OAI
Ohio Aerospace Institute

Symmetry eigensolutions on the Cheap

and

Going beyond "Gruppenpest"

Exploiting local symmetry algebra and geometry of a quantum "Mock-Mach" principle

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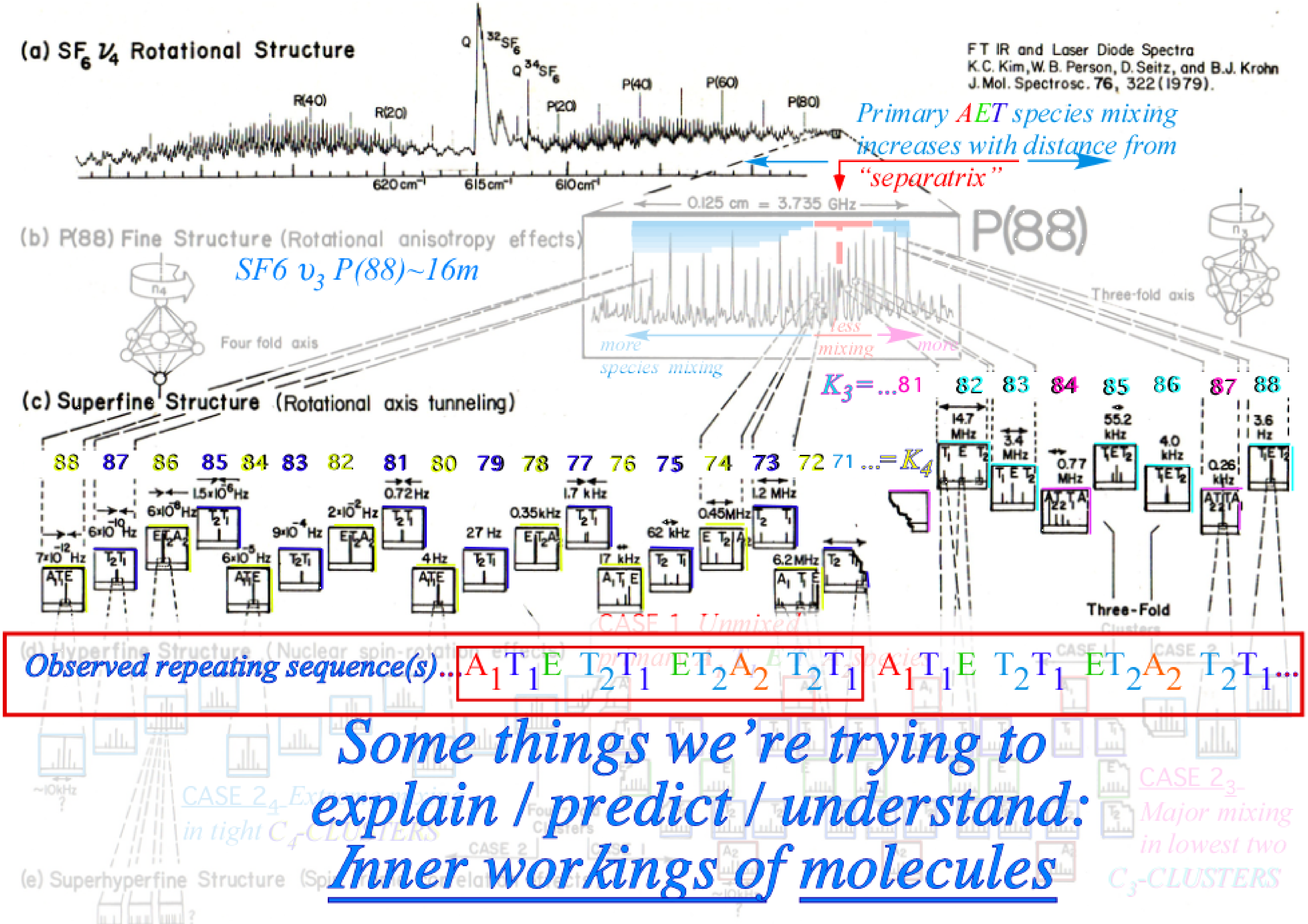
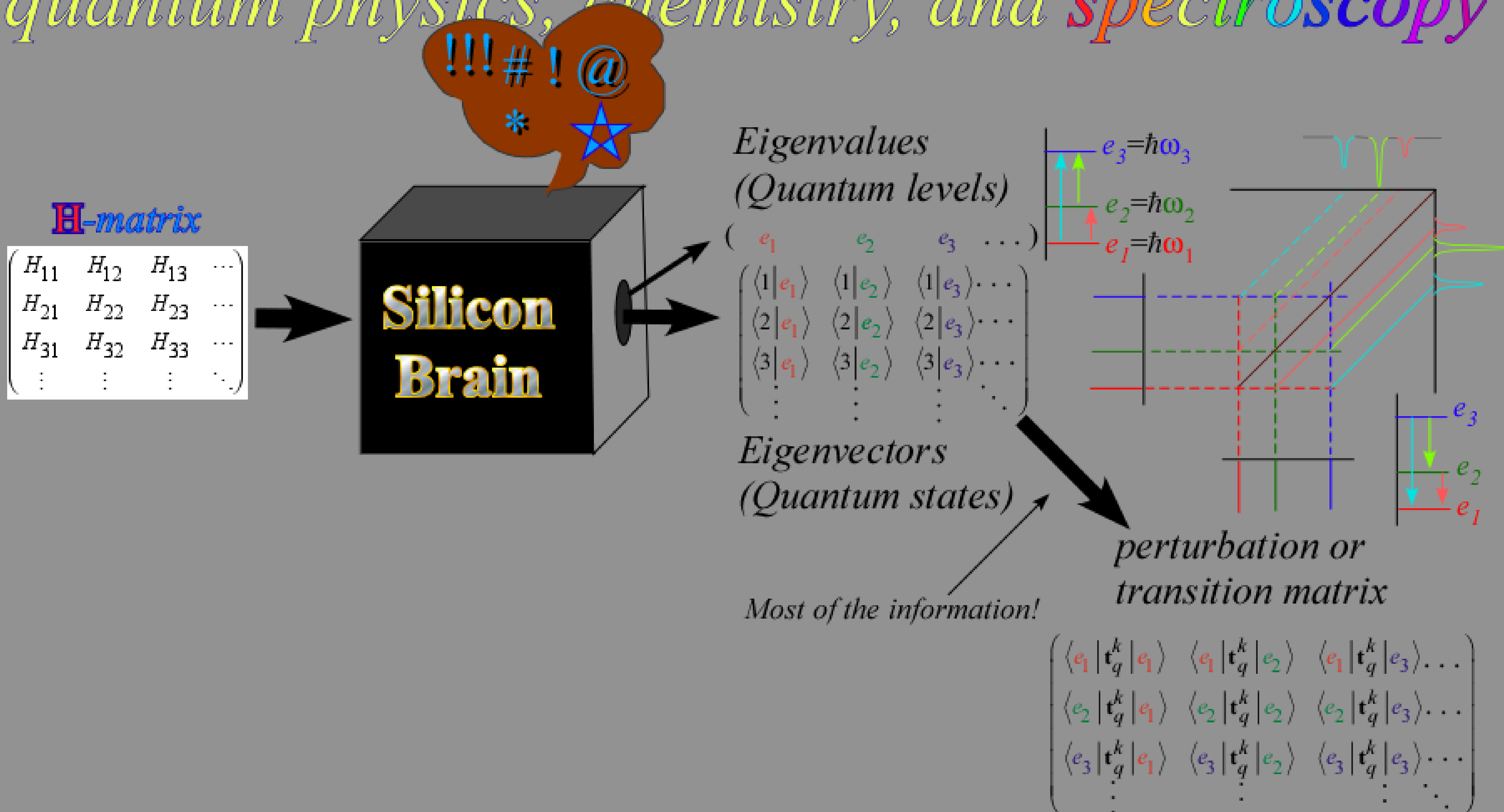
*...and friend**

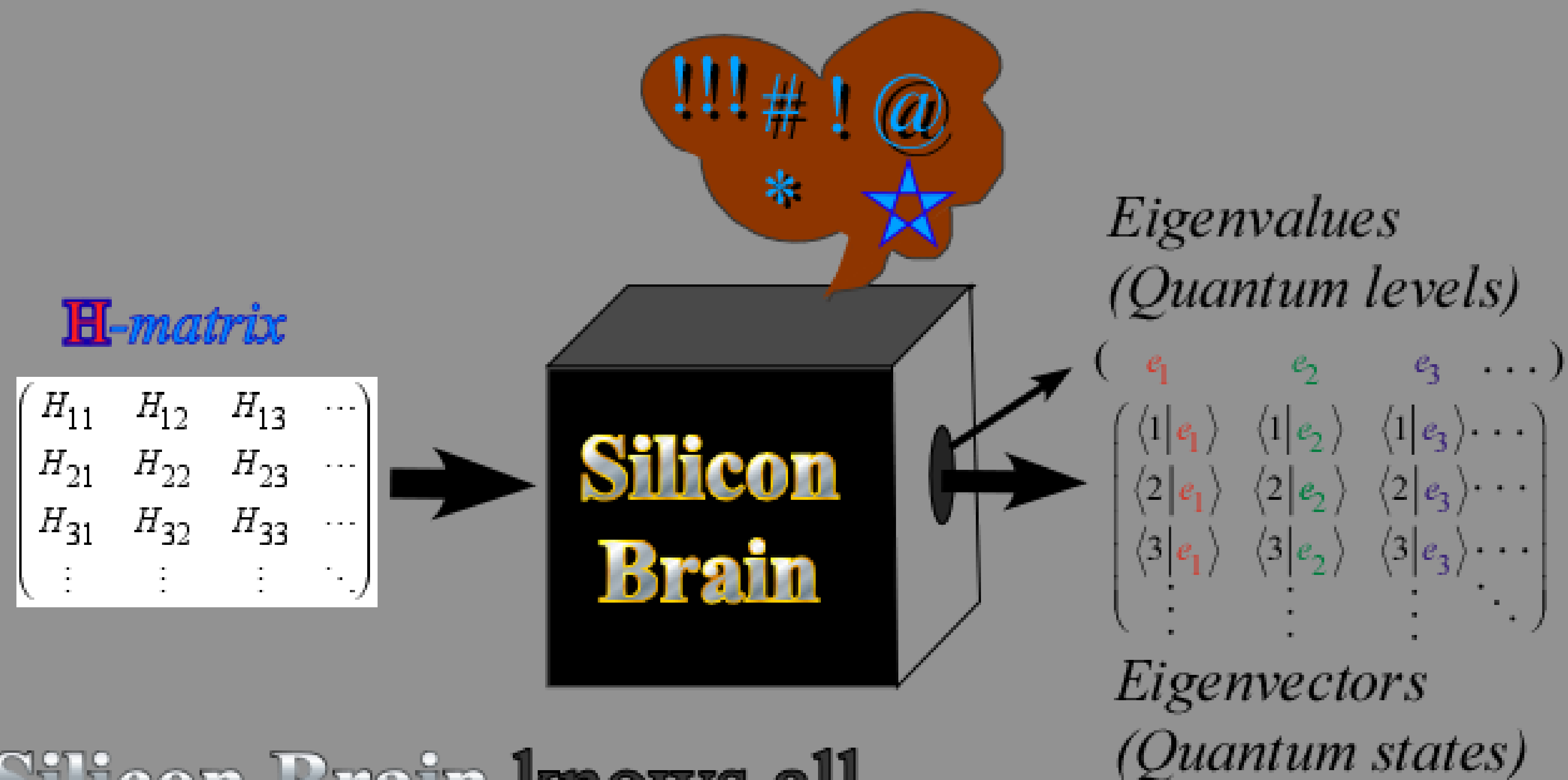
**(O_h slide rule)*


(a) SF6 ν4 Rotational Structure
Q 32SF6
Q 34SF6
R(40)
R(20)
P(20)
P(40)
P(60)
P(80)
620 cm-1
615 cm-1
610 cm-1
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
K3=...81 82 83 84 85 86 87 88
(c) Superfine Structure (Rotational axis tunneling)
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...
Some things we're trying to
explain / predict / understand:
Inner workings of molecules

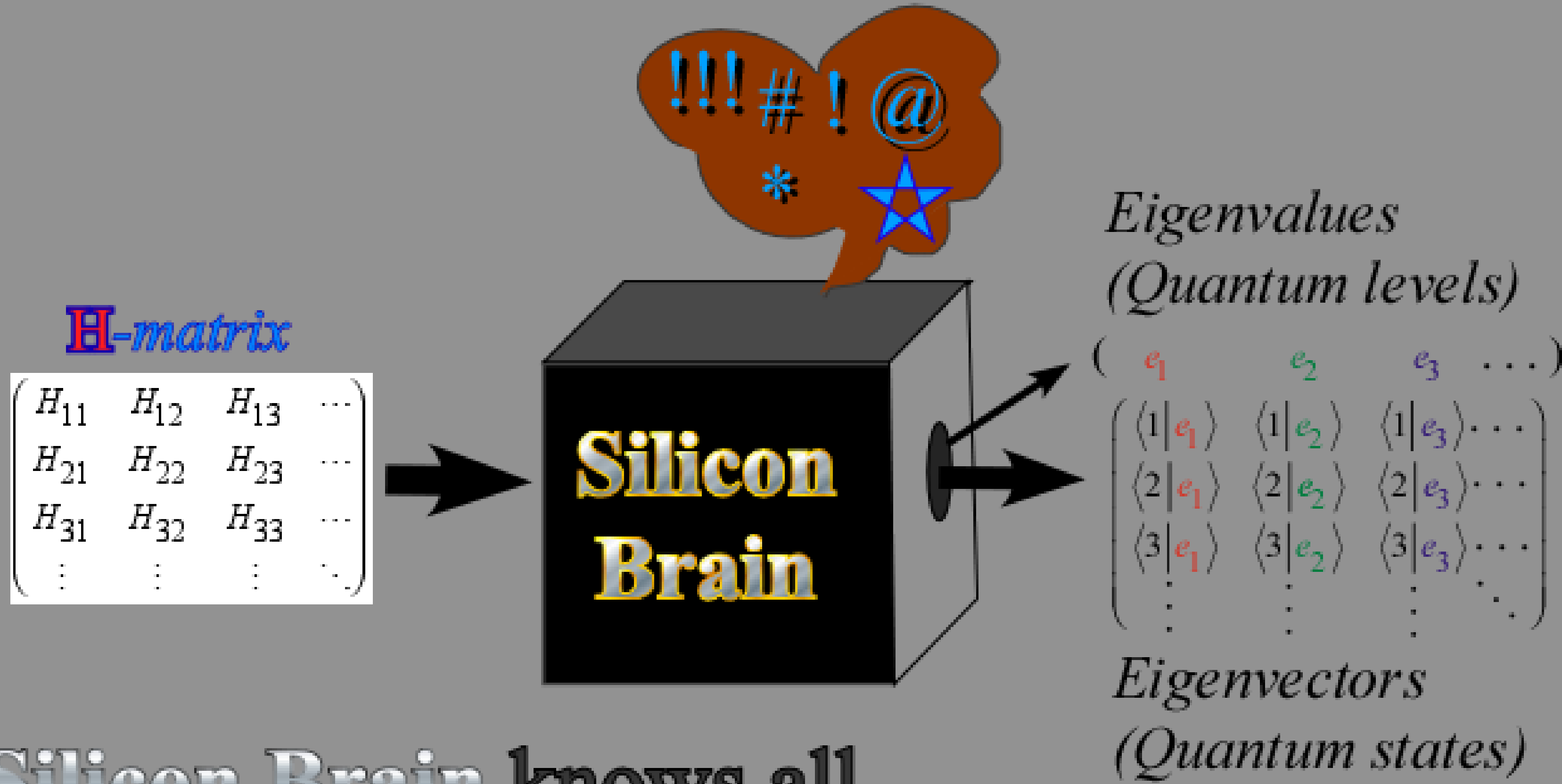
Matrix Diagonalization by computer:

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





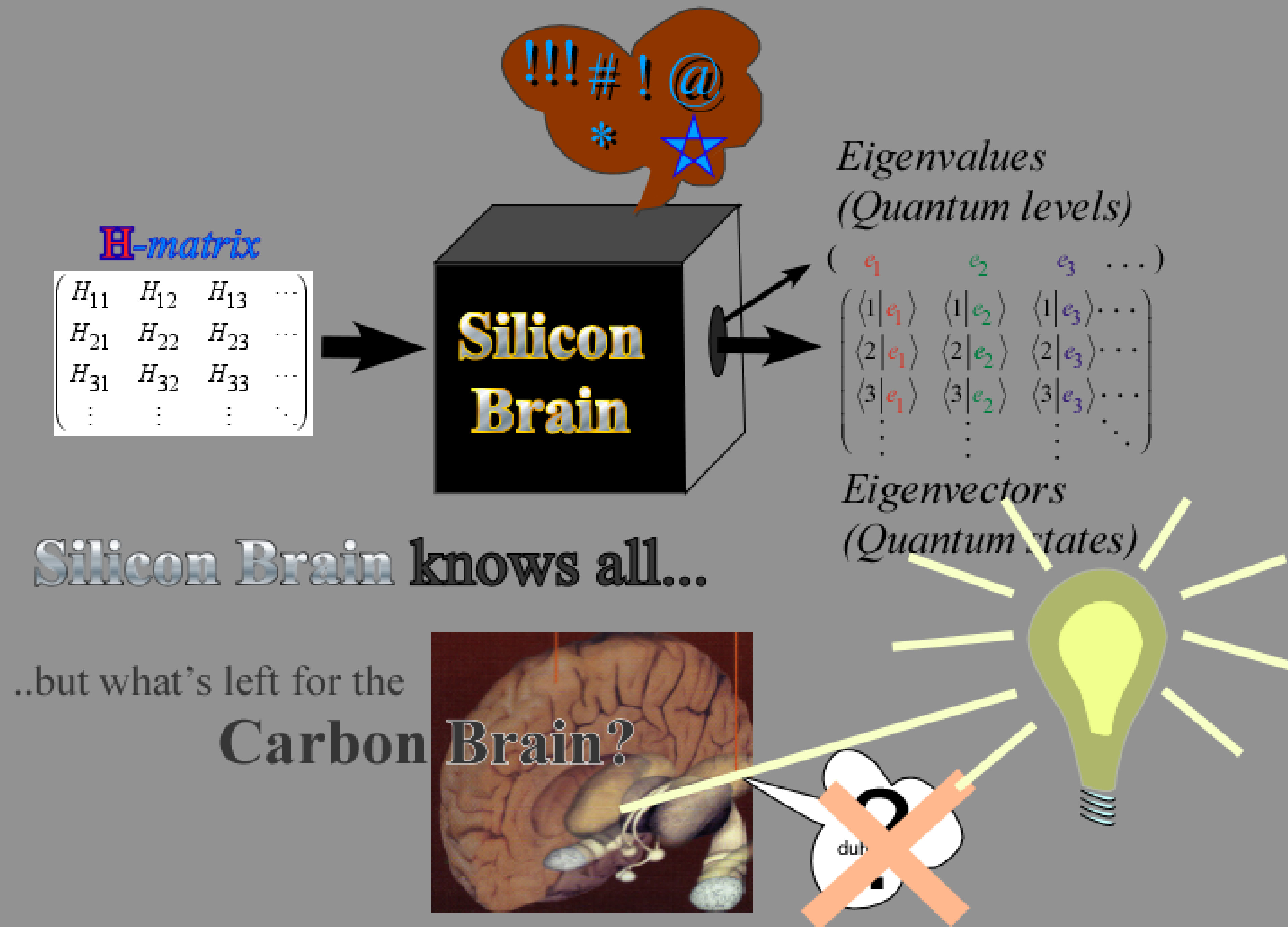
Silicon Brain knows all...



Silicon Brain knows all...

..but what's left for the

Carbon Brain?



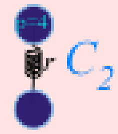
New symmetry analysis techniques

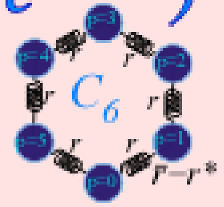
***come to rescue old* Carbon Brain!**

(Commuting)

- ***Abelian symmetry = Fourier analysis*** *(Back to our roots $1^{1/N} = e^{2\pi i m/N}$)*

  *Group product table => Hamiltonian **H**-matrices* *(C_2 and C_6 examples)*





  *Group roots => **H**-matrix spectral resolution by $P^{(m)}$ projectors*

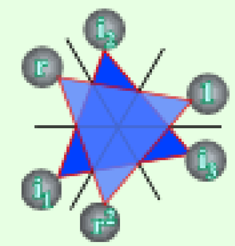
Commutivity conundrum... ? $\mathbf{H}\cdot g = g\cdot\mathbf{H}$?

- ***New symmetry insights:*** *Local vs. Global symmetry* *Projector invariance*

  "Mock-Mach" principle *Conway, et.al, May (2008)* *Cvitanovic, (2008)*

(Non-Commuting)

- ***Non-Abelian symmetry analysis I.*** *(Simplest example: D_3)*



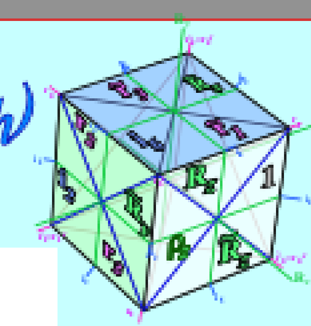
  *Local vs. Global product tables => **H**-matrices*

  All-commuting invariants => Global invariant (character) $P^{(\alpha)}$ projectors

  Mutually-commuting sets => Local vs. Global eigensolutions by $P^{(\alpha)}_{m,n}$ projectors

  *=> **H**-matrix spectral resolution by $P^{(\alpha)}_{m,n}$ projectors*

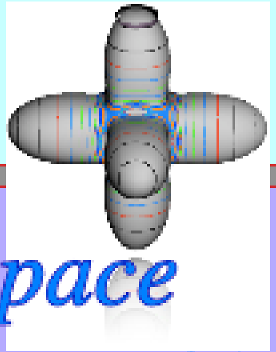
- ***Non-Abelian symmetry analysis II.*** *(Octahedral example: O_h)*

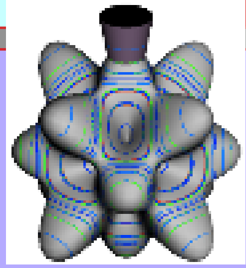


  *Global-local product tables => **H**-matrices...*

  ... and all the above ...

  => eigensolution formulas by local-symmetry defined $P^{(\alpha)}_{n,n}$ projectors



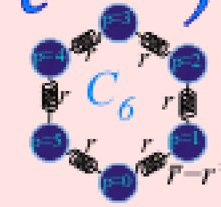


- ***Local vs Global symmetry in rovibronic phase space***

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

(Commuting)

- ***Abelian symmetry = Fourier analysis*** *(Back to our roots* $1^{1/N} = e^{2\pi i m/N}$*)*
  - *Group product table => Hamiltonian* $\hat{\mathbf{H}}$*-matrices* *(C_2 and C_6 examples)*
  - *Group roots =>* $\mathbf{H}$*-matrix spectral resolution by* $\mathrm{P}^{(m)}$*projectors*

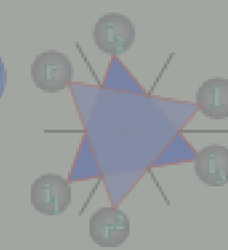


Commutivity conundrum... ? $\mathbf{H}\cdot g = g\cdot\mathbf{H}$?

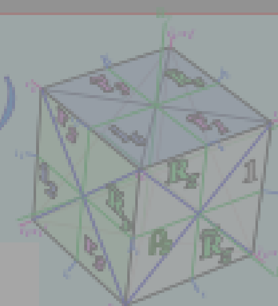
- ***New symmetry insights:*** *Local vs. Global symmetry* *Projector invariance*
  - *"Mock-Mach" principle* *Conway, et.al, May (2008)* *Cvitanovic, (2008)*

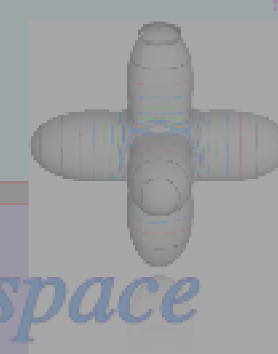
(Non-Commuting)

- ***Non-Abelian symmetry analysis I.*** *(Simplest example: D_3)*
  - *Local vs. Global product tables =>* $\hat{\mathbf{H}}$*-matrices*
  - *All-commuting invariants => Global invariant (character)* $\mathrm{P}^{(\alpha)}$*projectors*
  - *Mutually-commuting sets => Local vs. Global eigensolutions by* $\mathrm{P}^{(\alpha)}_{m,n}$ *projectors*
  - *=>* $\mathbf{H}$*-matrix spectral resolution by* $\mathrm{P}^{(\alpha)}_{m,n}$ *projectors*

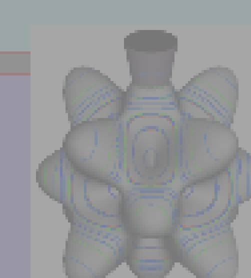


- ***Non-Abelian symmetry analysis II.*** *(Octahedral example: O_h)*
  - *Global-local product tables =>* $\mathbf{H}$*-matrices...*
  - *... and all the above ...*
  - *=> eigensolution formulas by local-symmetry defined* $\mathrm{P}^{(\alpha)}_{n,n}$ *projectors*





- ***Local vs Global symmetry in rovibronic phase space***
  - *How group operators analyze rovibronic tunneling effects at high J.* *(SF_6 examples)*



1^{st} Step

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($^{gg^\dagger}_{form}$)

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

(columns: $g^\dagger$; rows: g)

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

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

$$\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 r-matrices,...

1^{st} Step (contd.)

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($\frac{gg^\dagger}{form}$)*

$g^\dagger$ (columns), g (rows):

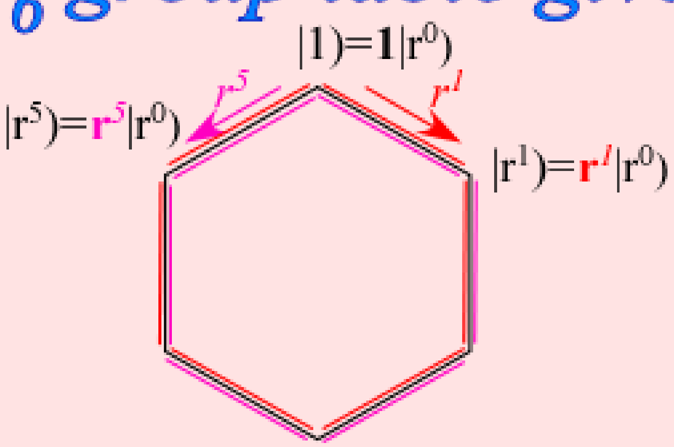
C_6	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{1}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$	$\mathbf{r}$
$\mathbf{r}$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^5$	$\mathbf{r}^4$	$\mathbf{r}^3$	$\mathbf{r}^2$
$\mathbf{r}^2$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

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

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

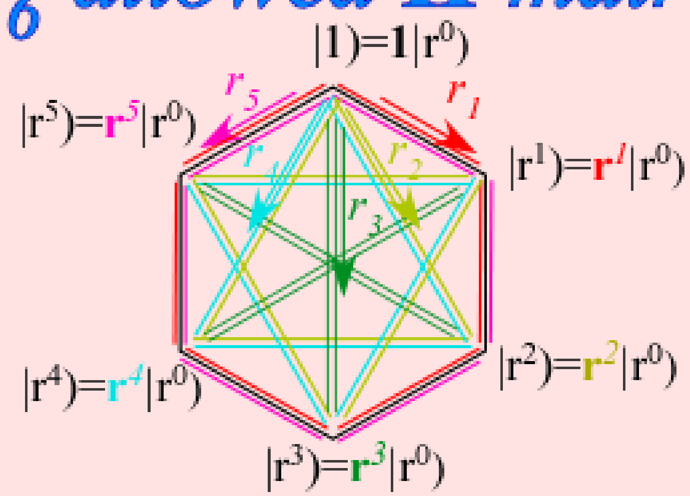
$$\begin{pmatrix} r_0 & r_5 & r_4 & r_3 & r_2 & r_1 \\ r_1 & r_0 & r_5 & r_4 & r_3 & r_2 \\ r_2 & r_1 & r_0 & r_5 & r_4 & r_3 \\ r_3 & r_2 & r_1 & r_0 & r_5 & r_4 \\ r_4 & r_3 & r_2 & r_1 & r_0 & r_5 \\ r_5 & r_4 & r_3 & r_2 & r_1 & r_0 \end{pmatrix} = r_0\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \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 **r**-*matrices,...C_6-allowed* **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

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*

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

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

$\psi_1^0 = 1$

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

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

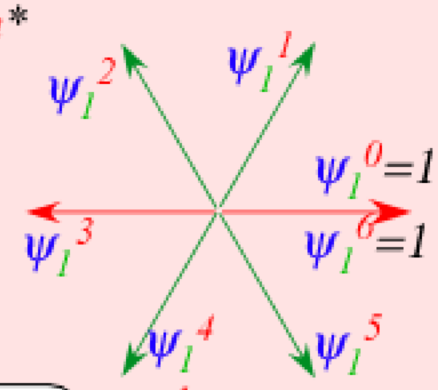
$\psi_1^3 = \psi_3^1 = -1$

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

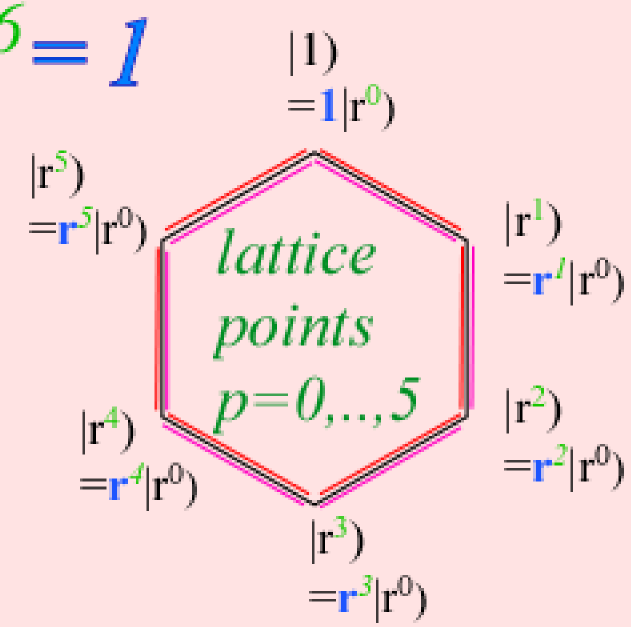
$\psi_1^5 = \psi_5^1 = \psi_1^{-1} = e^{-2\pi i/6}$

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 (contd.)

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

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

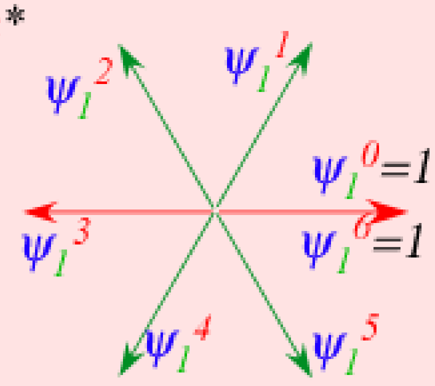
$$D^m(\mathbf{r}) = e^{-2\pi i m/6} = \chi_1{}^m = \psi_1{}^{m*}$$

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

p = power (exponent) or position point

m = momentum or wave-number

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



top-row flip not needed...

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

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

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

$$\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 $\mathbf{P}^{(m)}$ are eigenvalue "placeholders" having orthogonal-idempotent products, eigen-equations,

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

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

2^{nd} Step (contd.)

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

top-row flip not needed...

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

All $x = \mathbf{r}^p$ 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

$\psi_1^{\,0} = 1$

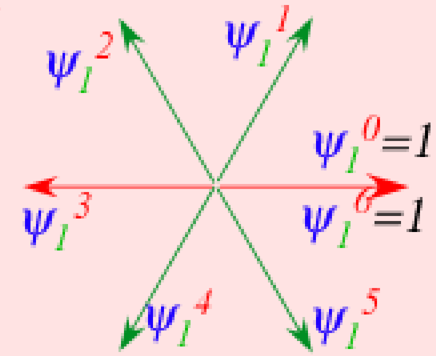
$\psi_1^{\,1} = e^{2\pi i/6}$

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

$\psi_1^{\,3} = \psi_3^{\,1} = -1$

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

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



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

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

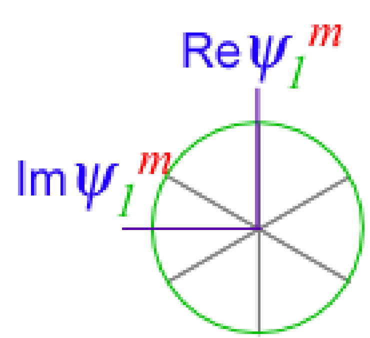
$$\begin{pmatrix}\chi_p^{\,0} & \cdot & \cdot & \cdot & \cdot & \cdot\\ \cdot & \chi_p^{\,1} & \cdot & \cdot & \cdot & \cdot\\ \cdot & \cdot & \chi_p^{\,2} & \cdot & \cdot & \cdot\\ \cdot & \cdot & \cdot & \chi_p^{\,3} & \cdot & \cdot\end{pmatrix} = \chi_p^{\,0}\begin{pmatrix}1 & \cdot & \cdots\\ \cdot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

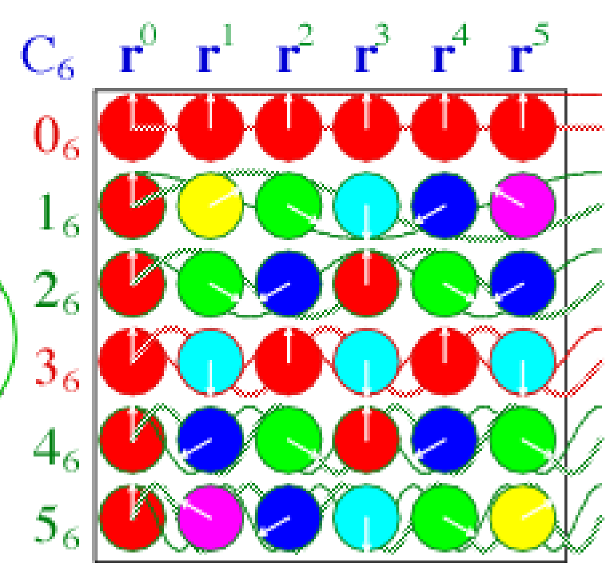
Inverse C_6 spectral resolution m-wave $\psi_p^{\,m} = D^{m*}(\mathbf{r}^p) = e^{+2\pi i m\cdot p/6}$:

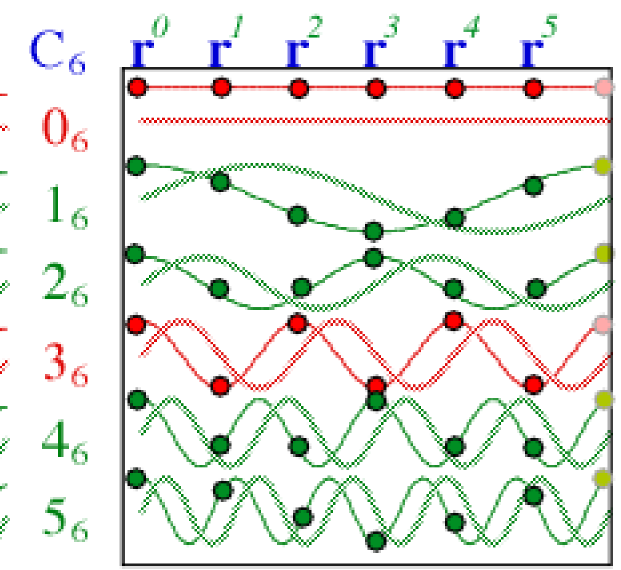
$$\mathbf{P}^{(m)} = \psi_0^{\,m}\,\mathbf{r}^0 + \psi_1^{\,m}\,\mathbf{r}^1 + \psi_2^{\,m}\,\mathbf{r}^2 + \psi_3^{\,m}\,\mathbf{r}^3 + \psi_4^{\,m}\,\mathbf{r}^4 + \psi_5^{\,m}\,\mathbf{r}^5$$

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

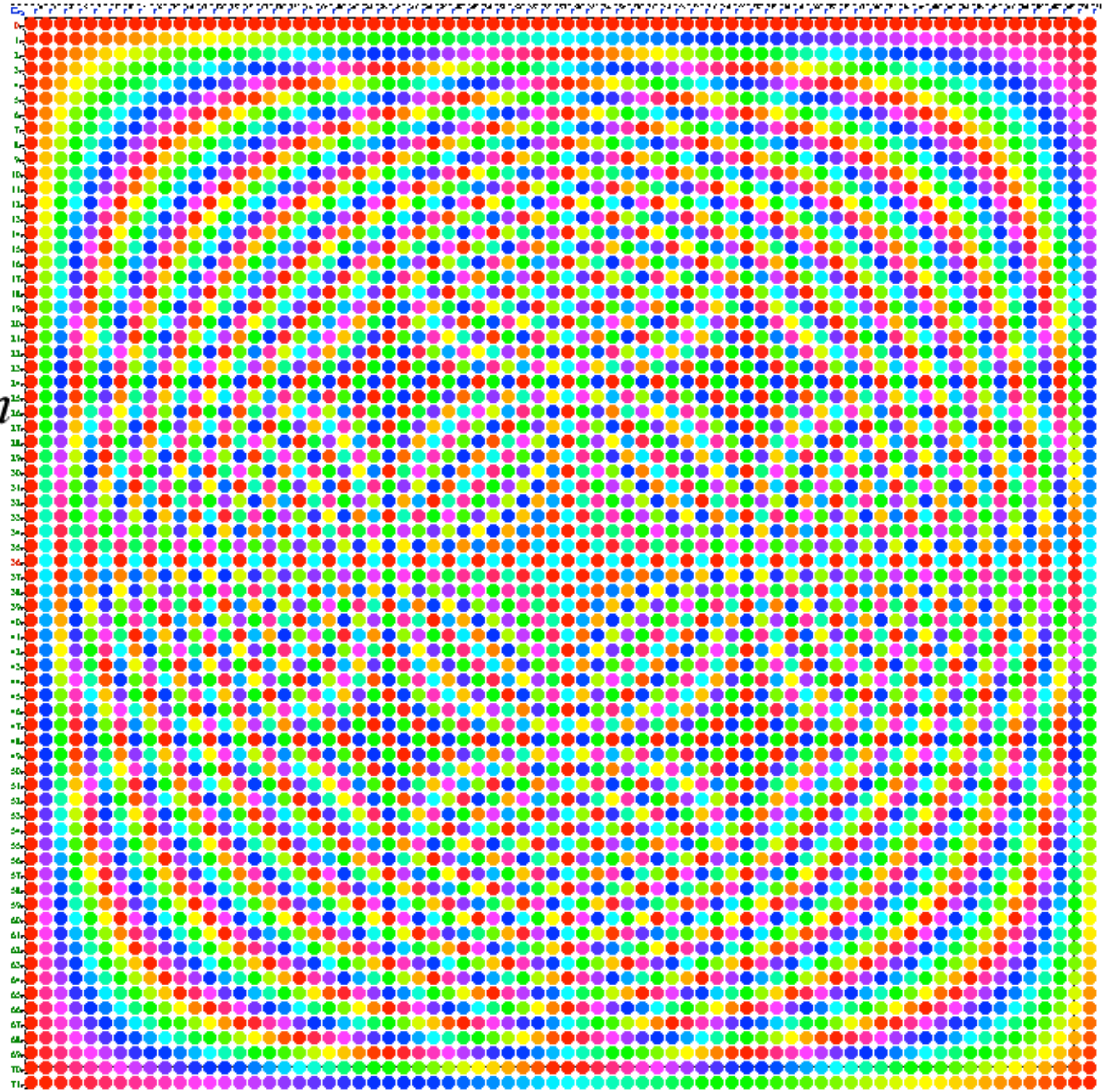
momentum m	$p=0$	1	2	3	4	5
$m=0$	$\psi_0^{\,0}$	$\psi_1^{\,0}$	$\psi_2^{\,0}$	$\psi_3^{\,0}$	$\psi_4^{\,0}$	$\psi_5^{\,0}$
$m=1$	$\psi_0^{\,1}$	$\psi_1^{\,1}$	$\psi_2^{\,1}$	$\psi_3^{\,1}$	$\psi_4^{\,1}$	$\psi_5^{\,1}$
$m=2$	$\psi_0^{\,2}$	$\psi_1^{\,2}$	$\psi_2^{\,2}$	$\psi_3^{\,2}$	$\psi_4^{\,2}$	$\psi_5^{\,2}$
$m=3$	$\psi_0^{\,3}$	$\psi_1^{\,3}$	$\psi_2^{\,3}$	$\psi_3^{\,3}$	$\psi_4^{\,3}$	$\psi_5^{\,3}$
$m=4$	$\psi_0^{\,4}$	$\psi_1^{\,4}$	$\psi_2^{\,4}$	$\psi_3^{\,4}$	$\psi_4^{\,4}$	$\psi_5^{\,4}$
$m=5$	$\psi_0^{\,5}$	$\psi_1^{\,5}$	$\psi_2^{\,5}$	$\psi_3^{\,5}$	$\psi_4^{\,5}$	$\psi_5^{\,5}$







C_{72}
Fourier transformation matrix

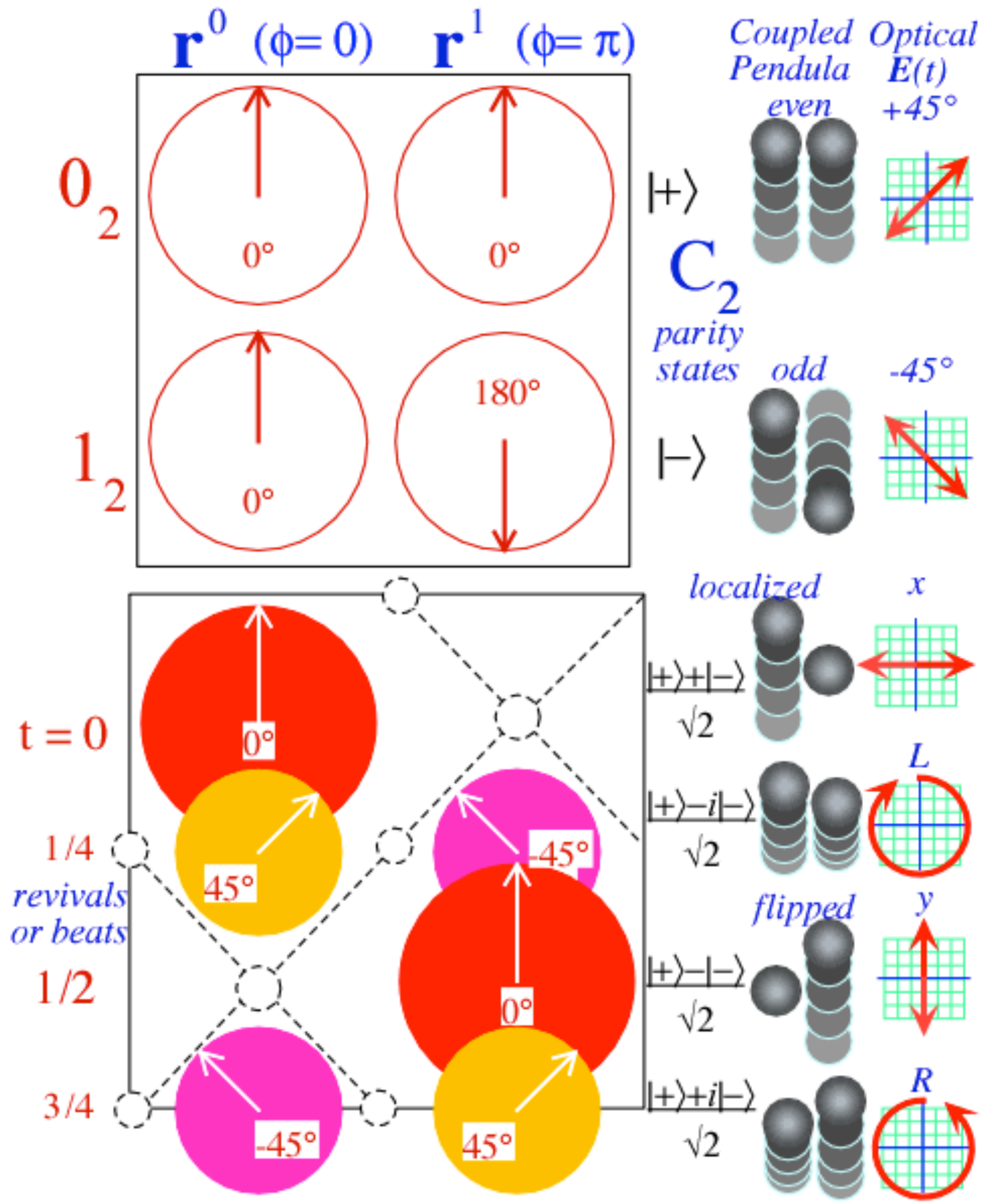


C_2

Fourier transformation matrix

and

dynamics



3rd Step

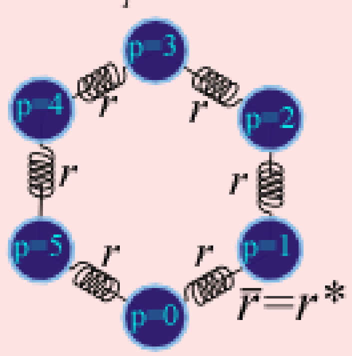
Display all eigensolutions for all possible C_6 symmetric real H

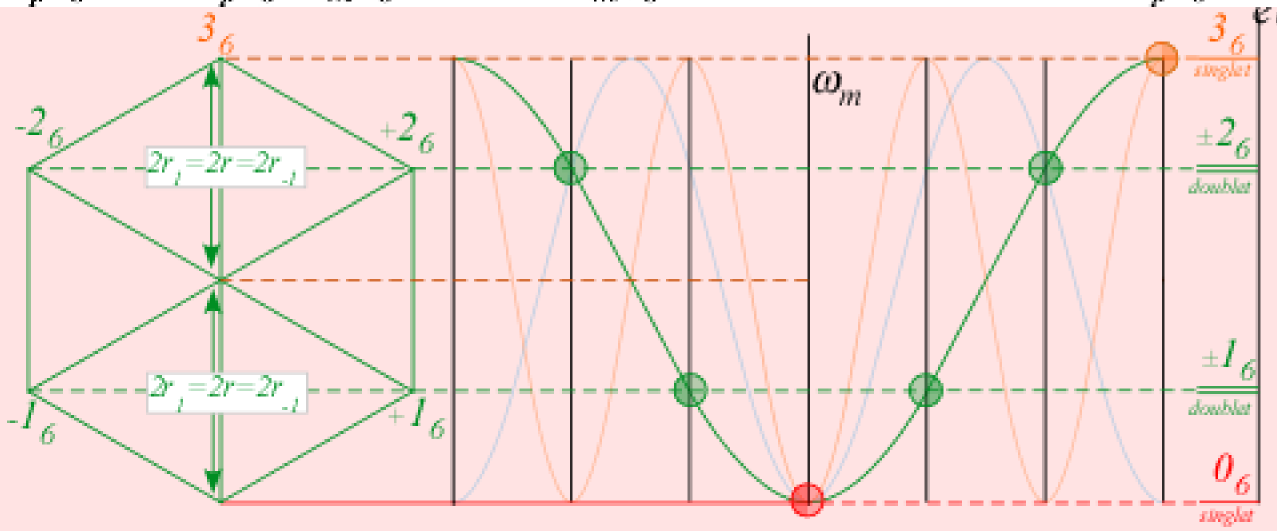
$$\mathbf{H}=\sum_{p=0}^{n-1} r_p \mathbf{r}^p=\sum_{p=0}^{n-1} r_p \sum_{m=0}^{n-1} \chi_p^m \mathbf{P}^{(m)}=\sum_{m=0}^{n-1} \omega^{(m)} \mathbf{P}^{(m)} \quad where: \omega^{(m)}=\sum_{p=0}^{n-1} r_p \chi_p^m=\omega(k_m)$$

(Dispersion function)

Elementary Bloch Model

$\mathbf{H}= H_1\mathbf{1} - r\mathbf{r} - r\mathbf{r}^{-1}$





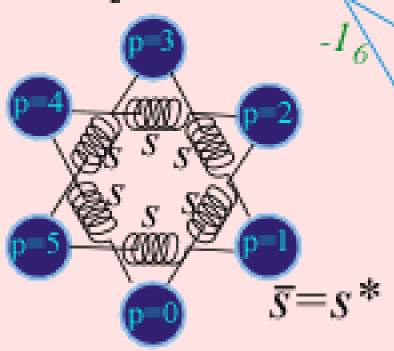
eigenvalues of $\mathbf{H}^{B1(6)}$

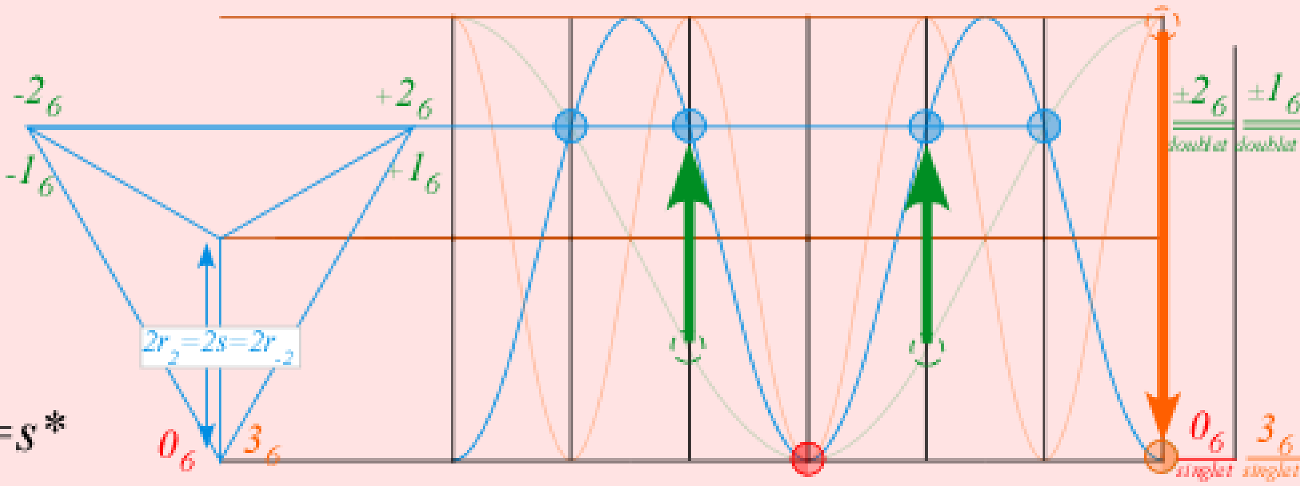
$$\begin{pmatrix} H_1 & -r & \cdot & \cdot & \cdot & -r \\ -r & H_1 & -r & \cdot & \cdot & \cdot \\ \cdot & -r & H_1 & -r & \cdot & \cdot \\ \cdot & \cdot & -r & H_1 & -r & \cdot \\ \cdot & \cdot & \cdot & -r & H_1 & -r \\ -r & \cdot & \cdot & \cdot & -r & H_1 \end{pmatrix}$$

$$\omega^{B1(n)}(k_m) = r_0\chi_0^m + r_1\chi_1^m + r_{-1}\chi_{-1}^m = H_1 - 2r\cos(2\pi m/6)$$

2nd Neighbor coupling

$\mathbf{H}= H_2\mathbf{1} - s\mathbf{r}^2 - s\mathbf{r}^{-2}$





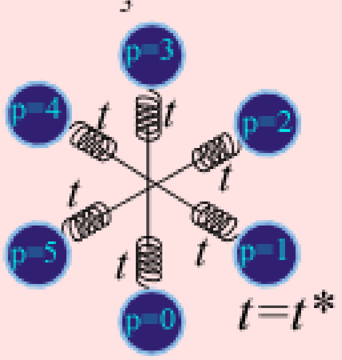
eigenvalues of $\mathbf{H}^{B2(6)}$

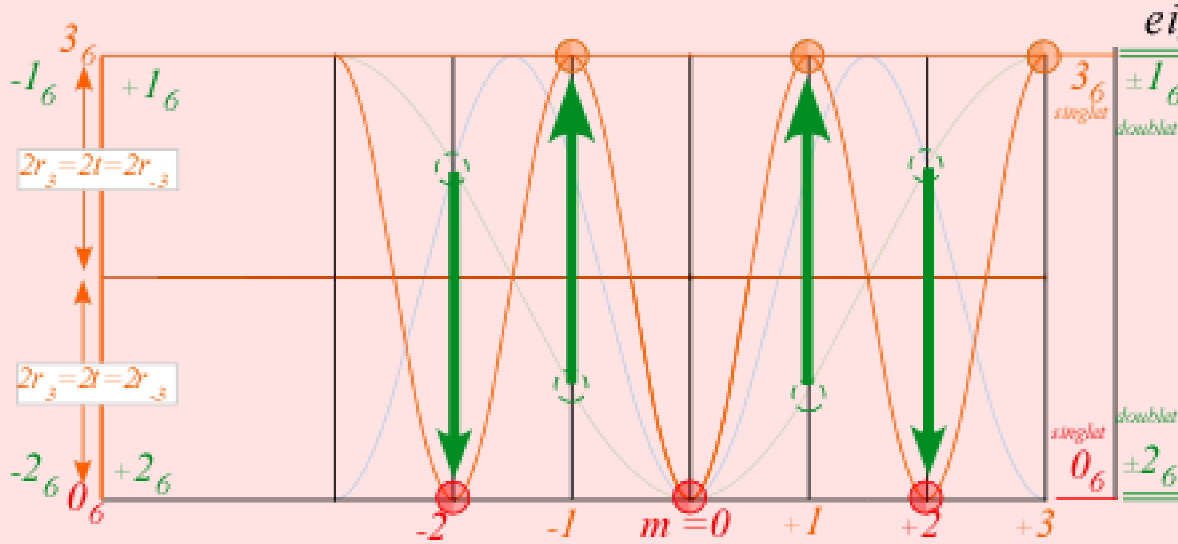
$$\begin{pmatrix} H_2 & \cdot & -s & \cdot & -s & \cdot \\ \cdot & H_2 & \cdot & -s & \cdot & -s \\ -s & \cdot & H_2 & \cdot & -s & \cdot \\ \cdot & -s & \cdot & H_2 & \cdot & -s \\ -s & \cdot & -s & \cdot & H_2 & \cdot \\ \cdot & -s & \cdot & -s & \cdot & H_2 \end{pmatrix}$$

$$\omega^{B2(n)}(k_m) = r_0\chi_0^m + r_2\chi_2^m + r_{-2}\chi_{-2}^m = H_2 - 2s\cos(4\pi m/6)$$

3rd Neighbor coupling

$\mathbf{H}= H_3\mathbf{1} - t\mathbf{r}^3 - t\mathbf{r}^{-3}$





eigenvalues of $\mathbf{H}^{B3(6)}$

$$\begin{pmatrix} H_3 & \cdot & \cdot & -t & \cdot & \cdot \\ \cdot & H_3 & \cdot & \cdot & -t & \cdot \\ \cdot & \cdot & H_3 & \cdot & \cdot & -t \\ -t & \cdot & \cdot & H_3 & \cdot & \cdot \\ \cdot & -t & \cdot & \cdot & H_3 & \cdot \\ \cdot & \cdot & -t & \cdot & \cdot & H_3 \end{pmatrix}$$

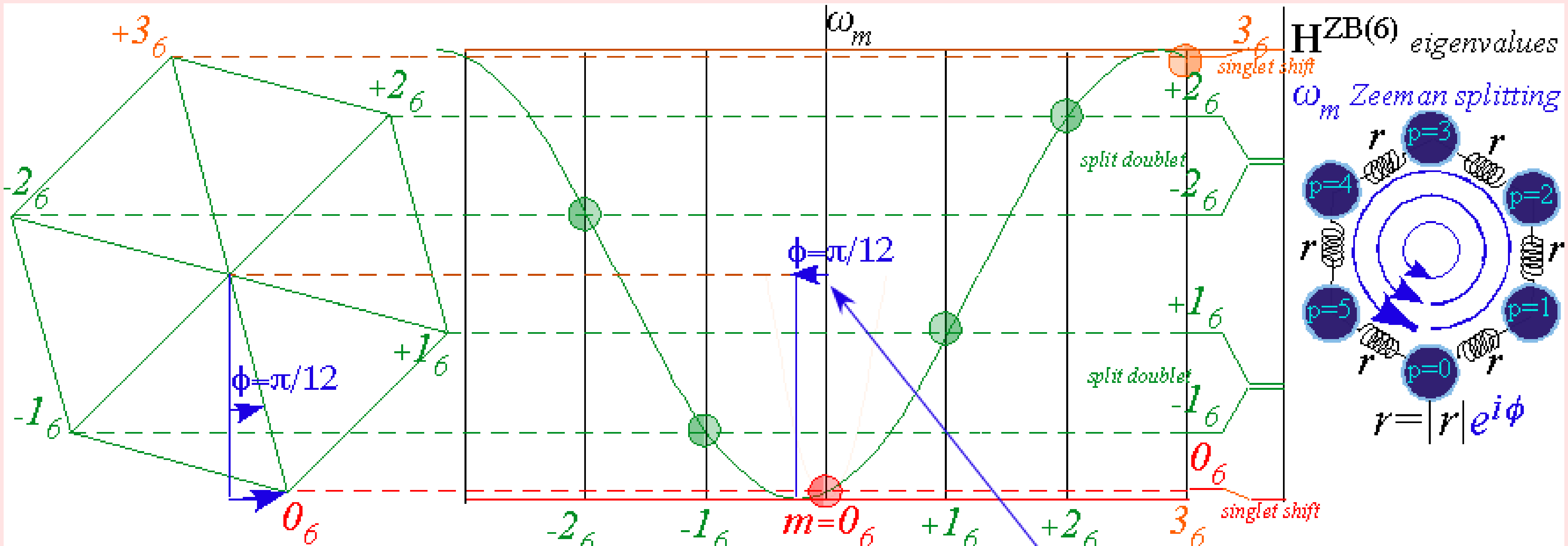
$$\omega^{B3(n)}(k_m) = r_0\chi_0^m + r_3\chi_3^m + r_{-3}\chi_{-3}^m = H_3 - 2t\,(-1)^m$$

3rd Step (contd.)

...eigensolutions for all possible C_6 symmetric complex H

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

(Dispersion function)



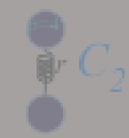
Note "gauge" shift

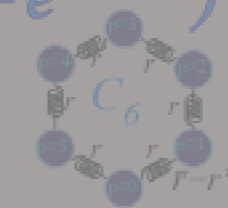
(Commuting)

- *Abelian symmetry = Fourier analysis* *(Back to our roots $1^{1/N}=e^{2\pi im/N}$)*

  Group product table => Hamiltonian $\hat{H}$-matrices *(C_2 and C_6 examples)*

  Group roots => $\hat{H}$-matrix spectral resolution by $P^{(m)}$projectors





Commutivity conundrum... ? $\hat{H}\cdot g=g\cdot\hat{H}$?

- ***New symmetry insights:*** ***Local vs. Global symmetry*** ***Projector invariance***

  "Mock-Mach" principle *Conway, et.al, May (2008)* *Cvitanovic, (2008)*

(Non-Commuting)

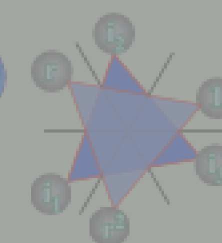
- *Non-Abelian symmetry analysis I.* *(Simplest example: D_3)*

  Local vs. Global product tables => $\hat{H}$-matrices

  All-commuting invariants => Global invariant (character) $P^{(\alpha)}$projectors

  Mutually-commuting sets => Local vs. Global eigensolutions by $P^{(\alpha)}_{m,n}$ projectors

  => $\hat{H}$-matrix spectral resolution by $P^{(\alpha)}_{m,n}$ projectors

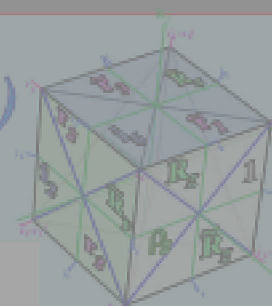


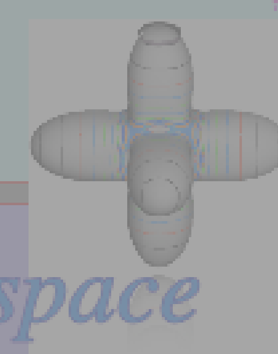
- *Non-Abelian symmetry analysis II.* *(Octahedral example: O_h)*

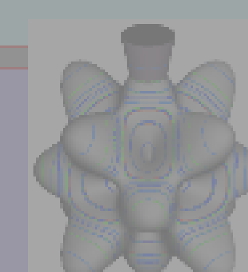
  Global-local product tables => $\hat{H}$-matrices...

  ... and all the above ...

  => eigensolution formulas by local-symmetry defined $P^{(\alpha)}_{n,n}$ projectors







- *Local vs Global symmetry in rovibronic phase space*

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

Abelian (Commutative) $C_2, C_2, \ldots, C_6 \ldots$

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) $D_3, O_h, \ldots$

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* **U** *?*

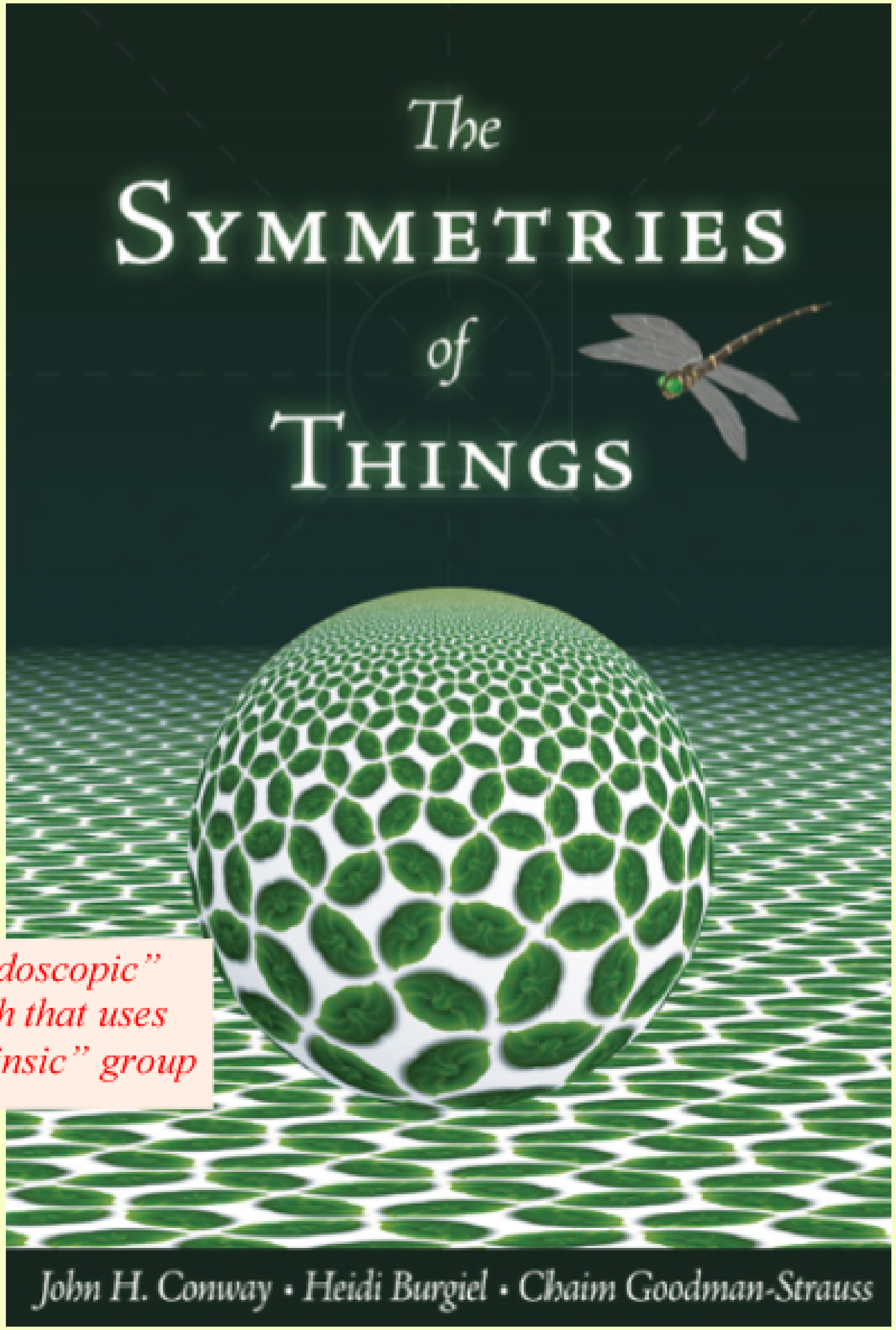
Time to examine how we..

...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

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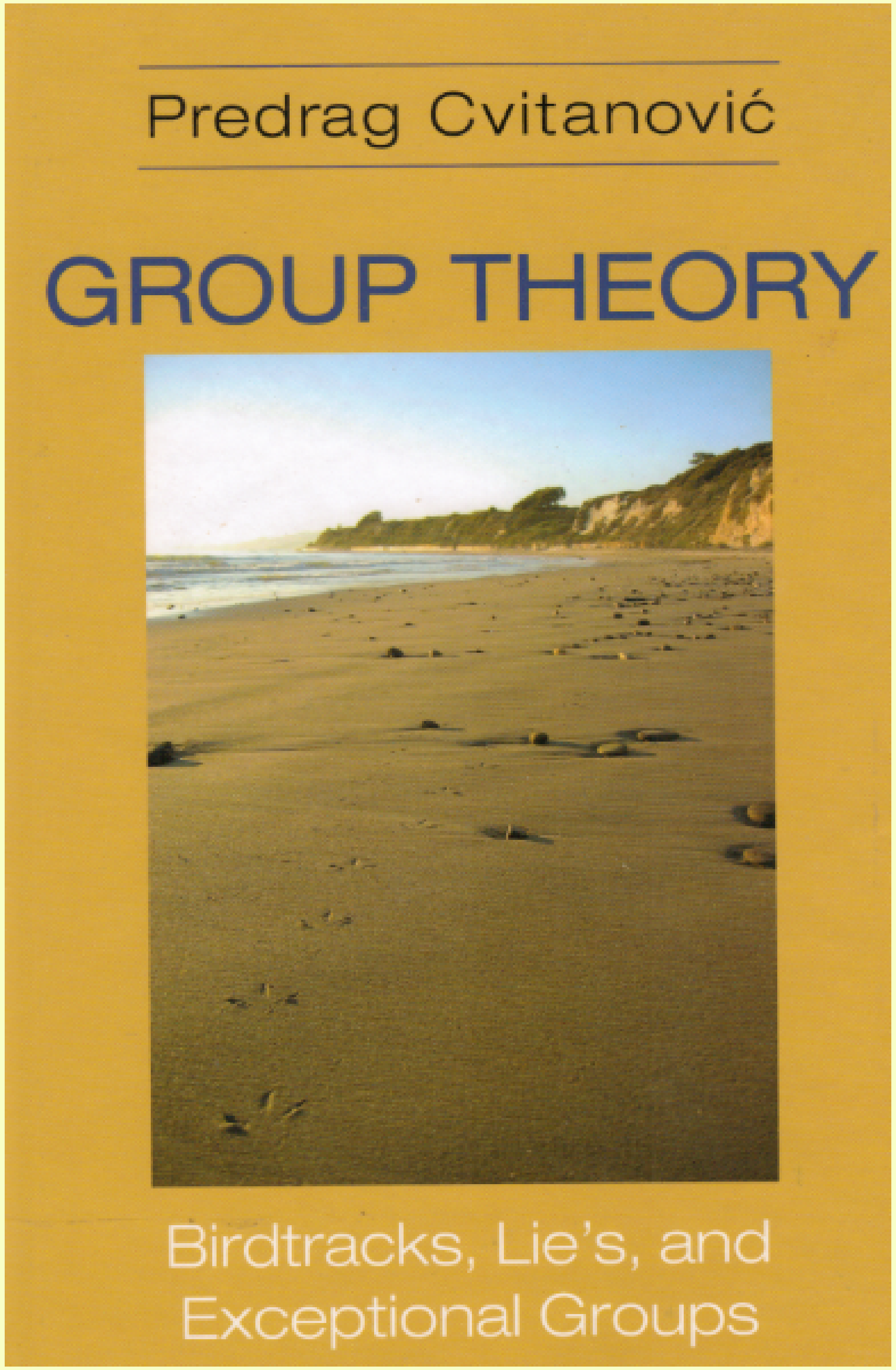
...from APPLIED(to string theory)...

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



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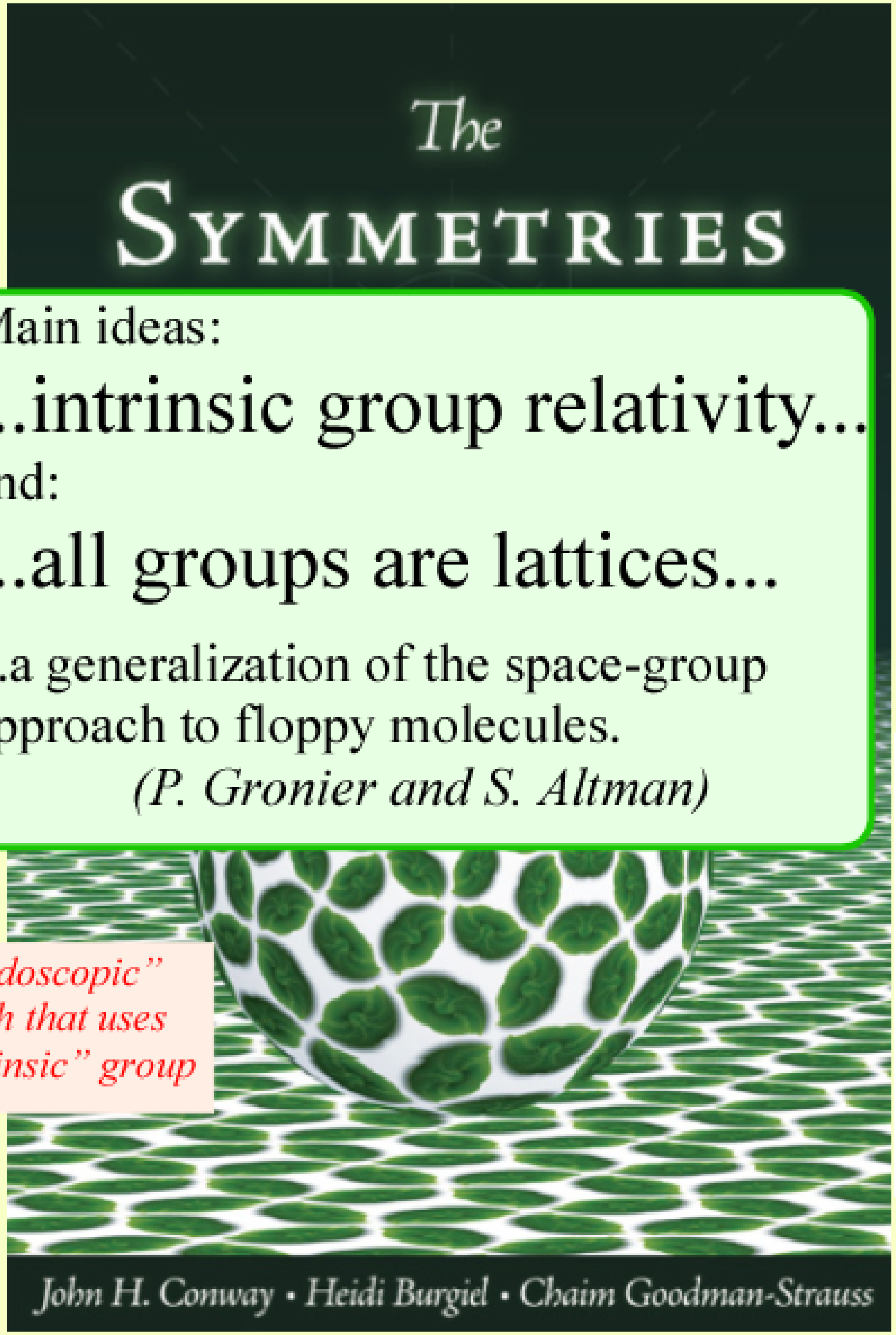
...from PURE group theory...

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

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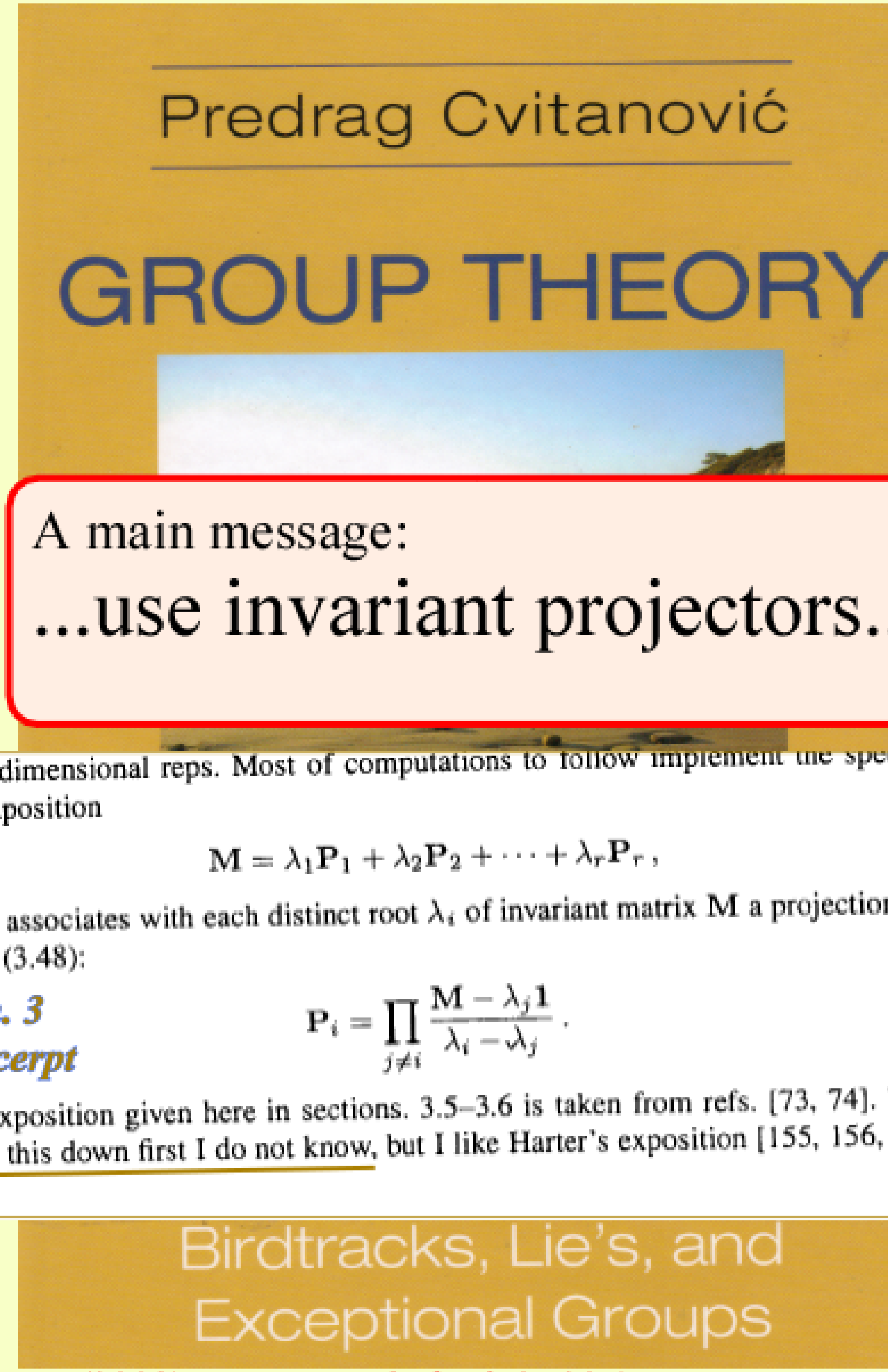
...from APPLIED (to supersymmetry)...

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.

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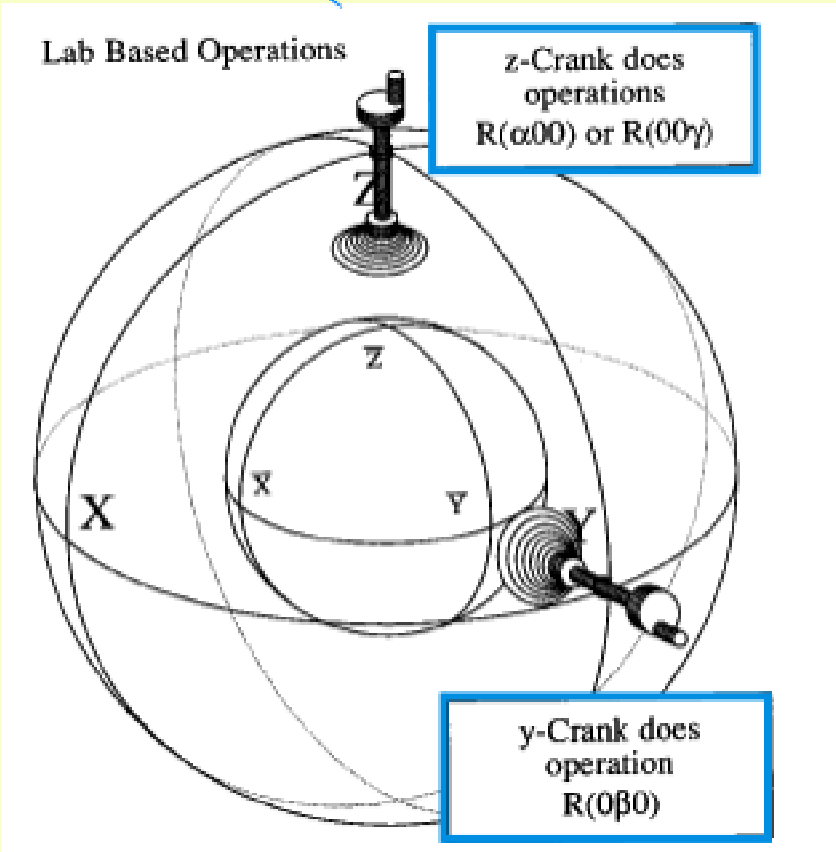
"Give me a place to stand...
and I will move the Earth"
Archimedes 287-212 B.C.E

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

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

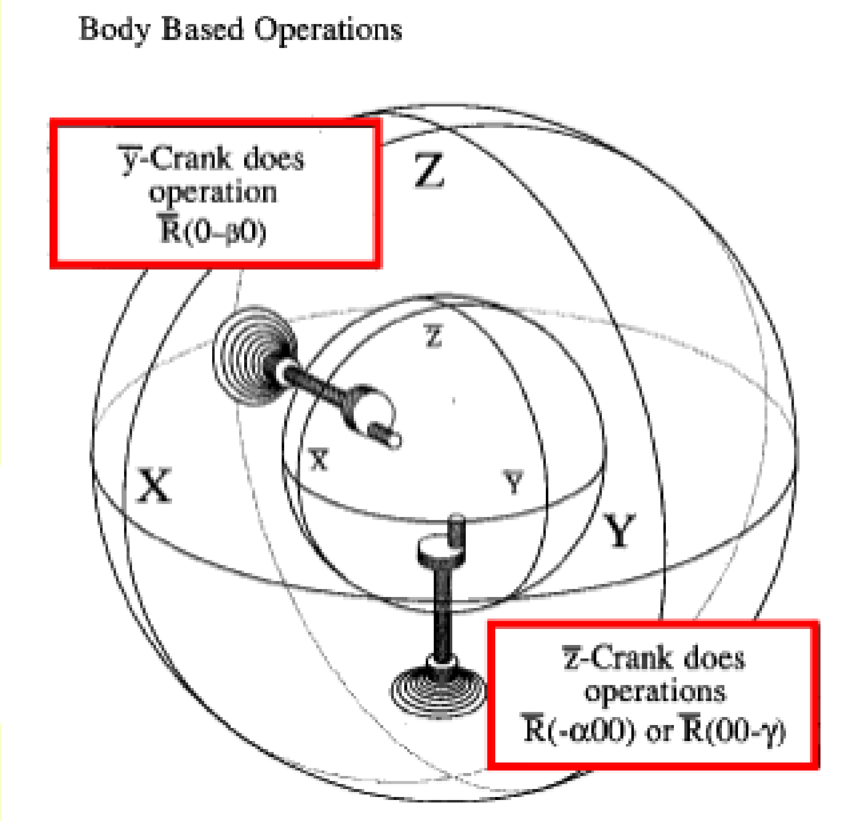


R *commutes* with *all* $\bar{\mathbf{R}}$

Mock-Mach relativity principle

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

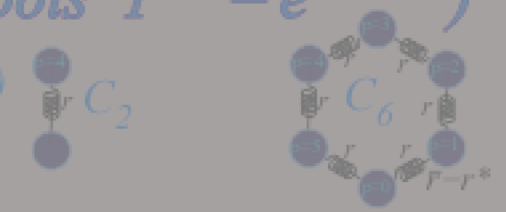
...for *one* state |1⟩ *only!*



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

(Commuting)

- *Abelian symmetry = Fourier analysis* *(Back to our roots $1^{1/N}=e^{2\pi i m/N}$)*
  *Group $\hat{\text{product}}$ table => Hamiltonian **H**-matrices* *(C_2 and C_6 examples)*
  *Group roots => **H**-matrix spectral resolution by $P^{(m)}$ projectors*



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(Non-Commuting)

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  *Local vs. Global $\hat{\text{product}}$ tables => **H**-matrices*
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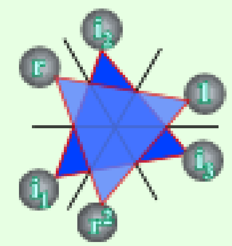
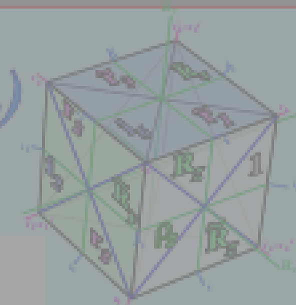
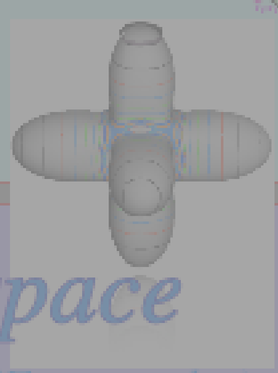
  Mutually-commuting sets => Local vs. Global eigensolutions by $P^{(\alpha)}_{m,n}$ projectors
  *=> **H**-matrix spectral resolution by $P^{(\alpha)}_{m,n}$ projectors*

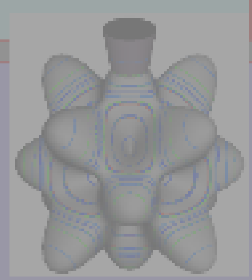


- *Non-Abelian symmetry analysis II.* *(Octahedral example: O_h)*
  *Global-local product tables => **H**-matrices...*
  ... and all the above ...
  => eigensolution formulas by local-symmetry defined $P^{(\alpha)}_{n,n}$ projectors

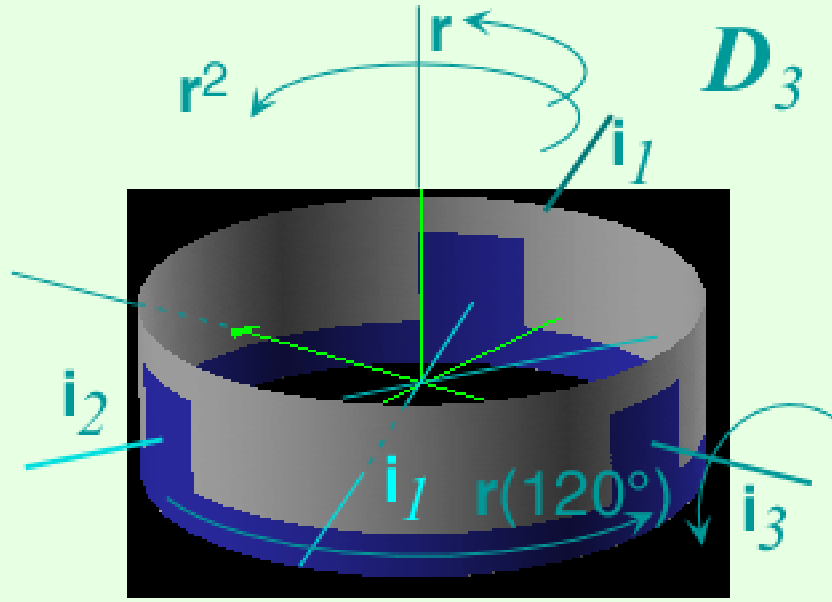




- *Local vs Global symmetry in rovibronic phase space*
  How group operators analyze rovibronic tunneling effects at high J. *(SF_6 examples)*



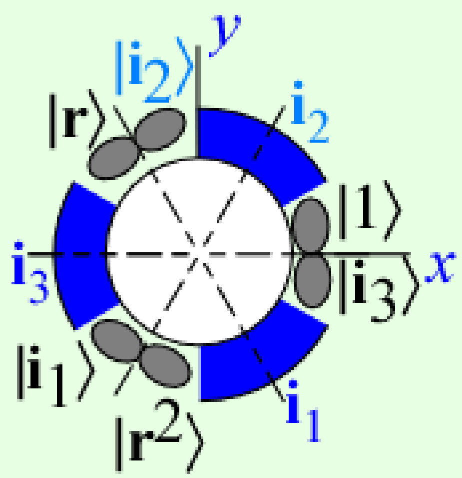
Example of GLOBAL vs LOCAL projector algebra for $D_3 \sim C_{3v}$

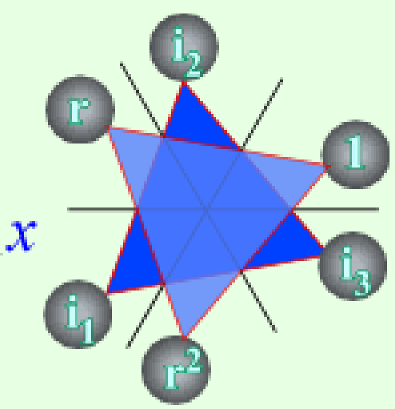


D_3

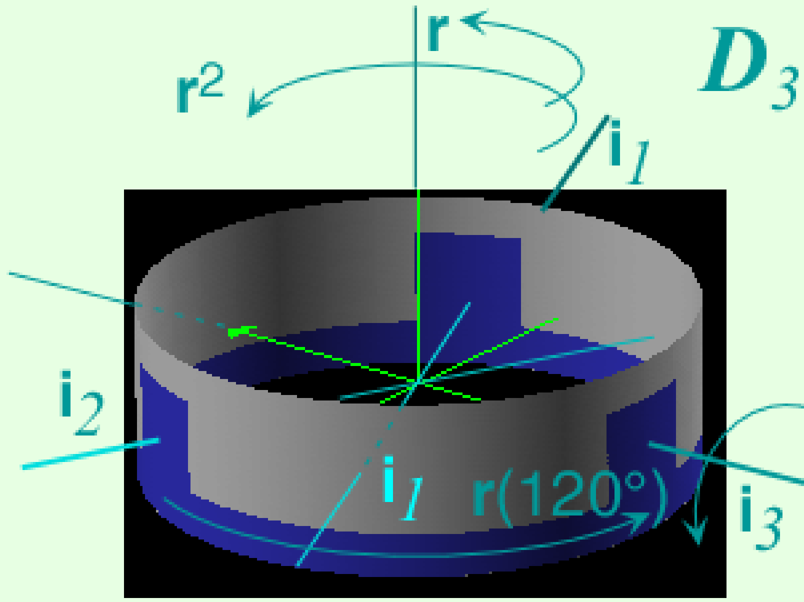
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

D_3-defined local-wave bases





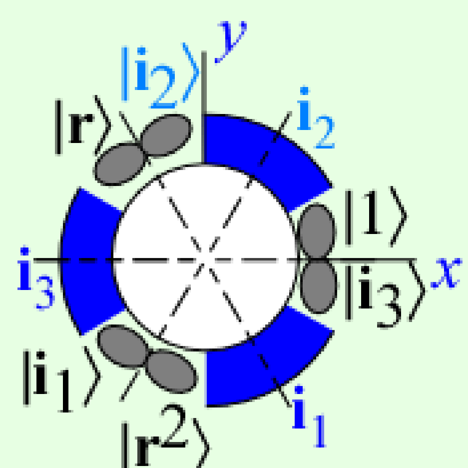
Example of GLOBAL vs LOCAL projector algebra for $D_3 \sim C_{3v}$

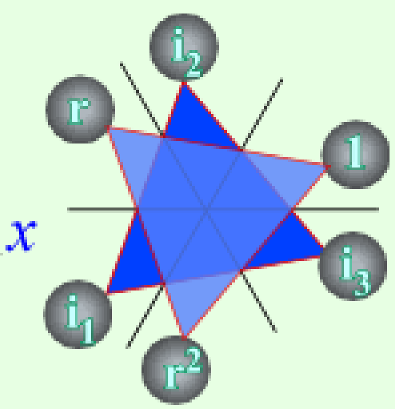


D_3

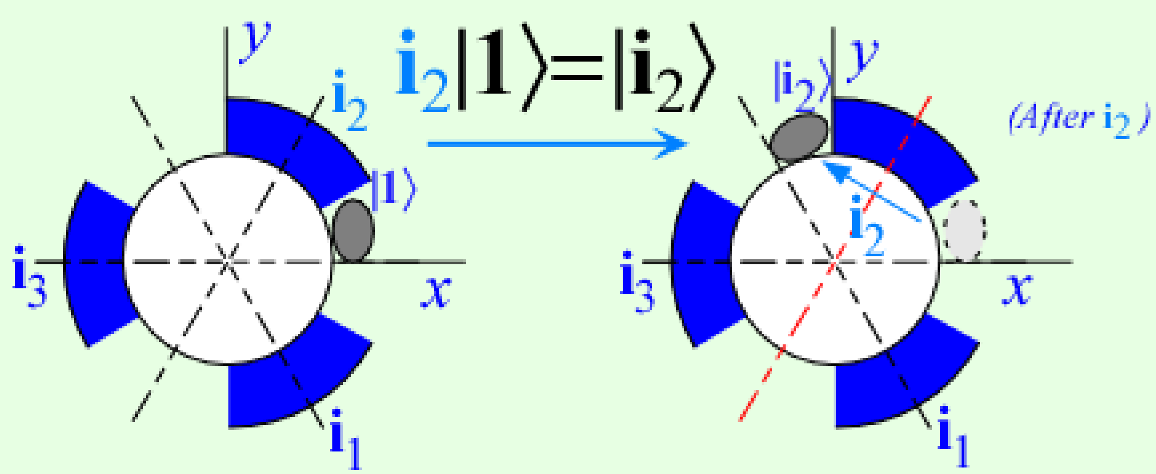
1	r^2	r	i_1	i_2	i_3
r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

D_3-defined local-wave bases





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



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

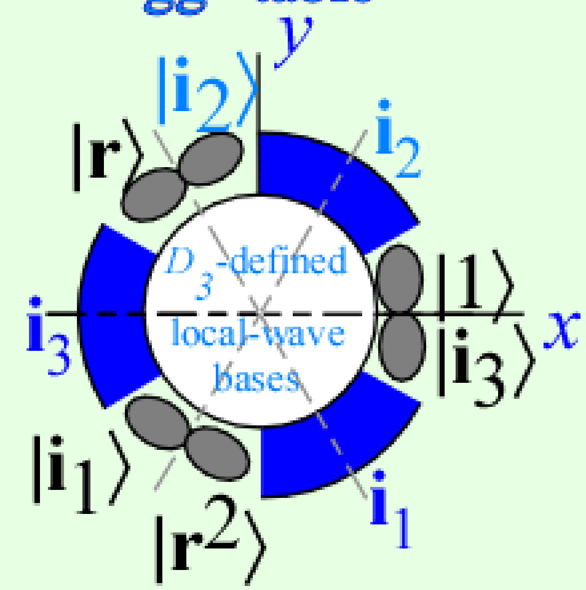
To represent *external* {..**T**,**U**,**V**,... }switch $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

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

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

1	$\mathbf{r}^2$	**r**	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
r	**1**	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	**r**	**1**	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	**1**	**r**	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{r}^2$	**1**	**r**
$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{i}_1$	**r**	$\mathbf{r}^2$	**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 $\mathbf{g} \leftrightarrows \mathbf{g}^\dagger$ on top of group table

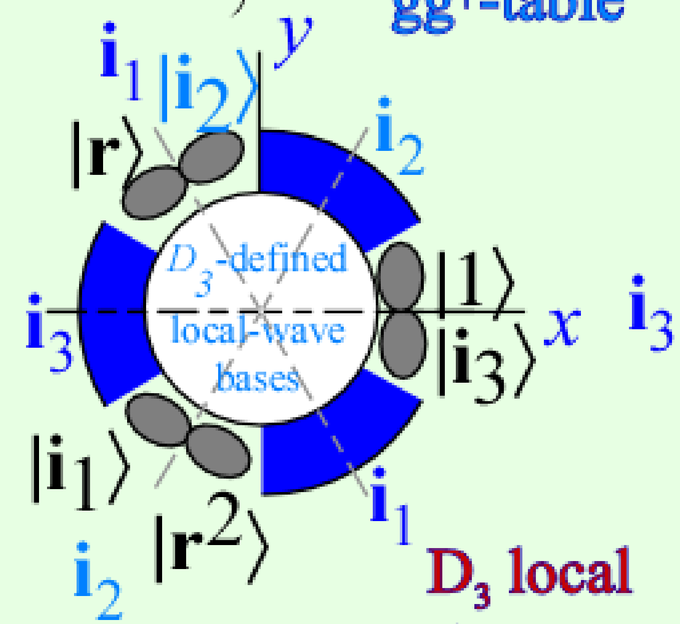
$R^G(\mathbf{1}) = \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$, $R^G(\mathbf{r}) = \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}$, $R^G(\mathbf{r}^2) = \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix}$, $R^G(\mathbf{i}_1) = \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix}$, $R^G(\mathbf{i}_2) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$, $R^G(\mathbf{i}_3) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$

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 $gg^\dagger$-table

RESULT:
Any *R(**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 $\bar{\mathbf{T}}\cdot\bar{\mathbf{U}}=\bar{\mathbf{V}}$.



D_3 local $g^\dagger g$-table

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

$R^G(\bar{\mathbf{1}}) = \begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$, $R^G(\bar{\mathbf{r}}) = \begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}$, $R^G(\bar{\mathbf{r}}^2) = \begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix}$, $R^G(\bar{\mathbf{i}}_1) = \begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$, $R^G(\bar{\mathbf{i}}_2) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix}$, $R^G(\bar{\mathbf{i}}_3) = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$

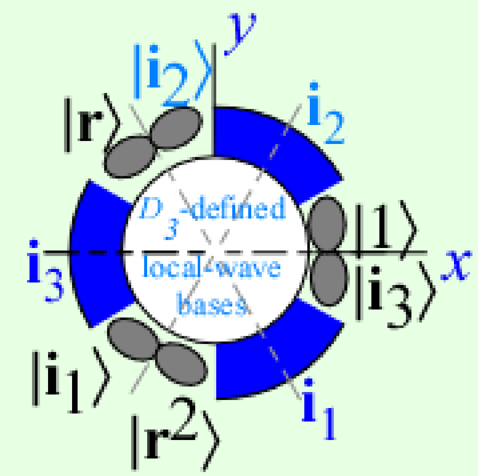
1	r	r^2	i_1	i_2	i_3
r^2	1	r	i_2	i_3	i_1
r	r^2	1	i_3	i_1	i_2
i_1	i_2	i_3	1	r	r^2
i_2	i_3	i_2	r^2	1	r
i_3	i_1	i_2	r	r^2	1

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

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

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

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



Local H matrix parametrized by ḡ's

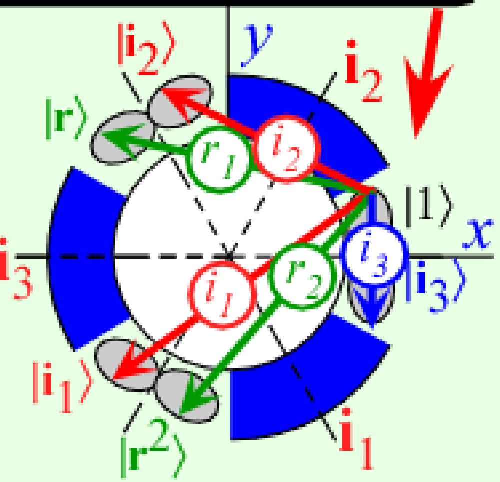
RESULT:
Any $R(\mathbf{T})$ *commute* with any $R(\overline{\mathbf{U}})$...

So an H*-matrix having* ***Global*** *symmetry* D_3

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

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

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



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

local D_3 defined Hamiltonian matrix

$\mathbb{H} \equiv$

	$\vert 1\rangle$	$\vert r\rangle$	$\vert r^2\rangle$	$\vert i_1\rangle$	$\vert i_2\rangle$	$\vert i_3\rangle$
$\langle 1\vert$	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_1	r_2	H	r_1
$\langle i_3\vert$	i_3	i_1	i_2	r_1	r_2	H

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

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

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

Example of RELATIVITY-DUALITY

To represent *external* {..**T**,**U**,**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

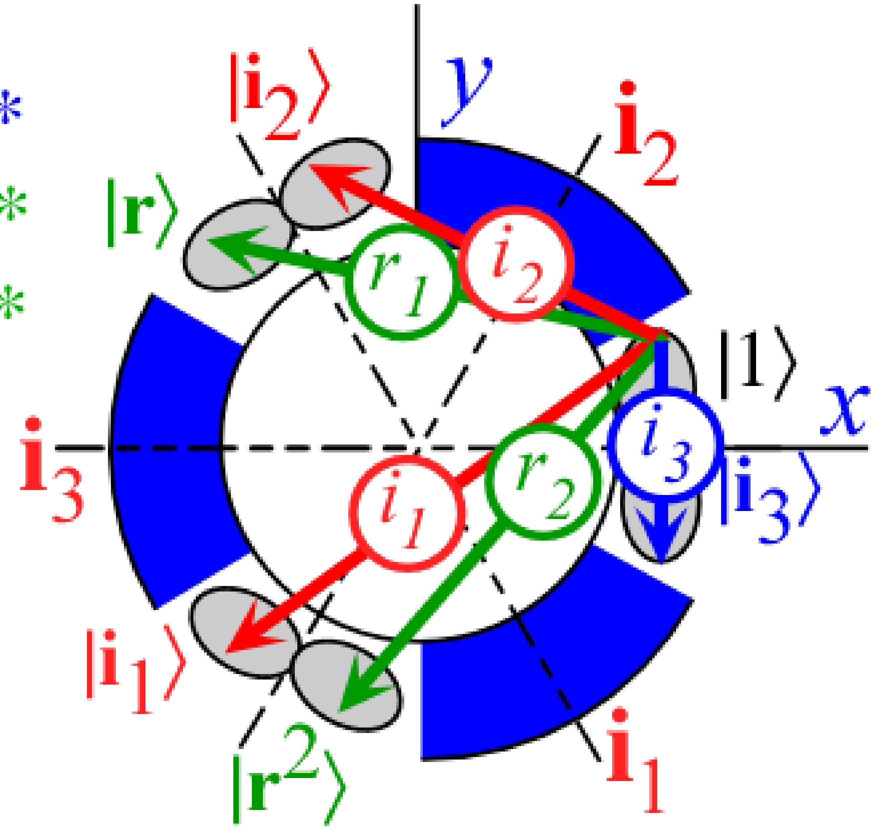
$$\mathbb{H}=H\mathbf{1}^0+r_1\bar{\mathbf{r}}^1+r_2\bar{\mathbf{r}}^2+i_1\bar{\mathbf{i}}_1+i_2\bar{\mathbf{i}}_2+i_3\bar{\mathbf{i}}_3$$

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

$\mathbb{H}=$

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

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

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

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

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

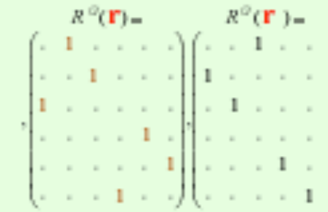
(3) Assemble

local-D_3-defined Hamiltonian matrix

$\mathbb{H} =$

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

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*

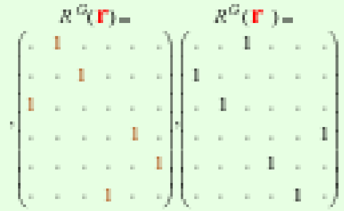
For symmetry group or algebra G

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?



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(2) Find commuting invariants (Using character projection algebra)
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local-D_3-defined Hamiltonian matrix

$\mathbb{H}=$	$\vert 1)$	$\vert r)$	$\vert r^2)$	$\vert i_1)$	$\vert i_2)$	$\vert i_3)$
$(1\vert$	H	r_1	r_2	i_1	i_2	i_3
$(r\vert$	r_2	H	r_1	i_2	i_3	i_1
$(r^2\vert$	r_1	r_2	H	i_3	i_1	i_2
$(i_1\vert$	i_1	i_2	i_3	H	r_1	r_2
$(i_2\vert$	i_2	i_3	i_1	r_2	H	r_1
$(i_3\vert$	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
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$\ell^\alpha =$ Irreducible representation (irrep) *dimension* or level *degeneracy*
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Rank: $\rho(G)=\Sigma_{irrep(\alpha)}(\ell^\alpha)^1$ =Number of irrep idempotents $\mathbf{P}^{(\alpha)}_{n,n}$, *mutually-commuting* ops

Order: $°(G)=\Sigma_{irrep(\alpha)}(\ell^\alpha)^2$ =*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: $°(D_3)=\Sigma_{(\alpha)}(\ell^\alpha)^0=1^2+1^2+2^2=6$

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

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 $\underline{\kappa}_k$ 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 $\mathbf{P}^{E}$

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

Algebra Center like cell nucleus;
Its invariants are made here.

- *characters* *(invariant)*
- *projectors* *(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)

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

$\rightarrow$

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

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
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$$0 = (\kappa_3 - 3\cdot\mathbf{1})\mathbf{P}^{A_1} \qquad \kappa_3\mathbf{P}^{A_1} = +3\cdot\mathbf{P}^{A_1}$$

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

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

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

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

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

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

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

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

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

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

D_3 Example

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

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

→

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

$\kappa_1 = \mathbf{1}$	$\kappa_2 = \mathbf{r}^1 + \mathbf{r}^2$	$\kappa_3 = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
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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 $\mathbf{P}^{E}$

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

$$0 = (\kappa_3 - 3\cdot\mathbf{1})\mathbf{P}^{A_1} \qquad 0 = (\kappa_3 + 3\cdot\mathbf{1})\mathbf{P}^{A_2} \qquad 0 = (\kappa_3 - 0\cdot\mathbf{1})\mathbf{P}^{E}$$

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

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

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

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

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

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)

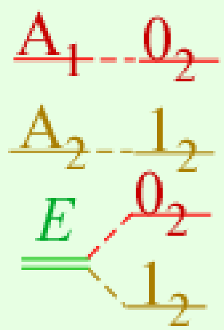
D_3 $\kappa=$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	1	1	1	/6
$\mathbf{P}^{A_2}=$	1	1	-1	/6
$\mathbf{P}^{E}=$	2	-1	0	/3

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

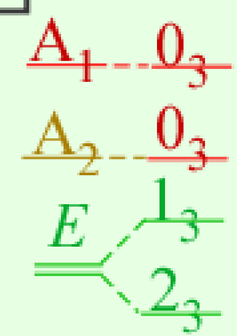
$\varepsilon = e^{2\pi i/3}$

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)

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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
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$n^{A_2}=$	·	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

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$\mathbf{P}^{A_1}=$	1	1	1	/6
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$\mathbf{P}^{E}=$	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 $\mathbf{P}^{(\alpha)}_{n,n}$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$\mathbf{P}^{E}$ 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 $\kappa_{\mathbf{i}_3}$

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

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

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

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

$\mathbf{P}^{E}$ 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 $\kappa_{\mathbf{r}^2}$

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 $\mathbf{P}^{(\alpha)}$

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

Centrum $\kappa(D_3)=3$ 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 $\kappa_{\mathbf{i}_3}$

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

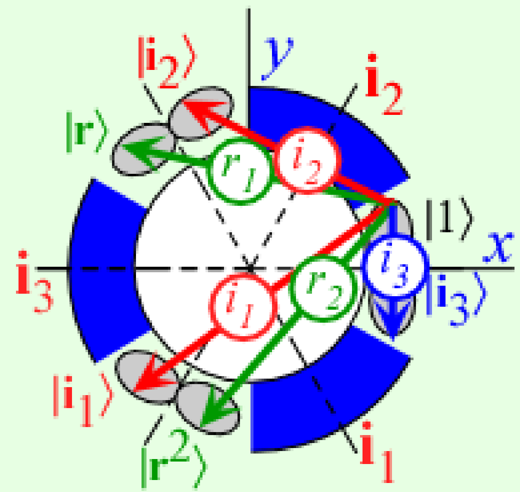
$\mathbf{P}^E$ splits into $\mathbf{P}^E=\mathbf{P}^E_{1_3 1_3}+\mathbf{P}^E_{2_3 2_3}$,

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

$r=r_2$ must equal r_1 $\quad$ $i=i_2$ 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	$\kappa=\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
$\mathbf{P}^{A_1}=$	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 $\mathbf{P}^{(\alpha)}_{n,n}$

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

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D3 :

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

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

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

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

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

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

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

	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

	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

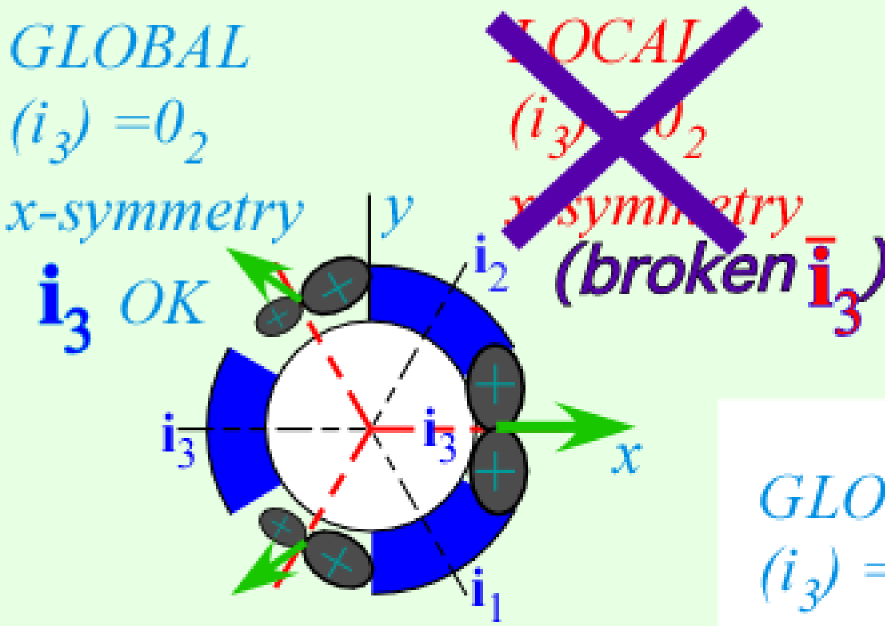
	1	$\mathbf{r}^1$	$\mathbf{r}^2$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$	
$\mathbf{P}^{E}_{x,y}=$	(0	-1	1	-1	+1	0)	/√3/2
$\mathbf{P}^{E}_{y,y}=$	(2	-1	-1	+1	+1	-2)	/6

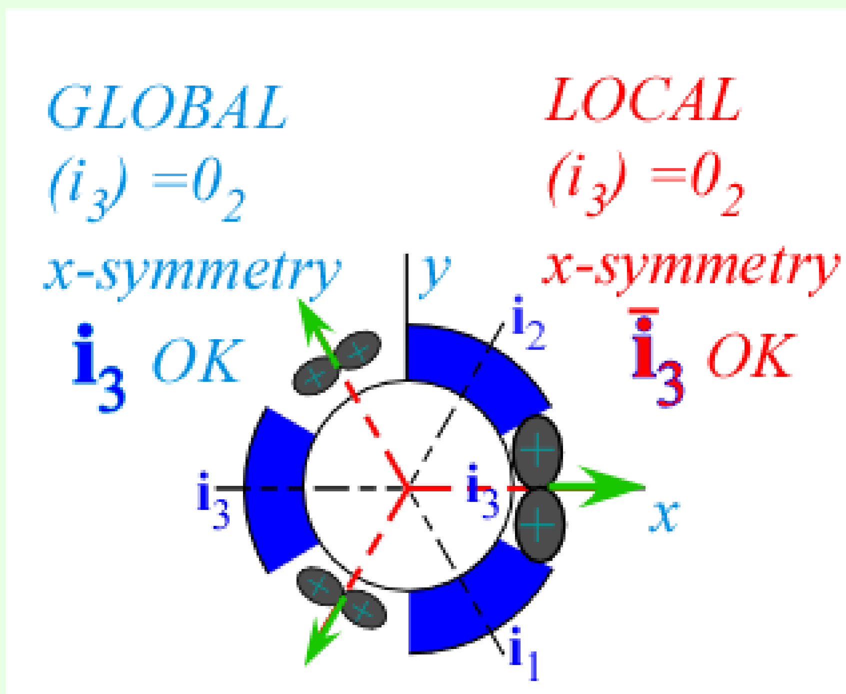
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|\mathbf{1}\right\rangle$$

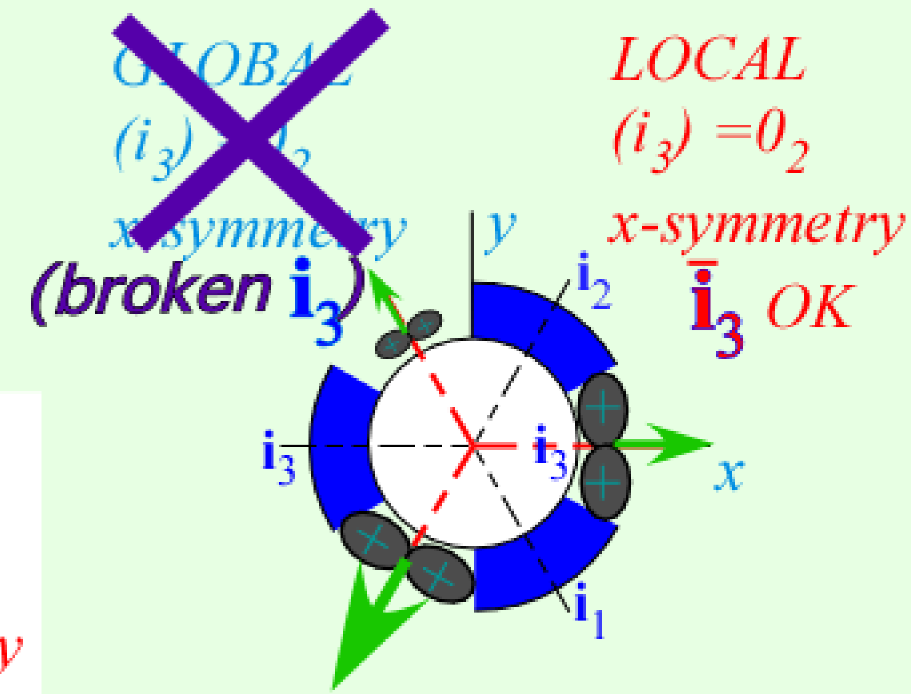
external LAB — *internal BOD*

symmety label-e — *symmety label-b*

GLOBAL — *LOCAL*







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

Global (LAB) symmetry

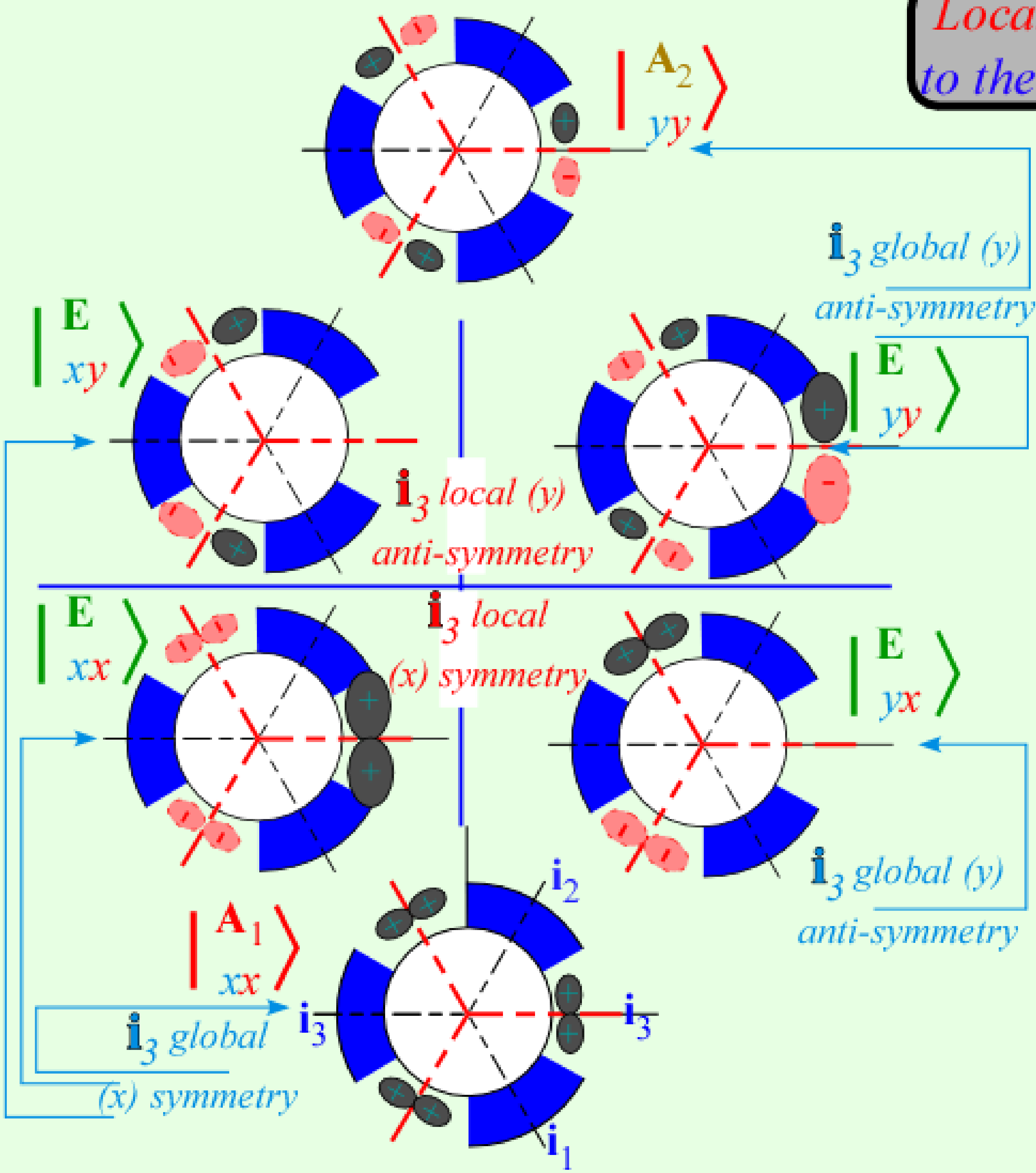
$$\mathbf{i}_3\left|{}^{(m)}_{eb}\right\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = (-1)^e \left|{}^{(m)}\right\rangle$$

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

Local (BOD) symmetry

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

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



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

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

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**

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

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: $H + 2r + 2i + i_3$

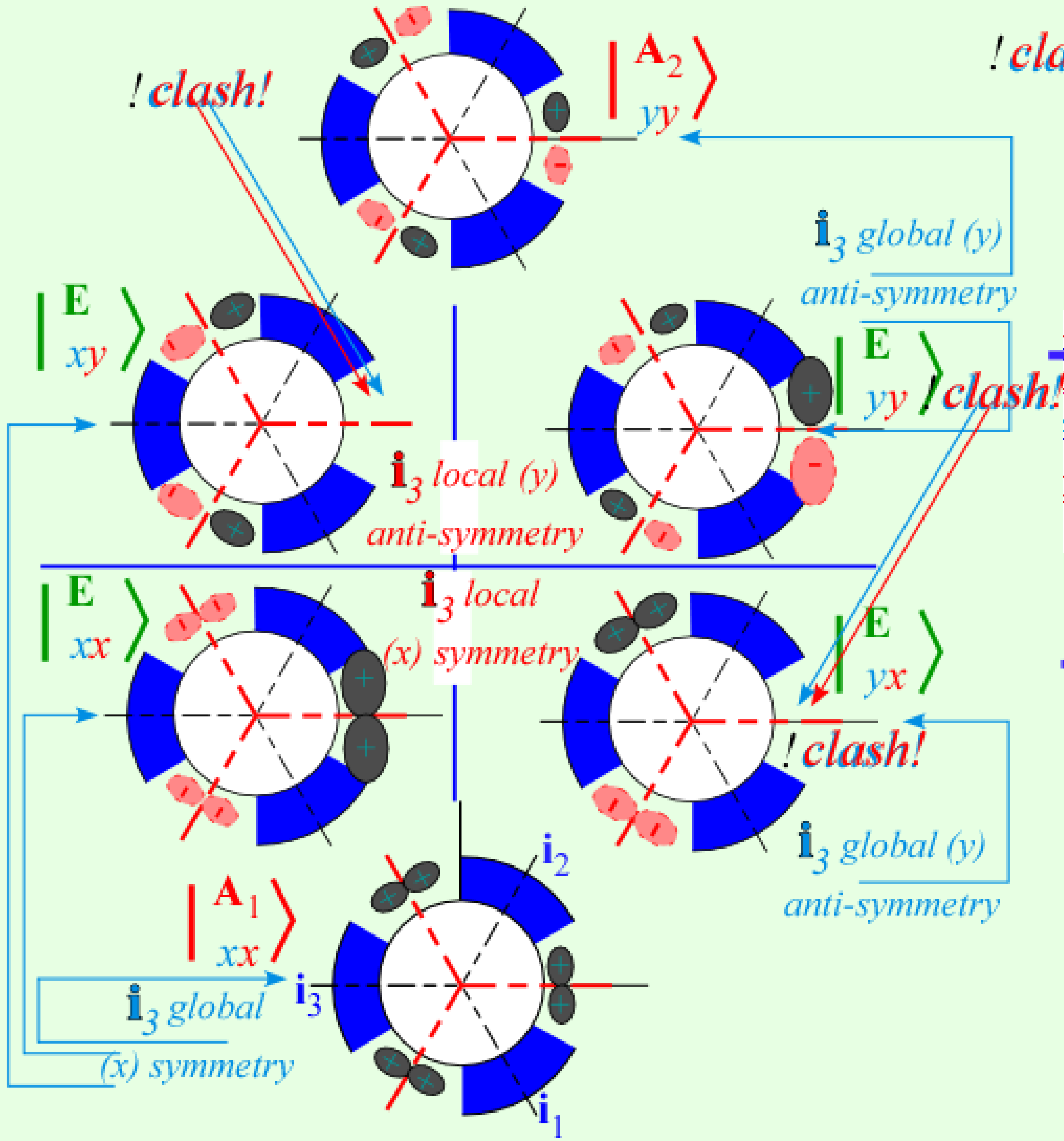
A_1-level: $H + 2r - 2i - i_3$

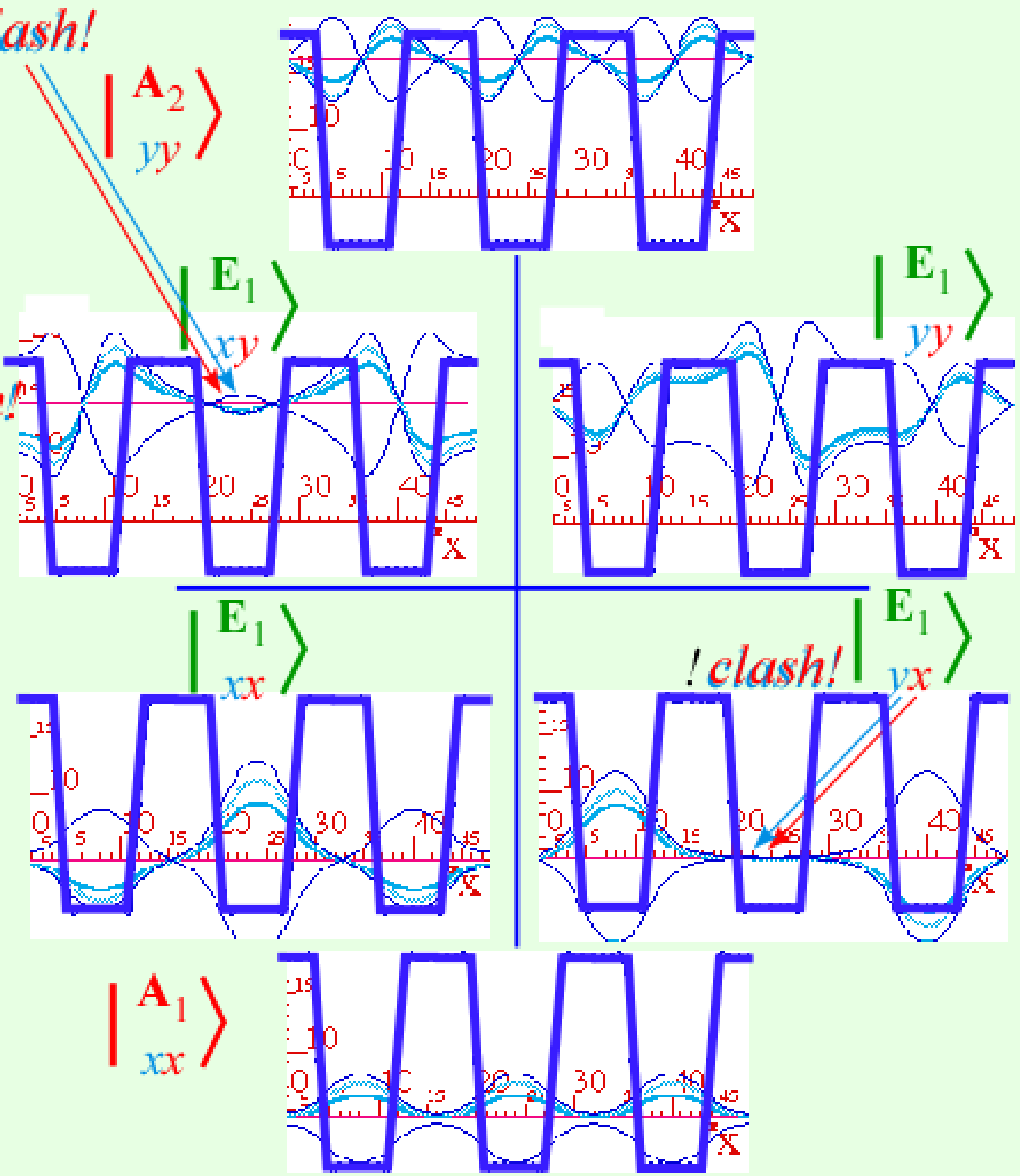
E_x-level: $H - r - i + i_3$

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

When there is no there, there...

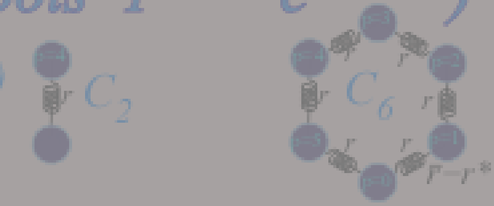
Nobody Home
where LOCAL
and GLOBAL





(Commuting)

- *Abelian symmetry = Fourier analysis* *(Back to our roots $1^{1/N} = e^{2\pi i m/N}$)*
  - *Group product table => Hamiltonian **H**-matrices* *(C_2 and C_6 examples)*
  - *Group roots => **H**-matrix spectral resolution by $P^{(m)}$ projectors*

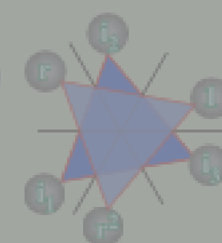


Commutivity conundrum... ? $\mathbf{H}\cdot g = g\cdot \mathbf{H}$?

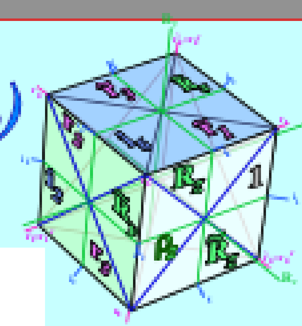
- *New symmetry insights:* *Local vs. Global symmetry* *Projector invariance*
  - *"Mock-Mach" principle* Conway, et.al, May (2008) Cvitanovic, (2008)

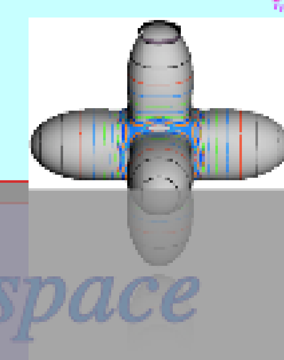
(Non-Commuting)

- *Non-Abelian symmetry analysis I.* *(Simplest example: D_3)*
  - *Local vs. Global product tables => **H**-matrices*
  - *All-commuting invariants => Global invariant (character) $P^{(\alpha)}$ projectors*
  - *Mutually-commuting sets => Local vs. Global eigensolutions by $P^{(\alpha)}_{m,n}$ projectors*
  - *=> **H**-matrix spectral resolution by $P^{(\alpha)}_{m,n}$ projectors*

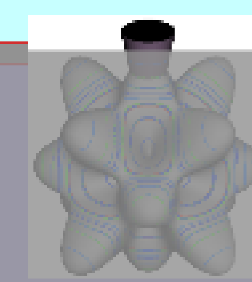


- ***Non-Abelian symmetry analysis II.*** ***(Octahedral example: O_h)***
  - *Global-local product tables => **H**-matrices...*
  - *... and all the above ...*
  - *=> eigensolution formulas by local-symmetry defined $P^{(\alpha)}_{n,n}$ projectors*





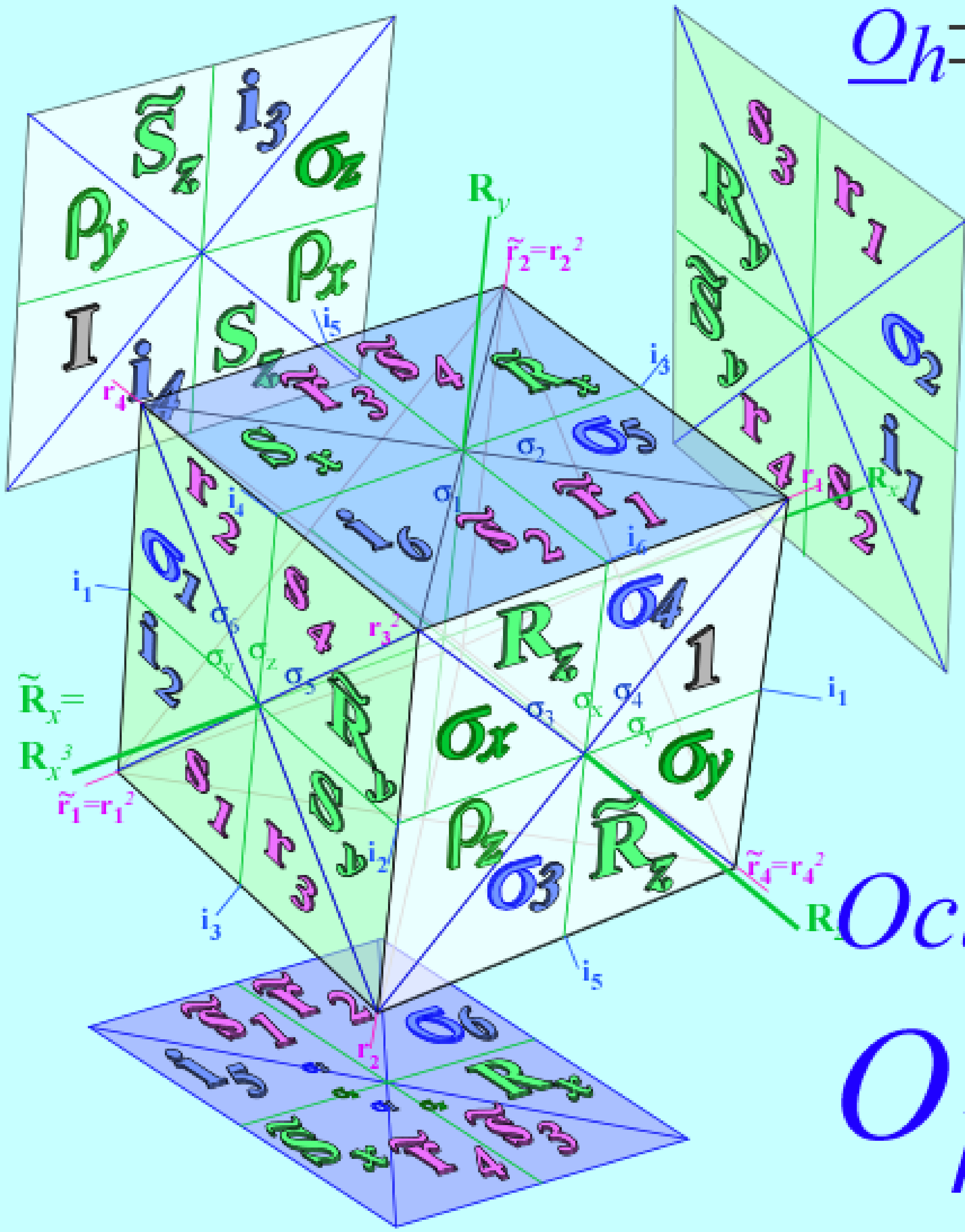
- *Local vs Global symmetry in rovibronic phase space*
  - *How group operators analyze rovibronic tunneling effects at high J.* *(SF_6 examples)*



Example of GLOBAL vs LOCAL projector algebra for

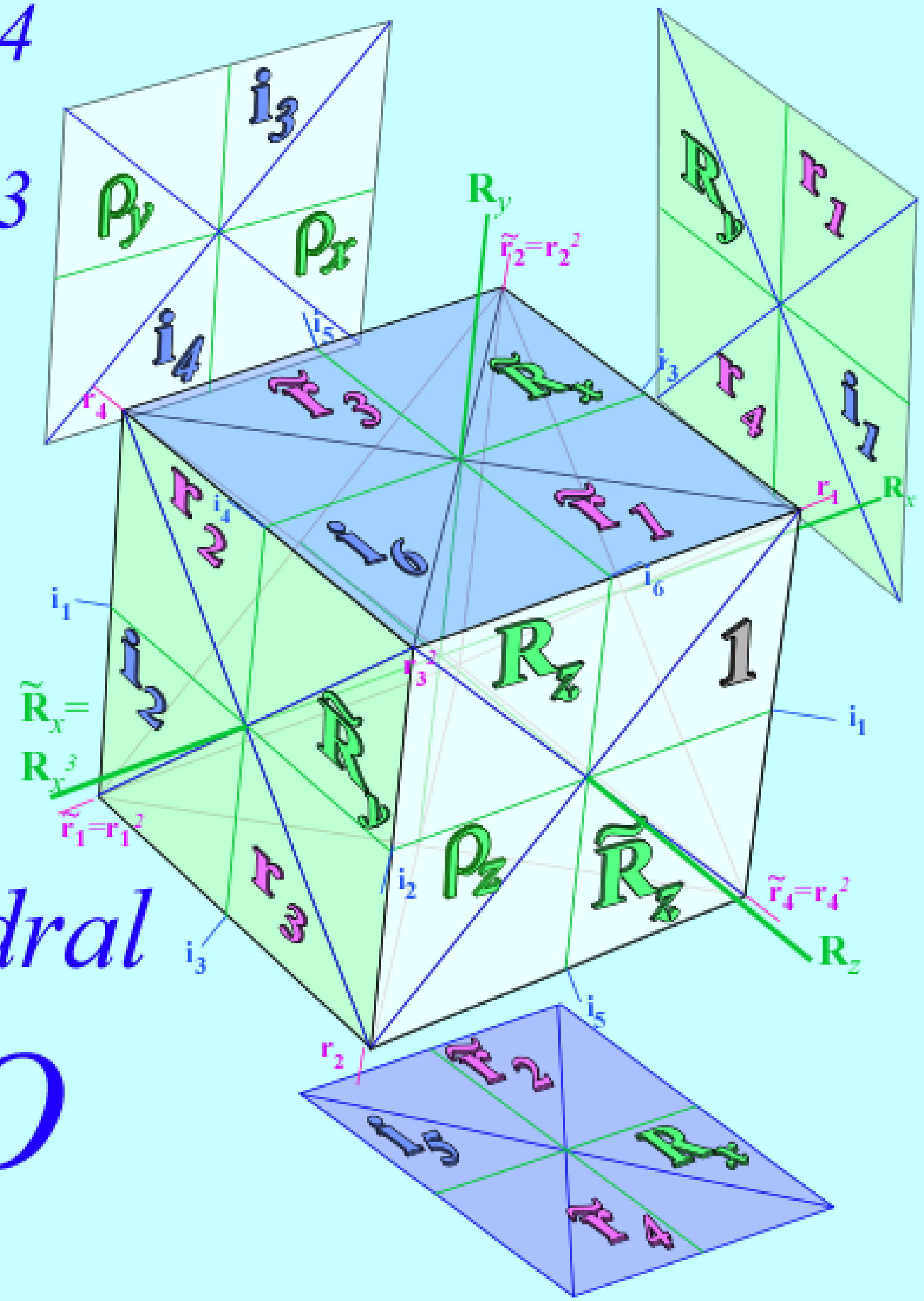
$\underline{O}_h \supset \underline{O} \supset \underline{C}_4$

or: $\supset \underline{C}_3$



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

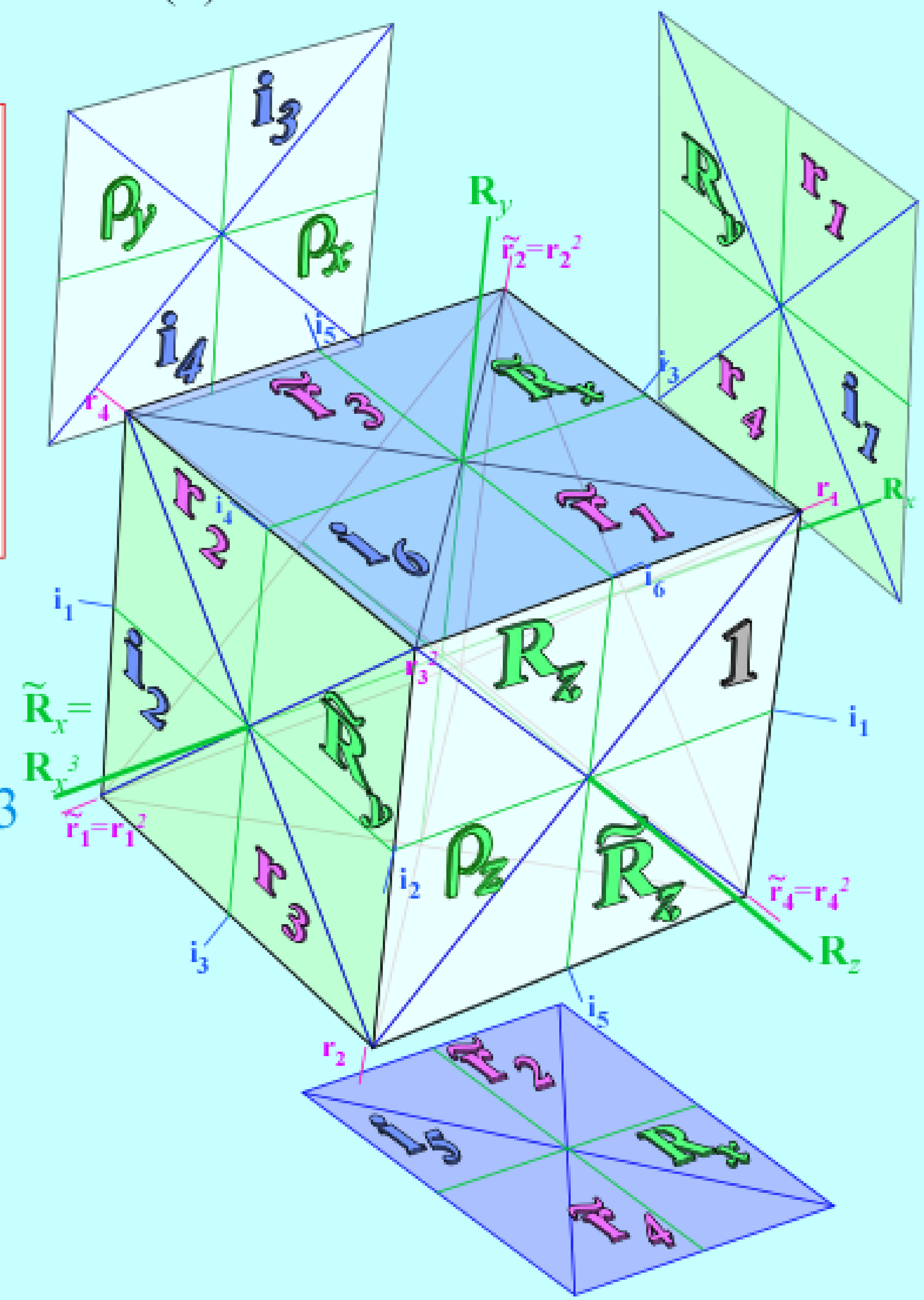
	O group $\chi^{\alpha}_{\kappa_g}$	$g=1$	r_{1-4} $\tilde{r}_{1-4}$	ρ_{xyz}	R_{xyz} $\tilde{R}_{xyz}$	i_{1-6}
s-orbital r^2	$\alpha=A_1$	1	1	1	1	1
	A_2	1	1	1	−1	−1
d-orbitals $\{x^2+y^2-2z^2, x^2-y^2\}$	E	2	−1	2	0	0
p-orbitals $\{x, y, z\}$	T_1	3	0	−1	1	−1
$\{xz,yz,xy\}$ d-orbitals	T_2	3	0	−1	−1	1

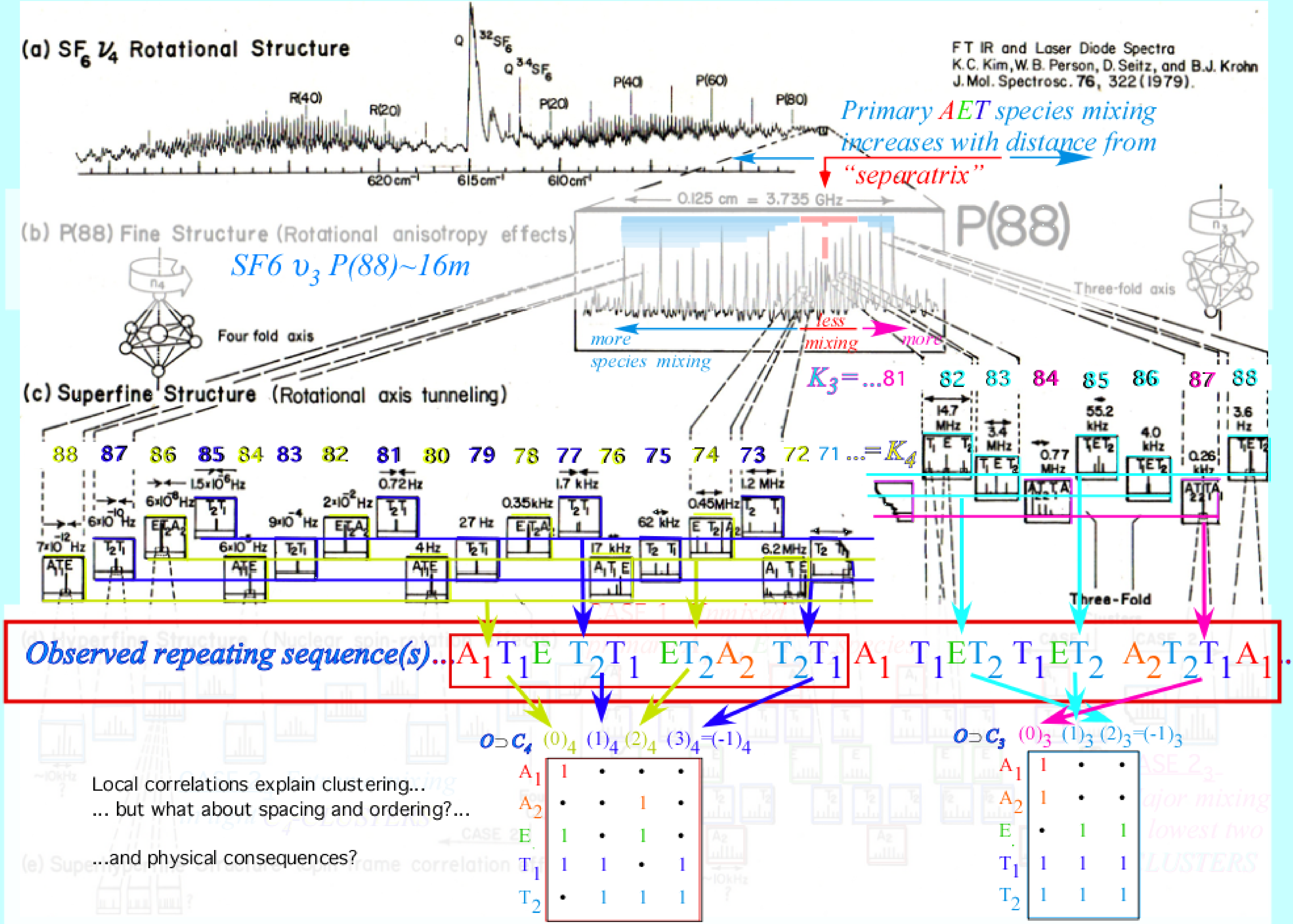
$O\supset C_4$

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

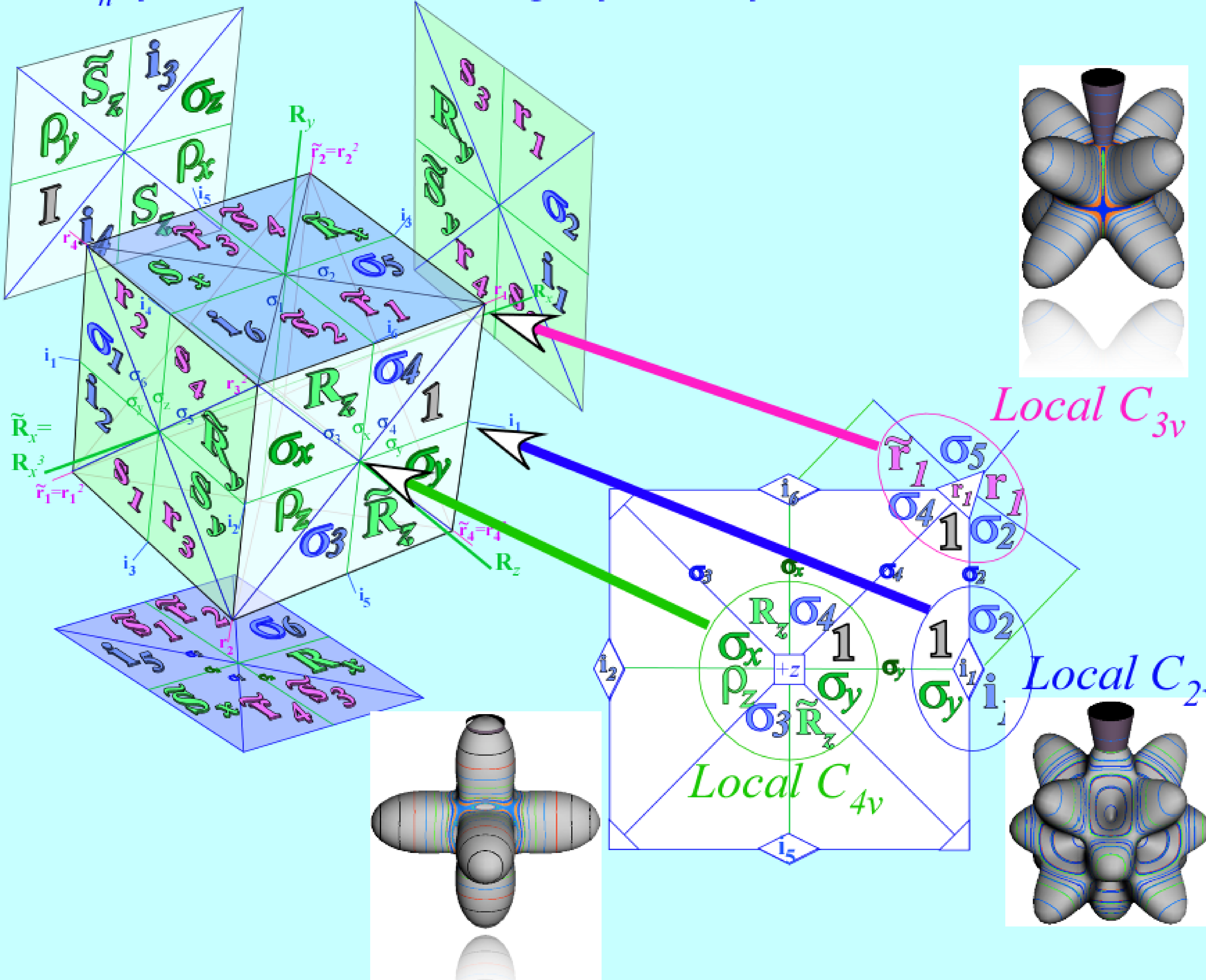
$O\supset C_3$

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




(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)...A1 T1 E T2 T1 E T2 A2 T2 T1 A1 T1 E T2 T1 E T2 A2 T2 T1 A1...
O⊃C4 (0)4 (1)4 (2)4 (3)4=(-1)4
O⊃C3 (0)3 (1)3 (2)3=(-1)3
Local correlations explain clustering...
... but what about spacing and ordering?...
...and physical consequences?

O_h operator slide rule and subgroup / coset-space structure



C_4 subgroup correlation to O (largest local symmetry => smallest level-clusters)

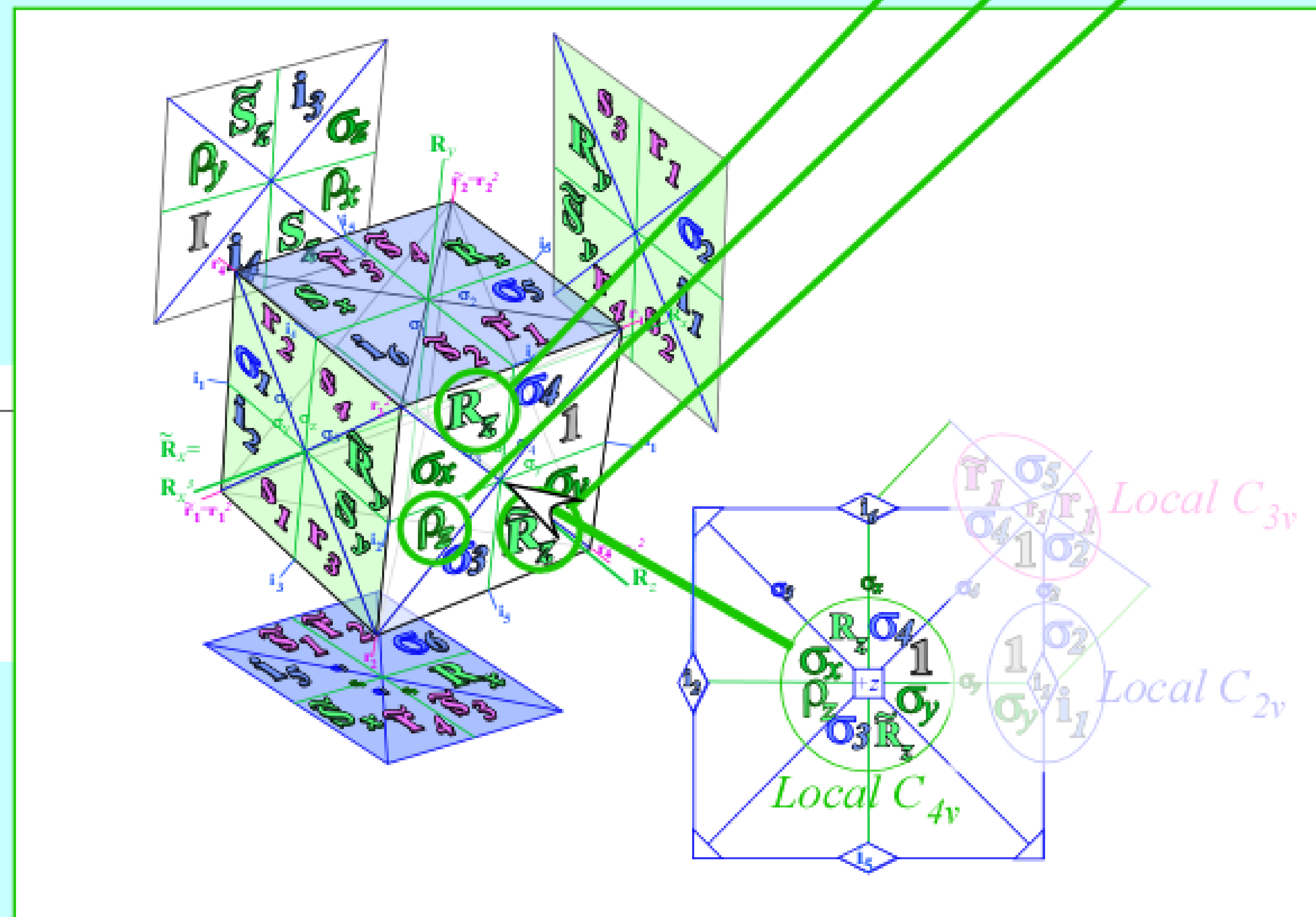
$O \supset C_4$

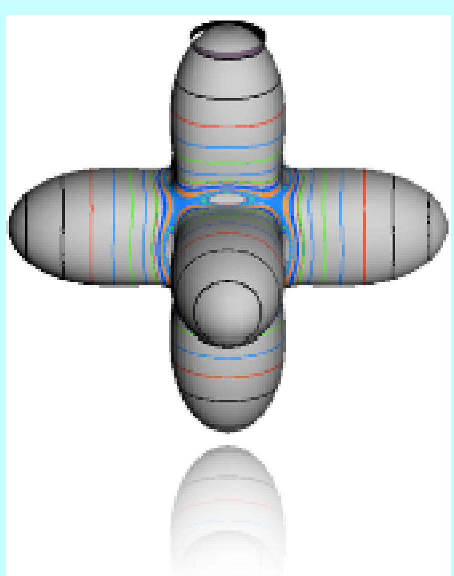
	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

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

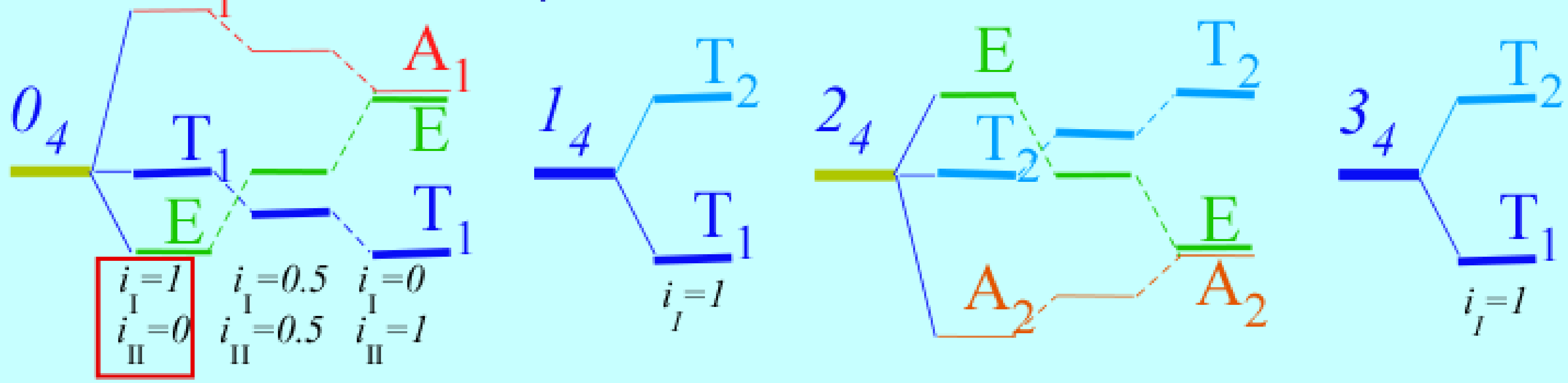
$$\mathbf{p}_{m_4} = \sum_{p=0}^{3} \frac{e^{2\pi i m\cdot p/4}}{4}\mathbf{R}_z^p = \begin{cases} \mathbf{p}_{0_4} = (\mathbf{1}+\mathbf{R}_z+\rho_z+\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{1_4} = (\mathbf{1}+i\mathbf{R}_z-\rho_z-i\tilde{\mathbf{R}}_z)/4 \\ \mathbf{p}_{2_4} = (\mathbf{1}-\mathbf{R}_z+\rho_z-\tilde{\mathbf{R}}_z)/4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

$\mathbf{1}\cdot\mathbf{P}^\alpha =$	$(\mathbf{p}_{0_4}$	$+\mathbf{p}_{1_4}$	$+\mathbf{p}_{2_4}$	$+\mathbf{p}_{3_4})\cdot\mathbf{P}^\alpha$
$\mathbf{1}\cdot\mathbf{P}^{A_1} =$	$\mathbf{P}^{A_1}_{0_40_4}$	$+0$	$+0$	$+0$
$\mathbf{1}\cdot\mathbf{P}^{A_2} =$	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

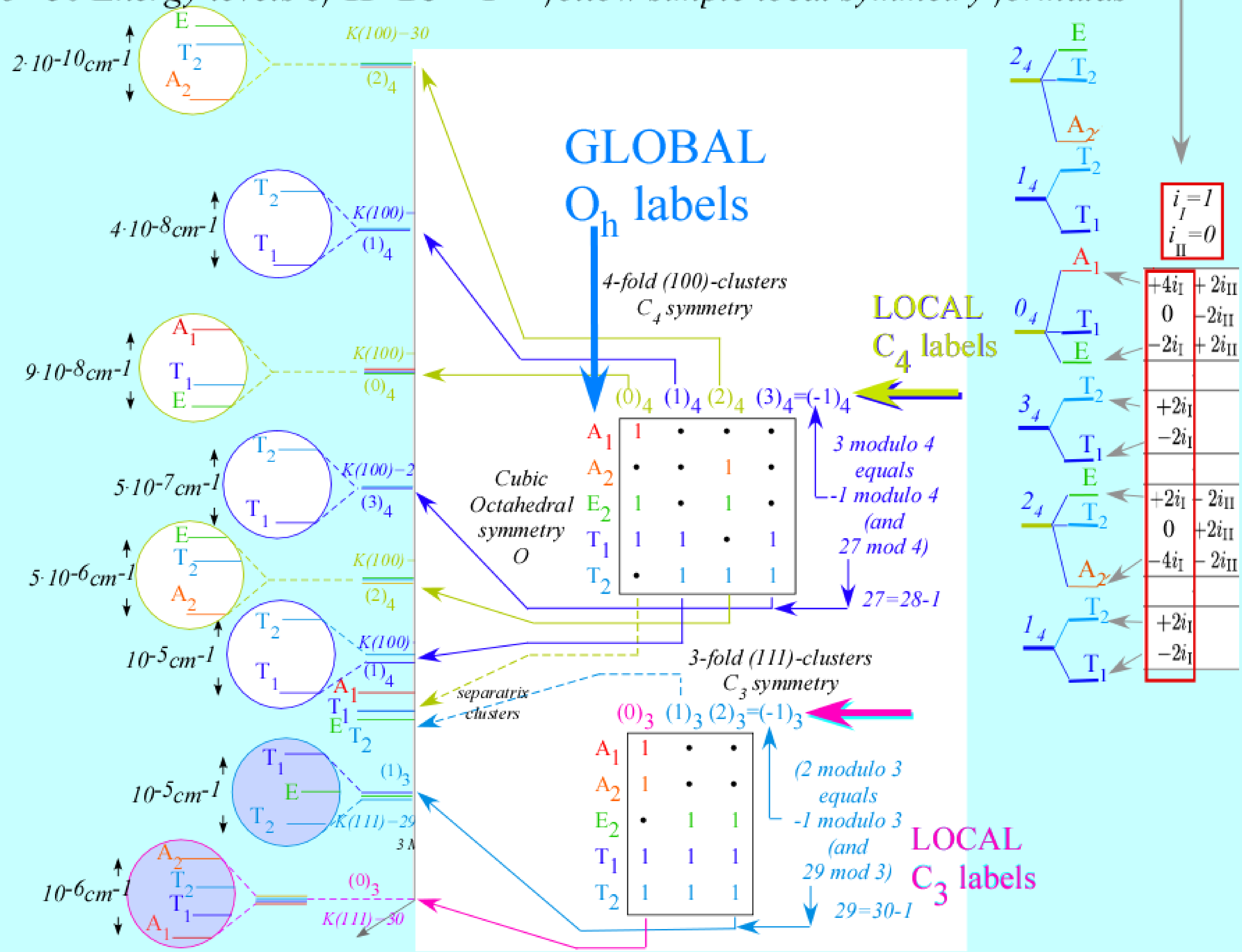
A_1 10 split $O \supset C_4$ octahedral e-vals ε^{α} versus 10 sub-class parameters



Sequence if $i_{\text{I}}=i_{1256}$ 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	$\cdot$	$r_{\text{I}} = \text{Re}\, r_{1234}$ $m_{\text{I}} = \text{Im}\, r_{1234}$	$\cdot$	$R_z = \text{Re}R_z$ $I_z = \text{Im}R_z$	$i_{\text{I}} = i_{1256}$ $i_{\text{II}} = i_{34}$	
$\varepsilon_{0_4}^{A_1} =$	g_0	$+4r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+4R_{xy} + 2R_z$	$+4i_{\text{I}} + 2i_{\text{II}}$	
$\varepsilon_{0_4}^{T_1}$	g_0	0	$-2\rho_{xy} + \rho_z$	$+2R_z$	$0 \quad -2i_{\text{II}}$	
$\varepsilon_{0_4}^{E}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-2R_{xy} - R_z$	$-2i_{\text{I}} + 2i_{\text{II}}$	
1_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon_{1_4}^{T_2}$	g_0	$+2m_{\text{I}}$	$-\rho_z$	$-R_{xy} - 2I_z$	$+2i_{\text{I}}$	
$\varepsilon_{1_4}^{T_1}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$+R_{xy} - 2I_z$	$-2i_{\text{I}}$	
2_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon_{2_4}^{E}$	g_0	$-2r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$+2R_{xy} - R_z$	$+2i_{\text{I}} - 2i_{\text{II}}$	
$\varepsilon_{2_4}^{T_2}$	g_0	0	$-2\rho_{xy} + \rho_z$	$-2R_z$	$0 \quad +2i_{\text{II}}$	
$\varepsilon_{2_4}^{A_2}$	g_0	$+4r_{\text{I}}$	$+2\rho_{xy} + \rho_z$	$-4R_{xy} - 2R_z$	$-4i_{\text{I}} - 2i_{\text{II}}$	
3_4	$\cdot$	$\cdot$	$\cdot$	$\cdot$	$\cdot$	
$\varepsilon_{3_4}^{T_2}$	g_0	$-2m_{\text{I}}$	$-\rho_z$	$-R_{xy} + 2I_z$	$+2i_{\text{I}}$	
$\varepsilon_{3_4}^{T_1}$	g_0	$+2m_{\text{I}}$	$-\rho_z$	$+R_{xy} + 2I_z$	$-2i_{\text{I}}$	

J=30 Energy levels of $\mathbf{H}=B\mathbf{J}^2+T^{[4]}$ follow simple local symmetry formulas



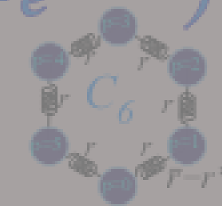
	$(0)_4$	$(1)_4$	$(2)_4$	$(3)_4=(-1)_4$
A_1	1	•	•	•
A_2	•	•	1	•
E_2	1	•	1	•
T_1	1	1	•	1
T_2	•	1	1	1

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

(Commuting)

- ***Abelian symmetry = Fourier analysis*** *(Back to our roots $1^{1/N}=e^{2\pi i m/N}$)*

  Group $\hat{\text{p}}$roduct table => Hamiltonian $\mathbf{H}$-matrices *(C_2 and C_6 examples)*



  Group roots => $\mathbf{H}$-matrix spectral resolution by $\mathrm{P}^{(m)}$projectors

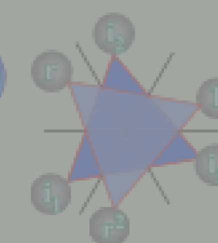
Commutivity conundrum... ? $\mathbf{H}\cdot g = g\cdot\mathbf{H}$?

- ***New symmetry insights:*** *Local vs. Global symmetry* *Projector invariance*

  "Mock-Mach" principle *Conway, et.al, May (2008)* *Cvitanovic, (2008)*

(Non-Commuting)

- ***Non-Abelian symmetry analysis I.*** *(Simplest example: D_3)*



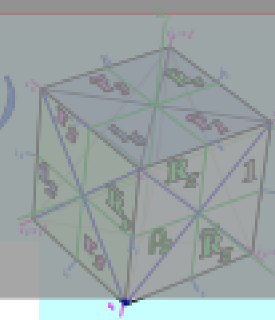
  Local vs. Global $\hat{\text{p}}$roduct tables => $\mathbf{H}$-matrices

  All-commuting invariants => Global invariant (character) $\mathrm{P}^{(\alpha)}$projectors

  Mutually-commuting sets => Local vs. Global eigensolutions by $\mathrm{P}^{(\alpha)}_{m,n}$ projectors

  => $\mathbf{H}$-matrix spectral resolution by $\mathrm{P}^{(\alpha)}_{m,n}$ projectors

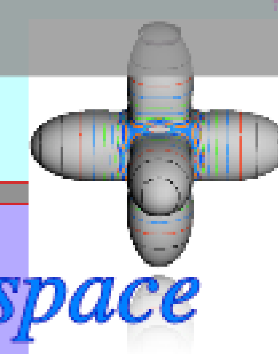
- ***Non-Abelian symmetry analysis II.*** *(Octahedral example: O_h)*

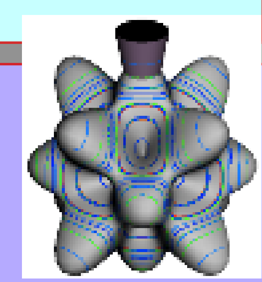


  Global-local product tables => $\mathbf{H}$-matrices...

  ... and all the above ...

  => eigensolution formulas by local-symmetry defined $\mathrm{P}^{(\alpha)}_{n,n}$ projectors

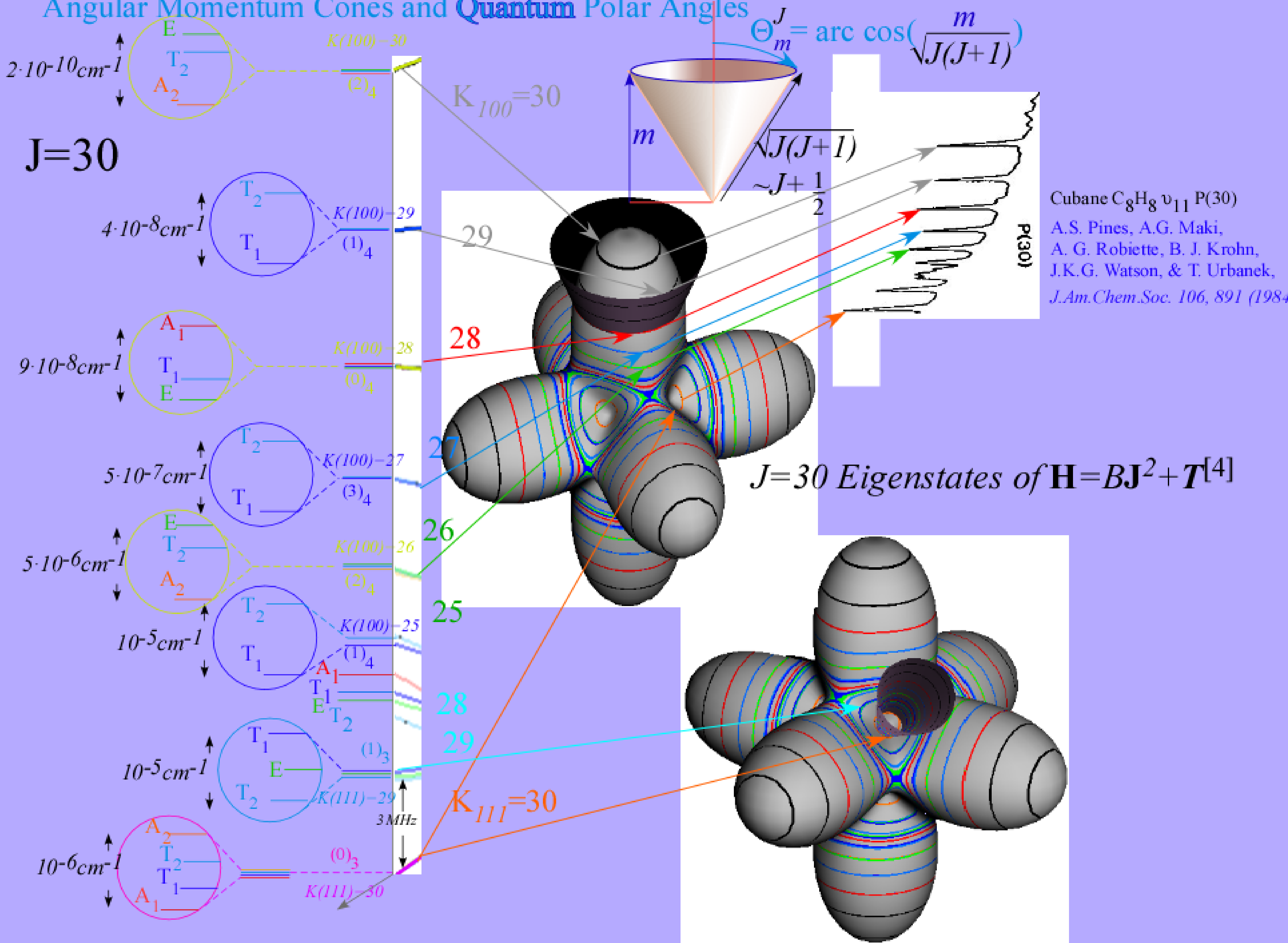




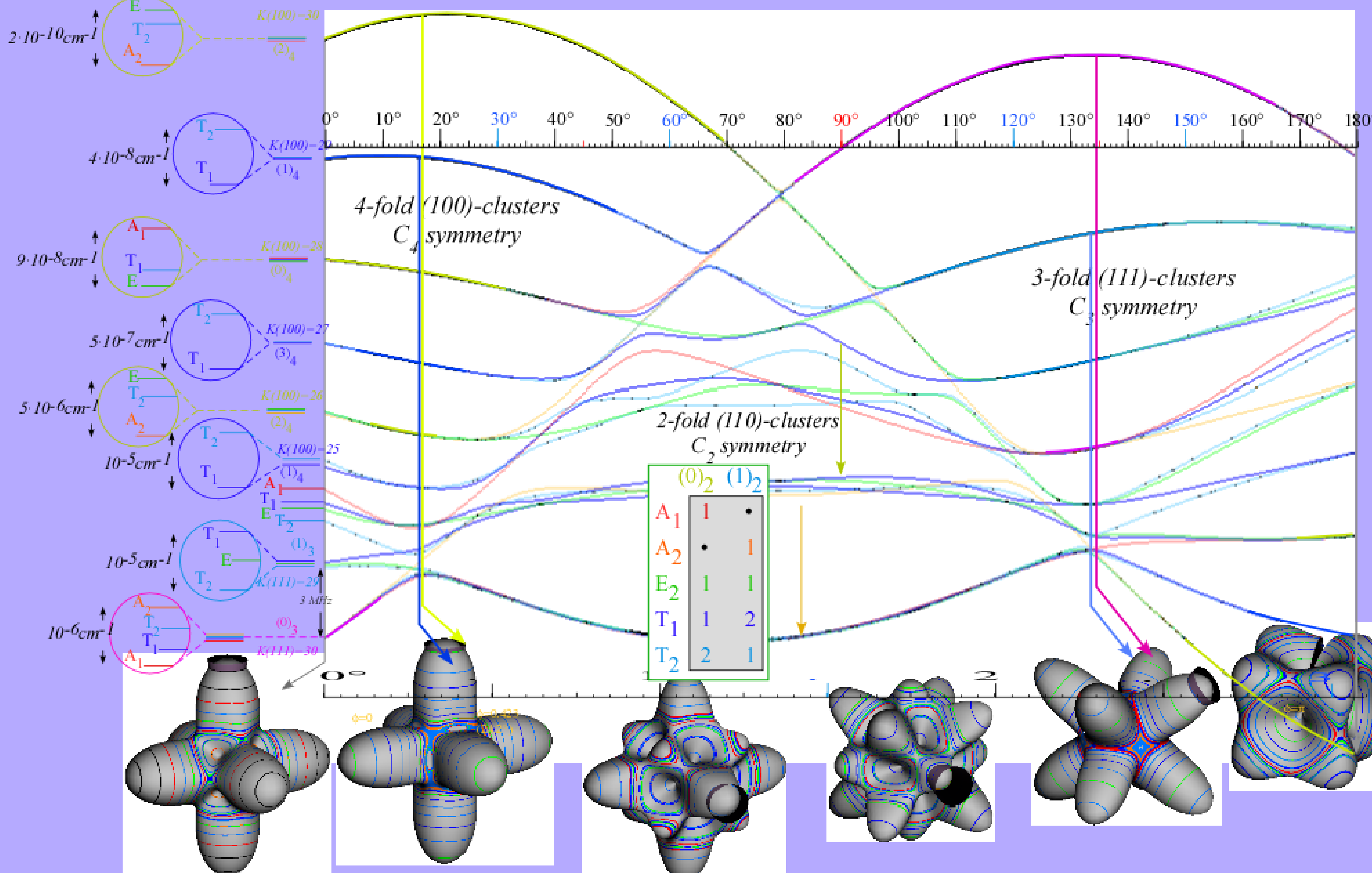
- ***Local vs Global symmetry in rovibronic phase space***

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

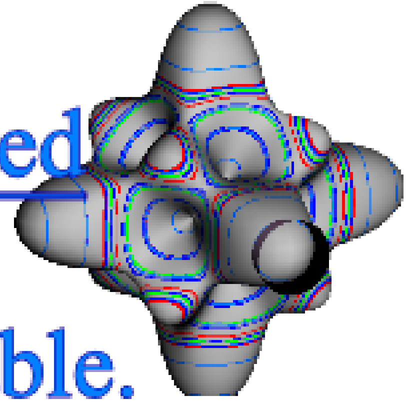
Angular Momentum Cones and Quantum Polar Angles



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



	$(0)_2$	$(1)_2$
A_1	1	•
A_2	•	1
E_2	1	1
T_1	1	2
T_2	2	1



Conclusion: H-matrix symmetry analysis greatly improved

Group space tunneling matrix defined nicely by group table.

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

When local symmetry conditions apply:

- Spectral algebra yields closed-form energies and statess (using same table!) .

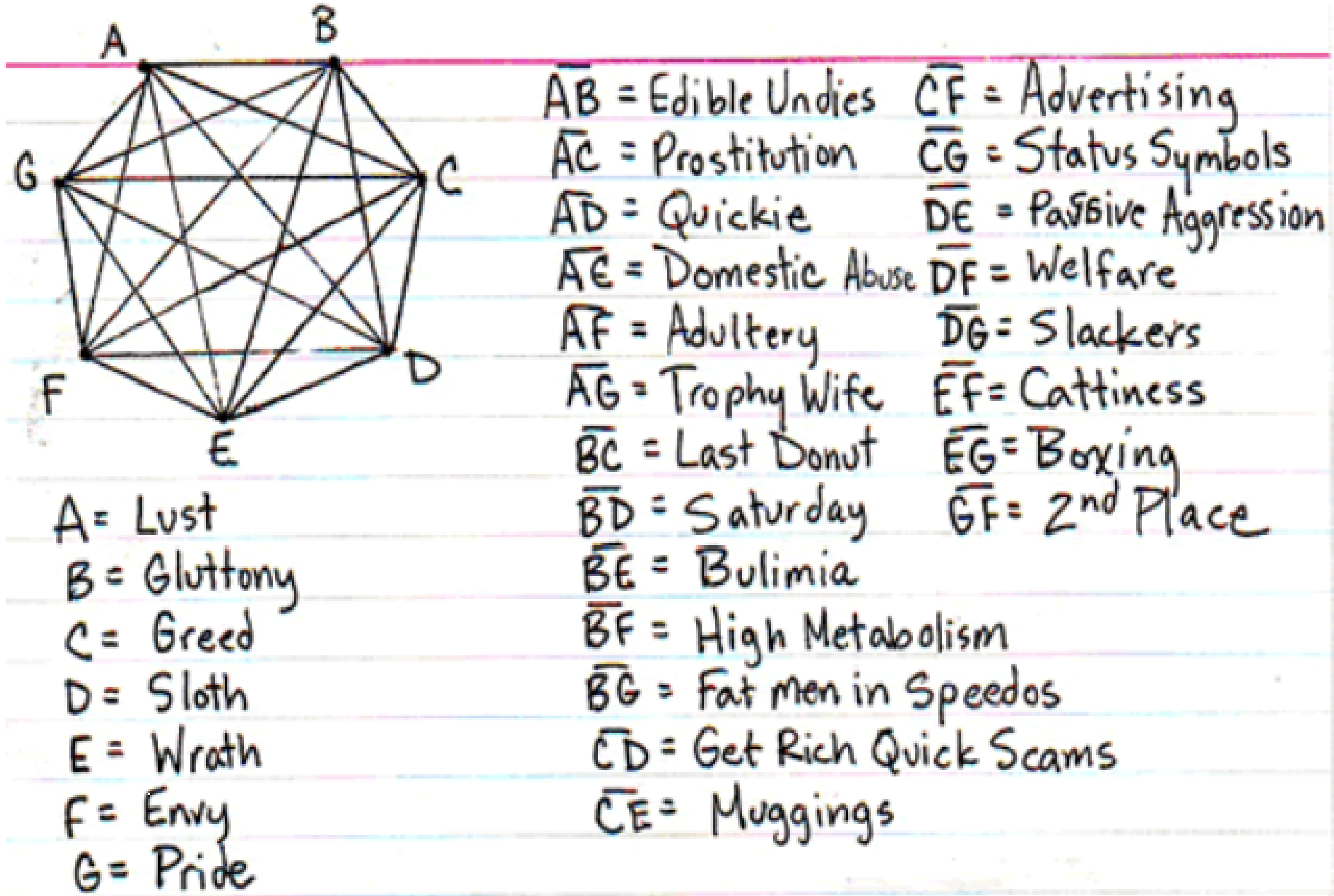
- Expressions easily deconvoluted (same table , again!).

Transitions between local symmetries clearly defined.

We can now do a D_7 example (Next slide :-)

Seven-Deadly-Sin Tunneling Theory

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



Effects of broken or transition local symmetry for i-class

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

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

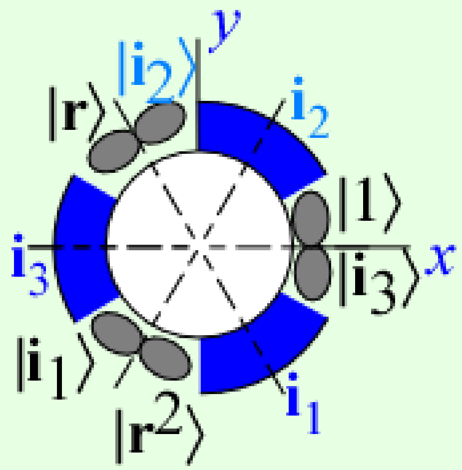
	0_4	2_4
0_4	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6) + i_3 + i_4$	$\frac{\sqrt{3}}{2}(i_1 + i_2 - i_5 - i_6)$
2_4	$h.c.$	$\frac{1}{2}(i_1 + i_2 + i_5 + i_6) - i_3 - i_4$

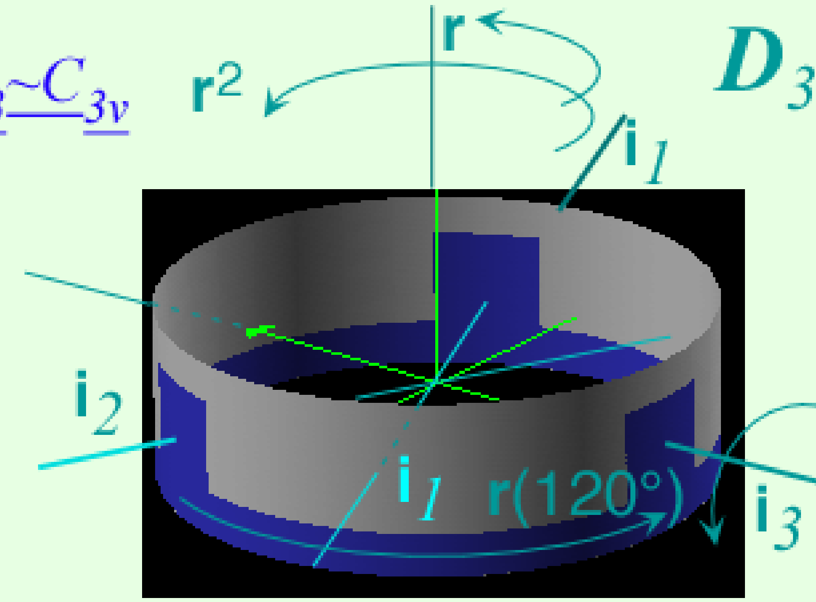
$D^{T_1^*}(i_k \mathbf{i}_\mathrm{k})$	1_4	3_4	0_4
1_4	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$-\frac{1}{2}(i_1 + i_2 - i_5 - i_6) - i(i_3 - i_4)$	$-\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5 - i_6)$
3_4	$h.c.$	$-\frac{1}{2}(i_1 + i_2 + i_5 + i_6)$	$+\frac{1}{\sqrt{2}}(i_1 - i_2) + \frac{i}{\sqrt{2}}(i_5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

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

D_3-defined local-wave bases



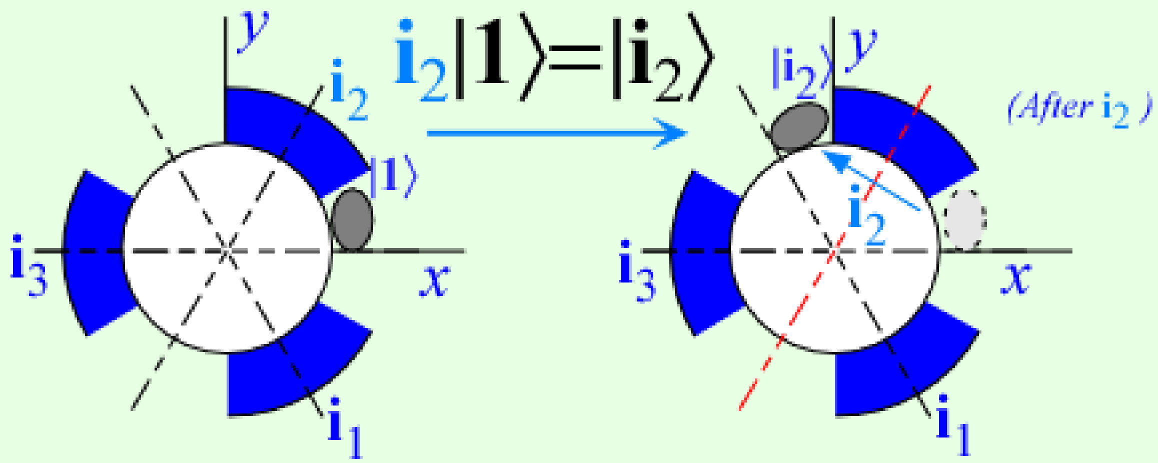


D_3

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

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

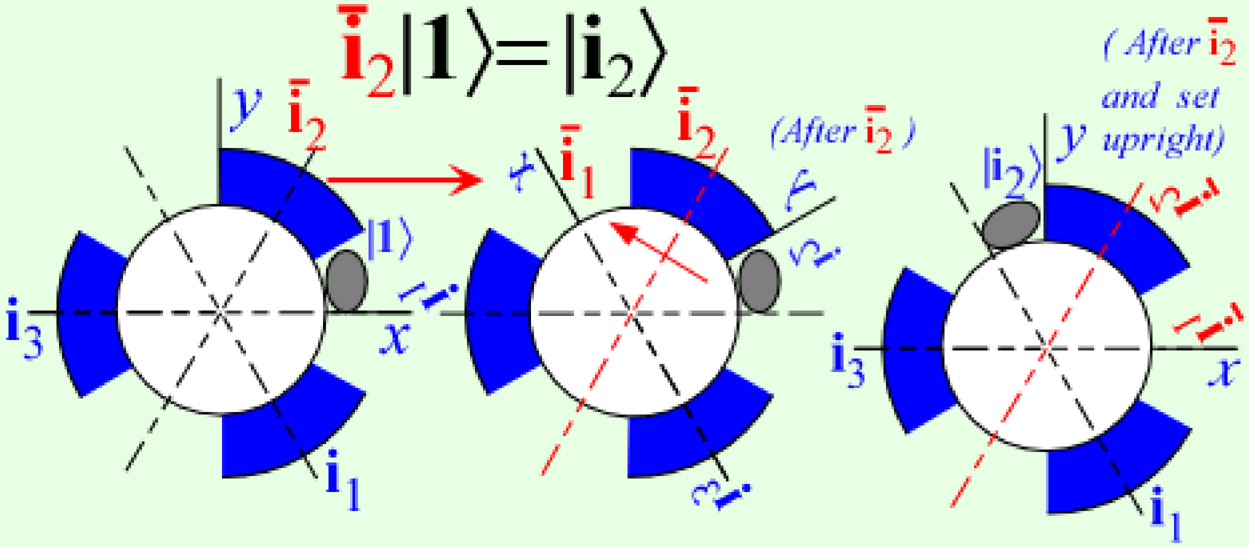


$i_1 i_2 = r$ implies: $\bar{i}_1 \bar{i}_2 = \bar{r}$

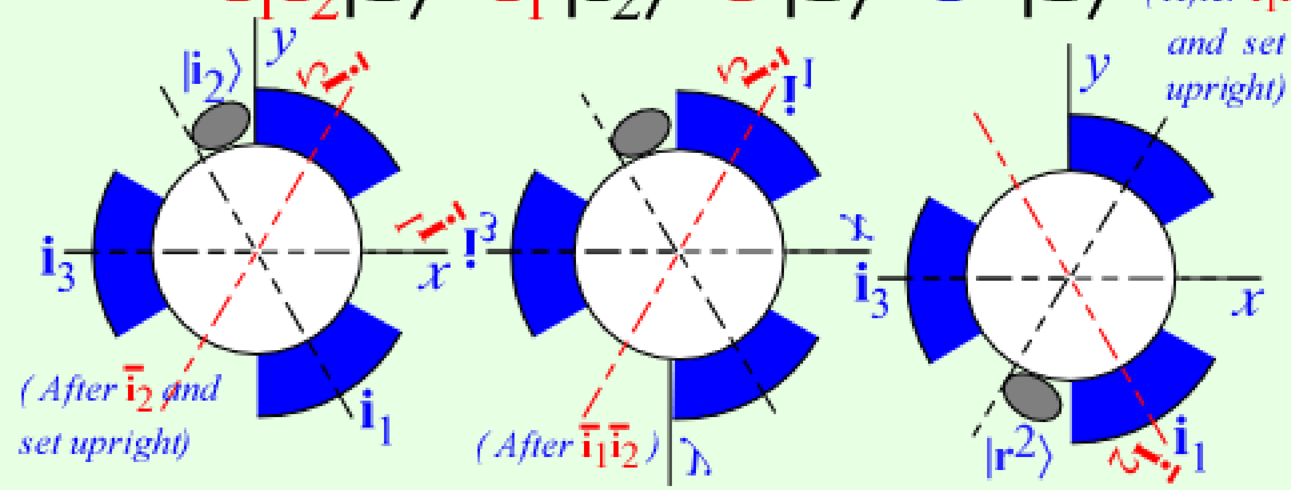
Body-fixed (Intrinsic-Local) operations appear to move their rotation axes (relative to lab)

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

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



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



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

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

(all others are self-conjugate)

D_3 local group product table

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

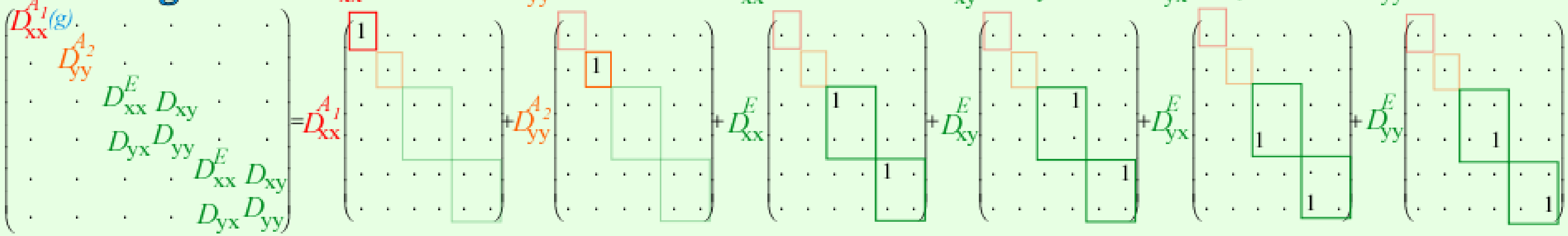
D_3 local projector product table

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

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

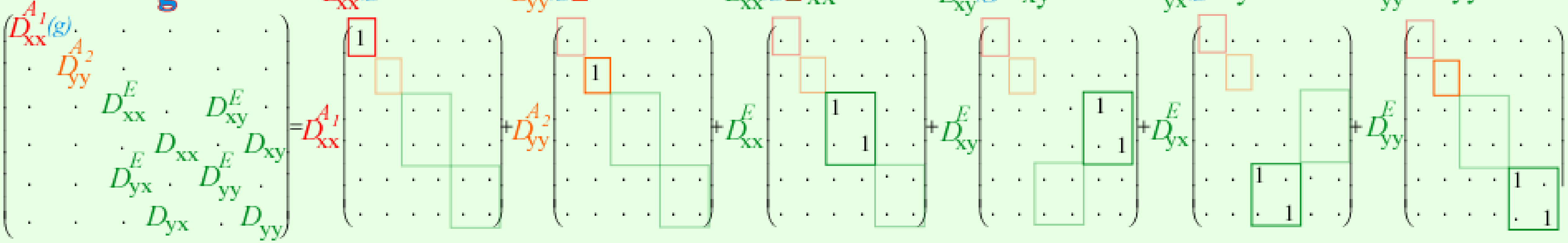
Matrix "Placeholders" $\mathbf{P}_{ab}^{(m)}$ for GLOBAL $\mathbf{g}$ operators in D_3

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



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

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



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

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