GROUP PARAMETRIZED TUNNELING
AND
LOCAL SYMMETRY CONDITIONS
(or: Powerful symmetry eigensolutions on the Cheap)

William G. Harter and Justin C. Mitchell
Department of Physics, University of Arkansas
Fayetteville, AR 72701

Dr. T. C. Reimer,

RJ-15 *speaker*

Justin Mitchell,

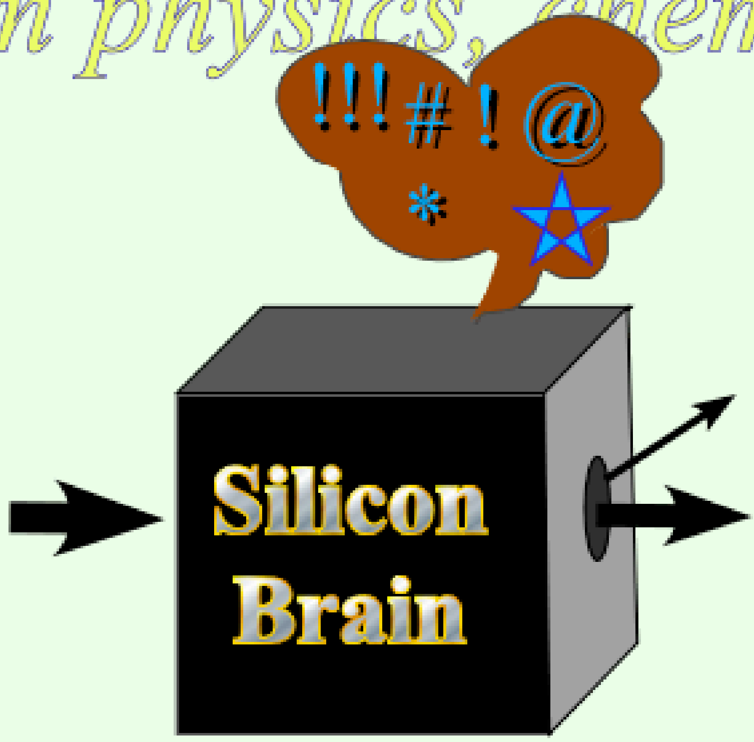
*...and friend**

**(O_h slide rule)*

Matrix Diagonalization by computer:

The **BLACK BOX** *of quantum physics, chemistry, and spectroscopy*

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



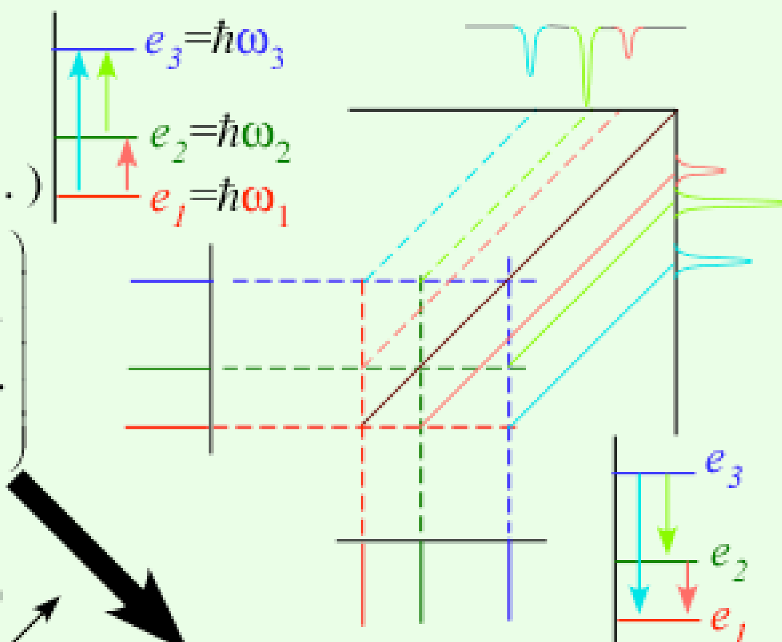
Eigenvalues (Quantum levels)

$$\begin{pmatrix} e_1 & e_2 & e_3 & \cdots \end{pmatrix}$$

$$\begin{pmatrix} \langle 1|e_1\rangle & \langle 1|e_2\rangle & \langle 1|e_3\rangle & \cdots \\ \langle 2|e_1\rangle & \langle 2|e_2\rangle & \langle 2|e_3\rangle & \cdots \\ \langle 3|e_1\rangle & \langle 3|e_2\rangle & \langle 3|e_3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Eigenvectors (Quantum states)

Most of the information!

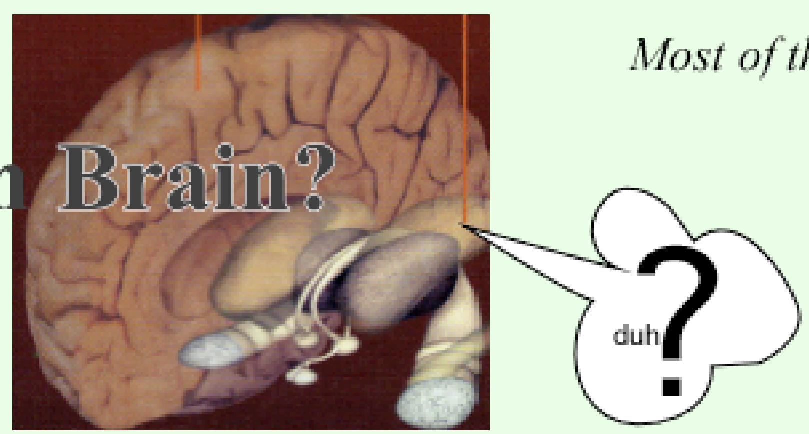


perturbation or transition matrix

$$\begin{pmatrix} \langle e_1|\mathbf{t}^k_q|e_1\rangle & \langle e_1|\mathbf{t}^k_q|e_2\rangle & \langle e_1|\mathbf{t}^k_q|e_3\rangle & \cdots \\ \langle e_2|\mathbf{t}^k_q|e_1\rangle & \langle e_2|\mathbf{t}^k_q|e_2\rangle & \langle e_2|\mathbf{t}^k_q|e_3\rangle & \cdots \\ \langle e_3|\mathbf{t}^k_q|e_1\rangle & \langle e_3|\mathbf{t}^k_q|e_2\rangle & \langle e_3|\mathbf{t}^k_q|e_3\rangle & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Silicon brain knows all...

..but what's left for the **Carbon Brain?**



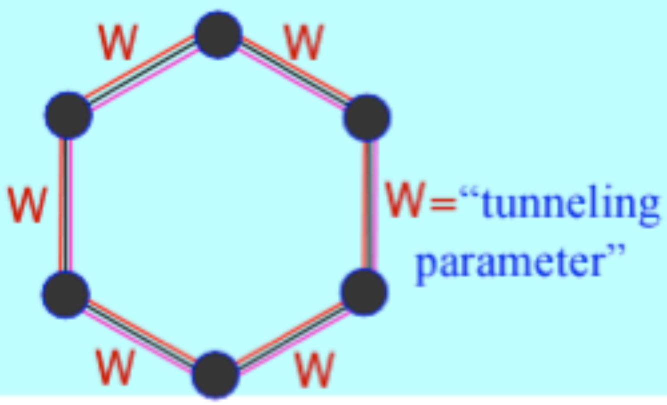
Hougen suggested tunneling matrix approach to spectral analysis (Columbus 2009 **RJ01**)

6 Benzene out-of-plane π orbitals

$$
H = \begin{bmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{bmatrix} \begin{matrix} |1;p_z\rangle \\ |2;p_z\rangle \\ |3;p_z\rangle \\ |4;p_z\rangle \\ |5;p_z\rangle \\ |6;p_z\rangle \end{matrix}
$$

Tunneling matrix has three kinds of elements: non-tunneling E, tunneling splitting W, and 0

Hougen suggested tunneling matrix approach to spectral analysis (Columbus 2009 **RJ01**)

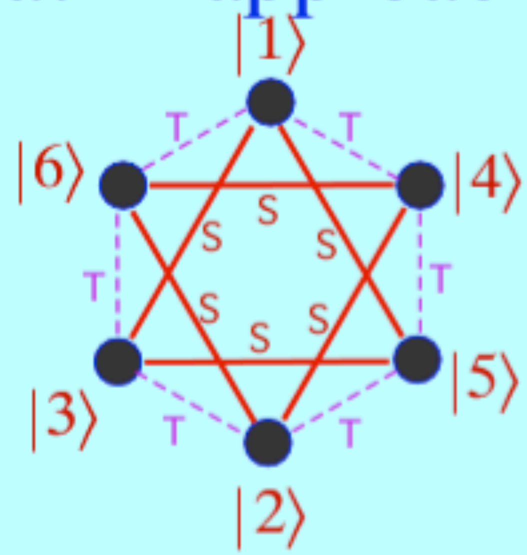


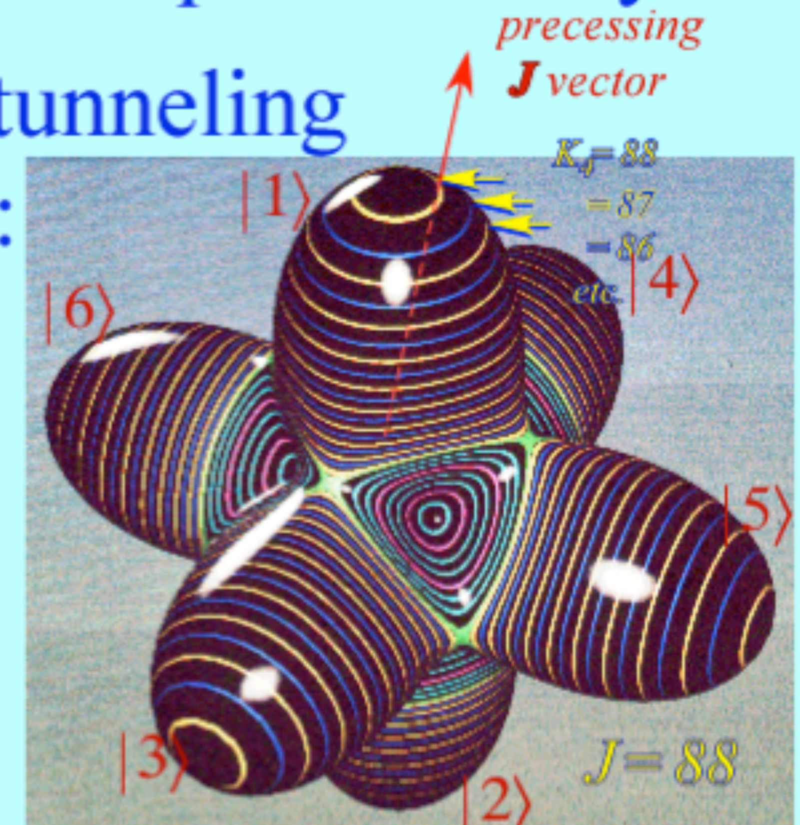
6 Benzene out-of-plane π orbitals

$$H = \begin{bmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{bmatrix} \begin{matrix} |1;p_z\rangle \\ |2;p_z\rangle \\ |3;p_z\rangle \\ |4;p_z\rangle \\ |5;p_z\rangle \\ |6;p_z\rangle \end{matrix}$$

Tunneling matrix has three kinds of elements:
non-tunneling E, tunneling splitting W, and 0

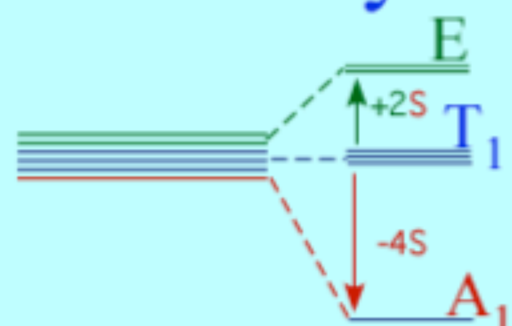
Another *ad hoc* tunneling matrix approach:





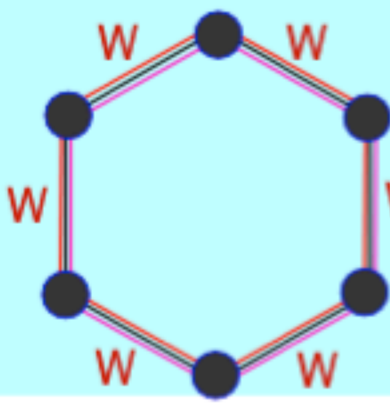
gives “ad hoc” theory of J-level clusters

$$H = \begin{matrix} |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle \end{matrix}$$
$$\begin{bmatrix} H & T & S & S & S & S \\ T & H & T & S & S & S \\ S & T & H & T & S & S \\ S & S & T & H & T & S \\ S & S & S & T & H & T \\ S & S & S & S & T & H \end{bmatrix}$$



Q: Are there “tunneling matrix” schemes that are less *ad hoc*?

Hougen suggested tunneling matrix approach to spectral analysis (Columbus 2009 **RJ01**)



W="tunneling parameter"

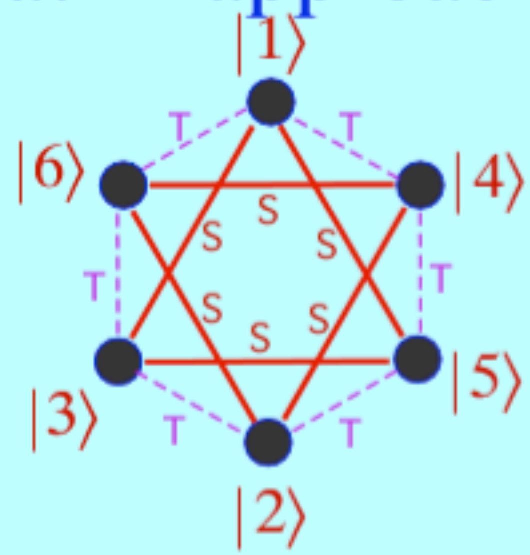
6 Benzene out-of-plane π orbitals

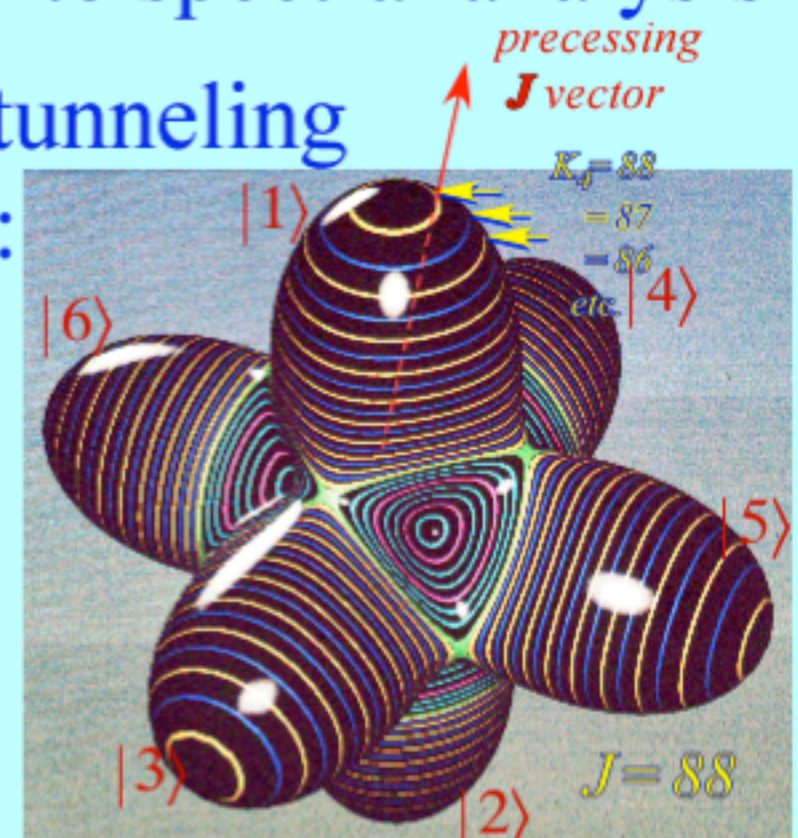
H =

E	W	0	0	0	W	$\|1;p_z\rangle$
W	E	W	0	0	0	$\|2;p_z\rangle$
0	W	E	W	0	0	$\|3;p_z\rangle$
0	0	W	E	W	0	$\|4;p_z\rangle$
0	0	0	W	E	W	$\|5;p_z\rangle$
W	0	0	0	W	E	$\|6;p_z\rangle$

Tunneling matrix has three kinds of elements: non-tunneling E, tunneling splitting W, and 0

Another *ad hoc* tunneling matrix approach:

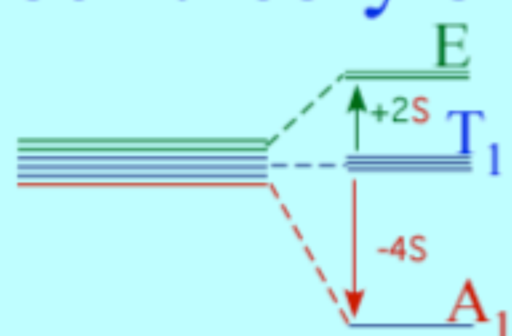




gives "ad hoc" theory of J-level clusters

H =

|1⟩	|2⟩	|3⟩	|4⟩	|5⟩	|6⟩
H	T	S	S	S	S
T	H	T	S	S	S
S	T	H	T	S	S
S	S	T	H	T	S
S	S	S	T	H	T
S	S	S	S	T	H



Q: Are there "tunneling matrix" schemes that are less *ad hoc*?

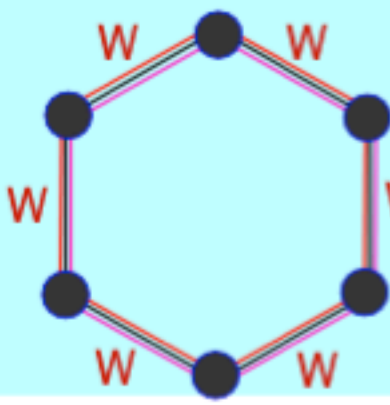
A: Yes. Examples in this talk **(RJ14)** and following talk **(RJ15)**...

Group Parametrization examples:

(1) C_6 band theory *(abelian)*

(2) D_3 group theory *(non-abelian)*

Hougen suggested tunneling matrix approach to spectral analysis (Columbus 2009 **RJ01**)

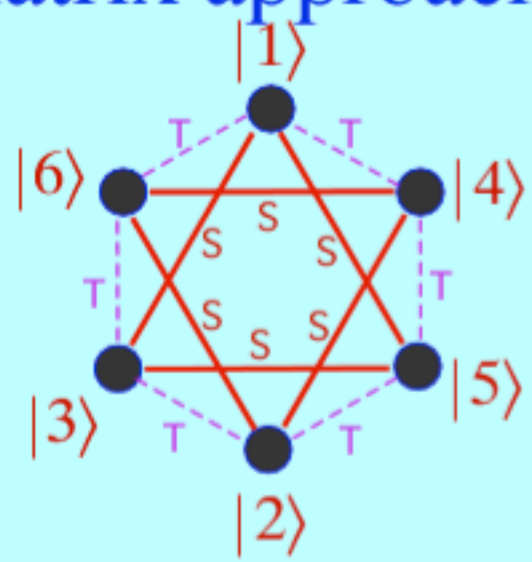


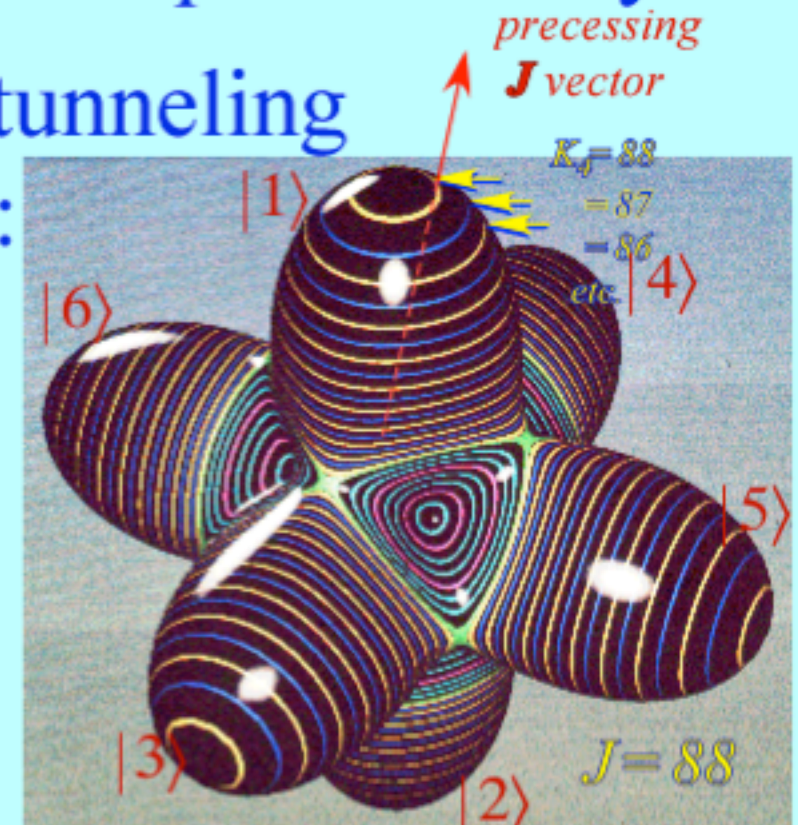
6 Benzene out-of-plane π orbitals

$$H = \begin{bmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{bmatrix} \begin{matrix} |1;p_z\rangle \\ |2;p_z\rangle \\ |3;p_z\rangle \\ |4;p_z\rangle \\ |5;p_z\rangle \\ |6;p_z\rangle \end{matrix}$$

Tunneling matrix has three kinds of elements: non-tunneling E, tunneling splitting W, and 0

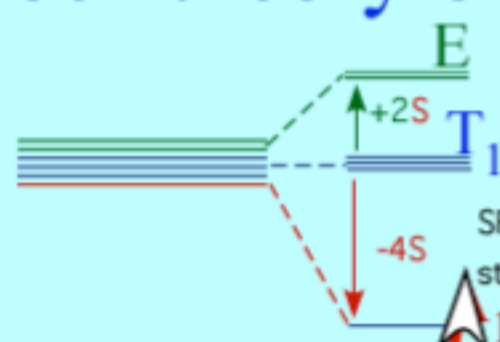
Another *ad hoc* tunneling matrix approach:





gives "ad hoc" theory of J-level clusters

$$H = \begin{matrix} |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle \end{matrix}$$
$$\begin{bmatrix} H & T & S & S & S & S \\ T & H & T & S & S & S \\ S & T & H & T & S & S \\ S & S & T & H & T & S \\ S & S & S & T & H & T \\ S & S & S & S & T & H \end{bmatrix}$$



SF_6 Angular momentum coherent states and superfine structure

Q: Are there "tunneling matrix" schemes that are less *ad hoc*?

A: Yes. Examples in this talk **(RJ14)** and following talk **(RJ15)**...

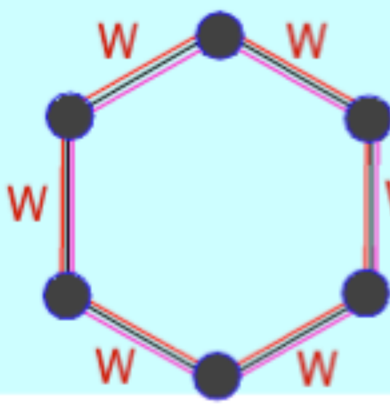
Group Parametrization examples:

(1) C_6 band theory *(abelian)*

(2) D_3 group theory *(non-abelian)*

(3) O_h "cluster bands" *SF_6 rank-4 tensor mononodromy*

Hougen suggested tunneling matrix approach to spectral analysis (Columbus 2009 **RJ01**)

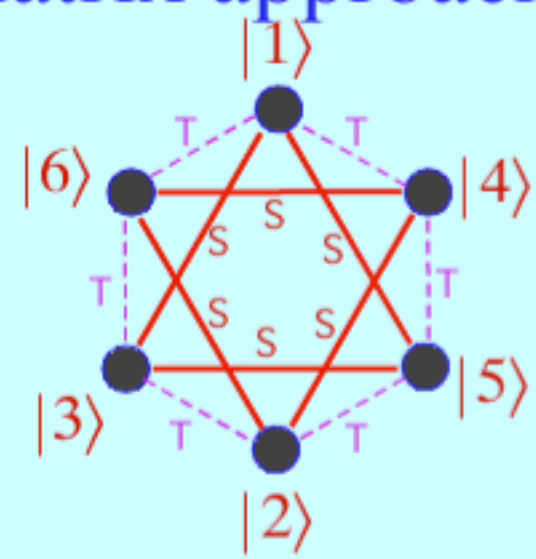


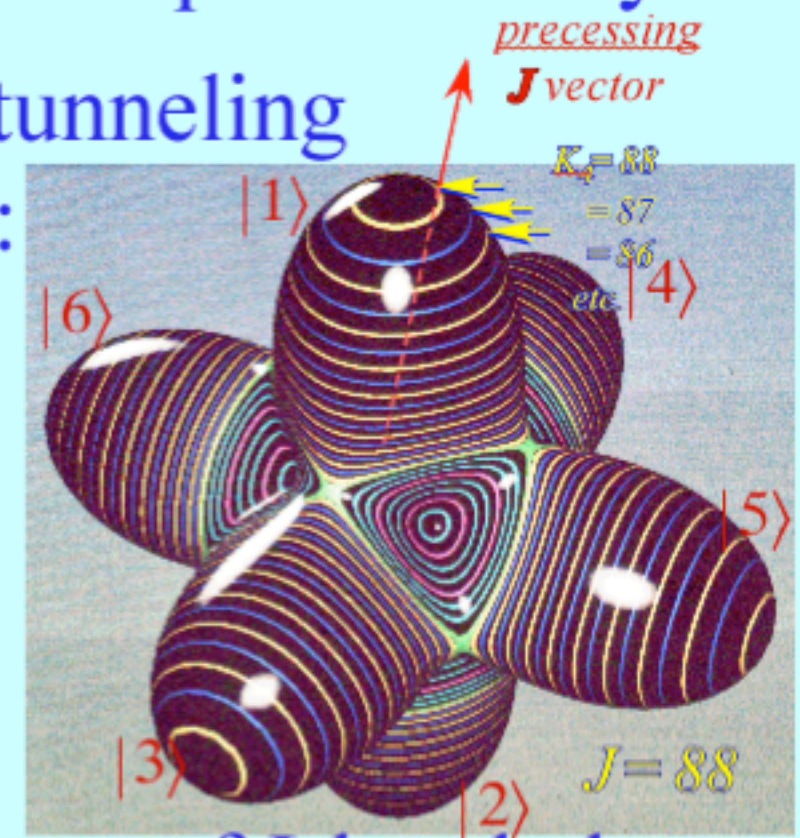
6 Benzene out-of-plane π orbitals

$$H = \begin{bmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{bmatrix} \begin{matrix} |1;p_z\rangle \\ |2;p_z\rangle \\ |3;p_z\rangle \\ |4;p_z\rangle \\ |5;p_z\rangle \\ |6;p_z\rangle \end{matrix}$$

Tunneling matrix has three kinds of elements: non-tunneling E, tunneling splitting W, and 0

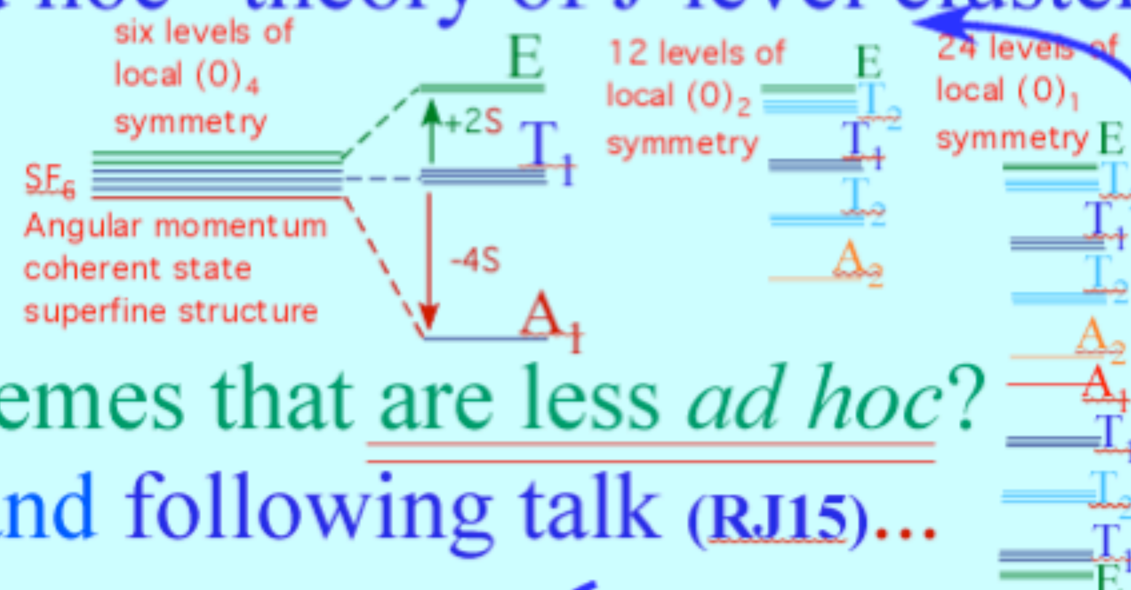
Another *ad hoc* tunneling matrix approach:





gives "ad hoc" theory of J-level clusters

$$H = \begin{bmatrix} H & T & S & S & S & S \\ T & H & T & S & S & S \\ S & T & H & T & S & S \\ S & S & T & H & T & S \\ S & S & S & T & H & T \\ S & S & S & S & T & H \end{bmatrix} \quad (|1\rangle\ |2\rangle\ |3\rangle\ |4\rangle\ |5\rangle\ |6\rangle)$$



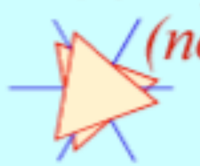
Q: Are there "tunneling matrix" schemes that are less *ad hoc*?

A: Yes. Examples in this talk **(RJ14)** and following talk **(RJ15)**...

Group Parametrization examples:

(1) C_6 band theory *(abelian)*

(2) D_3 group theory *(non-abelian)*



(3) O_h "cluster bands" *SF_6 rank-4 tensor monondromy*

(4) "monster-clusters" *CH_4 SiF_4 rank-4,6,8 T_1 polyad bands*

1^{st} Step Beyond *ad hoc*-ery

Expand C_6 symmetric $\mathbf{H}$= $\begin{bmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{bmatrix}$ ***using C_6 group table($^{gg^\dagger}_{form}$)***

$g^\dagger$

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

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

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

$$\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}$$

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

1^{st} Step Beyond *ad hoc*-ery

Expand C_6 symmetric $\mathbf{H}=\begin{pmatrix} E & W & 0 & 0 & 0 & W \\ W & E & W & 0 & 0 & 0 \\ 0 & W & E & W & 0 & 0 \\ 0 & 0 & W & E & W & 0 \\ 0 & 0 & 0 & W & E & W \\ W & 0 & 0 & 0 & W & E \end{pmatrix}$ *using C_6 group table* $\left(\frac{gg^\dagger}{form}\right)$

$g^\dagger$ across, g down:

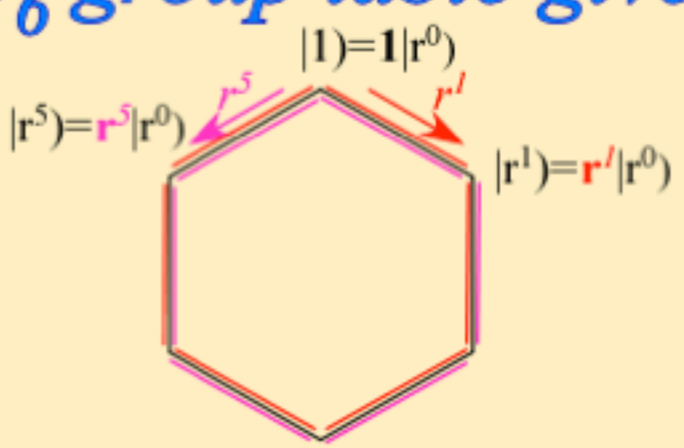
C_6	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{r}$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
$\mathbf{r}^2$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

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

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

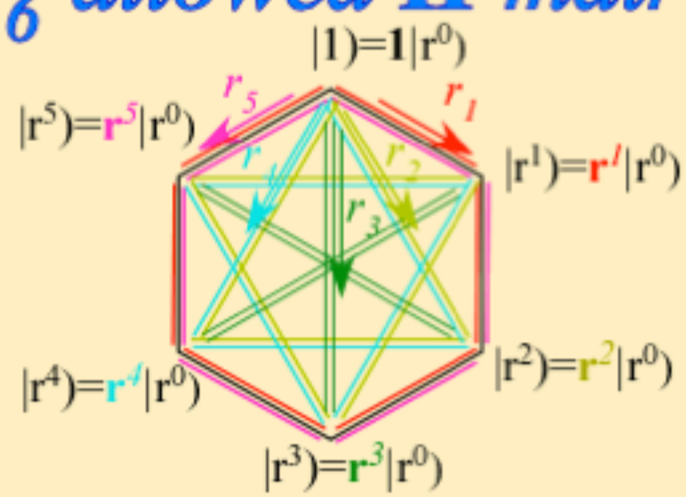
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot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

C_6 group table gives $\mathbf{r}$*-matrices,...C_6-allowed* $\mathbf{H}$*-matrices...*



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

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

2^{nd} Step Beyond *ad hoc*-ery

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

All $x = r^p$ satisfy $x^6 = 1$ and use **6^{th}-roots-of-1** *for eigenvalues*

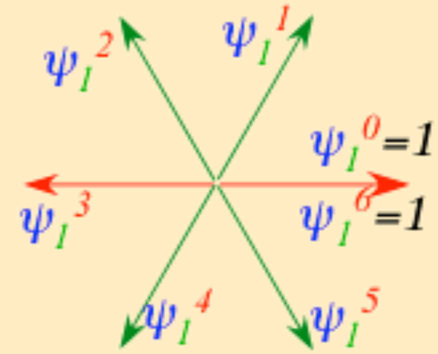
$\psi_1^{\,0} = 1$
$\psi_1^{\,1} = e^{2\pi i/6}$
$\psi_1^{\,2} = \psi_2^{\,1} = e^{4\pi i/6}$
$\psi_1^{\,3} = \psi_3^{\,1} = -1$
$\psi_1^{\,4} = \psi_4^{\,1} = \psi_1^{\,-2} = e^{-4\pi i/6}$
$\psi_1^{\,5} = \psi_5^{\,1} = \psi_1^{\,-1} = e^{-2\pi i/6}$

$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1^{\,m} = \psi_1^{\,m*}$

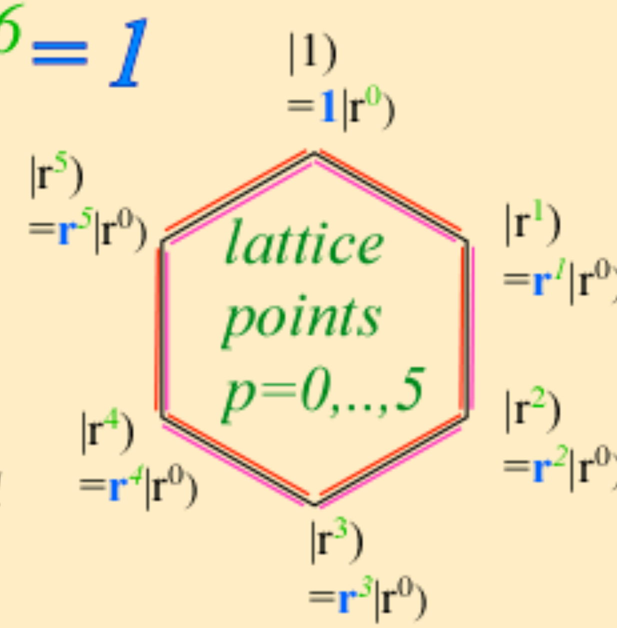
$D^m(\mathbf{r}^p) = e^{-2\pi i m \cdot p/6} = \chi_p^{\,m} = \psi_p^{\,m*}$

p = power (exponent)
or position point

m = momentum
or wave-number



6^{th} roots of 1
m=0,..,5



Groups "know" their roots and will tell you them if you ask nicely!
You efficiently get:

- *invariant projectors*
- *irreducible projectors*
- *irreducible representations (irreps)*
- *H eigenvalues*
- *H eigenvectors*
- *T matrices*
- *dispersion functions*

2^{nd} Step Beyond *ad hoc*-ery

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

top-row flip not needed...

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

All $x = r^p$ satisfy $x^6 = 1$ and use ***6^{th}-roots-of-1*** *for eigenvalues*

$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1^m = \psi_1^{m*}$

$D^m(\mathbf{r}^p) = e^{-2\pi i m \cdot p/6} = \chi_p^m = \psi_p^{m*}$

p = power (exponent) or position point

m = momentum or wave-number

$\psi_1^0 = 1$

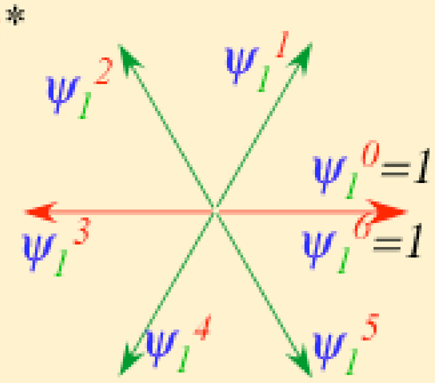
$\psi_1^1 = e^{2\pi i/6}$

$\psi_1^2 = \psi_2^1 = e^{4\pi i/6}$

$\psi_1^3 = \psi_3^1 = -1$

$\psi_1^4 = \psi_4^1 = \psi_1^{-2} = e^{-4\pi i/6}$

$\psi_1^5 = \psi_5^1 = \psi_1^{-1} = e^{-2\pi i/6}$



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

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

$$\begin{pmatrix} \chi_p^0 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \chi_p^1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \chi_p^2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \chi_p^3 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \chi_p^4 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \chi_p^5 \end{pmatrix} = \chi_p^0 \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} + \chi_p^1 \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} + \chi_p^2 \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} + \chi_p^3 \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} + \chi_p^4 \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} + \chi_p^5 \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}$$

Projectors $\mathbf{P}^{(m)}$ start out as eigenvalue "placeholders" with simple (orthogonal-idempotent) product rules

$$\mathbf{P}^{(m)}\mathbf{P}^{(n)} = \delta^{mn}\mathbf{P}^{(m)} \qquad \mathbf{r}^p\,\mathbf{P}^{(m)} = \chi_p^m \mathbf{P}^{(m)}$$

and one completeness rule: $\mathbf{P}^{(0)} + \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \ldots + \mathbf{P}^{(5)} = \mathbf{1}$

2^{nd} Step Beyond *ad hoc*-ery

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

All $x = r^p$ *satisfy* $x^6 = 1$ *and use* **6th-roots-of-1** *for eigenvalues*

$$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1^m = \psi_1^{m*}$$

$$D^m(\mathbf{r}^p) = e^{-2\pi i m\cdot p/6} = \chi_p^m = \psi_p^{m*}$$

p = power (exponent) or position point

m = momentum or wave-number

$\psi_1^0 = 1$

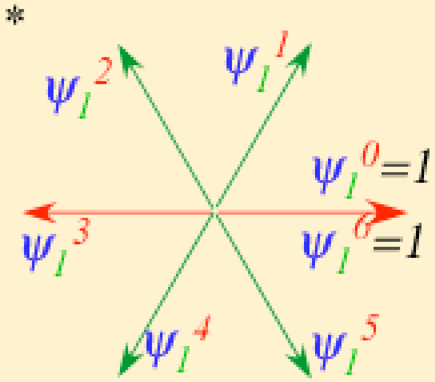
$\psi_1^1 = e^{2\pi i/6}$

$\psi_1^2 = \psi_2^1 = e^{4\pi i/6}$

$\psi_1^3 = \psi_3^1 = -1$

$\psi_1^4 = \psi_4^1 = \psi_1^{-2} = e^{-4\pi i/6}$

$\psi_1^5 = \psi_5^1 = \psi_1^{-1} = e^{-2\pi i/6}$

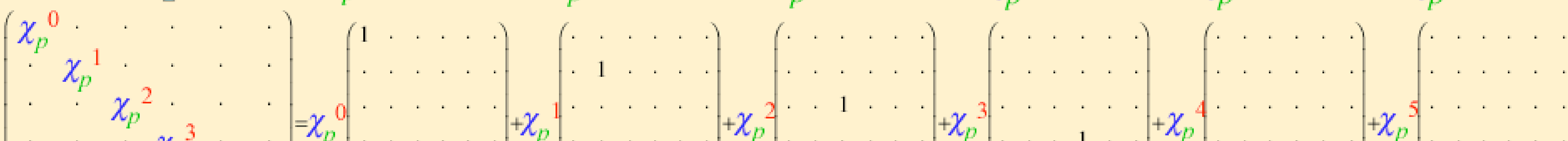


top-row flip not needed...

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

$_6$ ring	$\mathbf{P}^{(0)}$	$\mathbf{P}^{(1)}$	$\mathbf{P}^{(2)}$	$\mathbf{P}^{(3)}$	$\mathbf{P}^{(4)}$	$\mathbf{P}^{(5)}$
$^{(0)}$	$\mathbf{P}^{(0)}$	.	.	.	.	.
$\mathbf{P}^{(1)}$	.	$\mathbf{P}^{(1)}$	.	.	.	.
$\mathbf{P}^{(2)}$	.	.	$\mathbf{P}^{(2)}$	.	.	.
$\mathbf{P}^{(3)}$	.	.	.	$\mathbf{P}^{(3)}$	.	.
$\mathbf{P}^{(4)}$	.	.	.	.	$\mathbf{P}^{(4)}$	.
$\mathbf{P}^{(5)}$	.	.	.	.	.	$\mathbf{P}^{(5)}$

$$\mathbf{r}^p = \chi_p^0\,\mathbf{P}^{(0)} + \chi_p^1\,\mathbf{P}^{(1)} + \chi_p^2\,\mathbf{P}^{(2)} + \chi_p^3\,\mathbf{P}^{(3)} + \chi_p^4\,\mathbf{P}^{(4)} + \chi_p^5\,\mathbf{P}^{(5)}$$

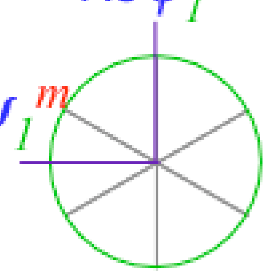


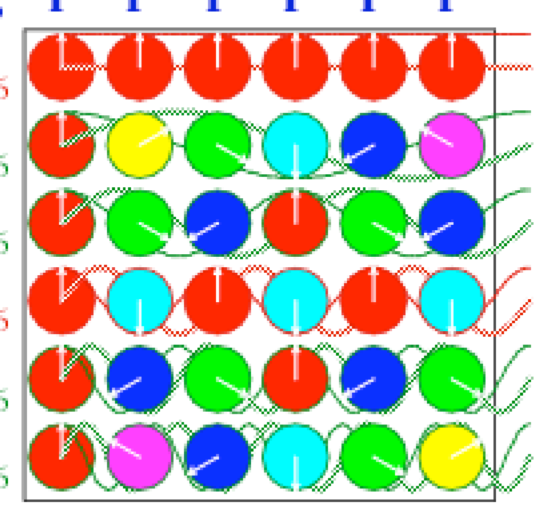
Inverse C_6 *spectral resolution m-wave* $\psi_p^m = D^{m*}(\mathbf{r}^p) = e^{+2\pi i m\cdot p/6}$:

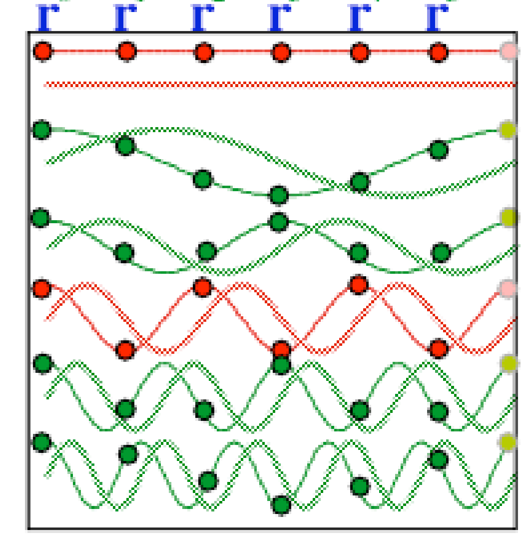
$$\mathbf{P}^{(m)} = \psi_0^m\,\mathbf{r}^0 + \psi_1^m\,\mathbf{r}^1 + \psi_2^m\,\mathbf{r}^2 + \psi_3^m\,\mathbf{r}^3 + \psi_4^m\,\mathbf{r}^4 + \psi_5^m\,\mathbf{r}^5$$

position p (or power of $\mathbf{r}^p$*)*

momentum m	p=0	1	2	3	4	5
m=0	ψ_0^0	ψ_1^0	ψ_2^0	ψ_3^0	ψ_4^0	ψ_5^0
m=1	ψ_0^1	ψ_1^1	ψ_2^1	ψ_3^1	ψ_4^1	ψ_5^1
m=2	ψ_0^2	ψ_1^2	ψ_2^2	ψ_3^2	ψ_4^2	ψ_5^2
m=3	ψ_0^3	ψ_1^3	ψ_2^3	ψ_3^3	ψ_4^3	ψ_5^3
m=4	ψ_0^4	ψ_1^4	ψ_2^4	ψ_3^4	ψ_4^4	ψ_5^4
m=5	ψ_0^5	ψ_1^5	ψ_2^5	ψ_3^5	ψ_4^5	ψ_5^5





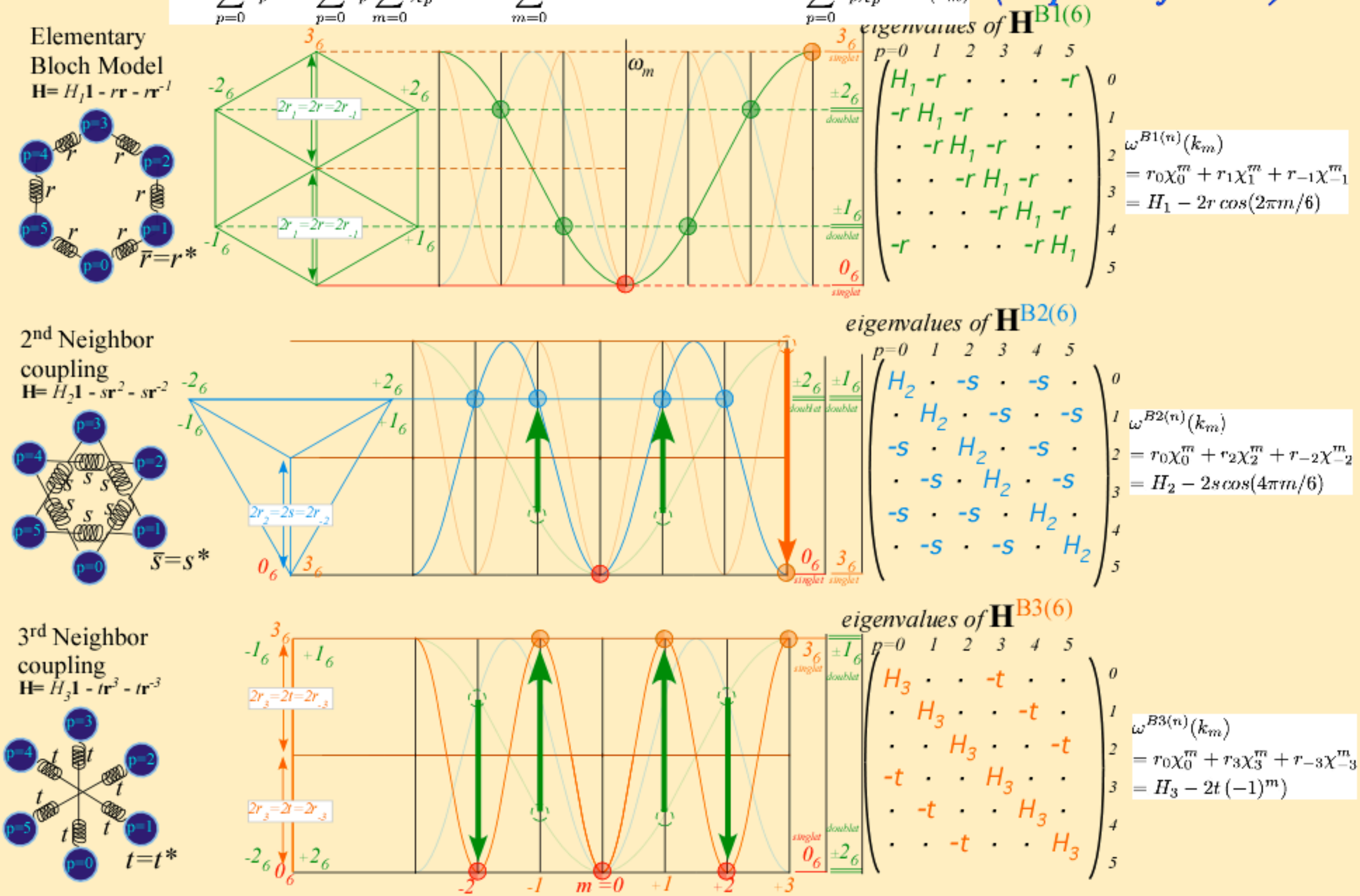


3^{rd} Step Beyond *ad hoc*-ery

Display all eigensolutions for all possible C_6 symmetric real H

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p=\sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)}=\sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)}=\sum_{p=0}^{n-1} r_p \chi_p^m=\omega(k_m)$$

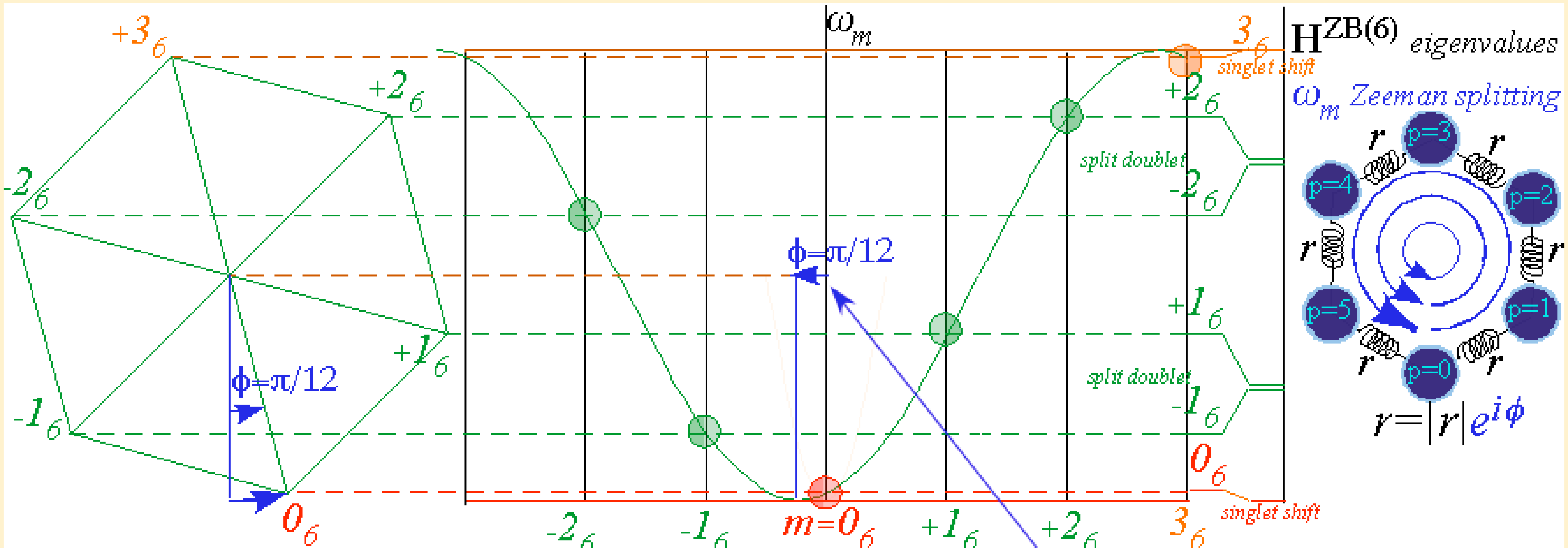
(Dispersion function)



3rd Step Beyond *ad hoc*-ery

...eigensolutions for all possible C_6 symmetric complex H

$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p = \sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)} = \sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where:\ \omega^{(m)} = \sum_{p=0}^{n-1} r_p \chi_p^m = \omega(k_m)$$ *(Dispersion function)*



Note "gauge" shift

Abelian (Commutative) C_2, C_2, ...,C_6 ...

H diagonalized by r^p *symmetry operators that COMMUTE with H* $(r^p H = H r^p)$,

and with each other $(r^p r^q = r^{p+q} = r^q r^p)$.

Versus...

Non-Abelian (do *not* commute) D_3, O_h,...

While all H symmetry operations COMMUTE with H $(\mathbf{U} H = H \mathbf{U})$

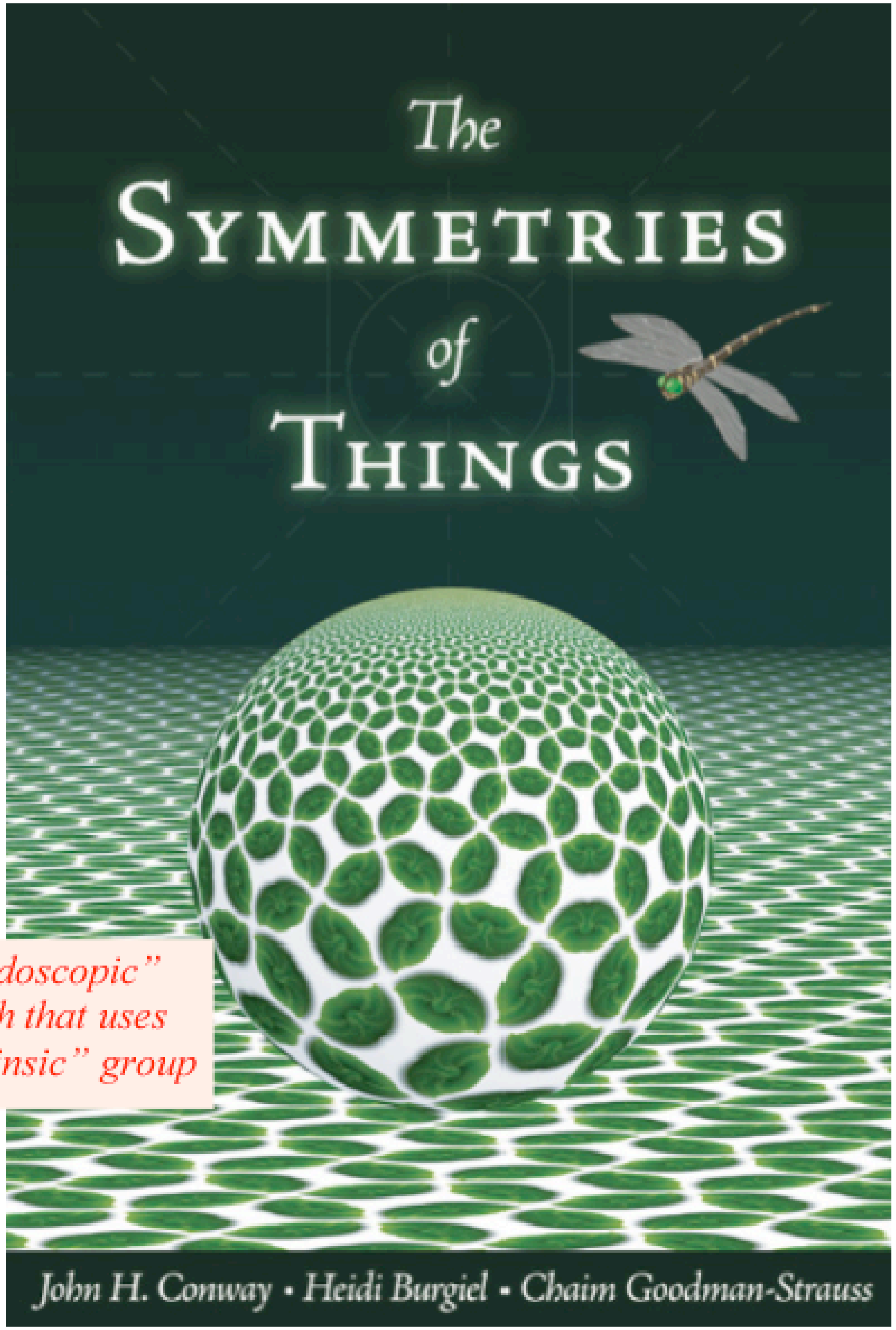
most do not with each other $(\mathbf{U}\mathbf{V} \neq \mathbf{V}\mathbf{U})$.

Q: *So how do we write* H *in terms of non-commutative* $\mathbf{U}$?

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

...from PURE group theory...

A revolutionary simplification to classify all groups and their algebras

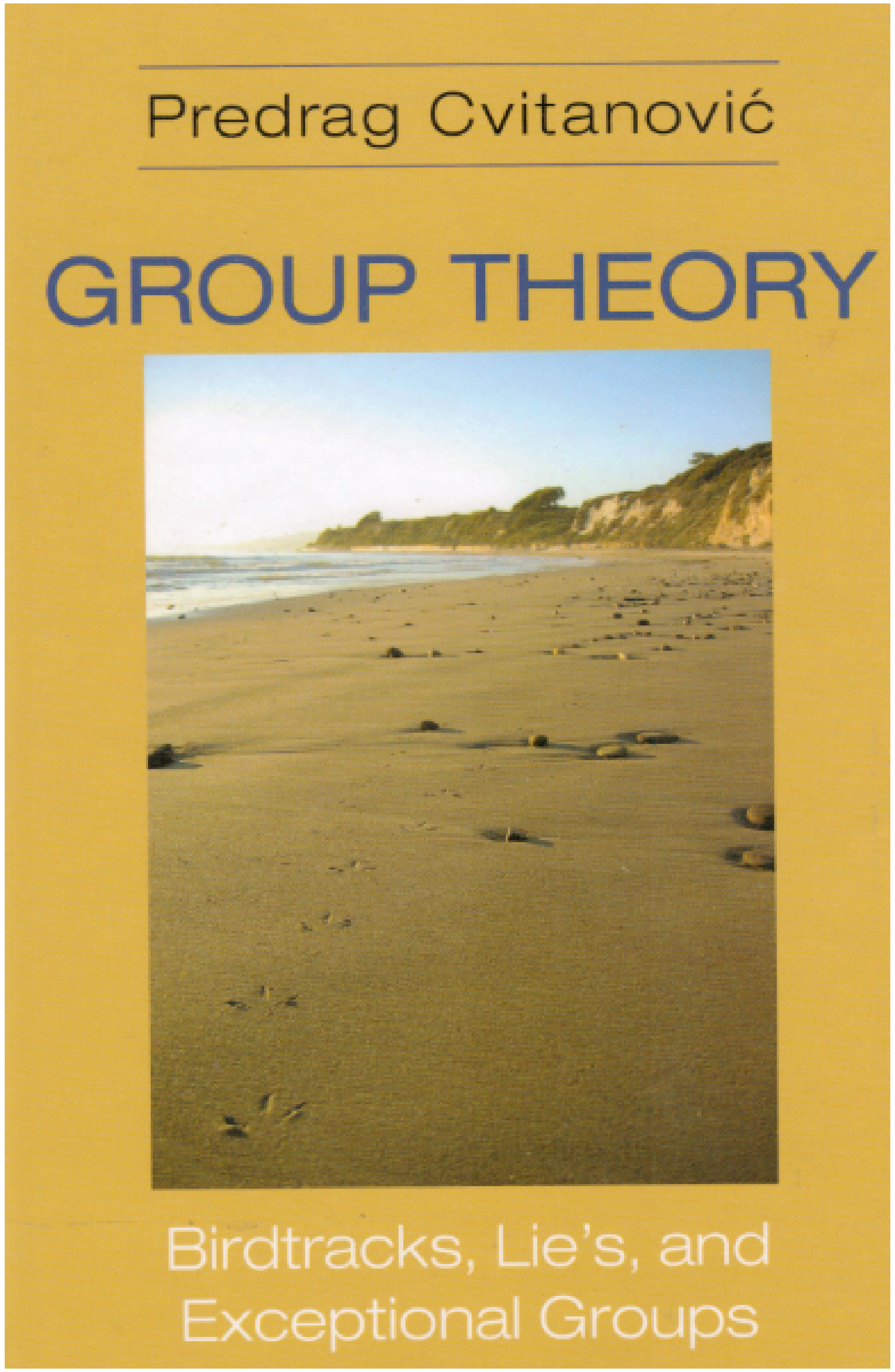


A "kaleidoscopic" approach that uses an "intrinsic" group

(2008) A.K. Peters Ltd. Wellesley, MA 02482

...from APPLIED*(to string theory)*...

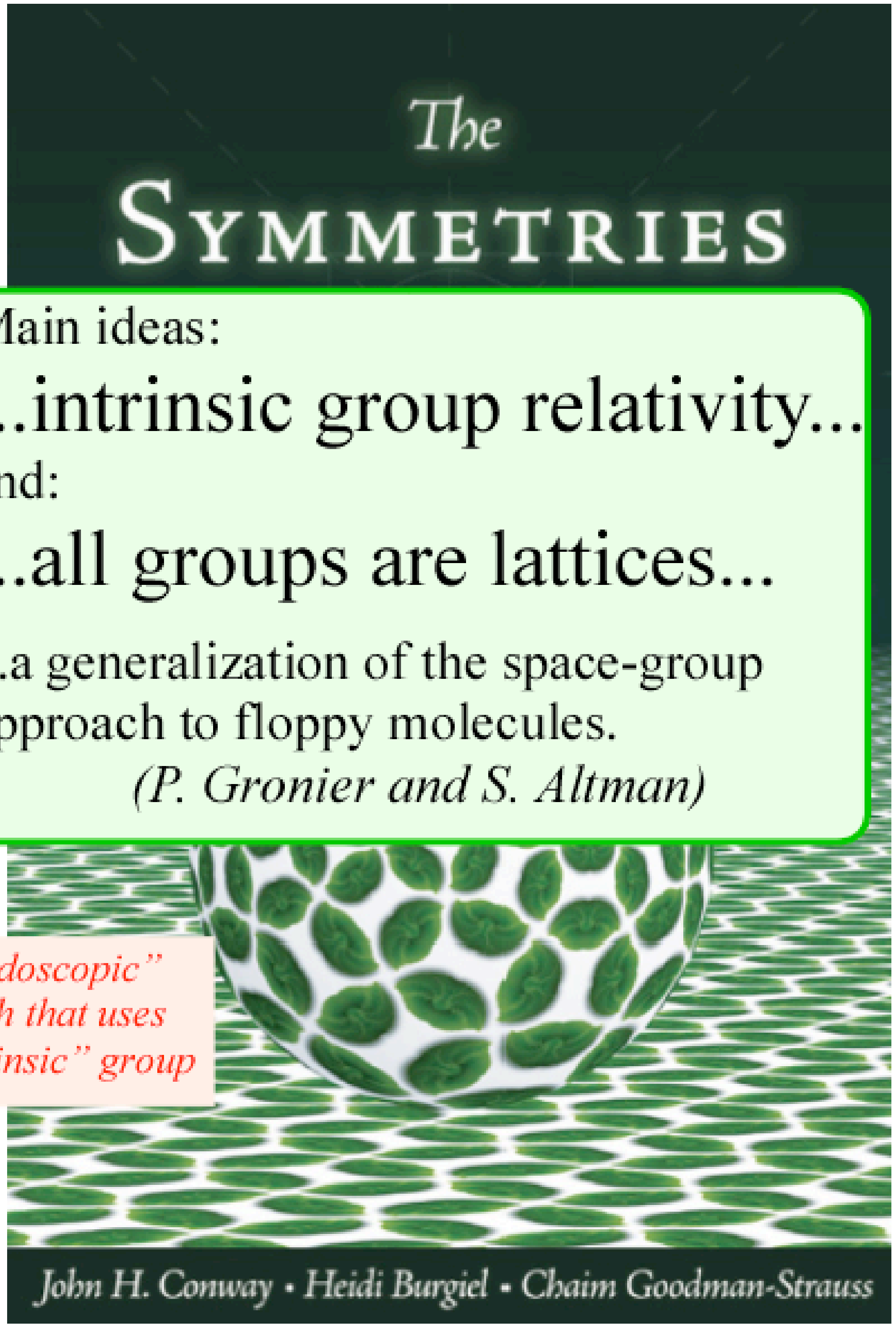
A new/old approach to Clebsch-Gordon-Racah-Yutsis invariants



(2008) Princeton. Oxford 0X20 1TW

...from PURE group theory...

A revolutionary simplification to classify all groups and their algebras



Main ideas:

...intrinsic group relativity...

and:

...all groups are lattices...

...a generalization of the space-group approach to floppy molecules.

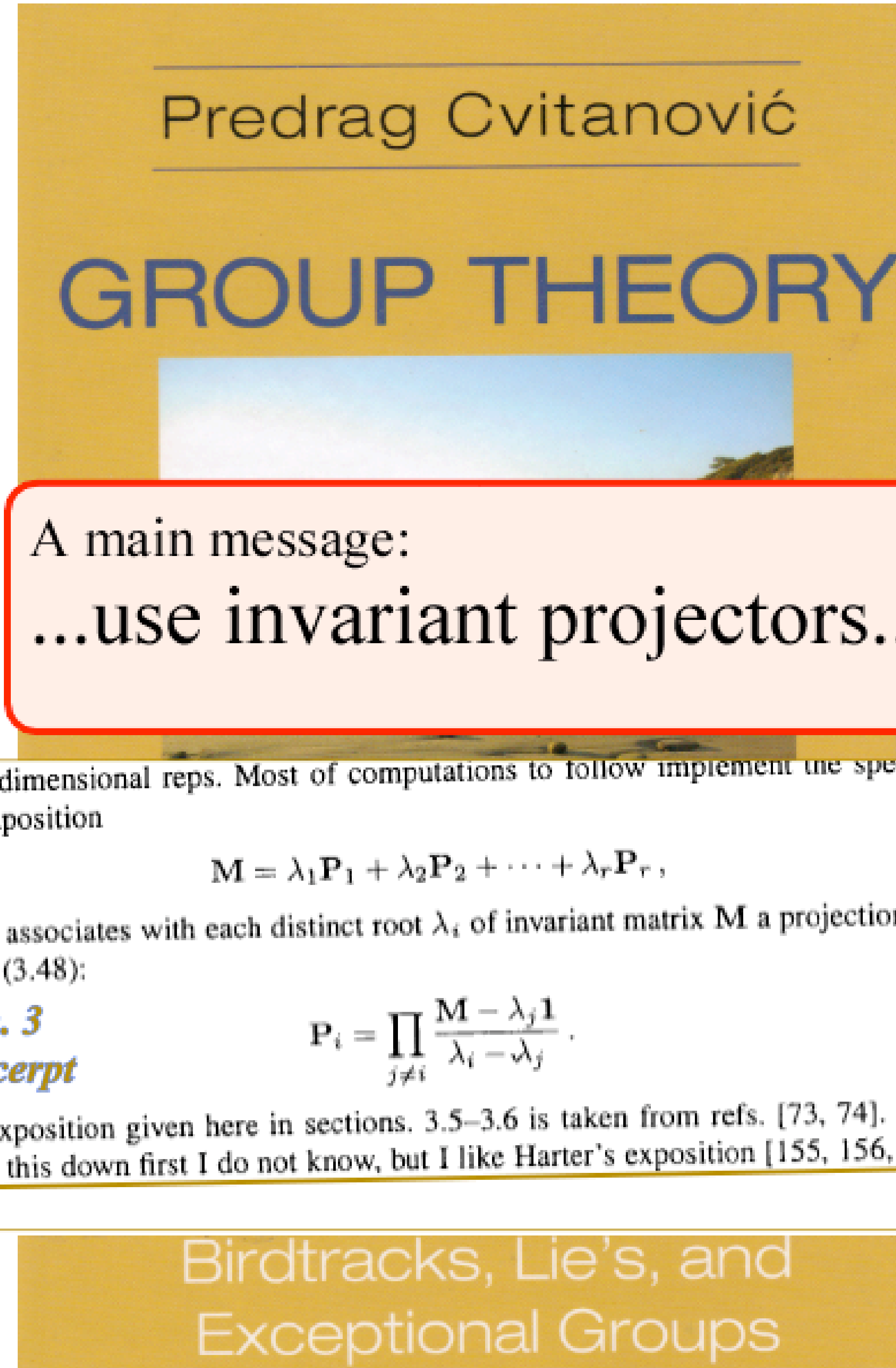
(P. Gronier and S. Altman)

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

(2008) A.K. Peters Ltd. Wellesley, MA 02482

...from APPLIED (to supersymmetry)...

A new/old approach to Clebsch-Gordon-Racah-Yutsis invariants



A main message:

...use invariant projectors...

lower-dimensional reps. Most of computations to follow implement the spectral decomposition

$$\mathbf{M} = \lambda_1 \mathbf{P}_1 + \lambda_2 \mathbf{P}_2 + \cdots + \lambda_r \mathbf{P}_r \,,$$

which associates with each distinct root λ_i of invariant matrix $\mathbf{M}$ a projection operator (3.48):

Ch. 3 excerpt

$$\mathbf{P}_i = \prod_{j \neq i} \frac{\mathbf{M} - \lambda_j \mathbf{1}}{\lambda_i - \lambda_j} \,.$$

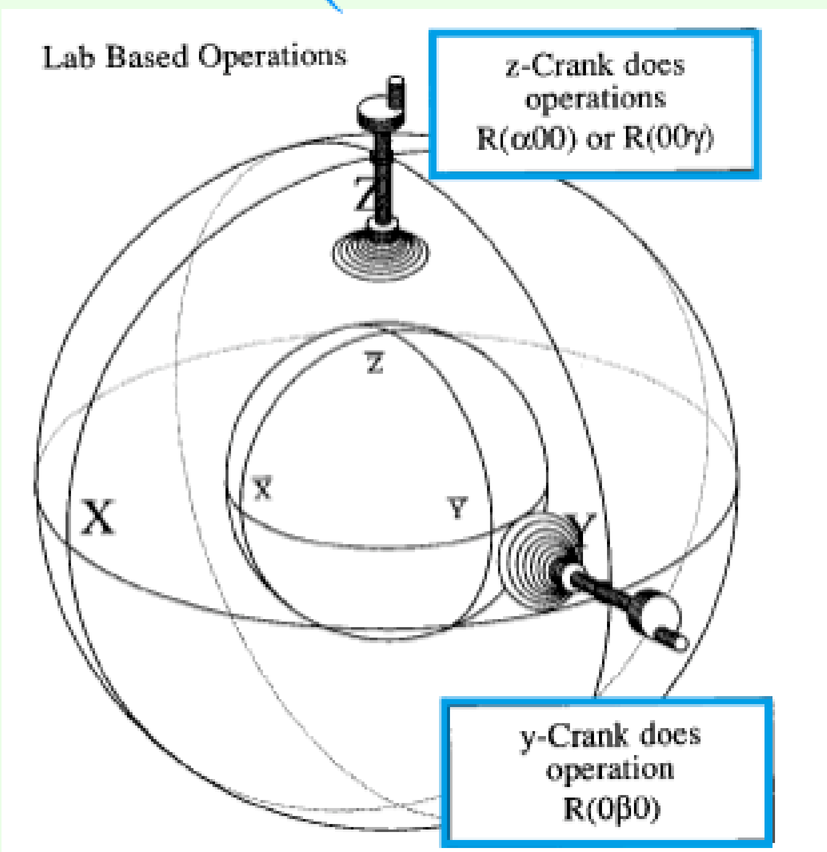
The exposition given here in sections. 3.5–3.6 is taken from refs. [73, 74]. Who wrote this down first I do not know, but I like Harter's exposition [155, 156, 157] best.

(2008) Princeton. Oxford 0X20 1TW

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

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

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

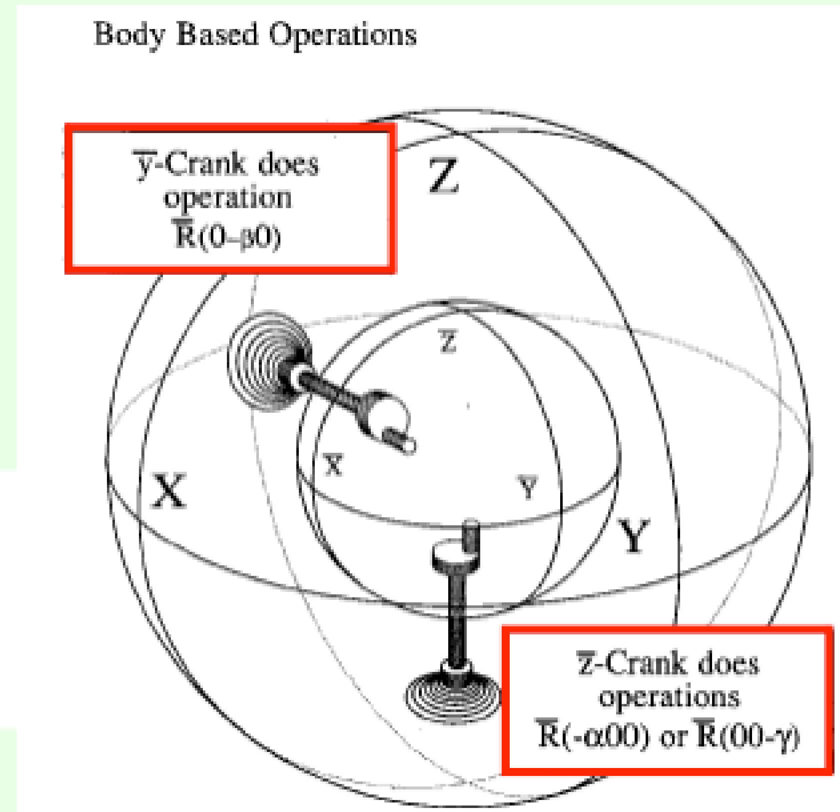


R *commutes* with *all* $\bar{\mathbf{R}}$

Mock-Mach relativity principle

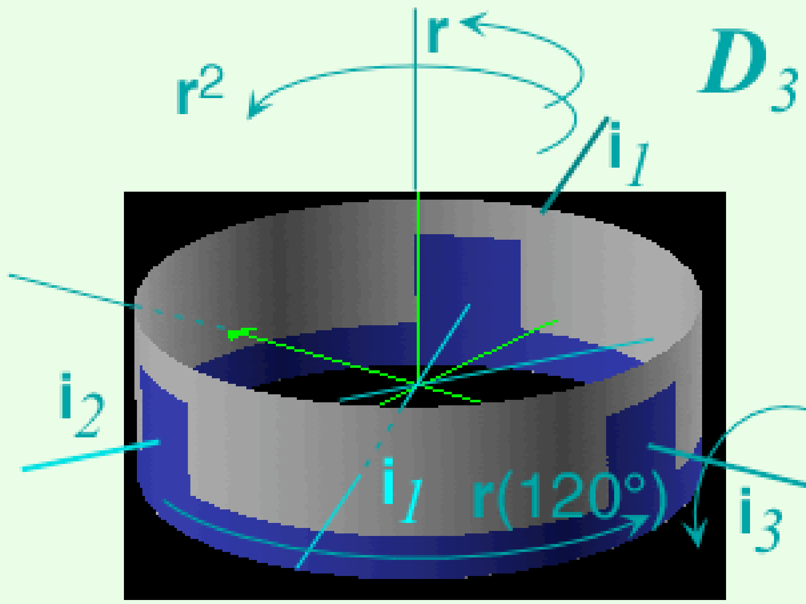
$$\mathbf{R}|1\rangle = \bar{\mathbf{R}}^{-1}|1\rangle$$

...for *one* state |1⟩ *only!*



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

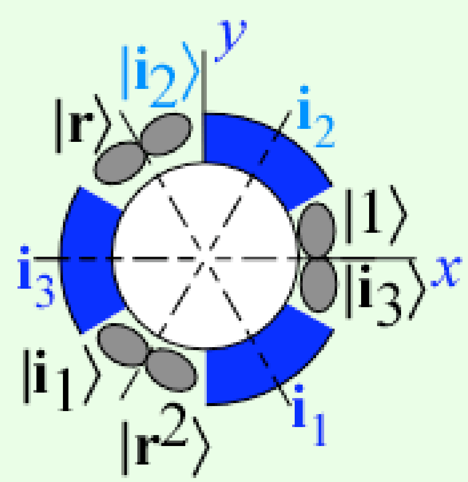
Example of GLOBAL vs LOCAL projector algebra for $D_3 \sim C_{3v}$

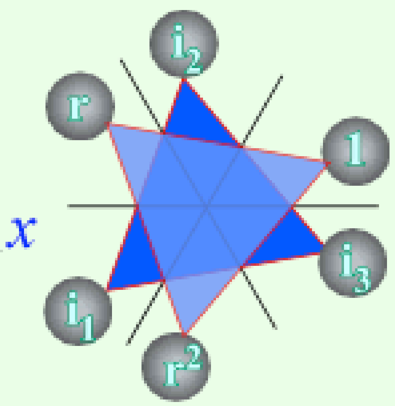


D_3

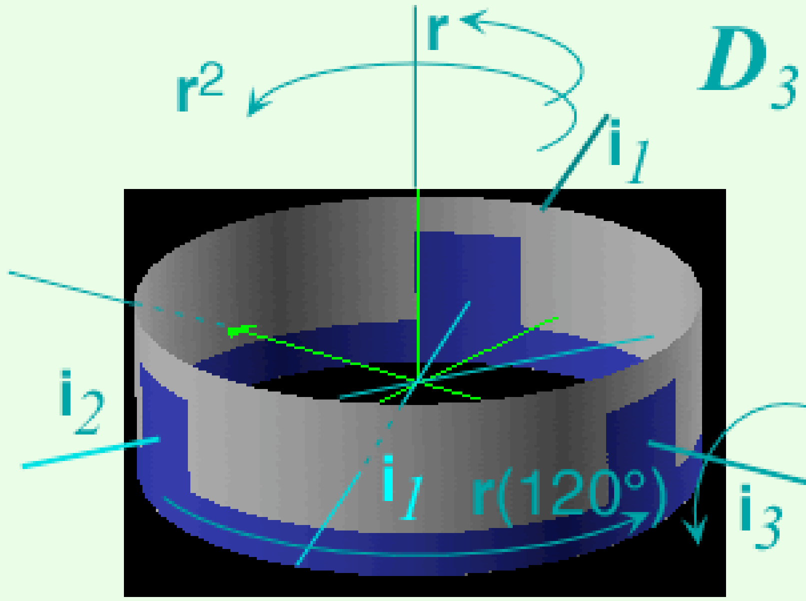
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

D_3-defined local-wave bases





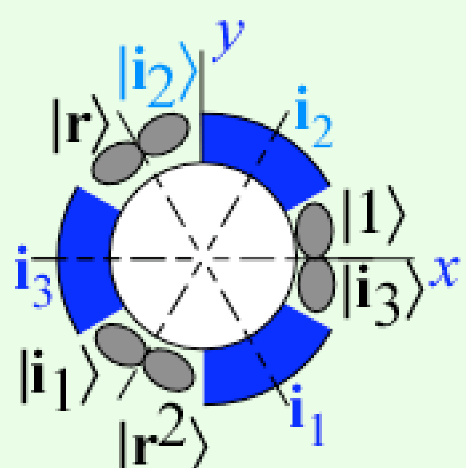
Example of GLOBAL vs LOCAL projector algebra for $D_3 \sim C_{3v}$

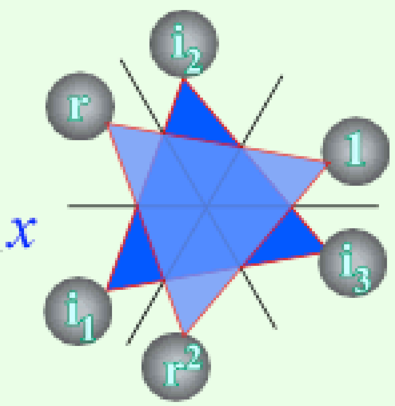


D_3

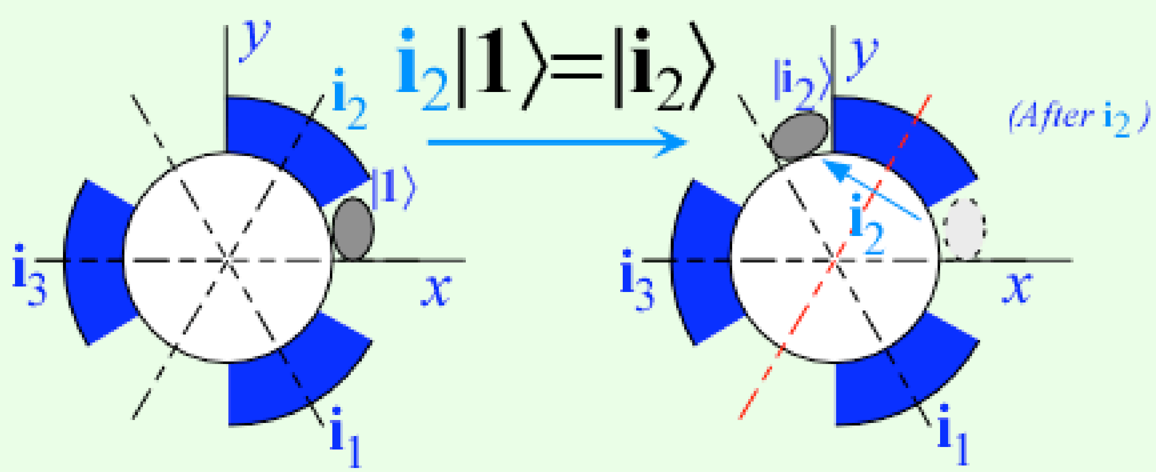
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

D_3-defined local-wave bases





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



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

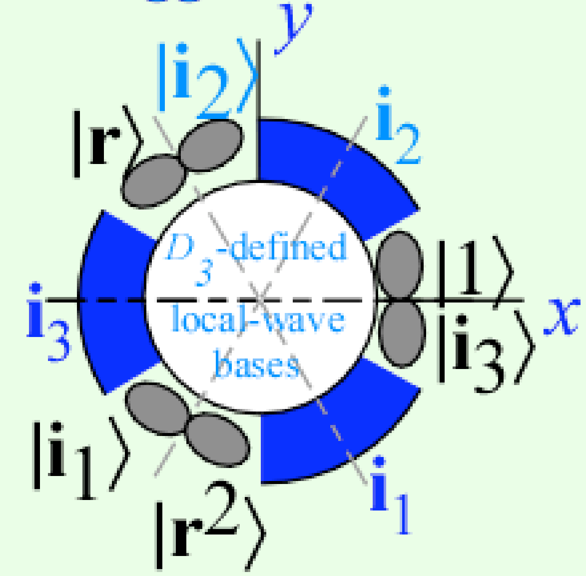
To represent *external* {..T,U,V,... }switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

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

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

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

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



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

To represent *external* {..**T**,**U**,**V**,... }switch **g** ⇄ **g**† on top of group table

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

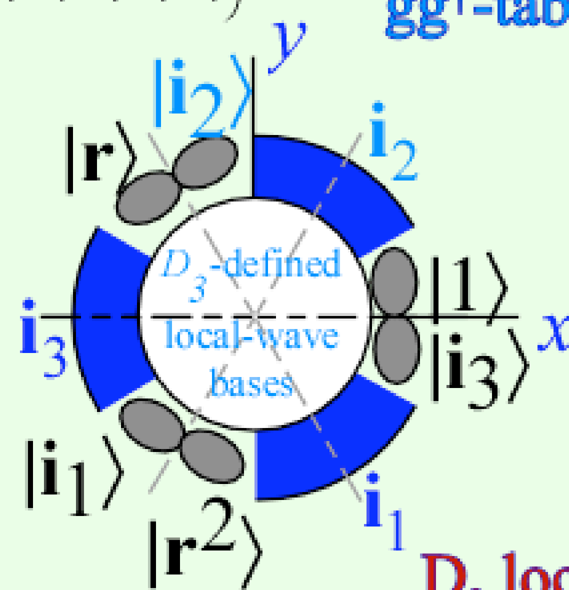
$$R^G(\mathbf{i}_1)=\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix},\ R^G(\mathbf{i}_2)=\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\cdot&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

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 gg†-table

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

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



D_3 local g†g-table

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

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

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

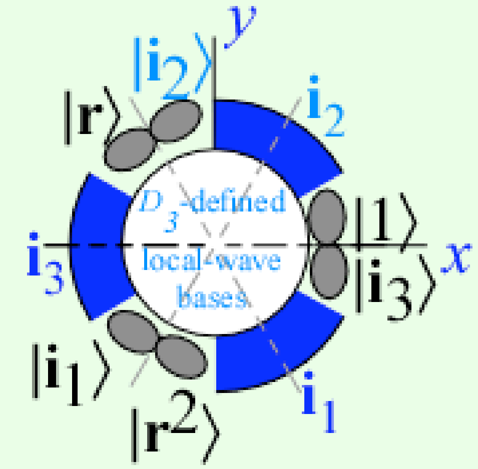
1	r	r^2	i_1	i_2	i_3
r^2	1	r	i_2	i_3	i_1
r	r^2	1	i_3	i_1	i_2
i_1	i_2	i_3	1	r	r^2
i_2	i_3	i_1	r^2	1	r
i_3	i_1	i_2	r	r^2	1

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

To represent *external* {..**T**,**U**,**V**,... }switch **g** ⇄ **g**†

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

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



Local ℍ matrix parametrized by ḡ's

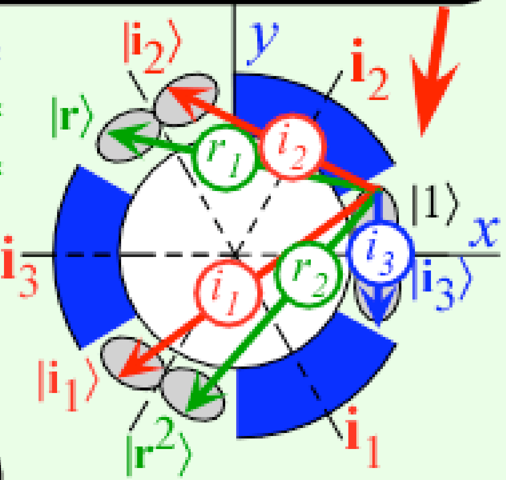
RESULT:
Any $R(\mathbf{T})$ commute with any $R(\overline{\mathbf{U}})$...

*So an 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*

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



local D_3 defined Hamiltonian matrix

*All these global **g** commute with general local ℍ matrix.*

To represent *internal* {..$\overline{\mathbf{T}}$,$\overline{\mathbf{U}}$,$\overline{\mathbf{V}}$,... } switch **g** ⇄ **g**†

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

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

ℍ ≡

	$\lvert 1)$	$\lvert r)$	$\lvert r^2)$	$\lvert i_1)$	$\lvert i_2)$	$\lvert i_3)$
$(1\lvert$	H	r_1	r_2	i_1	i_2	i_3
$(r\lvert$	r_2	H	r_1	i_2	i_3	i_1
$(r^2\lvert$	r_1	r_2	H	i_3	i_1	i_2
$(i_1\lvert$	i_1	i_2	i_3	H	r_1	r_2
$(i_2\lvert$	i_2	i_3	i_2	r_2	H	r_1
$(i_3\lvert$	i_3	i_1	i_2	r_1	r_2	H

Example of RELATIVITY-DUALITY

To represent *external* $\{..\mathbf{T},\mathbf{U},\mathbf{V},...\}$

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

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

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

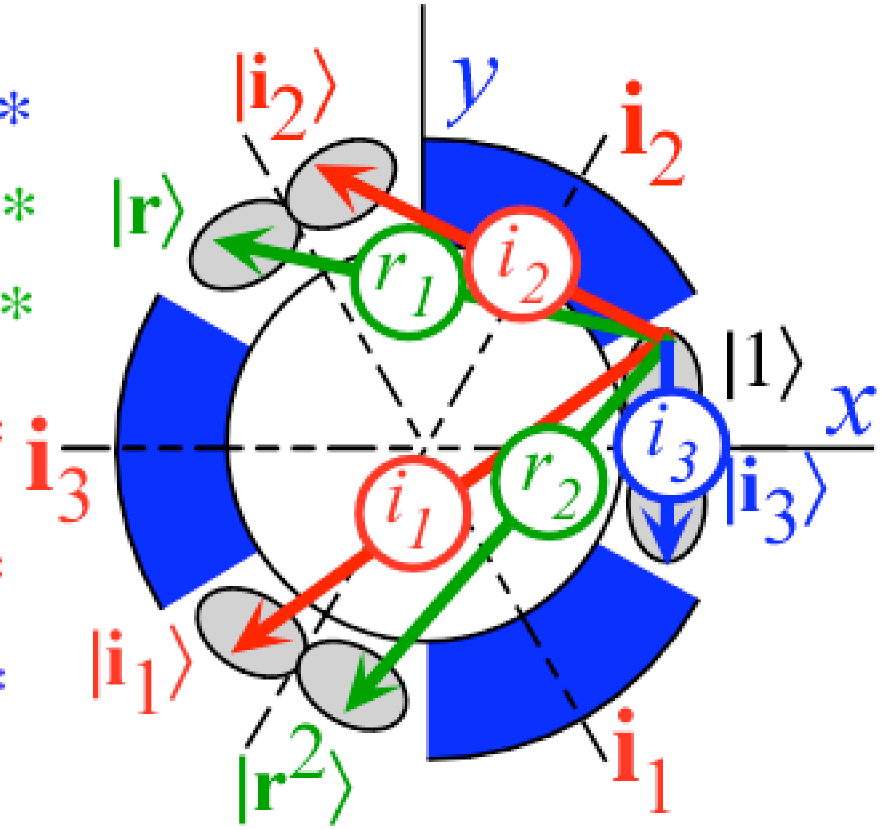
$$\mathbb{H} = H\mathbf{1}^0 + r_1\bar{\mathbf{r}}^1 + r_2\bar{\mathbf{r}}^2 + i_1\bar{\mathbf{i}}_1 + i_2\bar{\mathbf{i}}_2 + i_3\bar{\mathbf{i}}_3$$

is made from
Local *symmetry matrices*

To represent *internal* $\{..\bar{\mathbf{T}},\bar{\mathbf{U}},\bar{\mathbf{V}},...\}$ sy

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

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

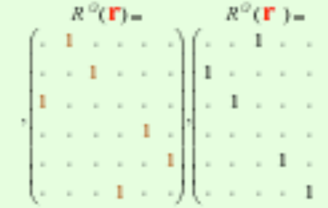


local-D_3-defined Hamiltonian matrix

$\mathbb{H} =$

	$\lvert\mathbf{1})$	$\lvert\mathbf{r})$	$\lvert\mathbf{r}^2)$	$\lvert\mathbf{i}_1)$	$\lvert\mathbf{i}_2)$	$\lvert\mathbf{i}_3)$
$(\mathbf{1}\rvert$	H	r_1	r_2	i_1	i_2	i_3
$(\mathbf{r}\rvert$	r_2	H	r_1	i_2	i_3	i_1
$(\mathbf{r}^2\rvert$	r_1	r_2	H	i_3	i_1	i_2
$(\mathbf{i}_1\rvert$	i_1	i_2	i_3	H	r_1	r_2
$(\mathbf{i}_2\rvert$	i_2	i_3	i_2	r_2	H	r_1
$(\mathbf{i}_3\rvert$	i_3	i_1	i_2	r_1	r_2	H

Q: How do you reduce/diagonalize all these matrices?



A: (1) Divide & Conquer (Use subgroup chains and sub-classes)

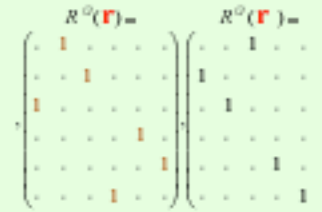
(2) Find commuting invariants (Using character projection algebra)

(3) Assemble

local-D_3-defined Hamiltonian matrix

$\mathbb{H}=$	$\vert 1\rangle$	$\vert r\rangle$	$\vert r^2\rangle$	$\vert i_1\rangle$	$\vert i_2\rangle$	$\vert i_3\rangle$
$\langle 1\vert$	H	r_1	r_2	i_1	i_2	i_3
$\langle r\vert$	r_2	H	r_1	i_2	i_3	i_1
$\langle r^2\vert$	r_1	r_2	H	i_3	i_1	i_2
$\langle i_1\vert$	i_1	i_2	i_3	H	r_1	r_2
$\langle i_2\vert$	i_2	i_3	i_2	r_2	H	r_1
$\langle i_3\vert$	i_3	i_1	i_2	r_1	r_2	H

Q: How do you reduce/diagonalize all these matrices?



A: (1) Divide & Conquer (Use subgroup chains and sub-classes)

(2) Find commuting invariants (Using character projection algebra)

(3) Assemble

local-D_3-defined Hamiltonian matrix

$\mathbf{H}=$

	$\|1)$	$\|r)$	$\|r^2)$	$\|i_1)$	$\|i_2)$	$\|i_3)$
$(1\|$	H	r_1	r_2	i_1	i_2	i_3
$(r\|$	r_2	H	r_1	i_2	i_3	i_1
$(r^2\|$	r_1	r_2	H	i_3	i_1	i_2
$(i_1\|$	i_1	i_2	i_3	H	r_1	r_2
$(i_2\|$	i_2	i_3	i_2	r_2	H	r_1
$(i_3\|$	i_3	i_1	i_2	r_1	r_2	H

D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

Important invariant numbers or "characters"

$\ell^{\alpha}=$ Irreducible representation (irrep) *dimension* or level *degeneracy*

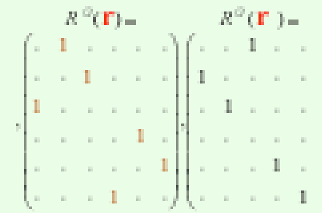
For symmetry group or algebra G

Centrum: $\kappa(G)=\Sigma_{irrep(\alpha)}(\ell^{\alpha})^0$ =Number of classes, invariants, irrep types, *all-commuting* ops

Rank: $\rho(G)=\Sigma_{irrep(\alpha)}(\ell^{\alpha})^1$ =Number of irrep idempotents $\mathbf{P}^{(\alpha)}_{n,n}$, *mutually-commuting* ops

Order: $^{o}(G)=\Sigma_{irrep(\alpha)}(\ell^{\alpha})^2$ =*Total* number of irrep projectors $\mathbf{P}^{(\alpha)}_{m,n}$ or symmetry ops

Q: How do you reduce/diagonalize all these matrices?



A: (1) Divide & Conquer (Use subgroup chains and sub-classes)
(2) Find commuting invariants (Using character projection algebra)
(3) Assemble

local-D_3-defined Hamiltonian matrix

$\mathbb{H}=$	$\vert 1\rangle$	$\vert r\rangle$	$\vert r^2\rangle$	$\vert i_1\rangle$	$\vert i_2\rangle$	$\vert i_3\rangle$
$\langle 1\vert$	H	r_1	r_2	i_1	i_2	i_3
$\langle r\vert$	r_2	H	r_1	i_2	i_3	i_1
$\langle r^2\vert$	r_1	r_2	H	i_3	i_1	i_2
$\langle i_1\vert$	i_1	i_2	i_3	H	r_1	r_2
$\langle i_2\vert$	i_2	i_3	i_2	r_2	H	r_1
$\langle i_3\vert$	i_3	i_1	i_2	r_1	r_2	H

Important invariant numbers or "characters"

D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

$\ell^\alpha=$ Irreducible representation (irrep) *dimension* or level *degeneracy*
For symmetry group or algebra G

Centrum: $\kappa(G)=\Sigma_{irrep(\alpha)}(\ell^\alpha)^0$ =Number of classes, invariants, irrep types, *all-commuting* ops

Rank: $\rho(G)=\Sigma_{irrep(\alpha)}(\ell^\alpha)^1$ =Number of irrep idempotents $\mathbf{P}^{(\alpha)}_{n,n}$, *mutually-commuting* ops

Order: $^o(G)=\Sigma_{irrep(\alpha)}(\ell^\alpha)^2$ =*Total* number of irrep projectors $\mathbf{P}^{(\alpha)}_{m,n}$ or symmetry ops

Example: $G=D_3$

Centrum: $\kappa(D_3)=\Sigma_{(\alpha)}(\ell^\alpha)^0=1^0+1^0+2^0=3$

Rank: $\rho(D_3)=\Sigma_{(\alpha)}(\ell^\alpha)^1=1^1+1^1+2^1=4$

Order: $^o(D_3)=\Sigma_{(\alpha)}(\ell^\alpha)^0=1^2+1^2+2^2=6$

$\ell^{A_1}=1$
$\ell^{A_2}=1$
$\ell^{E}=2$

Spectral analysis of non-commutative "Group-table Hamiltonian"

D_3 Example

1st Step: Spectral resolution of Center (Class algebra of D_3)

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

$\rightarrow$

Each class-sum κ_k commues with all of D_3.

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

Class products give spectral polynomial and all-commuting projectors $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, $\mathbf{P}^{A_2}$, and $\mathbf{P}^{E}$

$$0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3\cdot\mathbf{1})(\kappa_3 + 3\cdot\mathbf{1})(\kappa_3 - 0\cdot\mathbf{1})$$

Algebra Center like cell nucleus; everything's made here.

- *characters* *(invariant)*
- *H eigenvalues* *(depend on local sym.)*
- *H eigenvectors* *(depend on local sym.)*

Spectral analysis of non-commutative "Group-table Hamiltonian"

D_3 Example

1st Step: Spectral resolution of Center (Class algebra of D_3)

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

$\rightarrow$

Each class-sum $\underline{\kappa}_k$ commues with all of D_3.

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

Class products give spectral polynomial and all-commuting projectors $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, $\mathbf{P}^{A_2}$, and $\mathbf{P}^{E}$

$$0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3\cdot\mathbf{1})(\kappa_3 + 3\cdot\mathbf{1})(\kappa_3 - 0\cdot\mathbf{1})$$

$$0 = (\kappa_3 - 3\cdot\mathbf{1})\mathbf{P}^{A_1}$$
$$\kappa_3\mathbf{P}^{A_1} = +3\cdot\mathbf{P}^{A_1}$$

$$0 = (\kappa_3 + 3\cdot\mathbf{1})\mathbf{P}^{A_2}$$
$$\kappa_3\mathbf{P}^{A_2} = -3\cdot\mathbf{P}^{A_2}$$

$$0 = (\kappa_3 - 0\cdot\mathbf{1})\mathbf{P}^{E}$$
$$\kappa_3\mathbf{P}^{E} = +0\cdot\mathbf{P}^{E}$$

Class resolution into sum of eigenvalue · **Projector**

$$\kappa_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E}$$
$$\kappa_2 = 2\cdot\mathbf{P}^{A_1} - 2\cdot\mathbf{P}^{A_2} - 1\cdot\mathbf{P}^{E}$$
$$\kappa_3 = 3\cdot\mathbf{P}^{A_1} - 3\cdot\mathbf{P}^{A_2} + 0\cdot\mathbf{P}^{E}$$

$$\mathbf{P}^{A_1} = \frac{(\kappa_3+3\cdot\mathbf{1})(\kappa_3-0\cdot\mathbf{1})}{(+3+3)\ (+3-0)}$$

$$\mathbf{P}^{A_2} = \frac{(\kappa_3-3\cdot\mathbf{1})(\kappa_3-0\cdot\mathbf{1})}{(-3-3)\ (-3-0)}$$

$$\mathbf{P}^{E} = \frac{(\kappa_3-3\cdot\mathbf{1})(\kappa_3+3\cdot\mathbf{1})}{(+0-3)\ (+0+3)}$$

Spectral analysis of non-commutative "Group-table Hamiltonian"

D_3 Example

1st Step: Spectral resolution of Center (Class algebra of D_3)

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

$\rightarrow$

Each class-sum $\underline{\kappa}_k$ commues with all of D_3.

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_2	$2\kappa_1 + \kappa_2$	$2\kappa_3$
κ_3	$2\kappa_3$	$3\kappa_1 + 3\kappa_2$

Class products give spectral polynomial and all-commuting projectors $\mathbf{P}^{(\alpha)} = \mathbf{P}^{A_1}$, $\mathbf{P}^{A_2}$, and $\mathbf{P}^{E}$

$$0 = \kappa_3^3 - 9\kappa_3 = (\kappa_3 - 3\cdot\mathbf{1})(\kappa_3 + 3\cdot\mathbf{1})(\kappa_3 - 0\cdot\mathbf{1})$$

$$0 = (\kappa_3 - 3\cdot\mathbf{1})\mathbf{P}^{A_1} \qquad \kappa_3\mathbf{P}^{A_1} = +3\cdot\mathbf{P}^{A_1}$$

$$0 = (\kappa_3 + 3\cdot\mathbf{1})\mathbf{P}^{A_2} \qquad \kappa_3\mathbf{P}^{A_2} = -3\cdot\mathbf{P}^{A_2}$$

$$0 = (\kappa_3 - 0\cdot\mathbf{1})\mathbf{P}^{E} \qquad \kappa_3\mathbf{P}^{E} = +0\cdot\mathbf{P}^{E}$$

Class resolution into sum of eigenvalue · **Projector**

$$\kappa_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E}$$

$$\kappa_2 = 2\cdot\mathbf{P}^{A_1} - 2\cdot\mathbf{P}^{A_2} - 1\cdot\mathbf{P}^{E}$$

$$\kappa_3 = 3\cdot\mathbf{P}^{A_1} - 3\cdot\mathbf{P}^{A_2} + 0\cdot\mathbf{P}^{E}$$

$$\mathbf{P}^{A_1} = \frac{(\kappa_3+3\cdot\mathbf{1})(\kappa_3-0\cdot\mathbf{1})}{(+3+3)\ (+3-0)}$$

$$\mathbf{P}^{A_2} = \frac{(\kappa_3-3\cdot\mathbf{1})(\kappa_3-0\cdot\mathbf{1})}{(-3-3)\ (-3-0)}$$

$$\mathbf{P}^{E} = \frac{(\kappa_3-3\cdot\mathbf{1})(\kappa_3+3\cdot\mathbf{1})}{(+0-3)\ (+0+3)}$$

Inverse resolution gives D_3 Character Table

$$\mathbf{P}^{A_1} = (\kappa_1 + \kappa_2 + \kappa_3)/6 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2} = (\kappa_1 + \kappa_2 - \kappa_3)/6 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3)/6$$

$$\mathbf{P}^{E} = (2\kappa_1 - \kappa_2)/3 = (2\mathbf{1} - \mathbf{r}^1 - \mathbf{r}^2)/3$$

Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgoup(s) $C_2(\mathbf{i})$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)

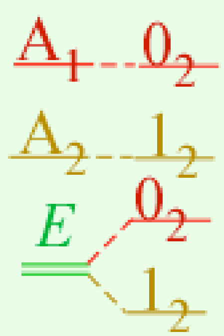
D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

C_2 $\kappa=$	$\mathbf{1}$	$\mathbf{i}_3$	
$p^{0_2}=$	1	1	/2
$p^{1_2}=$	1	-1	/2

C_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	
$p^{0_3}=$	1	1	1	/3
$p^{1_3}=$	1	ε	ε*	/3
$p^{2_3}=$	2	ε*	ε	/3

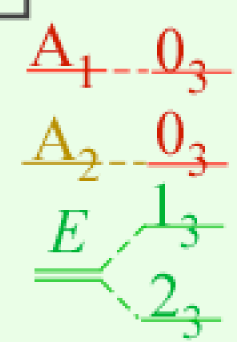
$\varepsilon=e^{2\pi i/3}$

level splitting



$D_3 \supset C_2$	0_2	1_2
$n^{A_1}=$	1	·
$n^{A_2}=$	·	1
$n^{E}=$	1	1
	A_1, E	A_2, E

level un-splitting or clustering



$D_3 \supset C_2$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1
	A_1, A_2	E	E

Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgoup(s) $C_2\{\mathbf{i}\}$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)

D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

C_2 $\kappa=$	$\mathbf{1}$	$\mathbf{i}_3$	
$p^{0_2}=$	1	1	/2
$p^{1_2}=$	1	-1	/2

C_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	
$p^{0_3}=$	1	1	1	/3
$p^{1_3}=$	1	ε	ε^*	/3
$p^{2_3}=$	2	ε^*	ε	/3

$\varepsilon=e^{2\pi i/3}$

$D_3\supset C_2$	0_2	1_2
$n^{A_1}=$	1	·
$n^{A_2}=$	·	1
$n^{E}=$	1	1

$D_3\supset C_2$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1

Correlation shows products of $\mathbf{P}^{(\alpha)}$ by the C_2-unit or by the C_3-unit make IRREDUCIBLE $\mathbf{P}^{(\alpha)}_{n,n}$

Rank $\rho(D_3)=4$ idempotent $\mathbf{P}^{(\alpha)}_{n_2 n_2}$

$\mathbf{1}=p^{0_2}+p^{1_2}$

$\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_2 0_2}$	·
$\mathbf{P}^{A_2}=$	·	$\mathbf{P}^{A_2}_{1_2 1_2}$
$\mathbf{P}^{E}=$	$\mathbf{P}^{E}_{0_2 0_2}$	$\mathbf{P}^{E}_{1_2 1_2}$

4 different idempotent $\mathbf{P}^{(\alpha)}_{n_3 n_3}$

$\mathbf{1}=p^{0_3}+p^{1_3}+p^{2_3}$

$\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_3 0_3}$	·	·
$\mathbf{P}^{A_2}=$	$\mathbf{P}^{A_2}_{0_3 0_3}$	·	·
$\mathbf{P}^{E}=$	·	$\mathbf{P}^{E}_{1_3 1_3}$	$\mathbf{P}^{E}_{2_3 2_3}$

Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

2nd Step: Spectral resolution of Class Projector(s) of D_3

Correlate D_3 characters with its subgoup(s) $C_2(\mathbf{i}\}$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)

D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

C_2 $\kappa=$	$\mathbf{1}$	$\mathbf{i}_3$	
$p^{0_2}=$	1	1	/2
$p^{1_2}=$	1	-1	/2

C_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	
$p^{0_3}=$	1	1	1	/3
$p^{1_3}=$	1	ε	ε^*	/3
$p^{2_3}=$	2	ε^*	ε	/3

$\varepsilon=e^{2\pi i/3}$

$D_3\supset C_2$	0_2	1_2
$n^{A_1}=$	1	·
$n^{A_2}=$	·	1
$n^{E}=$	1	1

$D_3\supset C_2$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1

Correlation shows products of $\mathbf{P}^{(\alpha)}$ by the C_2-unit or by the C_3-unit make IRREDUCIBLE $\mathbf{P}^{(\alpha)}_{n,n}$

$\mathbf{1}=p^{0_2}+p^{1_2}$

$\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_20_2}$	·
$\mathbf{P}^{A_2}=$	·	$\mathbf{P}^{A_2}_{1_21_2}$
$\mathbf{P}^{E}=$	$\mathbf{P}^{E}_{0_20_2}$	$\mathbf{P}^{E}_{1_21_2}$

$\mathbf{1}=p^{0_3}+p^{1_3}+p^{2_3}$

$\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_30_3}$	·	·
$\mathbf{P}^{A_2}=$	$\mathbf{P}^{A_2}_{0_30_3}$	·	·
$\mathbf{P}^{E}=$	·	$\mathbf{P}^{E}_{1_31_3}$	$\mathbf{P}^{E}_{2_32_3}$

Rank $\rho(D_3)=4$ idempotent $\mathbf{P}^{(\alpha)}_{n_2,n_2}$

$\mathbf{P}^{A_1}_{0_20_2}=\mathbf{P}^{A_1}p^{0_2}=\mathbf{P}^{A_1}(1+\mathbf{i}_3)/2=(1+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$

$\mathbf{P}^{A_2}_{1_21_2}=\mathbf{P}^{A_2}p^{1_2}=\mathbf{P}^{A_2}(1-\mathbf{i}_3)/2=(1+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$

$\mathbf{P}^{E}_{0_20_2}=\mathbf{P}^{E}p^{0_2}=\mathbf{P}^{E}(1+\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)/6$

$\mathbf{P}^{E}_{1_21_2}=\mathbf{P}^{E}p^{1_2}=\mathbf{P}^{E}(1-\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)/6$

4 different idempotent $\mathbf{P}^{(\alpha)}_{n_3,n_3}$

$\mathbf{P}^{A_1}_{0_30_3}=\mathbf{P}^{A_1}p^{0_3}=\mathbf{P}^{A_1}(1+\mathbf{r}^1+\mathbf{r}^2)/3=(1+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$

$\mathbf{P}^{A_2}_{0_30_3}=\mathbf{P}^{A_2}p^{0_3}=\mathbf{P}^{A_2}(1+\mathbf{r}^1+\mathbf{r}^2)/3=(1+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$

$\mathbf{P}^{E}_{1_31_3}=\mathbf{P}^{E}p^{1_3}=\mathbf{P}^{E}(1+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/3=(1+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/6$

$\mathbf{P}^{E}_{2_32_3}=\mathbf{P}^{E}p^{2_3}=\mathbf{P}^{E}(1+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/3=(1+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/6$

2nd Step: (contd.) While some class projectors $\mathbf{P}^{(\alpha)}$ split in two,

so ALSO DO some classes κ_k

D_3 κ = $\mathbf{1}$ | $\mathbf{r}^1+\mathbf{r}^2$ | $\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$

$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

Rank $\rho(D_3)=4$ idempotents $\mathbf{P}^{(\alpha)}$

Centrum $\kappa(D_3)=3$ idempotents $\mathbf{P}^{(\alpha)}$

4 *different* idempotent $\mathbf{P}^{(\alpha)}_{n,n}$

$$\mathbf{P}^{A_1}_{0_2 0_2}=\mathbf{P}^{A_1}p^{0_2}=\mathbf{P}^{A_1}(\mathbf{1}+\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}_{1_2 1_2}=\mathbf{P}^{A_2}p^{1_2}=\mathbf{P}^{A_2}(\mathbf{1}-\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

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

$$\mathbf{P}^{E}_{1_2 1_2}=\mathbf{P}^{E}p^{1_2}=\mathbf{P}^{E}(\mathbf{1}-\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)/6$$

$\mathbf{P}^E$ splits into $\mathbf{P}^E=\mathbf{P}^E_{0_2 0_2}+\mathbf{P}^E_{1_2 1_2}$,

class $\kappa_{\mathbf{i}}$ splits into $\kappa_{\mathbf{i}_{12}}$ and $\kappa_{\mathbf{i}_3}$

$$\mathbf{P}^{A_1}_{0_3 0_3}=\mathbf{P}^{A_1}p^{0_3}=\mathbf{P}^{A_1}(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2)/3=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}_{0_3 0_3}=\mathbf{P}^{A_2}p^{0_3}=\mathbf{P}^{A_2}(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2)/3=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

$$\mathbf{P}^{E}_{1_3 1_3}=\mathbf{P}^{E}p^{1_3}=\mathbf{P}^{E}(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/3=(\mathbf{1}+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/6$$

$$\mathbf{P}^{E}_{2_3 2_3}=\mathbf{P}^{E}p^{2_3}=\mathbf{P}^{E}(\mathbf{1}+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/3=(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/6$$

$\mathbf{P}^E$ splits into $\mathbf{P}^E=\mathbf{P}^E_{1_3 1_3}+\mathbf{P}^E_{2_3 2_3}$,

class $\kappa_{\mathbf{r}}$ splits into $\kappa_{\mathbf{r}^1}$ and $\kappa_{\mathbf{r}^2}$

2nd Step: (contd.) While some class projectors $\mathbf{P}^{(\alpha)}$ split in two, so ALSO DO some classes κ_k

D_3	$\kappa = \mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

Rank $\rho(D_3)=4$ idempotents $\mathbf{P}^{(\alpha)}$

$$\mathbf{P}^{A_1}_{0_2 0_2}=\mathbf{P}^{A_1}p^{0_2}=\mathbf{P}^{A_1}(1+\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}_{1_2 1_2}=\mathbf{P}^{A_2}p^{1_2}=\mathbf{P}^{A_2}(1-\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

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

$$\mathbf{P}^{E}_{1_2 1_2}=\mathbf{P}^{E}p^{1_2}=\mathbf{P}^{E}(1-\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)/6$$

$\mathbf{P}^E$ *splits into* $\mathbf{P}^E=\mathbf{P}^E_{0_2 0_2}+\mathbf{P}^E_{1_2 1_2}$,

class $\kappa_{\mathbf{i}}$ *splits into* $\kappa_{\mathbf{i}_{12}}$ *and* $\kappa_{\mathbf{i}_3}$

4 *different* idempotent $\mathbf{P}^{(\alpha)}_{n,n}$

Centrum $\kappa(D_3)=3$ idempotents $\mathbf{P}^{(\alpha)}$

$$\mathbf{P}^{A_1}_{0_3 0_3}=\mathbf{P}^{A_1}p^{0_3}=\mathbf{P}^{A_1}(1+\mathbf{r}^1+\mathbf{r}^2)/3=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}_{0_3 0_3}=\mathbf{P}^{A_2}p^{0_3}=\mathbf{P}^{A_2}(1+\mathbf{r}^1+\mathbf{r}^2)/3=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

$$\mathbf{P}^{E}_{1_3 1_3}=\mathbf{P}^{E}p^{1_3}=\mathbf{P}^{E}(1+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/3=(\mathbf{1}+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/6$$

$$\mathbf{P}^{E}_{2_3 2_3}=\mathbf{P}^{E}p^{2_3}=\mathbf{P}^{E}(1+\varepsilon\mathbf{r}^1+\varepsilon^*\mathbf{r}^2)/3=(\mathbf{1}+\varepsilon^*\mathbf{r}^1+\varepsilon\mathbf{r}^2)/6$$

$\mathbf{P}^E$ *splits into* $\mathbf{P}^E=\mathbf{P}^E_{1_3 1_3}+\mathbf{P}^E_{2_3 2_3}$,

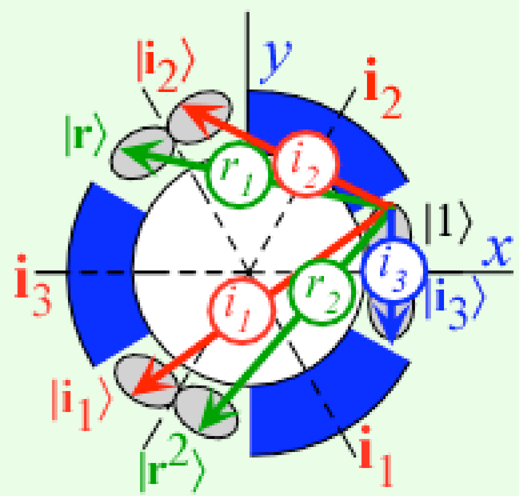
class $\kappa_{\mathbf{r}}$ *splits into* $\kappa_{\mathbf{r}^1}$ *and* $\kappa_{\mathbf{r}^2}$

$r=r_2$ must equal r_1

$i=i_2$ must equal i_1

For Local $D_3 \supset C_2(\mathbf{i}_3)$ symmetry

i_3 is free parameter



Rank $\rho(D_3)=4$ parameters in either case

$i=i_1=i_2=i_3$

For Local $D_3 \supset C_3(\mathbf{r}^p)$ symmetry

r_1 and r_2 are free

Centrum $\kappa(D_3)=3$
idempotents
$\mathbf{P}^{(\alpha)}$

D_3 κ = $\mathbf{1}$ | $\mathbf{r}^1+\mathbf{r}^2$ | $\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$

	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

Rank $\rho(D_3)=4$
idempotents
$\mathbf{P}^{(\alpha)}_{n,n}$

$\mathbf{P}^{A_1}_{x,x}=\mathbf{P}^{A_1}_{0_2 0_2}=\mathbf{P}^{A_1}p^{0_2}=\mathbf{P}^{A_1}(\mathbf{1}+\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

The old '**g**-equals-**1**-times-**g**-times-**1**' Trick

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

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

$$\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}=(\mathbf{P}^{A_1}_{x,x}+\mathbf{P}^{A_2}_{y,y}+\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{y,y})\cdot\mathbf{g}\cdot(\mathbf{P}^{A_1}_{x,x}+\mathbf{P}^{A_2}_{y,y}+\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{y,y})$$

$$\mathbf{g}=\mathbf{P}^{A_1}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}+\mathbf{P}^{A_2}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}+\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}+\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}$$

Order $^{\circ}(D_3)=6$
projectors
$\mathbf{P}^{(\alpha)}_{m,n}$

Six D_3 projectors: 4 idempotents + 2 nilpotents (off-diag.)

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

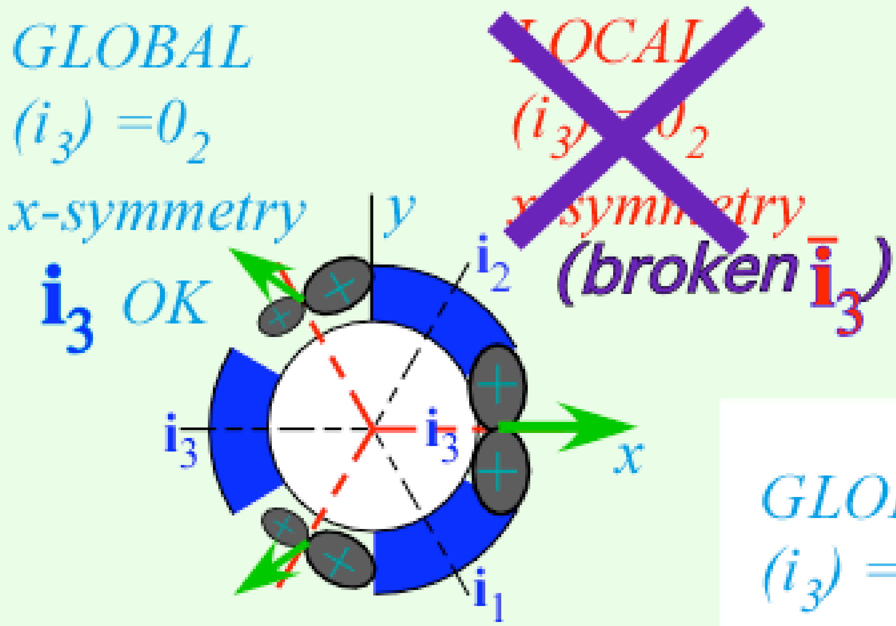
	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	
$\mathbf{P}^{E}_{x,y}=$	(0	-1	1	-1	+1	0)	/√3/2
$\mathbf{P}^{E}_{y,y}=$	(2	-1	-1	+1	+1	-2)	/6

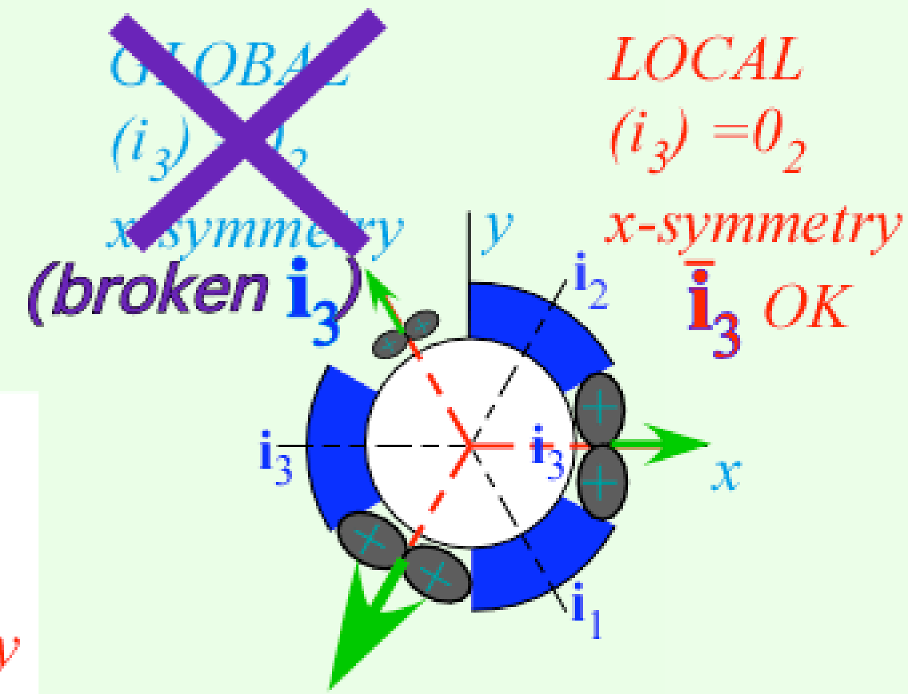
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|\mathbf{1}\right\rangle$$

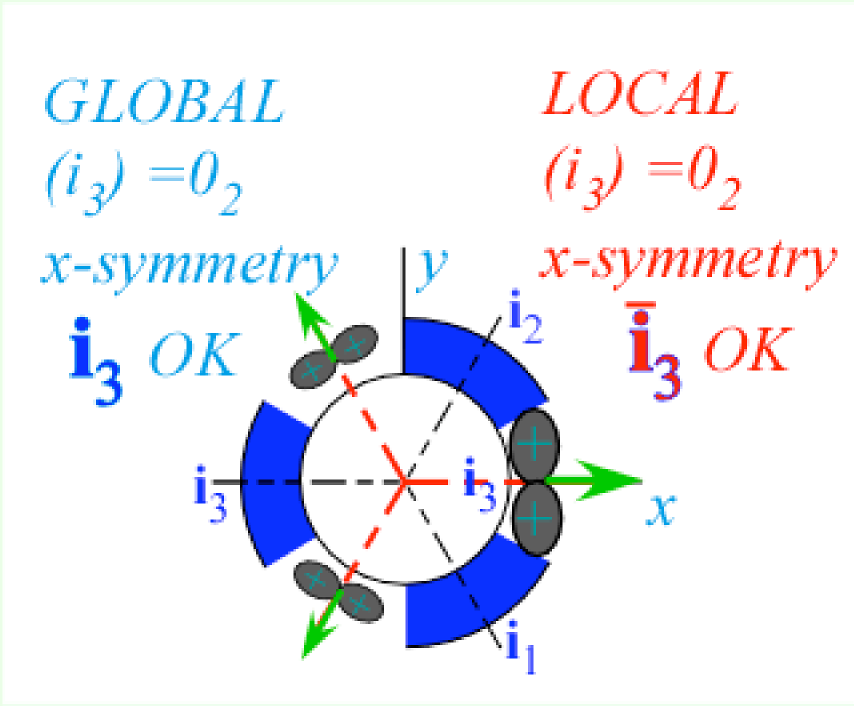
external LAB — *internal BOD*

symmety label-e — *symmety label-b*

GLOBAL — *LOCAL*







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

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

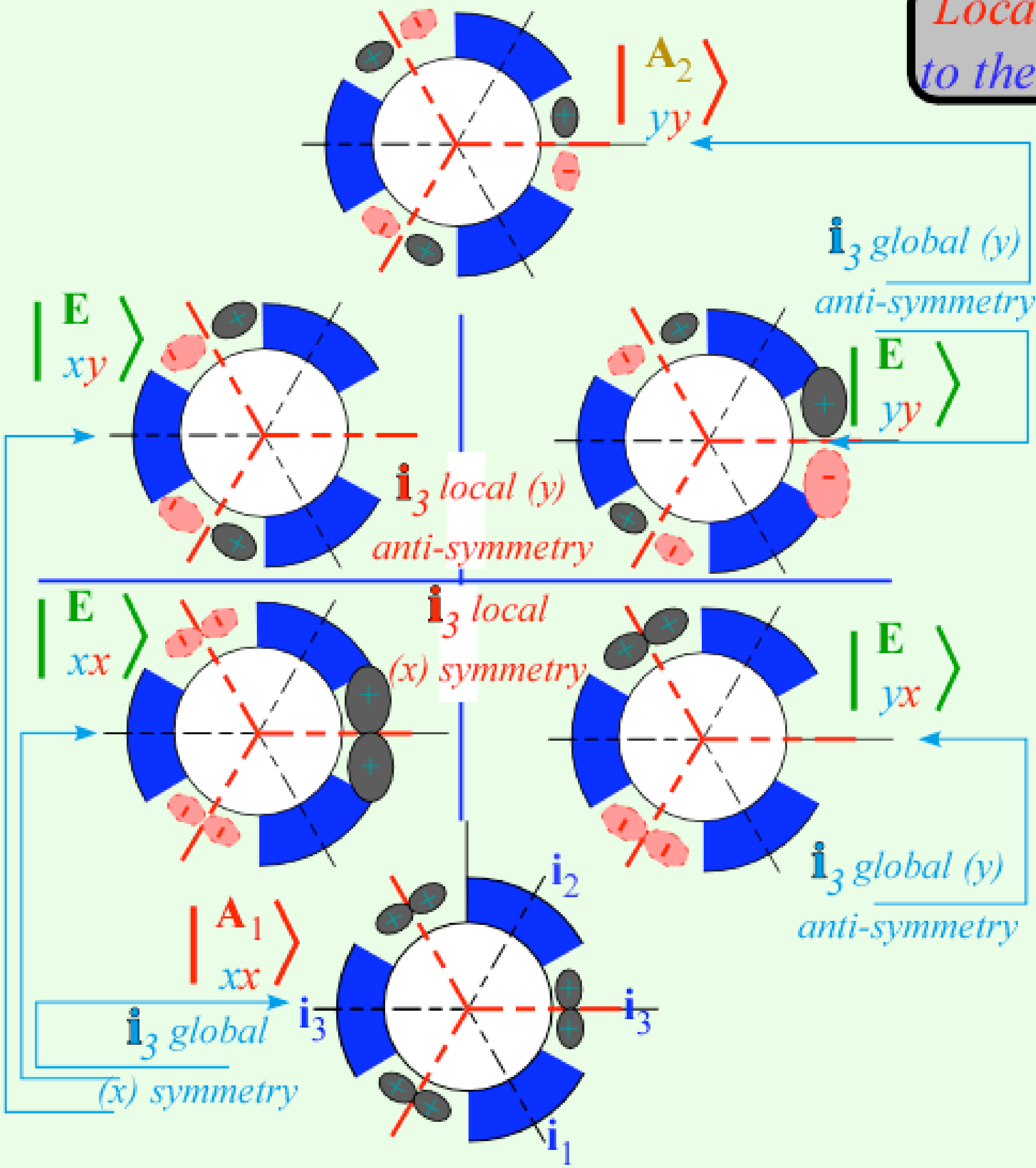
Global (LAB) symmetry

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

Local (BOD) symmetry

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

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



	$\mathbf{1}$	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	
$\mathbf{P}^{A_2}_{y,y}=$	(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

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

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 (previous slide)*
- *Complete Hamiltonian*

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

A_1-block

A_2-block

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

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

gives:

A_1-level: $H + 2r + 2i + i_3$

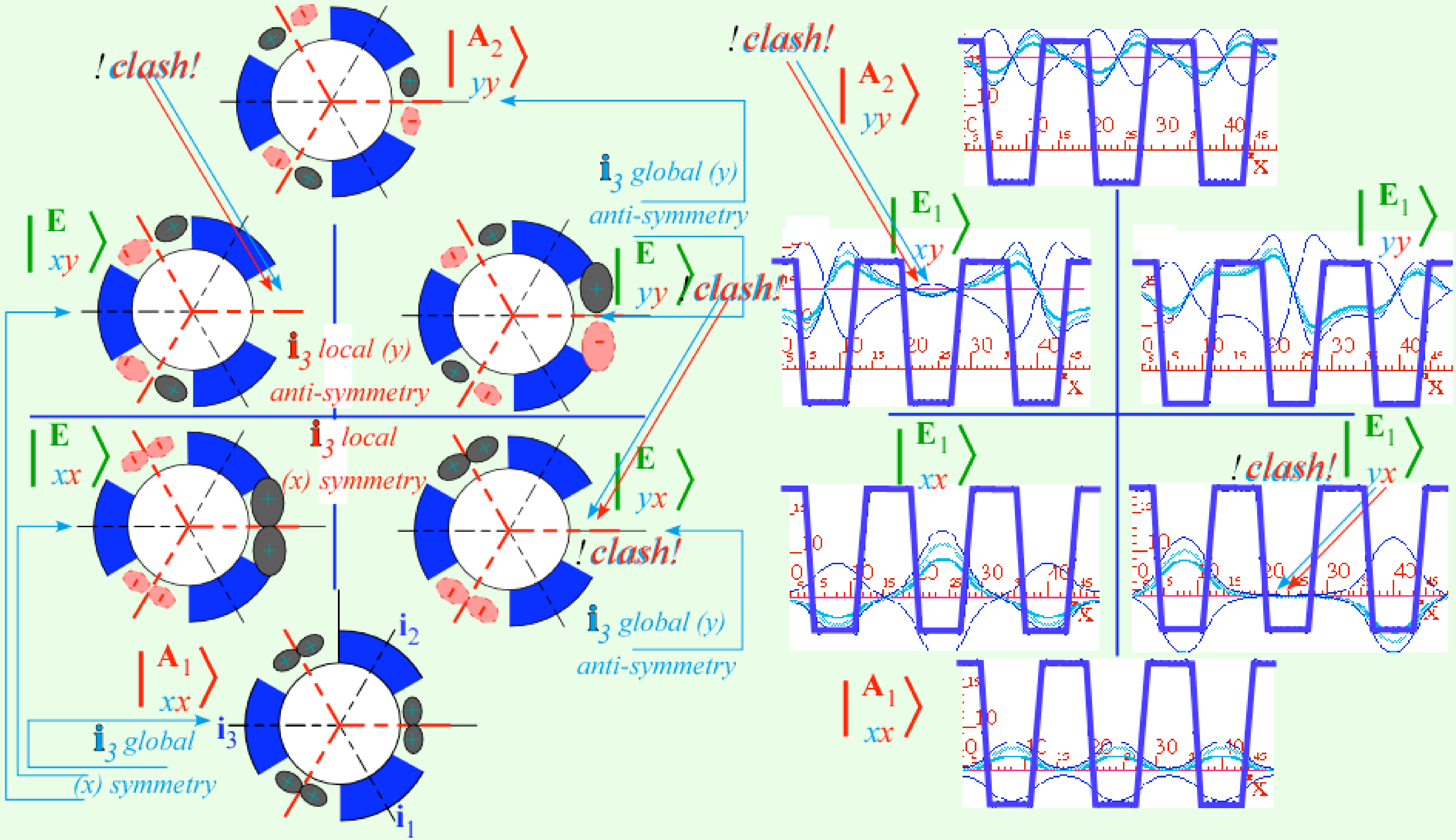
A_1-level: $H + 2r - 2i - i_3$

E_x-level: $H - r - i + i_3$

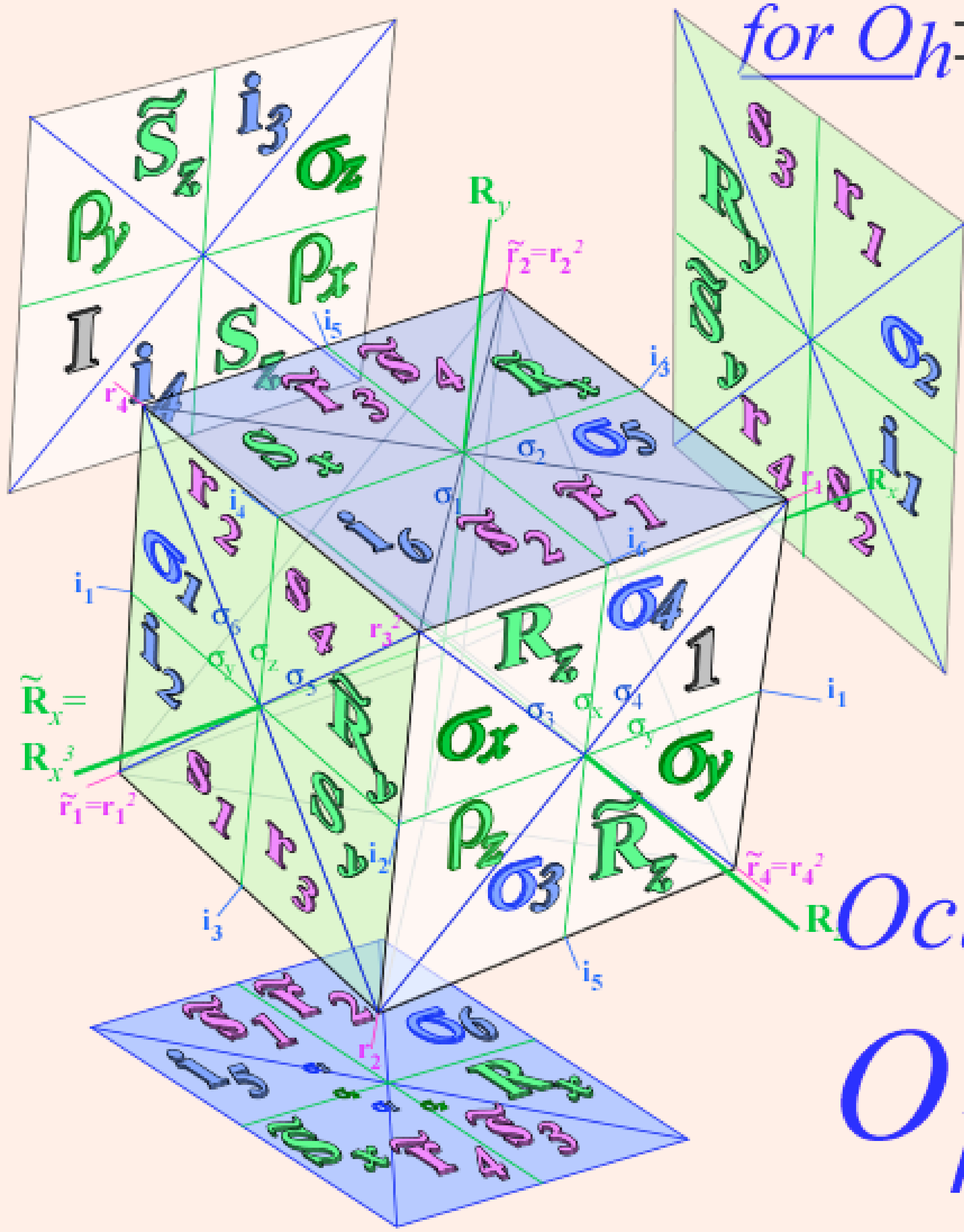
E_y-level: $H - r + i - i_3$

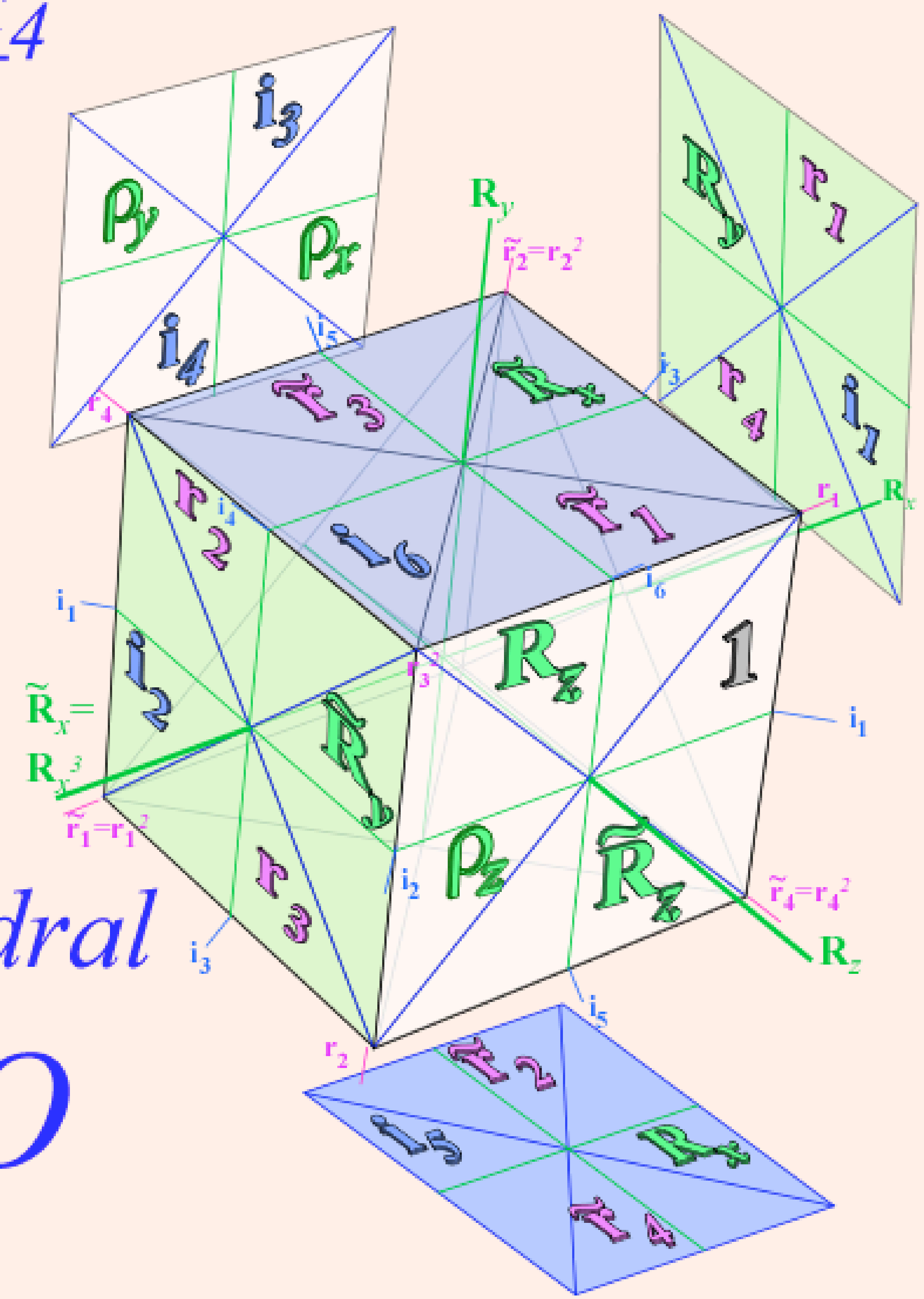
When there is no there, there...

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



Example of GLOBAL vs LOCAL projector algebra
for $O_h \supset O \supset C_4$





Octahedral

$O_h \supset O$

$\ell^{A_1}=1$

$\ell^{A_2}=1$

$\ell^{E}=2$

$\ell^{T_1}=3$

$\ell^{T_2}=3$

Example: $G=O$

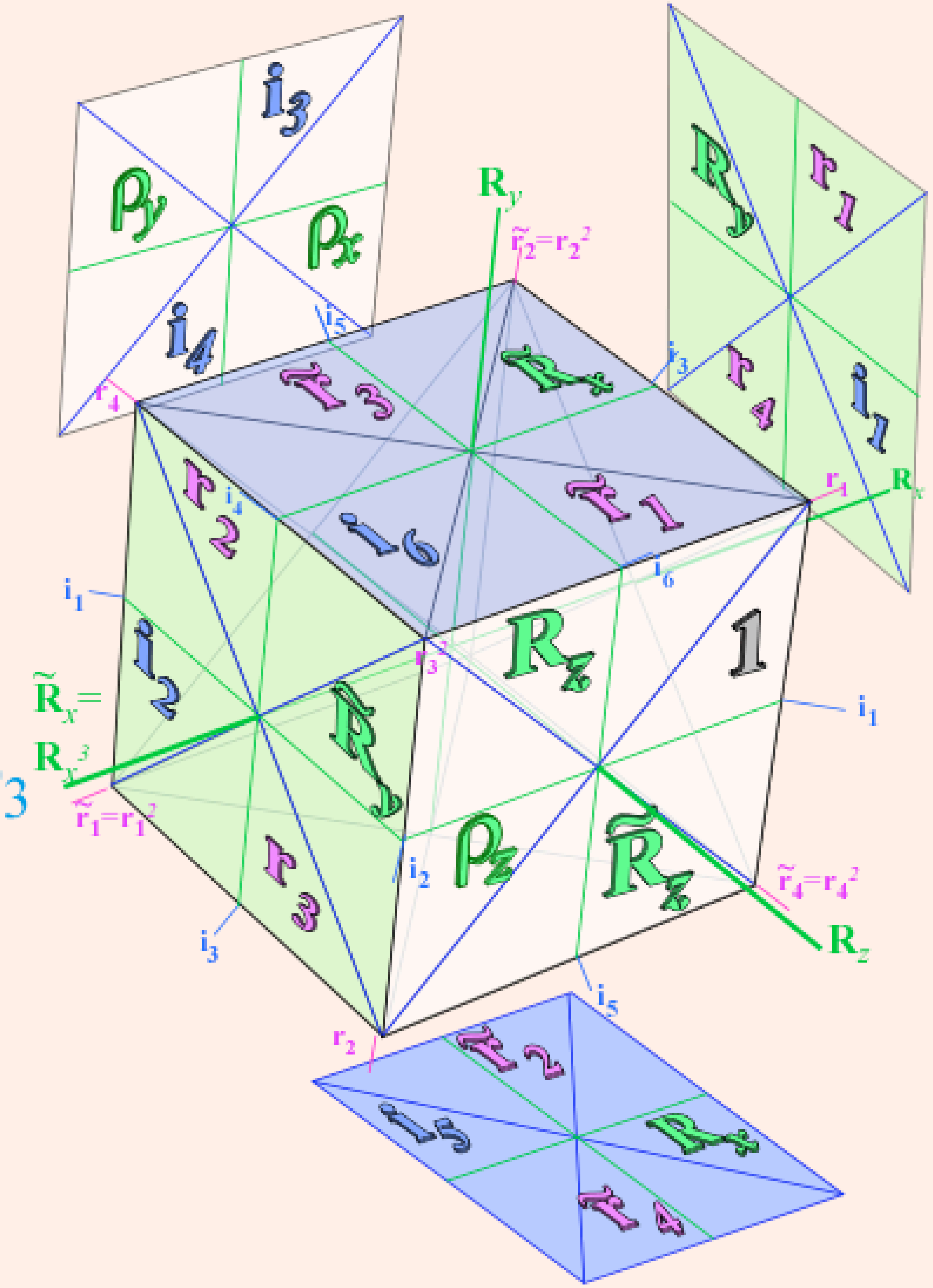
Cubic-Octahedral Group O

Centrum: $\kappa(O)=\Sigma_{(\alpha)}\,(\ell^{\alpha})^0 = 1^0+1^0+2^0+3^0+3^0=5$

Rank: $\rho(O)=\Sigma_{(\alpha)}\,(\ell^{\alpha})^1 = 1^1+1^1+2^1+3^1+3^1=10$

Order: $^{o}(O)=\Sigma_{(\alpha)}\,(\ell^{\alpha})^0 = 1^2+1^2+2^2+3^2+3^2=24$

O group $\chi^{\alpha}_{\kappa_g}$	$g=1$	r_{1-4} $\tilde{r}_{1-4}$	ρ_{xyz}	R_{xyz} $\tilde{R}_{xyz}$	i_{1-6}
$\alpha=A_1$	1	1	1	1	1
A_2	1	1	1	-1	-1
E	2	-1	2	0	0
T_1	3	0	-1	1	-1
T_2	3	0	-1	-1	1



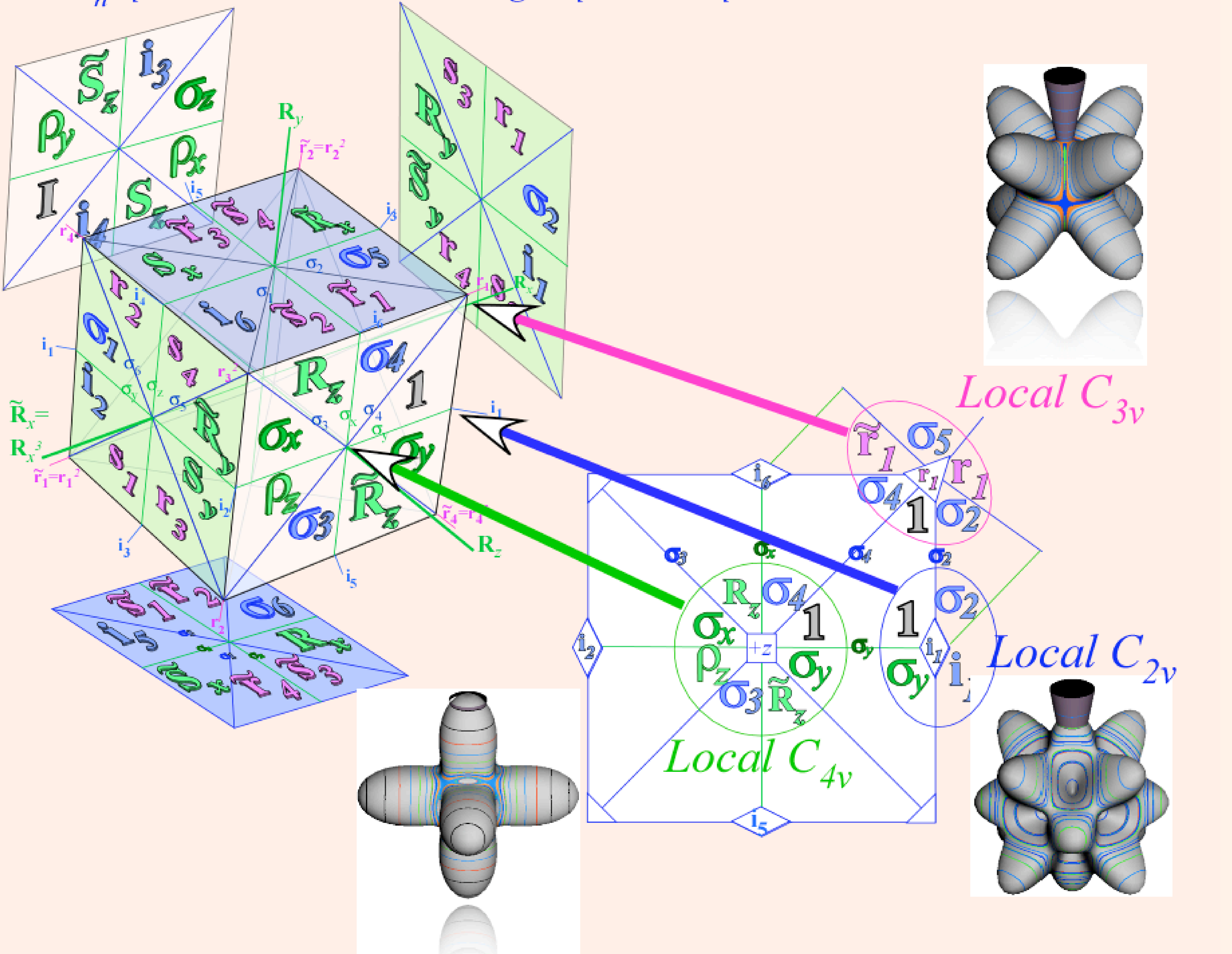
$O \supset C_4$

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

$O \supset C_3$

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

O_h operator slide rule and subgroup / coset-space structure



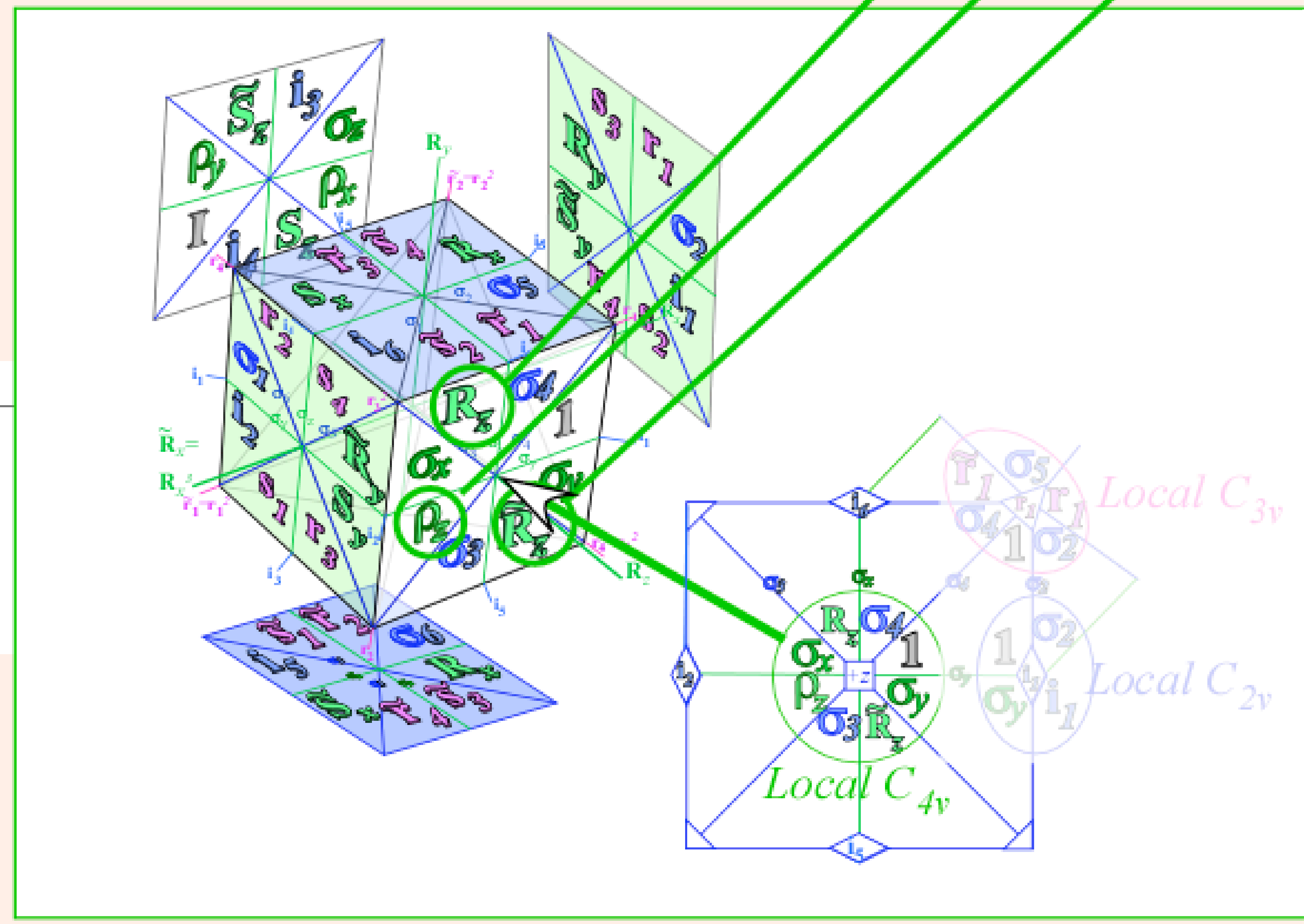
$O \supset C_4$

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

C_4 Projectors to split octahedral P^α

$$\mathbf{p}_{m_4} = \sum_{p=0}^{3} \frac{e^{2\pi i m \cdot p/4}}{4} \mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1} + \mathbf{R}_z + \rho_z + \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1} + i\mathbf{R}_z - \rho_z - i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1} - \mathbf{R}_z + \rho_z - \tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{3_4} = (\mathbf{1} - i\mathbf{R}_z - \rho_z + i\tilde{\mathbf{R}}_z)/4 \end{cases}$$

$\mathbf{1}\cdot\mathbf{P}^\alpha =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^\alpha$
$\mathbf{1}\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_4 0_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2} =$	0	$+0$	$+\mathbf{P}^{A_2}_{2_4 2_4}$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{E} =$	$\mathbf{P}^{E}_{0_4 0_4}$	$+0$	$+\mathbf{P}^{E}_{2_4 2_4}$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{T_1} =$	$\mathbf{P}^{T_1}_{0_4 0_4}$	$+\mathbf{P}^{T_1}_{1_4 1_4}$	$+0$	$+\mathbf{P}^{T_1}_{3_4 3_4}$
$\mathbf{1}\cdot\mathbf{P}^{T_2} =$	0	$+\mathbf{P}^{T_2}_{1_4 1_4}$	$+\mathbf{P}^{T_2}_{2_4 2_4}$	$+\mathbf{P}^{T_2}_{3_4 3_4}$



largest local symmetry C_4 => smallest level-clusters (6-levels)

C_4 subgroup correlation to O

$O\supset C_4$	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

C_4 Projectors to split octahedral P^α

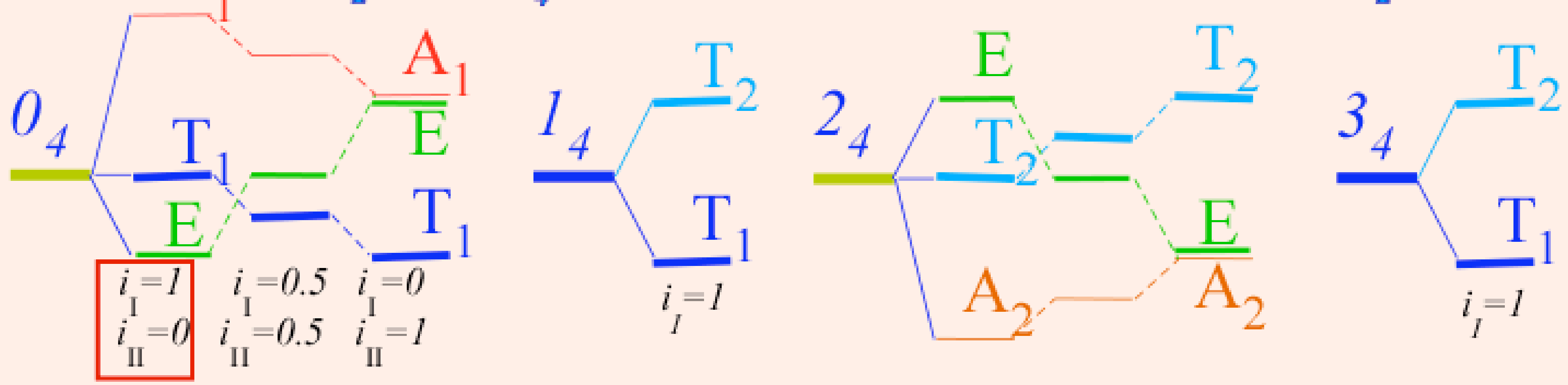
$$\mathbf{p}_{m_4}=\sum_{p=0}^{3}\frac{e^{2\pi i m\cdot p/4}}{4}\mathbf{R}_z^p=\begin{cases}\mathbf{p}_{0_4}=(\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{1_4}=(\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{2_4}=(\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4\\ \mathbf{p}_{3_4}=(\mathbf{1}-i\mathbf{R}_z-\rho_z+i\tilde{\mathbf{R}}_z)/4\end{cases}$$

$\mathbf{1}\cdot\mathbf{P}^\alpha=$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^\alpha$
$\mathbf{1}\cdot\mathbf{P}^{A_1}=$	$\mathbf{P}^{A_1}_{0_40_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2}=$	0	$+0$	$+\mathbf{P}^{A_2}_{2_42_4}$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{E}=$	$\mathbf{P}^{E}_{0_40_4}$	$+0$	$+\mathbf{P}^{E}_{2_42_4}$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{T_1}=$	$\mathbf{P}^{T_1}_{0_40_4}$	$+\mathbf{P}^{T_1}_{1_41_4}$	$+0$	$+\mathbf{P}^{T_1}_{3_43_4}$
$\mathbf{1}\cdot\mathbf{P}^{T_2}=$	0	$+\mathbf{P}^{T_2}_{1_41_4}$	$+\mathbf{P}^{T_2}_{2_42_4}$	$+\mathbf{P}^{T_2}_{3_43_4}$

10 split $O\supset C_4$ octahedral P^α related to 10 split sub-classes

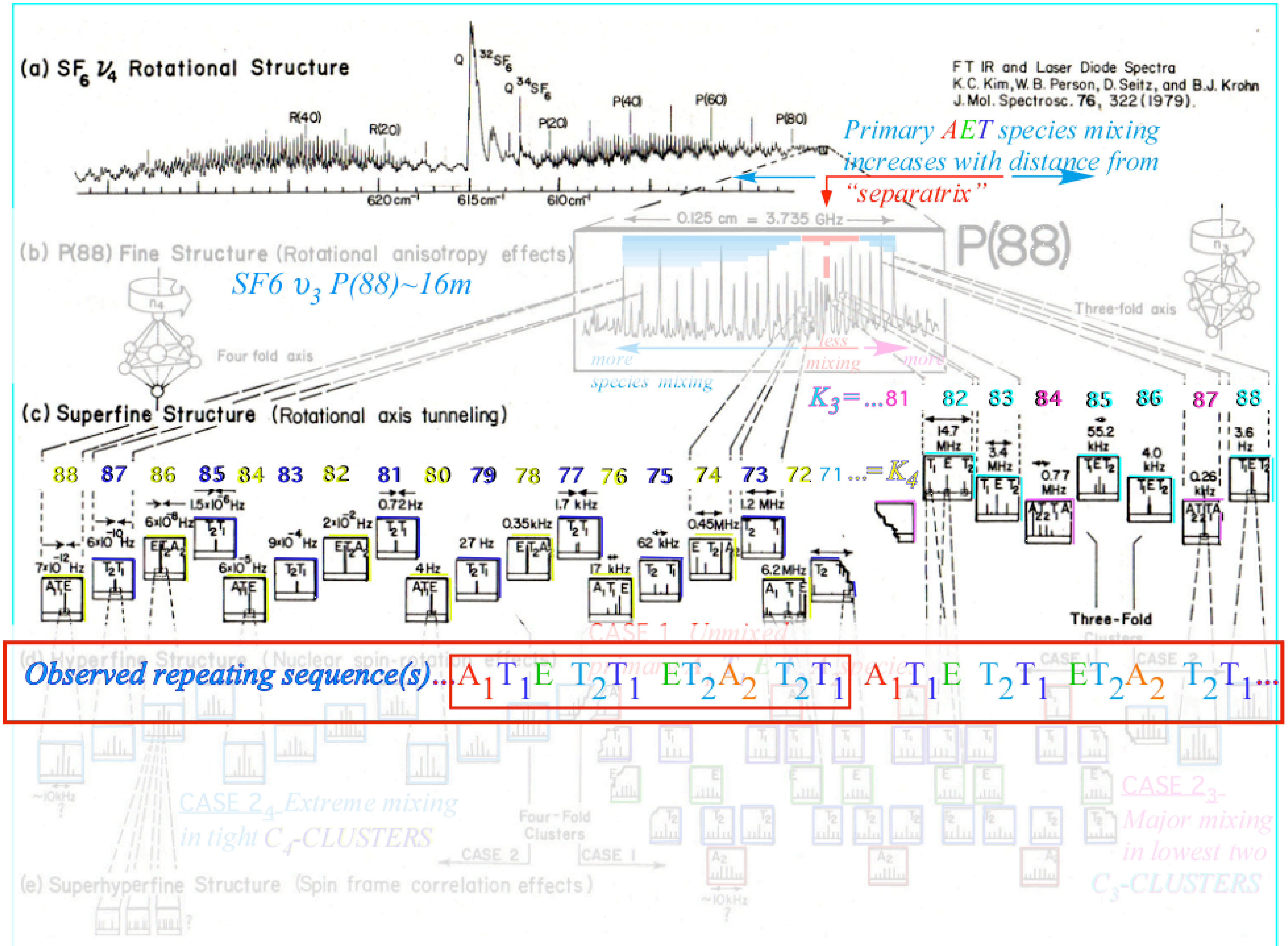
$\mathbf{P}^{(\alpha)}_{n_4n_4}(O\supset C_4)$	$\mathbf{1}$	$r_1r_2\tilde{r}_3\tilde{r}_4$	$\tilde{r}_1\tilde{r}_2r_3r_4$	$\rho_x\rho_y$	ρ_z	$R_x\tilde{R}_xR_y\tilde{R}_y$	R_z	$\tilde{R}_z$	$i_1i_2i_5i_6$	i_3i_4
$24\cdot\mathbf{P}^{A_1}_{0_40_4}$	1	1	1	1	1	1	1	1	1	1
$24\cdot\mathbf{P}^{A_2}_{2_42_4}$	1	1	1	1	1	-1	-1	-1	-1	-1
$12\cdot\mathbf{P}^{E}_{0_40_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1	1	$-\frac{1}{2}$	1
$12\cdot\mathbf{P}^{E}_{2_42_4}$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	1	1	$+\frac{1}{2}$	-1	-1	$+\frac{1}{2}$	-1
$8\cdot\mathbf{P}^{T_1}_{1_41_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$-i$	$+i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{3_43_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$+\frac{1}{2}$	$+i$	$-i$	$-\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_1}_{0_40_4}$	1	0	0	-1	1	0	1	1	0	-1
$8\cdot\mathbf{P}^{T_2}_{1_41_4}$	1	$+\frac{i}{2}$	$-\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$-i$	$+i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{3_43_4}$	1	$-\frac{i}{2}$	$+\frac{i}{2}$	0	-1	$-\frac{1}{2}$	$+i$	$-i$	$+\frac{1}{2}$	0
$8\cdot\mathbf{P}^{T_2}_{2_42_4}$	1	0	0	-1	1	0	-1	-1	0	1

10 split $O \supset C_4$ octahedral e-vals ε^{α} versus 10 sub-class parameters



Sequence if $i_I = i_{1256}$ only non-zero parameter: A_1T_1E T_2T_1 ET_2A_2 T_2T_1

$O \supset C_4$	$0°$	$r_n 120°$	$\rho_n 180°$	$R_n 90°$	$i_n 180°$	
0_4	$\cdot$	$r_I = \mathrm{Re}\, r_{1234}$ $m_I = \mathrm{Im}\, r_{1234}$	$\cdot$	$R_z = \mathrm{Re} R_z$ $I_z = \mathrm{Im} R_z$	$i_I = i_{1256}$ $i_{II} = i_{34}$	
$\varepsilon^{A_1}_{0_4} =$	g_0	$+4r_I$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_I + 2i_{II}$	
$\varepsilon^{T_1}_{0_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$-2i_{II}$	
$\varepsilon^{E}_{0_4}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_I + 2i_{II}$	
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon^{T_2}_{1_4}$	g_0	$+2m_I$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_I$	
$\varepsilon^{T_1}_{1_4}$	g_0	$-2m_I$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_I$	
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon^{E}_{2_4}$	g_0	$-2r_I$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_I - 2i_{II}$	
$\varepsilon^{T_2}_{2_4}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$+2i_{II}$	
$\varepsilon^{A_2}_{2_4}$	g_0	$+4r_I$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_I - 2i_{II}$	
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon^{T_2}_{3_4}$	g_0	$-2m_I$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_I$	
$\varepsilon^{T_1}_{3_4}$	g_0	$+2m_I$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_I$	


(a) SF6 ν4 Rotational Structure
FT IR and Laser Diode Spectra
K.C. Kim, W. B. Person, D. Seitz, and B.J. Krohn
J. Mol. Spectrosc. 76, 322 (1979).
Primary AET species mixing increases with distance from "separatrix"
0.125 cm = 3.735 GHz
P(88)
(b) P(88) Fine Structure (Rotational anisotropy effects)
SF6 υ3 P(88)~16m
Four fold axis
Three-fold axis
more species mixing
less mixing
more
(c) Superfine Structure (Rotational axis tunneling)
K3 = ...81 82 83 84 85 86 87 88
88 87 86 85 84 83 82 81 80 79 78 77 76 75 74 73 72 71 ...= K4
Three-Fold
Observed repeating sequence(s)...A1T1E T2T1 ET2A2 T2T1 A1T1E T2T1 ET2A2 T2T1...
CASE 1 Unmixed
(d) Hyperfine Structure (Nuclear spin-rotation effects)
CASE 2₄ Extreme mixing in tight C4-CLUSTERS
Four-Fold Clusters
CASE 2₃- Major mixing in lowest two C3-CLUSTERS
(e) Superhyperfine Structure (Spin frame correlation effects)

Effects of broken or transition local symmetry for i-class

$$D^{A_1}_{0_4 0_4}(i_k \mathbf{i}_\mathrm{k}) = i_1 + i_2 + i_3 + i_4 + i_5 + i_6$$
$$D^{A_2}_{2_4 2_4}(i_k \mathbf{i}_\mathrm{k}) = -(i_1 + i_2 + i_3 + i_4 + i_5 + i_6)$$

$D^{E}(i_k \mathbf{i}_\mathrm{k}) =$

	0_4	2_4
0_4	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6) + i_3 + i_4$	$\frac{\sqrt{3}}{2}(i_1 + i_2 - i_5 - i_6)$
2_4	$h.c.$	$\frac{1}{2}(i_1 + i_2 + i_5 + i_6) - i_3 - i_4$

$D^{T_1^*}(i_k \mathbf{i}_\mathrm{k})$	1_4	3_4	0_4
1_4	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$-\frac{1}{2}(i_1 + i_2 - i_5 - i_6) - i(i_3 - i_4)$	$-\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6)$
3_4	$h.c.$	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$+\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6)$
0_4	$h.c.$	$h.c.$	$-(i_3 + i_4)$

$D^{T_2^*}(i_k \mathbf{i}_\mathrm{k})$	1_4	3_4	2_4
1_4	$+\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$+\frac{1}{2}(i_1 + i_2 - i_5 - i_6) - i(i_3 - i_4)$	$+\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6)$
3_4	$h.c.$	$+\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$-\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6)$
0_4	$h.c.$	$h.c.$	$+(i_3 + i_4)$

Conclusion: H-matrix *Ad-hoc*-ery greatly reduced

Group space tunneling matrix defined nicely by group table.

Each tunneling path matched to group element (complete set of Feynman paths!)

Spectral algebra yields closed-form eigenvalues and eigenvectors (in same table!) when local symmetry conditions apply.

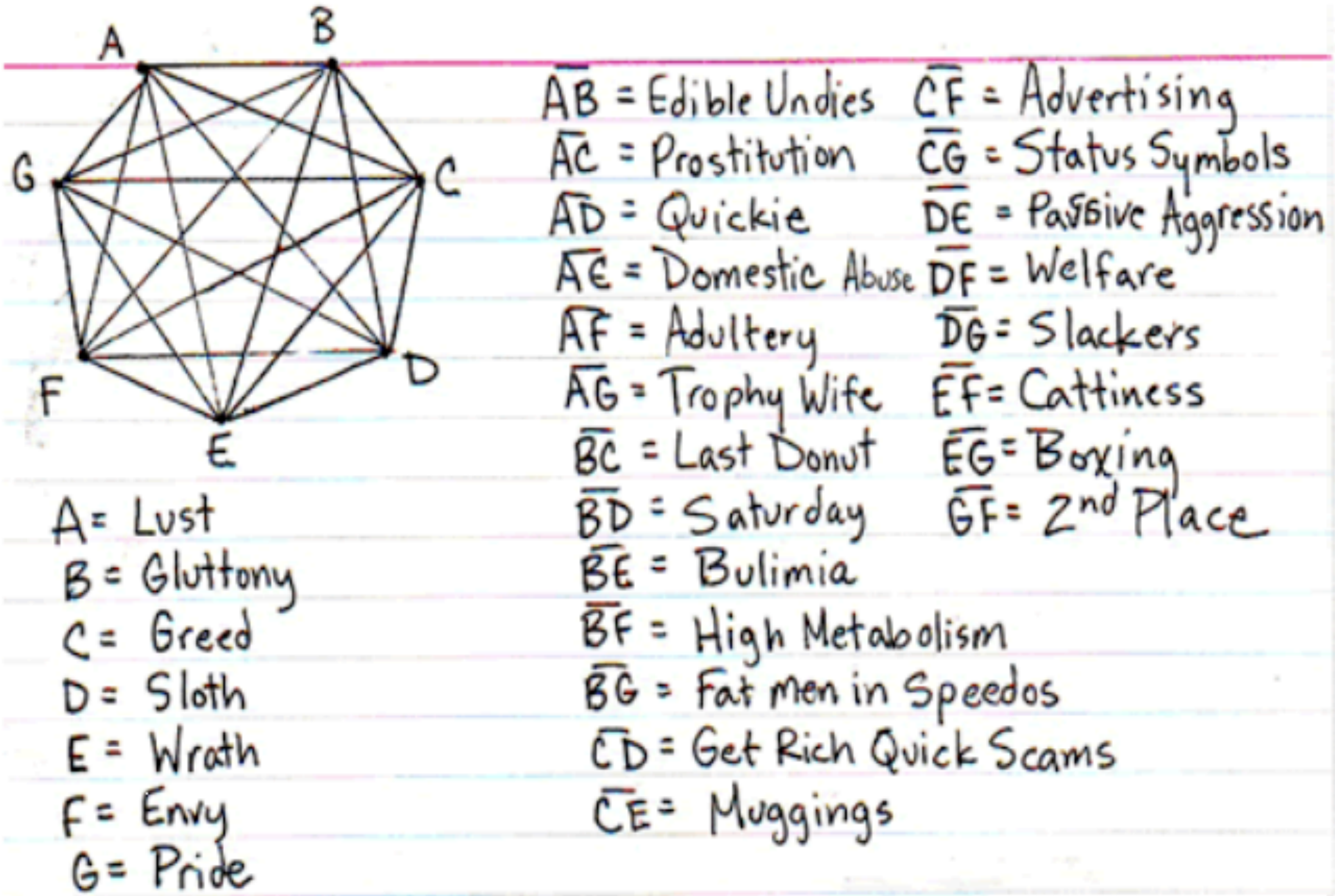
Expressions easily deconvoluted (essentially same table , again!).

Transitions to and from various local symmetries are shown.

Hougen could have done a D_7 example

Seven-Deadly-Sin Tunneling Theory

$D_7 \supset C_7$ sin calculator...(not recommended)



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-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 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

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

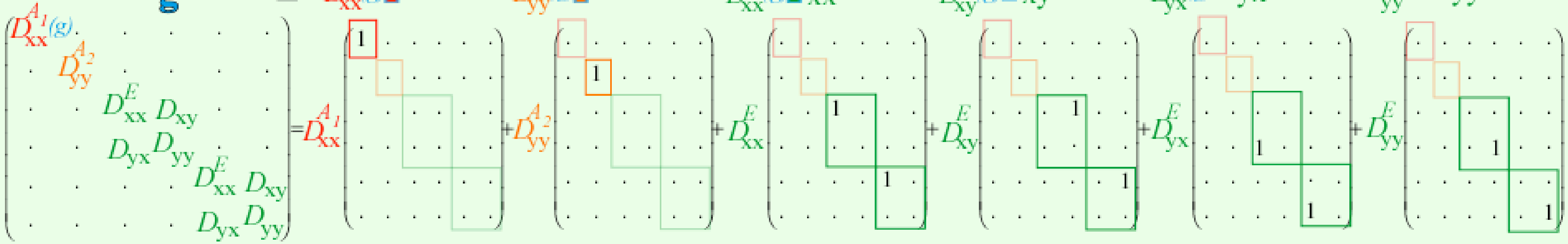
D_3 local projector product table

	$P^{A_1}_{xx}$	$P^{A_2}_{yy}$	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}

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

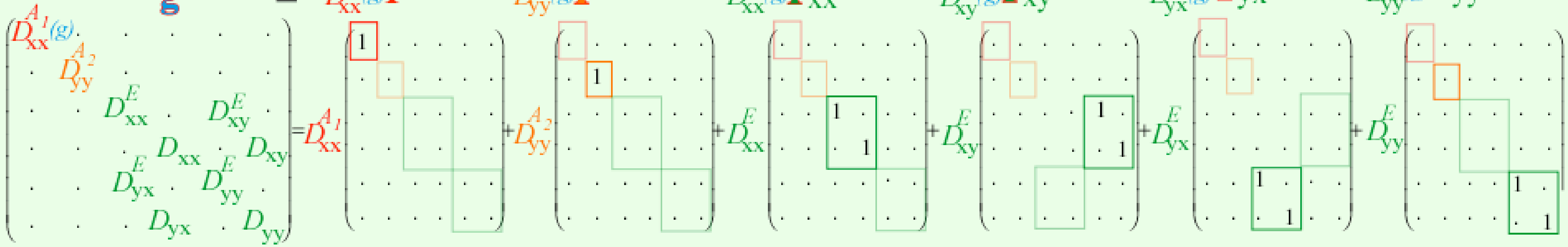
Matrix "Placeholders" $\mathbf{P}_{ab}^{(m)}$ *for GLOBAL* $\mathbf{g}$ *operators in* D_3

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



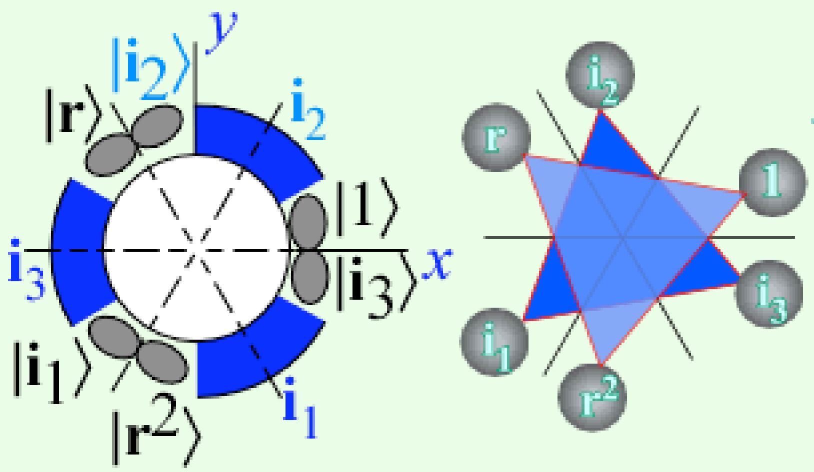
$\overline{\mathbf{P}}_{ab}^{(m)}$ *...for LOCAL* $\overline{\mathbf{g}}$ *operators in* $\overline{D}_3$

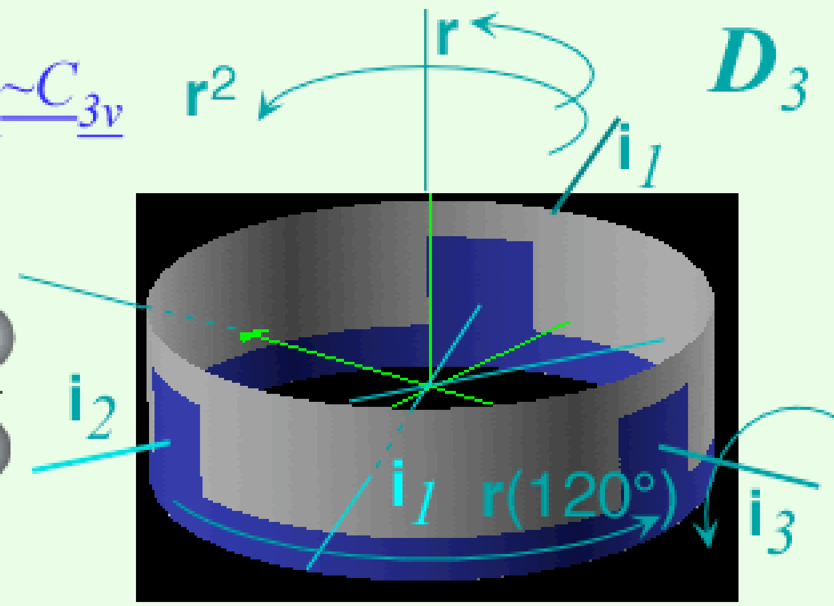
$$\overline{\mathbf{g}} = D_{xx}^{A_1}(g)\overline{\mathbf{P}}^{A_1} + D_{yy}^{A_2}(g)\overline{\mathbf{P}}^{A_2} + D_{xx}^{E}(g)\overline{\mathbf{P}}_{xx}^{E} + D_{xy}^{E}(g)\overline{\mathbf{P}}_{xy}^{E} + D_{yx}^{E}(g)\overline{\mathbf{P}}_{yx}^{E} + D_{yy}^{E}(g)\overline{\mathbf{P}}_{yy}^{E}$$



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

D_3-defined local-wave bases

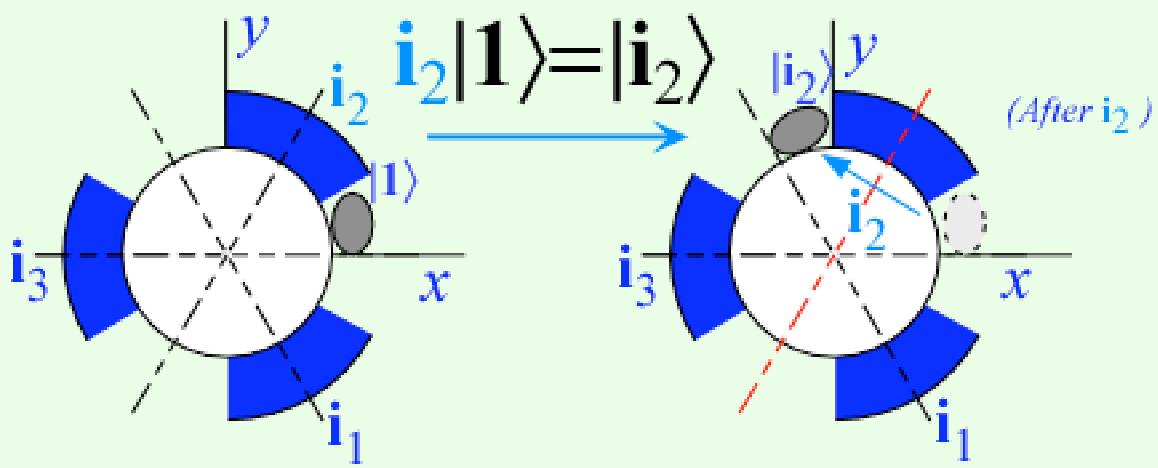




D_3

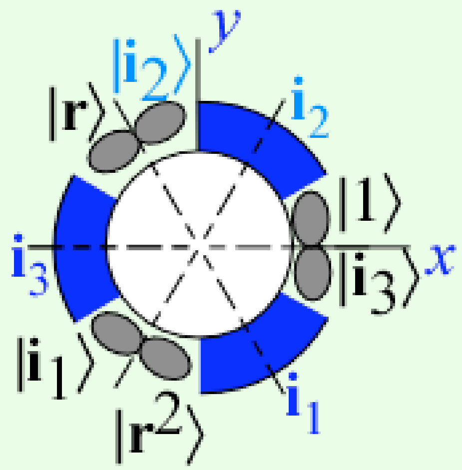
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

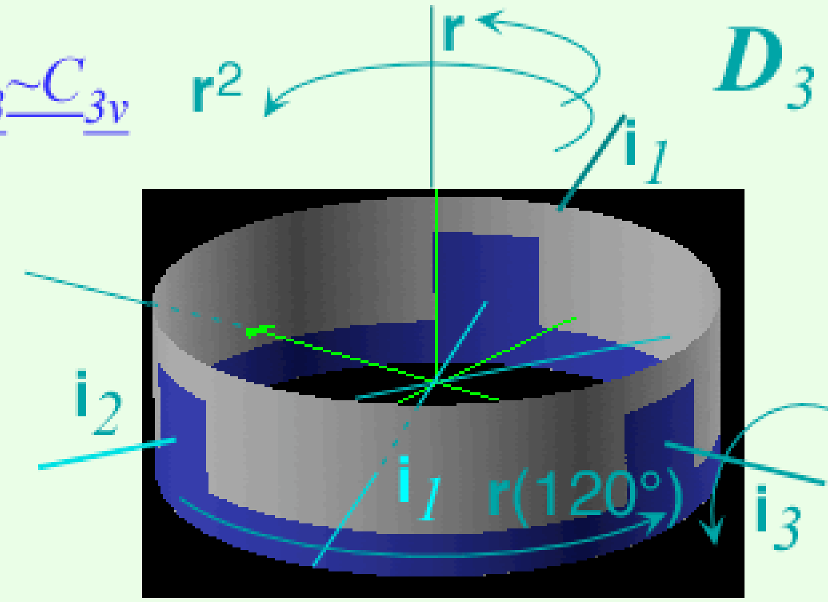
Lab-fixed (Extrinsic-Global) operations and rotation axes



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

D_3-defined local-wave bases



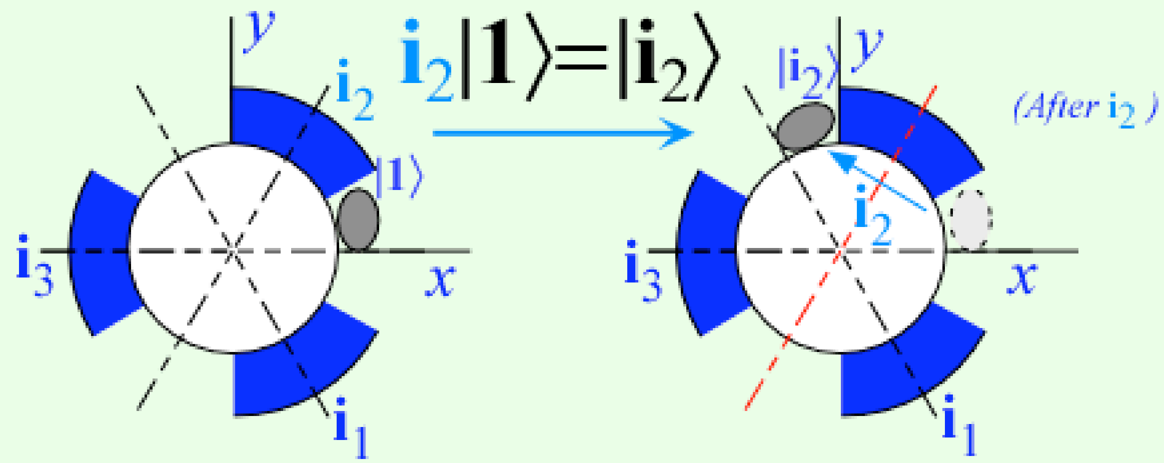


D_3

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

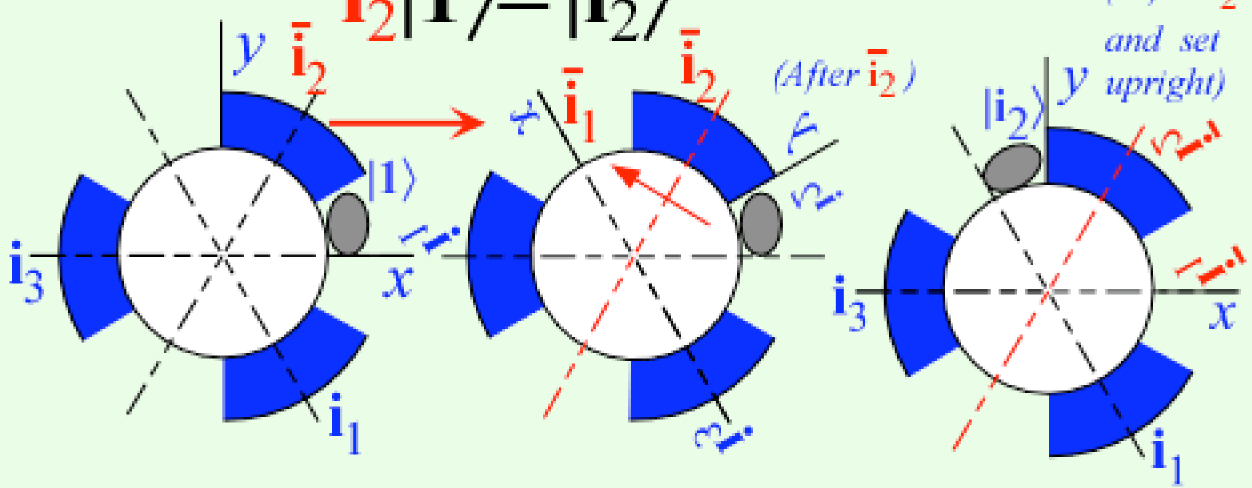
Lab-fixed (Extrinsic-Global) operations and rotation axes

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



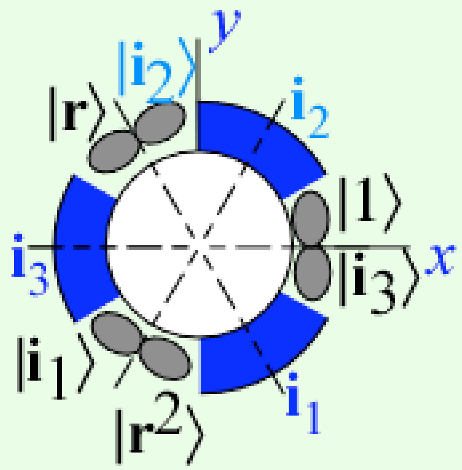
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

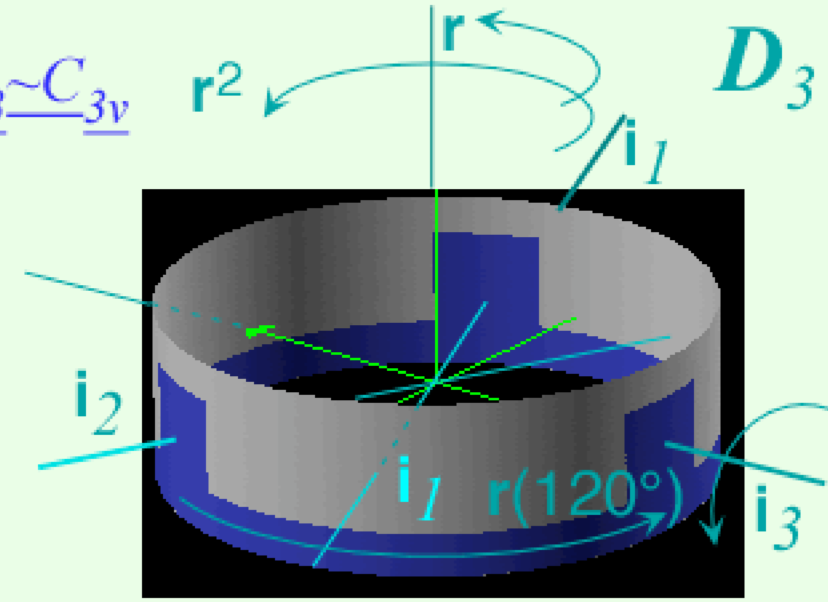
$\bar{i}_2|1\rangle = |i_2\rangle$



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

D_3-defined local-wave bases



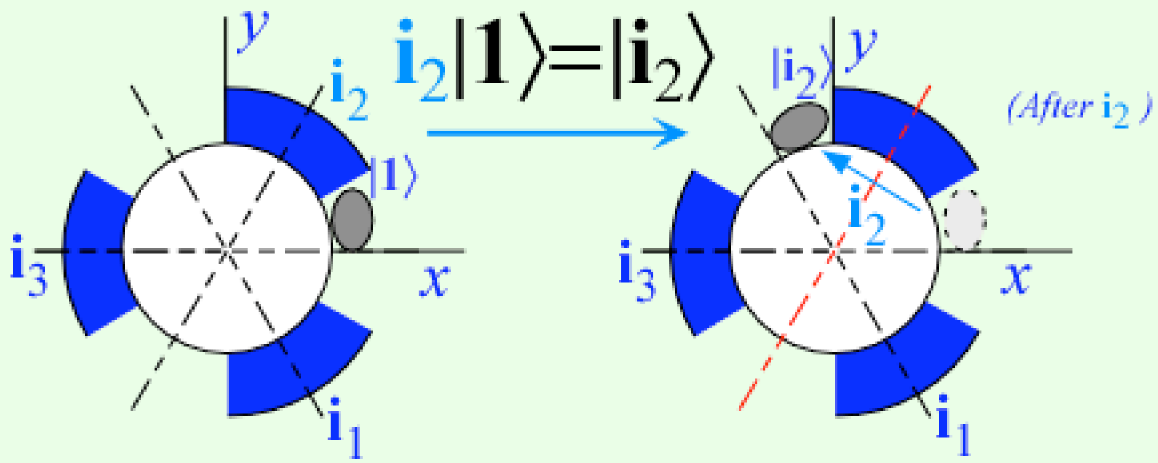


D_3

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

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

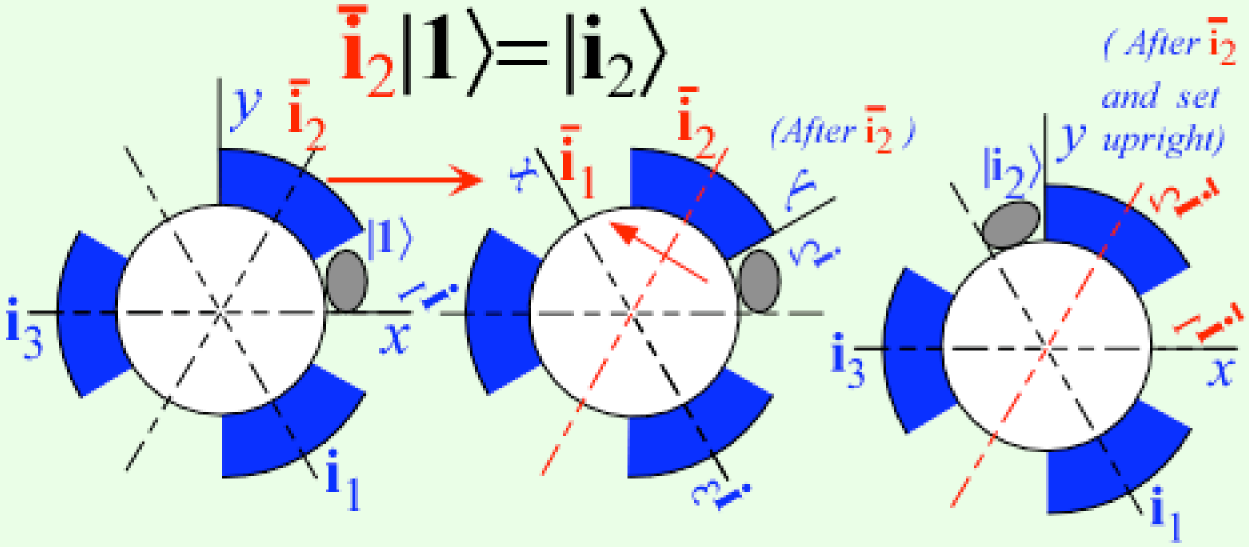
$$i_2|1\rangle=|i_2\rangle$$



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

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

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



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

$$\bar{i}_1\bar{i}_2|1\rangle=\bar{i}_1\,|i_2\rangle=\bar{r}\,|1\rangle=r^2\,|1\rangle$$