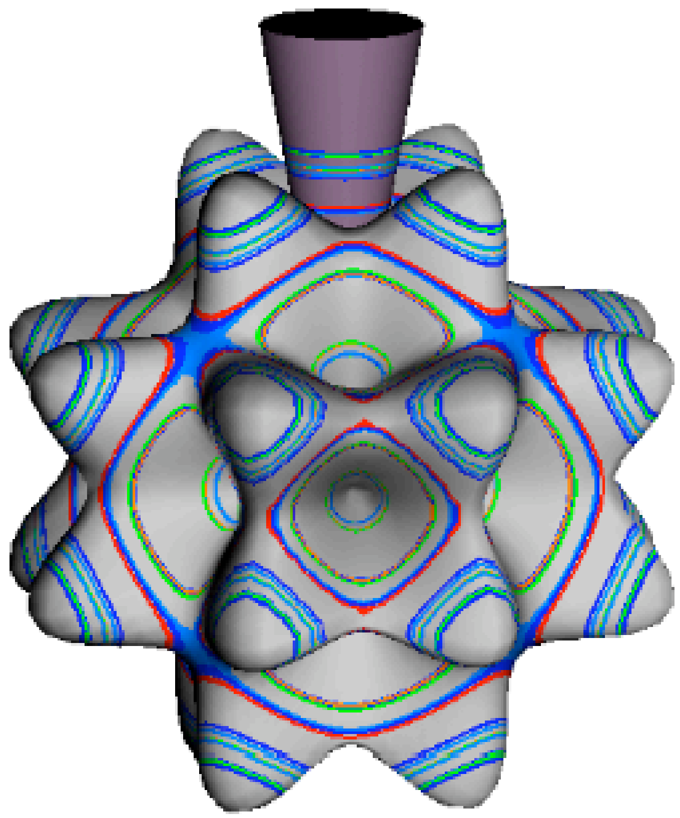
ROVIBRONIC ENERGY TOPOGRAPHY

local symmetry

II: Molecular ~~internal momentum~~ effects and multi-RES resonance in high symmetry molecules.



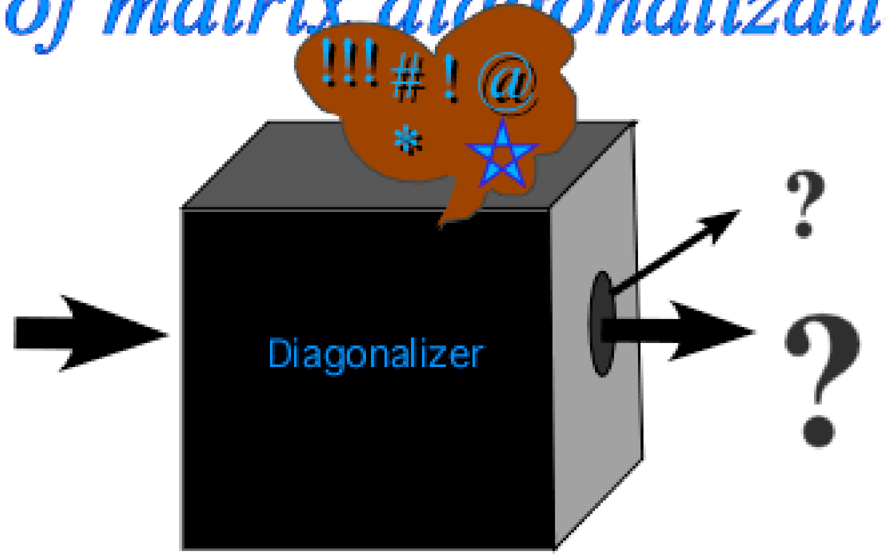
Bill Harter , Justin Mitchell - University of Arkansas

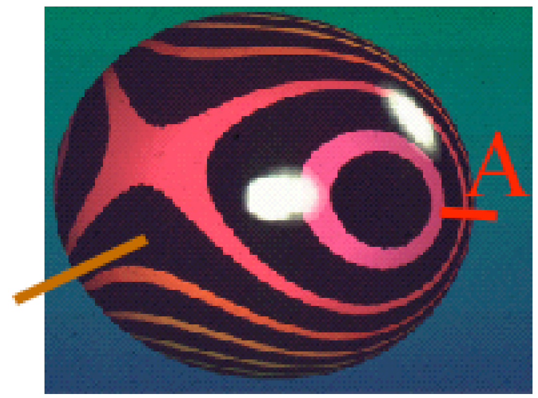
HARTER- *Soft*

Elegant Educational Tools Since 2001

Making sense of matrix diagonalization **BLACK BOX** *:*

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$





Express **H** *in terms that make <u>algebraic/geometric sense</u>*

- *Intro: Symmetry analysis is Fourier analysis on steroids*

  Going back to our (nth) roots (of unity: $\sqrt[n]{1}=e^{i2\pi m/n}$) *(C_6 example)*

- *Brand new approach to symmetry* *(Conway, Burgiel, Goodman-Strauss, May (2008))*

  A "group-theory-on-steroids" uses "local" symmetry effectively

- *Local vs Global symmetry analysis of quantum waves*

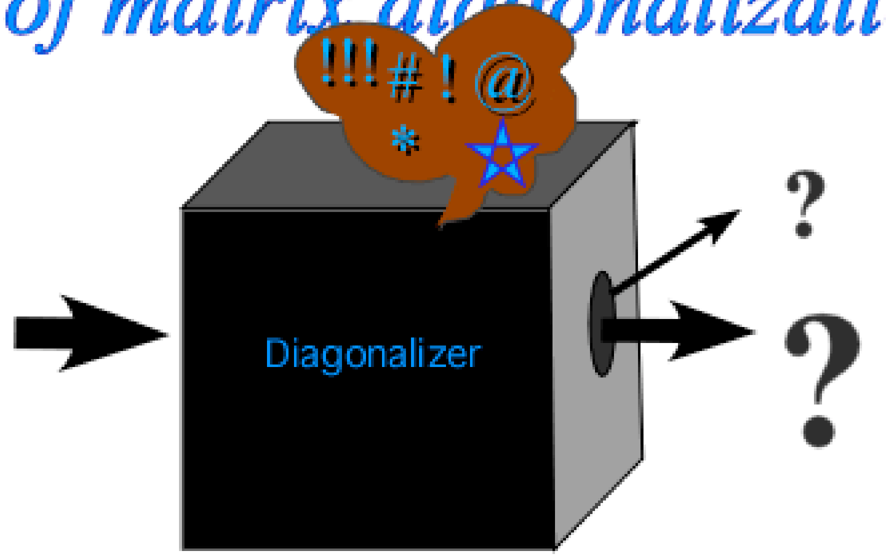
  How "group-theory-on-steroids" grows twice as big (and powerful) *(D_3 example)*

- *Local vs Global symmetry in rovibronic phase space*

  How group operators analyze rovibronic tunneling effects at high J. *(SF_6 examples)*

Making sense of matrix diagonalization **BLACK BOX** :

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



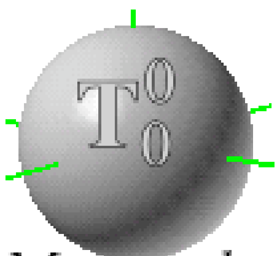
Express **H** *in terms that make algebraic/geometric sense*

Plotting 2^k-pole expansion of $\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$ *into Fano-Racah tensors*

scalar+ *+ vector+* *+ 2^2-tensor +...* *+ 2^k-tensor +..*

$$\mathbf{H}= a\mathbf{T}^0_0 + b\mathbf{T}^1_0 + c\mathbf{T}^1_1 + \ldots + d\mathbf{T}^2_0 + e\mathbf{T}^2_1 + \ldots = \Sigma c^k_q \mathbf{T}^k_q$$

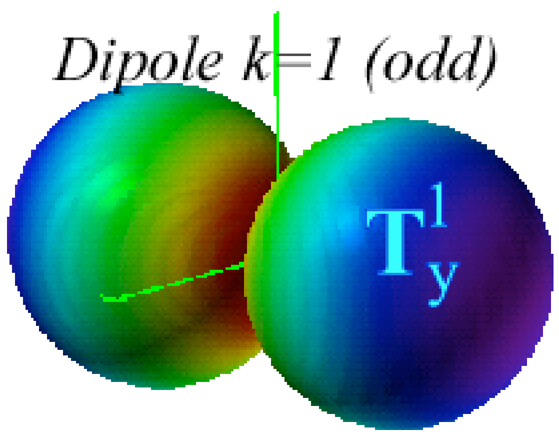
Generators of group U(n)



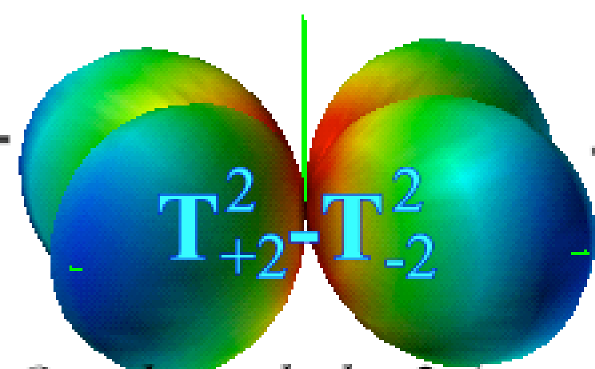
Monopole k=0 (even)

+

Dipole k=1 (odd)

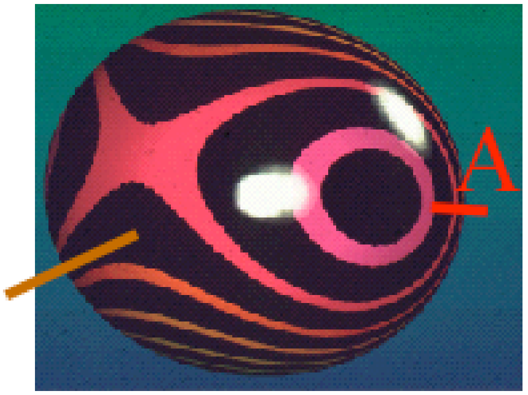


+



Quadrupole k=2 (even)

+... =



Expansion of C_n symmetric $\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \end{pmatrix}$ *by C_n operator powers* $\mathbf{r}^n$

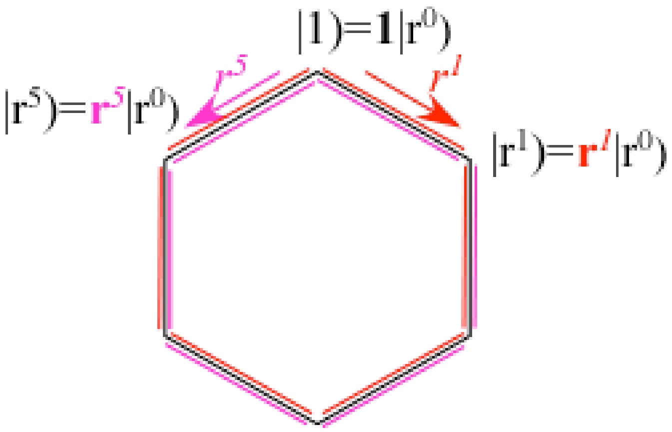
$$\mathbf{H}= r_0\mathbf{r}^0+ r_1\mathbf{r}^1+ r_2\mathbf{r}^2+ \ldots + r_{n-1}\mathbf{r}^{n-1}= \Sigma r_q\mathbf{r}^k$$

C_6 example:

$$\mathbf{H} \quad = r_0\mathbf{r}^0 \quad + r_1\mathbf{r}^1 \quad + r_2\mathbf{r}^2 \quad + r_3\mathbf{r}^3 \quad + r_4\mathbf{r}^4 \quad + r_5\mathbf{r}^5$$

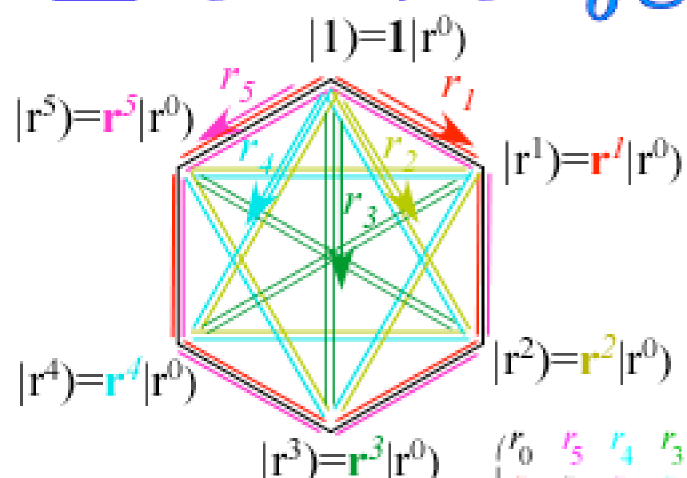
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0 \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix} + r_1 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix} + r_2 \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix} + r_3 \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix} + r_4 \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + r_5 \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Nearest neighbor coupling



$$\begin{pmatrix} r_0 & r_5 & & & & r_1 \\ r_1 & r_0 & r_5 & & & \\ & r_1 & r_0 & r_5 & & \\ & & r_1 & r_0 & r_5 & \\ & & & r_1 & r_0 & r_5 \\ r_5 & & & & r_1 & r_0 \end{pmatrix}$$

ALL neighbor coupling



$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix}$$

C_6 group-†-table gives $\mathbf{r}$*-matrices...*

...C_6-allowed $\mathbf{H}$*-matrices...*

C_6	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{1}=\mathbf{r}^0$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{r}$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
$\mathbf{r}^2$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$
$\mathbf{r}^3$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$
$\mathbf{r}^4$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$
$\mathbf{r}^5$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$

in top row flip g with $g^\dagger$

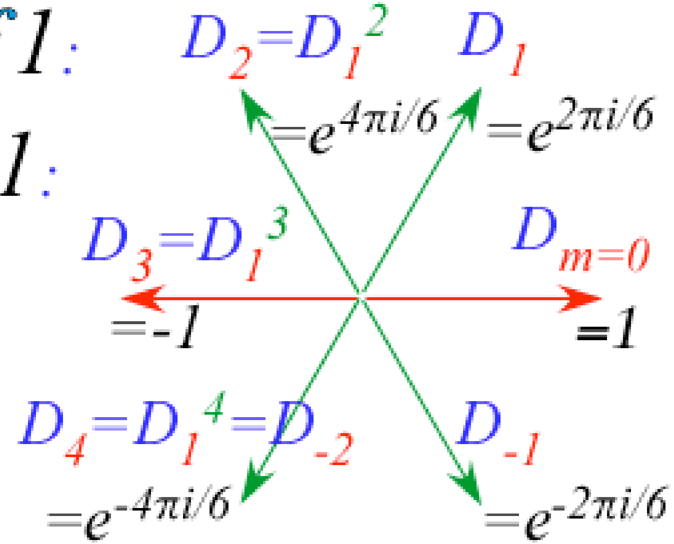
C_6 **“dagger-†-table”**

$$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$$

To diagonalize $\mathbf{H}$ *just diagonalize* $\mathbf{g} = \mathbf{r}, \mathbf{r}^2, \ldots$ *(All obey:* $\mathbf{g}^6 = \mathbf{1}$*)*

Eigenvalues $D_m^p = \psi_m^*(\mathbf{r}^p)$ ***of*** $\mathbf{r}^p$ ***are 6 th roots of 1:***

Eigenfunctions $\psi_m(\mathbf{r}^p) = D_m^{*p}$ ***of*** $\mathbf{r}^p$ ***are 6 th roots of 1:***



$$\psi_m(\mathbf{r}) = (1^m)^{1/6} = (e^{2\pi i m})^{1/6} = e^{2\pi i m/6}$$

$$\psi_m(\mathbf{r}^2) = (e^{2\pi i m/6})^2$$

$$\psi_m(\mathbf{r}^3) = (e^{2\pi i m/6})^3$$

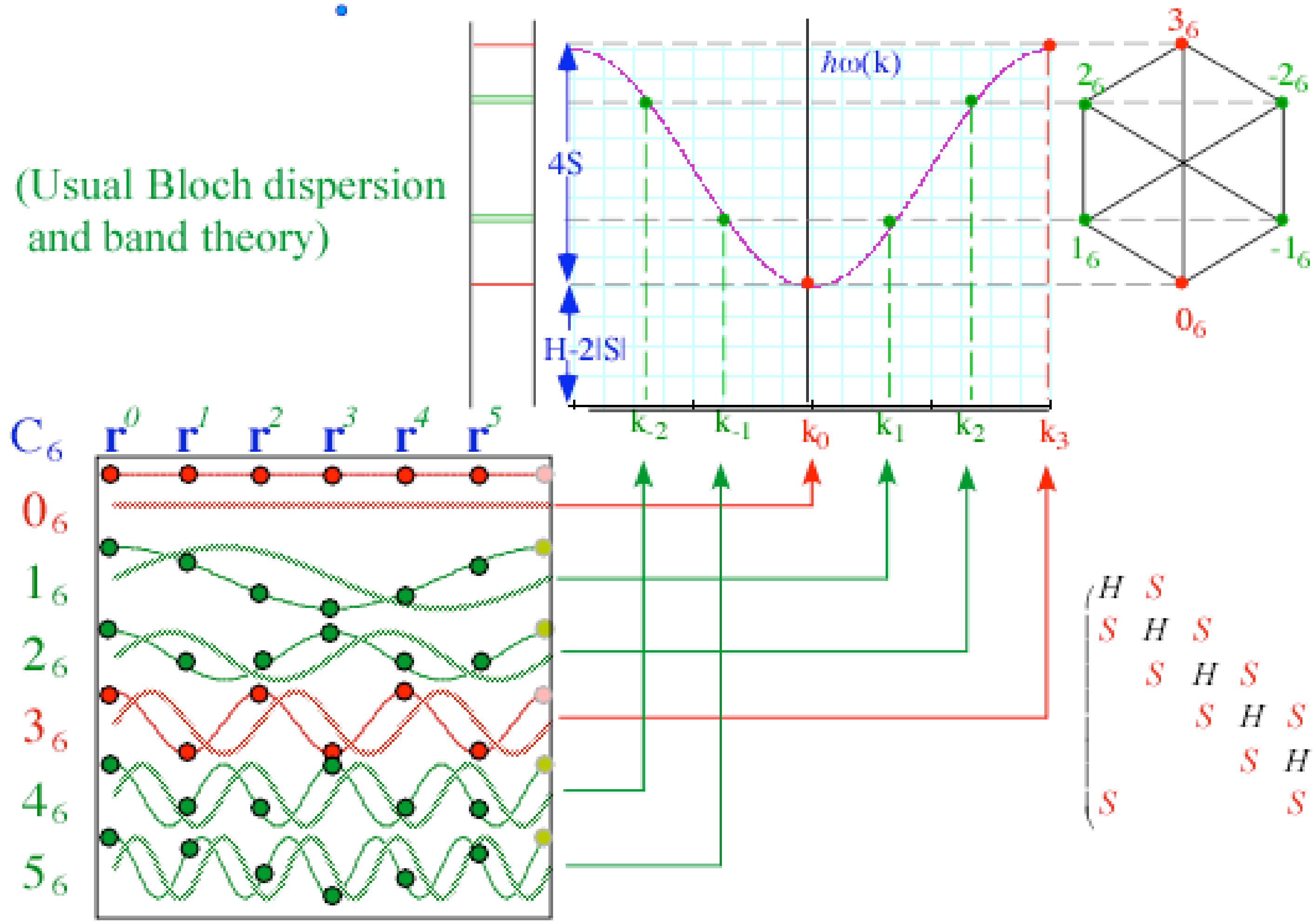
$$\vdots$$

power or position point p

$$\boxed{\psi_m(\mathbf{r}^p) = (e^{2\pi i m/6})^p = e^{2\pi i m\cdot p/6} = D_m^{*p}}$$

momentum number m

(Usual Bloch dispersion and band theory)



$$\begin{pmatrix} H & S & & & & S \\ S & H & S & & & \\ & S & H & S & & \\ & & S & H & S & \\ & & & S & H & S \\ S & & & & S & H \end{pmatrix}$$

Key Idea

C_N ***"roots"*** $D_m^p = e^{-2\pi i m\cdot p/N}$ ***are***
everything!

trans-matrix elements
eigenvectors
eigenvalues...
...

$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$

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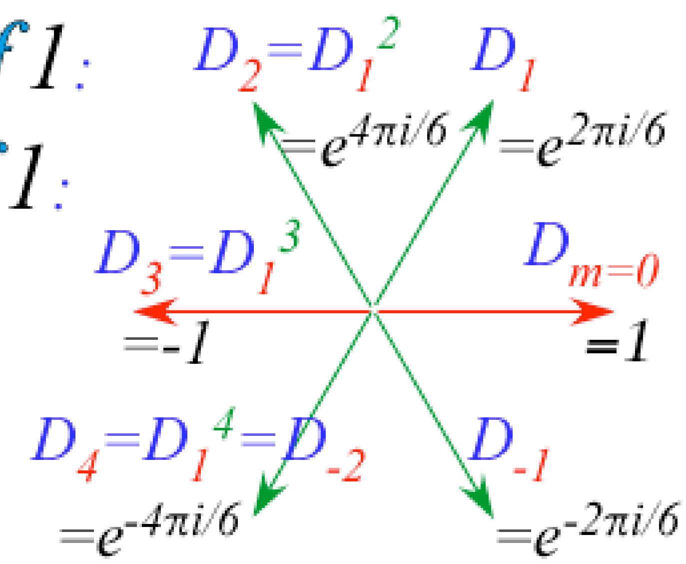

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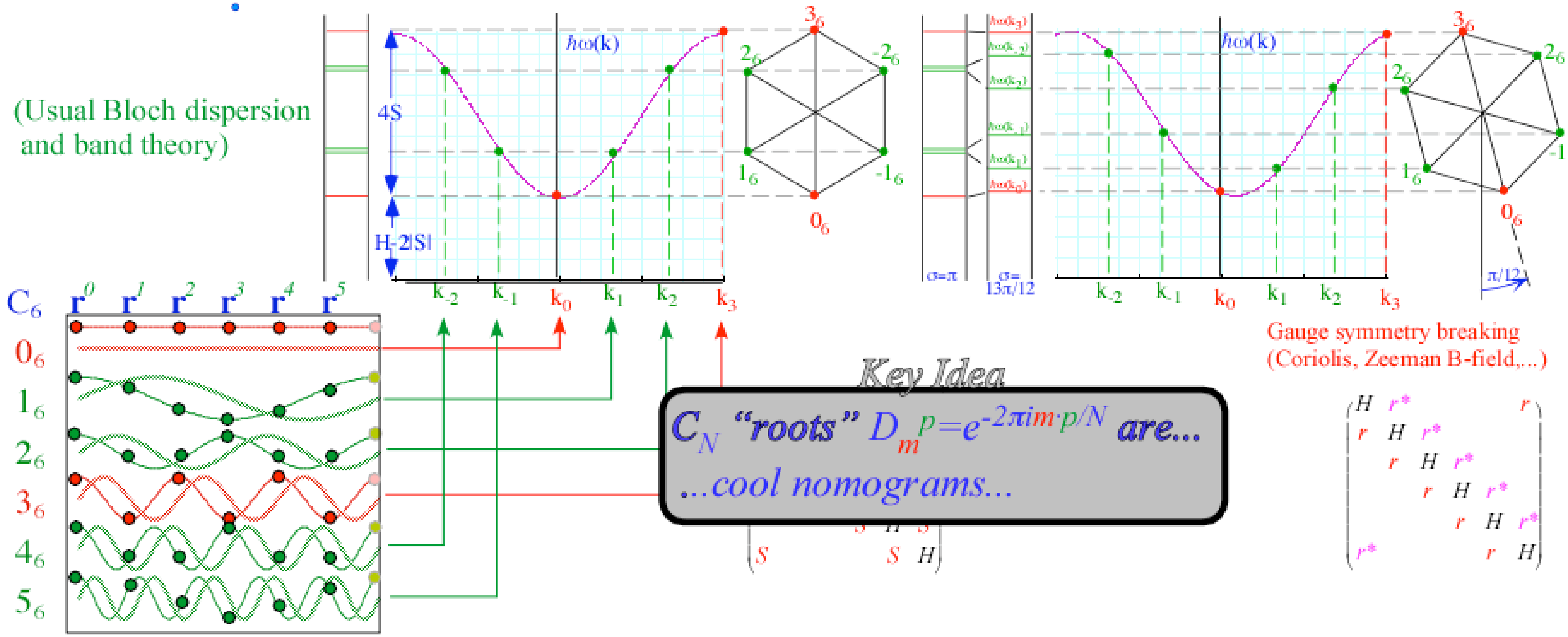


Gauge symmetry breaking (Coriolis, Zeeman B-field,...)

Key Idea

C_N ***"roots"*** $D_m^p = e^{-2\pi i m \cdot p/N}$ ***are...***

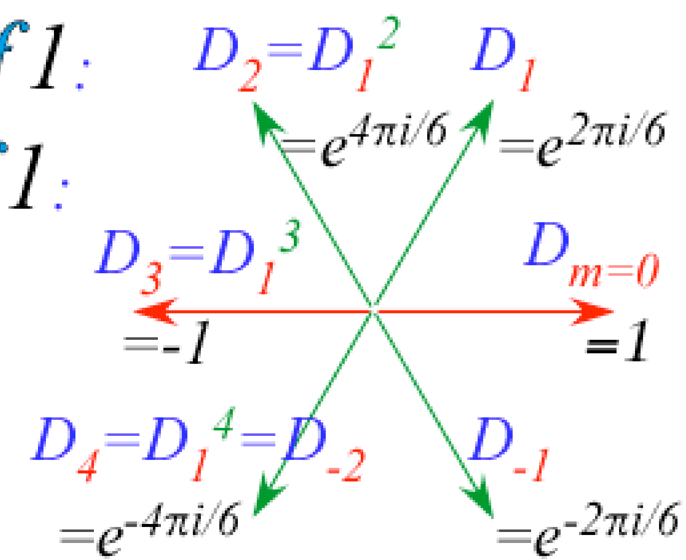
...cool nomograms...

$\mathbf{H} = r_0\mathbf{r}^0 + r_1\mathbf{r}^1 + r_2\mathbf{r}^2 + r_3\mathbf{r}^3 + r_4\mathbf{r}^4 + r_5\mathbf{r}^5$

To diagonalize $\mathbf{H}$ *just diagonalize* $\mathbf{g} = \mathbf{r}, \mathbf{r}^2, \ldots$ *(All obey:* $\mathbf{g}^6 = 1$*)*

Eigenvalues $D_m^{\ p} = \psi_m^*(\mathbf{r}^p)$ ***of*** $\mathbf{r}^p$ ***are*** 6^{th} ***roots of*** 1:

Eigenfunctions $\psi_m(\mathbf{r}^p) = D_m^{*p}$ ***of*** $\mathbf{r}^p$ ***are*** 6^{th} ***roots of*** 1:



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$$\psi_m(\mathbf{r}^3) = (e^{2\pi i m/6})^3$$

$$\vdots$$

power or position point p

$$\boxed{\psi_m(\mathbf{r}^p) = (e^{2\pi i m/6})^p = e^{2\pi i m\cdot p/6} = D_m^{*p}} = (p|m) = (m|p)^*$$

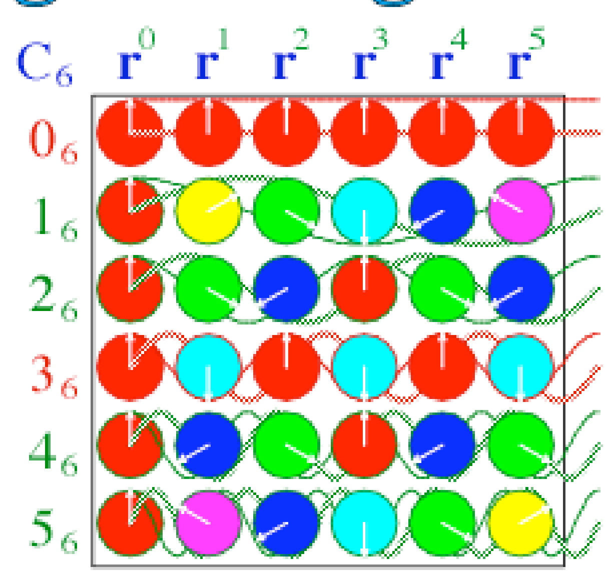
momentum number m

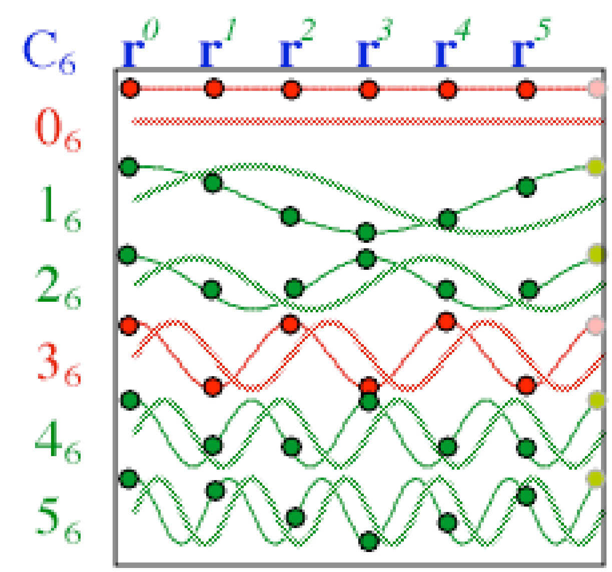
Key Idea

C_N ***"roots"*** $D_m^{\ p} = e^{-2\pi i m\cdot p/N}$ ***are...***
..character tables...

$D_m^{\ p} = \psi_m^*(\mathbf{r}^p)$ ***give Fourier diagonalizing transform matrix***

$\rho_m^{p*} = \psi_m^p$	$\mathbf{r}^0$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{r}^3$	$\mathbf{r}^4$	$\mathbf{r}^5$
m=(0)	1	1	1	1	1	1
(1)	1	ψ_1	$(\psi_1)^2$	$(\psi_1)^3$	$(\psi_1)^4$	$(\psi_1)^5$
(2)	1	ψ_2	$(\psi_2)^2$	$(\psi_2)^3$	$(\psi_2)^4$	$(\psi_2)^5$
(3)	1	ψ_3	$(\psi_3)^2$	$(\psi_3)^3$	$(\psi_3)^4$	$(\psi_3)^5$
(4)	1	ψ_4	$(\psi_4)^2$	$(\psi_4)^3$	$(\psi_4)^4$	$(\psi_4)^5$
(5)	1	ψ_5	$(\psi_5)^2$	$(\psi_5)^3$	$(\psi_5)^4$	$(\psi_5)^5$





H diagonalized by spectral resolution of r, $r^2, \ldots, r^6 = 1$

$$(\mathbf{r})^p = D_0^p \mathbf{P}^{(0)} + D_1^p \mathbf{P}^{(1)} + D_2^p \mathbf{P}^{(2)} + D_3^p \mathbf{P}^{(3)} + D_4^p \mathbf{P}^{(4)} + D_5^p \mathbf{P}^{(5)}$$

$$\begin{pmatrix} D_0^p & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & D_1^p & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & D_2^p & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & D_3^p & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & D_4^p & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & D_5^p \end{pmatrix} = D_0^p \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D_1^p \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D_2^p \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D_3^p \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D_4^p \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + D_5^p \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

Inverse C_6 spectral resolution by $\psi_m{}^p = D_m{}^{p*} = e^{-2\pi i m \cdot p/6}$:

$$\mathbf{P}^{(m)} = \psi_m{}^0 \mathbf{r}^0 + \psi_m{}^1 \mathbf{r}^1 + \psi_m{}^2 \mathbf{r}^2 + \psi_m{}^3 \mathbf{r}^3 + \psi_m{}^4 \mathbf{r}^4 + \psi_m{}^5 \mathbf{r}^5$$

...gives "Placeholder" Projectors $\mathbf{P}^{(m)}$ and "crushed" group table

top-row flip g with $g^\dagger$

C_6	1	r^5	r^4	r^3	r^2	r
$1=r^0$	1	r^5	r^4	r^3	r^2	r
$r=r^1$	r	1	r^5	r^4	r^3	r^2
r^2	r^2	r	1	r^5	r^4	r^3
r^3	r^3	r^2	r	1	r^5	r^4
r^4	r^4	r^3	r^2	r	1	r^5
r^5	r^5	r^4	r^3	r^2	r	1

($\mathbf{r}$'s go *everywhere*!)

"crunch!"

$$\mathbf{P}^{(m)}\mathbf{P}^{(n)} = \delta^{mn}\,\mathbf{P}^{(m)} = \mathbf{P}^{(n)}\mathbf{P}^{(m)}$$

Key Idea

$D_m{}^p = e^{-2\pi i m \cdot p/N}$ *placement* or "*book-keeping*" of *processes* is crucial to understanding QM.

$..P_m = |m)(m|$ - projectors ...

C_6 ring	$\mathbf{P}^{(0)}$	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$	$\mathbf{P}^{(4)}$	$\mathbf{P}^{(5)}$
$\mathbf{P}^{(0)}$	$\mathbf{P}^{(0)}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\mathbf{P}^{(1)}$	$\cdot$	$\mathbf{P}^{(1)}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$
$\mathbf{P}^{(2)}$	$\cdot$	$\cdot$	$\mathbf{P}^{(2)}$	$\cdot$	$\cdot$	$\cdot$
$\mathbf{P}^{(3)}$	$\cdot$	$\cdot$	$\cdot$	$\mathbf{P}^{(3)}$	$\cdot$	$\cdot$
$\mathbf{P}^{(4)}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\mathbf{P}^{(4)}$	$\cdot$
$\mathbf{P}^{(5)}$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\mathbf{P}^{(5)}$

($\mathbf{P}$'s go *NOwhere*!)

top-row flip not needed...

$$\mathbf{P}^{(m)} = \mathbf{P}^{(m)\dagger}$$

GOOD News

H diagonalized by $\mathbf{r}^p$ *symmetry operators that COMMUTE*
with H ($\mathbf{r}^p H = H\,\mathbf{r}^p$),
and with each other ($\mathbf{r}^p\mathbf{r}^q = \mathbf{r}^{p+q} = \mathbf{r}^q\mathbf{r}^p$). (called ABELIAN symmetry)

BAD News

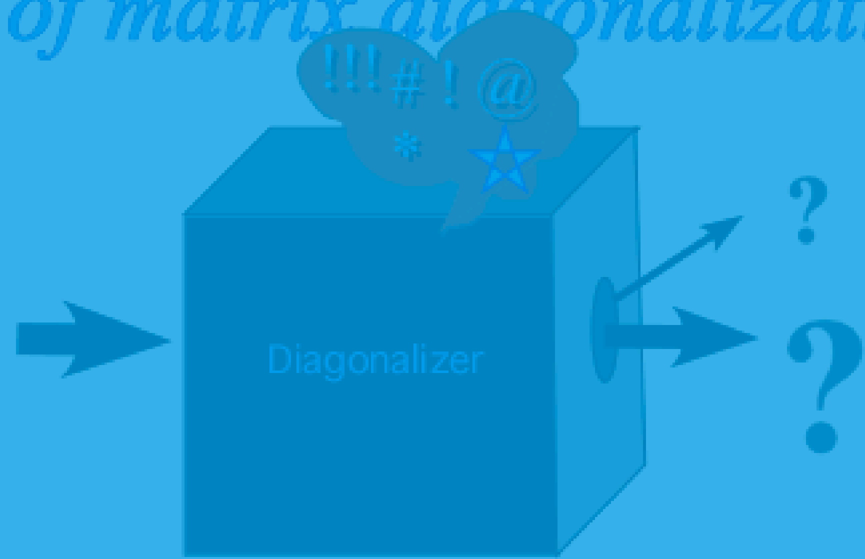
While all H symmetry operations COMMUTE
with H ($\mathbf{U}\,H = H\,\mathbf{U}$)
most do not with each other ($\mathbf{U}\,\mathbf{V} \neq \mathbf{V}\mathbf{U}$). (called NON-ABELIAN symmetry)

Key Idea

Time to change..
...how we classify symmetry
...how we apply it ...

Making sense of matrix diagonalization **BLACK BOX** :

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



Express **H** *in terms that make algebraic/geometric sense*

• *Intro: Symmetry analysis is Fourier analysis on steroids*

Going back to our (nth) roots (of unity: $\sqrt[n]{1}=e^{i2\pi m/n}$ *)* *(C_6 example)*

• *Brand new approach to symmetry* *(Conway, Burgiel, Goodman-Strauss, May (2008))*

A "group-theory-on-steroids" uses "local" symmetry effectively

..and a not quite so new approach...

• *Local vs Global symmetry analysis of quantum waves*

How "group-theory-on-steroids" grows twice as big (and powerful) *(D_3 example)*

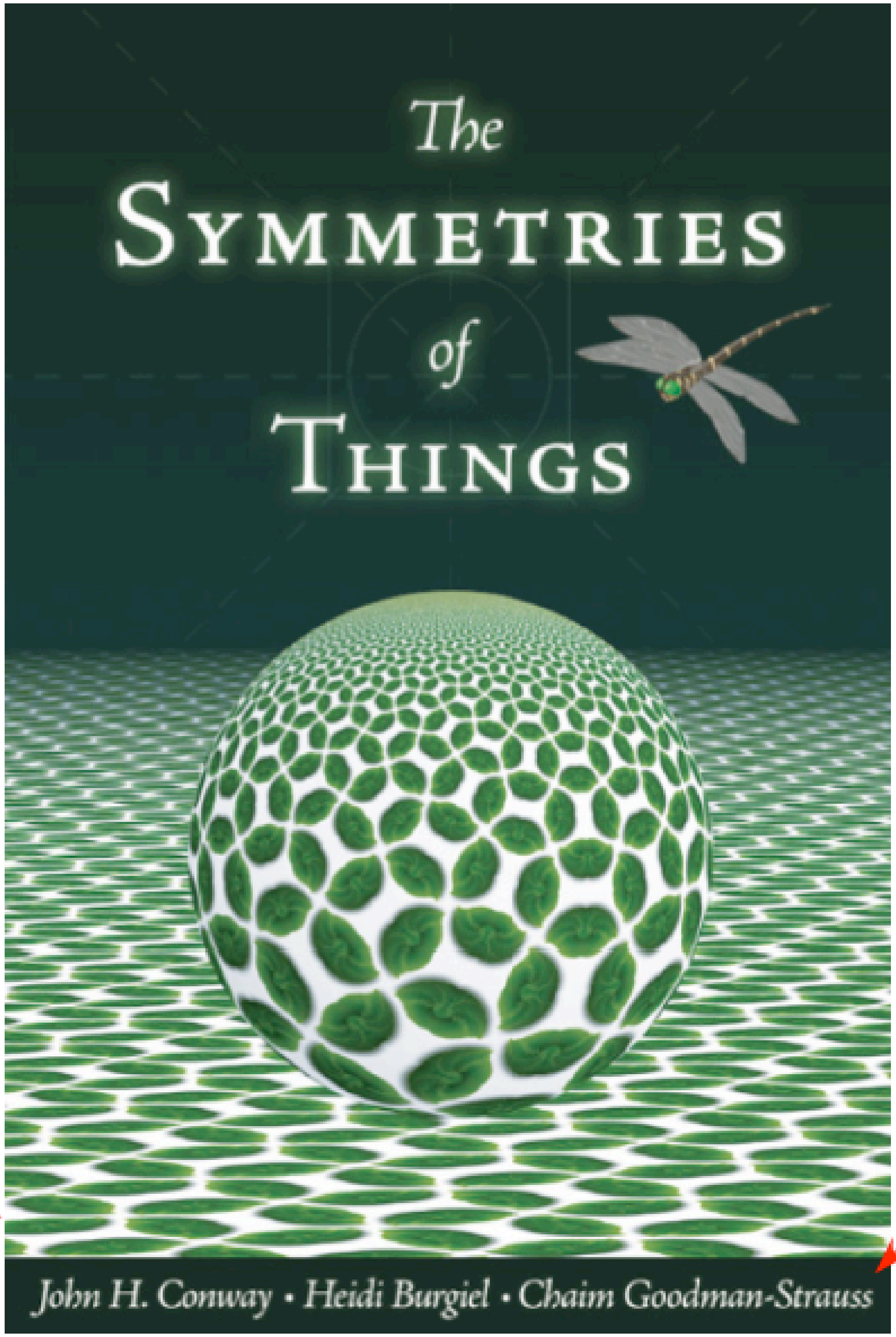
We interrupt this program to bring an important announcement
from the makers of
PURE and APPLIED group theory...

(drum-roll, Please...)

...from PURE group theory...

A revolutionary simplification to classify all groups and their algebras

A "kaleidoscopic" approach that uses an "intrinsic" group



May be useful for space-group models of floppy molecules by P. Groner and S. Altman

A.K. Peters Ltd.
Wellesley, MA
02482

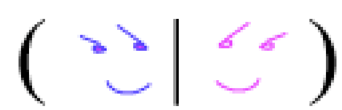
Disclosure 1:
Chaim Goodman-Strauss is a colleague at University of Arkansas (He's in math across the street.)

...from APPLIED group theory...

Group theory of wave mechanics is twice as big as you might think...

...due to RELATIVITY-DUALITY...

"It takes two to tango!"



(bra-ket)

...from APPLIED group theory...

Group theory of wave mechanics is twice as big as you might think...

APPLIED RELATIVITY-DUALITY THEOREM:

For each *external* group $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ there is an *internal* group $\{..\bar{\mathbf{T}},\bar{\mathbf{U}},\bar{\mathbf{V}},...\}$

satisfing *duality:*

$\mathbf{T}|1)=|T)=\bar{\mathbf{T}}^{-1}|1)$,

$\mathbf{U}|1)=|U)=\bar{\mathbf{U}}^{-1}|1)$,

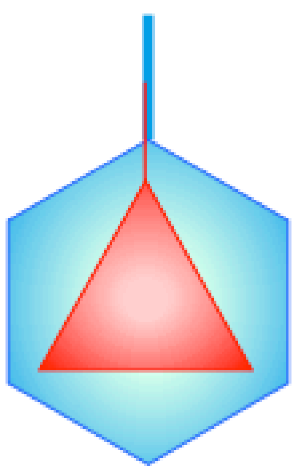
etc.,

and *commutivity:*

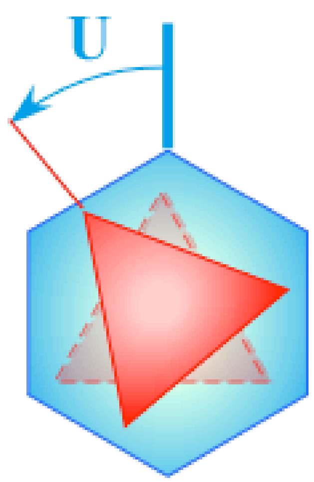
$\mathbf{T}\bar{\mathbf{U}}=\bar{\mathbf{T}}\mathbf{U}$, $\mathbf{T}\bar{\mathbf{V}}=\bar{\mathbf{V}}\mathbf{U}$,..

$\mathbf{U}\bar{\mathbf{V}}=\bar{\mathbf{V}}\mathbf{U}$, ..*etc.*,

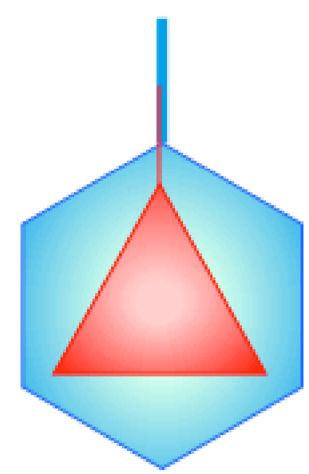
$|1)$



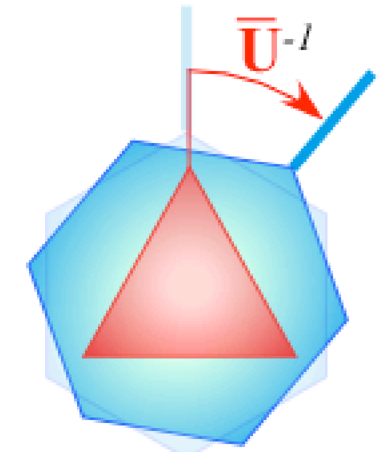
$|U)=\mathbf{U}|1)$



$|1)$



$|U)=\bar{\mathbf{U}}^{-1}|1)$



$|1)$ moved by $\mathbf{U}$ to $\mathbf{U}|1)$ yields same *relative* position $|U)$ as $|1)$ moved by $\bar{\mathbf{U}}^{-1}$ to $\bar{\mathbf{U}}^{-1}|1)$

...and wave interference depends on *relative* position only.

Key Idea

Think of global and local as
independent waves for which
only relative position is relevant.

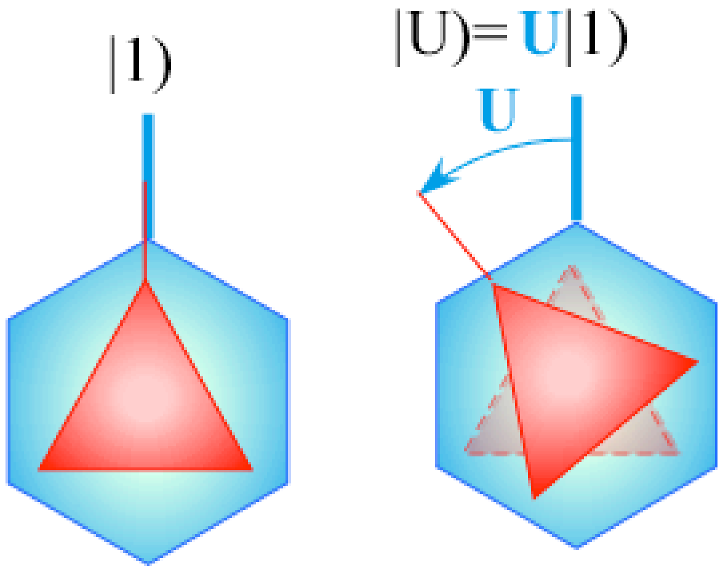
"It's all relative!"

...from APPLIED group theory...

Group theory of wave mechanics is twice as big as you might think...

APPLIED RELATIVITY-DUALITY THEOREM:

For each *external* group $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ there is an *internal* group $\{..\bar{\mathbf{T}},\bar{\mathbf{U}},\bar{\mathbf{V}},...\}$



satisfing *duality:*

$\mathbf{T}|1)=|T)=\bar{\mathbf{T}}^{-1}|1)$,

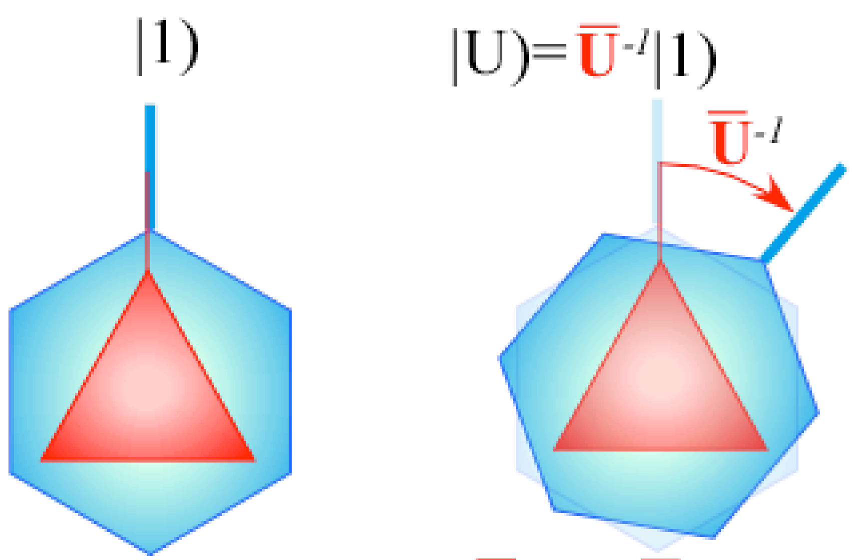
$\mathbf{U}|1)=|U)=\bar{\mathbf{U}}^{-1}|1)$,

etc.,

and *commutivity:*

$\mathbf{T}\bar{\mathbf{U}}=\bar{\mathbf{T}}\mathbf{U}$, $\mathbf{T}\bar{\mathbf{V}}=\bar{\mathbf{V}}\mathbf{U}$,..

$\mathbf{U}\bar{\mathbf{V}}=\bar{\mathbf{V}}\mathbf{U}$, *..etc.*,



|1) moved by $\mathbf{U}$ to $\mathbf{U}$|1) yields same *relative* position |U) as |1) moved by $\bar{\mathbf{U}}^{-1}$ to $\bar{\mathbf{U}}^{-1}$|1)

...and wave interference depends on *relative* position only.

RELATIVITY-DUALITY also known as:

LAB vs *BODY* *(molecular theory)*

STATE vs *PARTICLE* *(nuclear shell theory)*

GLOBAL vs *LOCAL* *(gauge theory)*

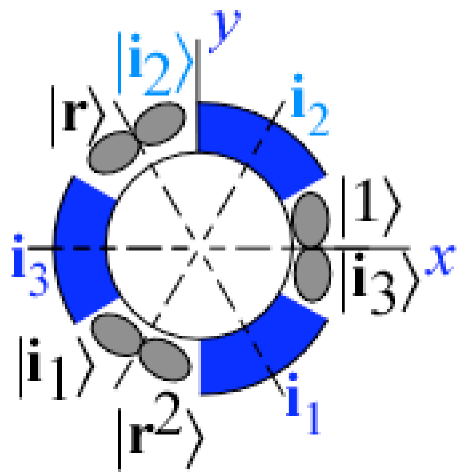
Disclosure 2:

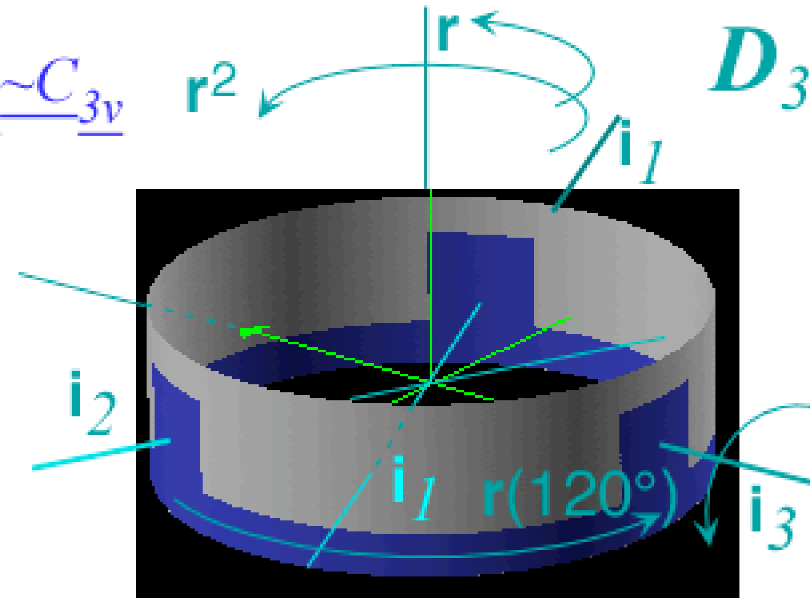
Duality issues lie somewhere between a hobby and obsession for me.

(Rev.Mod.Phys.50,37(1978), Phys.Rev.A, 24,192 (1981))

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

D_3-defined local-wave bases

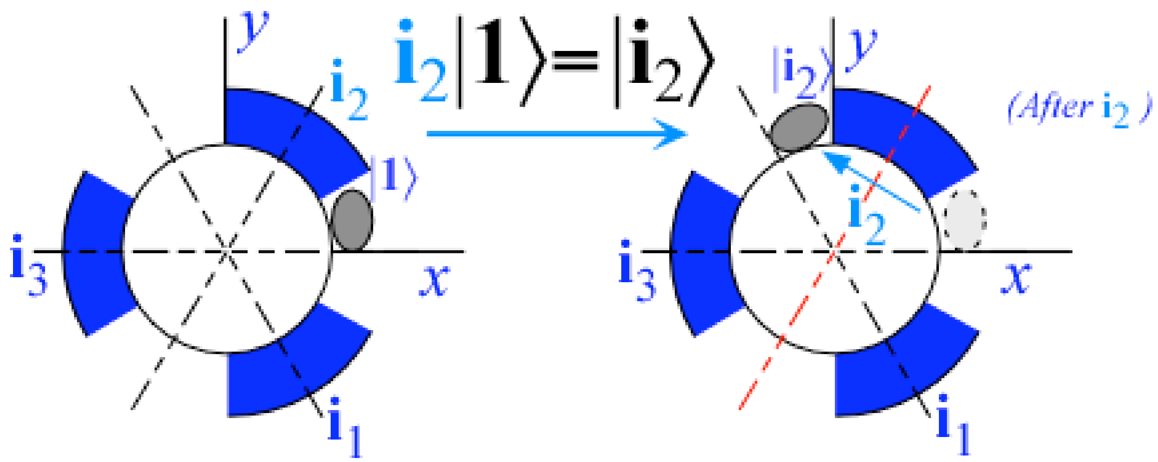




***D*$_3$**

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

Lab-fixed (Extrinsic-Global) operations and rotation axes



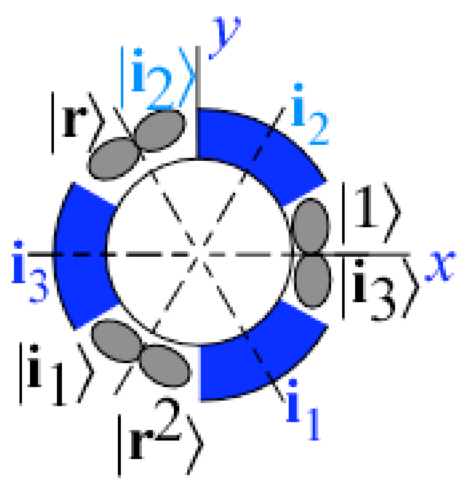
Key Idea

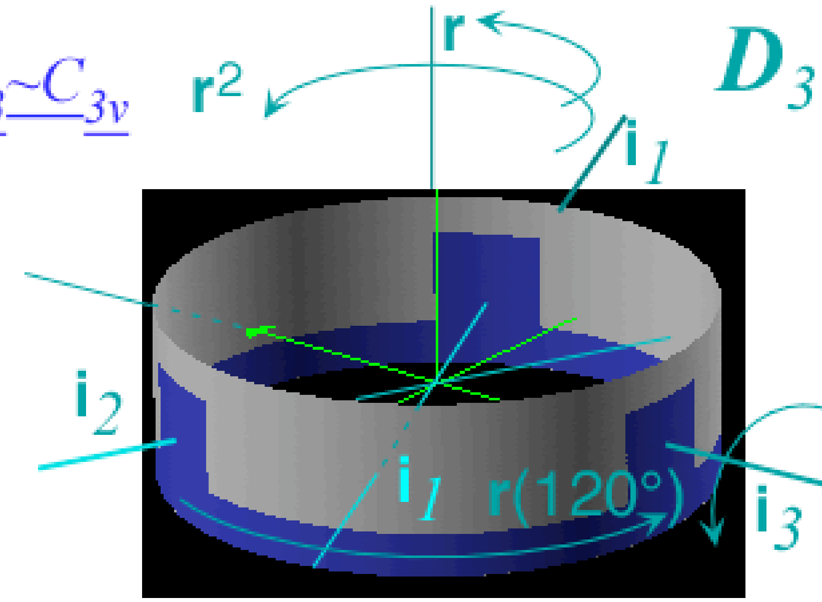
Let global group label...

...localized wave arrangements

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

D_3-defined local-wave bases



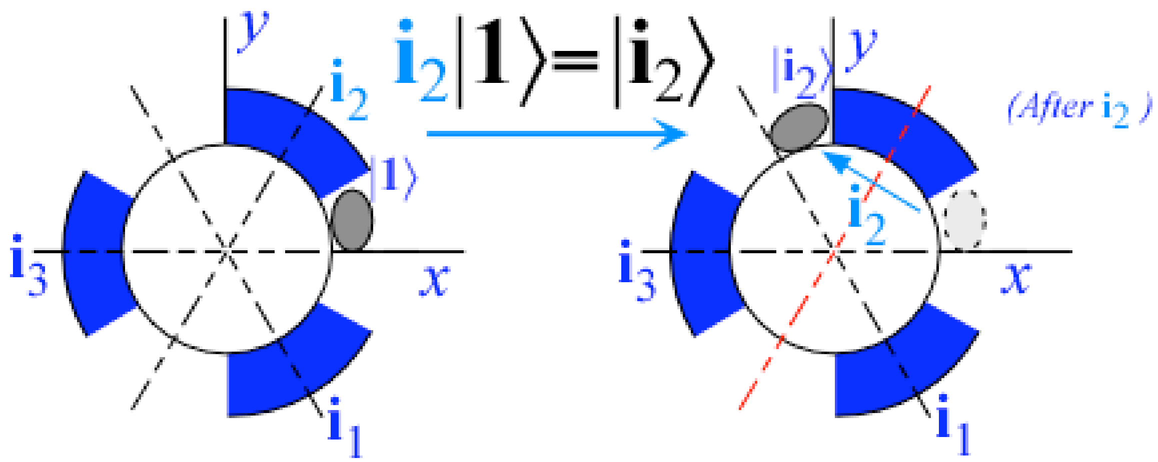


D_3

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

Lab-fixed (Extrinsic-Global) operations and rotation axes

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



Key Idea

Let global group label...

...localized wave arrangements

Let commuting local group ...

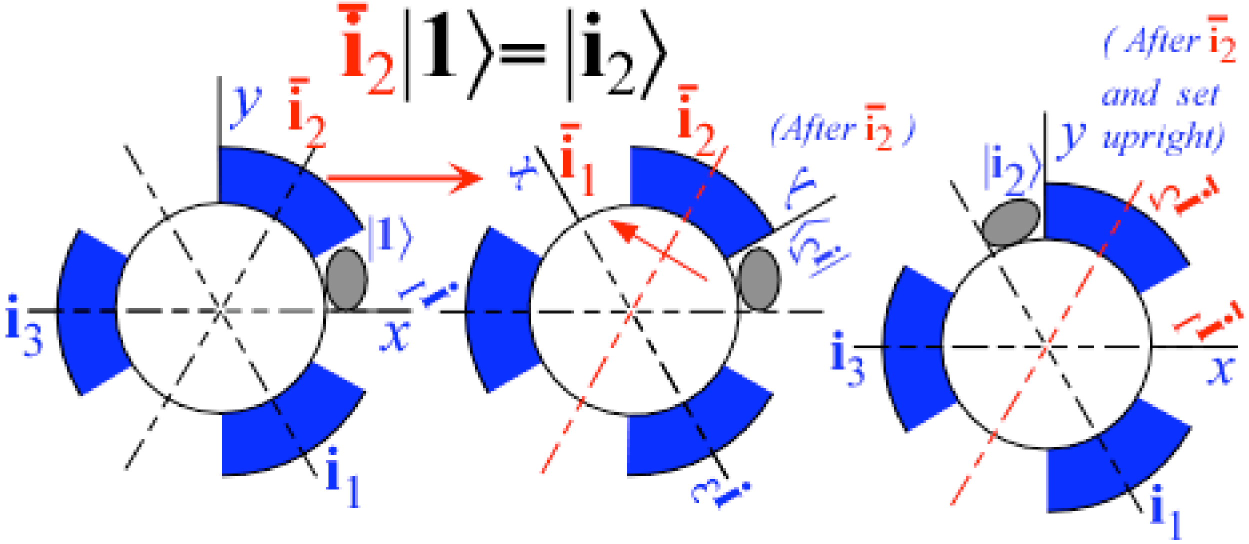
...do essentially the same...

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

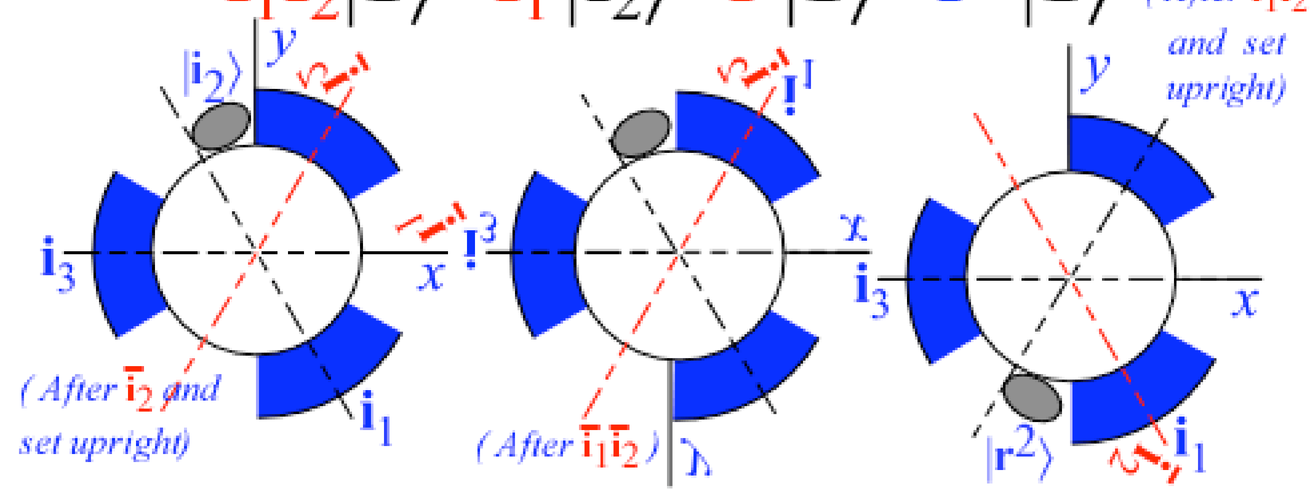
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

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

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



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



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

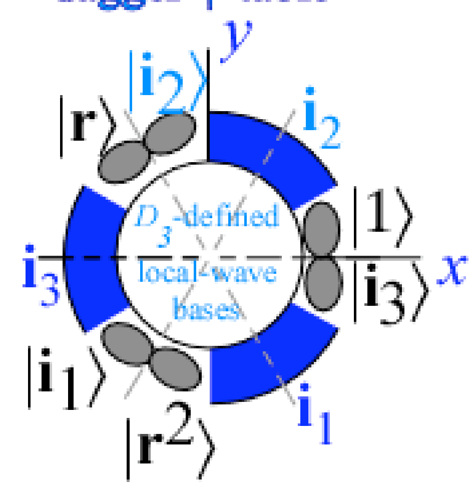
To represent *external* $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

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

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

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

D_3 global "dagger-†-table"



Key Idea (A "Placement" trick)

> ***Global group multiplication table***
> *defines global matrix operators*
> ***Local †-group multiplication table***
> *defines local matrix operators*
> ***Global and Local † commute***

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

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

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

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

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

D_3 local "dagger-†-table"

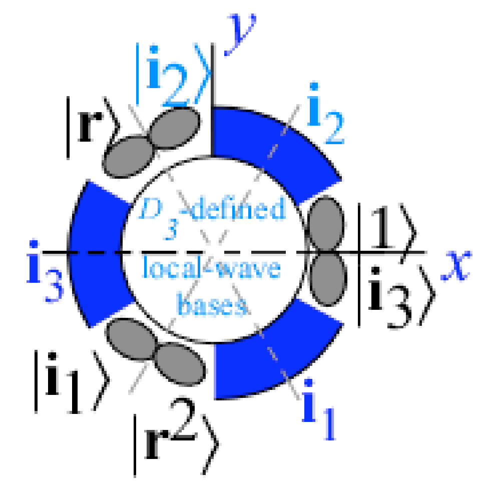
1	r	r^2	i_1	i_2	i_3
r^2	1	r	i_2	i_3	i_1
r	r^2	1	i_3	i_1	i_2
i_1	i_2	i_3	1	r	r^2
i_2	i_3	i_2	r^2	1	r
i_3	i_1	i_2	r	r^2	1

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

To represent *external* $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$ switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$

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

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



Local $\mathbb{H}$ ***matrix parametrized by*** $\mathbf{g}$***'s***

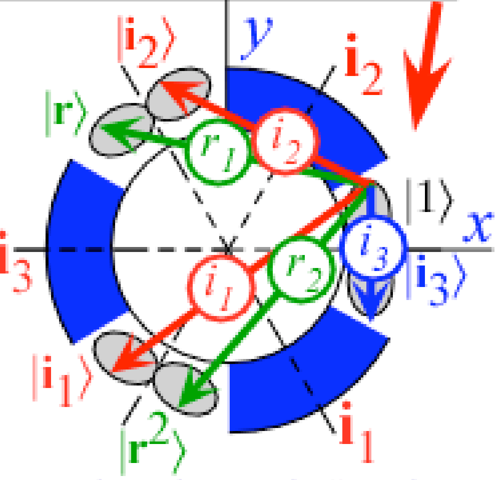
RESULT:
Any $R(\mathbf{T})$
commute
with any $R(\bar{\mathbf{U}})$...

So an $\mathbb{H}$*-matrix having* ***Global*** *symmetry* D_3

$$\mathbb{H} = H\bar{\mathbf{1}}^0 + r_1\bar{\mathbf{r}}^1 + r_2\bar{\mathbf{r}}^2 + i_1\bar{\mathbf{i}}_1 + i_2\bar{\mathbf{i}}_2 + i_3\bar{\mathbf{i}}_3$$

is made from ***Local*** *symmetry matrices*

$H = \langle 1|\mathbb{H}|1\rangle = H^*$
$r_1 = \langle \mathrm{r}|\mathbb{H}|1\rangle = r_2^*$
$r_2 = \langle \mathrm{r}^2|\mathbb{H}|1\rangle = r_1^*$
$i_1 = \langle \mathrm{i}_1|\mathbb{H}|1\rangle = i_1^*$
$i_2 = \langle \mathrm{i}_2|\mathbb{H}|1\rangle = i_2^*$
$i_3 = \langle \mathrm{i}_3|\mathbb{H}|1\rangle = i_3^*$



All these global $\mathbf{g}$ *commute with general local* $\mathbb{H}$ *matrix.*

local D_3 defined Hamiltonian matrix

$\mathbb{H}=$

	$\vert 1\rangle$	$\vert \mathrm{r}\rangle$	$\vert \mathrm{r}^2\rangle$	$\vert \mathrm{i}_1\rangle$	$\vert \mathrm{i}_2\rangle$	$\vert \mathrm{i}_3\rangle$
$\langle 1\vert$	H	r_1	r_2	i_1	i_2	i_3
$\langle \mathrm{r}\vert$	r_2	H	r_1	i_2	i_3	i_1
$\langle \mathrm{r}^2\vert$	r_1	r_2	H	i_3	i_1	i_2
$\langle \mathrm{i}_1\vert$	i_1	i_2	i_3	H	r_1	r_2
$\langle \mathrm{i}_2\vert$	i_2	i_3	i_1	r_2	H	r_1
$\langle \mathrm{i}_3\vert$	i_3	i_1	i_2	r_1	r_2	H

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

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

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

The Devil-in-the-Details part of this talk

(We've got to skip a lot here.)

Local $\mathbb{H}$ matrix made of **g***'s is spectrally reduced by resolving* **g***'s into group projectors* $\mathbf{P}^{(m)}_{eb}$.

$$\mathbf{g} = \Sigma_m \Sigma_e \Sigma_b D^{(m)}_{eb}(g)\, \mathbf{P}^{(m)}_{eb}$$

$$\mathbf{P}^{(m)} = {}_{(norm)}\Sigma_{\mathbf{g}} D^{(m)*}_{eb}(g)\, \mathbf{g}$$

The $D^{(m)}_{eb}$ are the "do-everything" numbers called the irreducible representations.

Bad-news: *There are about a gadzillion ways to do this.*

GOOD-news: *Local-symmetry sub-group chains provide road maps.*

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

external LAB *internal BOD*

symmety label-e *symmety label-b*

GLOBAL *LOCAL*

$D_3 > C_2$-local Hamiltonian in group-basis $|\mathbf{g}) = \mathbf{g}|\mathbf{1})$

$$
\mathbb{H} = \begin{array}{c|ccc|ccc|}
 & |\mathbf{1}) & |\mathbf{r}) & |\mathbf{r}^2) & |\mathbf{i}_1) & |\mathbf{i}_2) & |\mathbf{i}_3) \\ \hline
(\mathbf{1}| & H & r_1 & r_2 & i_1 & i_2 & i_3 \\ \hline
(\mathbf{r}| & r_2 & H & r_1 & i_2 & i_3 & i_1 \\
(\mathbf{r}^2| & r_1 & r_2 & H & i_3 & i_1 & i_2 \\ \hline
(\mathbf{i}_1| & i_1 & i_2 & i_3 & H & r_1 & r_2 \\
(\mathbf{i}_2| & i_2 & i_3 & i_2 & r_2 & H & r_1 \\
(\mathbf{i}_3| & i_3 & i_1 & i_2 & r_1 & r_2 & H
\end{array}
$$

$$
= H\begin{pmatrix}1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\end{pmatrix}
+ r_1\begin{pmatrix}\cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\end{pmatrix}
+ r_2\begin{pmatrix}\cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\end{pmatrix}
+ i_1\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\end{pmatrix}
+ i_2\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix}
+ i_3\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\end{pmatrix}
$$

$$
\mathbb{H} = H\,\bar{\mathbf{1}} + r_1\bar{\mathbf{r}}^1 + r_2\bar{\mathbf{r}}^2 + i_1\bar{\mathbf{i}}_1 + i_2\bar{\mathbf{i}}_2 + i_3\bar{\mathbf{i}}_3
$$

$$
= H\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&0&\cdot&\cdot\\ \cdot&\cdot&0&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&0\\ \cdot&\cdot&\cdot&\cdot&0&1\end{pmatrix}
+ r_1\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}&\cdot&\cdot\\ \cdot&\cdot&\frac{\sqrt{3}}{2}&\frac{-1}{2}&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\ \cdot&\cdot&\cdot&\cdot&\frac{\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}
+ r_2\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}&\cdot&\cdot\\ \cdot&\cdot&\frac{-\sqrt{3}}{2}&\frac{-1}{2}&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}\\ \cdot&\cdot&\cdot&\cdot&\frac{-\sqrt{3}}{2}&\frac{-1}{2}\end{pmatrix}
+ i_1\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{-1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}&\cdot&\cdot\\ \cdot&\cdot&\frac{-\sqrt{3}}{2}&\frac{1}{2}&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\frac{-1}{2}&\frac{-\sqrt{3}}{2}\\ \cdot&\cdot&\cdot&\cdot&\frac{-\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}
+ i_2\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{-1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}&\cdot&\cdot\\ \cdot&\cdot&\frac{\sqrt{3}}{2}&\frac{1}{2}&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\frac{-1}{2}&\frac{\sqrt{3}}{2}\\ \cdot&\cdot&\cdot&\cdot&\frac{\sqrt{3}}{2}&\frac{1}{2}\end{pmatrix}
+ i_3\begin{pmatrix}\boxed{1}&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\boxed{-1}&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&0&\cdot&\cdot\\ \cdot&\cdot&0&-1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&0\\ \cdot&\cdot&\cdot&\cdot&0&-1\end{pmatrix}
$$

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

A_1-block

A_2-block

E-block (appears twice)

$D_3 > C_2$-local Hamiltonian in projector-basis $\left|{}^{(m)}_{ab}\right) = \mathbf{P}^{(m)}_{ab}|\mathbf{1})$

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

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

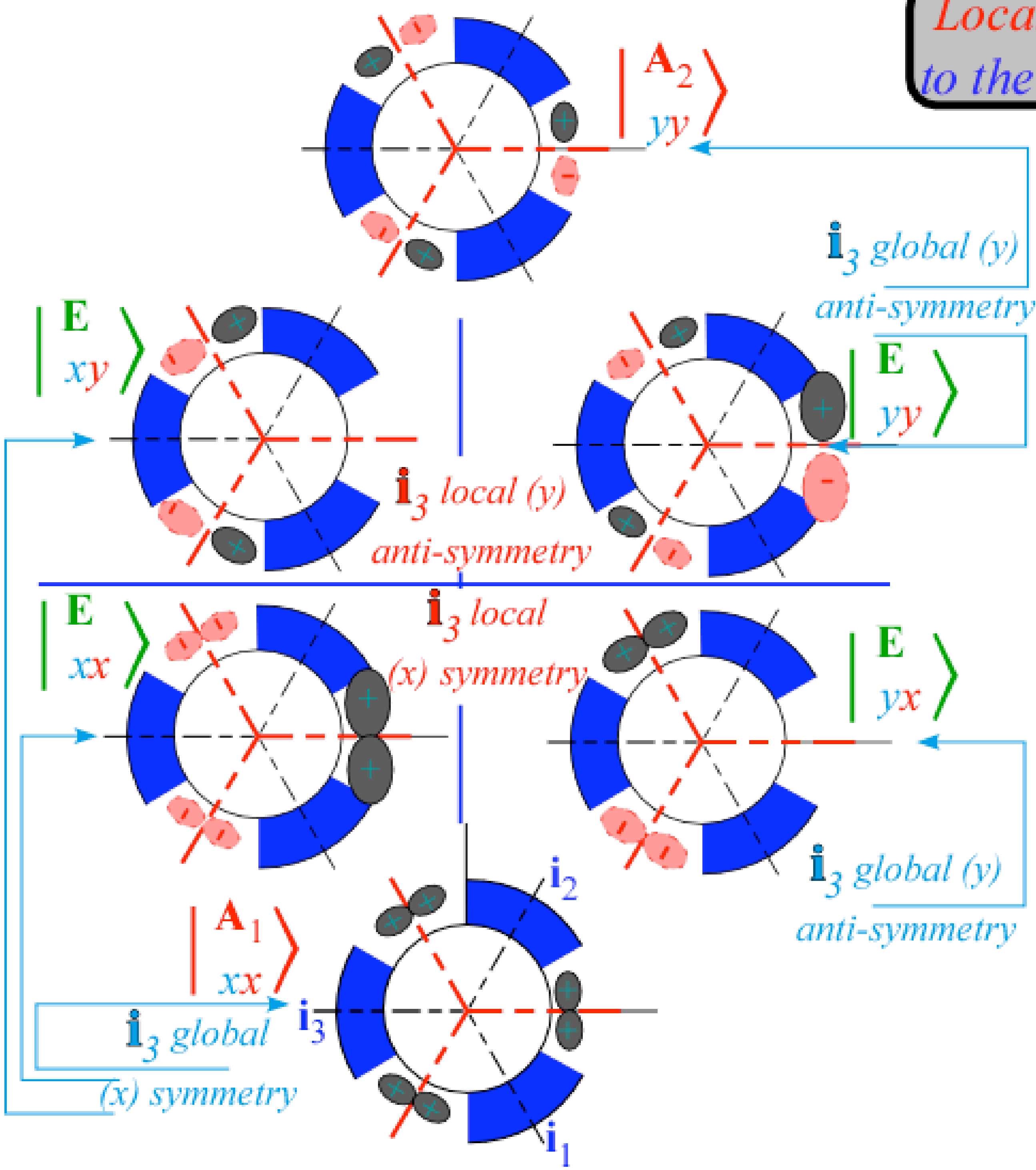
Global (LAB) symmetry

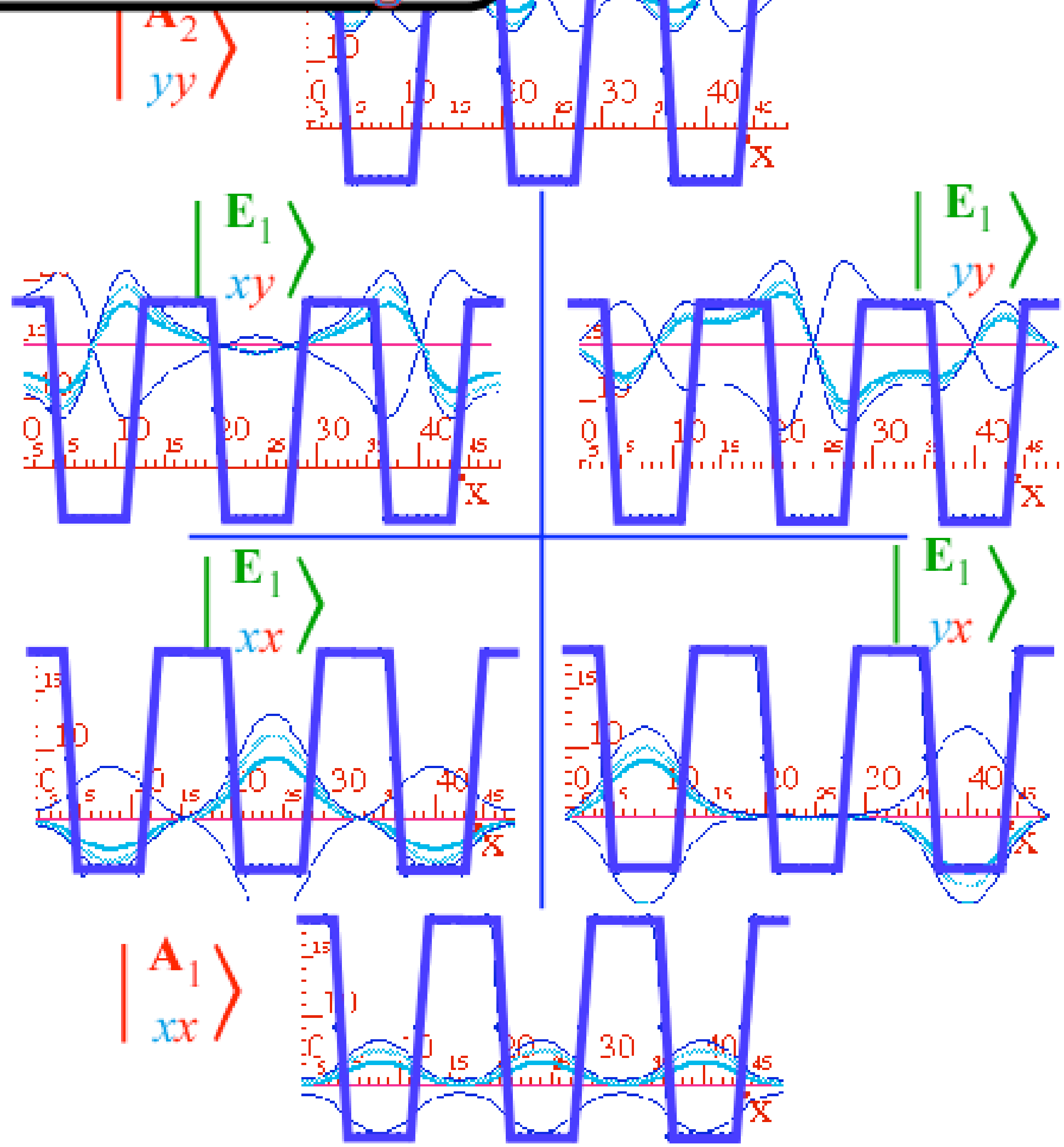
$$\mathbf{i}_3|^{(m)}_{eb}\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}|1\rangle$$
$$= (-1)^e\,|^{(m)}\rangle$$

Local (BOD) symmetry

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

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

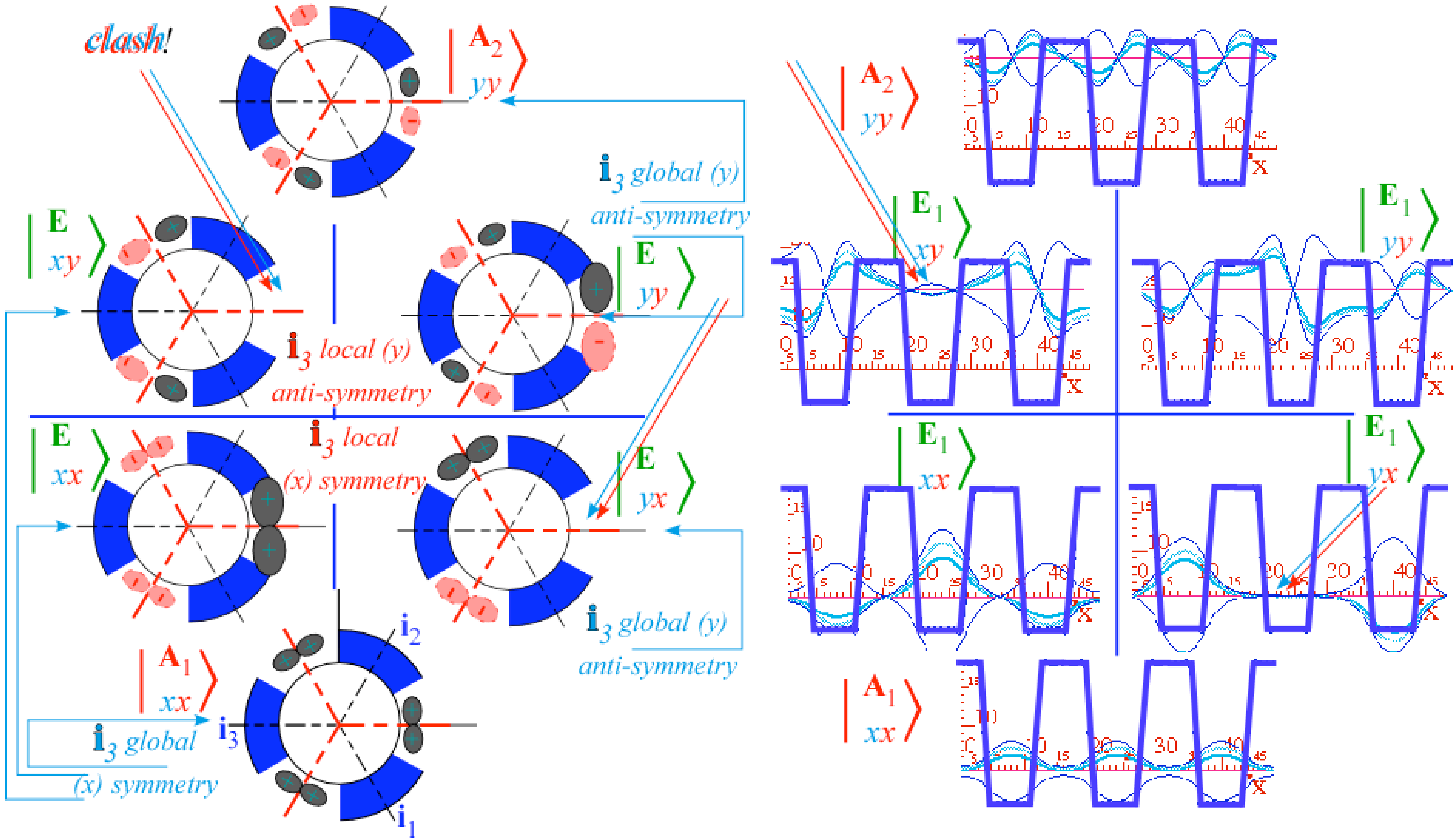




When there is no there, there...

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

.. leads to Local symmetry conditions...

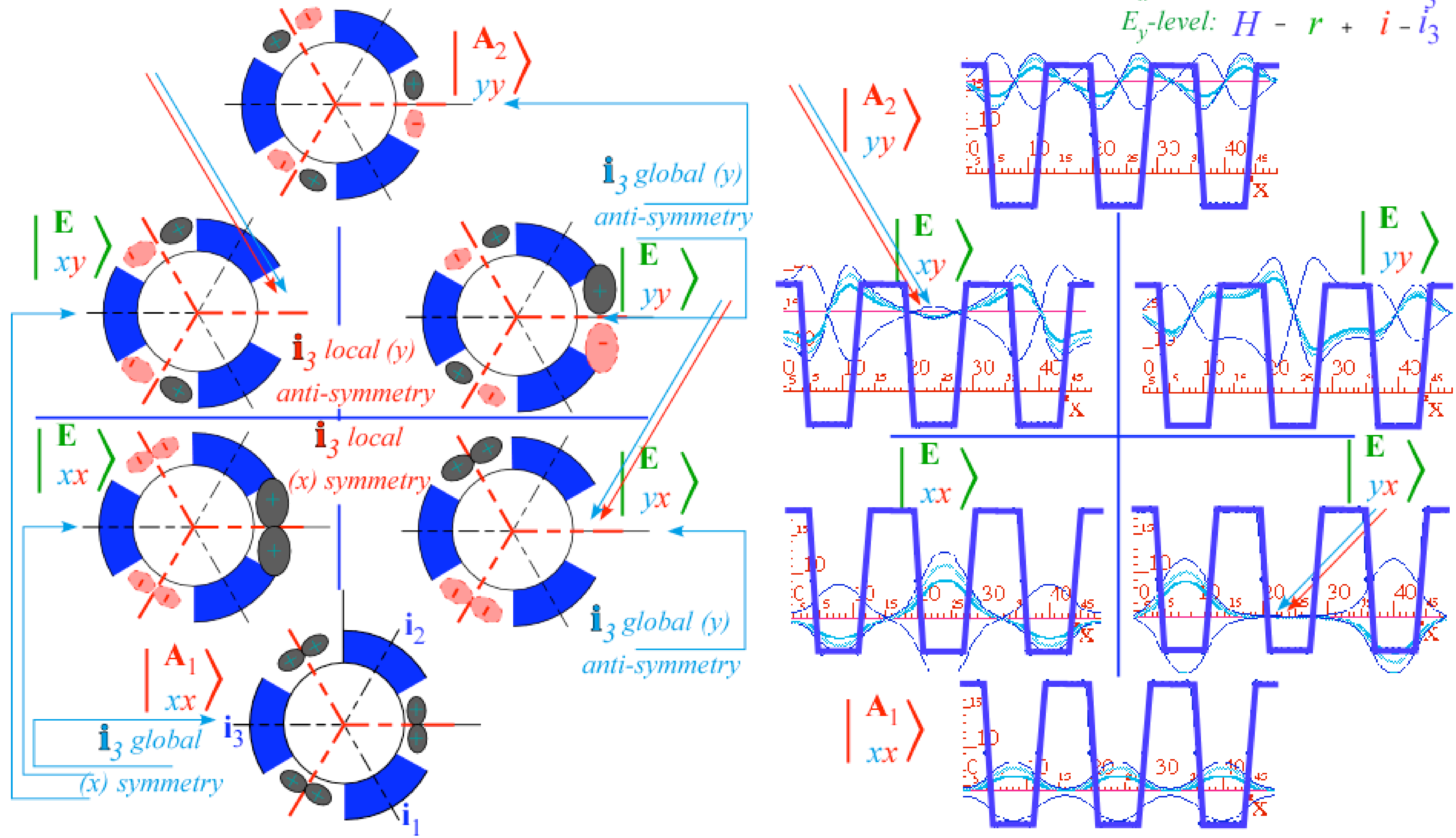


Local symmetry conditions

$$\left(\begin{array}{cccc} \boxed{H+r_1+r_2+i_1+i_2+i_3} & & & \\ A_1\text{-block} & \boxed{H+r_1+r_2-i_1-i_2-i_3} & & \\ & A_2\text{-block} & H-\frac{1}{2}r_1-\frac{1}{2}r_2-\frac{1}{2}i_1-\frac{1}{2}i_2+i_3 & \frac{\sqrt{3}}{2}(-r_1+r_2-i_1+i_2) \\ & & \frac{\sqrt{3}}{2}(+r_1-r_2-i_1+i_2) & H-\frac{1}{2}r_1-\frac{1}{2}r_2+\frac{1}{2}i_1+\frac{1}{2}i_2-i_3 \end{array}\right.$$

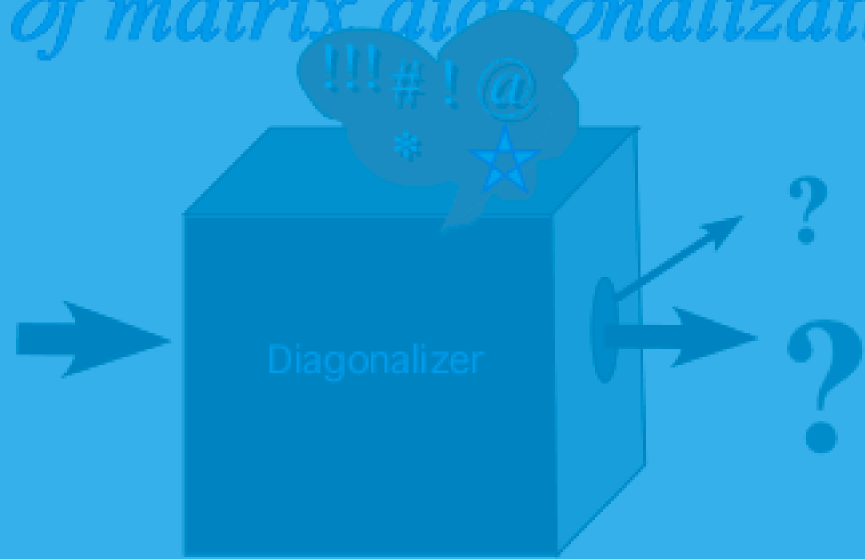
Set off-diagonal to zero. $r_1 = r_2 = -r_1{}^* = r, \quad i_1 = i_2 = -i_1{}^* = i$

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



Making sense of matrix diagonalization **BLACK BOX** :

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



Express **H** *in terms that make algebraic/geometric sense*

- *Intro: Symmetry analysis is Fourier analysis on steroids*

  Going back to our (nth) roots (of unity: $\sqrt[n]{1}= e^{i2\pi m/n}$) (*C_6 example*)

- *Brand new approach to symmetry* (*Conway, Burgiel, Goodman-Strauss, May (2008)*)

  A "group-theory-on-steroids" uses "local" symmetry effectively

..and a not quite so new approach...

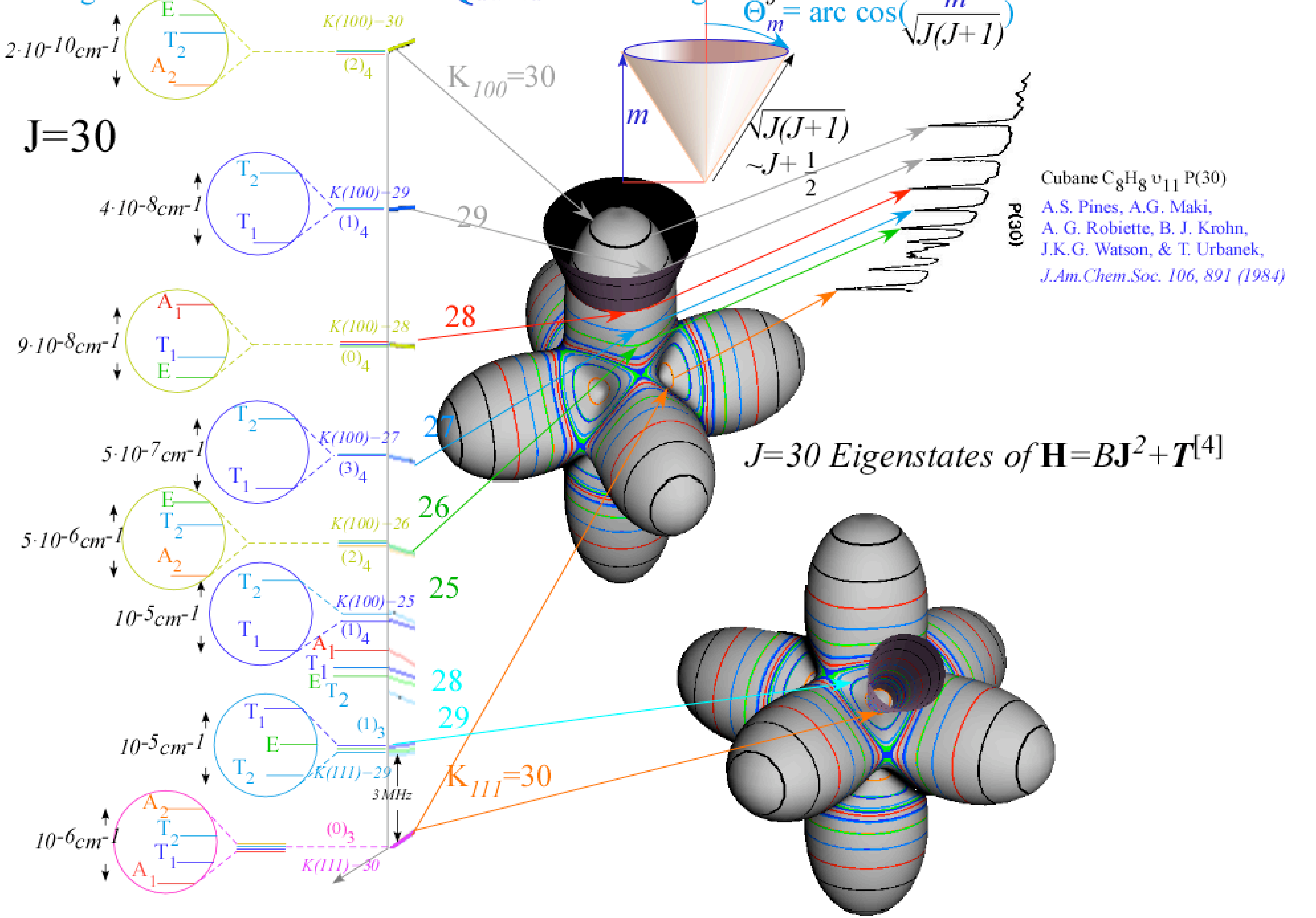
- *Local vs Global symmetry analysis of quantum waves*

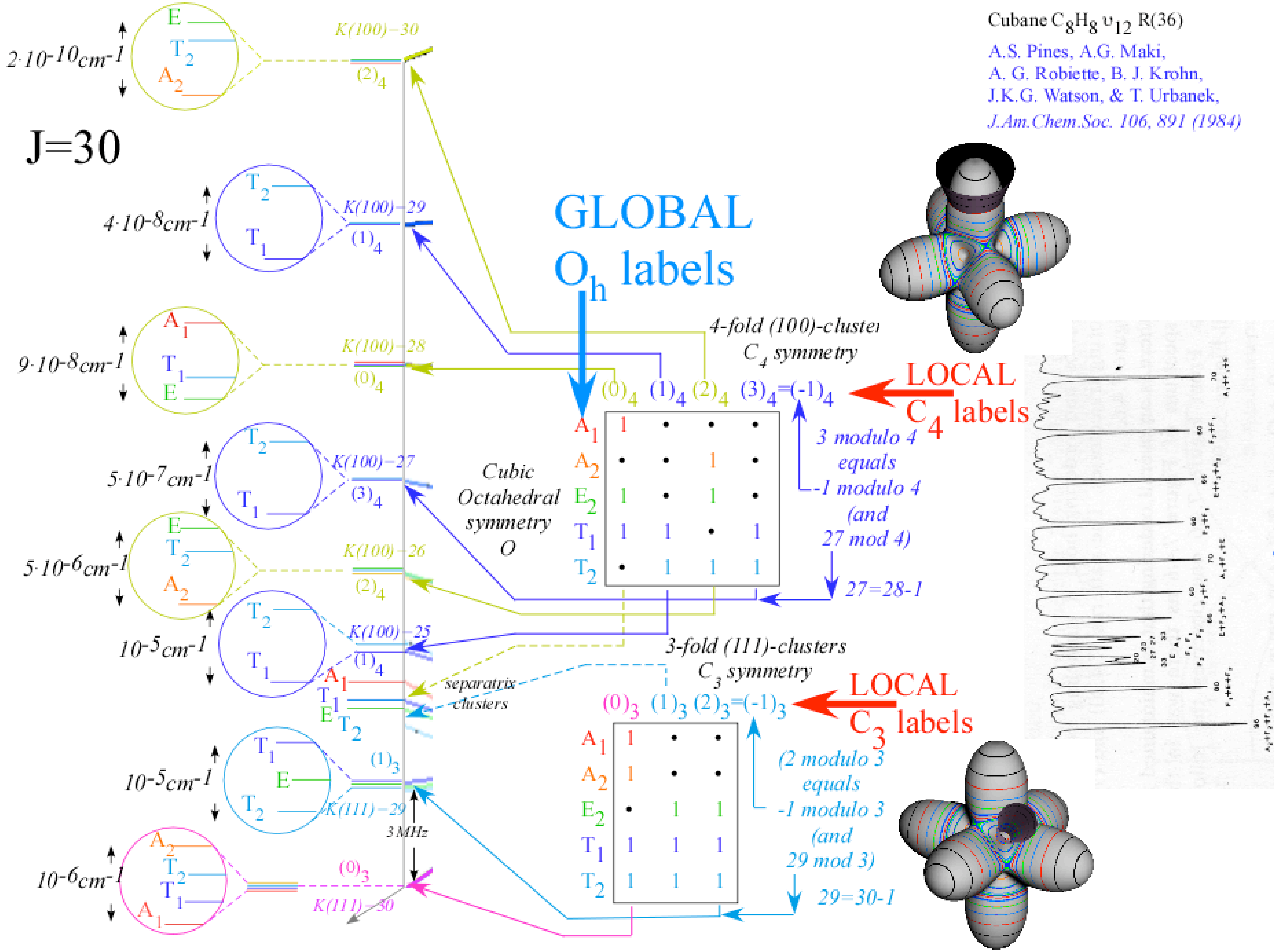
  How "group-theory-on-steroids" grows twice as big (and powerful) (*D_3 example*)

- *Local vs Global symmetry in rovibronic phase space*

  How group operators analyze rovibronic tunneling effects at high J. (*SF_6 examples*)

Angular Momentum Cones and Quantum Polar Angles

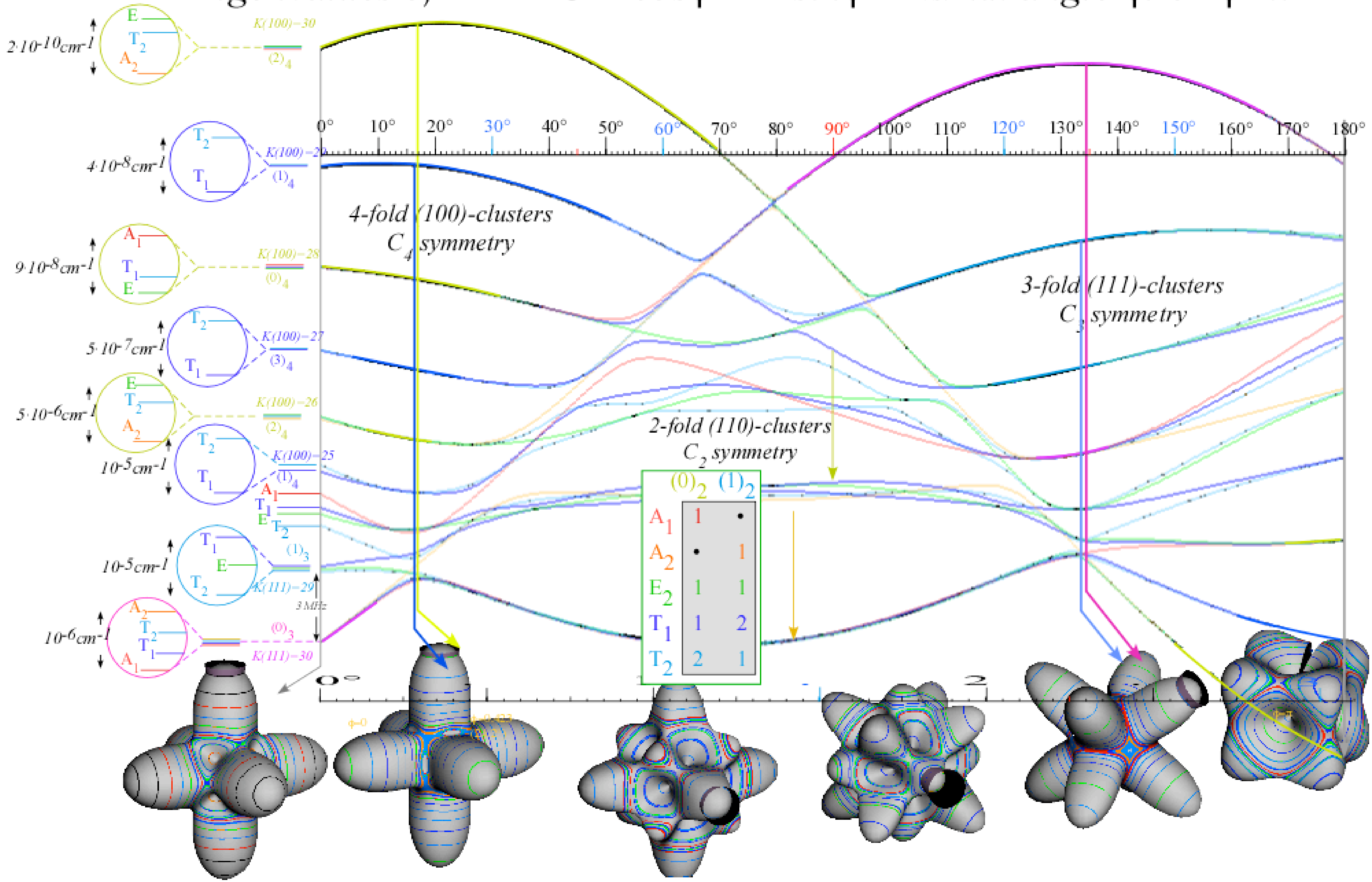




	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E_2	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

	$(0)_3$	$(1)_3$	$(2)_3=(-1)_3$
A_1	1	•	•
A_2	1	•	•
E_2	•	1	1
T_1	1	1	1
T_2	1	1	1

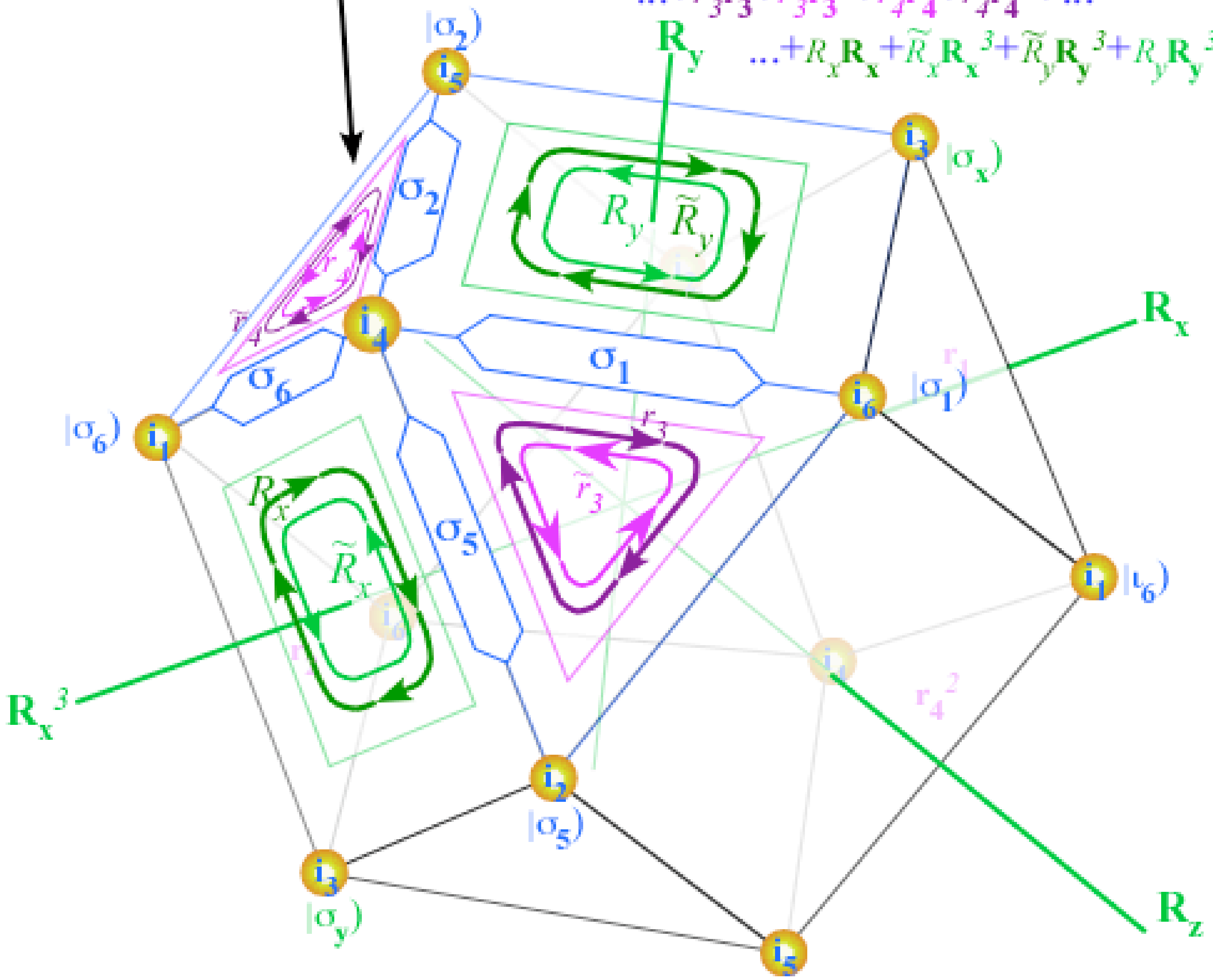
Eigenvalues of $\mathbf{H}=BJ^2+\cos\phi\,\mathbf{T}^{[4]}+\sin\phi\,\mathbf{T}^{[6]}$ *vs. mix angle* ϕ: $0<\phi<\pi$



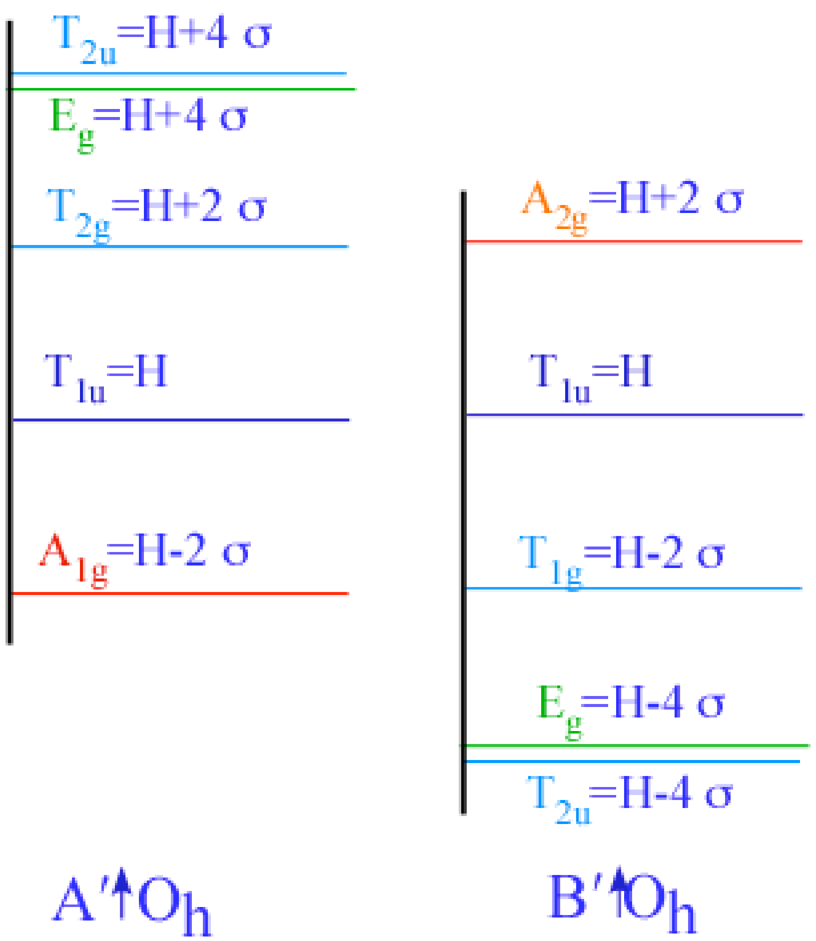
C_{2v} Clustering (Preliminary analysis)

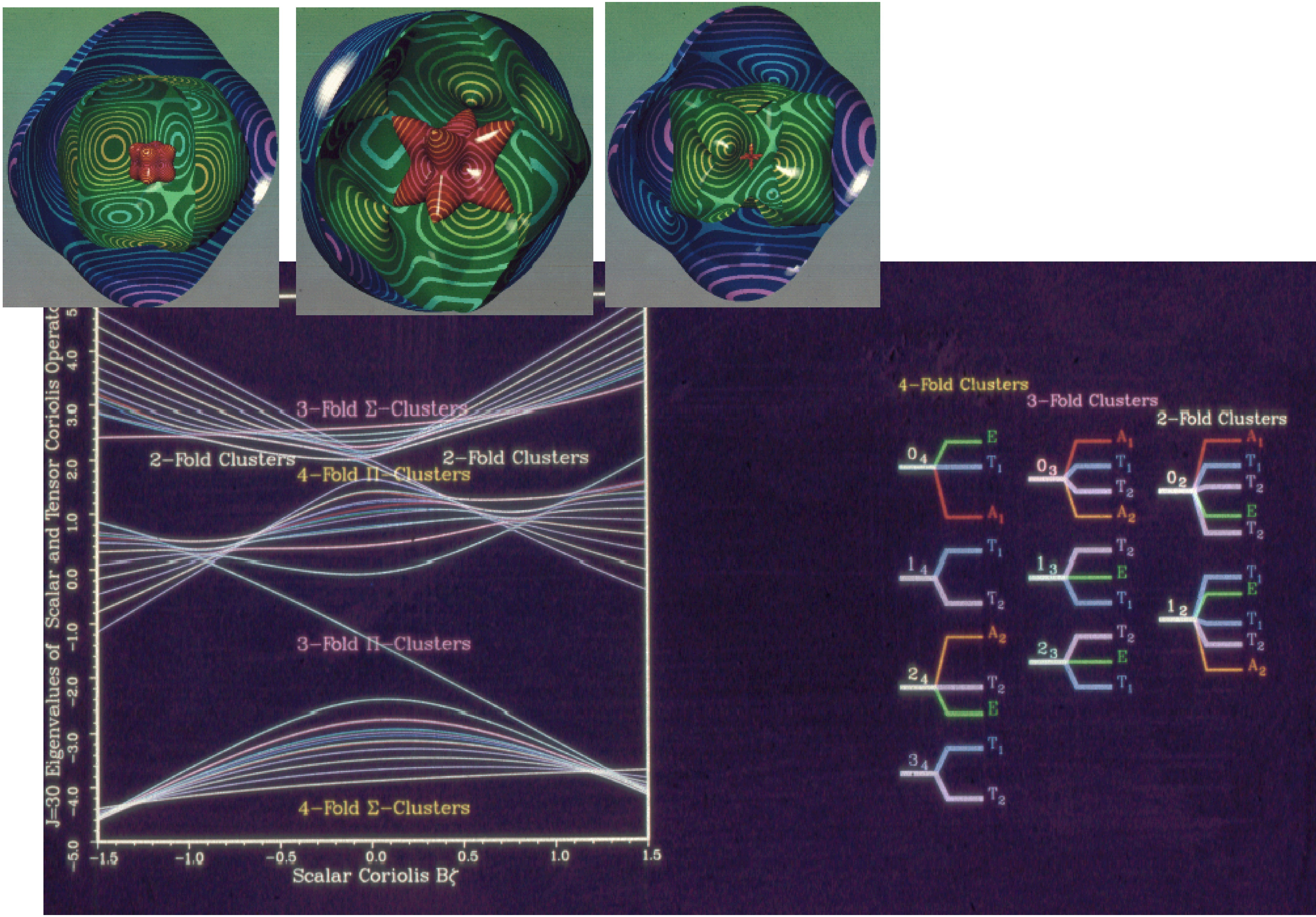
C_2 ($\mathbf{i}_4$)-based O_h symmetry operations
connect $|\mathbf{1})=|i_4)$ on $\mathbf{i}_4$-axis to $|\sigma_1)$, $|\sigma_2)$, $|\sigma_5)$, $|\sigma_6)$,...,$|\sigma_x)$, $|\sigma_y)$, ...

$$\mathbf{H}=\ldots\sigma_1\boldsymbol{\sigma}_1+\sigma_2\boldsymbol{\sigma}_2+\sigma_5\boldsymbol{\sigma}_5+\sigma_6\boldsymbol{\sigma}_6+\ldots$$
$$\ldots+r_3\mathbf{r}_3+\tilde{r}_3\mathbf{r}_3^{\,2}+r_4\mathbf{r}_4+\tilde{r}_4\mathbf{r}_4^{\,2}+\ldots$$
$$\ldots+R_x\mathbf{R}_x+\tilde{R}_x\mathbf{R}_x^{\,3}+\tilde{R}_y\mathbf{R}_y^{\,3}+R_y\mathbf{R}_y^{\,3}+\ldots$$



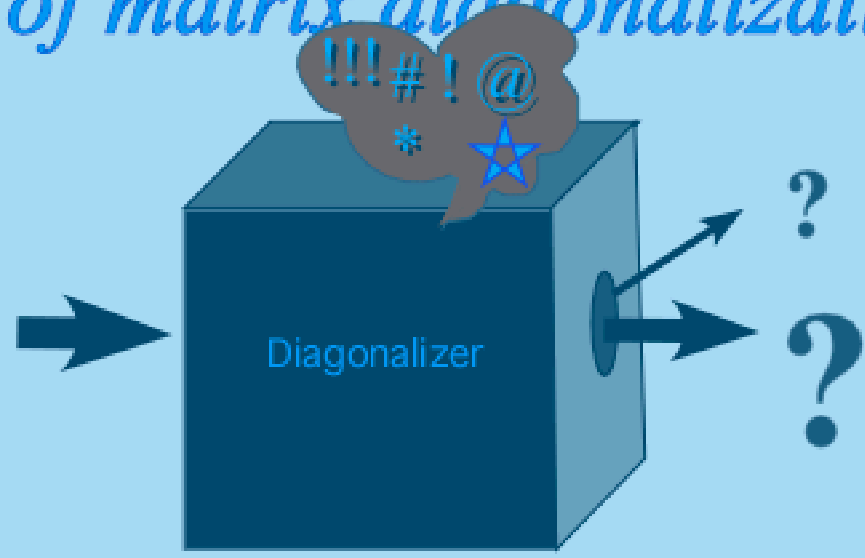
C_{2v} ($\mathbf{i}_4$)-based O_h symmetry clusters
(Reflection tunneling only)

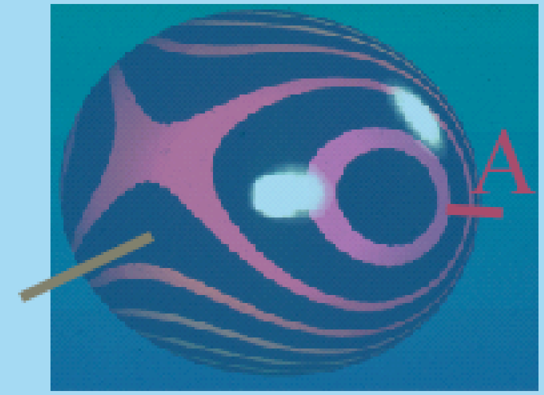



3-Fold Σ-Clusters
2-Fold Clusters
2-Fold Clusters
4-Fold Π-Clusters
3-Fold Π-Clusters
4-Fold Σ-Clusters
J=30 Eigenvalues of Scalar and Tensor Coriolis Operato
Scalar Coriolis Bζ
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
4-Fold Clusters
3-Fold Clusters
2-Fold Clusters
0_4 E T_1 A_1
1_4 T_1 T_2
2_4 A_2 T_2 E
3_4 T_1 T_2
0_3 A_1 T_1 T_2 A_2
1_3 T_2 E T_1
2_3 T_2 E T_1
0_2 A_1 T_1 T_2 E T_2
1_2 T_1 E T_1 T_2 A_2

Making sense of matrix diagonalization **BLACK BOX** :

$$\mathbf{H}=\begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$





Express **H** *in terms that make algebraic/geometric sense*

- *Intro: Symmetry analysis is Fourier analysis on steroids*
  - *Going back to our (nth) roots (of unity: $\sqrt[n]{1}=e^{i2\pi m/n}$)* *(C_6 example)*
- *Brand new approach to symmetry* *(Conway, Burgiel, Goodman-Strauss, May (2008))*
  - *A "group-theory-on-steroids" uses "local" symmetry effectively*

..and a not quite so new approach...

- *Local vs Global symmetry analysis of quantum waves*
  - *How "group-theory-on-steroids" grows twice as big (and powerful)* *(D_3 example)*

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

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

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

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

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

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

D_3 global group multiplication 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 multiplication table

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

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

Change Global to Local by switching

...column-g with column-$g^\dagger$

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

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

D_3 local group table

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

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

D_3 local projector "placeholder" table

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

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