Group Theory in Quantum Mechanics

Lecture 18 *(4.04.17)*

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 and tight-binding modes*
- *Induced rep* $d^{a}(C_6)\uparrow D_6 = D^{\alpha} \oplus D^{\beta} \oplus ..$ *correlation*
  - *Global vs.Local symmetry effects and U(12) super-degeneracy*

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 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	$P^{A_1}_{xx}$	$P^{A_2}_{yy}$	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†

....and row-P with row-P†

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

(all others are self-conjugate)

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

D_3 local group product 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

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

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

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

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

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

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

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

***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- $\mathbf{H}$ 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:*

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

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

$$H^{A_1}=r_0D^{A_1*}(1)+r_1D^{A_1*}(r^1)+r_1^*D^{A_1*}(r^2)+i_1D^{A_1*}(i_1)+i_2D^{A_1*}(i_2)+i_3D^{A_1*}(i_3)\;=r_0+r_1+r_1^*+i_1+i_2+i_3\qquad =r_0+2r_1+2i_{12}+i_3$$

$$H^{A_2}=r_0D^{A_2*}(1)+r_1D^{A_2*}(r^1)+r_1^*D^{A_2*}(r^2)+i_1D^{A_2*}(i_1)+i_2D^{A_2*}(i_2)+i_3D^{A_2*}(i_3)\;=r_0+r_1+r_1^*-i_1-i_2-i_3\qquad =r_0+2r_1\;-2i_{12}\;-i_3$$

$$H^{E_1}_{xx}=r_0D^{E*}_{xx}(1)+r_1D^{E*}_{xx}(r^1)+r_1^*D^{E*}_{xx}(r^2)+i_1D^{E*}_{xx}(i_1)+i_2D^{E*}_{xx}(i_2)+i_3D^{E*}_{xx}(i_3)\;=(2r_0-r_1-r_1^*-i_1-i_2+2i_3)/2\qquad =r_0\;-r_1\;\;-i_{12}+i_3$$

$$H^{E_1}_{xy}=r_0D^{E*}_{xy}(1)+r_1D^{E*}_{xy}(r^1)+r_1^*D^{E*}_{xy}(r^2)+i_1D^{E*}_{xy}(i_1)+i_2D^{E*}_{xy}(i_2)+i_3D^{E*}_{xy}(i_3)\;=\sqrt{3}(-r_1+r_1^*-i_1+i_2)/2=H^{E*}_{yx}\qquad =0$$

$$H^{E_1}_{yy}=r_0D^{E*}_{yy}(1)+r_1D^{E*}_{yy}(r^1)+r_1^*D^{E*}_{yy}(r^2)+i_1D^{E*}_{yy}(i_1)+i_2D^{E*}_{yy}(i_2)+i_3D^{E*}_{yy}(i_3)\;=(2r_0-r_1-r_1^*+i_1+i_2-2i_3)/2\qquad =r_0\;-r_1\;\;+i_{12}\;-i_3$$

$C_2=\{\mathbf{1},\mathbf{i_3}\}$
Local symmetry determines all levels and eigenvectors with just 4 real parameters

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

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

Choosing local $C_2=\{\mathbf{1},\mathbf{i_3}\}$ *symmetry with local constraints* $r_1=r_1{}^*=r_2$ *and* $i_1=i_2$

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

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

	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	
$\mathbf{P}^{A_1}_{x,x}=$	(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:

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

$\mathbf{P}^{\mu}_{mn}$ 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

Global (LAB) symmetry

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

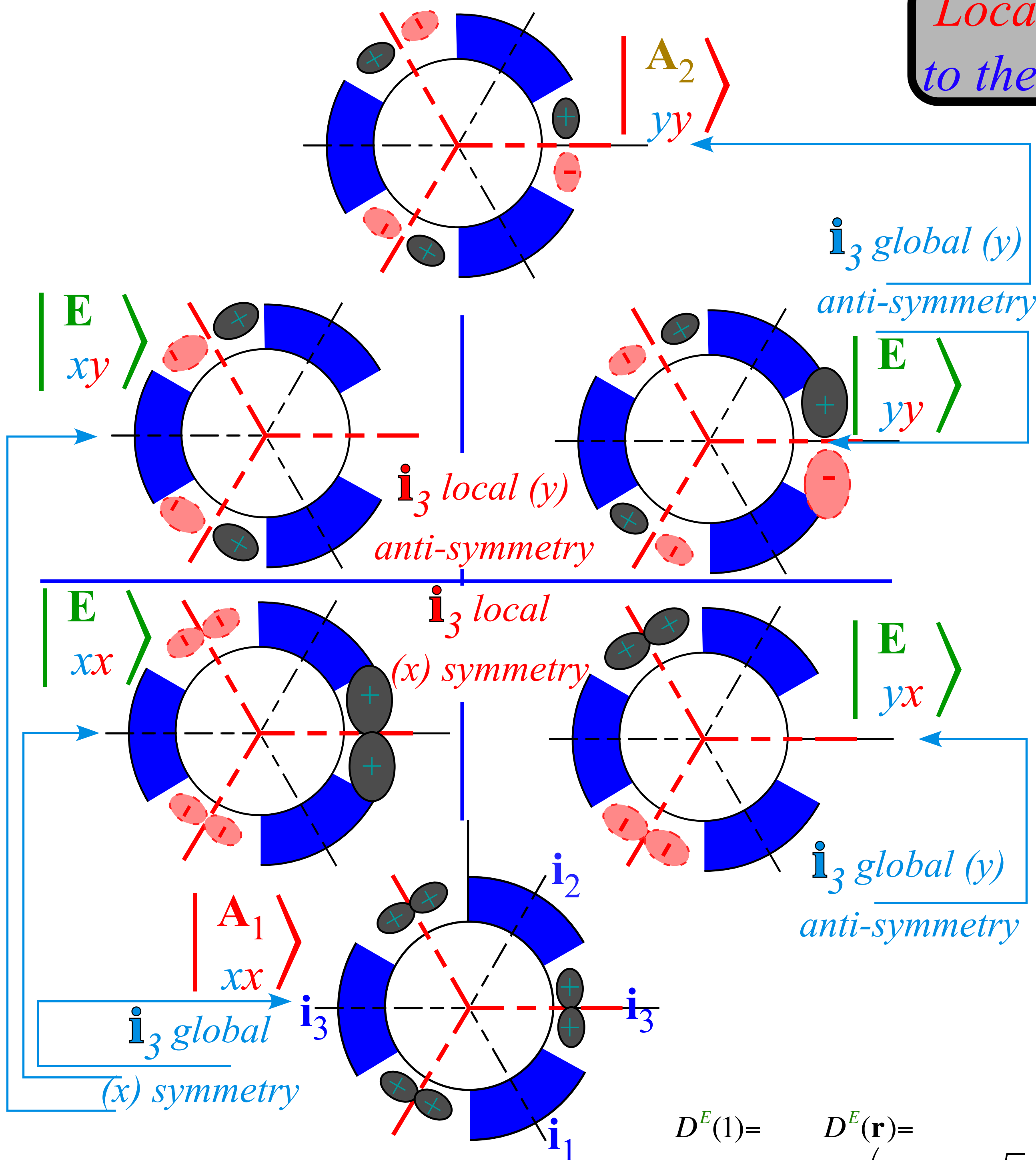
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

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

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

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

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

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

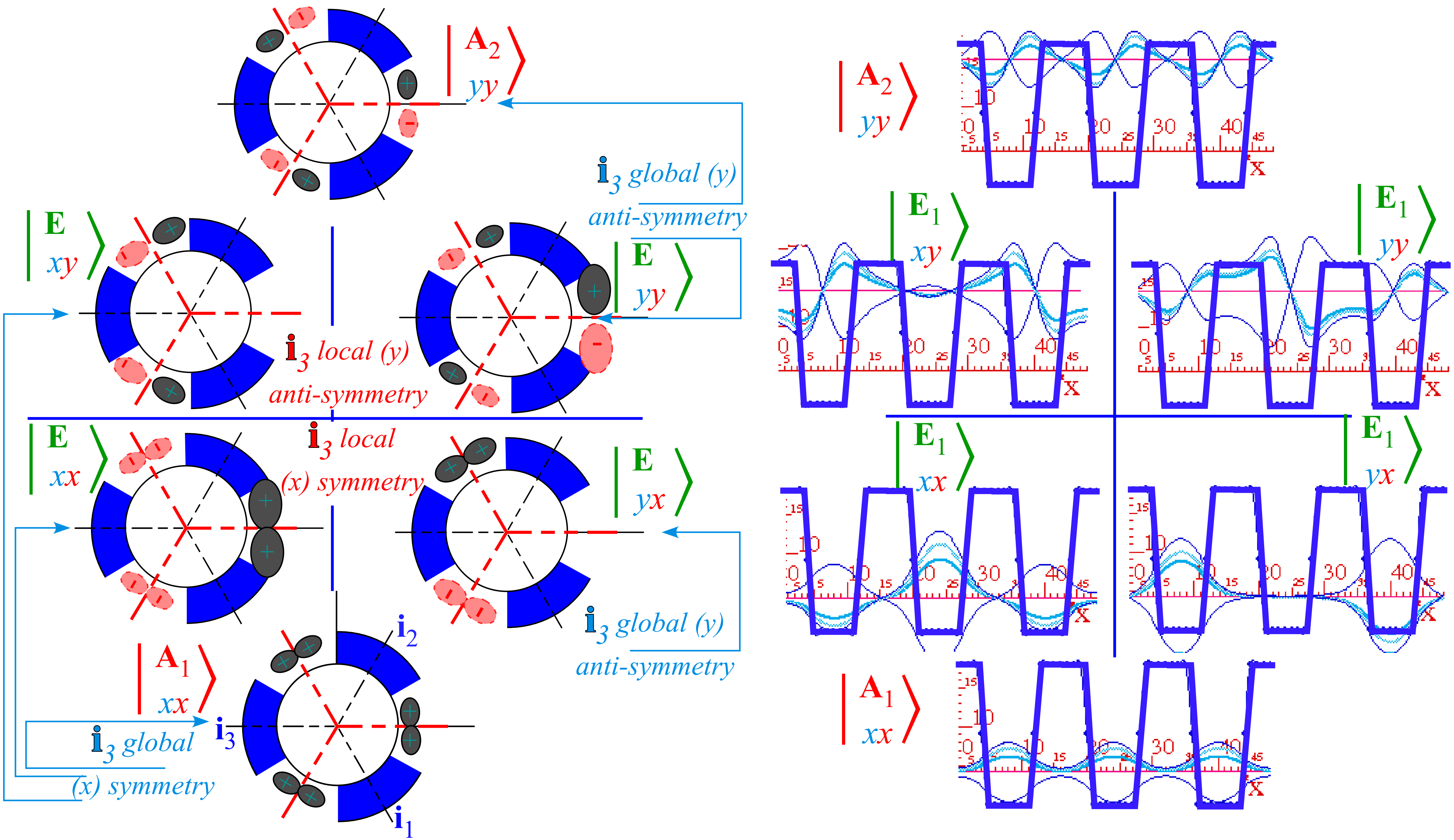
$$|{}^{(m)}_{eb}\rangle = \mathbf{P}^{(m)}_{eb}|1\rangle$$

Global (LAB) symmetry

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

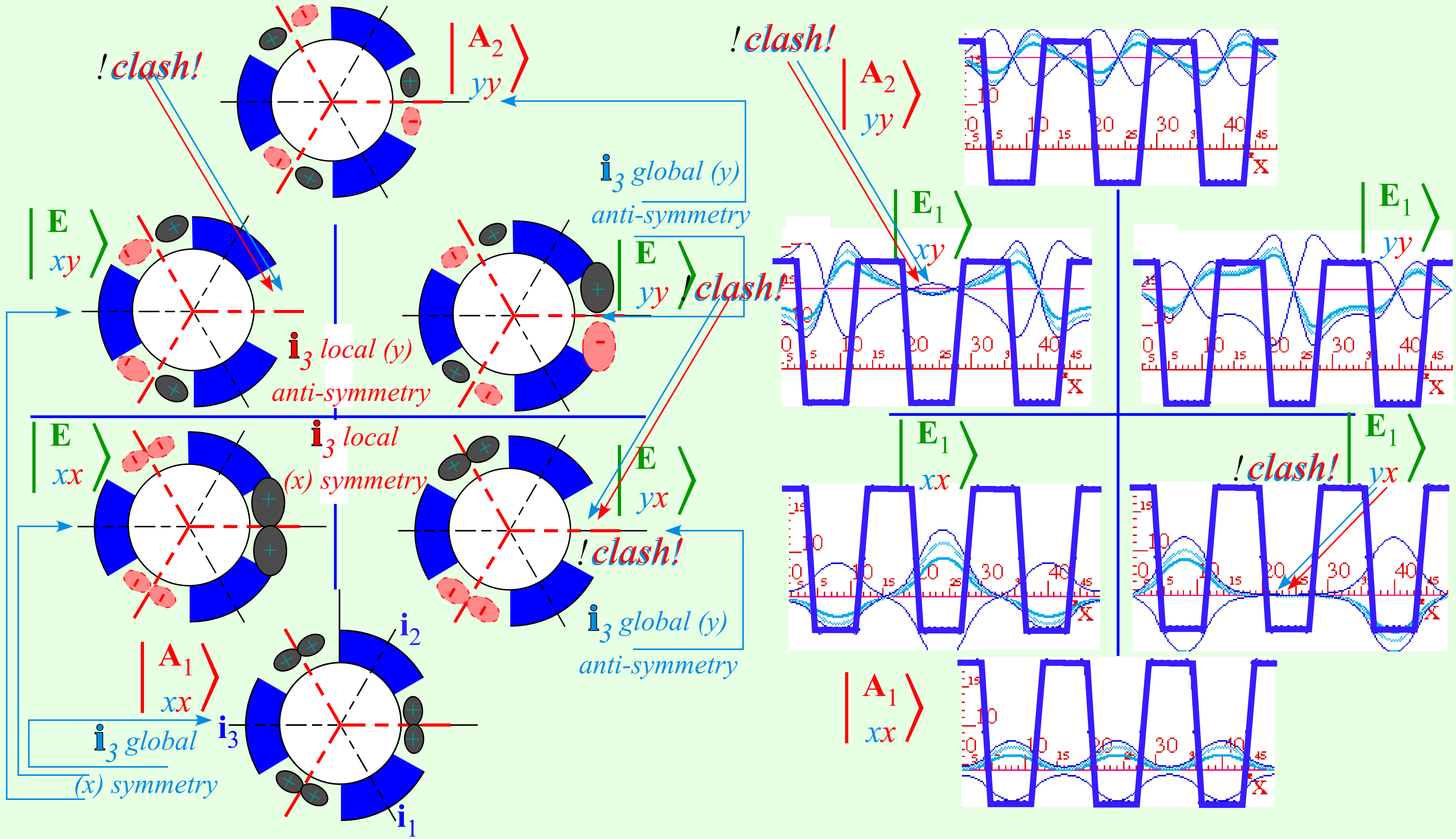
Local (BOD) symmetry

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



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

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

Molecular vibrational modes vs. Hamiltonian eigenmodes

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.

$$-M\partial_t^2 x^a = \frac{\partial V}{\partial x^a} = \sum_b K_{ab} x^b$$

Molecular vibrational modes vs. Hamiltonian eigenmodes

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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Compare classical equation to Schrodinger's equation for quantum motion.†

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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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Molecular K-matrix construction

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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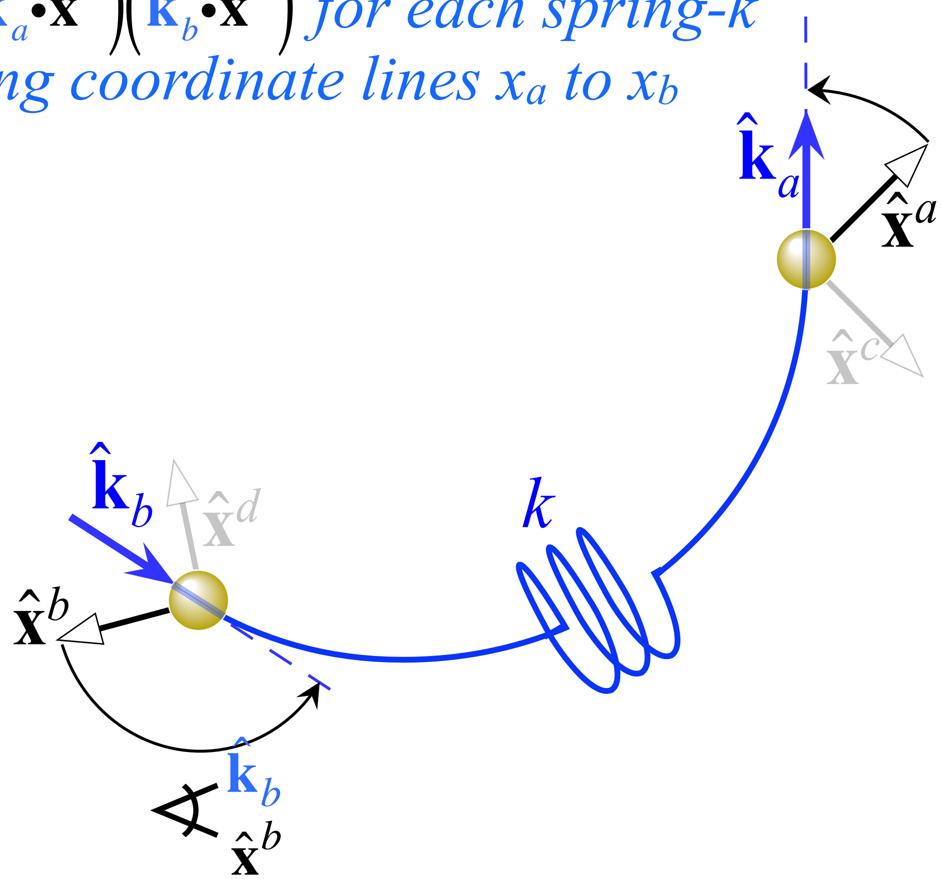
Sum $k\cdot(\hat{\mathbf{k}}_a\bullet\hat{\mathbf{x}}^a)(\hat{\mathbf{k}}_b\bullet\hat{\mathbf{x}}^b)$ *for each spring-k connecting coordinate lines* x_a *to* x_b



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Diagonal $K_{aa}{=}\langle a|\mathbf{K}|a\rangle$
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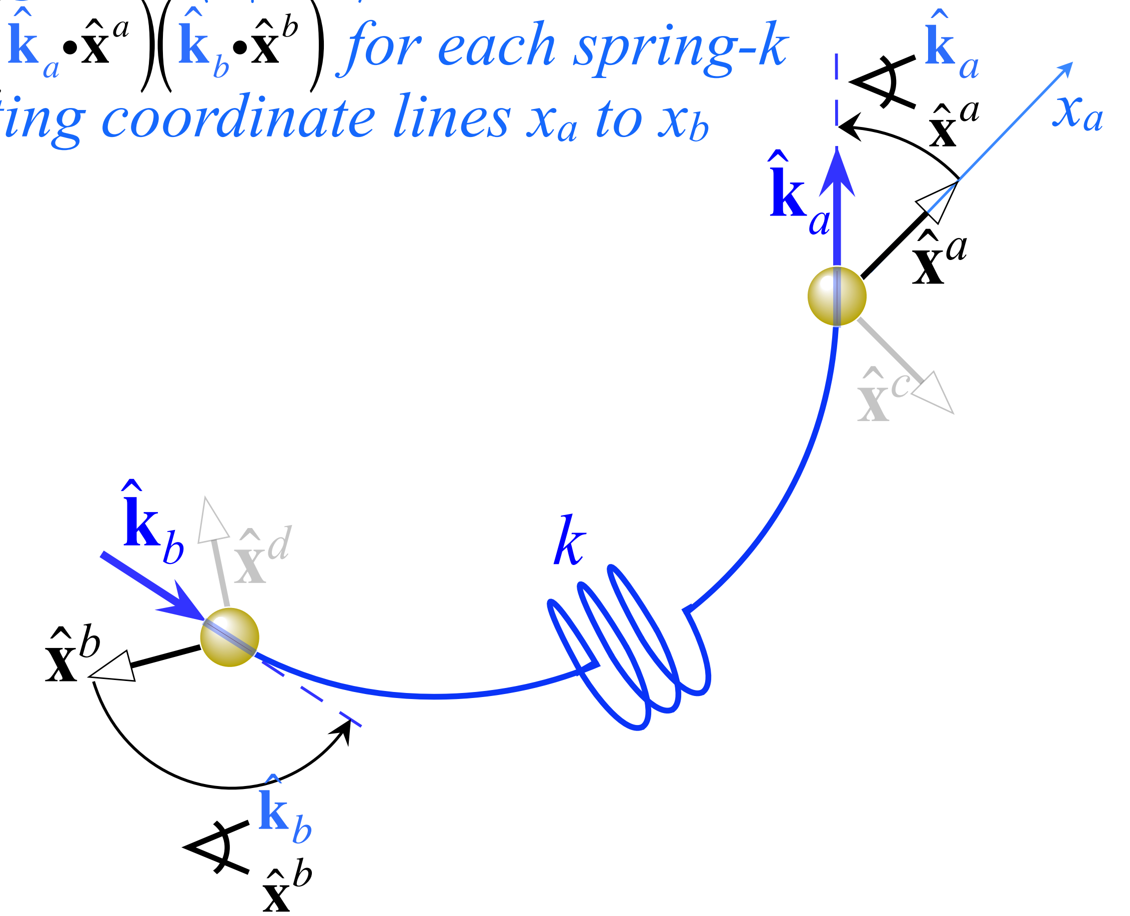
connected to coordinate line x_a



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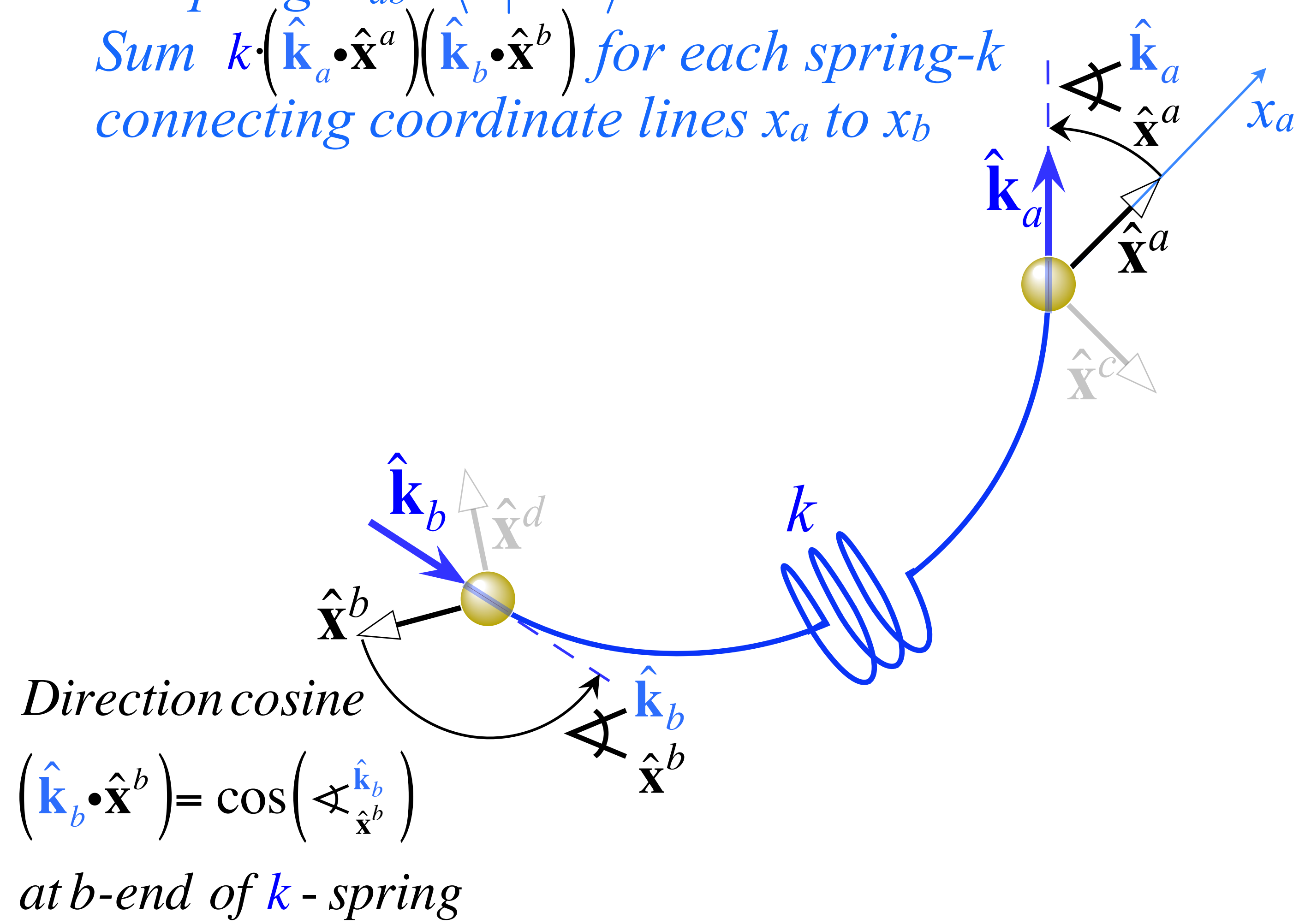

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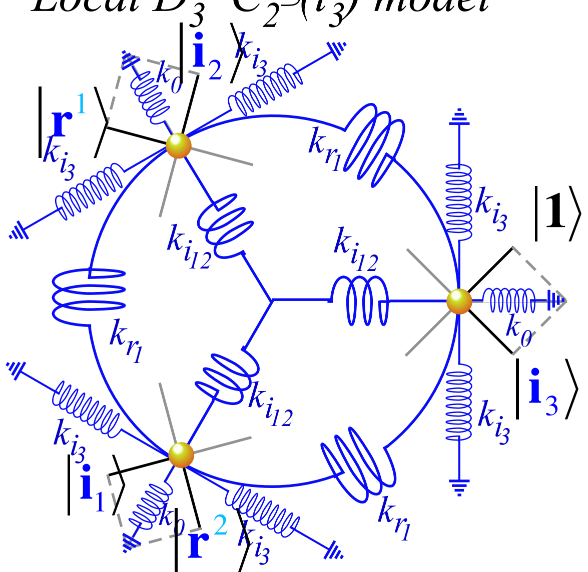
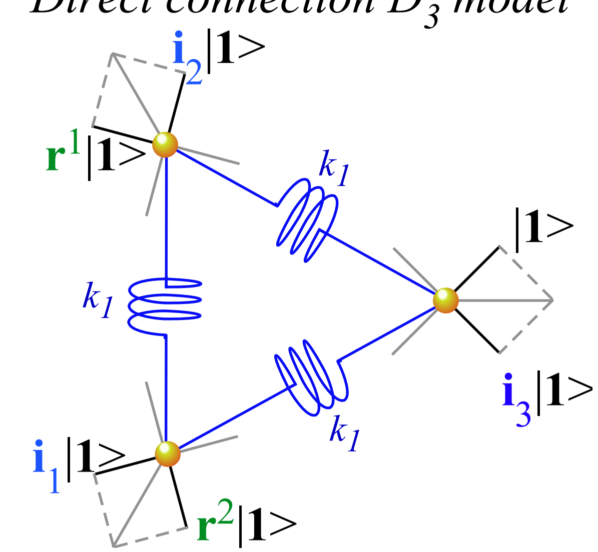
Local D_3 $C_2 \supset (i_3)$ model



Direct connection D_3 model



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

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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

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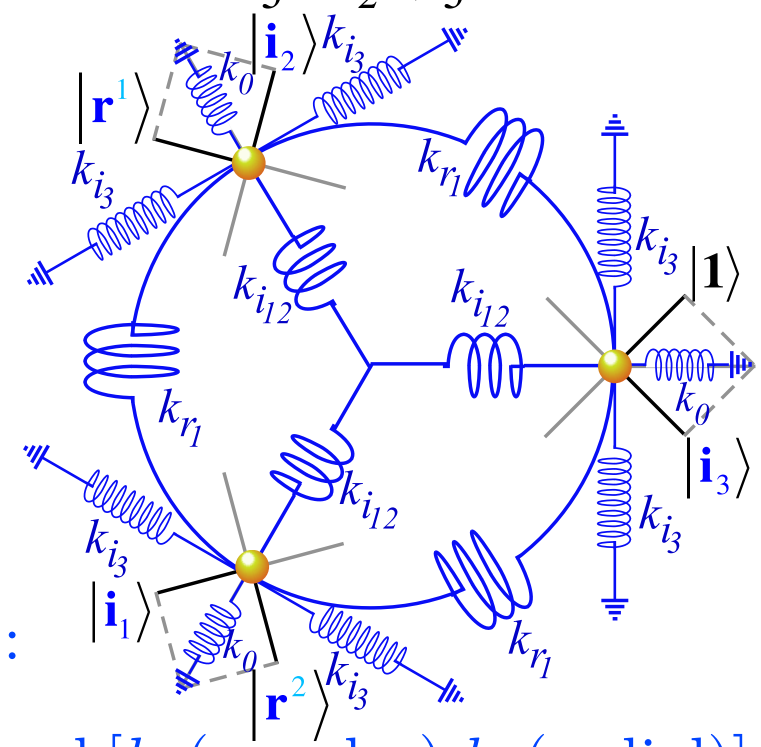

Generic **K***-matrix (Top row)*

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

$D_3 \supset C_2(i_3)$ 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.

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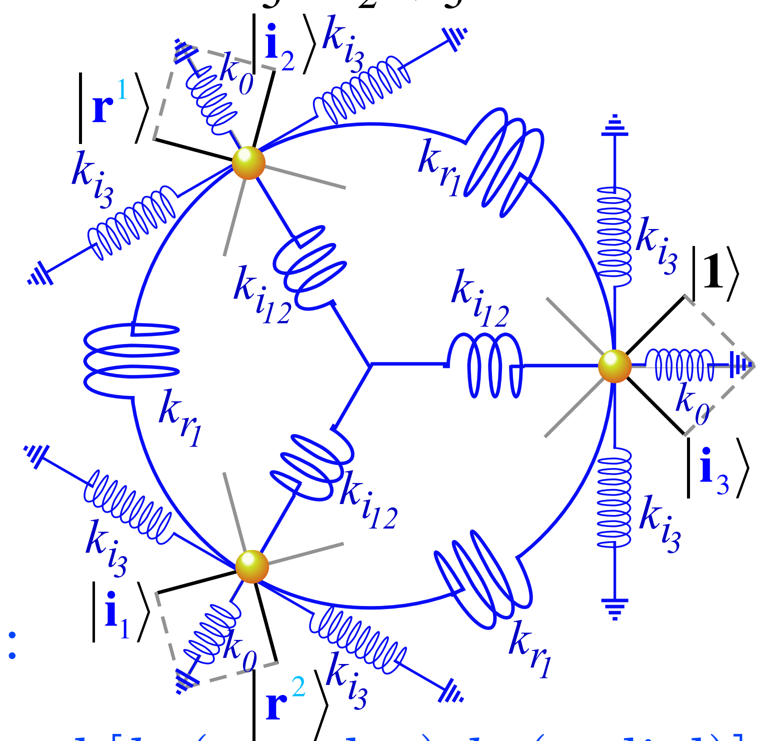

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$\vert g_b\rangle$	$\vert\mathbf{1}\rangle$	$\vert\mathbf{r}^1\rangle$	$\vert\mathbf{r}^2\rangle$	$\vert\mathbf{i}_1\rangle$	$\vert\mathbf{i}_2\rangle$	$\vert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\vert\,\mathbf{K}\,\vert g_b\rangle =$	$k_i/2$ $+k_r$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

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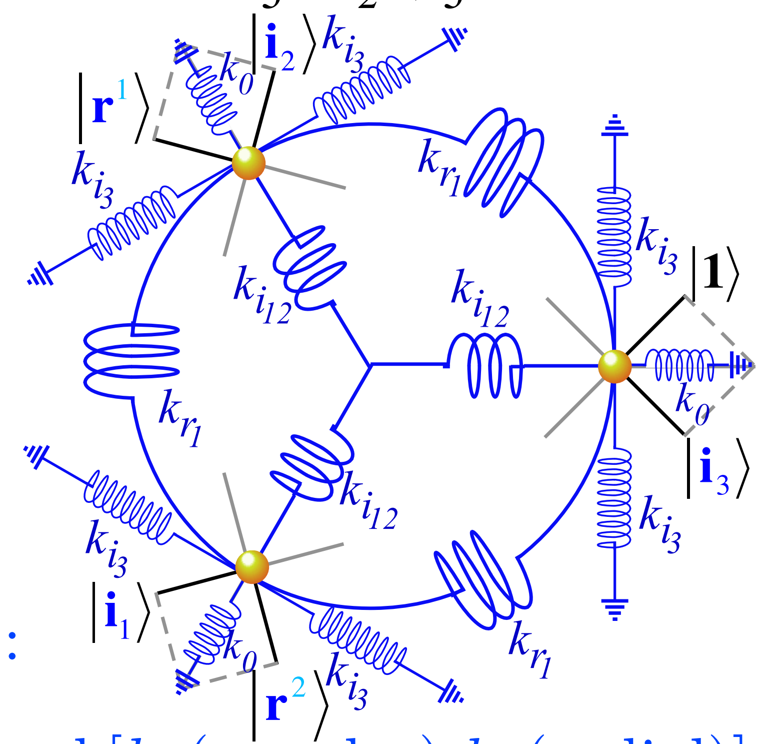

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$$\langle \mathbf{1} | \mathbf{K} | \mathbf{g}_b \rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

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

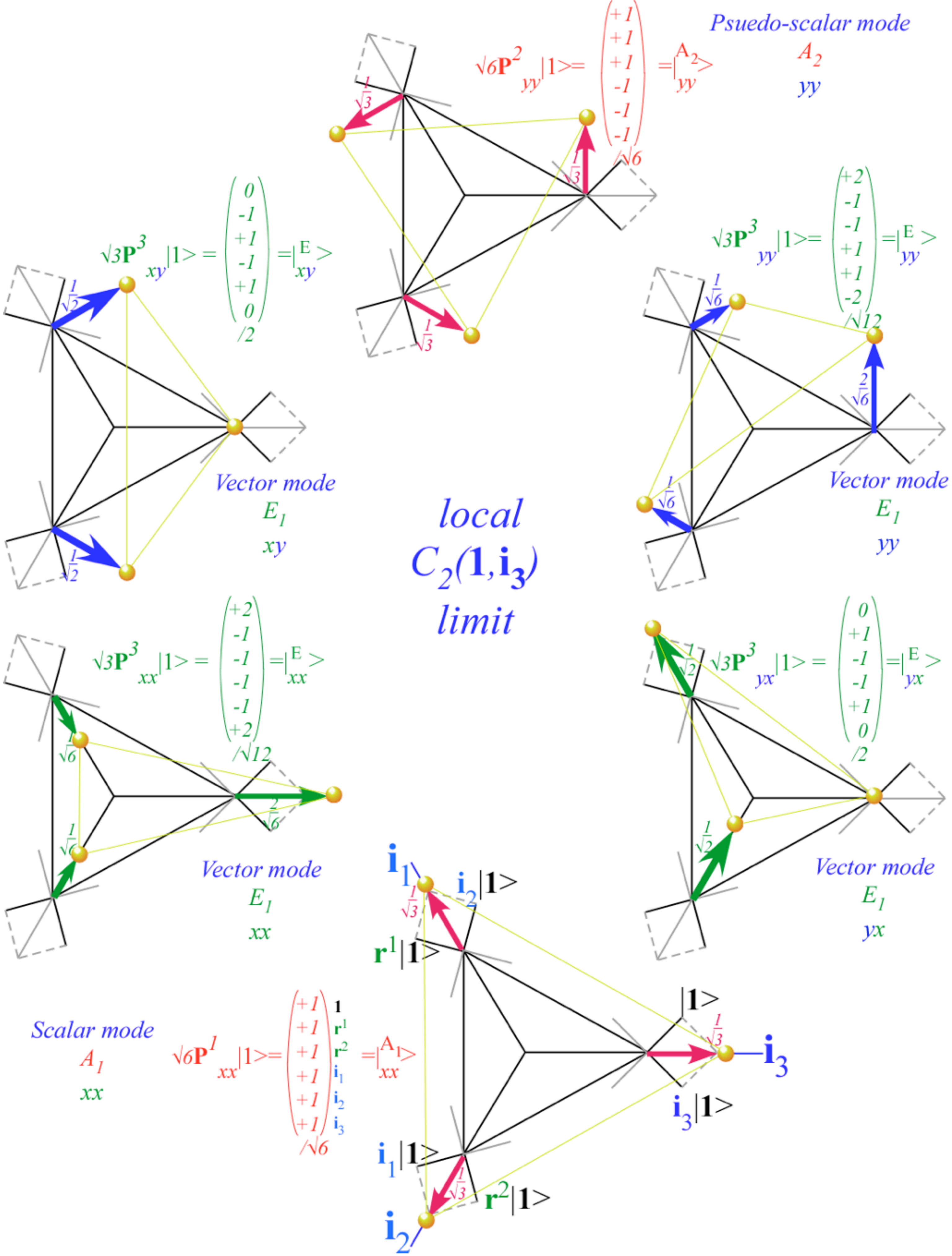
$\lvert g_b \rangle$	$\lvert \mathbf{1} \rangle$	$\lvert \mathbf{r}^1 \rangle$	$\lvert \mathbf{r}^2 \rangle$	$\lvert \mathbf{i}_1 \rangle$	$\lvert \mathbf{i}_2 \rangle$	$\lvert \mathbf{i}_3 \rangle$
$\langle \mathbf{1} \lvert \mathbf{K} \rvert g_b \rangle =$	$k_i/2$ $+k_r$ $+k_3$ $+k_0/2$	$k_i/2$ $-k_r/2$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

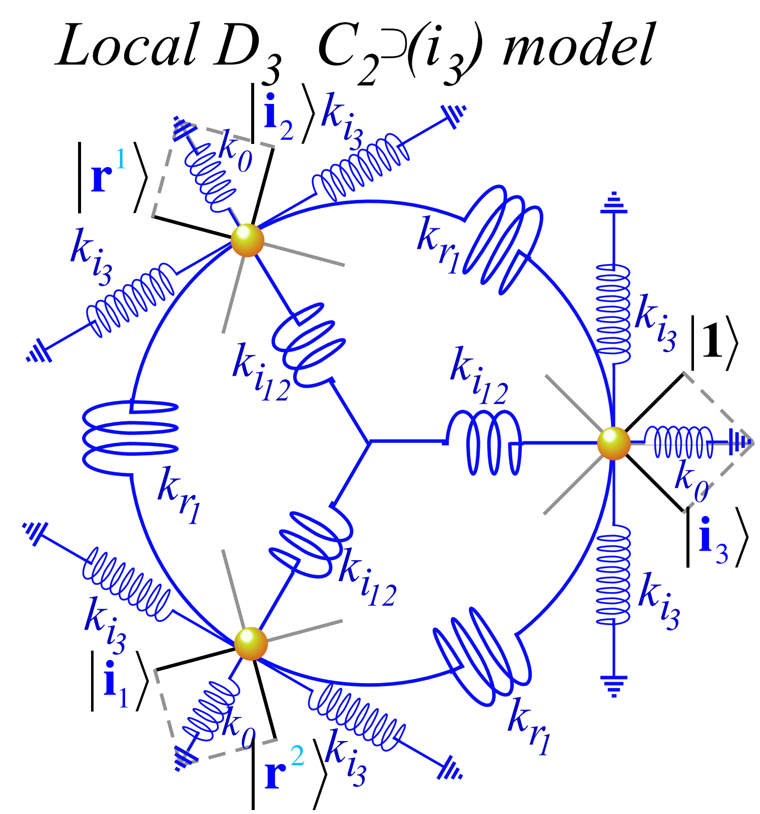
$D_3 \supset C_2(i_3)$ local-symmetry vibrational K-matrix eigenvalues $K_m/M = \omega_m^2$

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

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

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


Psuedo-scalar mode
A2
yy
√6P²yy|1>=(+1, +1, +1, -1, -1, -1)/√6 =|A2 yy>
√3P³xy|1> = (0, -1, +1, -1, +1, 0)/2 =|E xy>
Vector mode
E1
xy
√3P³yy|1>=(+2, -1, -1, +1, +1, -2)/√12 =|E yy>
Vector mode
E1
yy
local
C2(1,i3)
limit
√3P³xx|1> = (+2, -1, -1, -1, -1, +2)/√12 =|E xx>
Vector mode
E1
xx
√3P³yx|1> = (0, +1, -1, -1, +1, 0)/2 =|E yx>
Vector mode
E1
yx
Scalar mode
A1
xx
√6P¹xx|1>=(+1, +1, +1, +1, +1, +1)/√6 =|A1 xx>
1
r¹
r²
i1
i2
i3
i1
i2|1>
r¹|1>
|1>
i3
i3|1>
i1|1>
r²|1>
i2


Local D3 C2⊃(i3) model
|i2⟩
|r1⟩
|1⟩
|i3⟩
|i1⟩
|r2⟩
k0
ki3
kr1
ki12

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

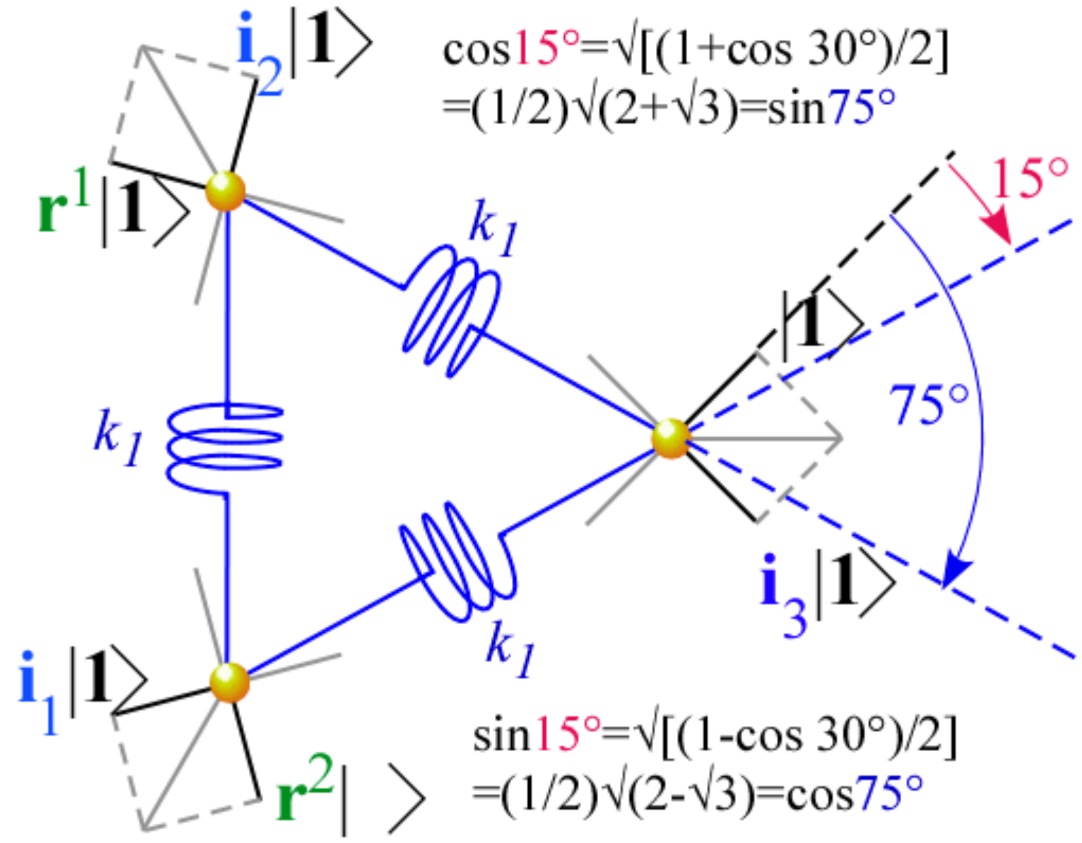
D_6 symmetry and Hexagonal Bands

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)*

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



D₃-direct-connection vibrational K-matrix

D_3-direct-connection K-matrix eigensolutions

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

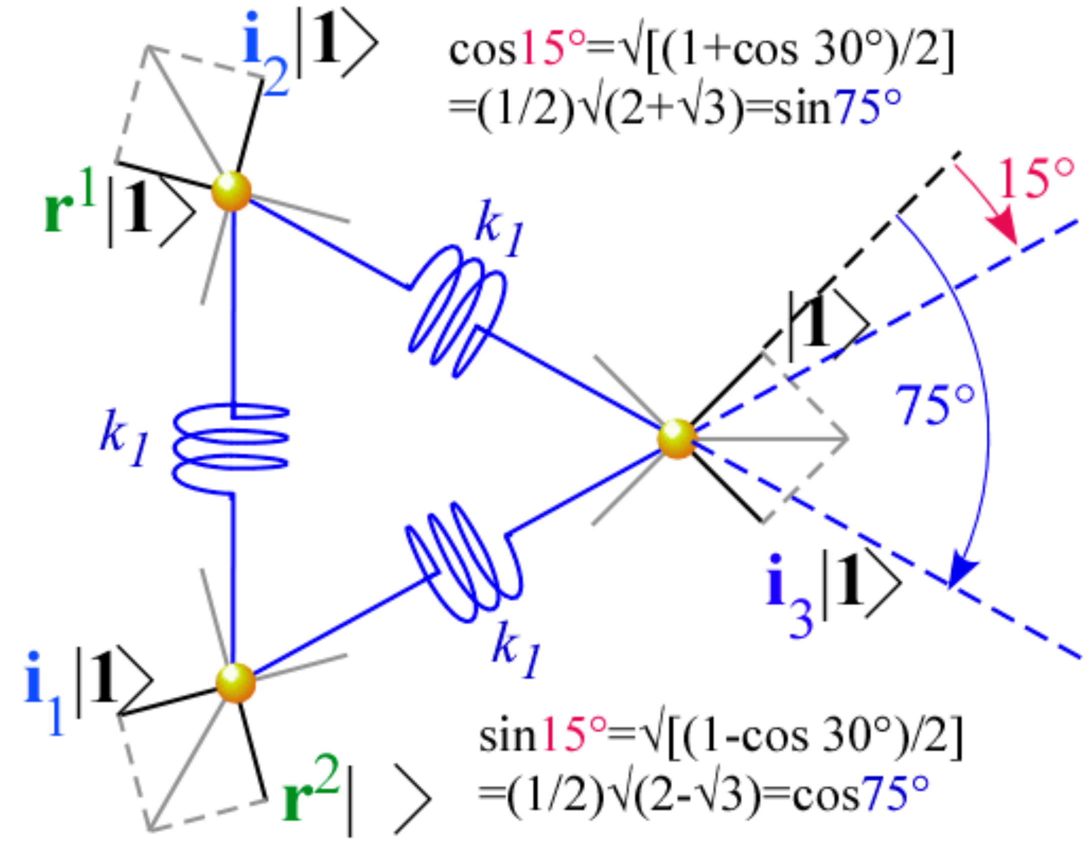
$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

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

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

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

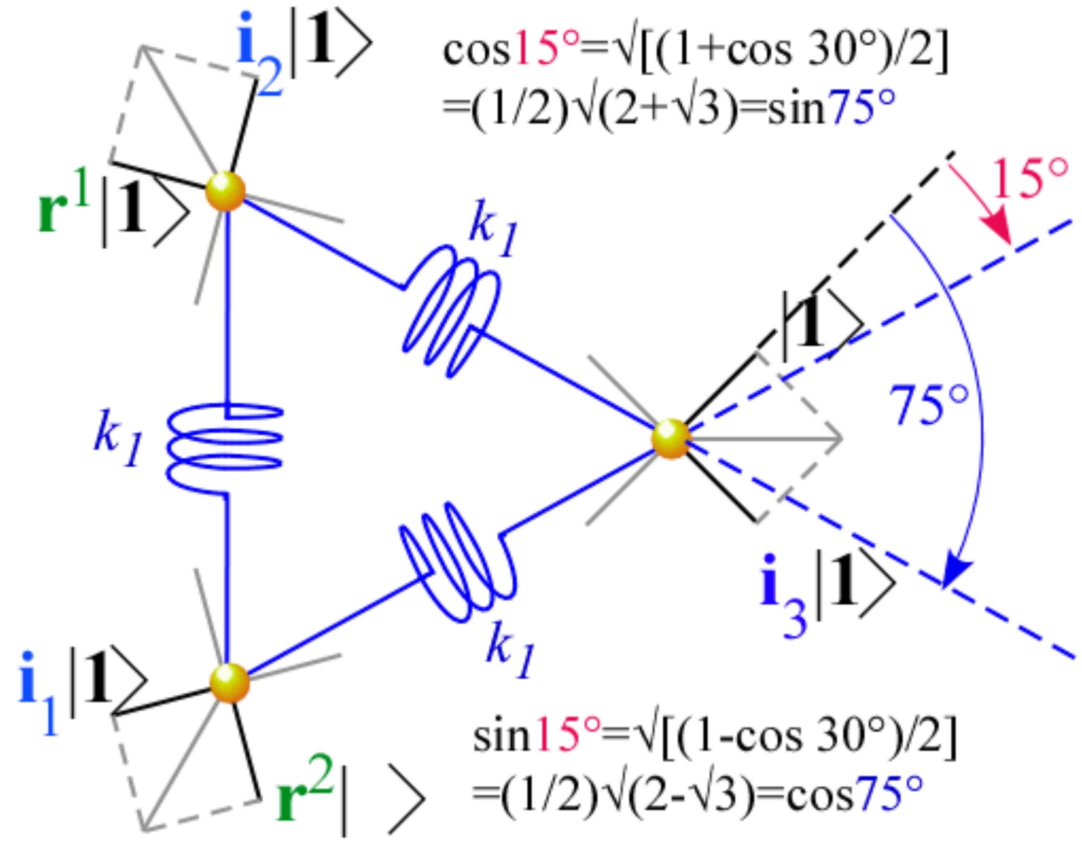
$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}$$



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

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

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

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

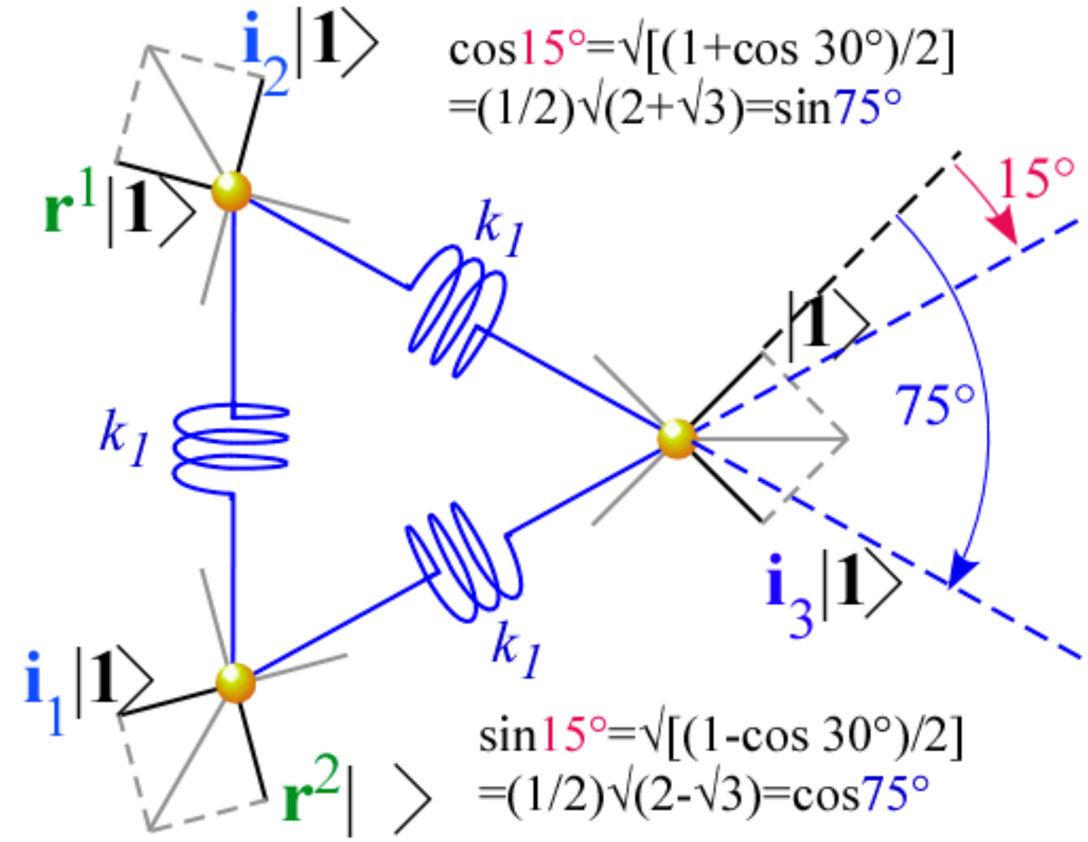
D_3-direct-connection vibrational K-matrix

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

D_3-direct-connection K-matrix eigensolutions

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

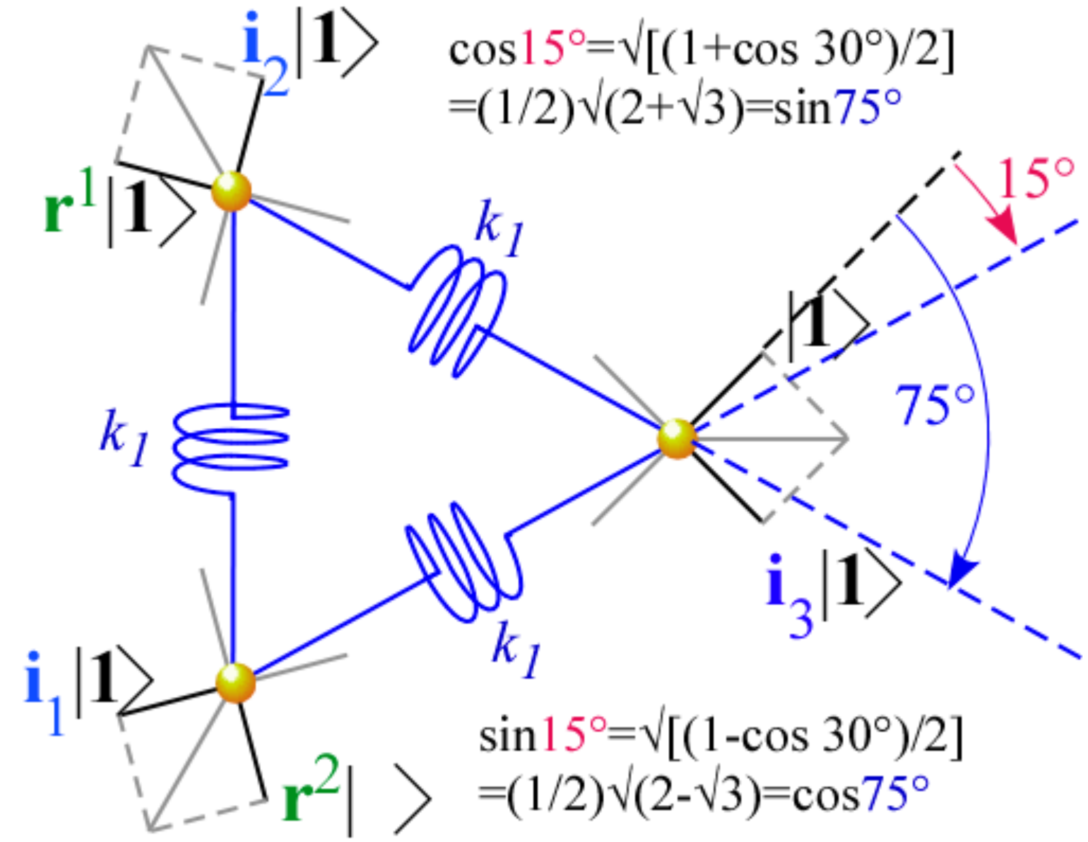
$\vert g_b\rangle$	$\vert\mathbf{1}\rangle$	$\vert\mathbf{r}^1\rangle$	$\vert\mathbf{r}^2\rangle$	$\vert\mathbf{i}_1\rangle$	$\vert\mathbf{i}_2\rangle$	$\vert\mathbf{i}_3\rangle$
$\langle\mathbf{1}\vert\,\mathbf{K}\,\vert g_b\rangle =$	$k_1(\cos^2 75° + \cos^2 15°) = k_1$	$k_1 \cos 75° \cdot \cos 15°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

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

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)

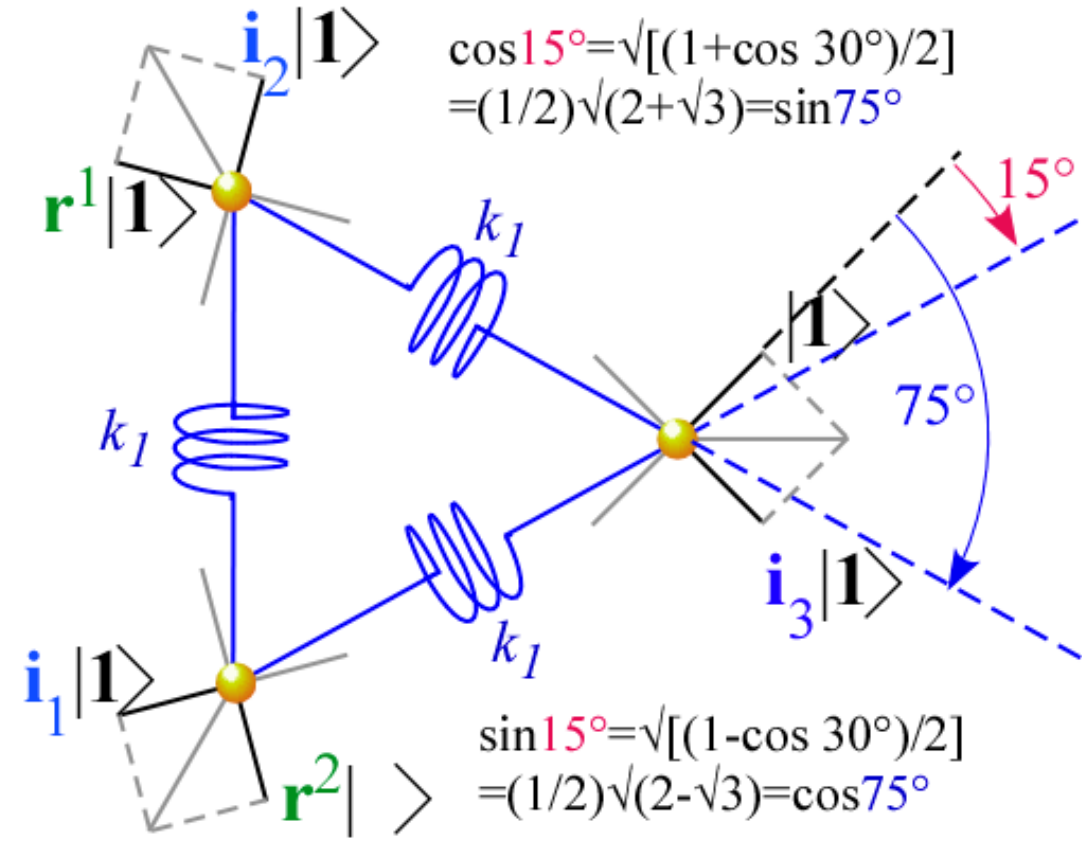
$$\langle \mathbf{1}|\mathbf{K}|\mathbf{g}_b\rangle = \begin{bmatrix} r_0 & r_1 & r_2 & i_1 & i_2 & i_3 \end{bmatrix}$$

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 $K_m/M=\omega_m^2$

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

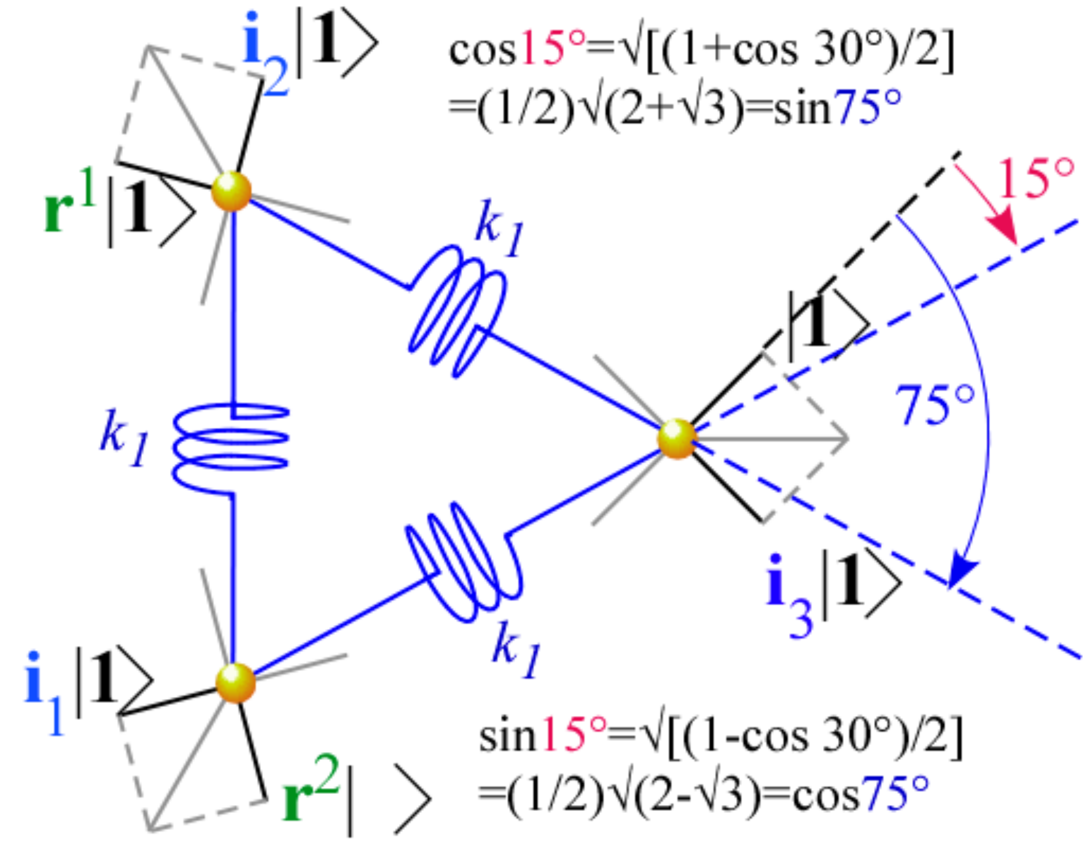
$$K_{yy}^{A_2} = 0$$

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

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 $K_m/M=\omega_m^2$

$$K^{A_1}_{xx} = 3k_1$$
$$K^{A_2}_{yy} = 0$$

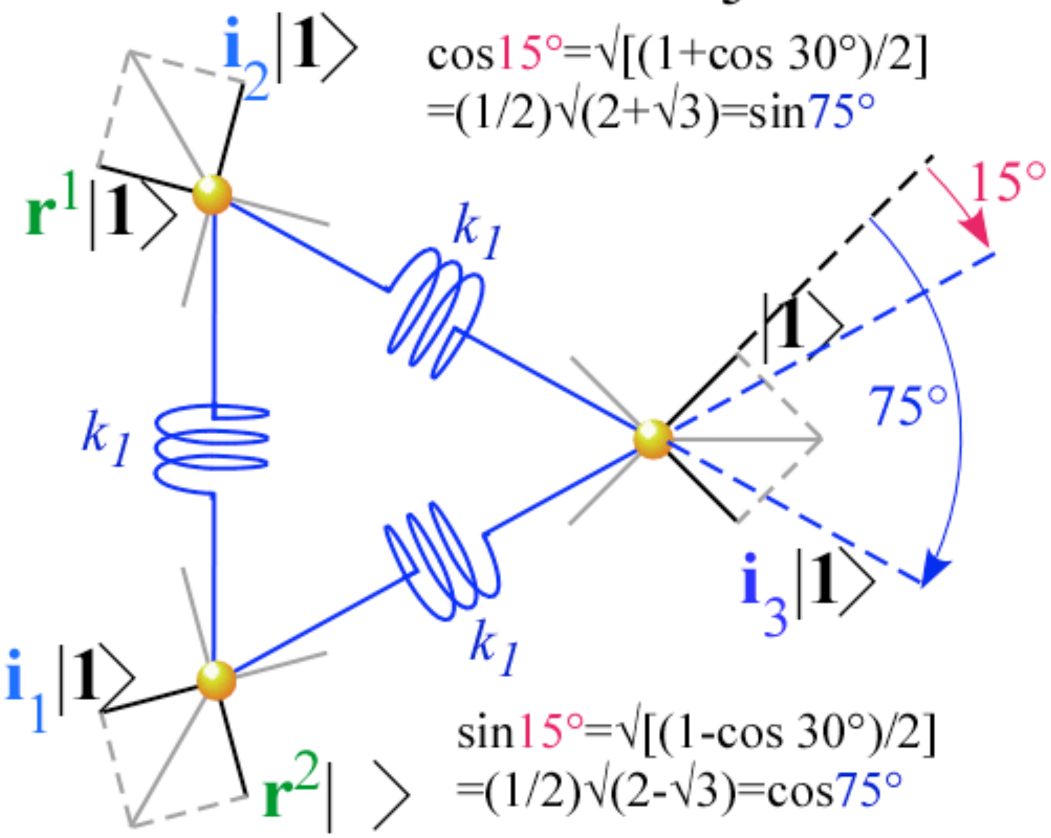
$$\begin{pmatrix} K^{E_1}_{xx} & K^{E_1}_{xy} \\ K^{E_1}_{yx} & K^{E_1}_{yy} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

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

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

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

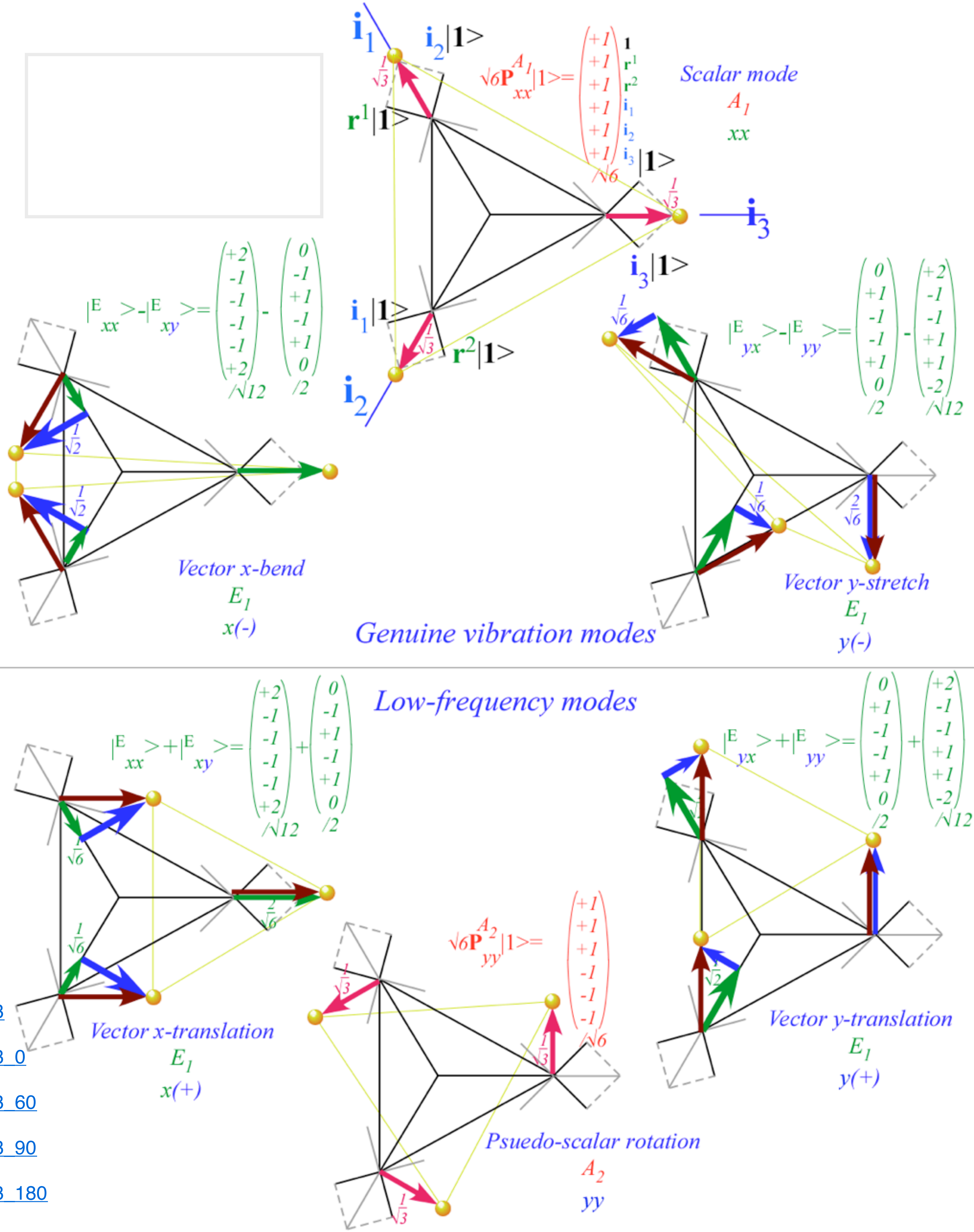
Mixed local symmetry D_3 model



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

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

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



http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3

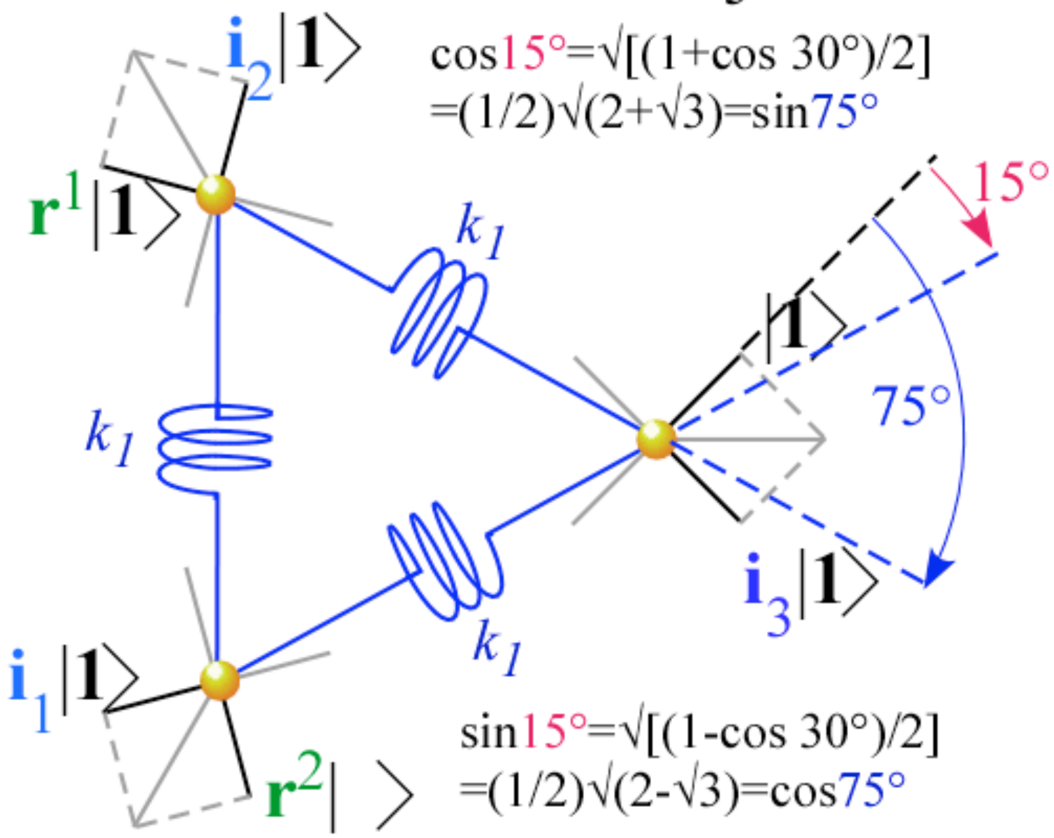
http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_0

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_60

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_90

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_180

Mixed local symmetry D_3 model



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

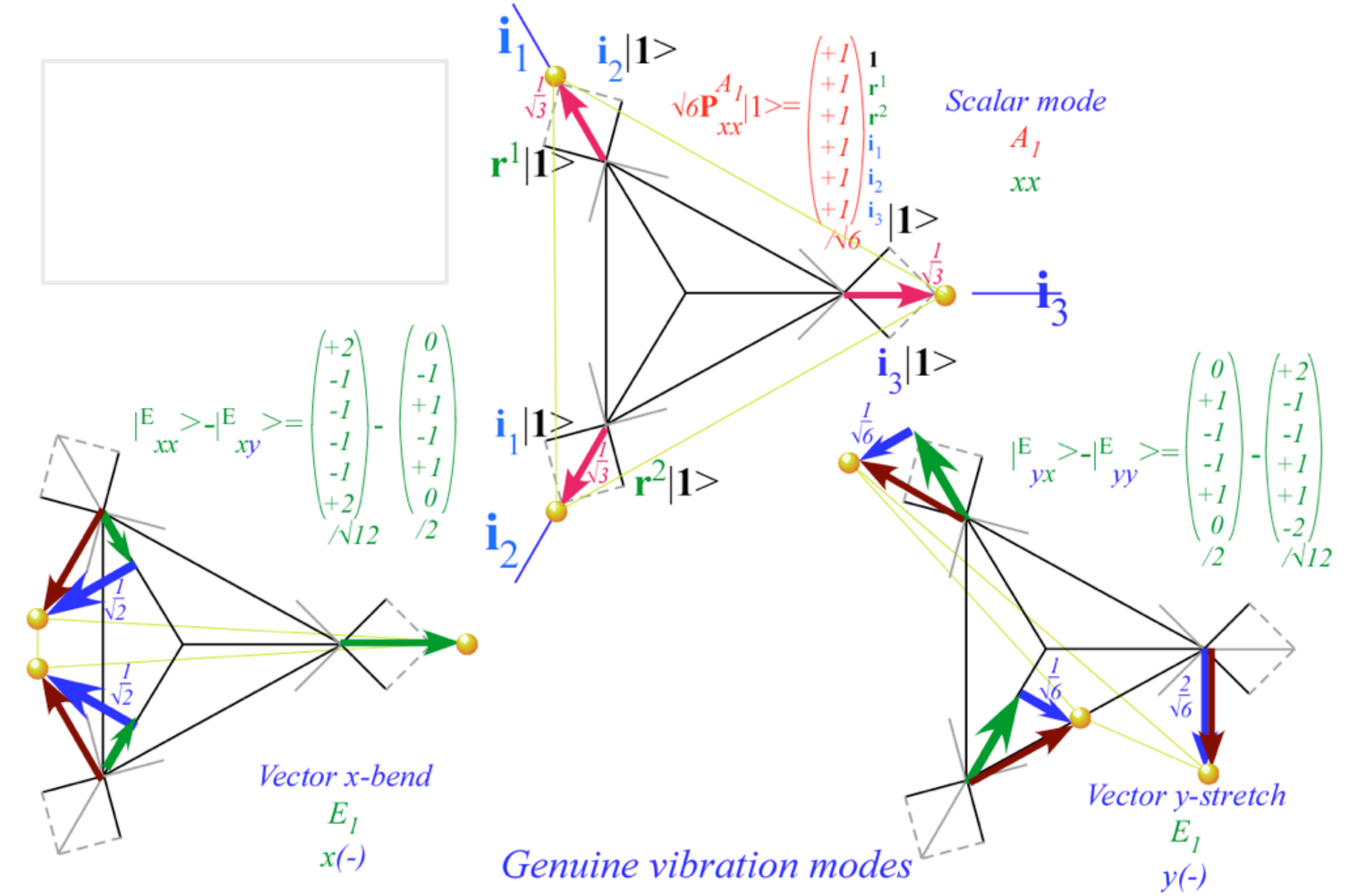
$$K_{yy}^{A_2} = 0$$

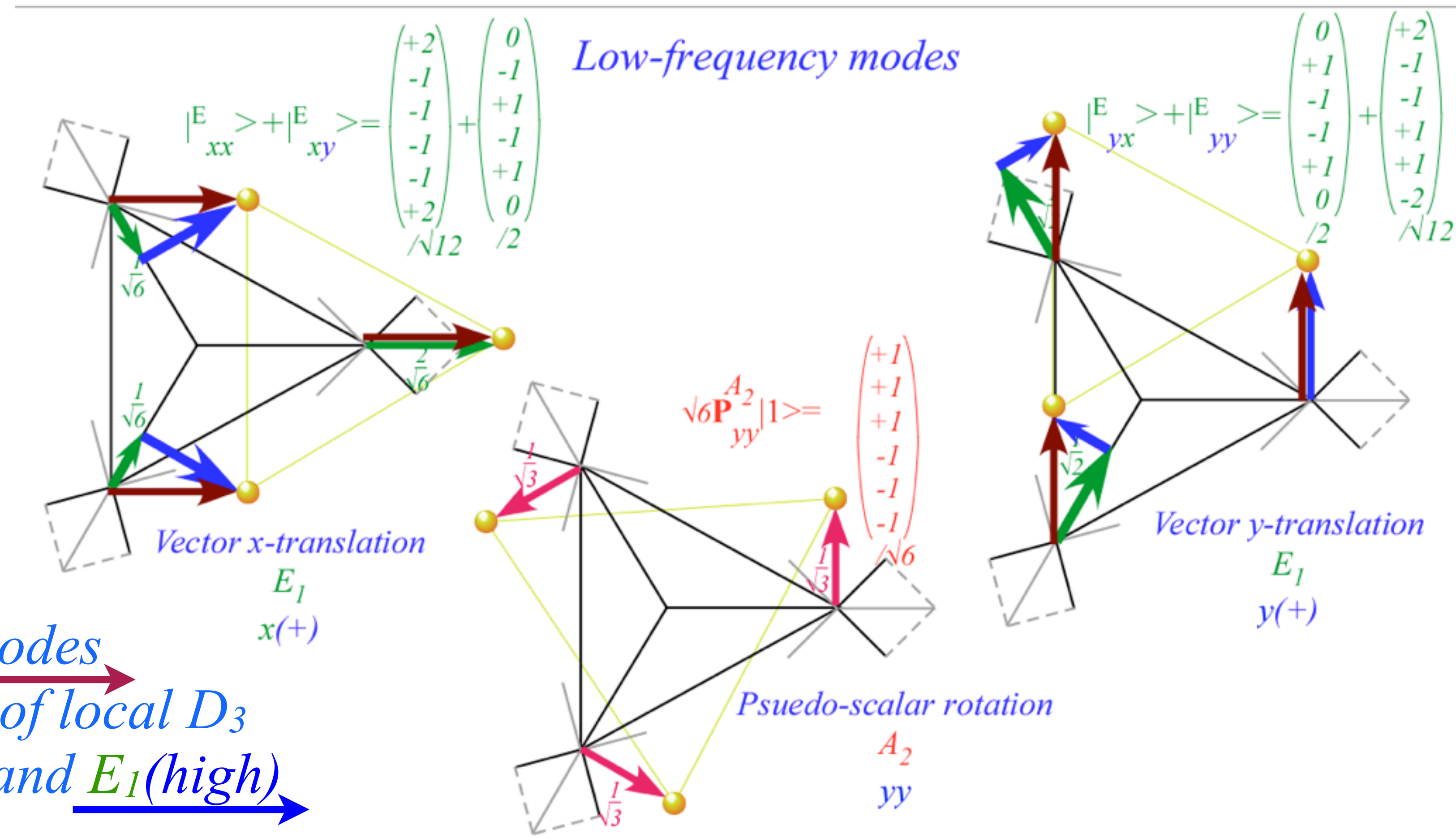
$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \begin{pmatrix} \frac{3k_1}{4} & \frac{3k_1}{4} \\ \frac{3k_1}{4} & \frac{3k_1}{4} \end{pmatrix}$$

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*

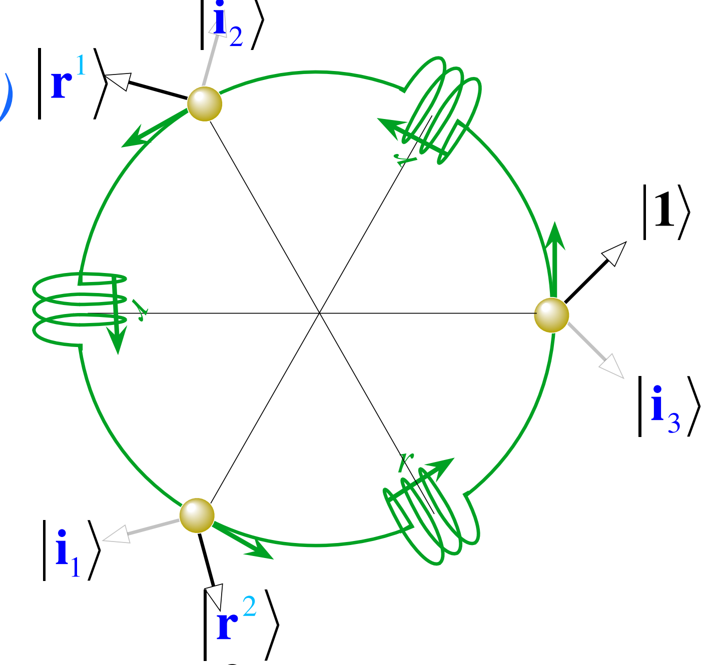
Cross product of the C_2 *and* D_3 *characters gives all* $D_6 = D_3 \times C_2$ *characters and ireps*

$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ 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: $i_1 = i_2 = i_3 = 0$

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

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

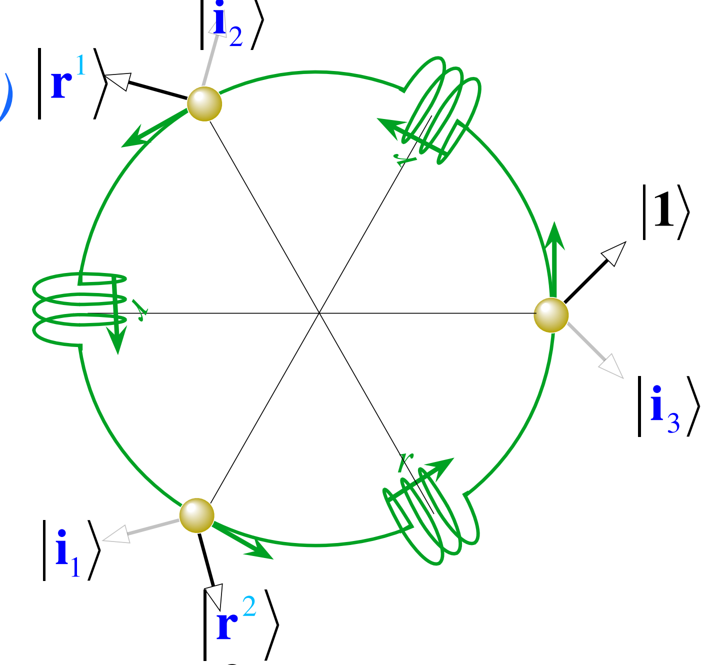
$$\begin{pmatrix} K_{xx}^{E_1} & K_{xy}^{E_1} \\ K_{yx}^{E_1} & K_{yy}^{E_1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2r_0 - r_1 - r_1^* - i_1 - i_2 + 2i_3 & \sqrt{3}(-r_1 + r_1^* - i_1 + i_2) \\ \sqrt{3}(-r_1^* + r_1 - i_1 + i_2) & 2r_0 - r_1 - r_1^* + i_1 + i_2 - 2i_3 \end{pmatrix}_{\substack{r_1=r=-r_2^*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

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

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

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

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



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

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 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

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

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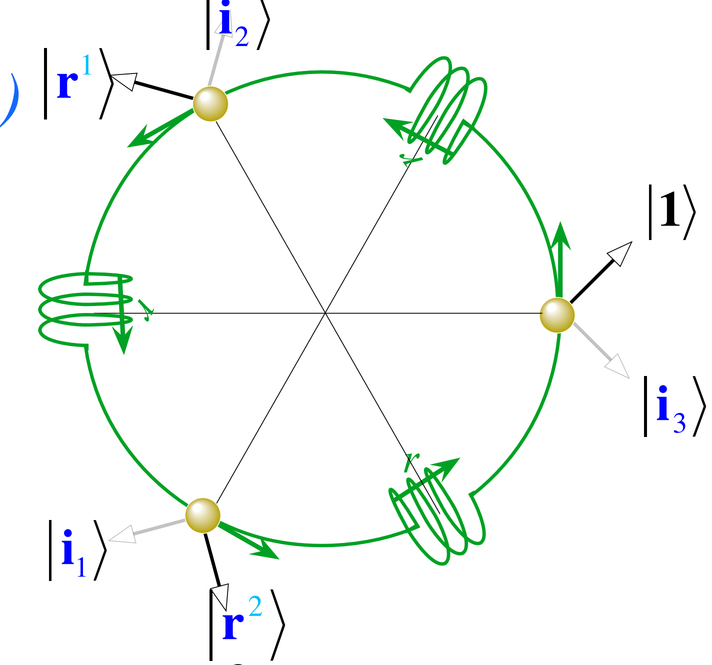
$D_3 \supset C_3(\mathbf{r}^{\pm 1})$ local symmetry model



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

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

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

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

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

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

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

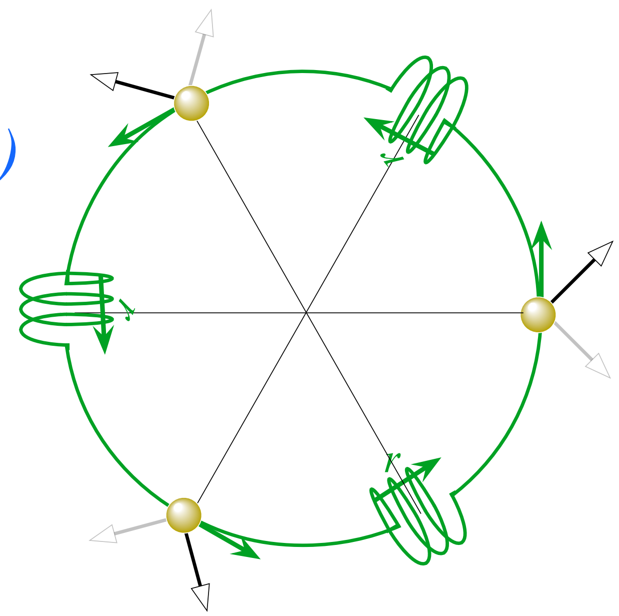
E_1 Eigenvectors in terms of $D_3 \supset C_2(i_3)$ E_1-vectors

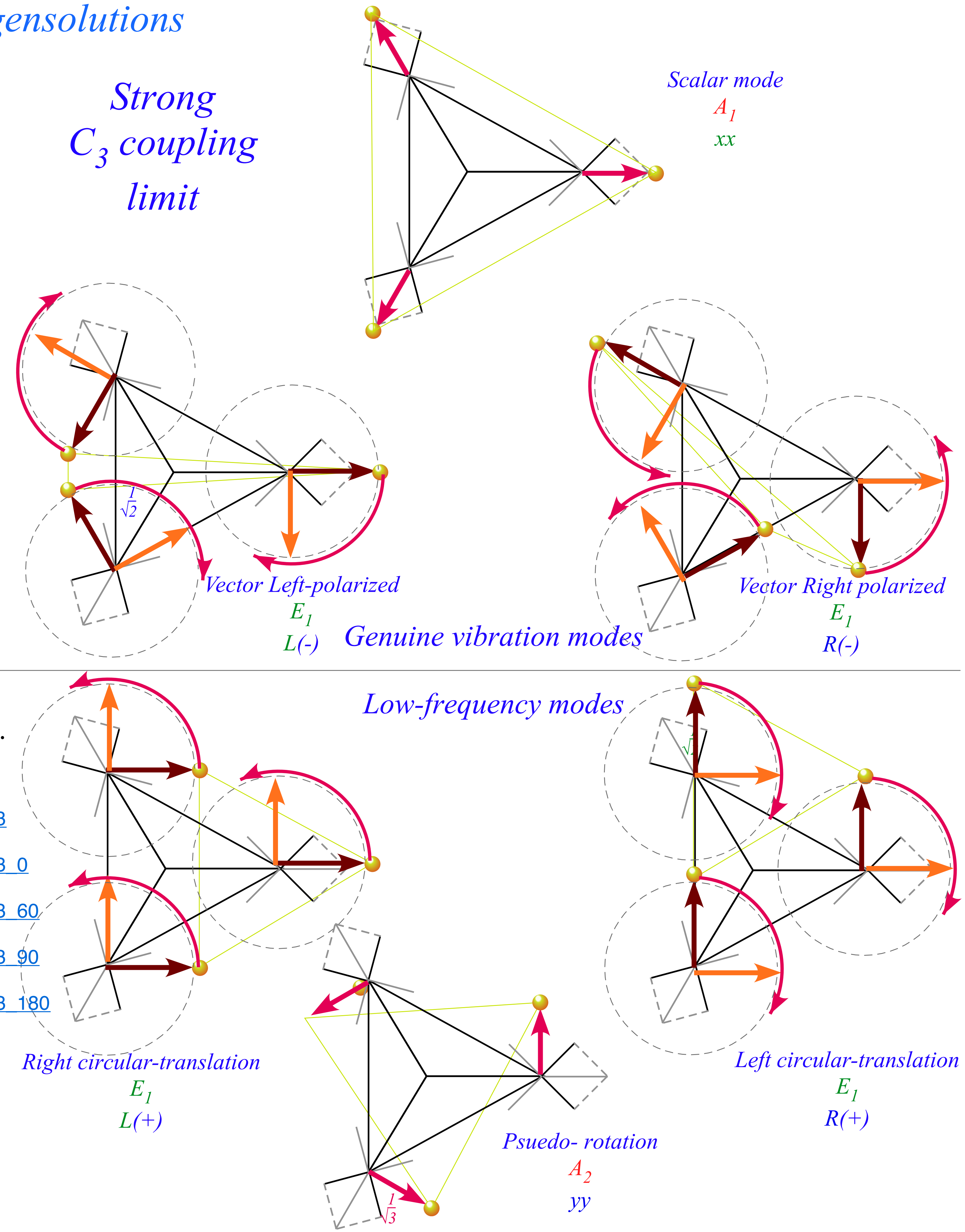
$$\mathbf{K}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle = \mathbf{K}\left(\left|\begin{matrix} E_1 \\ gx \end{matrix}\right\rangle + i\left|\begin{matrix} E_1 \\ gy \end{matrix}\right\rangle\right)\frac{1}{\sqrt{2}} = +r\frac{\sqrt{3}}{2}\left|\begin{matrix} E_1 \\ g(1)_3 \end{matrix}\right\rangle,$$

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

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

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





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

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

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_0

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_60

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_90

http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C3vN3_180

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

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- *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*

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

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

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

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

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

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

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

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

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

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A_1	$\mathbf{P}^{A_1}=\mathbf{P}^{A_1}\mathbf{P}^{0_3}=\mathbf{P}^{A_1}_{0_3 0_3}$	$\Rightarrow D^{A_1}\downarrow C_3 \sim d^{0_3}$	$\Rightarrow \omega^{A_1} \rightarrow \omega^{0_3}$
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	$\mathbf{P}^{E_1}=\mathbf{P}^{E_1}\mathbf{P}^{1_3}+\mathbf{P}^{E_1}\mathbf{P}^{2_3}$	$\Rightarrow D^{E_1}\downarrow C_3 \sim$	$\Rightarrow \omega^{E_1} \rightarrow \omega^{1_3}$
	$=\mathbf{P}^{E_1}_{1_3 1_3}+\mathbf{P}^{E_1}_{2_3 2_3}$	$d^{1_3}\oplus d^{2_3}$	$\searrow \omega^{2_3}$

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

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- *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*

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

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

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

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

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

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

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

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*

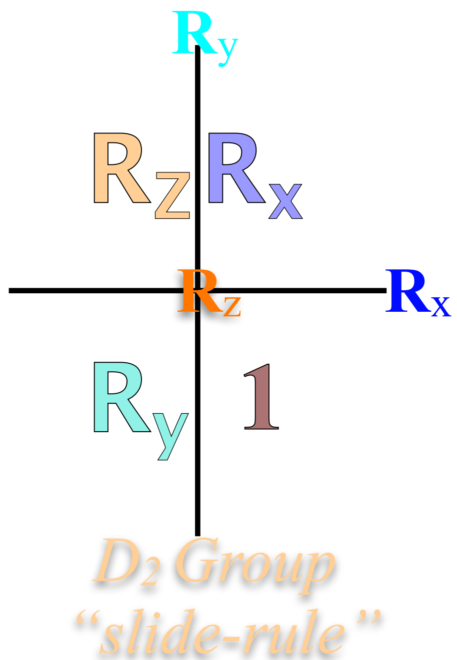
Spontaneous symmetry breaking and clustering: Frobenius Reciprocity , band structure

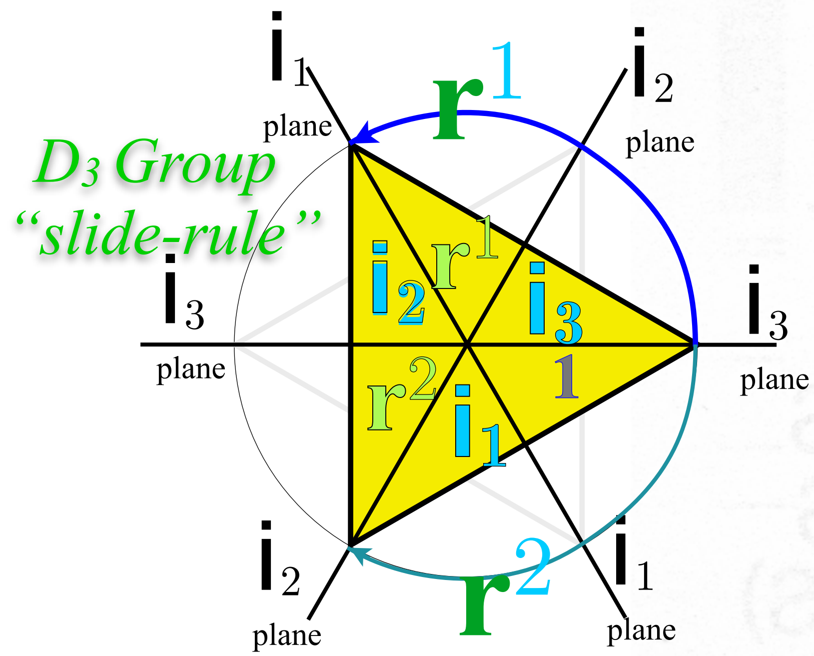
- *Induced rep $d^{a}(C_2)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation*
- *Induced rep $d^{a}(C_3)\uparrow D^3 = D^{\alpha} \oplus D^{\beta} \oplus ..$ correlation*

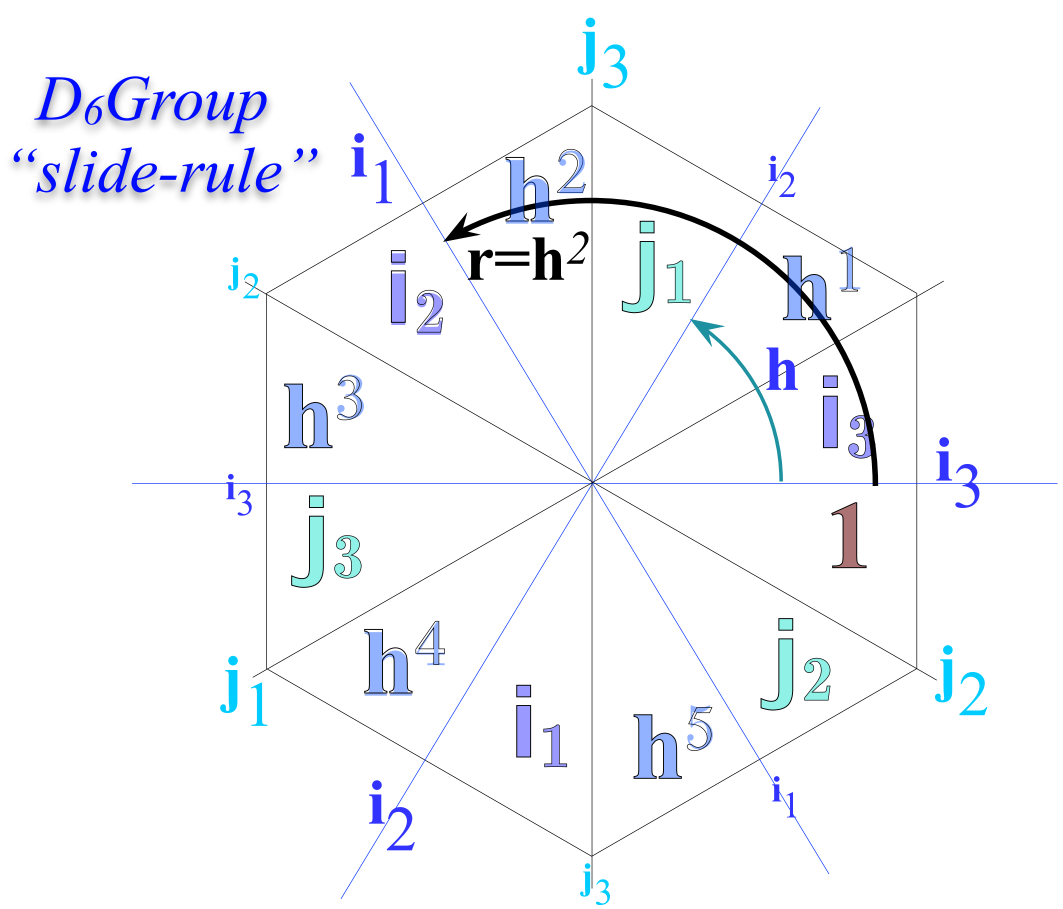
D_6 symmetry and Hexagonal Bands

- *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







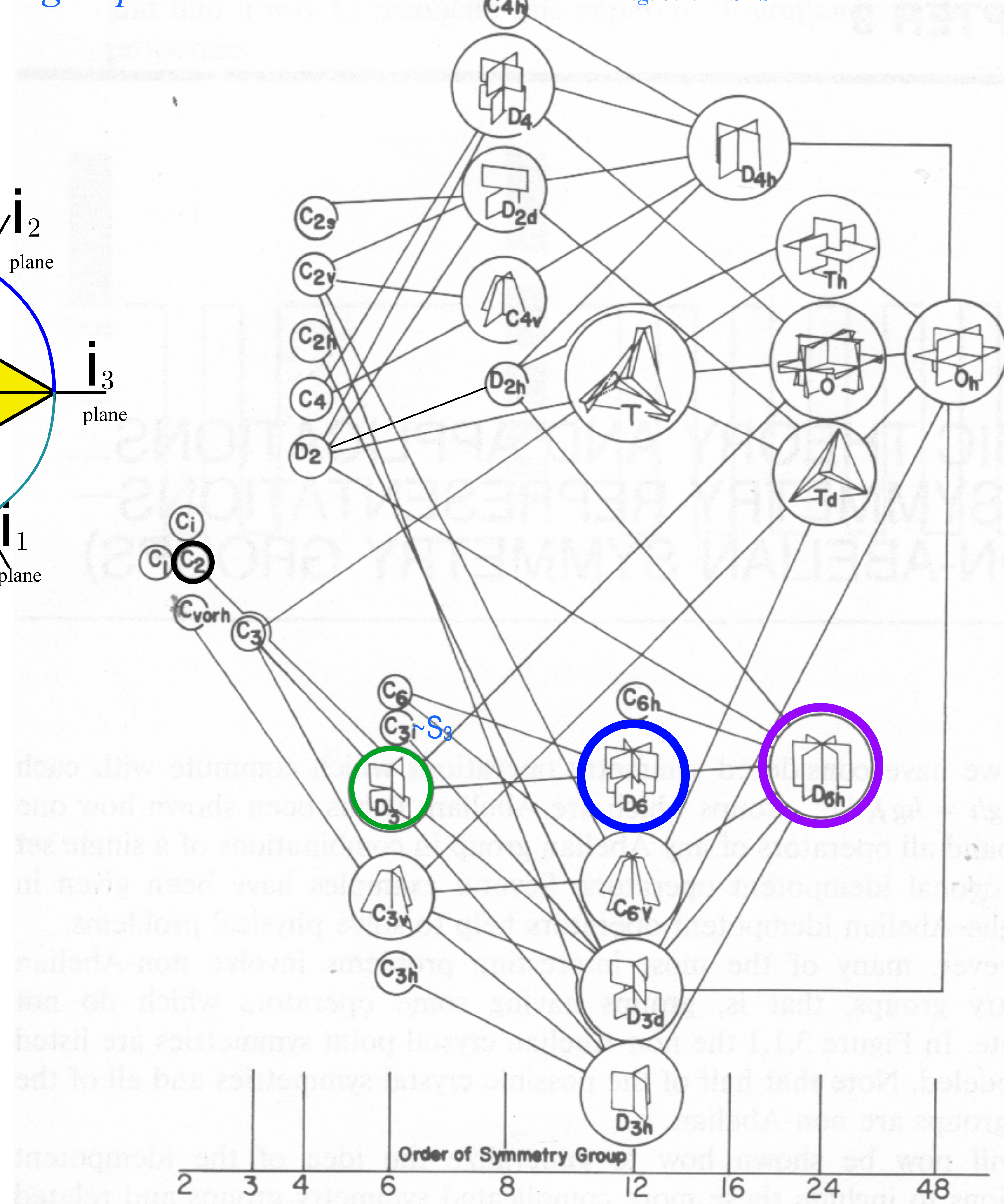


Fig. 3.1.1 PSDS

D_6 *symmetry and Hexagonal Bands*

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

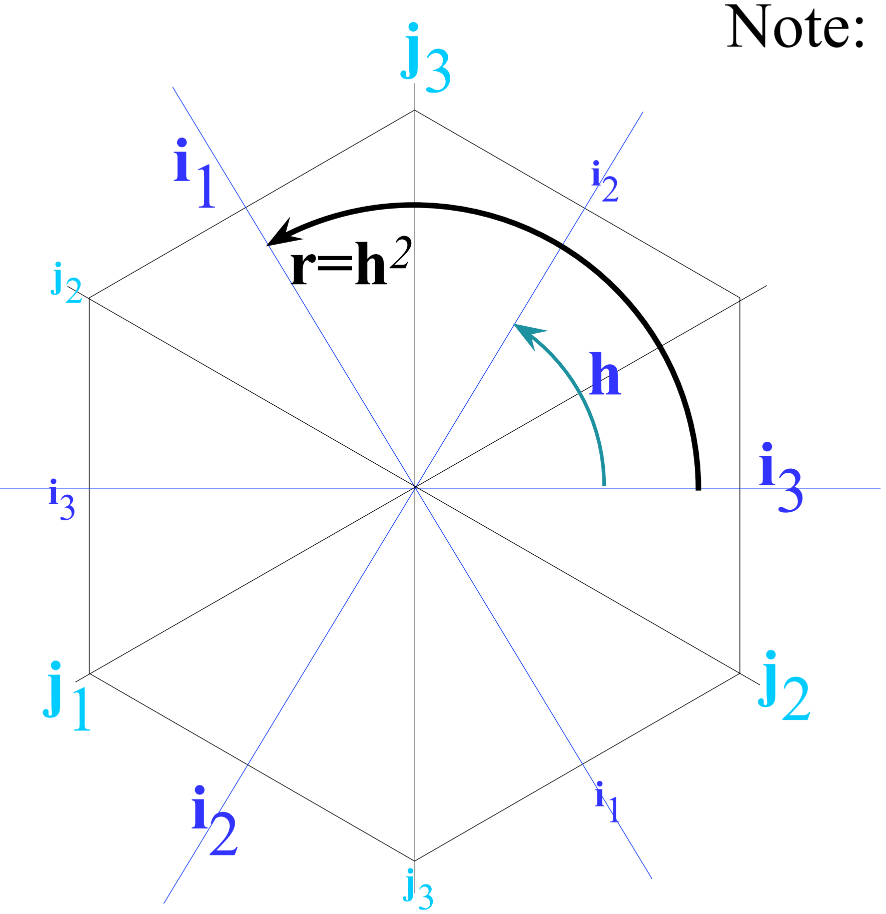
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$$

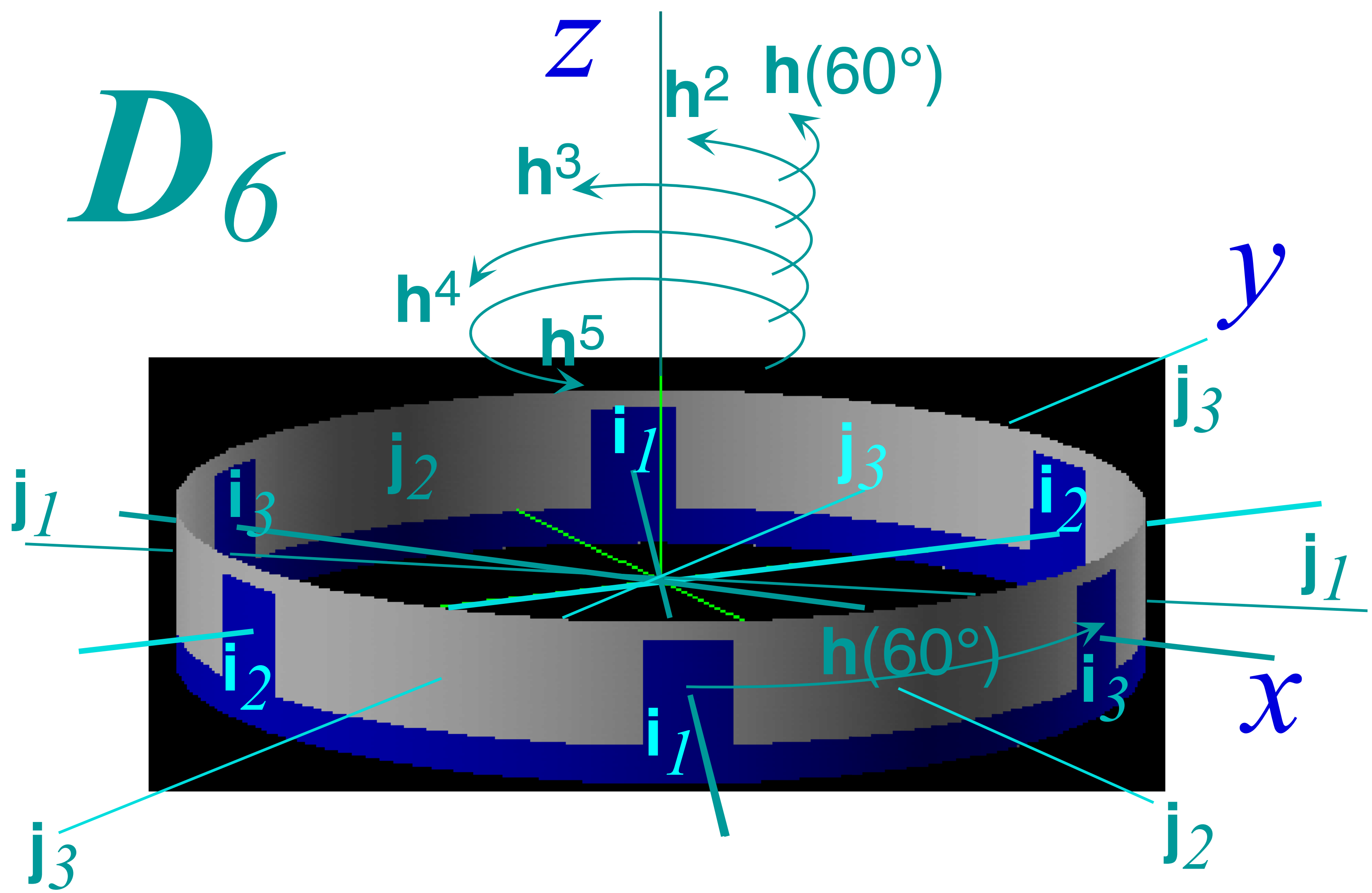
$\times$ product and D_6 operators. Define *hexagonal generator* **h** of subgroup $C_6 = \{\mathbf{1}, \mathbf{h}, \mathbf{h}^2, \mathbf{h}^3, \mathbf{h}^4\ \mathbf{h}^5\}$

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

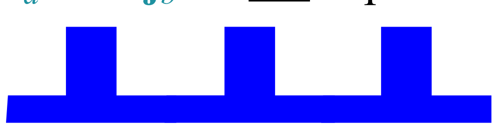
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{h}^2, \mathbf{h}^4, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{h}^3, \mathbf{h}^5, \mathbf{h}, \mathbf{j}_1, \mathbf{j}_2, \mathbf{j}_3\}$$

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 <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.

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.)

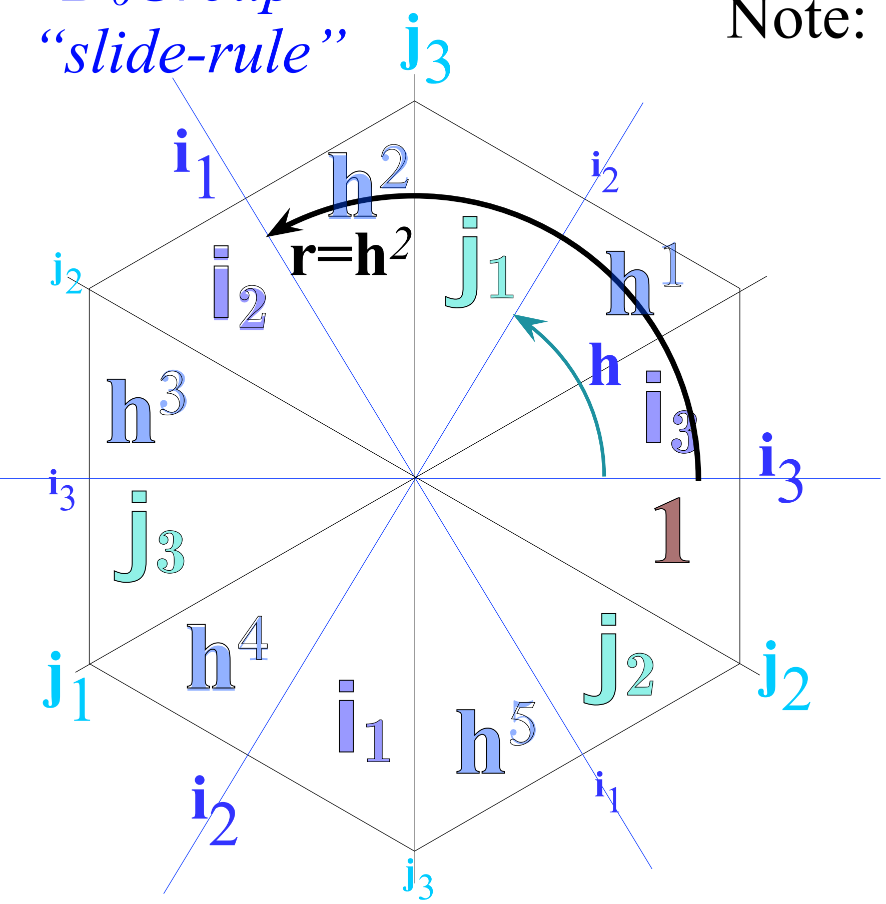
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\} \times \{\mathbf{1}, \mathbf{R}_z\}$$

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

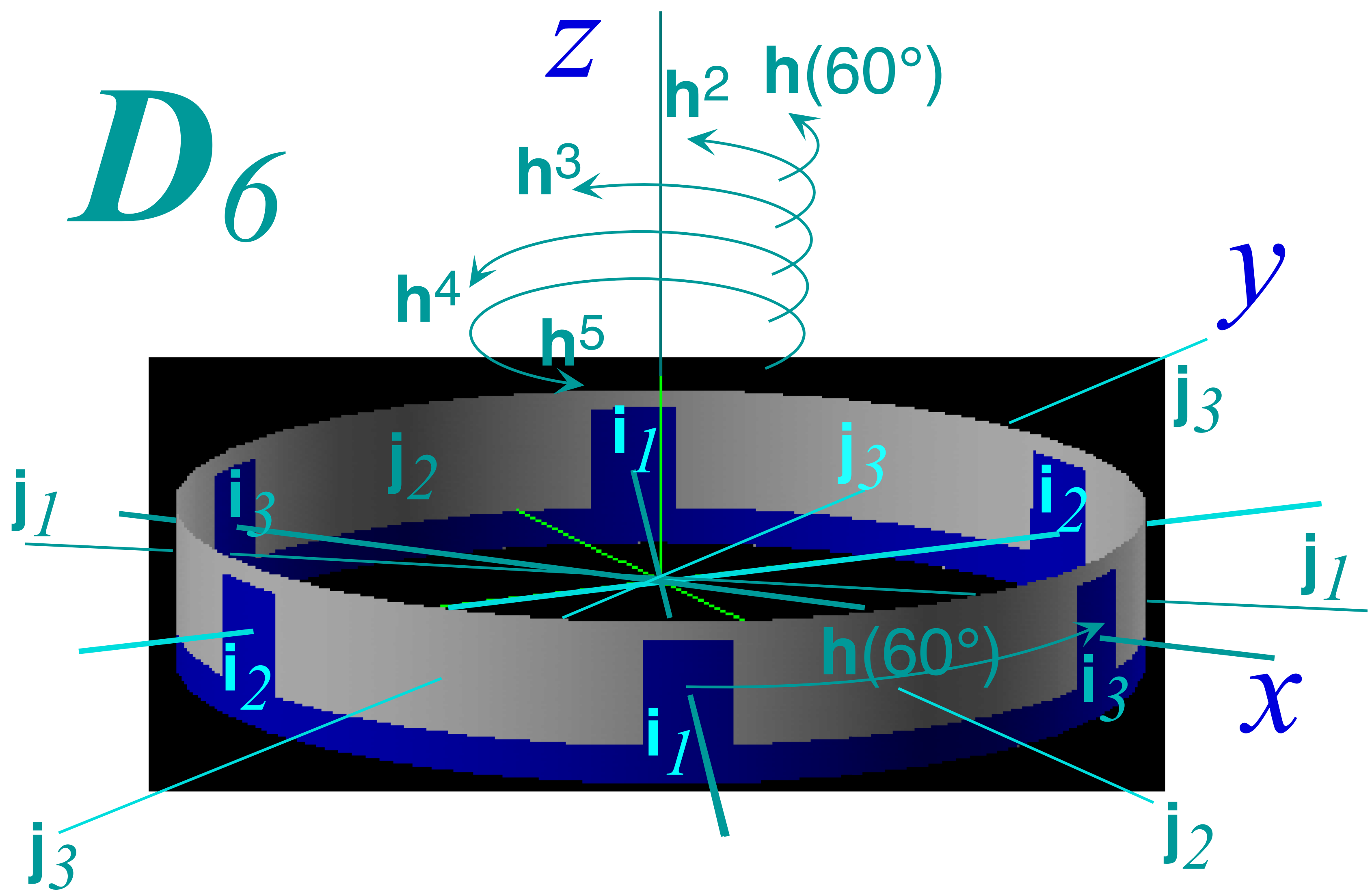
$$D_6 = D_3 \times C_2 = \{\mathbf{1}, \mathbf{r}, \mathbf{r}^2, \mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{1}\cdot\mathbf{R}_z, \mathbf{r}\cdot\mathbf{R}_z, \mathbf{r}^2\cdot\mathbf{R}^z, \mathbf{i}_1\cdot\mathbf{R}_z, \mathbf{i}_2\cdot\mathbf{R}_z, \mathbf{i}_3\cdot\mathbf{R}_z\}$$

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

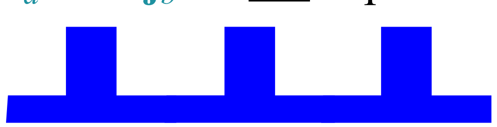
D_6Group “slide-rule”



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.

Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 14.5 p.80*)

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
+	1	1
−	1	−1

×

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
+	1	1
−	1	−1

=

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot1$	$1\cdot1$	$1\cdot1$	$1\cdot1$
$-\cdot+$	$1\cdot1$	$-1\cdot1$	$1\cdot1$	$-1\cdot1$
$+\cdot-$	$1\cdot1$	$1\cdot1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot1$	$-1\cdot1$	$1\cdot(-1)$	$-1\cdot(-1)$

=

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++ = A_1$	1	1	1	1
$-+ = A_2$	1	-1	1	-1
$+- = B_1$	1	1	−1	−1
$-- = B_2$	1	-1	−1	1

↑ *Note common notation*

Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 14.5 p.80*)

C_2^x	$\mathbf{1}$	$\mathbf{R}_x$
$+$	1	1
$-$	1	-1

$\times$

C_2^y	$\mathbf{1}$	$\mathbf{R}_y$
$+$	1	1
$-$	1	-1

$=$

$C_2^x \times C_2^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{R}_x\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{R}_y$	$\mathbf{R}_x\cdot\mathbf{R}_y$
$+\cdot+$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$-\cdot+$	$1\cdot 1$	$-1\cdot 1$	$1\cdot 1$	$-1\cdot 1$
$+\cdot-$	$1\cdot 1$	$1\cdot 1$	$1\cdot(-1)$	$1\cdot(-1)$
$-\cdot-$	$1\cdot 1$	$-1\cdot 1$	$1\cdot(-1)$	$-1\cdot(-1)$

$=$

D_2	$\mathbf{1}$	$\mathbf{R}_x$	$\mathbf{R}_y$	$\mathbf{R}_z$
$++ = A_1$	1	1	1	1
$-+ = A_2$	1	-1	1	-1
$+- = B_1$	1	1	-1	-1
$-- = B_2$	1	-1	-1	1

↑ *Note common notation*

$C_2 \times C_3 = C_6$ characters made of C_2 x C_3 Cartesian product

C_2^x	$\mathbf{1}$	ρ
0_2	1	1
1_2	1	-1

$\times$

C_3^y	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$
0_3	1	1	1
1_3	1	ε	ε^*
2_3	1	ε^*	ε

$=$

$C_2^x \times C_3^y$	$\mathbf{1}\cdot\mathbf{1}$	$\mathbf{1}\cdot\mathbf{r}^1$	$\mathbf{1}\cdot\mathbf{r}^2$	$\rho\cdot\mathbf{1}$	$\rho\cdot\mathbf{r}^1$	$\rho\cdot\mathbf{r}^2$
$0_2\cdot 0_3$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
$0_2\cdot 1_3$	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$
$0_2\cdot 2_3$	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$
$1_2\cdot 0_3$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$-1\cdot 1$	$-1\cdot 1$	$-1\cdot 1$
$1_2\cdot 1_3$	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$-1\cdot 1$	$-1\cdot\varepsilon$	$-1\cdot\varepsilon^*$
$1_2\cdot 2_3$	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$-1\cdot 1$	$-1\cdot\varepsilon^*$	$-1\cdot\varepsilon$

$=$

C_6^{xy}	0°	120°	240°	180°	-60°	60°
0_6	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$
2_6	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$
4_6	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$
3_6	$1\cdot 1$	$1\cdot 1$	$1\cdot 1$	$-1\cdot 1$	$-1\cdot 1$	$-1\cdot 1$
5_6	$1\cdot 1$	$1\cdot\varepsilon$	$1\cdot\varepsilon^*$	$-1\cdot 1$	$-1\cdot\varepsilon$	$-1\cdot\varepsilon^*$
1_6	$1\cdot 1$	$1\cdot\varepsilon^*$	$1\cdot\varepsilon$	$-1\cdot 1$	$-1\cdot\varepsilon^*$	$-1\cdot\varepsilon$

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

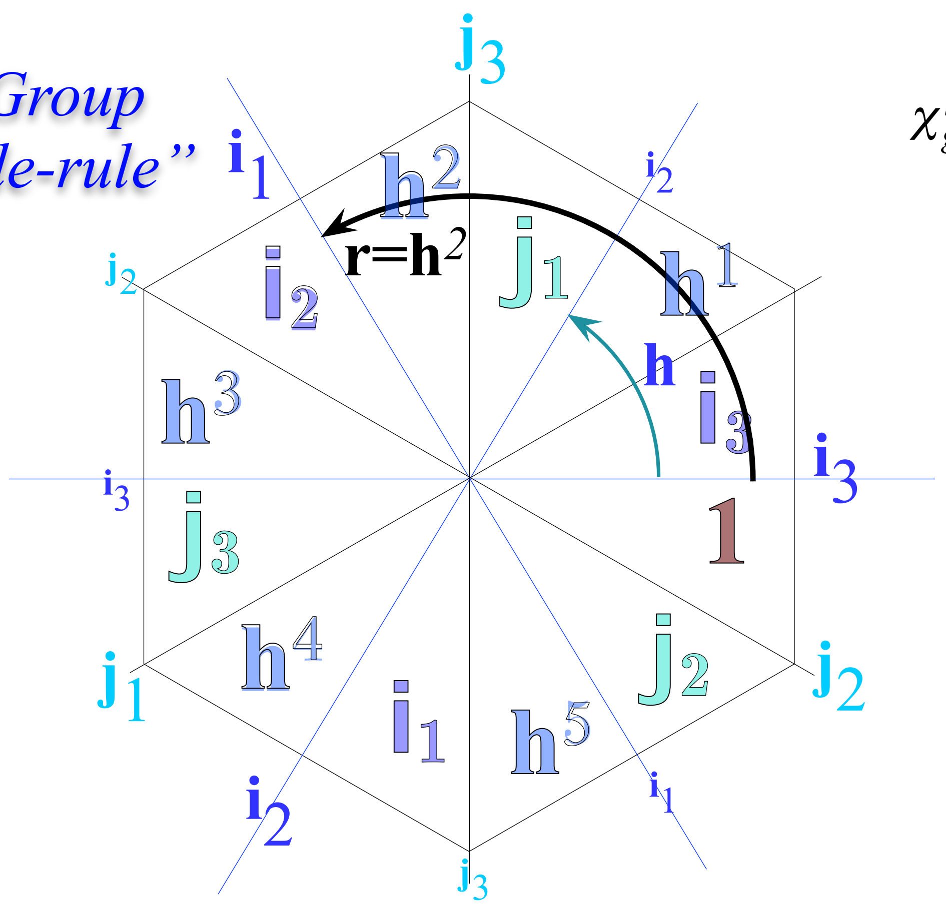
=

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

$\chi_g^\mu(D_6) =$

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

D_6 Group "slide-rule"



Recall $C_2 \times C_2 = D_2$ characters made of two C_2 groups (*Lecture 14.5 p.80*)

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

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

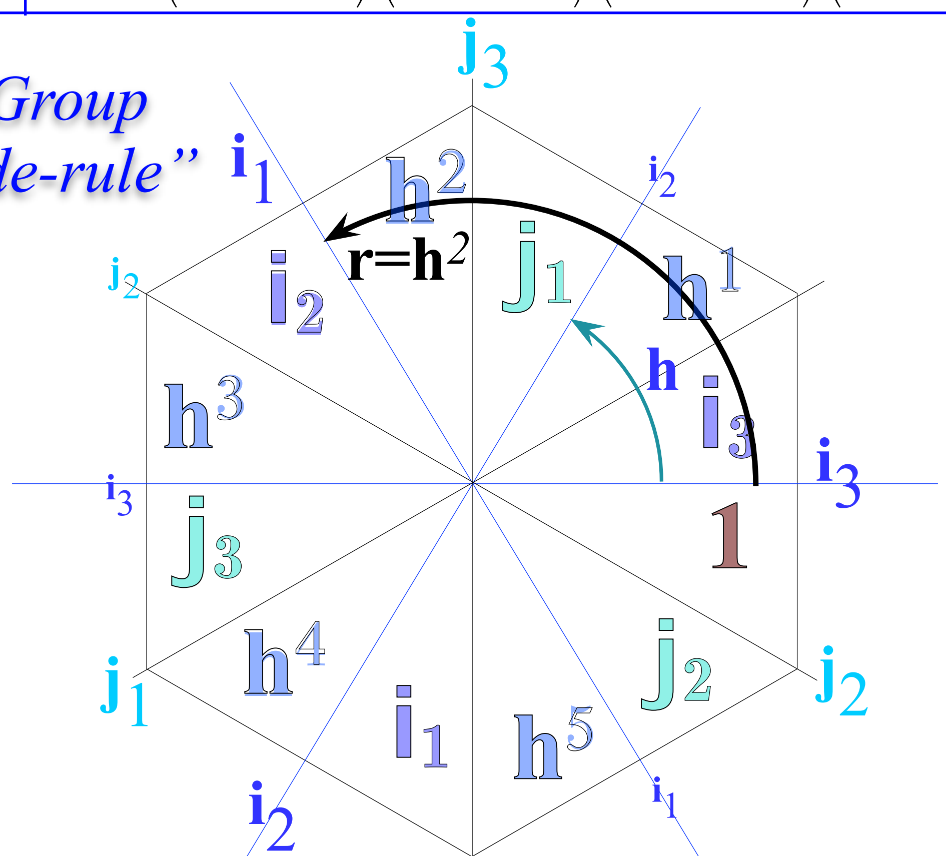
Odd vs Even

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

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

	0°	z 120°	z -120°	180°	180°	x 180°	z 180°	z -60°	z +60°	180°	180°	y 180°
g =	**1**	$\mathbf{r=h^2}$	$\mathbf{r^2=h^4}$	$\mathbf{i_1}$	$\mathbf{i_2}$	$\mathbf{i_3}$	$\mathbf{h^3}$	$\mathbf{h^3r=h^5}$	$\mathbf{h^3r^2=h^1}$	$\mathbf{h^3i_1=j_1}$	$\mathbf{h^3i_2=j_2}$	$\mathbf{h^3i_3=j_3}$
$D^{A_1}(g)=$	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
$D^{E_2}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$
$D^{B_2}(g)=$	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
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{\sqrt3}{2}\\\frac{\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{1}{2}&\frac{-\sqrt3}{2}\\\frac{-\sqrt3}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$

D_6 Group “slide-rule”



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.

	0°	z 120°	z -120°	180°	180°	x 180°
g =	**1**	**r=h²**	**r²=h⁴**	$\mathbf{i_1}$	$\mathbf{i_2}$	$\mathbf{i_3}$
$D^{A_1}(g)=$	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
$D^{E_1}(g)=$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}\frac{-1}{2}&\frac{\sqrt{3}}{2}\\\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}$	$\begin{pmatrix}1&0\\0&-1\end{pmatrix}$

	z 180°	z -60°	z +60°	180°	180°	y 180°
g =	**h³**	**h³r=h⁵**	**h³r²=h¹**	$\mathbf{h^3 i_1 = j_1}$	$\mathbf{h^3 i_2 = j_2}$	$\mathbf{h^3 i_3 = j_3}$
$D^{A_1}(g)=$	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**
determines
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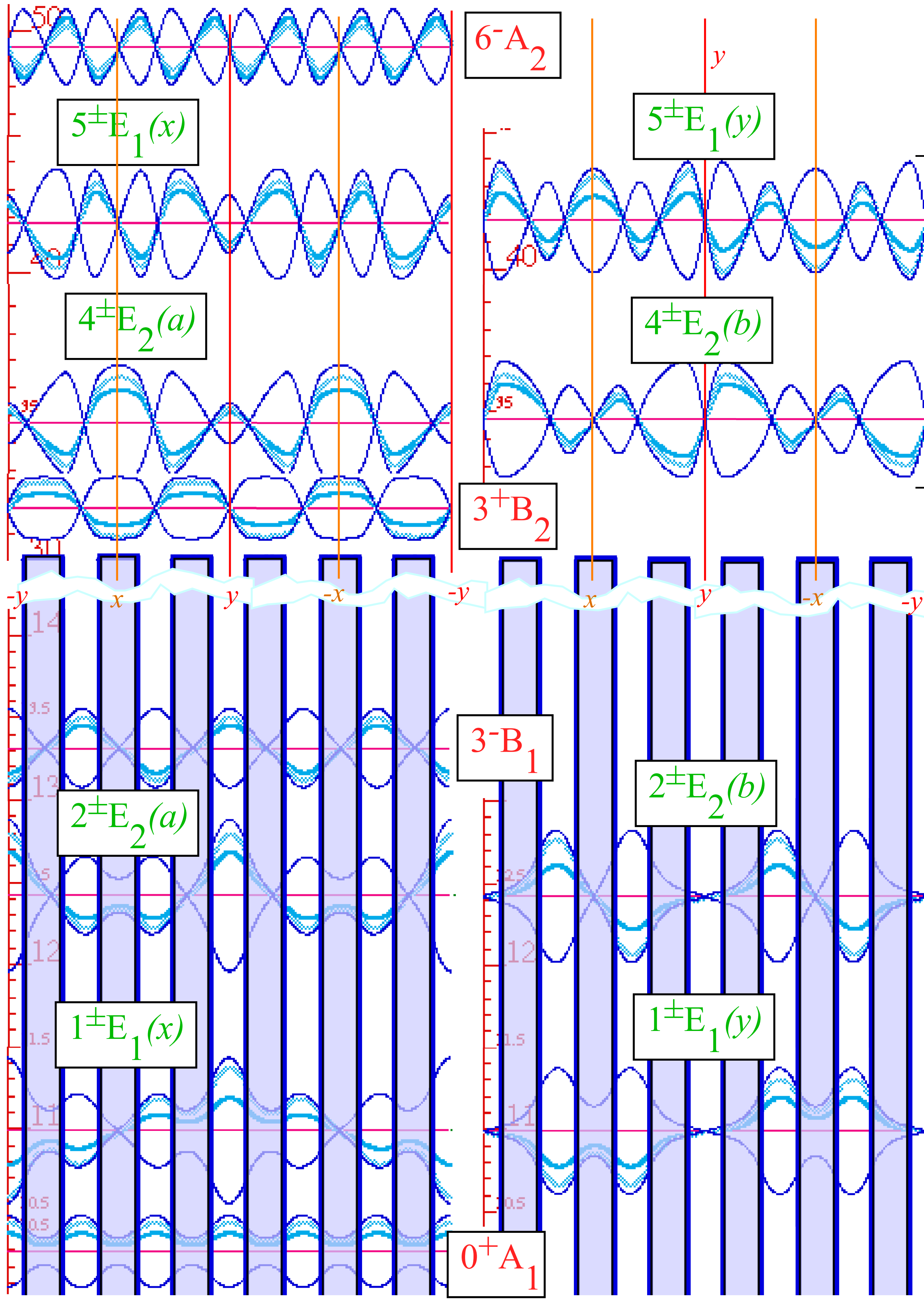
X_1 vs X_2
(+1) vs (-1)

$D_6 \supset C_2(j_3)$	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 (Mac OS-9)



$D_6 \supset C_3(h)$	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

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

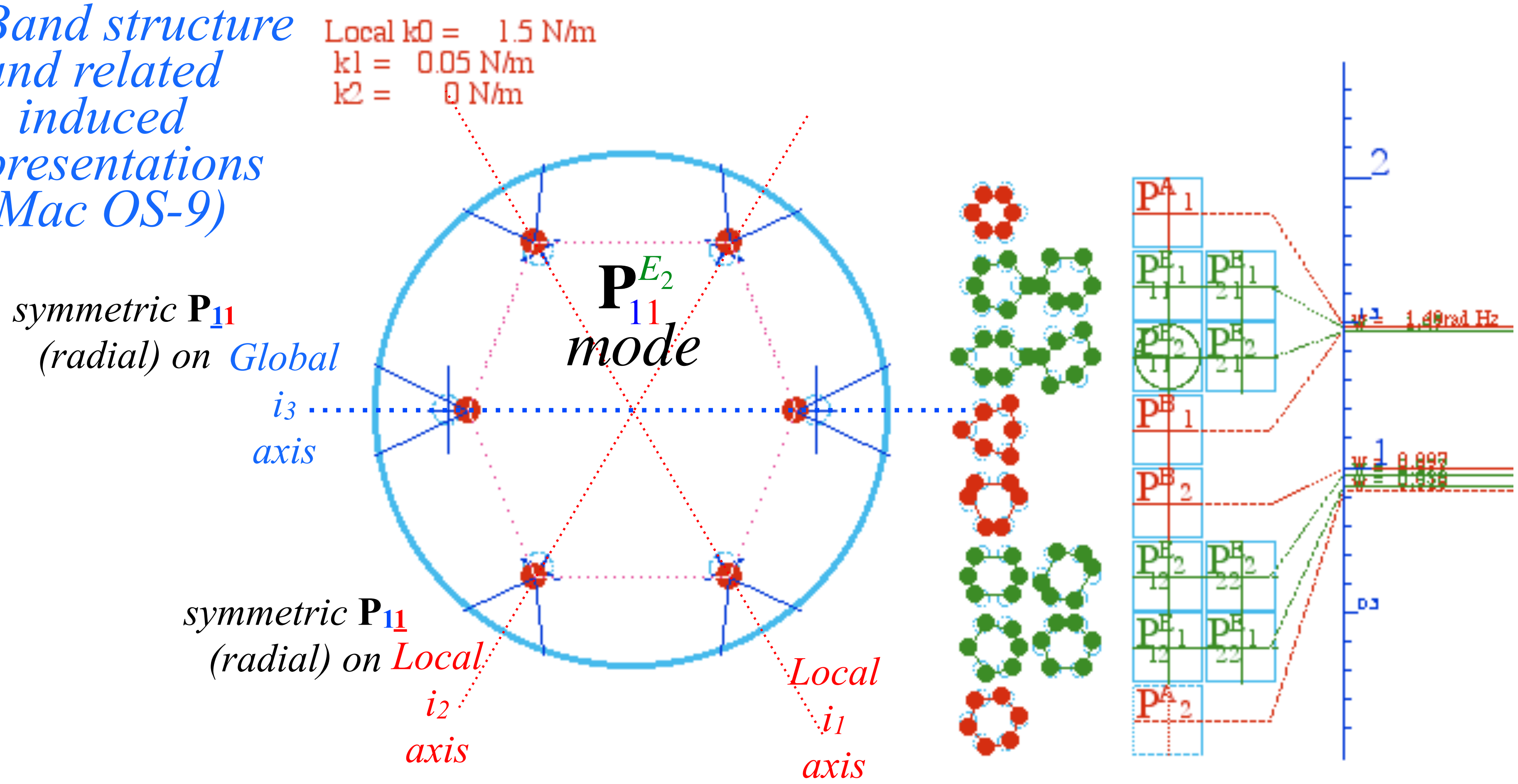
Odd Band or Cluster

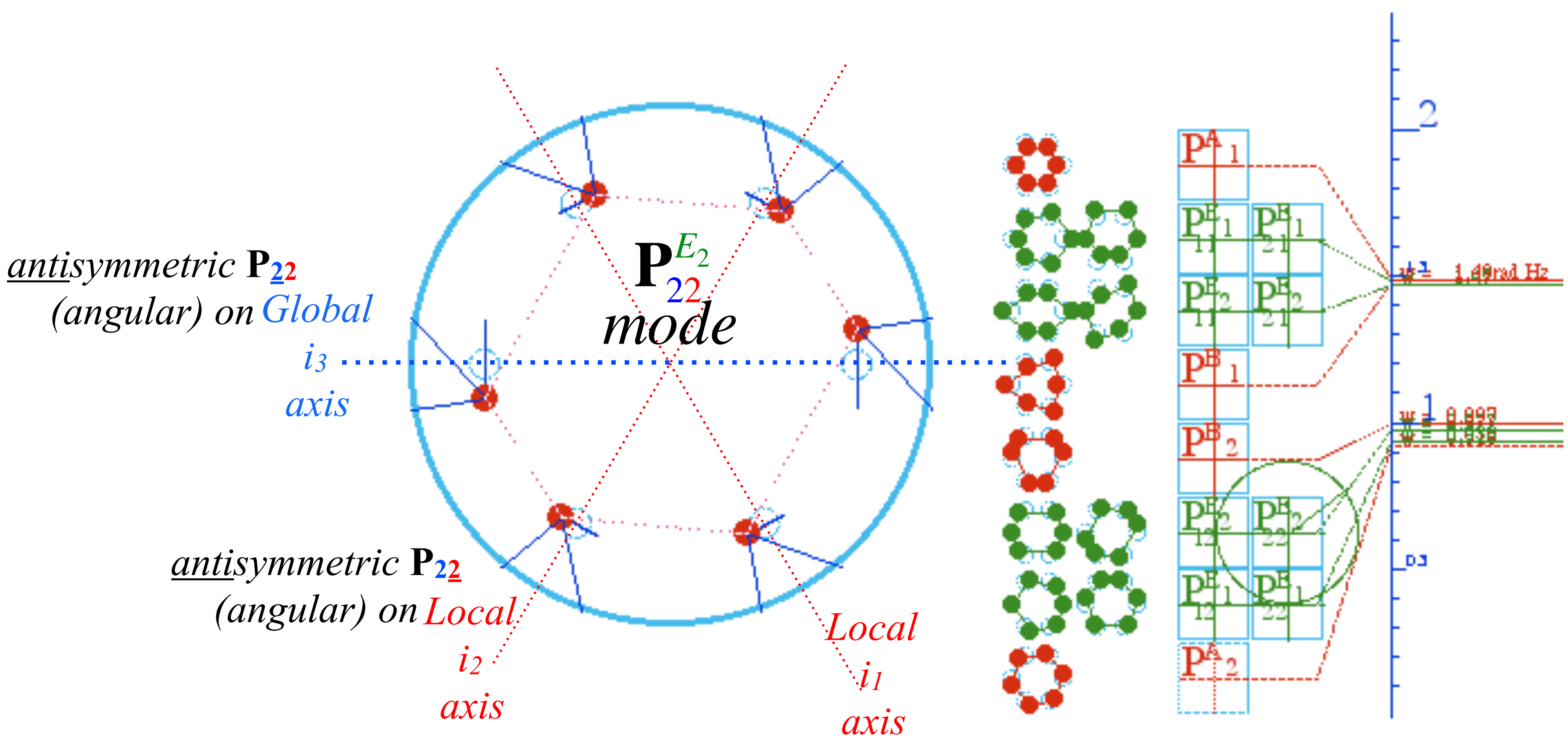
$0_2 \uparrow D_3 \sim A_1 \oplus E_1 \oplus E_2 \oplus B_1$

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

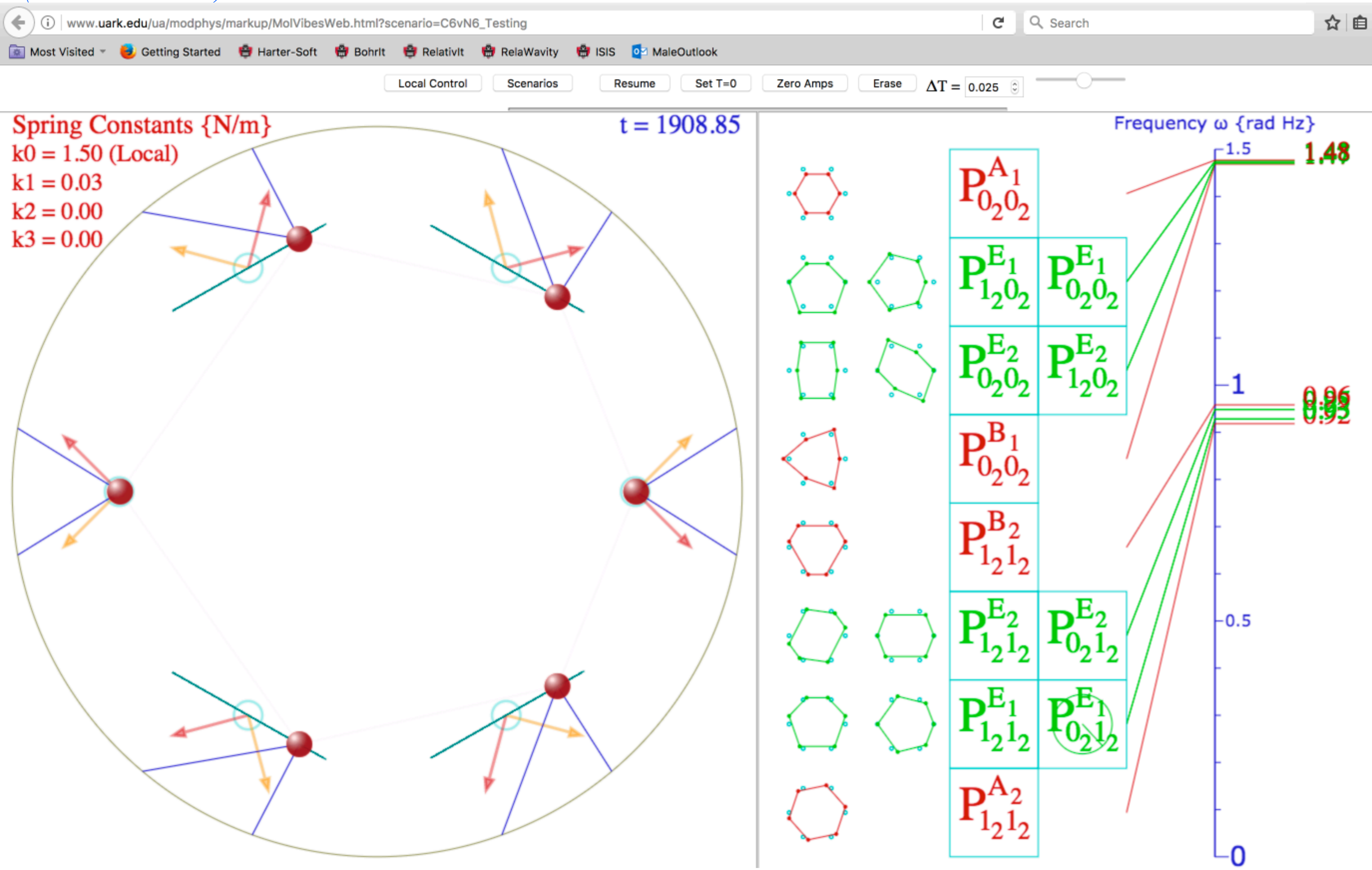
D_6 Band structure and related induced representations (Mac OS-9)

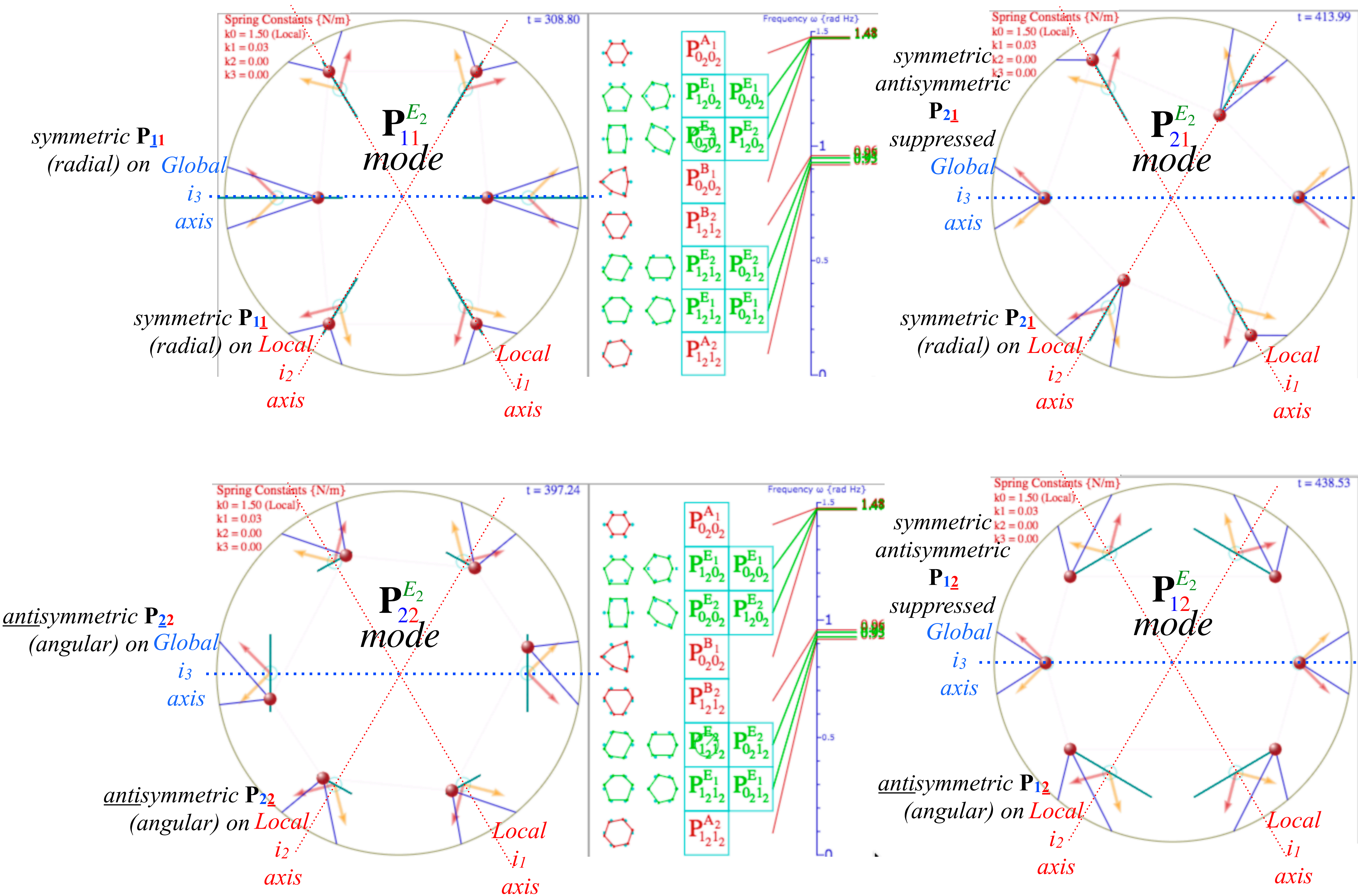




D_6 *Band structure and related induced representations (Web MolVibes)*

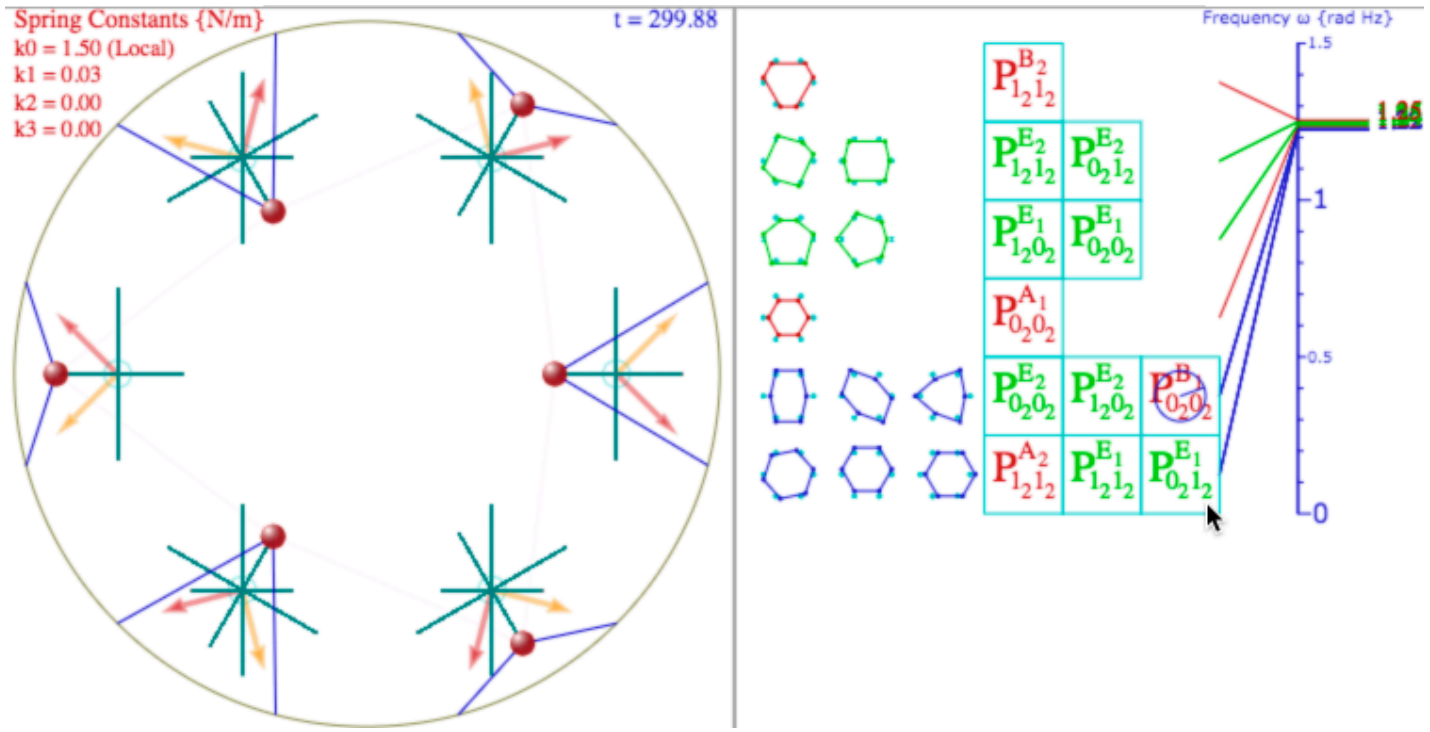
The testing config:
http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html?scenario=C6vN6_Testing



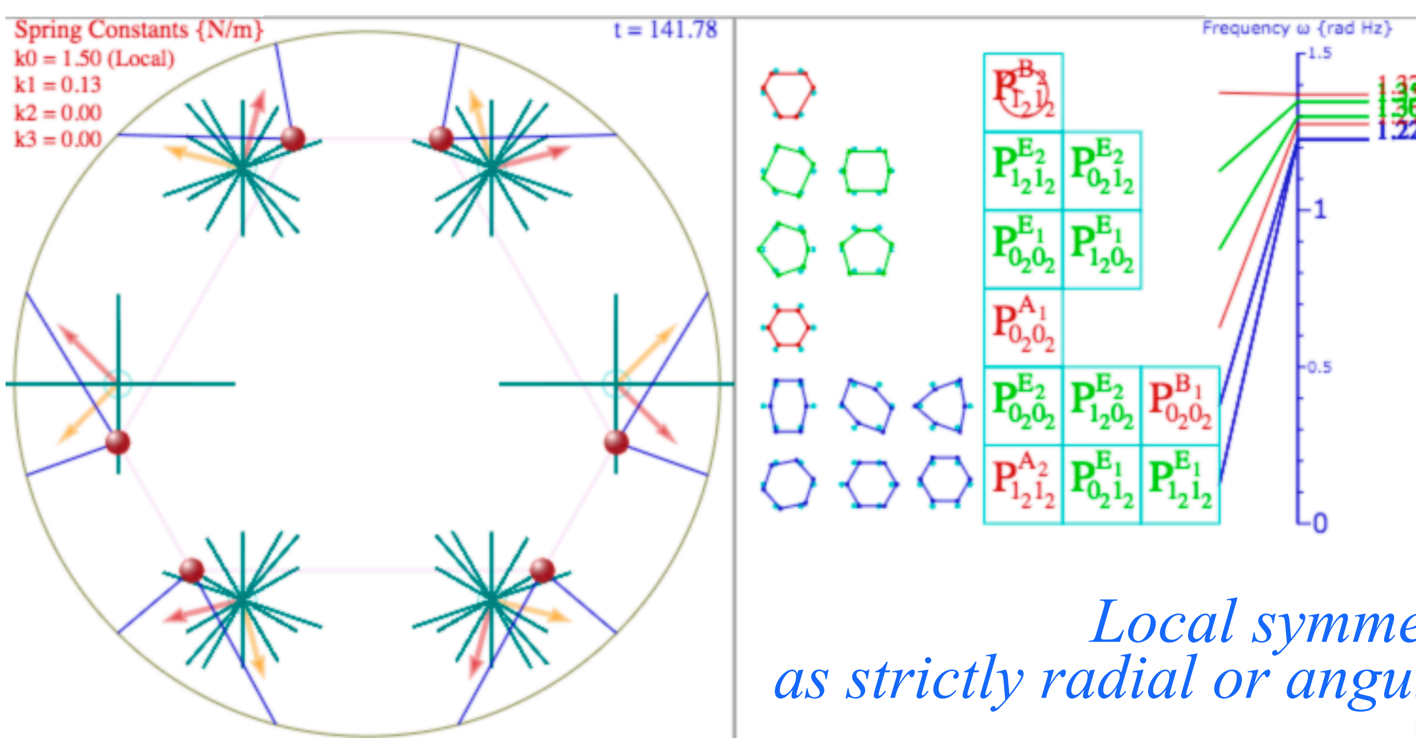


Spring Constants (N/m)
k0 = 1.50 (Local)
k1 = 0.03
k2 = 0.00
k3 = 0.00
t = 308.80
symmetric P11 (radial) on Global i3 axis
symmetric P11 (radial) on Local i2 axis
Local i1 axis
P11 E2 mode
Frequency ω (rad Hz)
1.48
0.96
0.93
symmetric antisymmetric P21 suppressed Global i3 axis
P21 E2 mode
t = 413.99
symmetric P21 (radial) on Local i2 axis
Local i1 axis
t = 397.24
antisymmetric P22 (angular) on Global i3 axis
P22 E2 mode
antisymmetric P22 (angular) on Local i2 axis
Local i1 axis
t = 438.53
symmetric antisymmetric P12 suppressed Global i3 axis
P12 E2 mode
antisymmetric P12 (angular) on Local i2 axis
Local i1 axis

U(12)-Supersymmetry: When D_6 Band structure approaches single 12-fold degeneracy
Setting mutually orthogonal external k_0 connection springs (and tiny k_1, k_2,.. coupling)



Even moderate k_1 coupling lifts a band of single-doublet-doublet-singlet above 6-fold degenerate sextet



Local symmetry-asymmetry is well broken
as strictly radial or angular paths are avoided by masses off x-axis