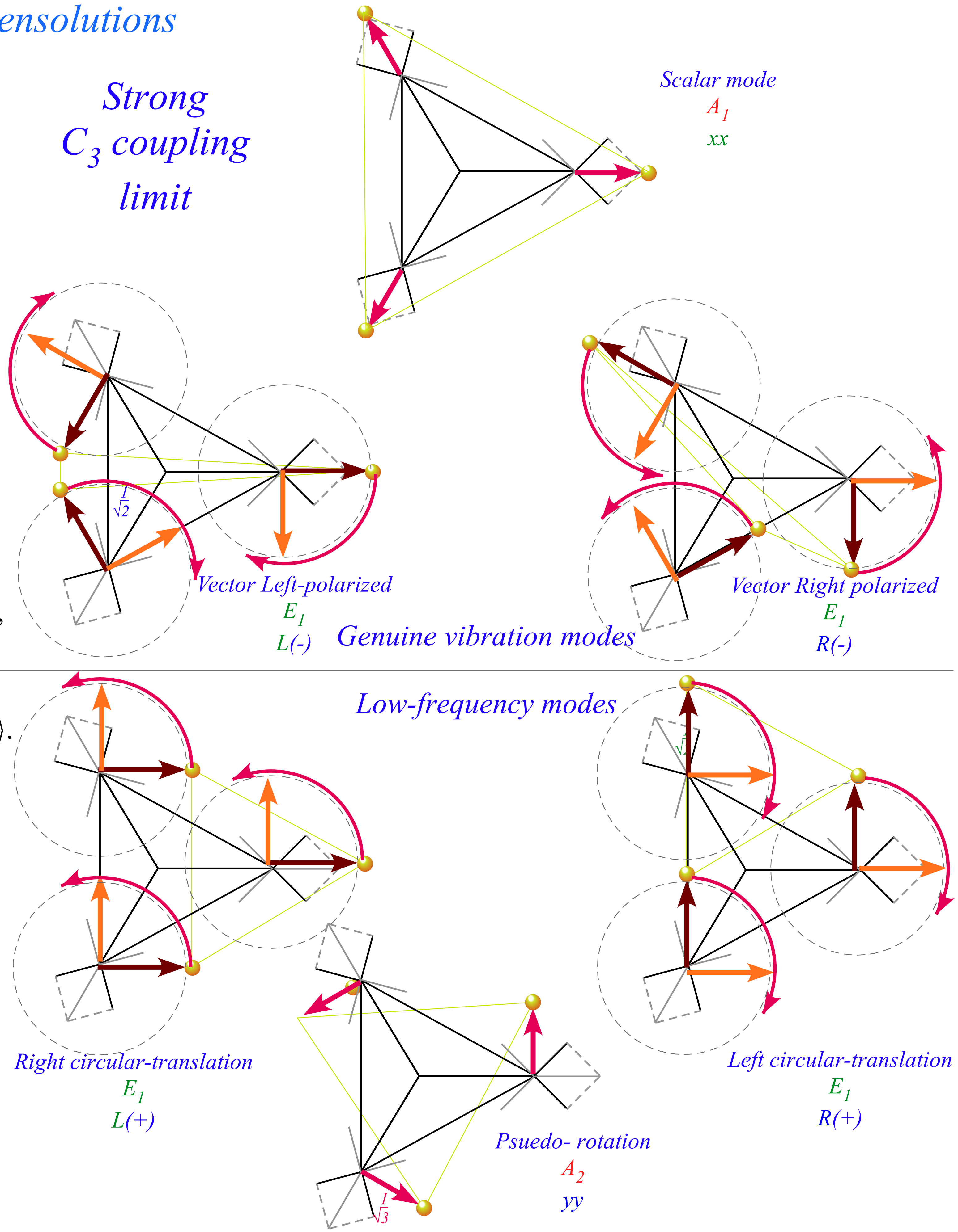

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Applied symmetry reduction and splitting

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

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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

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

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

$D_3 \supset C_2$	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
A_1	$\mathbf{P}^{A_1} = \mathbf{P}^{A_1}\mathbf{P}^{0_2} = \mathbf{P}^{A_1}_{0_2 0_2}$	$\Rightarrow D^{A_1}\downarrow C_2 \sim d^{0_2}$	$\Rightarrow \omega^{A_1} \to \omega^{0_2}$
A_2	$\mathbf{P}^{A_2} = \mathbf{P}^{A_2}\mathbf{P}^{1_2} = \mathbf{P}^{A_2}_{1_2 1_2}$	$\Rightarrow D^{A_2}\downarrow C_2 \sim d^{1_2}$	$\Rightarrow \omega^{A_2} \to \omega^{1_2}$
E_1	$\mathbf{P}^{E_1} = \mathbf{P}^{E_1}\mathbf{P}^{0_2} + \mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $= \mathbf{P}^{E_1}_{0_2 0_2} + \mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim d^{0_2} \oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \to \omega^{0_2}$ $\searrow \omega^{1_2}$

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

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	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{0_2}+\mathbf{P}^{E_1}\mathbf{P}^{1_2}$ $=\mathbf{P}^{E_1}_{0_2 0_2}+\mathbf{P}^{E_1}_{1_2 1_2}$	$\Rightarrow D^{E_1}\downarrow C_2 \sim$ $d^{0_2}\oplus d^{1_2}$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{0_2}$ $\searrow \omega^{1_2}$

$D_3 \supset C_2$	0_2	1_2
A_1	1	·
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$D_3 \supset C_3$	0_3	1_3	2_3
A_1	1	·	·
A_2	1	·	·
E_1	·	1	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Frobenius Reciprocity Theorem

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

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..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

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

D_6 symmetry and Hexagonal Bands

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

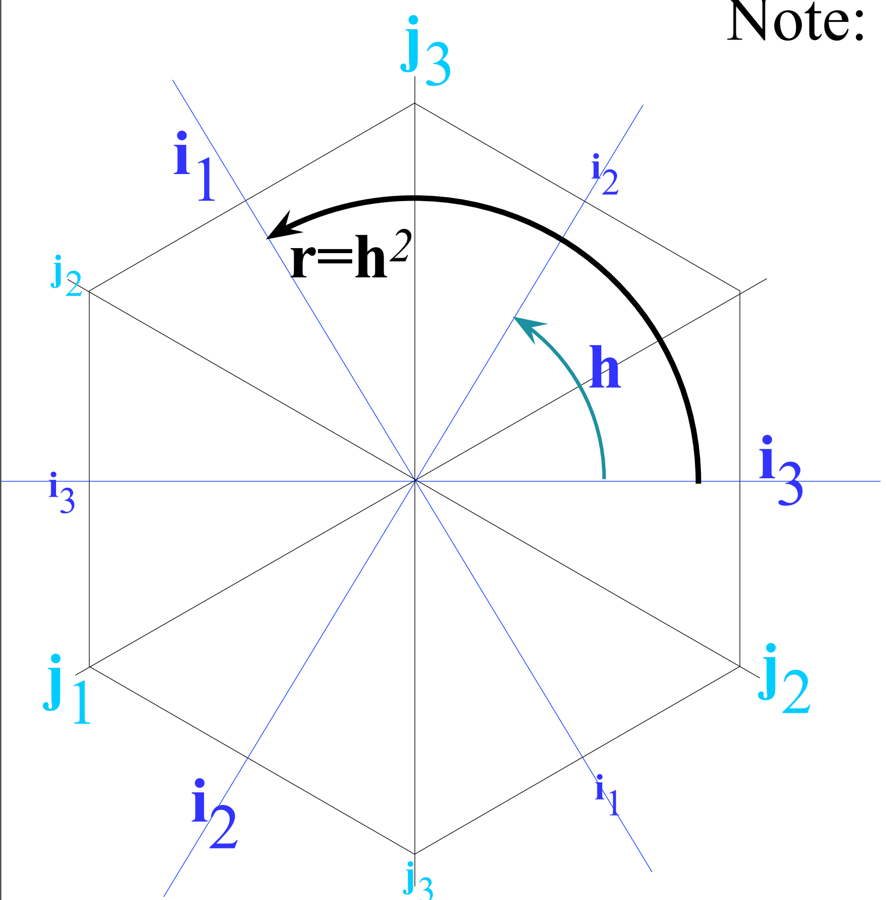
$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$

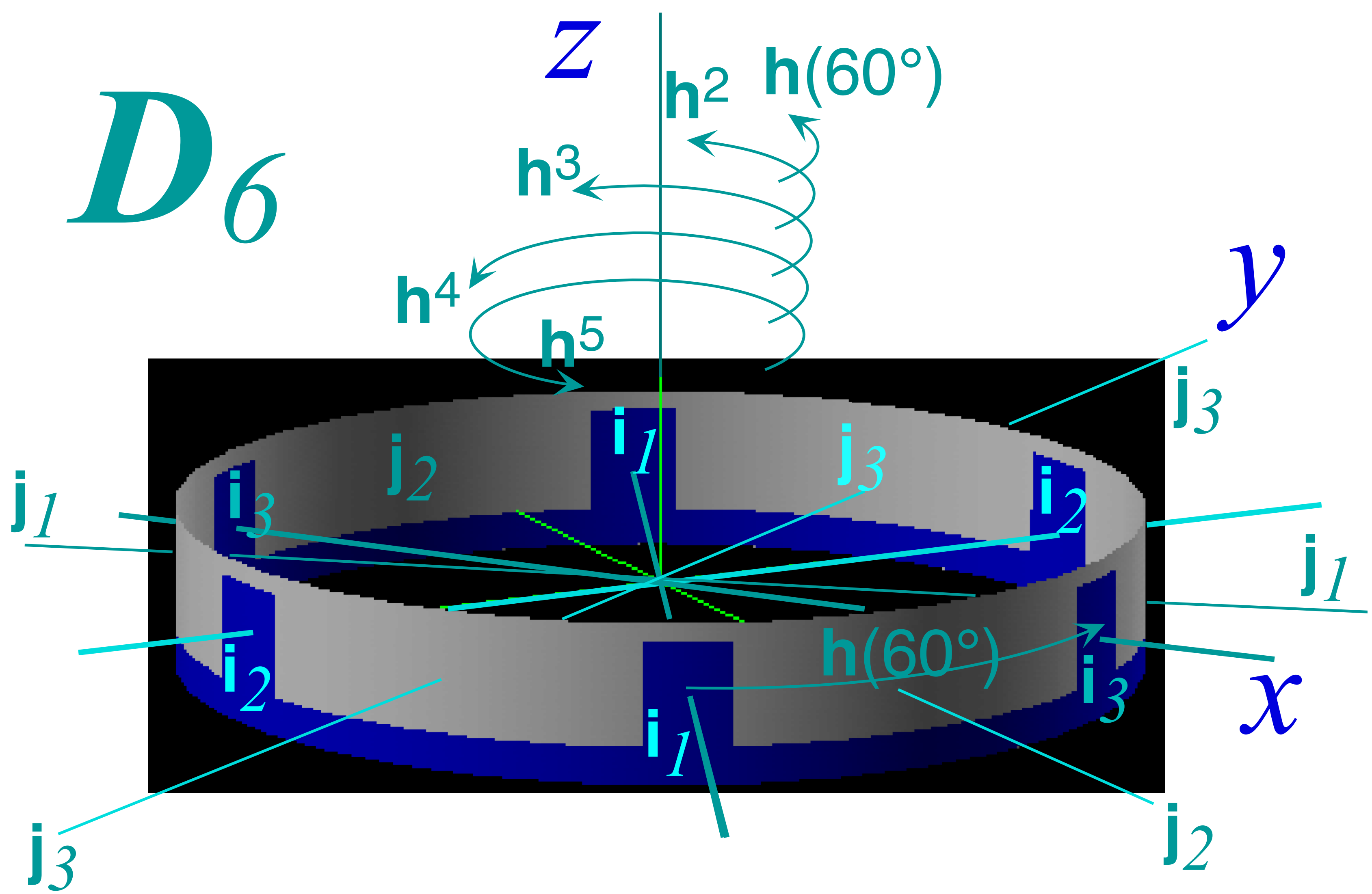
$\times$ product and D_6 operators. Define *hexagonal generator* **h** of subgroup $C_6 = \{\mathbf{1}, \mathbf{h}, \mathbf{h}^2, \mathbf{h}^3, \mathbf{h}^4\ \mathbf{h}^5\}$

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

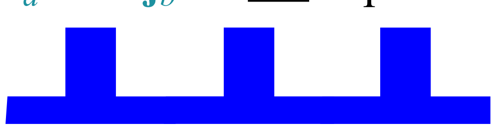
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$$

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 not 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.

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

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

Unit translation
or
60° *hex rotation* **h**
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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.

$g =$	1	$r=h^2$	$r^2=h^4$	i_1	i_2	i_3	h^3	$h^3r=h^5$	$h^3r^2=h^1$	$h^3i_1=j_1$	$h^3i_2=j_2$	$h^3i_3=j_3$
$D^{A_1}(g)=$	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
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

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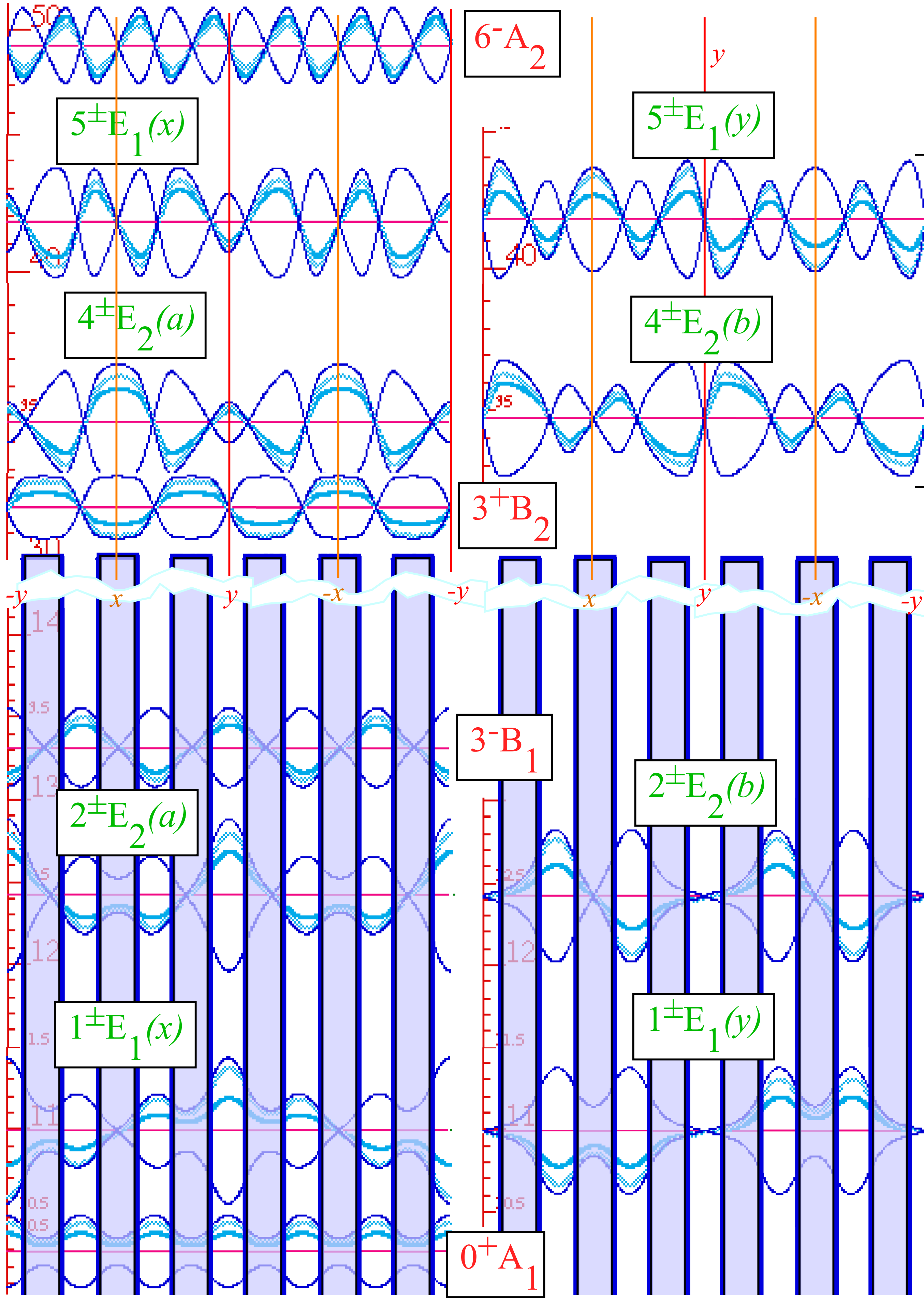
(+1) vs (-1)

$D_6 \supset C_2(j_3)$	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