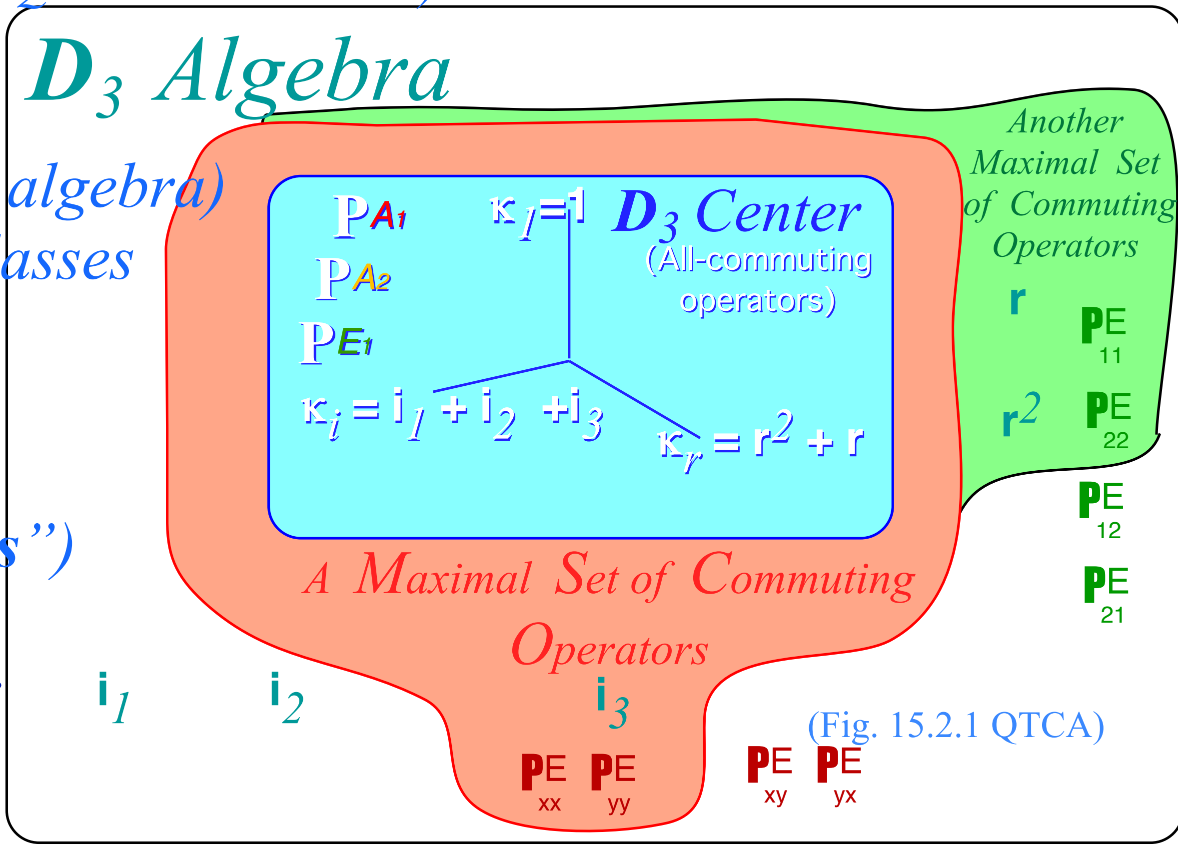
Group Theory in Quantum Mechanics

Lecture 16 (3.14.17)

Spectral decomposition of groups $D_3 \sim C_{3v}$

(Int.J.Mol.Sci, 14, 714(2013) p.755-774 , QTCA Unit 5 Ch. 15)
(PSDS - Ch. 3)



(Fig. 15.2.1 QTCA)

Review: 1st-Stage Spectral resolution of **D_3 Center** (Class algebra)
- Group theory of equivalence transformations and classes
  - Lagrange theorems
- All-commuting class projectors

D_3-invariant character ortho-completeness
Spectral resolution to **irreducible representations** (“**ireps**”)
foretold by **characters** or traces
- Subgroup splitting or correlation frequency formula:
  - $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$
  - Atomic ℓ-level or $2\ell+1$-multiplet splitting
    - D_3 examples for ℓ=1-6
- Group invariant numbers: Centrum, Rank, and Order

2^{nd}-Stage spectral decompositions of global/local D_3
- Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$
  - Splitting classes

3^{rd}-stage spectral resolution to **irreducible representations** (ireps) and Hamiltonian eigensolutions
- Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

Review: Spectral resolution of ***D_3 Center*** *(Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

Spectral resolution to ***irreducible representations*** *(or "**irreps**") foretold by* ***characters*** *or* <u>*traces*</u>

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for ℓ=1-6

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Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

Review: 1st-Stage Spectral resolution of ***D*₃ Center** *(Class algebra)*

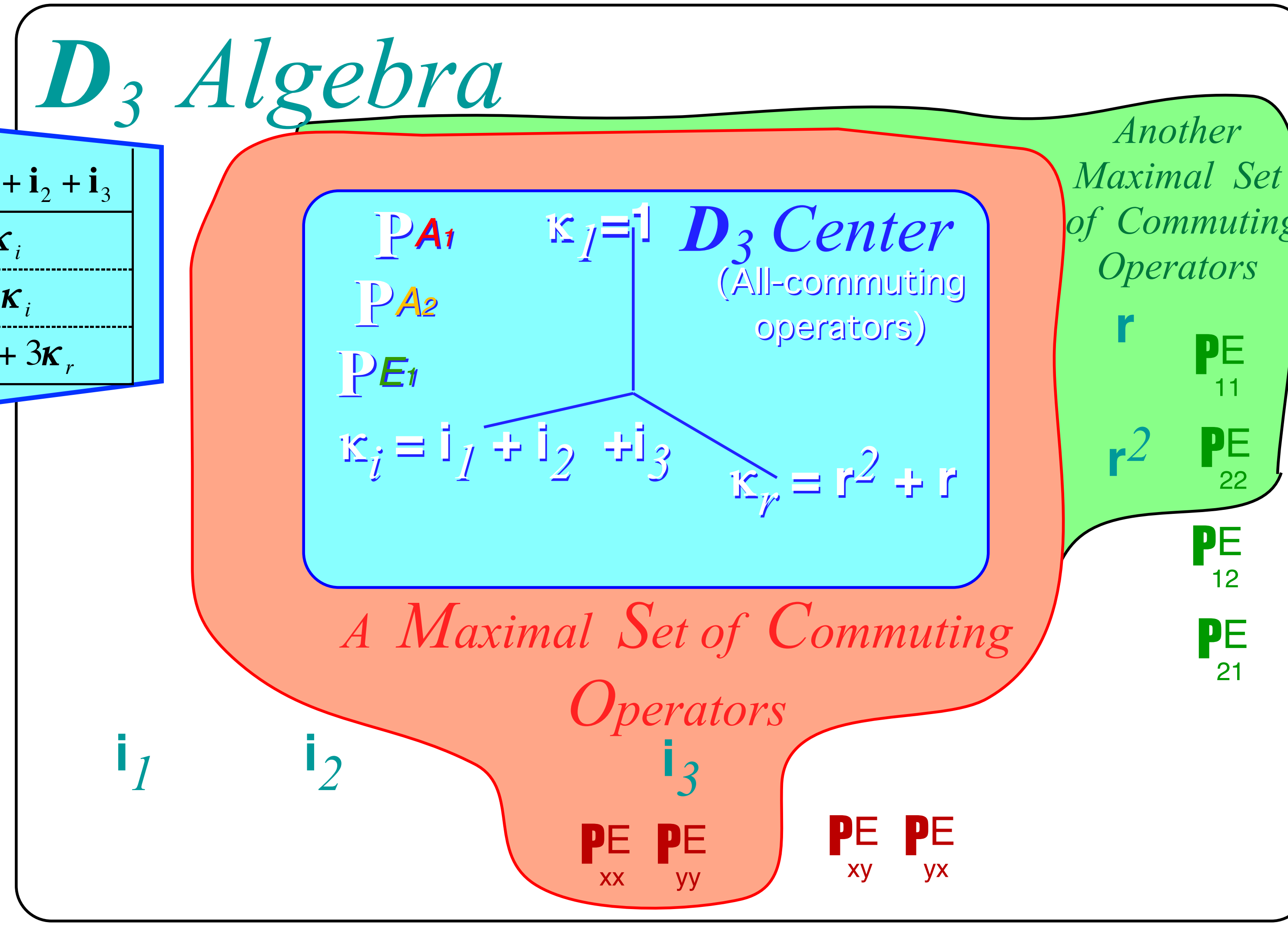
$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{i}_1$	$\mathbf{i}_2$	$\mathbf{i}_3$
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t \boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k \mathbf{g}_t$



*Review: 1^{st}-Stage Spectral resolution of **D_3 Center** (Class algebra)*

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

$\rightarrow$

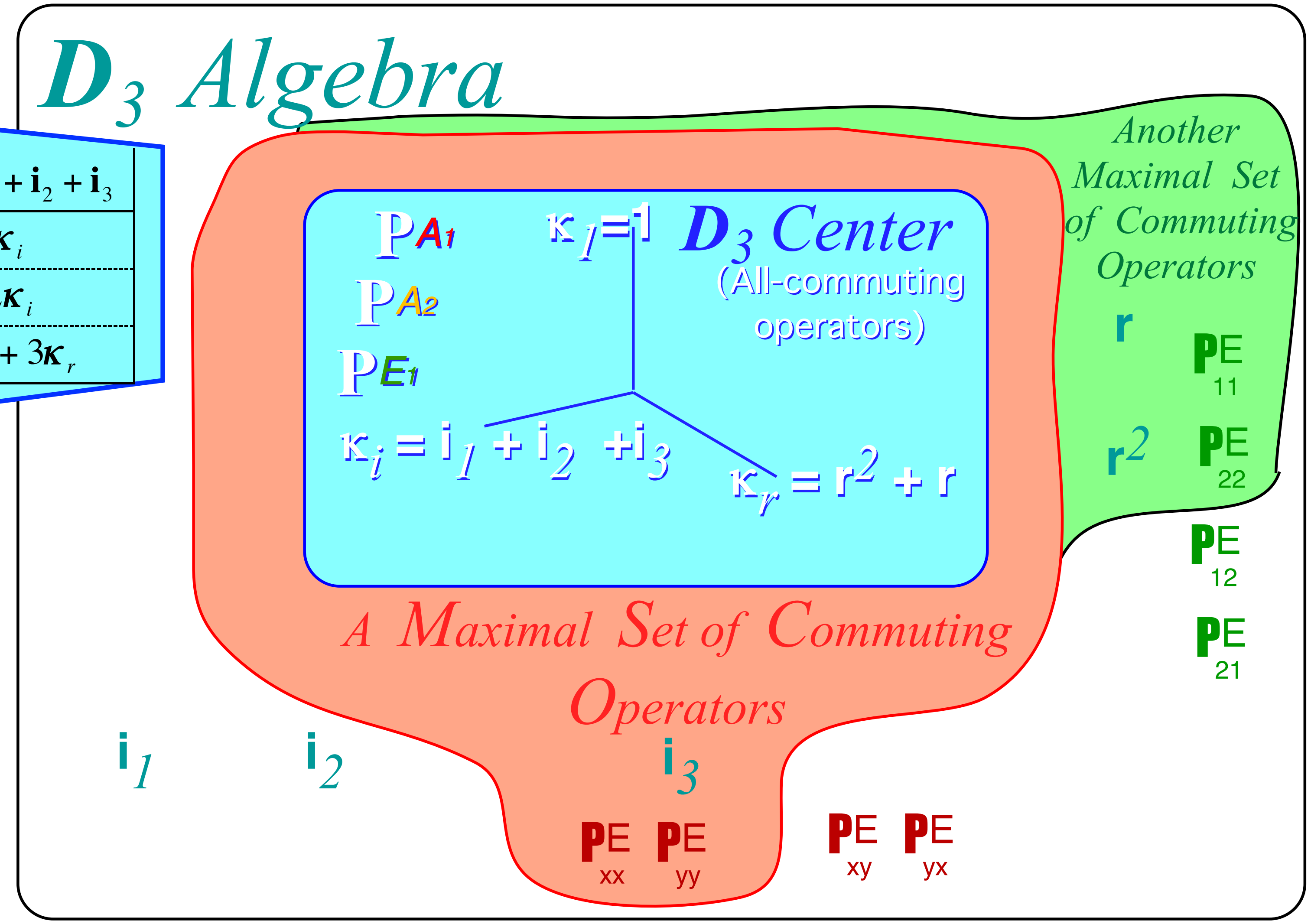
	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$^\circ G$ = order of group: $({}^\circ D_3 = 6)$

$^\circ\kappa_k$ = order of class κ_k: $({}^\circ\kappa_1 = 1,\ {}^\circ\kappa_r = 2,\ {}^\circ\kappa_i = 3)$



Review: *1^{st}-Stage Spectral resolution of **D_3 Center** (Class algebra)*

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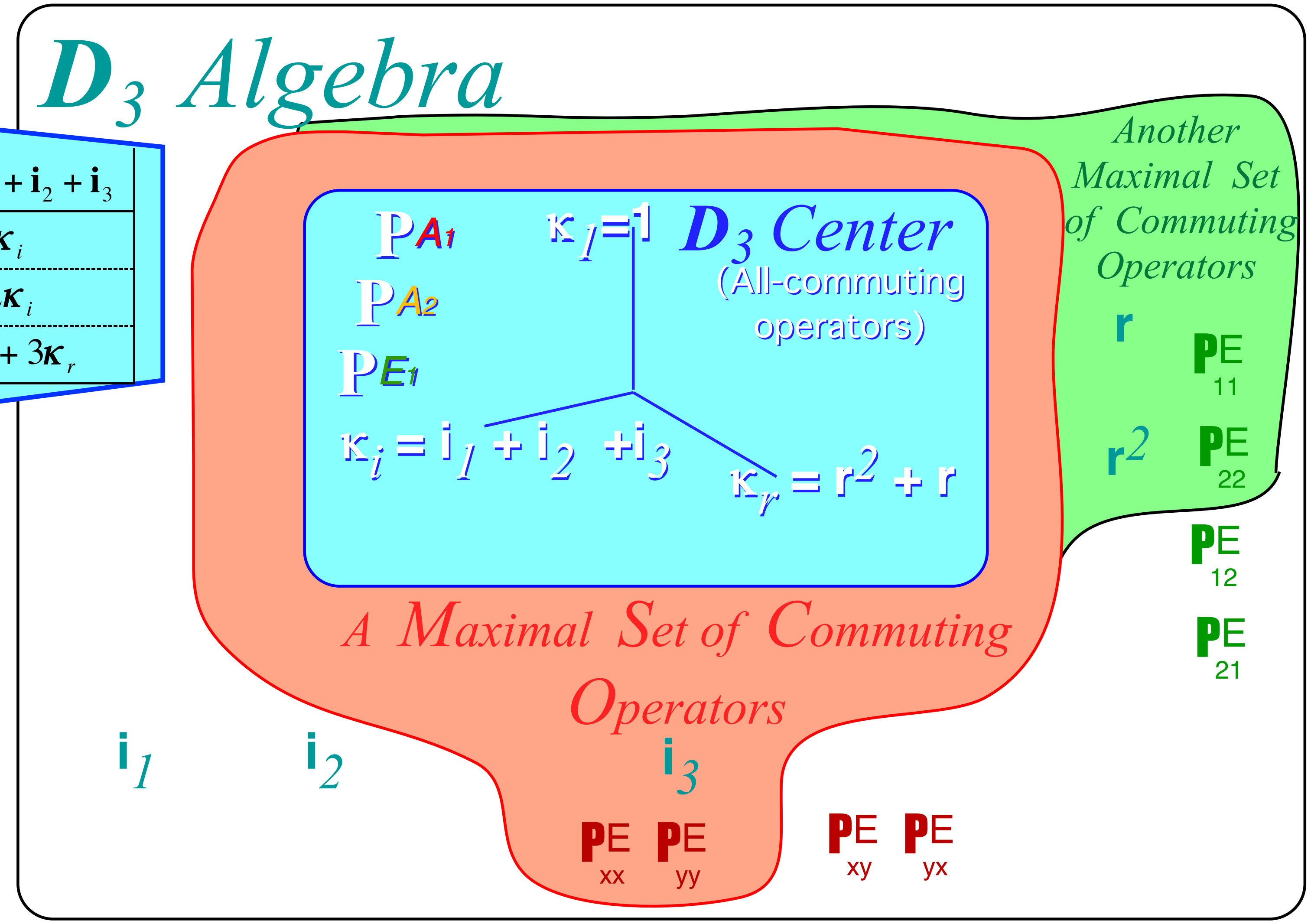
$\mathbf{r}$	$\mathbf{1}$	$\mathbf{r}^2$	$\mathbf{i}_3$	$\mathbf{i}_1$	$\mathbf{i}_2$
$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

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$°G$ = order of group: $(°D_3 = 6)$

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$\mathbf{g}_t \boldsymbol{\kappa}_k \mathbf{g}_t^{-1} = \boldsymbol{\kappa}_k$ where: $\boldsymbol{\kappa}_\mathbf{k} = \sum_{j=1}^{j=°\kappa_k} \mathbf{g}_j$

Review: 1^{st}-Stage Spectral resolution of $\mathbf{D_3}$ Center (Class algebra)

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

$\rightarrow$

	$\boldsymbol{\kappa}_1 = \mathbf{1}$	$\boldsymbol{\kappa}_r = \mathbf{r} + \mathbf{r}^2$	$\boldsymbol{\kappa}_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
$\boldsymbol{\kappa}_1$	$\boldsymbol{\kappa}_1$	$\boldsymbol{\kappa}_r$	$\boldsymbol{\kappa}_i$
$\boldsymbol{\kappa}_r$	$\boldsymbol{\kappa}_r$	$2\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_r$	$2\boldsymbol{\kappa}_i$
$\boldsymbol{\kappa}_i$	$\boldsymbol{\kappa}_i$	$2\boldsymbol{\kappa}_i$	$3\boldsymbol{\kappa}_1 + 3\boldsymbol{\kappa}_r$

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$$\mathbf{g}_t\boldsymbol{\kappa}_k\mathbf{g}_t^{-1} = \boldsymbol{\kappa}_k \quad \text{where: } \boldsymbol{\kappa}_k = \sum_{j=1}^{j=^\circ\kappa_k}\mathbf{g}_j = \frac{1}{^\circ s_k}\sum_{t=1}^{t=^\circ G}\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}$$

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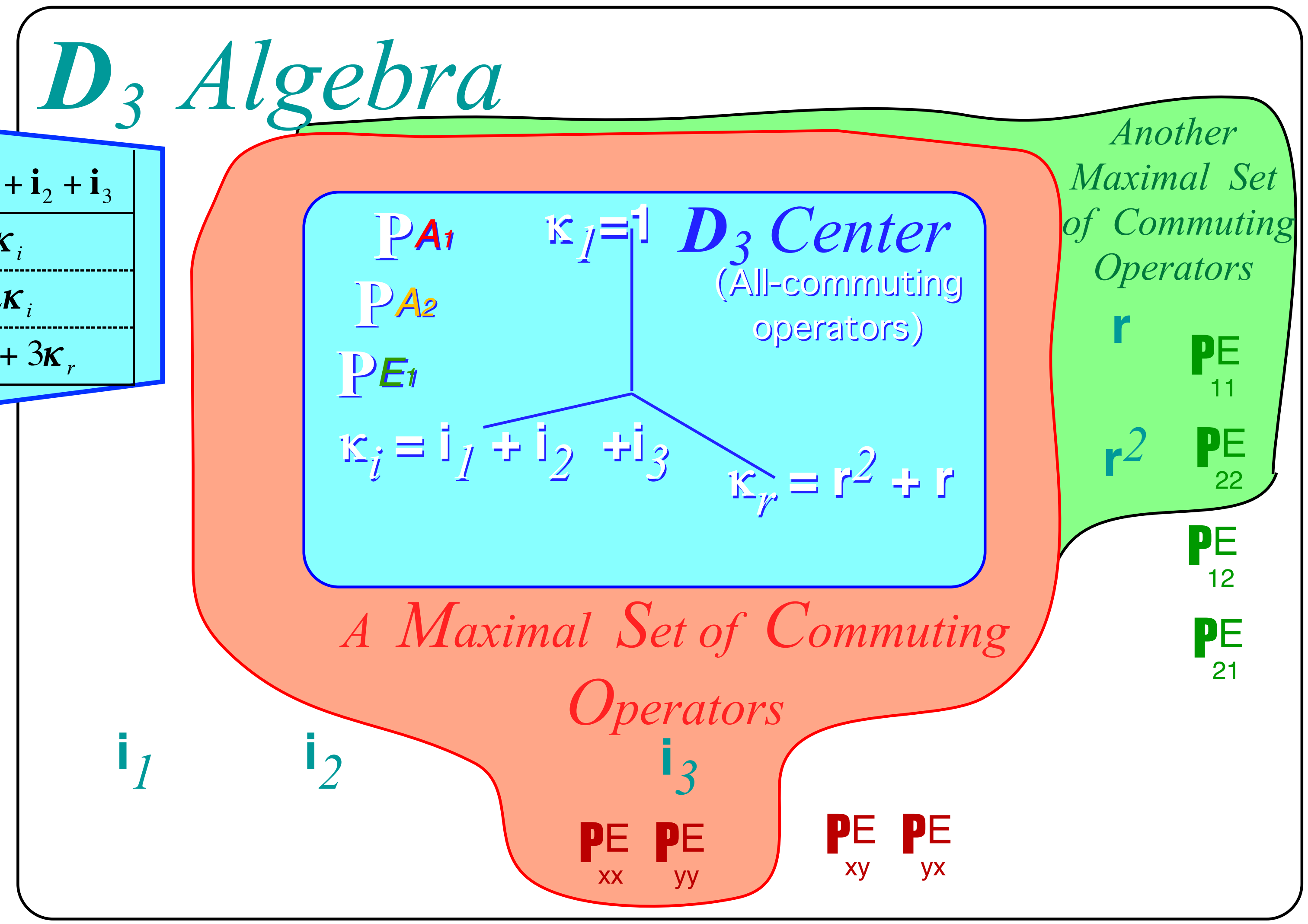

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$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}$
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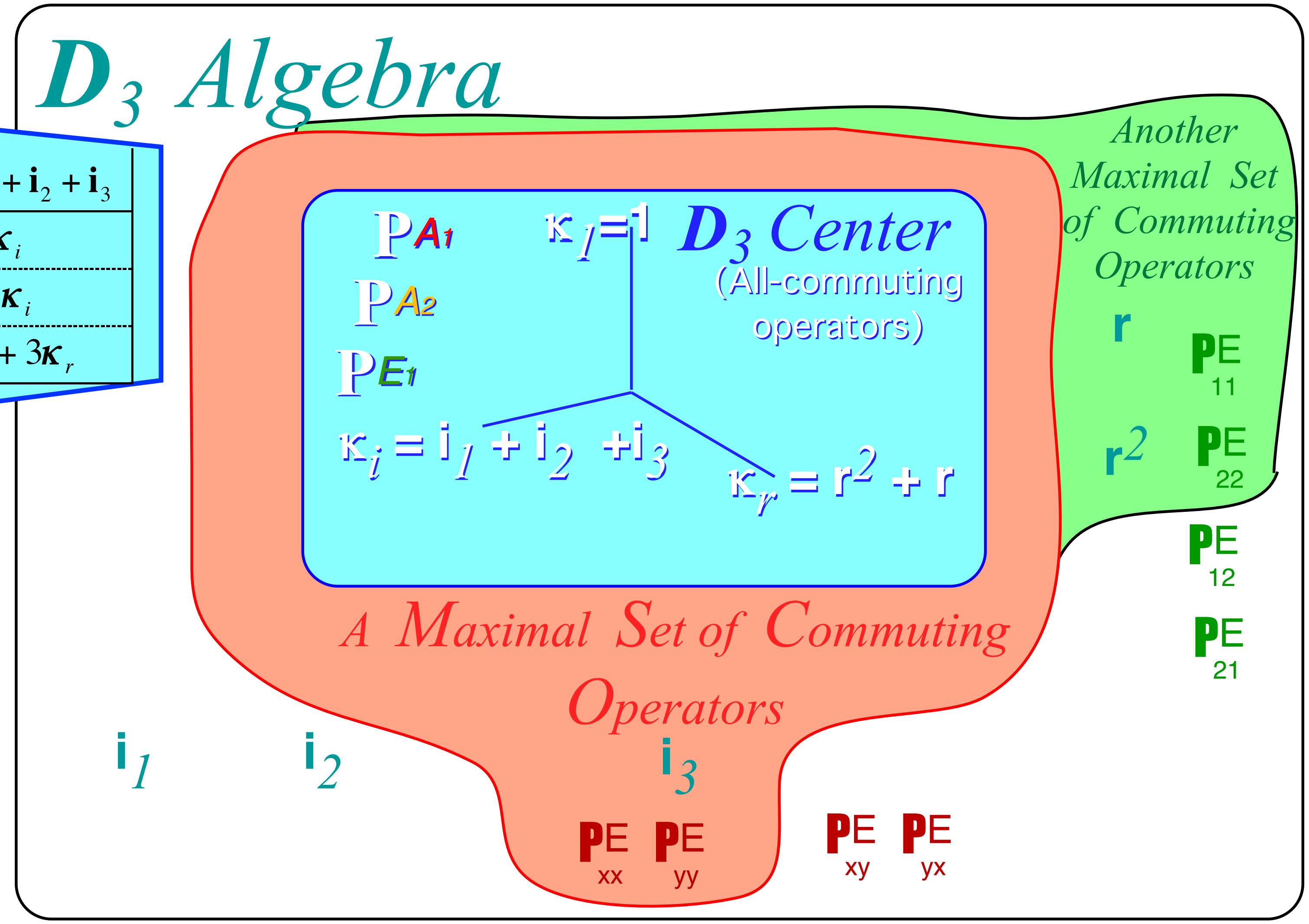

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$\mathbf{r}^2$	$\mathbf{r}$	$\mathbf{1}$	$\mathbf{i}_2$	$\mathbf{i}_3$	$\mathbf{i}_1$
$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{i}_2$	$\mathbf{1}$	$\mathbf{r}$	$\mathbf{r}^2$
$\mathbf{i}_2$	$\mathbf{i}_1$	$\mathbf{i}_3$	$\mathbf{r}^2$	$\mathbf{1}$	$\mathbf{r}$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

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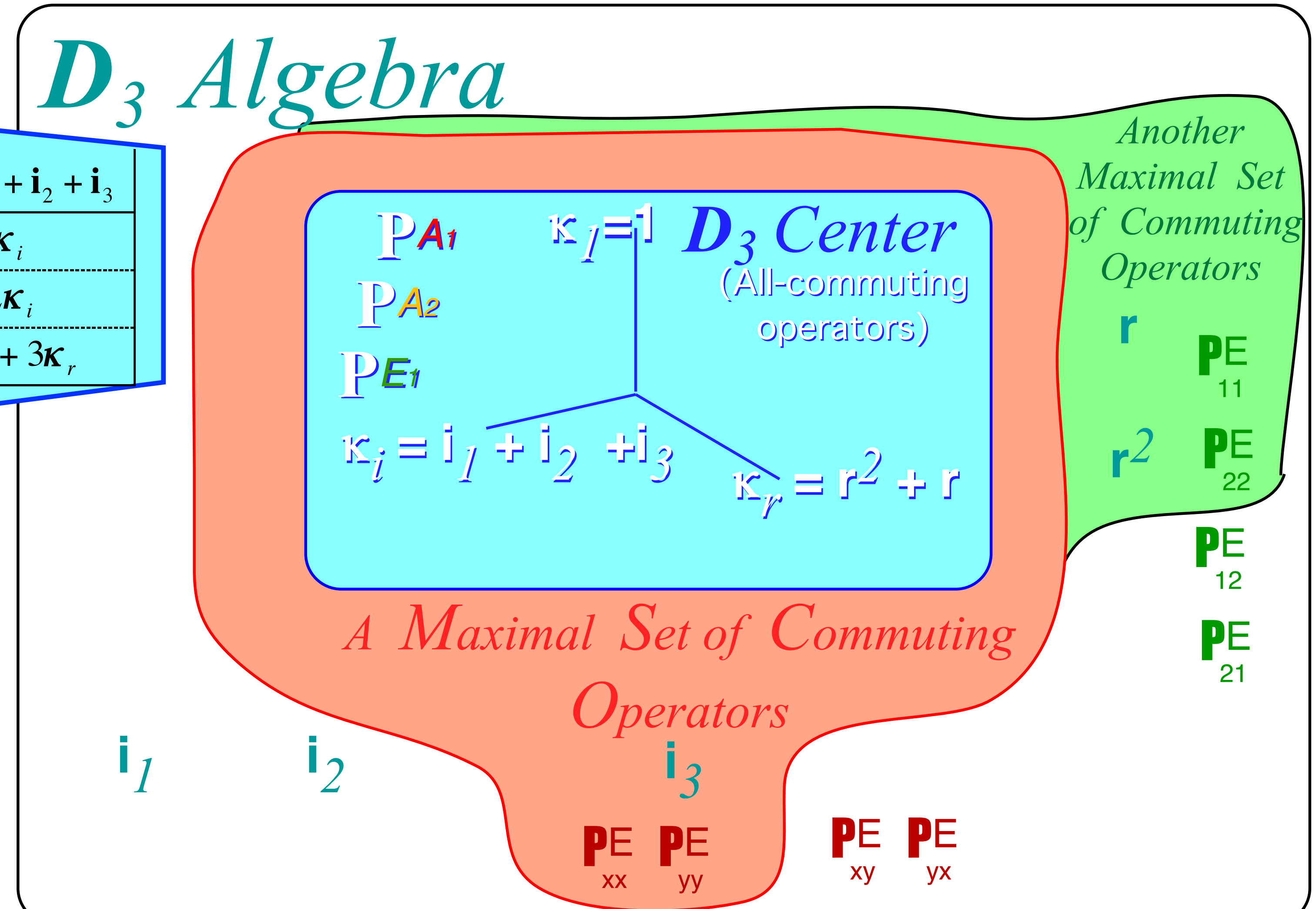

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$°s_k$=order of $\mathbf{g}_k$-self-symmetry: $(°s_1 = 6,\ °s_r = 3,\ °s_i = 2)$

$°s_k = °G / °\kappa_k$ *$°s_k$ is an integer count of D_3 operators $\mathbf{g}_s$ that commute with $\mathbf{g}_k$.*

Review: 1^{st}-Stage Spectral resolution of D_3 Center (Lagrange subgroup/class theorems)

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

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	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
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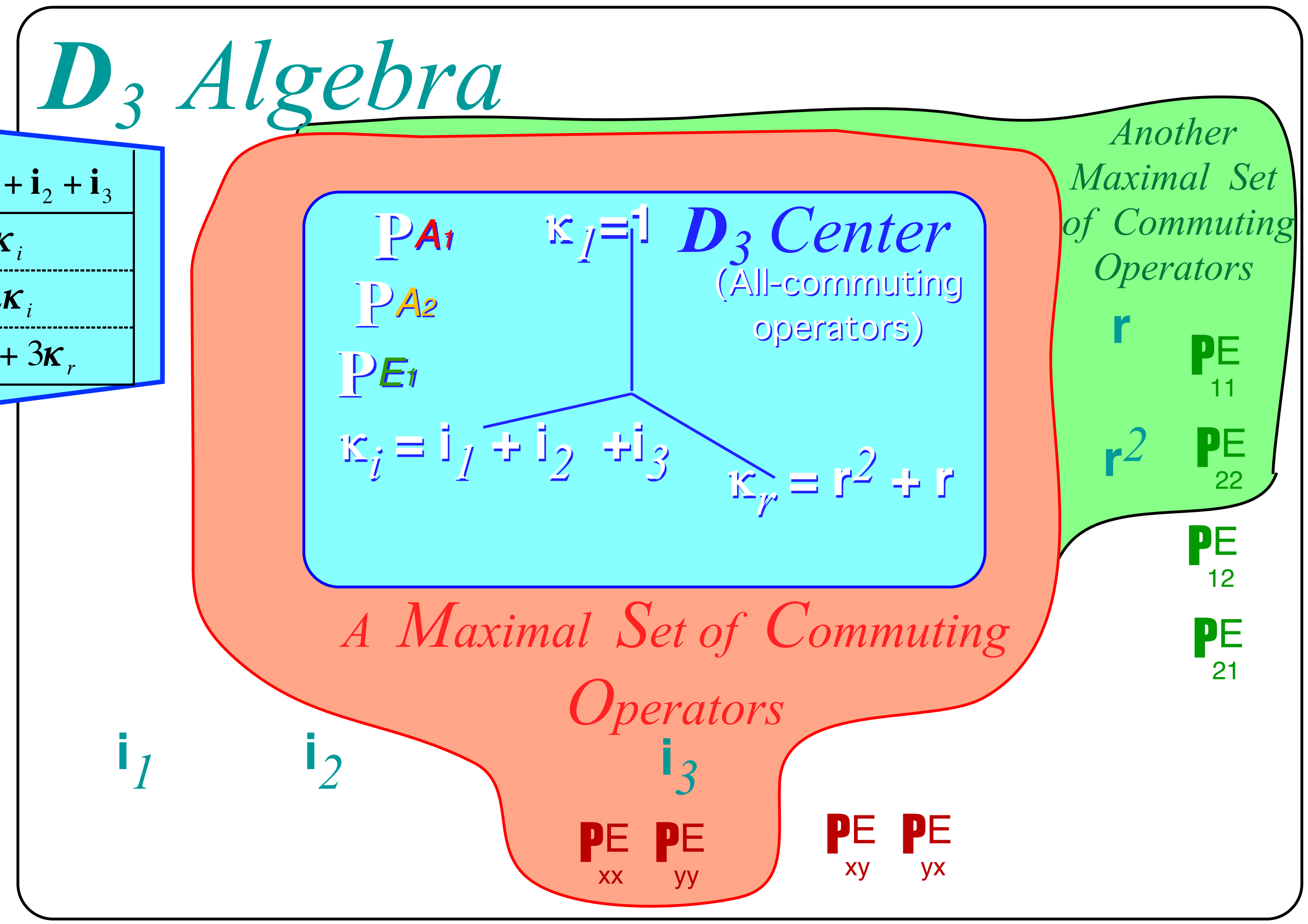
These operators $\mathbf{g}_s$ form the $\mathbf{g}_k$-self-symmetry group s_k . Each $\mathbf{g}_s$ transforms $\mathbf{g}_k$ into itself: $\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}=\mathbf{g}_k$



Review: *1^{st}-Stage Spectral resolution of D_3 Center (Lagrange subgroup/class theorems)*

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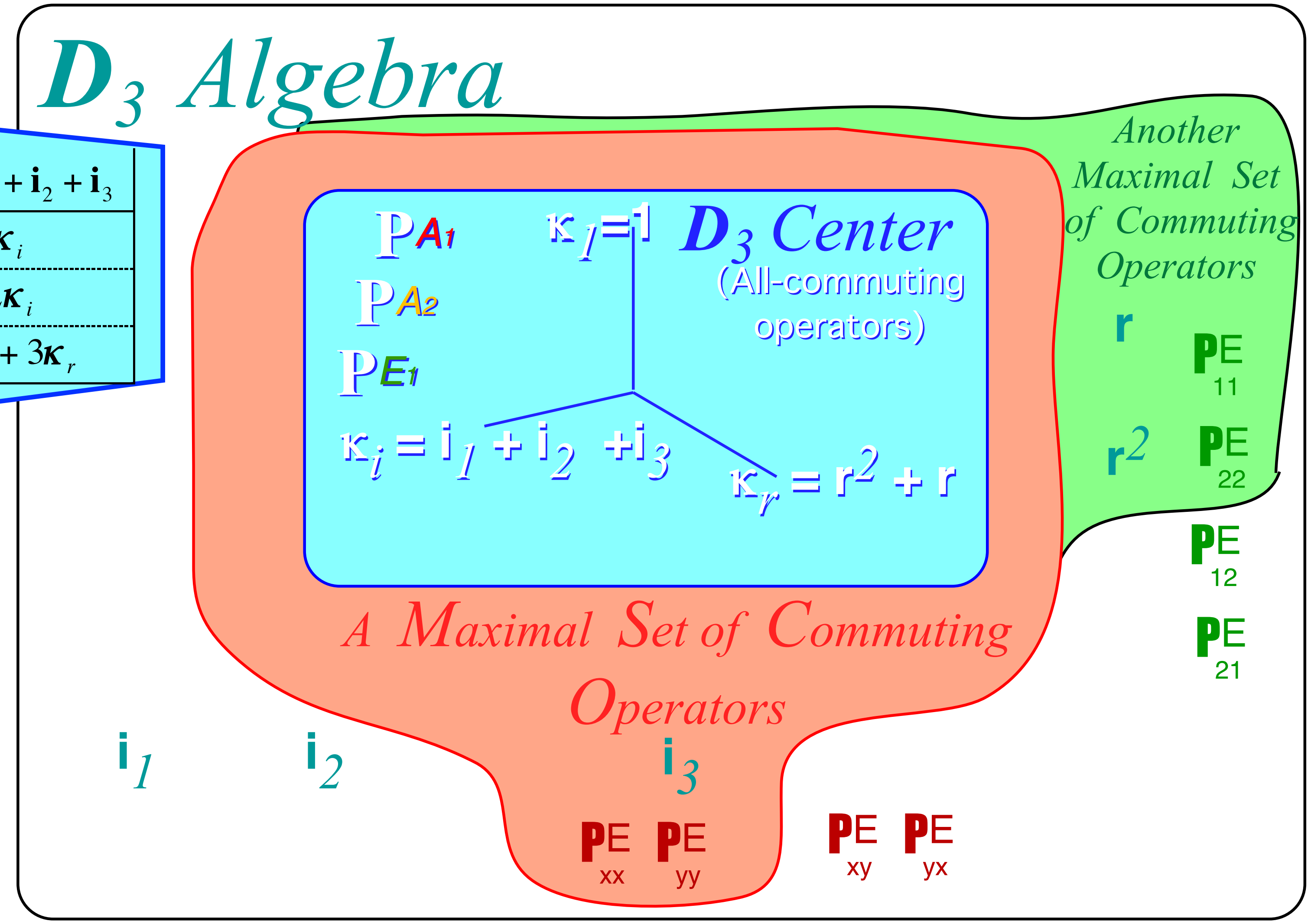

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If an operator $\mathbf{g}_t$ transforms $\mathbf{g}_k$ into a different element $\mathbf{g}'_k$ of its class: $\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$, then so does $\mathbf{g}_t\mathbf{g}_s$.
that is: $\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k(\mathbf{g}_t\mathbf{g}_s)^{-1}=\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}\mathbf{g}_t^{-1}=\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$,

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

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κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

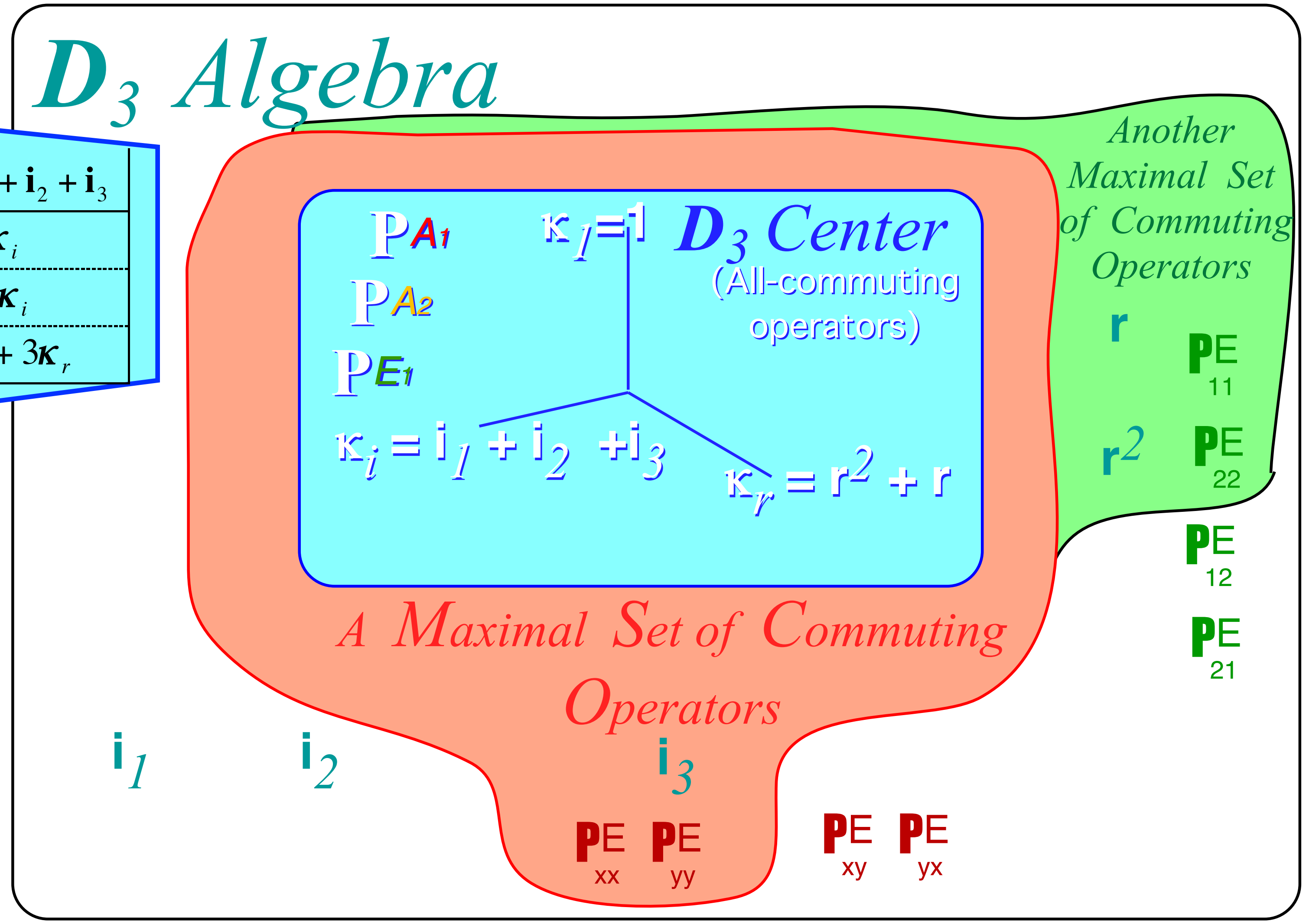
$^\circ G$ = order of group: $(^\circ D_3 = 6)$

$^\circ\kappa_k$ = order of class κ_k: $(^\circ\kappa_1 = 1,\ ^\circ\kappa_r = 2,\ ^\circ\kappa_i = 3)$

$$\mathbf{g}_t\boldsymbol{\kappa}_k\mathbf{g}_t^{-1} = \boldsymbol{\kappa}_k \quad \text{where: } \boldsymbol{\kappa}_\mathbf{k} = \sum_{j=1}^{j=^\circ\kappa_k}\mathbf{g}_j = \frac{1}{^\circ s_k}\sum_{t=1}^{t=^\circ G}\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}$$

$^\circ s_k$=order of $\mathbf{g}_k$-self-symmetry: $(^\circ s_1 = 6,\ ^\circ s_r = 3,\ ^\circ s_i = 2)$

$^\circ s_k = {^\circ G} / {^\circ\kappa_k}$ $\quad$ $^\circ s_k$ *is an integer count of* D_3 *operators* $\mathbf{g}_s$ *that commute with* $\mathbf{g}_k$.



These operators $\mathbf{g}_s$ *form the* $\mathbf{g}_k$*-self-symmetry group* s_k . *Each* $\mathbf{g}_s$ *transforms* $\mathbf{g}_k$ *into itself:* $\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}=\mathbf{g}_k$

If an operator $\mathbf{g}_t$ *transforms* $\mathbf{g}_k$ *into a different element* $\mathbf{g}'_k$ *of its class:* $\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$, *then so does* $\mathbf{g}_t\mathbf{g}_s$.

that is: $\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k(\mathbf{g}_t\mathbf{g}_s)^{-1}=\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}\mathbf{g}_t^{-1}=\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$,

Subgroup $s_k=\{\mathbf{g}_0=\mathbf{1},\ \mathbf{g}_1=\mathbf{g}_k,\ \mathbf{g}_2,\ldots\}$ *has* $\ell=(^\circ\kappa_k\text{-}1)$ ***Left Cosets*** (one coset for each member of class κ_k).

Review: *1^{st}-Stage Spectral resolution of **D_3 Center** (Lagrange subgroup/class theorems)*

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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r}+\mathbf{r}^2$	$\kappa_i = \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\quad \mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

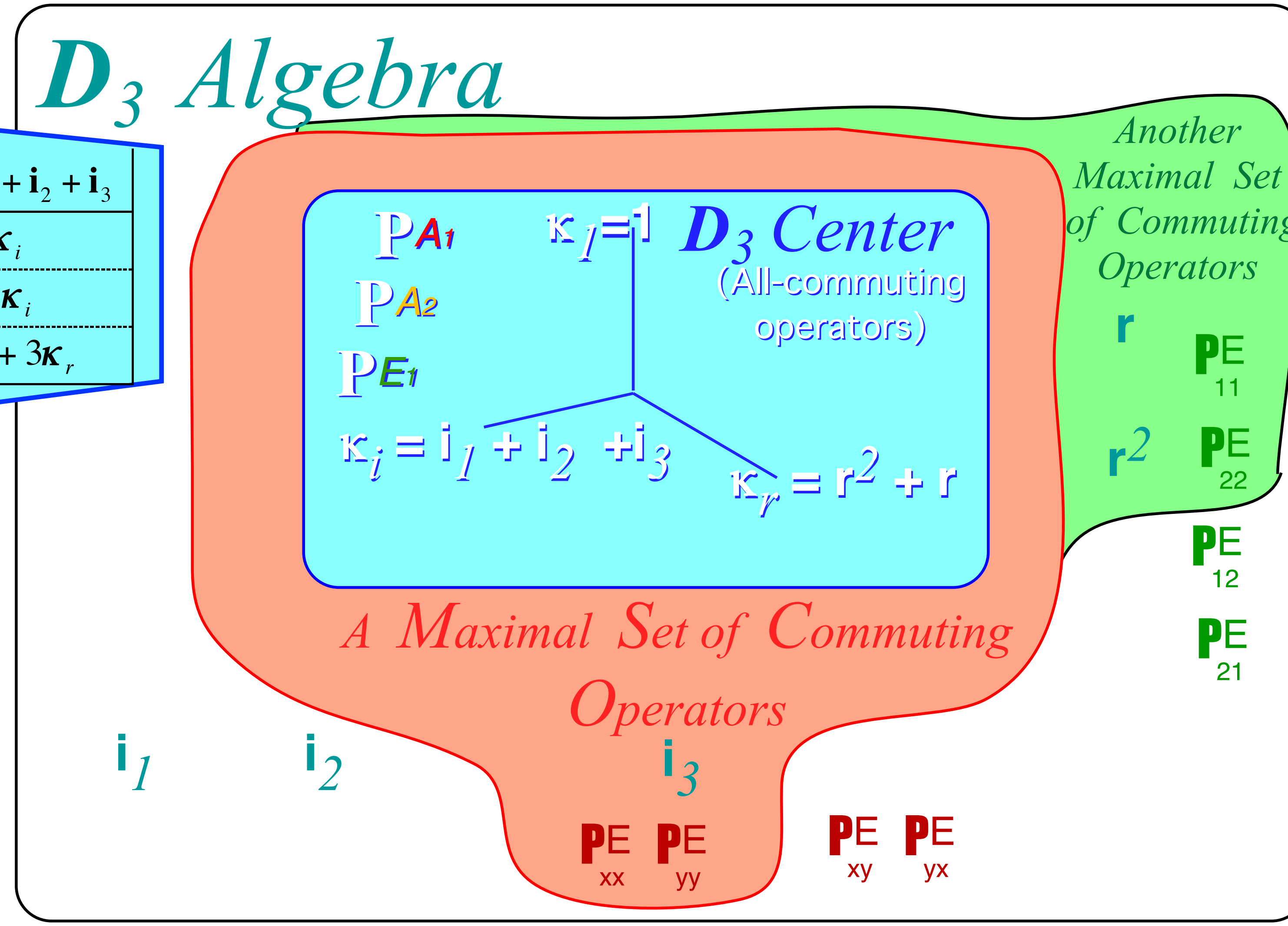
$°G$ = order of group: $\quad (°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $\quad (°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

$$\mathbf{g}_t\boldsymbol{\kappa}_k\mathbf{g}_t^{-1} = \boldsymbol{\kappa}_k \quad \text{where: } \boldsymbol{\kappa}_\mathbf{k} = \sum_{j=1}^{j=°\kappa_k}\mathbf{g}_j = \frac{1}{°s_k}\sum_{t=1}^{t=°G}\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}$$

$°s_k$=order of $\mathbf{g}_k$-self-symmetry:$(°s_1 = 6,\ °s_r = 3,\ °s_i = 2)$

$°s_k = °G\,/\,°\kappa_k$ *$\quad °s_k$ is an integer count of D_3 operators $\mathbf{g}_s$ that commute with $\mathbf{g}_k$.*



These operators $\mathbf{g}_s$ form the $\mathbf{g}_k$-self-symmetry group s_k . Each $\mathbf{g}_s$ transforms $\mathbf{g}_k$ into itself: $\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}=\mathbf{g}_k$

If an operator $\mathbf{g}_t$ transforms $\mathbf{g}_k$ into a different element $\mathbf{g}'_k$ of its class: $\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$, then so does $\mathbf{g}_t\mathbf{g}_s$.

that is: $\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k(\mathbf{g}_t\mathbf{g}_s)^{-1}=\mathbf{g}_t\mathbf{g}_s\mathbf{g}_k\mathbf{g}_s^{-1}\mathbf{g}_t^{-1}=\mathbf{g}_t\mathbf{g}_k\mathbf{g}_t^{-1}=\mathbf{g}'_k$,

*Subgroup $s_k=\{\mathbf{g}_0=\mathbf{1},\ \mathbf{g}_1=\mathbf{g}_k,\ \mathbf{g}_2,\dots\}$ has $\ell=(°\kappa_k-1)$ **Left Cosets*** (one coset for each member of class κ_k).

$$°\kappa_k\begin{cases}\mathbf{g}_1\, s_k = \mathbf{g}_1\{\mathbf{g}_0=1,\ \mathbf{g}_1=\mathbf{g}_k,\ \mathbf{g}_2,\dots\},\\ \mathbf{g}_2\, s_k = \mathbf{g}_2\underbrace{\{\mathbf{g}_0=1,\ \mathbf{g}_1=\mathbf{g}_k,\ \mathbf{g}_2,\dots\}}_{°s_k},\dots\end{cases}$$

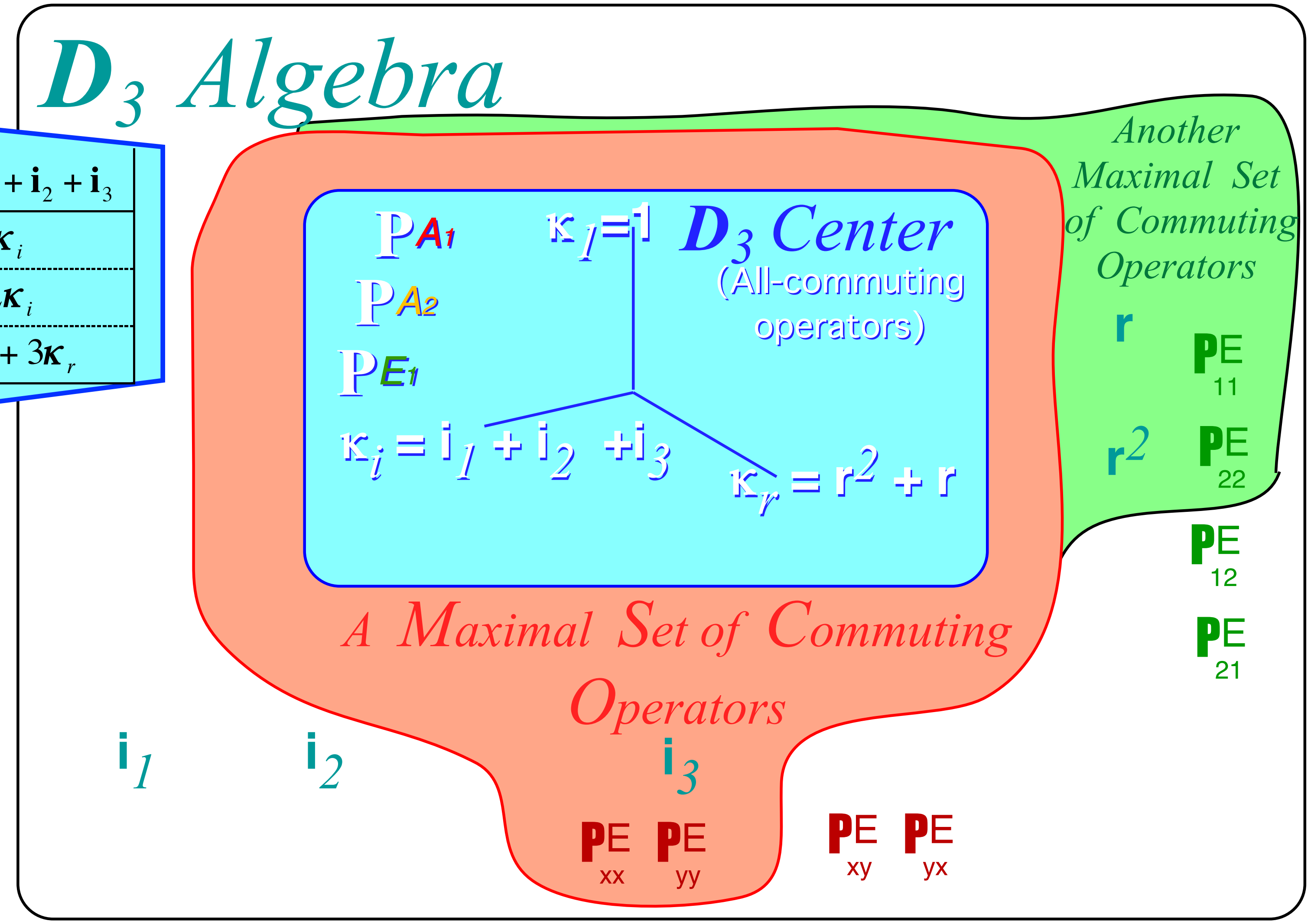
They will divide the group of order $°D_3 = °\kappa_k\cdot°s_k$ evenly into $°\kappa_k$ subsets each of order $°s_k$.

Review: *1st-Stage Spectral resolution of **D_3 Center** (Lagrange subgroup/class theorems)*

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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t \boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k \mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

$$\boxed{\mathbf{g}_t \boldsymbol{\kappa}_k \mathbf{g}_t^{-1} = \boldsymbol{\kappa}_k \quad \text{where: } \boldsymbol{\kappa}_\mathbf{k} = \sum_{j=1}^{j=°\kappa_k} \mathbf{g}_j = \frac{1}{°s_k} \sum_{t=1}^{t=°G} \mathbf{g}_t \mathbf{g}_k \mathbf{g}_t^{-1}}$$

$°s_k$=order of $\mathbf{g}_k$-self-symmetry: $(°s_1 = 6,\ °s_r = 3,\ °s_i = 2)$

$\boxed{°s_k = °G / °\kappa_k}$ *$°s_k$ is an integer count of D_3 operators $\mathbf{g}_s$ that commute with $\mathbf{g}_k$.*

These operators $\mathbf{g}_s$ form the $\mathbf{g}_k$-self-symmetry group s_k . Each $\mathbf{g}_s$ transforms $\mathbf{g}_k$ into itself: $\mathbf{g}_s \mathbf{g}_k \mathbf{g}_s^{-1} = \mathbf{g}_k$

If an operator $\mathbf{g}_t$ transforms $\mathbf{g}_k$ into a different element $\mathbf{g}'_k$ of its class: $\mathbf{g}_t \mathbf{g}_k \mathbf{g}_t^{-1} = \mathbf{g}'_k$, then so does $\mathbf{g}_t \mathbf{g}_s$.

that is: $\mathbf{g}_t \mathbf{g}_s \mathbf{g}_k (\mathbf{g}_t \mathbf{g}_s)^{-1} = \mathbf{g}_t \mathbf{g}_s \mathbf{g}_k \mathbf{g}_s^{-1} \mathbf{g}_t^{-1} = \mathbf{g}_t \mathbf{g}_k \mathbf{g}_t^{-1} = \mathbf{g}'_k$,

*Subgroup $s_k = \{\mathbf{g}_0 = \mathbf{1},\ \mathbf{g}_1 = \mathbf{g}_k,\ \mathbf{g}_2, \dots\}$ has $\ell = (°\kappa_k - 1)$ **Left Cosets*** (one coset for each member of class κ_k).

$$°\kappa_k \left\{ \begin{array}{l} \mathbf{g}_1 s_k = \mathbf{g}_1 \{\mathbf{g}_0 = 1,\ \mathbf{g}_1 = \mathbf{g}_k,\ \mathbf{g}_2, \dots\}, \\ \mathbf{g}_2 s_k = \mathbf{g}_2 \underbrace{\{\mathbf{g}_0 = 1,\ \mathbf{g}_1 = \mathbf{g}_k,\ \mathbf{g}_2, \dots\}}_{°s_k}, \dots \\ \vdots \end{array} \right.$$

*These results are known as **Lagrange's Coset Theorem(s)***

They will divide the group of order $\boxed{°D_3 = °\kappa_k \cdot °s_k}$ evenly into $°\kappa_k$ subsets each of order $°s_k$.

Review: *Spectral resolution of* ***D_3 Center*** *(Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

Spectral resolution to ***irreducible representations*** *(or "**irreps**") foretold by* ***characters*** *or* <u>*traces*</u>

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for $\ell=1$-6

Group invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$

3rd-stage spectral resolution to ***irreducible representations*** *(ireps) and Hamiltonian eigensolutions*

Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

Review: *1st-Stage Spectral resolution of **D_3 Center** (All-commuting class projectors)*

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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

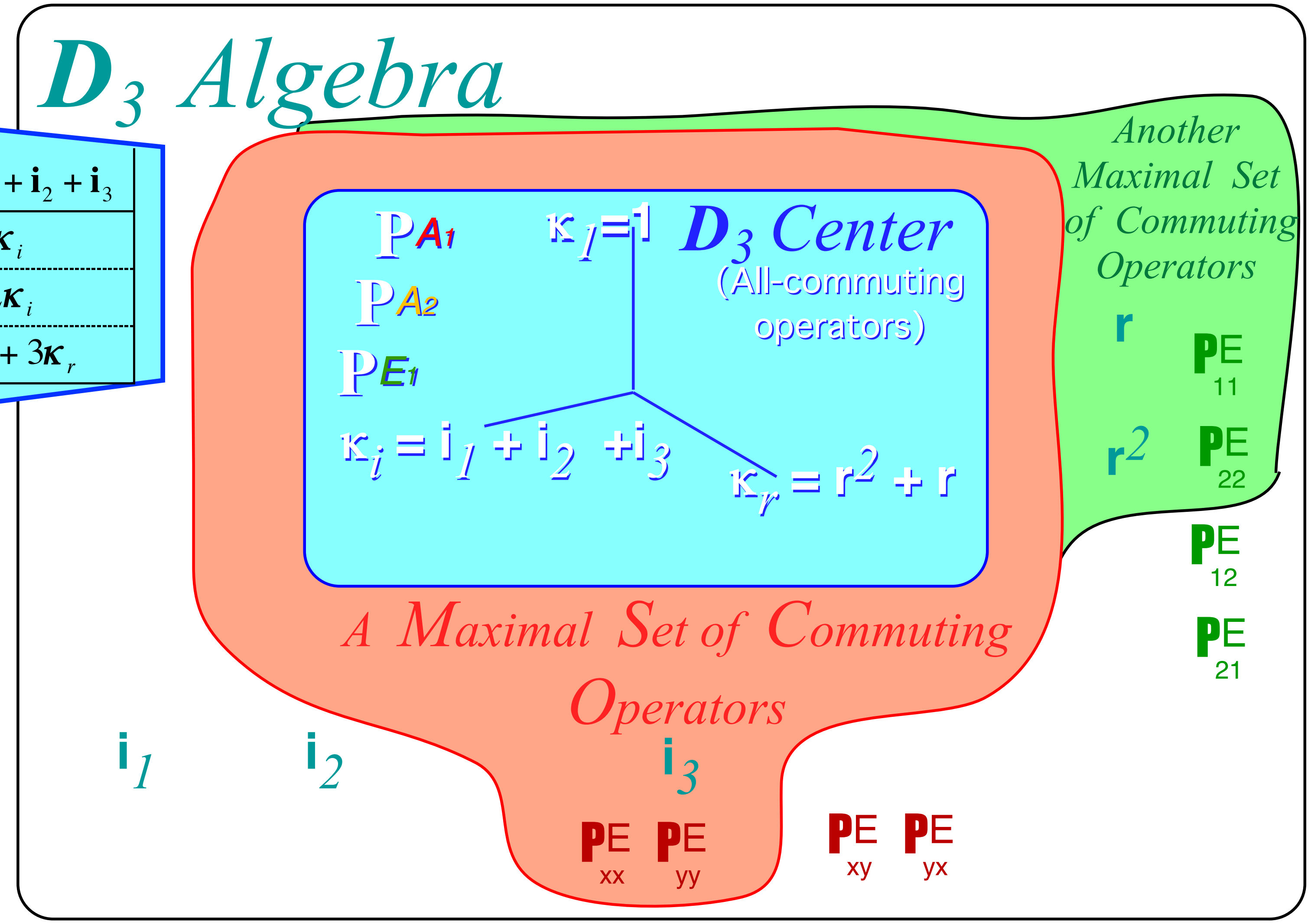
Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

Class minimal equation



Review: 1st-Stage Spectral resolution of $\mathbf{D_3}$ Center (All-commuting class projectors)

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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum κ_k commutes with all $\mathbf{g}_t$

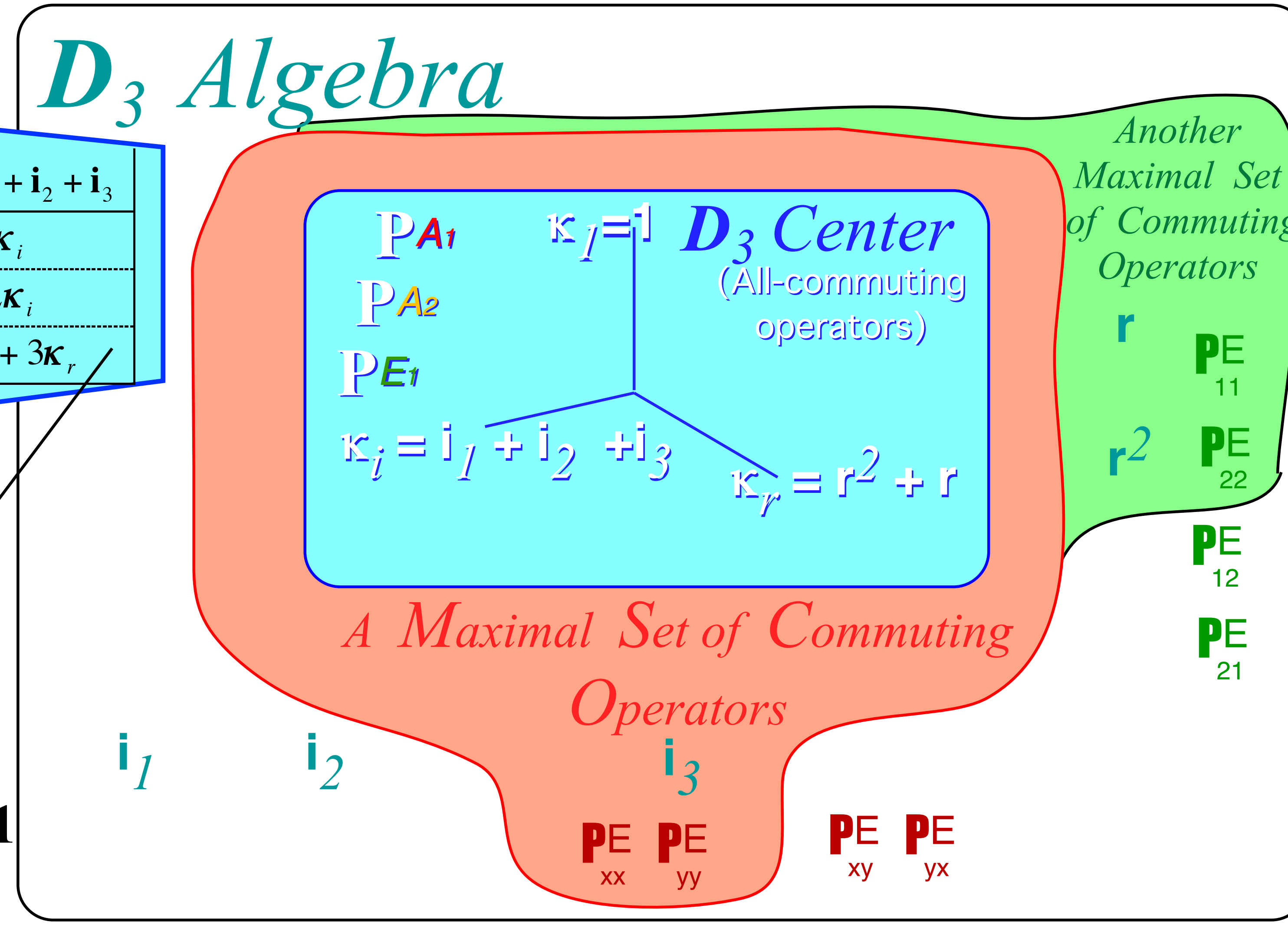
Class-sum κ_k invariance: $\mathbf{g}_t \kappa_k = \kappa_k \mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

Class minimal equation

$$\kappa^2{}_i = 3\cdot\kappa_r + 3\cdot\mathbf{1}$$



Review: 1st-Stage Spectral resolution of D_3 Center (All-commuting class projectors)

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

$\rightarrow$

	$\boldsymbol{\kappa}_1 = \mathbf{1}$	$\boldsymbol{\kappa}_r = \mathbf{r} + \mathbf{r}^2$	$\boldsymbol{\kappa}_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
$\boldsymbol{\kappa}_1$	$\boldsymbol{\kappa}_1$	$\boldsymbol{\kappa}_r$	$\boldsymbol{\kappa}_i$
$\boldsymbol{\kappa}_r$	$\boldsymbol{\kappa}_r$	$2\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_r$	$2\boldsymbol{\kappa}_i$
$\boldsymbol{\kappa}_i$	$\boldsymbol{\kappa}_i$	$2\boldsymbol{\kappa}_i$	$3\boldsymbol{\kappa}_1 + 3\boldsymbol{\kappa}_r$

Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t \boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k \mathbf{g}_t$

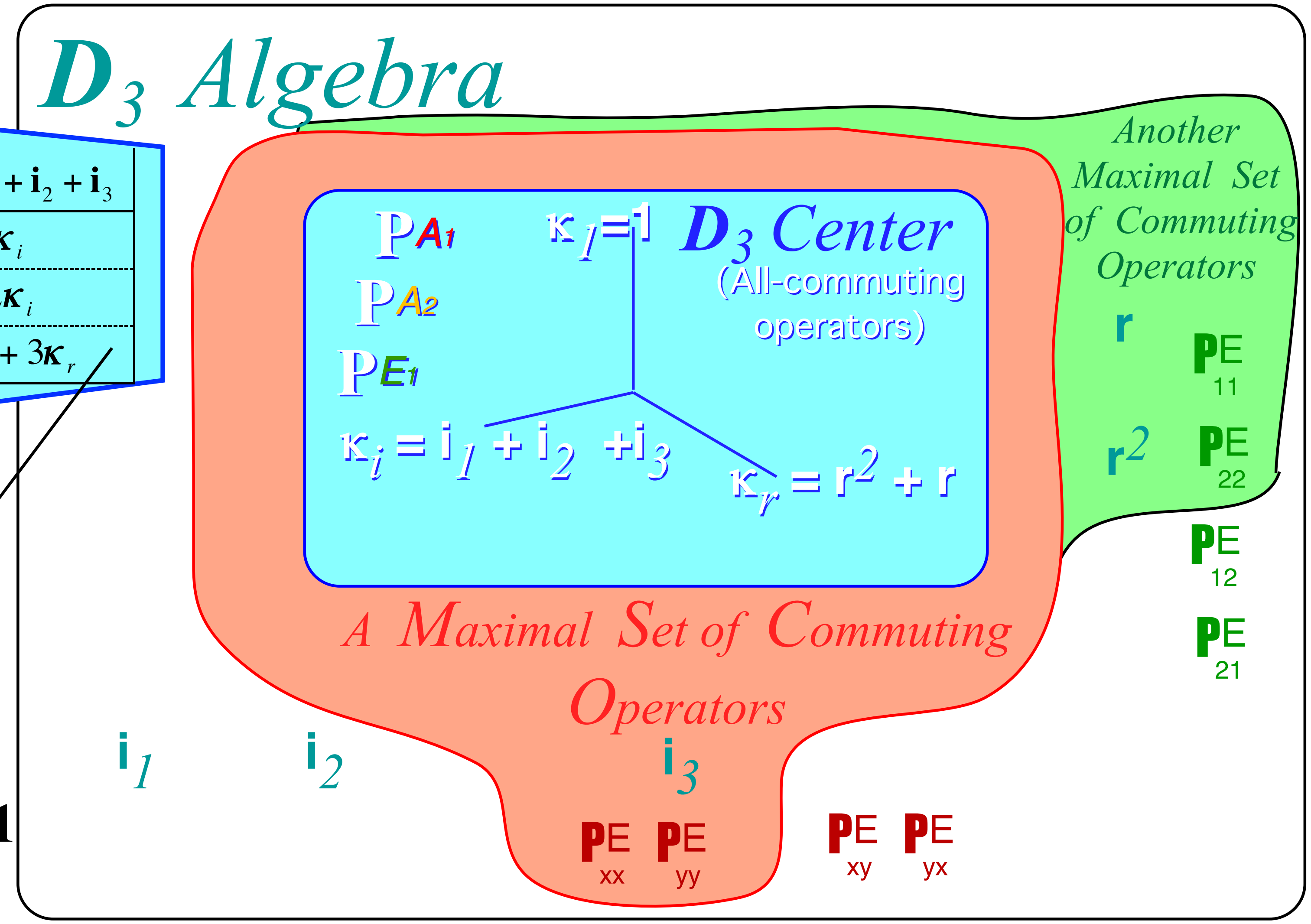
$^\circ G$ = order of group: $(^\circ D_3 = 6)$

$^\circ \kappa_k$ = order of class κ_k: $(^\circ\kappa_1 = 1,\ ^\circ\kappa_r = 2,\ ^\circ\kappa_i = 3)$

Class minimal equation

$$\boldsymbol{\kappa}^2{}_i = 3\cdot\boldsymbol{\kappa}_r + 3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3{}_i = 3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i + 3\cdot\boldsymbol{\kappa}_i = 9\cdot\boldsymbol{\kappa}_i$$



Review: 1^{st}-Stage Spectral resolution of D_3 Center (All-commuting class projectors)

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**

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t \boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k \mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

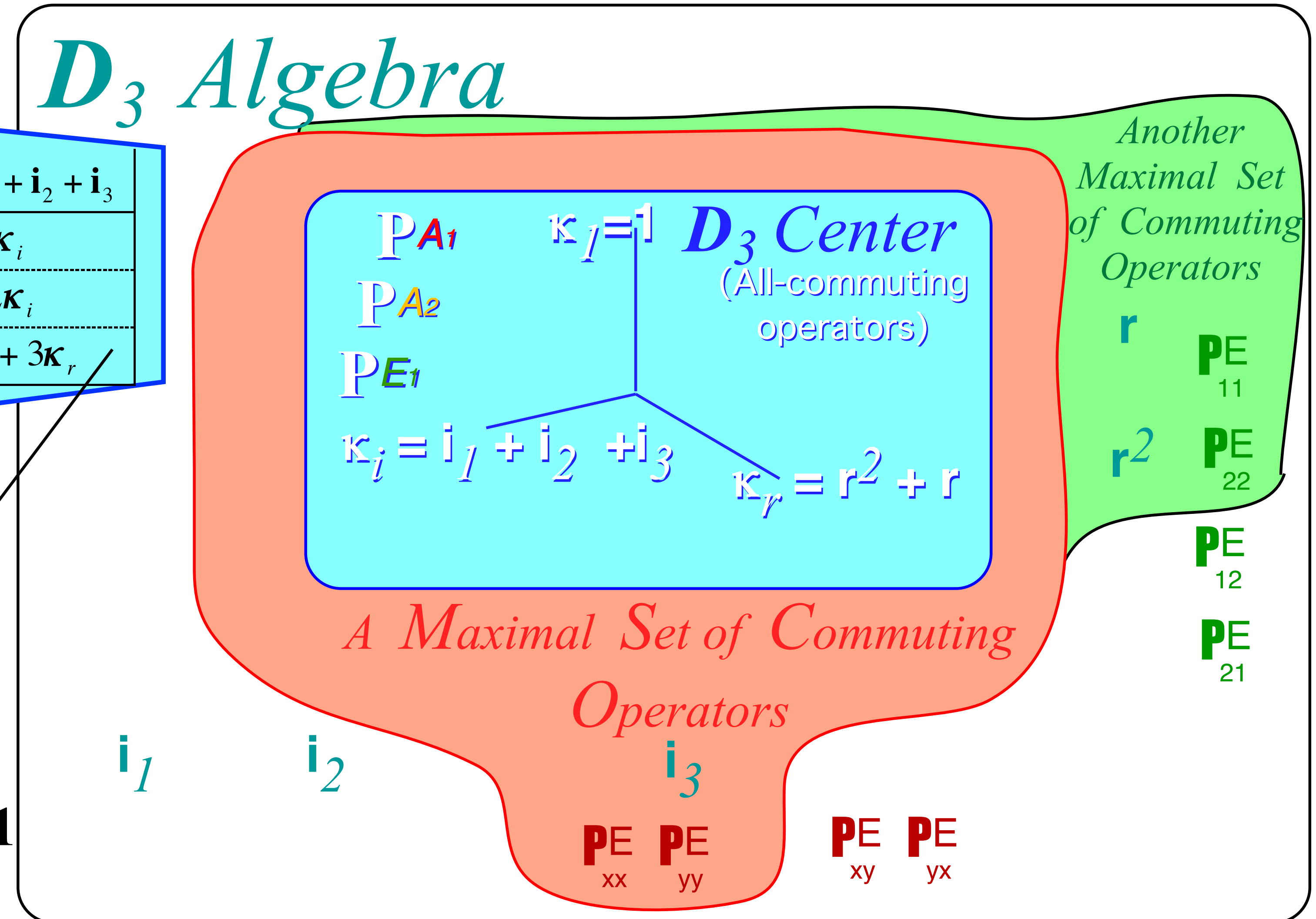
$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

Class minimal equation

$$\boldsymbol{\kappa}^2_i = 3\cdot\boldsymbol{\kappa}_r + 3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3_i = 3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i + 3\cdot\boldsymbol{\kappa}_i = 9\cdot\boldsymbol{\kappa}_i$$

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

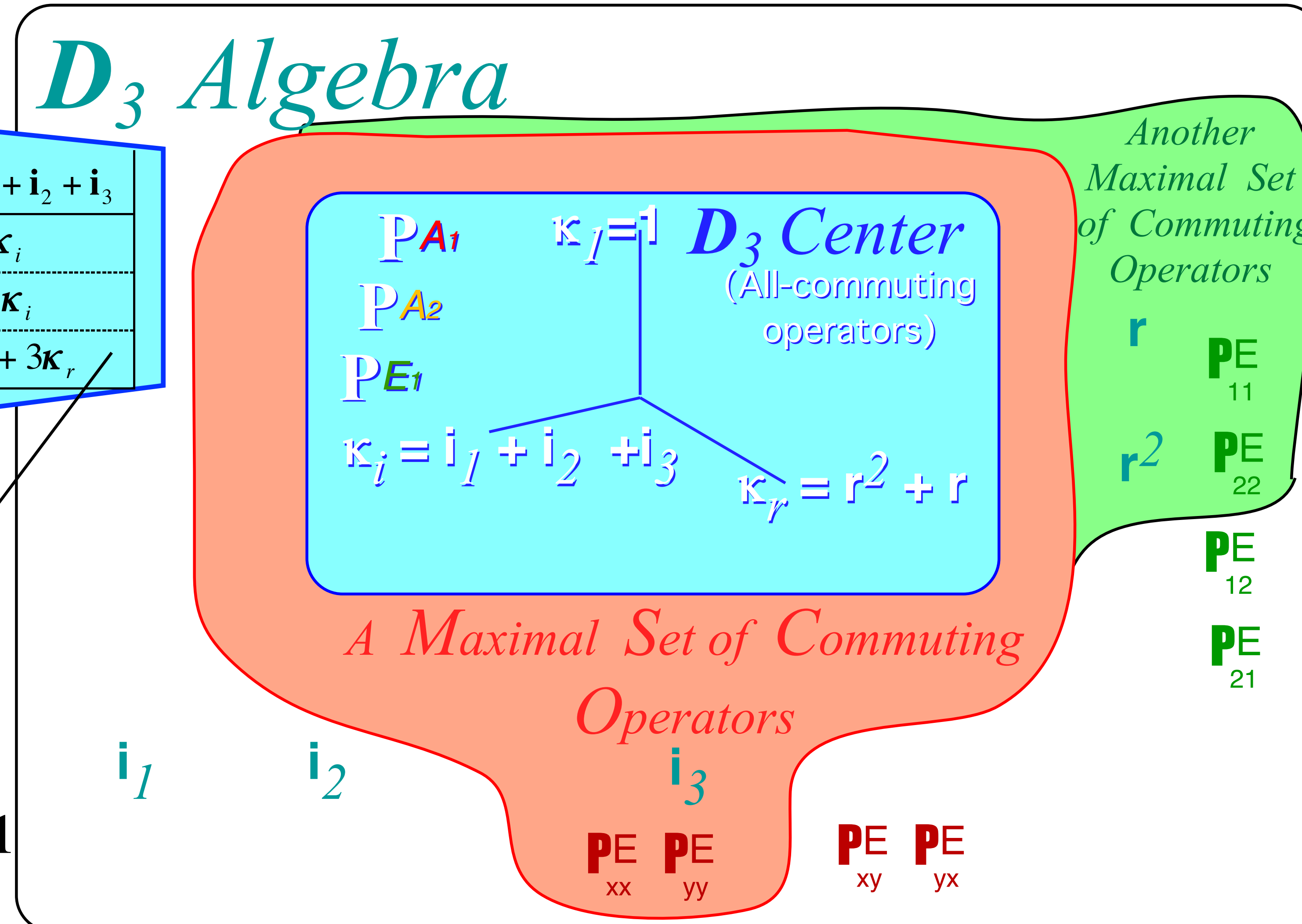


Review: 1^{st}-Stage Spectral resolution of D_3 Center (All-commuting class projectors)

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

$\rightarrow$

	$\kappa_1=\mathbf{1}$	$\kappa_r=\mathbf{r}+\mathbf{r}^2$	$\kappa_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

Class minimal equation

$$\boldsymbol{\kappa}^2_i = 3\cdot\boldsymbol{\kappa}_r + 3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3_i = 3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i + 3\cdot\boldsymbol{\kappa}_i = 9\cdot\boldsymbol{\kappa}_i$$

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

$$\boldsymbol{\kappa}_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E} = \mathbf{1}$$ *(Completeness)*

$$\boldsymbol{\kappa}_r = 2\cdot\mathbf{P}^{A_1} + 2\cdot\mathbf{P}^{A_2} - 1\cdot\mathbf{P}^{E} \longleftarrow \boldsymbol{\kappa}^2_r = \boldsymbol{\kappa}_r + 2\cdot\mathbf{1} \Rightarrow (\boldsymbol{\kappa}_r - 2\cdot\mathbf{1})(\boldsymbol{\kappa}_r + \mathbf{1}) = \mathbf{0}$$

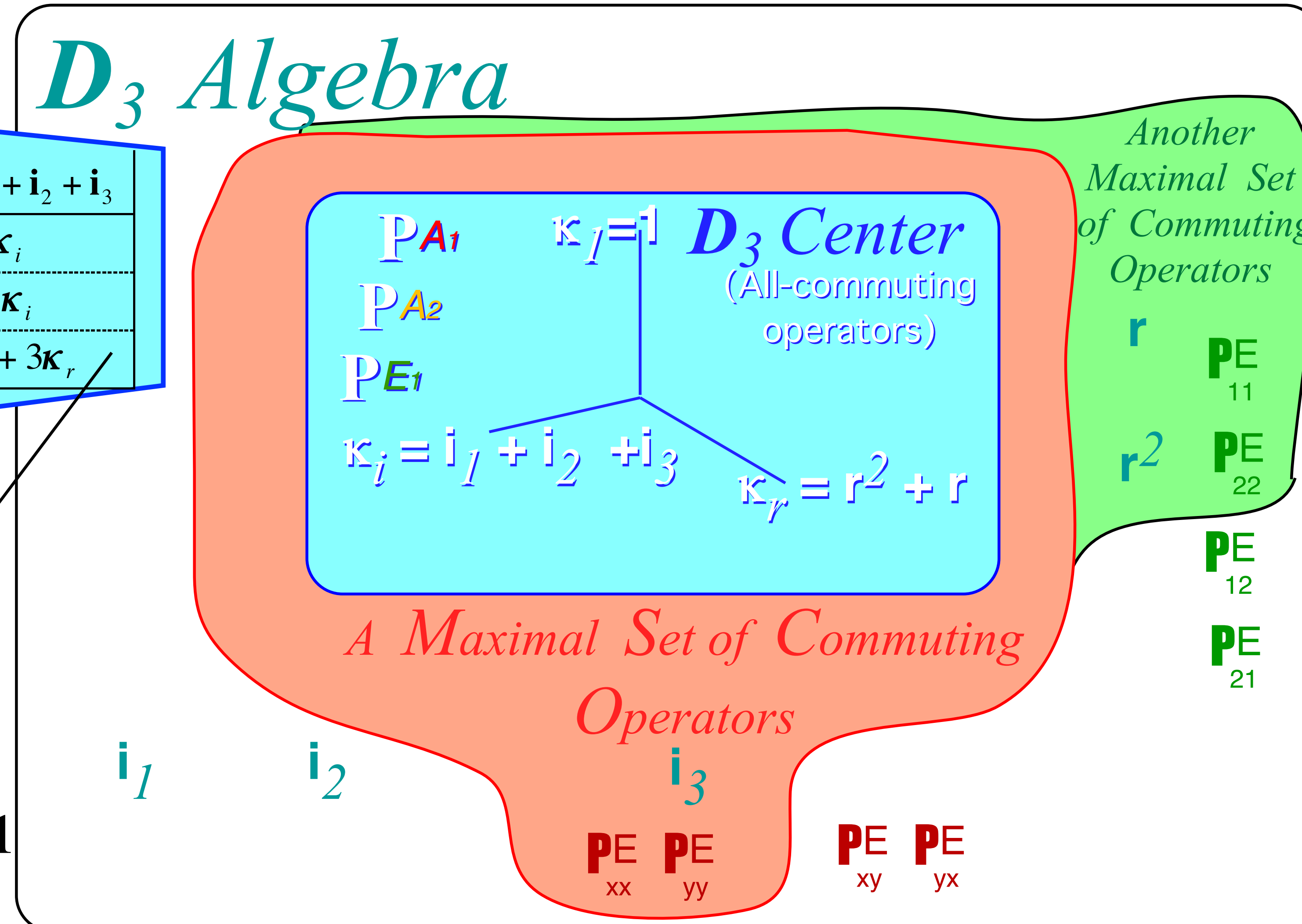
$$\boldsymbol{\kappa}_i = 3\cdot\mathbf{P}^{A_1} - 3\cdot\mathbf{P}^{A_2} + 0\cdot\mathbf{P}^{E}$$

Review: *1^{st}-Stage Spectral resolution of **D_3 Center** (All-commuting class projectors)*

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

$\rightarrow$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r}+\mathbf{r}^2$	$\kappa_i = \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ commutes with all $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$

Class minimal equation

$$\boldsymbol{\kappa}^2_i = 3\cdot\boldsymbol{\kappa}_r + 3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3_i = 3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i + 3\cdot\boldsymbol{\kappa}_i = 9\cdot\boldsymbol{\kappa}_i$$

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

$$\boldsymbol{\kappa}_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E} = \mathbf{1} \quad \textit{(Completeness)}$$

$$\boldsymbol{\kappa}_r = 2\cdot\mathbf{P}^{A_1} + 2\cdot\mathbf{P}^{A_2} - 1\cdot\mathbf{P}^{E}$$

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

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

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

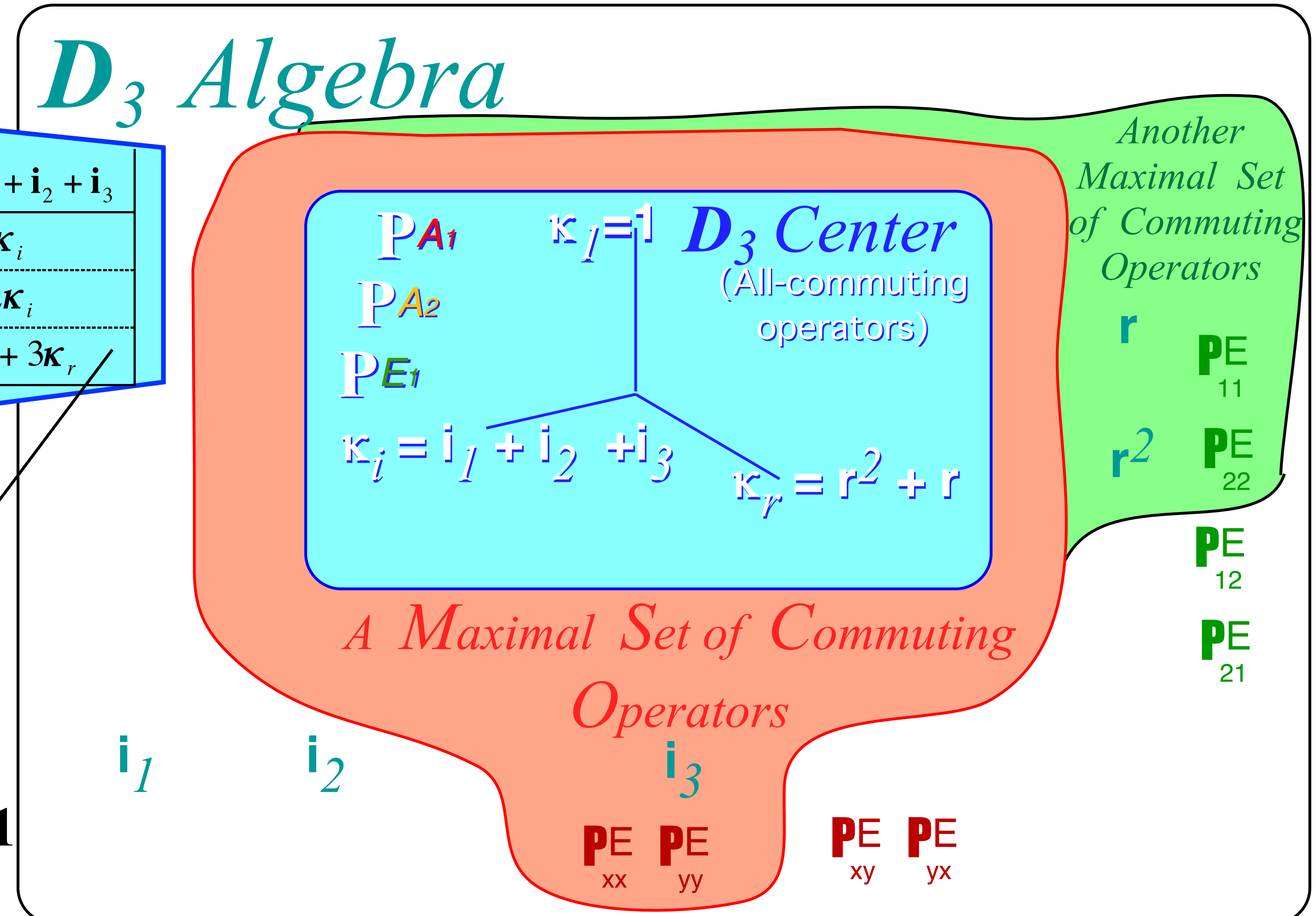
$$\mathbf{P}^{E} = \frac{(\boldsymbol{\kappa}_i - 3\cdot\mathbf{1})(\boldsymbol{\kappa}_i + 3\cdot\mathbf{1})}{(+0-3)(+0+3)}$$

Review: *1st-Stage Spectral resolution of* ***D₃ Center*** *(All-commuting class projectors)*

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

→

	$\kappa_1=\mathbf{1}$	$\kappa_r=\mathbf{r}+\mathbf{r}^2$	$\kappa_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k=\boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3=6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1=1,\ °\kappa_r=2,\ °\kappa_i=3)$

Class minimal equation

$$\boldsymbol{\kappa}^2_i=3\cdot\boldsymbol{\kappa}_r+3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3_i=3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i+3\cdot\boldsymbol{\kappa}_i=9\cdot\boldsymbol{\kappa}_i$$

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

Class ortho-complete **P**κ *relations*

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

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

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

$$\boldsymbol{\kappa}_1=1\cdot\mathbf{P}^{A_1}+1\cdot\mathbf{P}^{A_2}+1\cdot\mathbf{P}^{E}=\mathbf{1}\quad\textit{(Completeness)}$$

$$\boldsymbol{\kappa}_r=2\cdot\mathbf{P}^{A_1}+2\cdot\mathbf{P}^{A_2}-1\cdot\mathbf{P}^{E}$$

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

$$\mathbf{P}^{A_1}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r+\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r-\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

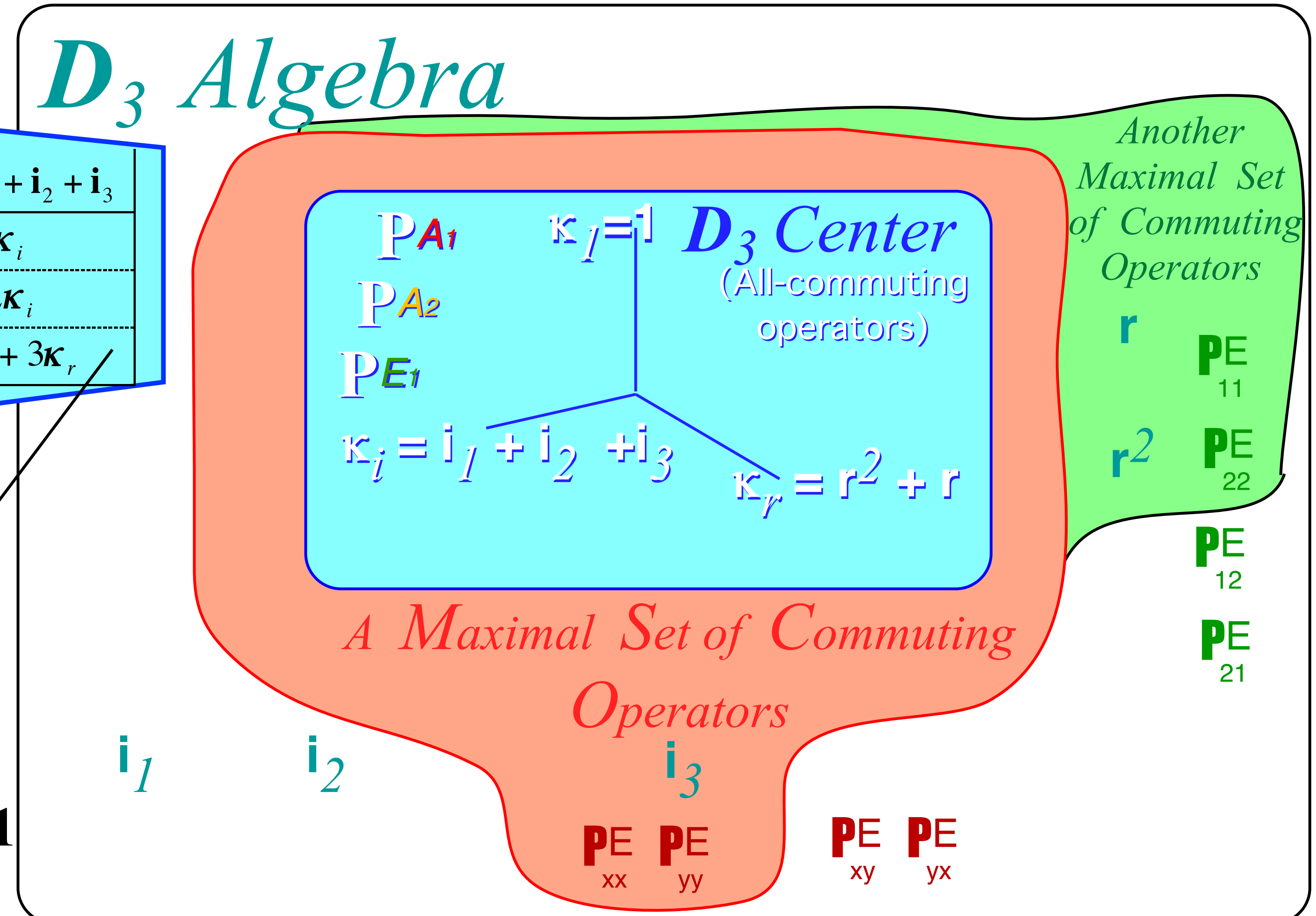
$$\mathbf{P}^{E}=(2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_r+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

Review: *1st-Stage Spectral resolution of* ***D₃ Center*** *(All-commuting class projectors)*

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

$\rightarrow$

	$\kappa_1=\mathbf{1}$	$\kappa_r=\mathbf{r}+\mathbf{r}^2$	$\kappa_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$



Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k=\boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3=6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1=1,\ °\kappa_r=2,\ °\kappa_i=3)$

Class minimal equation

$$\boldsymbol{\kappa}^2_i=3\cdot\boldsymbol{\kappa}_r+3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}^3_i=3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i+3\cdot\boldsymbol{\kappa}_i=9\cdot\boldsymbol{\kappa}_i$$

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

Class ortho-complete $\mathbf{P}\boldsymbol{\kappa}$ *relations*

$$\boldsymbol{\kappa}_1=1\cdot\mathbf{P}^{A_1}+1\cdot\mathbf{P}^{A_2}+1\cdot\mathbf{P}^{E}=\mathbf{1}\quad\text{(Completeness)}$$

$$\boldsymbol{\kappa}_r=2\cdot\mathbf{P}^{A_1}+2\cdot\mathbf{P}^{A_2}-1\cdot\mathbf{P}^{E}$$

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

$$\mathbf{P}^{A_1}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r+\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_r-\boldsymbol{\kappa}_i)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$

$$\mathbf{P}^{E}=(2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_r+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

$$\boldsymbol{\kappa}_k=\sum_{(\alpha)}\frac{°\kappa_k\chi_k^{(\alpha)}}{\ell^{(\alpha)}}\mathbf{P}^{(\alpha)}$$

irrep characters: $\chi_k^{(\alpha)}$
and dimensions: $\ell^{(\alpha)}$

$$\mathbf{P}^{(\alpha)}=\frac{\ell^{(\alpha)}}{°G}\sum_k\chi_k^{(\alpha)*}\boldsymbol{\kappa}_k=\frac{\ell^{(\alpha)}}{°G}\sum_{g=1}^{°G}\chi_g^{(\alpha)*}\mathbf{g}$$

χ_k^α	χ_1^α	χ_r^α	χ_i^α
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	−1
$\alpha=E$	2	−1	0

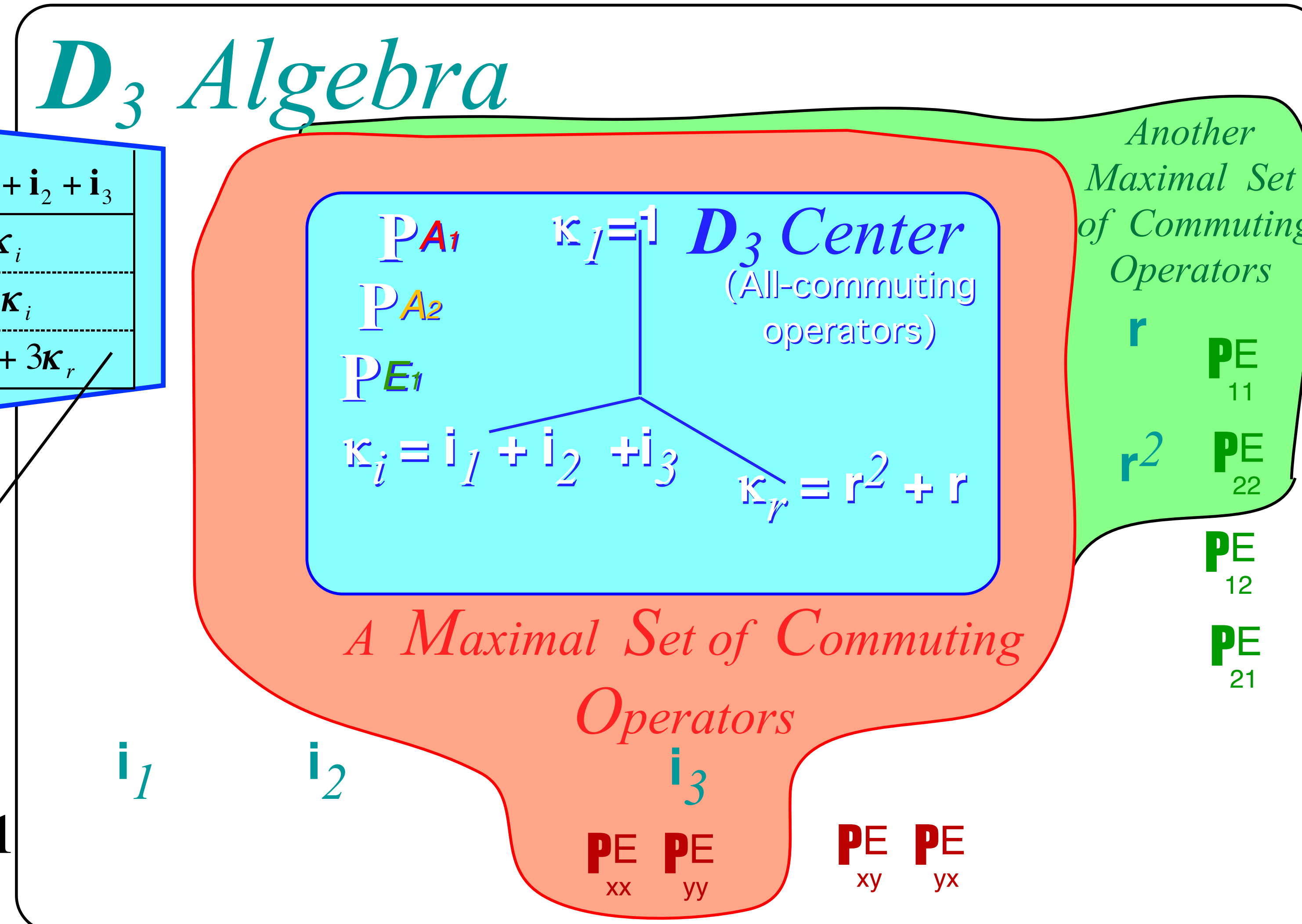
See $\mathbf{P}^{(\alpha)}{}_{vs}\boldsymbol{\kappa}_k$ *derivation in Lect 17 p. 77-89*

Review: 1^{st}-Stage Spectral resolution of D_3 Center (All-commuting class projectors)

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

$\rightarrow$

	$\kappa_1=\mathbf{1}$	$\kappa_r=\mathbf{r}+\mathbf{r}^2$	$\kappa_i=\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$



Class-sum κ_k commutes with all $\mathbf{g}_t$

Class-sum κ_k invariance: $\mathbf{g}_t\kappa_k=\kappa_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3=6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1=1,\ °\kappa_r=2,\ °\kappa_i=3)$

Class minimal equation

$$\kappa^2_i=3\cdot\kappa_r+3\cdot\mathbf{1}$$

$$\kappa^3_i=3\cdot\kappa_r\kappa_i+3\cdot\kappa_i=9\cdot\kappa_i$$

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

Class ortho-complete $\mathbf{P}\kappa$ relations

$$\kappa_1=1\cdot\mathbf{P}^{A_1}+1\cdot\mathbf{P}^{A_2}+1\cdot\mathbf{P}^{E}=\mathbf{1}\quad\text{(Completeness)}$$

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

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

$\chi_k^{(\alpha)}$=Trace $D^{(\alpha)}(\mathbf{g}_k)$

$\ell^{(\alpha)}$=Trace $D^{(\alpha)}(\mathbf{1})$

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

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

$$\mathbf{P}^{E}=(2\kappa_1-\kappa_r+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2)/3$$

$$\kappa_k=\sum_{(\alpha)}\frac{°\kappa_k\chi_k^{(\alpha)}}{\ell^{(\alpha)}}\mathbf{P}^{(\alpha)}$$

irrep characters: $\chi_k^{(\alpha)}$
and dimensions: $\ell^{(\alpha)}$

$$\mathbf{P}^{(\alpha)}=\frac{\ell^{(\alpha)}}{°G}\sum_k\chi_k^{(\alpha)*}\kappa_k=\frac{\ell^{(\alpha)}}{°G}\sum_{g=1}^{°G}\chi_g^{(\alpha)*}\mathbf{g}$$

χ_k^{α}	χ_1^{α}	χ_r^{α}	χ_i^{α}
$\alpha=A_1$	1	1	1
$\alpha=A_2$	1	1	−1
$\alpha=E$	2	−1	0

See $\mathbf{P}^{(\alpha)}{}_{vs}\kappa_k$ derivation in Lect 17 p. 77-89

Review: *1st-Stage Spectral resolution of* ***D_3 Center*** *(All-commuting class projectors)*

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

$\rightarrow$

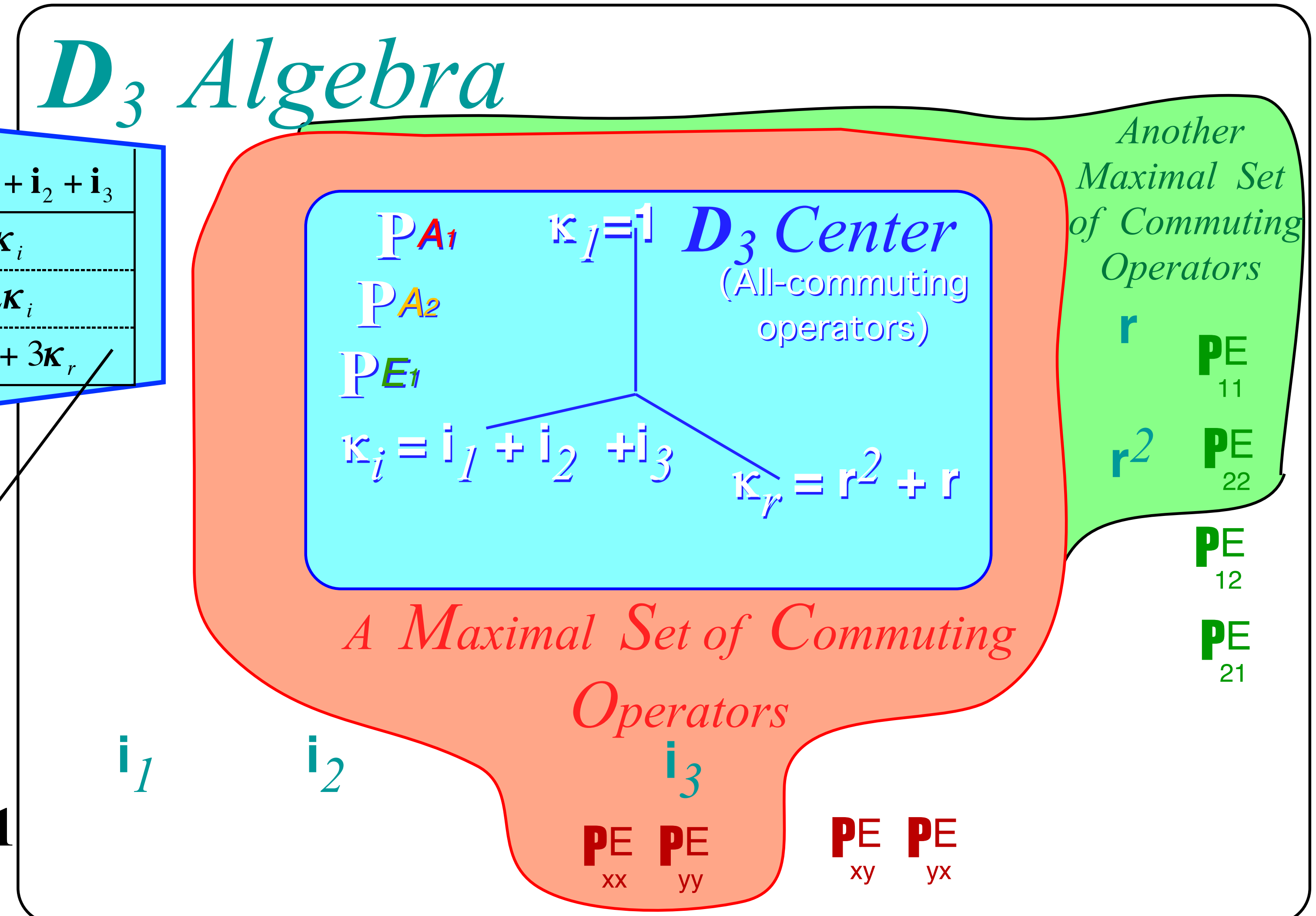
	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r}+\mathbf{r}^2$	$\kappa_i = \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1+\kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1+3\kappa_r$

Class-sum $\boldsymbol{\kappa}_k$ *commutes with all* $\mathbf{g}_t$

Class-sum $\boldsymbol{\kappa}_k$ invariance: $\mathbf{g}_t\boldsymbol{\kappa}_k = \boldsymbol{\kappa}_k\mathbf{g}_t$

$°G$ = order of group: $(°D_3 = 6)$

$°\kappa_k$ = order of class κ_k: $(°\kappa_1 = 1,\ °\kappa_r = 2,\ °\kappa_i = 3)$



Class minimal equation

$$\boldsymbol{\kappa}_i^2 = 3\cdot\boldsymbol{\kappa}_r + 3\cdot\mathbf{1}$$

$$\boldsymbol{\kappa}_i^3 = 3\cdot\boldsymbol{\kappa}_r\boldsymbol{\kappa}_i + 3\cdot\boldsymbol{\kappa}_i = 9\cdot\boldsymbol{\kappa}_i$$

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

Class ortho-complete $\mathbf{P}\kappa$ *relations*

$$\boldsymbol{\kappa}_1 = 1\cdot\mathbf{P}^{A_1} + 1\cdot\mathbf{P}^{A_2} + 1\cdot\mathbf{P}^{E} = \mathbf{1} \quad \textit{(Completeness)}$$

$$\boldsymbol{\kappa}_r = 2\cdot\mathbf{P}^{A_1} + 2\cdot\mathbf{P}^{A_2} - 1\cdot\mathbf{P}^{E}$$

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

$\chi_k^{(\alpha)}$=Trace $D^{(\alpha)}(\mathbf{g}_k)$

$\ell^{(\alpha)}$=Trace $D^{(\alpha)}(\mathbf{1})$

$$\boldsymbol{\kappa}_k = \sum_{(\alpha)} \frac{°\kappa_k\chi_k^{(\alpha)}}{\ell^{(\alpha)}}\mathbf{P}^{(\alpha)}$$

irrep characters: $\chi_k^{(\alpha)}$

and dimensions: $\ell^{(\alpha)}$

$$\mathbf{P}^{(\alpha)} = \frac{\ell^{(\alpha)}}{°G}\sum_k \chi_k^{(\alpha)*}\boldsymbol{\kappa}_k$$

$$= \frac{\ell^{(\alpha)}}{°G}\sum_{g=1}^{°G} \chi_g^{(\alpha)*}\mathbf{g}$$

χ_k^α	χ_1^α	χ_r^α	χ_i^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

Find $\chi_1^{(\alpha)*} = \ell^{(\alpha)}$ *using* $\boxed{\kappa_1 \textit{ coefficient}}$

$$\mathbf{P}^{(\alpha)} = \boxed{\frac{(\ell^{(\alpha)})^2}{°G}}\kappa_1 + \ldots$$

$$\mathbf{P}^{A_1} = (\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_r + \boldsymbol{\kappa}_i)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3)/6$$

$$\mathbf{P}^{A_2} = (\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_r - \boldsymbol{\kappa}_i)/6 = (\mathbf{1} + \mathbf{r} + \mathbf{r}^2 - \mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3)/6$$

$$\mathbf{P}^{E} = (2\boldsymbol{\kappa}_1 - \boldsymbol{\kappa}_r + 0)/3 = (2\mathbf{1} - \mathbf{r} - \mathbf{r}^2)/3$$

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

*Spectral resolution to **irreducible representations** (or "**irreps**") foretold by **characters** or traces*

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for ℓ=1-6

Group invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$

*3rd-stage spectral resolution to **irreducible representations** (ireps) and Hamiltonian eigensolutions*

Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

Spectral resolution to ***irreducible representations*** *(or "**irreps**") foretold by* ***characters*** *or* *<u>traces</u>*

$$
\begin{array}{c} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{array}
\overset{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}},
\overset{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}},
\overset{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}},
\overset{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}},
\overset{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}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix}
\cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\cdot & \cdot & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot \\
\cdot & 1 & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
1 & \cdot & \cdot & \cdot & \cdot & \cdot
\end{pmatrix}}
$$

$$
\mathbf{P}^{A_1} = (\boldsymbol{\kappa}_1 + \boldsymbol{\kappa}_2 + \boldsymbol{\kappa}_3)/6 = (\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1}) = \begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & 1 & 1 & 1
\end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_1}) = 1
$$

Spectral resolution to ***irreducible representations*** *(or "****irreps****") is foretold by* ***characters*** *or* *traces*

$$
\begin{array}{c} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1 \end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix} \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix} \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix} \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}}
$$

Min-eq. of all $\mathbf{P}$*'s :* $\mathbf{P}^2=\mathbf{P}$ *or* $(\mathbf{P}-\mathbf{1})\mathbf{P}=\mathbf{0}$

Allowed ***P*** *eigenvalues: 1 or 0*

$$
\mathbf{P}^{A_1}=(\kappa_1+\kappa_2+\kappa_3)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1})=\begin{pmatrix} 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1 \end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_1})=1
$$

So: $R(\mathbf{P}^{A_1})$ reduces to: $\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}$

*Spectral resolution to **irreducible representations** (or "**irreps**") is foretold by **characters** or <u>traces</u>*

$$
\begin{array}{c} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1 \end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix} \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix} \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix} \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}}
$$

Min-eq. of all $\mathbf{P}$*'s :* $\mathbf{P}^2=\mathbf{P}$ *or* $(\mathbf{P}-\mathbf{1})\mathbf{P}=\mathbf{0}$

Allowed $\mathbf{P}$ *eigenvalues: 1 or 0*

$$\mathbf{P}^{A_1}=(\kappa_1+\kappa_2+\kappa_3)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1})=\begin{pmatrix} 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1\\ 1&1&1&1&1&1 \end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_1})=1$$

So: $R(\mathbf{P}^{A_1})$ reduces to: $\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}$

$$\mathbf{P}^{A_2}=(\kappa_1+\kappa_2-\kappa_3)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_2})=\begin{pmatrix} 1&1&1&-1&-1&-1\\ 1&1&1&-1&-1&-1\\ 1&1&1&-1&-1&-1\\ -1&-1&-1&1&1&1\\ -1&-1&-1&1&1&1\\ -1&-1&-1&1&1&1 \end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_2})=1$$

So: $R(\mathbf{P}^{A_2})$ reduces to: $\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}$

Spectral resolution to ***irreducible representations*** *(or "****irreps****") is foretold by* ***characters*** *or* *<u>traces</u>*

$$R^G(\mathbf{1})= \qquad R^G(\mathbf{r})= \qquad R^G(\mathbf{r}^2)= \qquad R^G(\mathbf{i}_1)= \qquad R^G(\mathbf{i}_2)= \qquad R^G(\mathbf{i}_3)=$$

$$\begin{array}{c} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{array}
\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix},
\begin{pmatrix} \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix},
\begin{pmatrix} \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \end{pmatrix},
\begin{pmatrix} \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \end{pmatrix},
\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix},
\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

Min-eq. of all $\mathbf{P}$*'s :* $\mathbf{P}^2=\mathbf{P}$ *or* $(\mathbf{P}-\mathbf{1})\mathbf{P}=\mathbf{0}$

Allowed $\boldsymbol{P}$ *eigenvalues: 1 or 0*

$$\mathbf{P}^{A_1}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_2+\boldsymbol{\kappa}_3)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_1})=\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_1})=1$$

So: $R(\mathbf{P}^{A_1})$ reduces to:
$$\begin{pmatrix} 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\mathbf{P}^{A_2}=(\boldsymbol{\kappa}_1+\boldsymbol{\kappa}_2-\boldsymbol{\kappa}_3)/6=(\mathbf{1}+\mathbf{r}+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6 \Rightarrow R(\mathbf{P}^{A_2})=\begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix}/6 \qquad Trace R(\mathbf{P}^{A_2})=1$$

So: $R(\mathbf{P}^{A_2})$ reduces to:
$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}$$

$$\mathbf{P}^{E}=(2\boldsymbol{\kappa}_1-\boldsymbol{\kappa}_2+0)/3=(2\mathbf{1}-\mathbf{r}-\mathbf{r}^2+0+0+0)/3 \Rightarrow R(\mathbf{P}^{E})=\begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix}/3 \qquad Trace R(\mathbf{P}^{E})=4$$

So: $R(\mathbf{P}^{E})$ reduces to:
$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & 1 \end{pmatrix}$$

Review: *Spectral resolution of* ***D_3 Center*** *(Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

Spectral resolution to ***irreducible representations*** *(or "**irreps**") foretold by* ***characters*** *or <u>traces</u>*

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for ℓ=1-6

Group invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$

3rd-stage spectral resolution to ***irreducible representations*** *(ireps) and Hamiltonian eigensolutions*

Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

Spectral resolution to ***irreducible representations*** *(or "****irreps****") is foretold by* ***characters*** *or* <u>*traces*</u>

$$
\begin{array}{c}
1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3
\end{array}
\quad
R^G(\mathbf{1})=\begin{pmatrix}
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1
\end{pmatrix},\;
R^G(\mathbf{r})=\begin{pmatrix}
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot
\end{pmatrix},\;
R^G(\mathbf{r}^2)=\begin{pmatrix}
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot
\end{pmatrix},
$$

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

$$
R(\mathbf{P}^{A_1})=\begin{pmatrix}
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1
\end{pmatrix}/6 \;\Rightarrow\; TraceR(\mathbf{P}^{A_1})=1 \qquad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to: }
\begin{pmatrix}
D^{A_1}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}
$$

$$
R(\mathbf{P}^{A_2})=\begin{pmatrix}
1&1&1&-1&-1&-1\\
1&1&1&-1&-1&-1\\
1&1&1&-1&-1&-1\\
-1&-1&-1&1&1&1\\
-1&-1&-1&1&1&1\\
-1&-1&-1&1&1&1
\end{pmatrix}/6 \;\Rightarrow\; TraceR(\mathbf{P}^{A_2})=1
$$

$$
R(\mathbf{P}^{E})=\begin{pmatrix}
2&-1&-1&0&0&0\\
-1&2&-1&0&0&0\\
-1&-1&2&0&0&0\\
0&0&0&2&-1&-1\\
0&0&0&-1&2&-1\\
0&0&0&-1&-1&1
\end{pmatrix}/3 \;\Rightarrow\; TraceR(\mathbf{P}^{E})=4
$$

Spectral resolution to ***irreducible representations*** *(or “****irreps****”) is foretold by* ***characters*** *or* <u>*traces*</u>

$$
\begin{array}{c}
1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3
\end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix}
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1
\end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix}
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix}
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}}
$$

$$
R(\mathbf{P}^{A_1})=\begin{pmatrix}
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1\\
1&1&1&1&1&1
\end{pmatrix}/6 \quad\Rightarrow\quad TraceR(\mathbf{P}^{A_1})=1 \qquad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to:}
\begin{pmatrix}
D^{A_1}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}
$$

$$
R(\mathbf{P}^{A_2})=\begin{pmatrix}
1&1&1&-1&-1&-1\\
1&1&1&-1&-1&-1\\
1&1&1&-1&-1&-1\\
-1&-1&-1&1&1&1\\
-1&-1&-1&1&1&1\\
-1&-1&-1&1&1&1
\end{pmatrix}/6 \quad\Rightarrow\quad TraceR(\mathbf{P}^{A_2})=1 \qquad \text{So: } R(\mathbf{P}^{A_2}\mathbf{g}) \text{ reduces to:}
\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&D^{A_2}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}
$$

$$
R(\mathbf{P}^{E})=\begin{pmatrix}
2&-1&-1&0&0&0\\
-1&2&-1&0&0&0\\
-1&-1&2&0&0&0\\
0&0&0&2&-1&-1\\
0&0&0&-1&2&-1\\
0&0&0&-1&-1&1
\end{pmatrix}/3 \quad\Rightarrow\quad TraceR(\mathbf{P}^{E})=4
$$

Spectral resolution to ***irreducible representations*** *(or "****irreps****") is foretold by* ***characters*** *or* *traces*

$$
\begin{array}{c}1\\r^1\\r^2\\i_1\\i_2\\i_3\end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix}1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix}\cdot&\cdot&1&\cdot&\cdot&\cdot\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\cdot&1&\cdot&\cdot\end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix}\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix}\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\\1&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix}\cdot&\cdot&\cdot&\cdot&\cdot&1\\\cdot&\cdot&\cdot&1&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&1&\cdot\\\cdot&1&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&1&\cdot&\cdot&\cdot\\1&\cdot&\cdot&\cdot&\cdot&\cdot\end{pmatrix}}
$$

$$
R(\mathbf{P}^{A_1})=\begin{pmatrix}1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\end{pmatrix}/6 \;\Rightarrow\; TraceR(\mathbf{P}^{A_1})=1 \quad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{ reduces to:} \begin{pmatrix}D^{A_1}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\end{pmatrix}
$$

$$
R(\mathbf{P}^{A_2})=\begin{pmatrix}1&1&1&-1&-1&-1\\1&1&1&-1&-1&-1\\1&1&1&-1&-1&-1\\-1&-1&-1&1&1&1\\-1&-1&-1&1&1&1\\-1&-1&-1&1&1&1\end{pmatrix}/6 \;\Rightarrow\; TraceR(\mathbf{P}^{A_2})=1 \quad \text{So: } R(\mathbf{P}^{A_2}\mathbf{g}) \text{ reduces to:} \begin{pmatrix}\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&D^{A_2}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\end{pmatrix}
$$

$$
R(\mathbf{P}^{E})=\begin{pmatrix}2&-1&-1&0&0&0\\-1&2&-1&0&0&0\\-1&-1&2&0&0&0\\0&0&0&2&-1&-1\\0&0&0&-1&2&-1\\0&0&0&-1&-1&1\end{pmatrix}/3 \;\Rightarrow\; TraceR(\mathbf{P}^{E})=4 \quad \text{So: } R(\mathbf{P}^{E}\mathbf{g}) \text{ reduces to:} \begin{pmatrix}\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\\cdot&\cdot&D^E_{11}&D^E_{12}&\cdot&\cdot\\\cdot&\cdot&D^E_{21}&D^E_{22}&\cdot&\cdot\\\cdot&\cdot&\cdot&\cdot&D^E_{11}&D^E_{12}\\\cdot&\cdot&\cdot&\cdot&D^E_{21}&D^E_{22}\end{pmatrix}
$$

Spectral resolution to ***irreducible representations*** *(or “****irreps****”) foretold by* ***characters*** *or* *<u>traces</u>*

$$
\begin{array}{c}
1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3
\end{array}
\quad
R^G(\mathbf{1})=\begin{pmatrix}
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1
\end{pmatrix},\;
R^G(\mathbf{r})=\begin{pmatrix}
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot
\end{pmatrix},\;
R^G(\mathbf{r}^2)=\begin{pmatrix}
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot
\end{pmatrix},
$$

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

$TraceR(\mathbf{P}^{A_1}) = 1$ So: $R(\mathbf{P}^{A_1}\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
D^{A_1}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}
$$

$TraceR(\mathbf{P}^{A_2}) = 1$ So: $R(\mathbf{P}^{A_2}\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&D^{A_2}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}
$$

$TraceR(\mathbf{P}^{E}) = 4$ So: $R(\mathbf{P}^{E}\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&D^E_{11}&D^E_{12}&\cdot&\cdot\\
\cdot&\cdot&D^E_{21}&D^E_{22}&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&D^E_{11}&D^E_{12}\\
\cdot&\cdot&\cdot&\cdot&D^E_{21}&D^E_{22}
\end{pmatrix}
$$

So: $R(\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
D^{A_1}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&D^{A_2}(\mathbf{g})&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&D^E_{11}&D^E_{12}&\cdot&\cdot\\
\cdot&\cdot&D^E_{21}&D^E_{22}&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&D^E_{11}&D^E_{12}\\
\cdot&\cdot&\cdot&\cdot&D^E_{21}&D^E_{22}
\end{pmatrix}
$$

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

*Spectral resolution to **irreducible representations** (or "**irreps**") foretold by **characters** or <u>traces</u>*

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Spectral resolution to ***irreducible representations*** *(or "**ireps**") foretold by* ***characters*** *or* <u>*traces*</u>

$$
\begin{array}{c} 1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3 \end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix} 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1 \end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix} \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix} \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix} \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot \end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix} \cdot&\cdot&\cdot&\cdot&\cdot&1\\ \cdot&\cdot&\cdot&1&\cdot&\cdot\\ \cdot&\cdot&\cdot&\cdot&1&\cdot\\ \cdot&1&\cdot&\cdot&\cdot&\cdot\\ \cdot&\cdot&1&\cdot&\cdot&\cdot\\ 1&\cdot&\cdot&\cdot&\cdot&\cdot \end{pmatrix}}
$$

$\{R^G(\mathbf{g})\}$ has lots of empty space and looks like it could be reduced.

But, $\{R^G(\mathbf{g})\}$ cannot be diagonalized all-at-once. (Not all $\mathbf{g}$ commute.)

Nevertheless, $\{R^G(\mathbf{g})\}$ can be *block-diagonalized* *all-at-once* into *"**ireps**"* A_1, A_2, and *two* E_1's

$R(\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot\\
\cdot & \cdot & D^{E}_{11} & D^{E}_{12} & \cdot & \cdot\\
\cdot & \cdot & D^{E}_{21} & D^{E}_{22} & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & D^{E}_{11} & D^{E}_{12}\\
\cdot & \cdot & \cdot & \cdot & D^{E}_{21} & D^{E}_{22}
\end{pmatrix}
$$

Spectral resolution to ***irreducible representations*** *(or "**ireps**") foretold by* ***characters*** *or* *traces*

$$
\begin{array}{c}
1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3
\end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix}
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1
\end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix}
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix}
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}}
$$

$\{R^G(\mathbf{g})\}$ has lots of empty space and looks like it could be reduced.

But, $\{R^G(\mathbf{g})\}$ cannot be diagonalized all-at-once. (Not all $\mathbf{g}$ commute.)

Nevertheless, $\{R^G(\mathbf{g})\}$ can be *block-diagonalized all-at-once* into ***"ireps"*** A_1, A_2, and *two* E_1's

We relate traces of $\{R^G(\mathbf{g})\}$:

$(\mathbf{g})=$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$Trace R^G(\mathbf{g})=$	6	0	0

to D_3 character table:

$(\mathbf{g})=$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})=$	1	1	1
$\chi^{A_2}(\mathbf{g})=$	1	1	-1
$\chi^{E_1}(\mathbf{g})=$	2	-1	0

$\chi^{A_1}(\mathbf{g})$	1	1	1
$+\chi^{A_2}(\mathbf{g})$	1	1	-1
$+2\chi^{E_1}(\mathbf{g})$	$2\cdot 2$	$-2\cdot 1$	0
	6	0	0

$R(\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot\\
\cdot & \cdot & D^E_{11} & D^E_{12} & \cdot & \cdot\\
\cdot & \cdot & D^E_{21} & D^E_{22} & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & D^E_{11} & D^E_{12}\\
\cdot & \cdot & \cdot & \cdot & D^E_{21} & D^E_{22}
\end{pmatrix}
$$

*Spectral resolution to **irreducible representations** (or "**ireps**") foretold by **characters** or traces*

$$
\begin{array}{c}
1\\ r^1\\ r^2\\ i_1\\ i_2\\ i_3
\end{array}
\overset{R^G(\mathbf{1})=}{\begin{pmatrix}
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1
\end{pmatrix}},
\overset{R^G(\mathbf{r})=}{\begin{pmatrix}
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{r}^2)=}{\begin{pmatrix}
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_1)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_2)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}},
\overset{R^G(\mathbf{i}_3)=}{\begin{pmatrix}
\cdot&\cdot&\cdot&\cdot&\cdot&1\\
\cdot&\cdot&\cdot&1&\cdot&\cdot\\
\cdot&\cdot&\cdot&\cdot&1&\cdot\\
\cdot&1&\cdot&\cdot&\cdot&\cdot\\
\cdot&\cdot&1&\cdot&\cdot&\cdot\\
1&\cdot&\cdot&\cdot&\cdot&\cdot
\end{pmatrix}}
$$

$\{R^G(\mathbf{g})\}$ has lots of empty space and looks like it could be reduced.

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We relate traces of $\{R^G(\mathbf{g})\}$:

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$Trace R^G(\mathbf{g})=$	6	0	0

to D_3 character table:

$(\mathbf{g})=$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
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$\chi^{A_1}(\mathbf{g})$	1	1	1
$+\chi^{A_2}(\mathbf{g})$	1	1	-1
$+2\chi^{E_1}(\mathbf{g})$	$2\cdot 2$	$-2\cdot 1$	0
	6	0	0

$R(\mathbf{g})$ reduces to:

$$
\begin{pmatrix}
D^{A_1}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot & \cdot\\
\cdot & D^{A_2}(\mathbf{g}) & \cdot & \cdot & \cdot & \cdot\\
\cdot & \cdot & D^{E}_{11} & D^{E}_{12} & \cdot & \cdot\\
\cdot & \cdot & D^{E}_{21} & D^{E}_{22} & \cdot & \cdot\\
\cdot & \cdot & \cdot & \cdot & D^{E}_{11} & D^{E}_{12}\\
\cdot & \cdot & \cdot & \cdot & D^{E}_{21} & D^{E}_{22}
\end{pmatrix}
$$

So $\{R^G(\mathbf{g})\}$ can be *block-diagonalized* into a ***direct sum*** $\oplus$ of *"**ireps**"* $R^G(\mathbf{g})=D^{A_1}(\mathbf{g})\oplus D^{A_2}(\mathbf{g})\oplus 2D^{E_1}(\mathbf{g})$

Review: *Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

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Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

(irep ≡ irreducible representation)

Symmetry reduction of G to H⊂G involves splitting of G-ireps $D^{(\alpha)}(G)$ into smaller H-ireps $d^{(a)}(H)$

$$D^{(\alpha)}(G)\downarrow H \equiv D^{(\alpha)}(H) \text{ is reducible to: } T_{reducer}\, D^{(\alpha)}(H) T^{\dagger}_{reducer} = f^{(a)} d^{(a)}(H) \oplus f^{(b)} d^{(b)}(H) \oplus \ldots$$

$$T_{reducer} D^{(\alpha)}(h) T^{\dagger}_{reducer} = \begin{pmatrix} d^{(a)} & & & & \\ & d^{(a)} & & & \\ & & d^{(a)} & & \\ & & & d^{(b)} & \\ & & & & d^{(b)} \end{pmatrix} \qquad \begin{matrix} f^{(a)}=3 \\ \\ f^{(b)}=2 \end{matrix}$$

The following derives formulae for integral H⊂G correlation coefficients $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

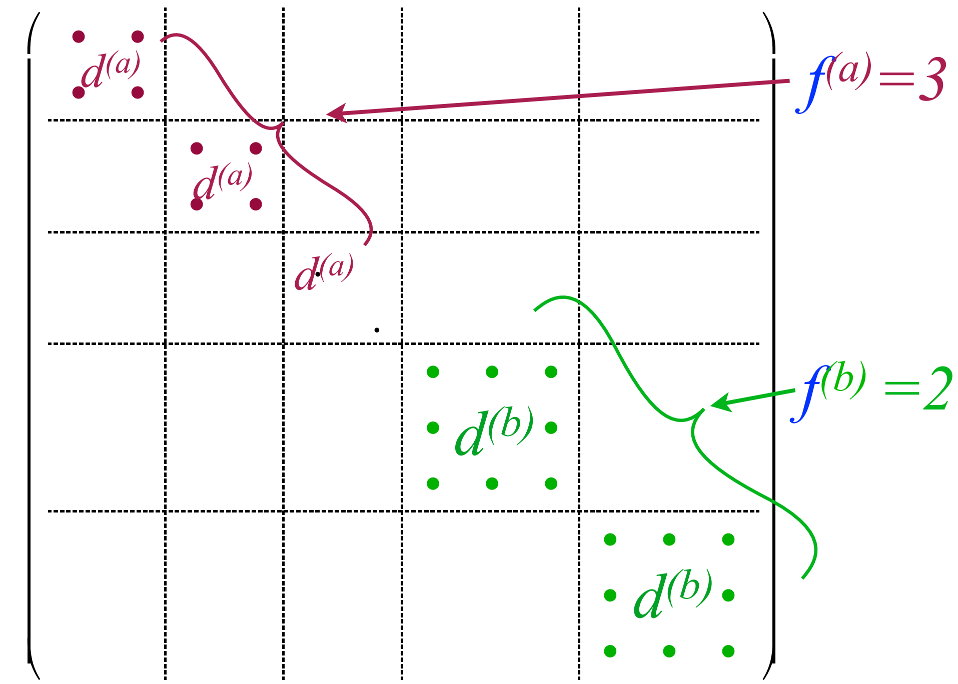
Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

(irep ≡ irreducible representation)

Symmetry reduction of G to $H\subset G$ involves splitting of G-ireps $D^{(\alpha)}(G)$ into smaller H-ireps $d^{(a)}(H)$

$$D^{(\alpha)}(G)\downarrow H \equiv D^{(\alpha)}(H) \text{ is reducible to: } T_{reducer}\, D^{(\alpha)}(H) T^{\dagger}_{reducer} = f^{(a)} d^{(a)}(H) \oplus f^{(b)} d^{(b)}(H) \oplus \ldots$$

$$T_{reducer} D^{(\alpha)}(h) T^{\dagger}_{reducer} =$$



The following derives formulae for integral $H\subset G$ correlation coefficients $f^{(b)}(D^{(\alpha)}(G)\downarrow H)$

$$Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = f^{(b)} \cdot \ell^{(b)}$$ *Since each $d^{(b)}(\mathbf{P}^{(b)})$ is an $\ell^{(b)}$-by-$\ell^{(b)}$ unit matrix*

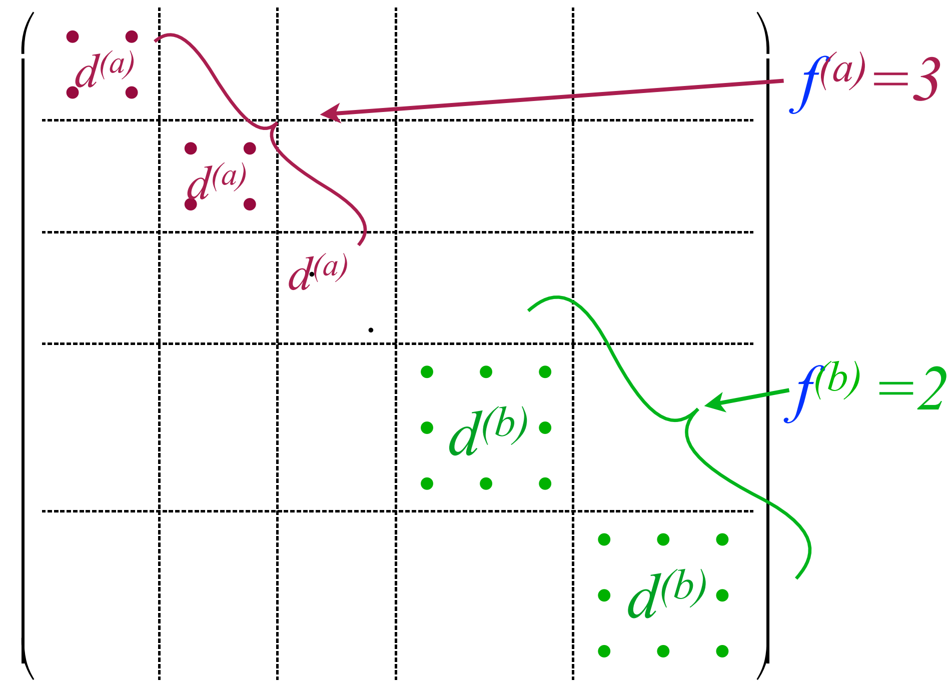
Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

(irep ≡ irreducible representation)

Symmetry reduction of G to H⊂G involves splitting of G-ireps $D^{(\alpha)}(G)$ into smaller H-ireps $d^{(a)}(H)$

$$D^{(\alpha)}(G)\downarrow H \equiv D^{(\alpha)}(H) \text{ is reducible to: } T_{reducer}\, D^{(\alpha)}(H) T^{\dagger}_{reducer} = f^{(a)} d^{(a)}(H) \oplus f^{(b)} d^{(b)}(H) \oplus \ldots$$

$$T_{reducer} D^{(\alpha)}(h) T^{\dagger}_{reducer} =$$



The following derives formulae for integral H⊂G correlation coefficients $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

$$Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = f^{(b)} \cdot \ell^{(b)}$$ *Since each $d^{(b)}(\mathbf{P}^{(b)})$ is an $\ell^{(b)}$-by-$\ell^{(b)}$ unit matrix*

$$f^{(b)} = \frac{1}{\ell^{(b)}} Trace D^{(\alpha)}(\mathbf{P}^{(b)})$$

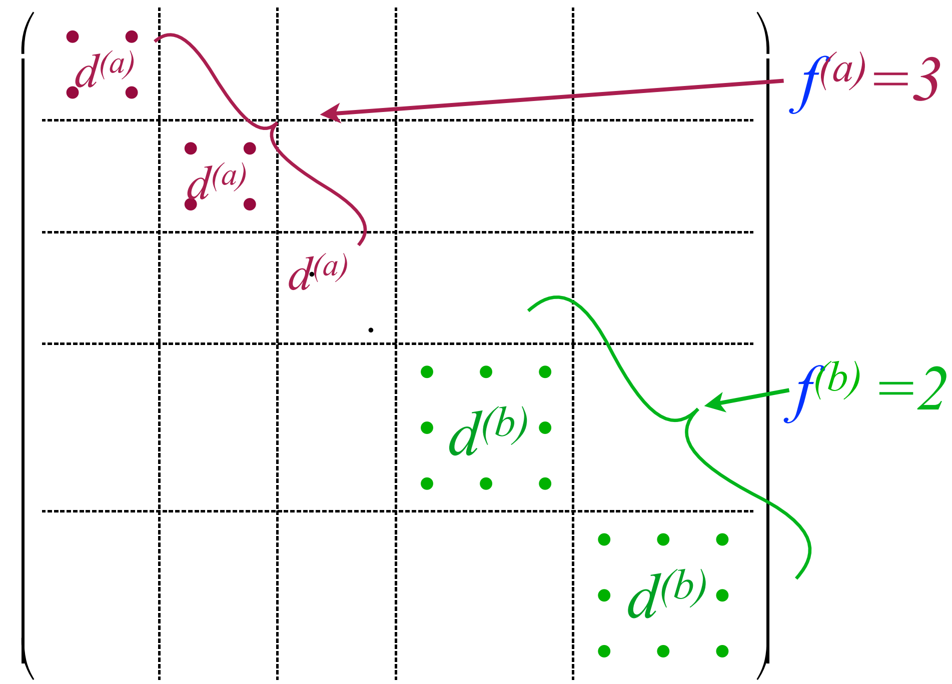
Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

(irep ≡ irreducible representation)

Symmetry reduction of G to H⊂G involves splitting of G-ireps $D^{(\alpha)}(G)$ *into smaller H-ireps* $d^{(a)}(H)$

$$D^{(\alpha)}(G)\downarrow H \equiv D^{(\alpha)}(H) \text{ is reducible to: } T_{reducer}\, D^{(\alpha)}(H) T^{\dagger}_{reducer} = f^{(a)} d^{(a)}(H) \oplus f^{(b)} d^{(b)}(H) \oplus \ldots$$

$$T_{reducer} D^{(\alpha)}(h) T^{\dagger}_{reducer} =$$



The following derives formulae for integral H⊂G correlation coefficients $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Class ortho-complete projector relations (p.24)

$$\mathbf{P}^{(\alpha)} = \frac{\ell^{(\alpha)}}{{}^\circ G} \sum_{k \in G} \chi_k^{(\alpha)*} \boldsymbol{\kappa}_k$$

$$\mathbf{P}^{(b)} = \frac{\ell^{(b)}}{{}^\circ H} \sum_{k \in H} \chi_k^{(b)*} \boldsymbol{\kappa}_k$$

$$Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = f^{(b)} \cdot \ell^{(b)}$$ *Since each* $d^{(b)}(\mathbf{P}^{(b)})$ *is an* $\ell^{(b)}$*-by-*$\ell^{(b)}$ *unit matrix*

$$f^{(b)} = \frac{1}{\ell^{(b)}} Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = \frac{1}{\ell^{(b)}} \frac{\ell^{(b)}}{{}^\circ H} \sum_{\substack{classes \\ \boldsymbol{\kappa}_k \in H}} \chi_k^{(b)*} Trace D^{(\alpha)}(\boldsymbol{\kappa}_k)$$

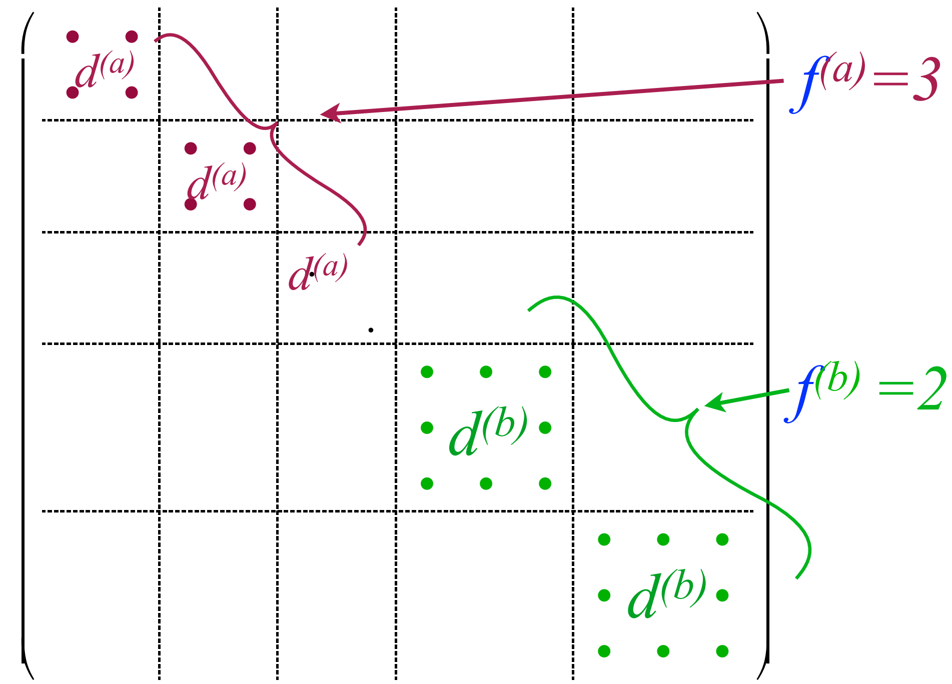
Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

($irep \equiv$ *irreducible representation*)

Symmetry reduction of G to $H\subset G$ involves splitting of G-ireps $D^{(\alpha)}(G)$ into smaller H-ireps $d^{(a)}(H)$

$$D^{(\alpha)}(G)\downarrow H \equiv D^{(\alpha)}(H) \text{ is reducible to: } T_{reducer}\, D^{(\alpha)}(H) T^{\dagger}_{reducer} = f^{(a)} d^{(a)}(H) \oplus f^{(b)} d^{(b)}(H) \oplus \ldots$$

$$T_{reducer} D^{(\alpha)}(h) T^{\dagger}_{reducer} =$$



The following derives formulae for integral $H\subset G$ correlation coefficients $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

$$Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = f^{(b)} \cdot \ell^{(b)}$$ *Since each $d^{(b)}(\mathbf{P}^{(b)})$ is an $\ell^{(b)}$-by-$\ell^{(b)}$ unit matrix*

Class ortho-complete projector relations (p.24)

$$\boxed{\begin{aligned} \mathbf{P}^{(\alpha)} &= \frac{\ell^{(\alpha)}}{{}^\circ G} \sum_{k\in G} \chi_k^{(\alpha)*} \boldsymbol{\kappa}_k \\ \mathbf{P}^{(b)} &= \frac{\ell^{(b)}}{{}^\circ H} \sum_{k\in H} \chi_k^{(b)*} \boldsymbol{\kappa}_k \end{aligned}}$$

$$f^{(b)} = \frac{1}{\ell^{(b)}} Trace D^{(\alpha)}(\mathbf{P}^{(b)}) = \frac{1}{\ell^{(b)}} \frac{\ell^{(b)}}{{}^\circ H} \sum_{\substack{classes \\ \boldsymbol{\kappa}_k \in H}} \chi_k^{(b)*} \underbrace{Trace D^{(\alpha)}(\boldsymbol{\kappa}_k)}_{\chi^{(\alpha)}(\boldsymbol{\kappa}_k) = {}^\circ\kappa_k \chi_k^{(\alpha)}}$$

$$\boxed{f^{(b)} = \frac{1}{{}^\circ H} \sum_{\substack{classes \\ \boldsymbol{\kappa}_k \in H}} {}^\circ\kappa_k \chi_k^{(b)*} \chi_k^{(\alpha)}}$$

Character relation for frequency $f^{(b)}$ of $d^{(b)}$ of subgroup H in $D^{(\alpha)}\downarrow H$ of G

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

*Spectral resolution to **irreducible representations** (or "**irreps**") foretold by **characters** or <u>traces</u>*

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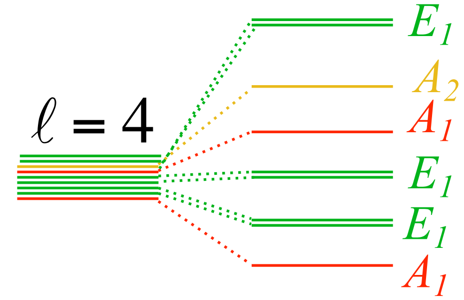
Atomic ℓ-level or 2ℓ+1-multiplet splitting

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



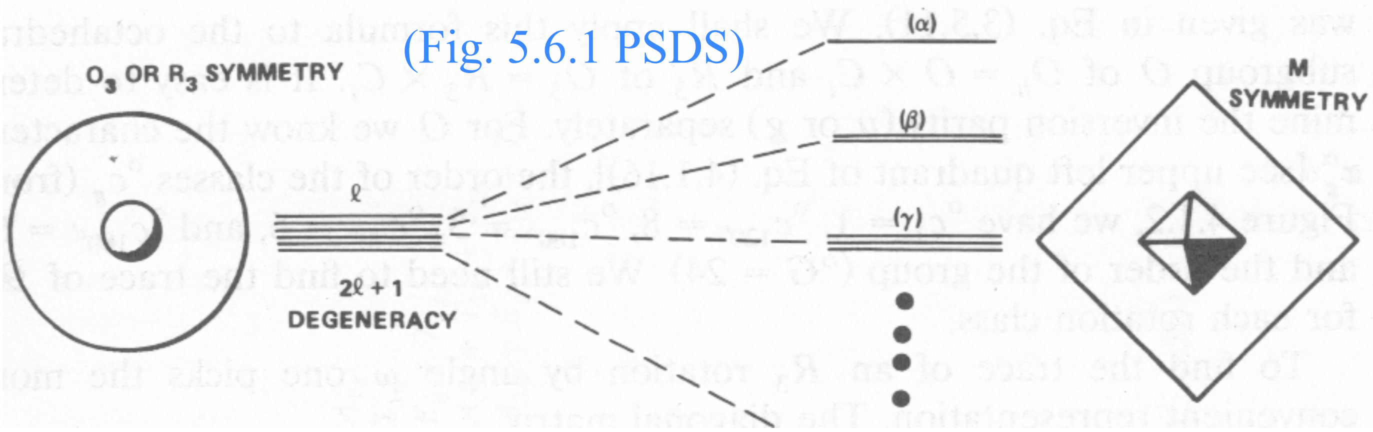
ℓ=0, s-singlet

2ℓ+1=1

ℓ=1, p-triplet

2ℓ+1=3

Crystal-field splitting: O(3)⊃D₃ symmetry reduction



(Fig. 5.6.1 PSDS)

Atomic ℓ-level or $2\ell+1$-multiplet splitting

Formula from p.44

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{\text{classes} \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \, \chi_k^{(b)*} \chi_k^{(\ell)}$$

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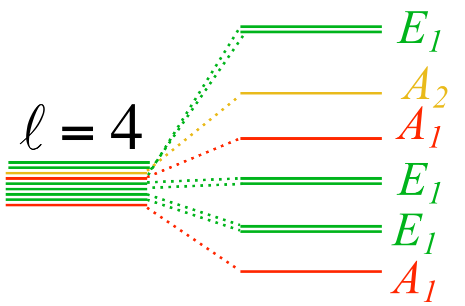

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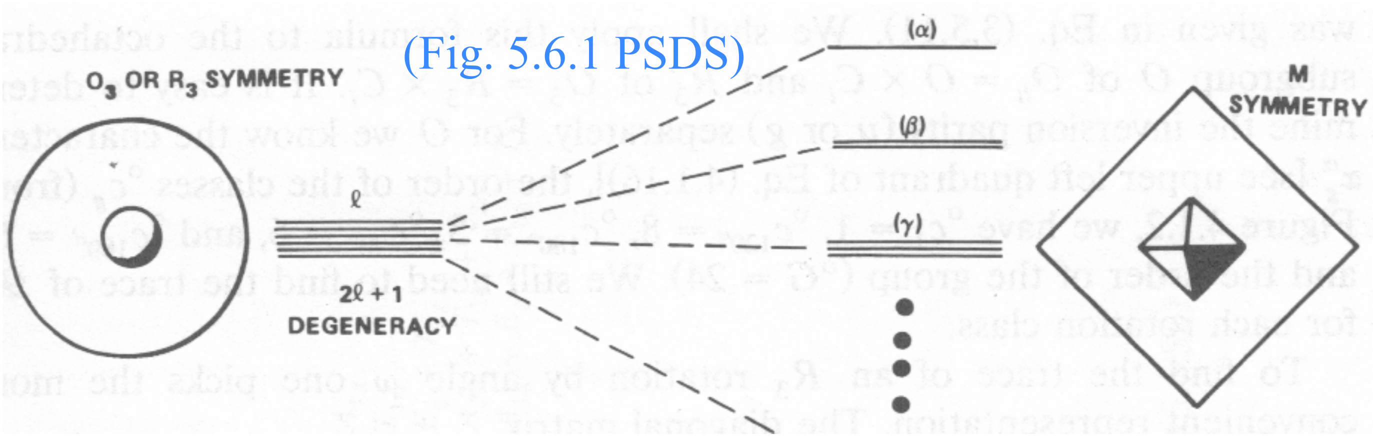
Crystal-field splitting: $O(3)\supset D_3$ symmetry reduction



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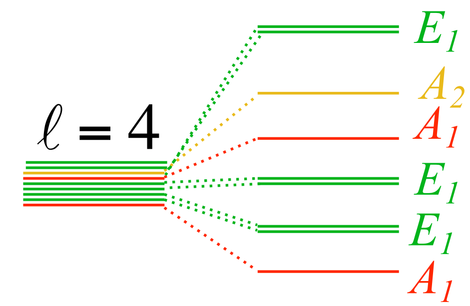

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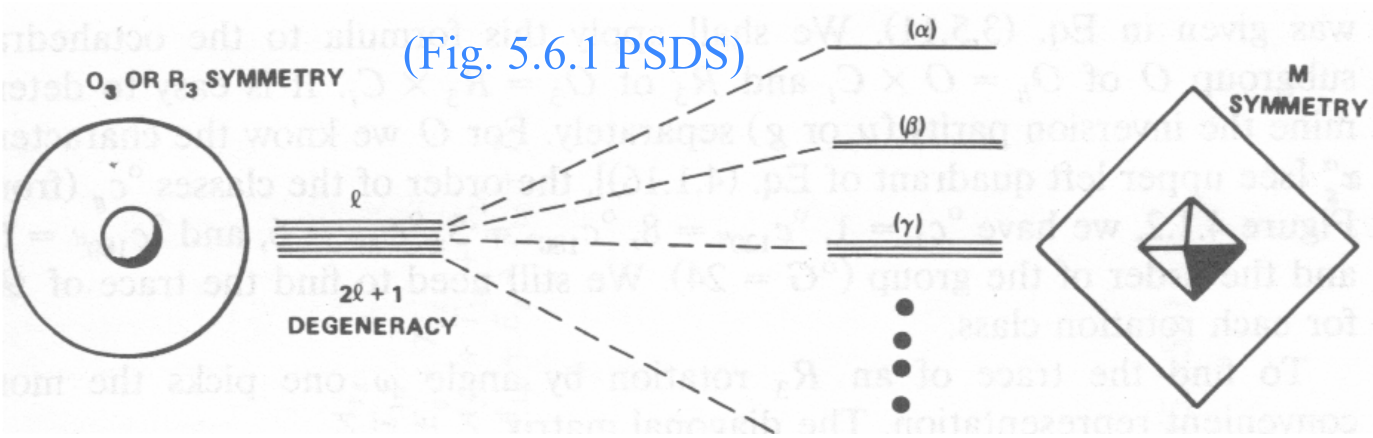

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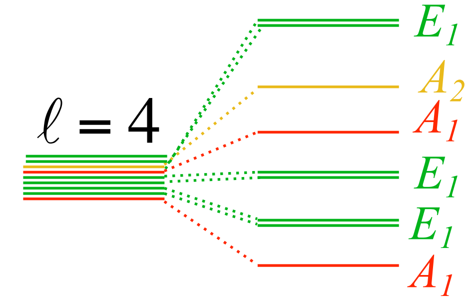
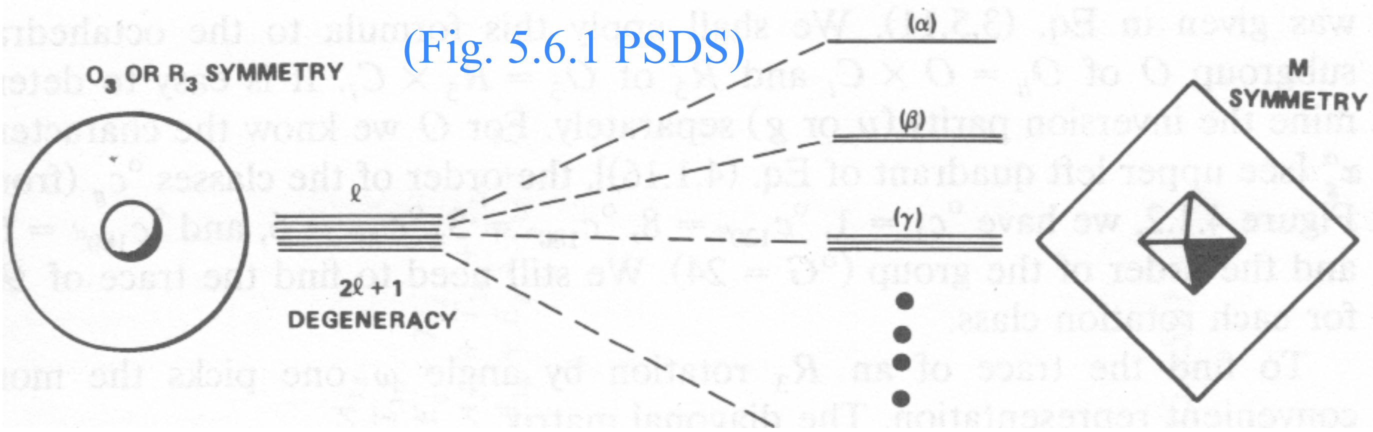


Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction

(Fig. 5.6.1 PSDS)



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Atomic ℓ-level or $2\ell+1$-multiplet splitting

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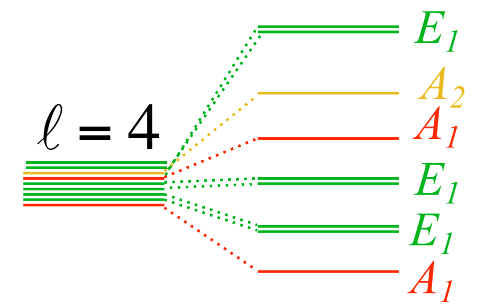
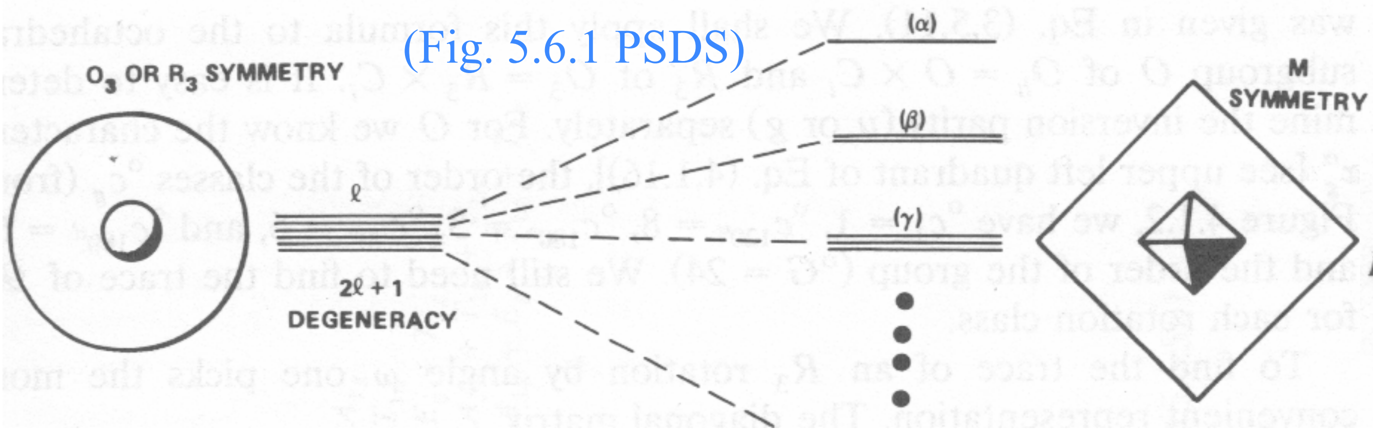
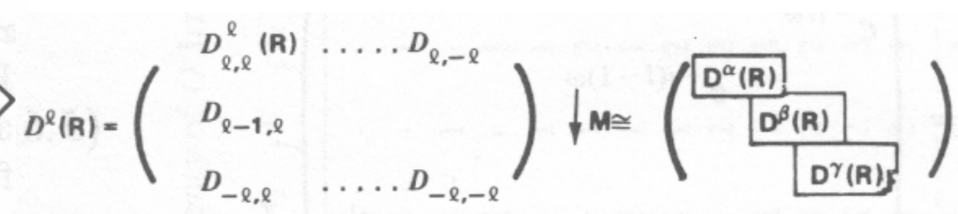


Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^{\ell} \downarrow D_3$ splitting

(Fig. 5.6.1 PSDS)





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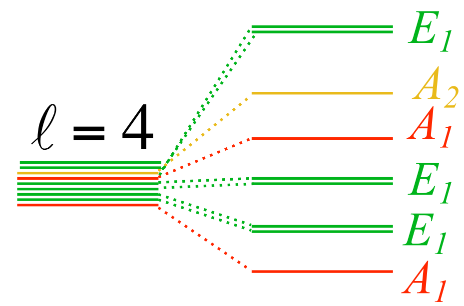

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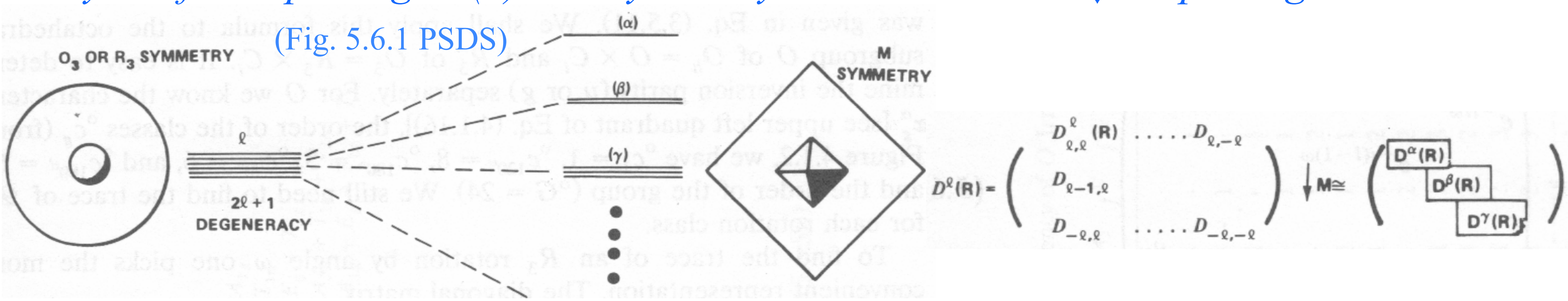
Crystal-field splitting: O(3)⊃D₃ symmetry reduction and $D^{\ell}\downarrow D_3$ splitting

(Fig. 5.6.1 PSDS)



U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$$\chi^{\ell}\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

R(3) character
where: 2ℓ+1
is ℓ-orbital dimension

Atomic ℓ-level or 2ℓ+1-multiplet splitting

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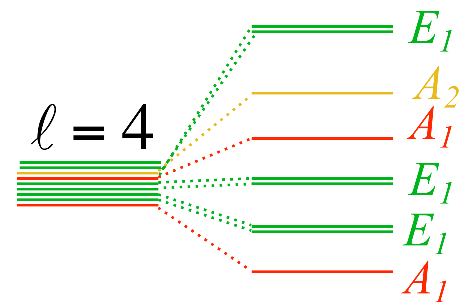

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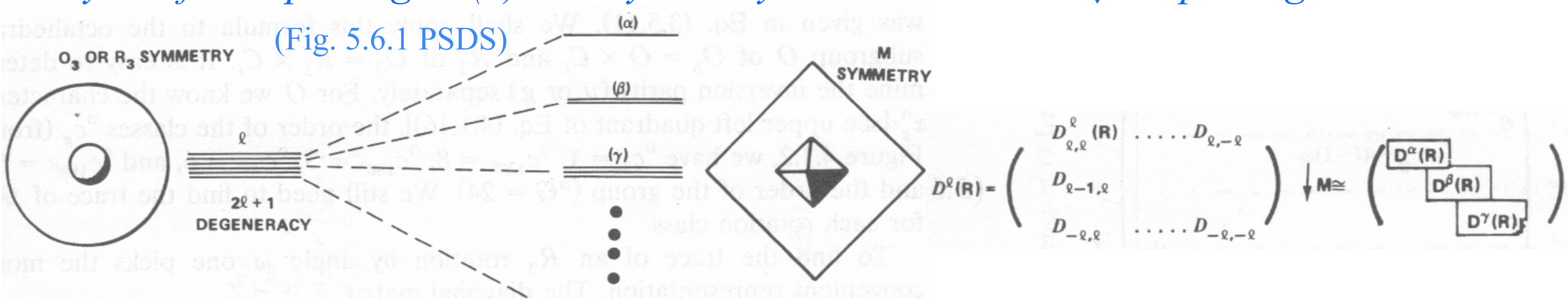
Crystal-field splitting: O(3)⊃D3 symmetry reduction and $D^{\ell}\downarrow D_3$ splitting



(Fig. 5.6.1 PSDS)

U(2) characters
from Lecture 14.5 p.93:
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$\chi^{\ell}(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

R(3) character
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is ℓ-orbital dimension

Atomic ℓ-level or $2\ell+1$-multiplet splitting
Formula from p.44

Example: (ℓ=4)

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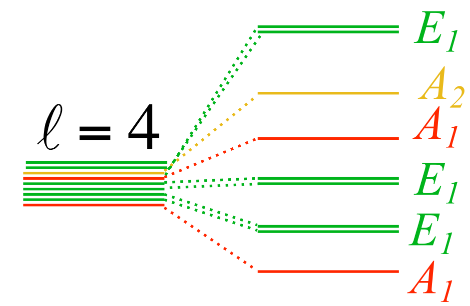

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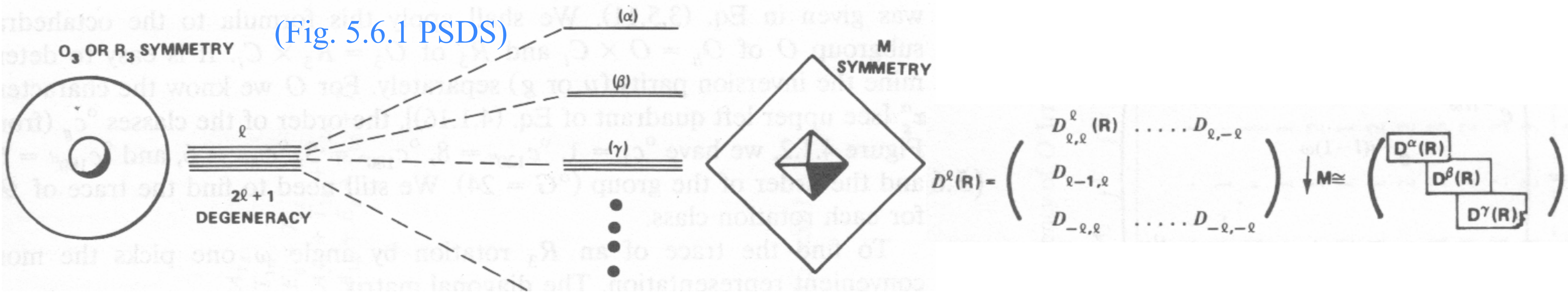
Crystal-field splitting: $O(3)\supset D_3$ symmetry reduction and $D^{\ell}\downarrow D_3$ splitting

(Fig. 5.6.1 PSDS)



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R(3) character where: $2\ell+1$ is ℓ-orbital dimension

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5	11	−1	−1
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...and *D₃* character table from p. 24:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

*Review:Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

*Spectral resolution to **irreducible representations** (or "**irreps**") foretold by **characters** or traces*

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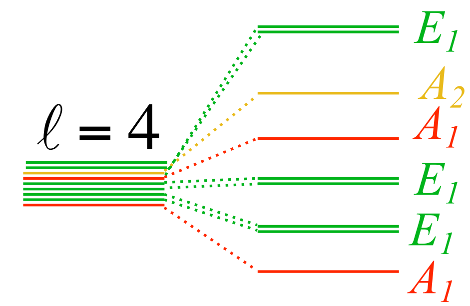

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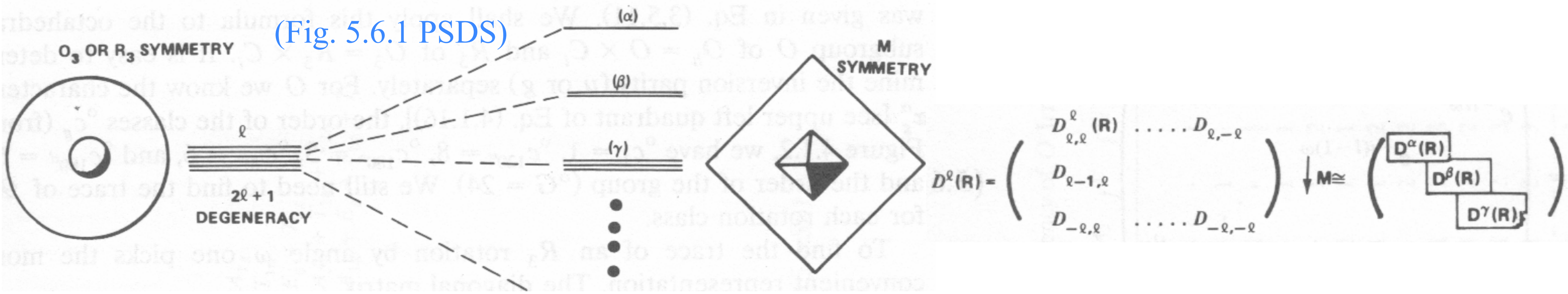
Crystal-field splitting: $O(3)\supset D_3$ symmetry reduction and $D^{\ell}\downarrow D_3$ splitting

(Fig. 5.6.1 PSDS)



U(2) characters
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R(3) character
where: $2\ell+1$
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$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell=0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$

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Example: (ℓ=4)

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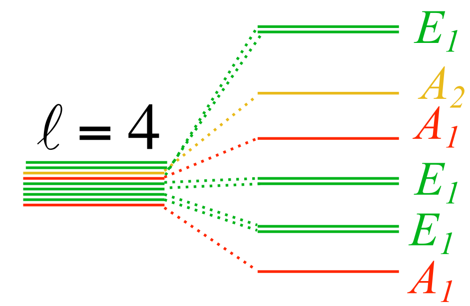

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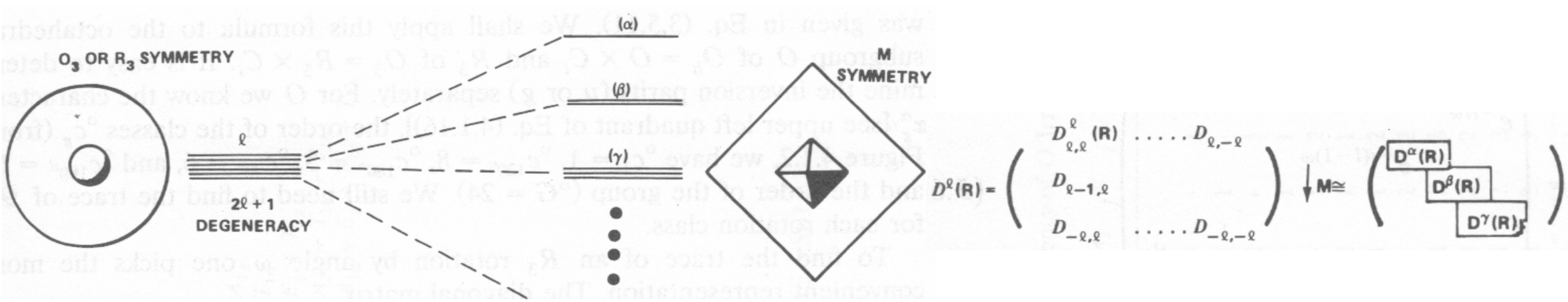

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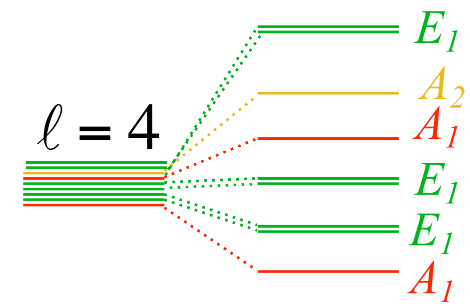

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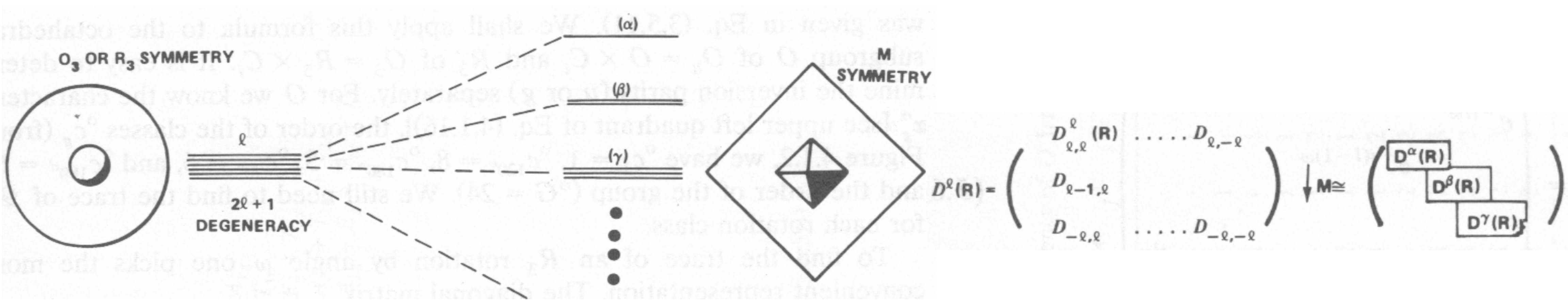

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2	1	·	2	$1A_1 \quad \oplus 2E_1$

...and D_3 character table from p. 24:

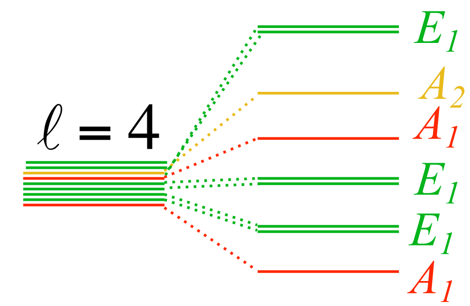
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

Atomic ℓ-level or $2\ell+1$-multiplet splitting

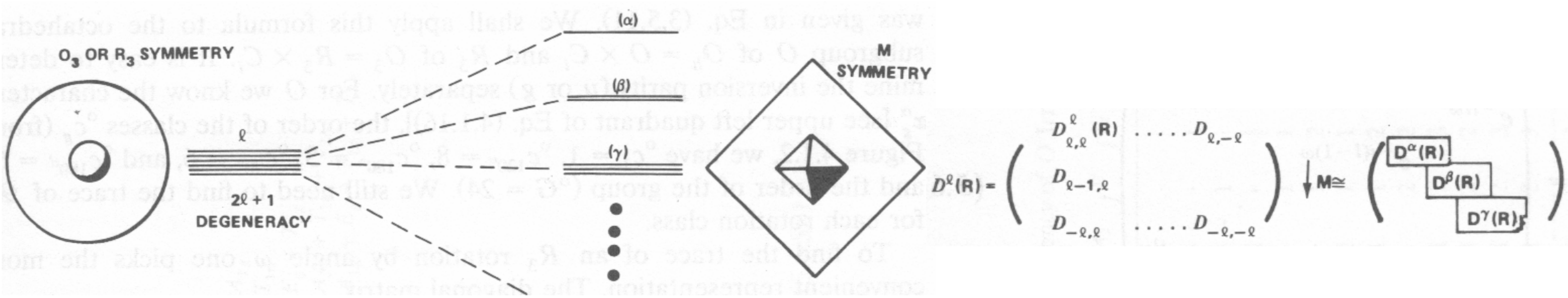
Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=0, s-singlet
$2\ell+1$=1
ℓ=1, p-triplet
$2\ell+1$=3
ℓ=2, d-quintet
$2\ell+1$=5
ℓ=3, f-septet
$2\ell+1$=7
ℓ=4, g-nonet
$2\ell+1$=9
ℓ=5, h-(11)-let
$2\ell+1$=11
...



U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta=0$	$\frac{2\pi}{3}$	π
$\ell=0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

R(3) character
where: $2\ell+1$
is ℓ-orbital dimension

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell=0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$

...and D_3 character table from p. 24:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

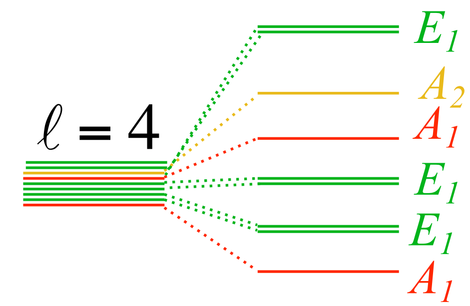
	5	−1	1
$1\chi^{A_1}(\mathbf{g}) =$	1	1	1
$0\chi^{A_2}(\mathbf{g}) =$	0	0	0
$2\chi^{E_1}(\mathbf{g}) =$	4	−2	0

Atomic ℓ-level or 2ℓ+1-multiplet splitting

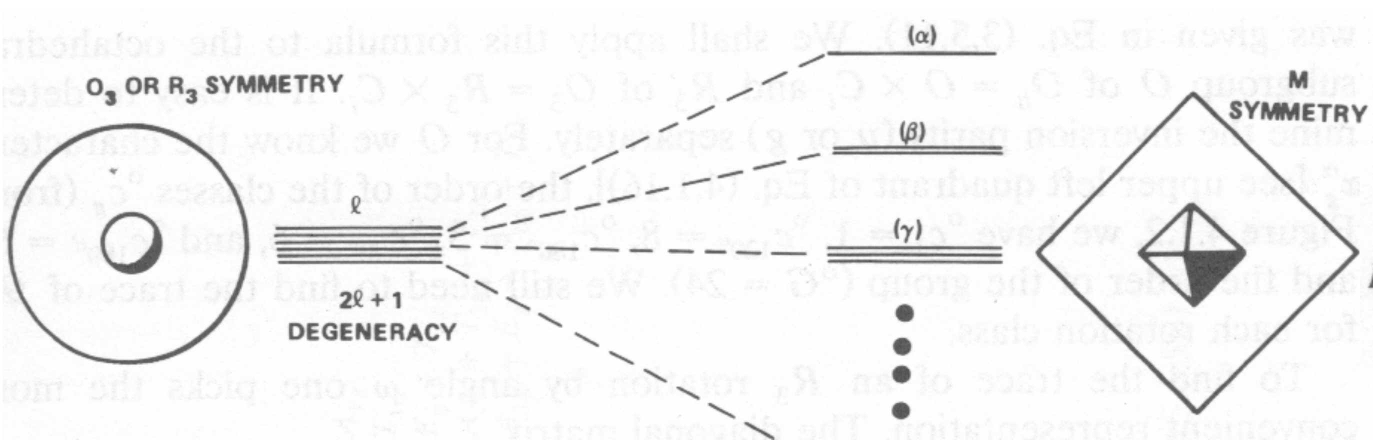
Formula from p.44

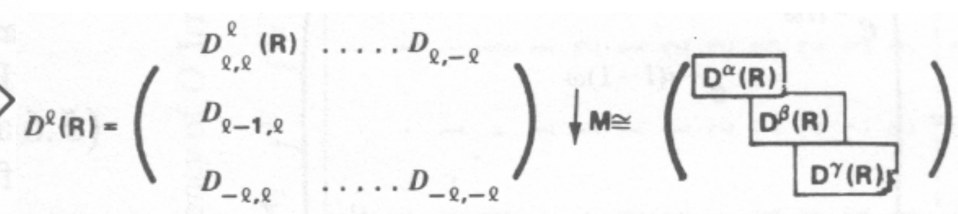
Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=0, s-singlet
2ℓ+1=1
ℓ=1, p-triplet
2ℓ+1=3
ℓ=2, d-quintet
2ℓ+1=5
ℓ=3, f-septet
2ℓ+1=7
ℓ=4, g-nonet
2ℓ+1=9
ℓ=5, h-(11)-let
2ℓ+1=11
...





U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

R(3) character
where: 2ℓ+1
is ℓ-orbital dimension

...and *D₃* character table from p. 24:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

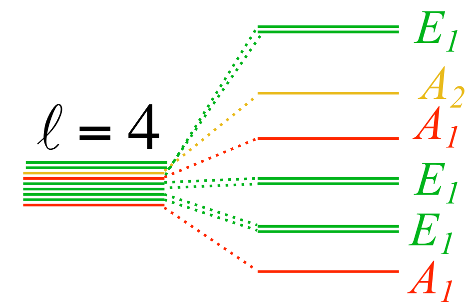
$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

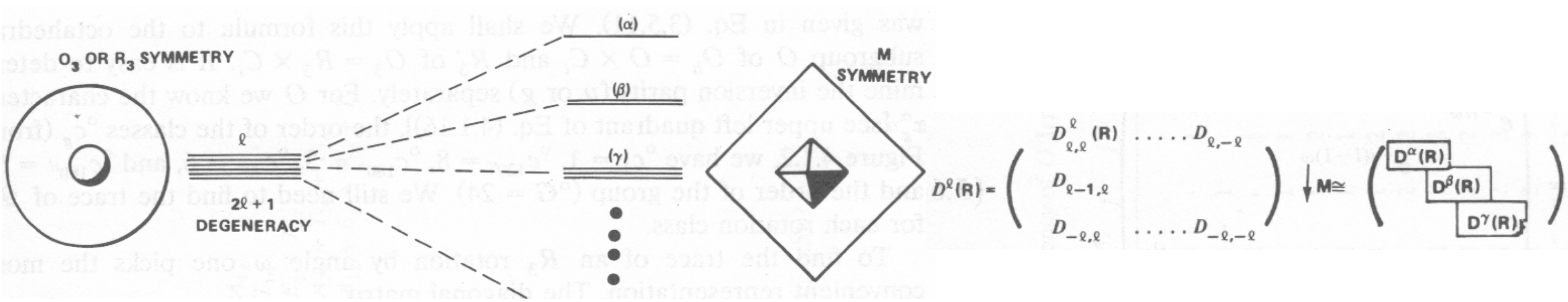
Formula from p.44

Example: ($\ell=4$)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



$\ell=0$, s-singlet
$2\ell+1=1$
$\ell=1$, p-triplet
$2\ell+1=3$
$\ell=2$, d-quintet
$2\ell+1=5$
$\ell=3$, f-septet
$2\ell+1=7$
$\ell=4$, g-nonet
$2\ell+1=9$
$\ell=5$, h-(11)-let
$2\ell+1=11$
...



U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

R(3) character
where: $2\ell+1$
is ℓ-orbital dimension

...and *D_3* character table from p. 24:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

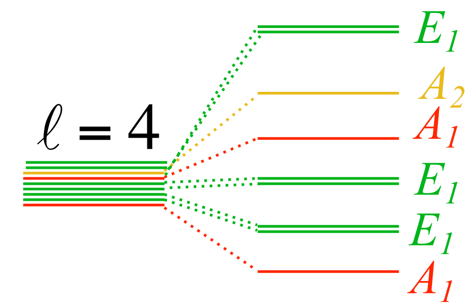
$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$

	7	1	−1
$1\chi^{A_1}(\mathbf{g}) =$	1	1	1
$2\chi^{A_2}(\mathbf{g}) =$	2	2	−2
$2\chi^{E_1}(\mathbf{g}) =$	4	−2	0

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=4, g-nonet
2ℓ+1=9

$$f^{(E_1)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(E_1)*} \chi_k^{(\ell=4)} = \frac{1}{{}^{\circ}D_3}\left({}^{\circ}\kappa_{0^\circ} \chi_{0^\circ}^{(E_1)*} \chi_{0^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{120^\circ} \chi_{120^\circ}^{(E_1)*} \chi_{120^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{180^\circ} \chi_{180^\circ}^{(E_1)*} \chi_{180^\circ}^{(\ell=4)} \right)$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and D_3 character table from p. 24:

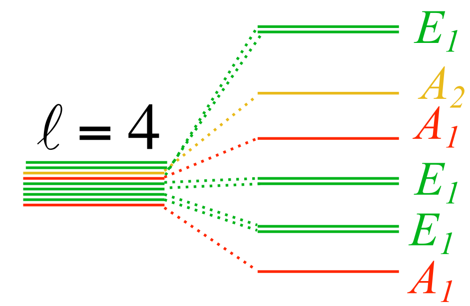
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	

Formula from p.44

Example: (ℓ=4)

$$f^{(b)}=\frac{1}{{}^{\circ}D_3}\sum_{\substack{classes\\ \kappa_k\in D_3}}{}^{\circ}\kappa_k\,\chi_k^{(b)*}\chi_k^{(\ell)}$$



ℓ=4, g-nonet
$2\ell+1=9$

$$f^{(E_1)}=\frac{1}{{}^{\circ}D_3}\sum_{\substack{classes\\ \kappa_k\in D_3}}{}^{\circ}\kappa_k\,\chi_k^{(E_1)*}\chi_k^{(\ell=4)}=\frac{1}{{}^{\circ}D_3}\left({}^{\circ}\kappa_{0^\circ}\chi_{0^\circ}^{(E_1)*}\chi_{0^\circ}^{(\ell=4)}+{}^{\circ}\kappa_{120^\circ}\chi_{120^\circ}^{(E_1)*}\chi_{120^\circ}^{(\ell=4)}+{}^{\circ}\kappa_{180^\circ}\chi_{180^\circ}^{(E_1)*}\chi_{180^\circ}^{(\ell=4)}\right)$$

$$=\frac{1}{6}\left(1\cdot 2^*\cdot 9\quad+\quad 2\cdot -1^*\cdot 0\quad+\quad 3\cdot 0^*\cdot 1\right)$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta=0$	$\frac{2\pi}{3}$	π
$\ell=0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}(\Theta)=\frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and *D₃* character table from p. 24:

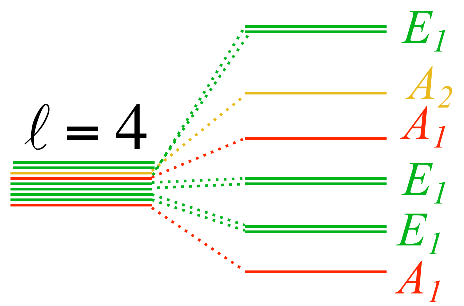
$(\mathbf{g})=$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g})=$	1	1	1
$\chi^{A_2}(\mathbf{g})=$	1	1	−1
$\chi^{E_1}(\mathbf{g})=$	2	−1	0

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell=0$	1	·	·	$1A_1$
1	·	1	1	$0A_1\oplus A_2\oplus E_1$
2	1	·	2	$1A_1\quad\oplus 2E_1$
3	1	2	2	$1A_1\oplus 2A_2\oplus 2E_1$
4	1	2	3	

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=4, g-nonet
2ℓ+1=9

$$f^{(E_1)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes \\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(E_1)*} \chi_k^{(\ell=4)} = \frac{1}{{}^{\circ}D_3}\left({}^{\circ}\kappa_{0^\circ} \chi_{0^\circ}^{(E_1)*} \chi_{0^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{120^\circ} \chi_{120^\circ}^{(E_1)*} \chi_{120^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{180^\circ} \chi_{180^\circ}^{(E_1)*} \chi_{180^\circ}^{(\ell=4)} \right)$$

$$= \frac{1}{6}\left(1 \cdot 2^* \cdot 9 \quad + \quad 2 \cdot -1^* \cdot 0 \quad + \quad 3 \cdot 0^* \cdot 1 \right)$$

$$f^{(E_1)} = 3$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^{\ell}(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^{\ell}(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and *D*₃ character table from p. 24:

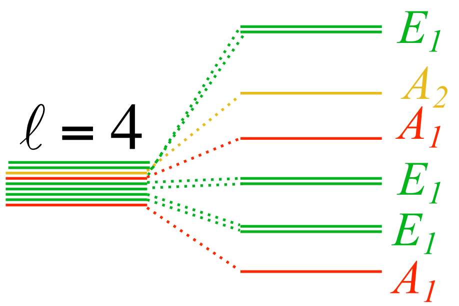
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	2	1	3	$\oplus 3E_1$

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{\text{classes}\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=4, g-nonet
2ℓ+1=9

$$f^{(E_1)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{\text{classes}\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(E_1)*} \chi_k^{(\ell=4)} = \frac{1}{{}^{\circ}D_3}\left({}^{\circ}\kappa_{0^\circ} \chi_{0^\circ}^{(E_1)*} \chi_{0^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{120^\circ} \chi_{120^\circ}^{(E_1)*} \chi_{120^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{180^\circ} \chi_{180^\circ}^{(E_1)*} \chi_{180^\circ}^{(\ell=4)} \right)$$

$$= \frac{1}{6}\left(1 \cdot 2^* \cdot 9 \quad + \quad 2 \cdot -1^* \cdot 0 \quad + \quad 3 \cdot 0^* \cdot 1 \right)$$

$$f^{(E_1)} = 3$$

$$f^{(A_2)} = \frac{1}{6}\left(1 \cdot 1^* \cdot 9 \quad + \quad 2 \cdot 1^* \cdot 0 \quad + \quad 3 \cdot -1^* \cdot 1 \right) = 1$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^\ell(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and D_3 character table from p. 24:

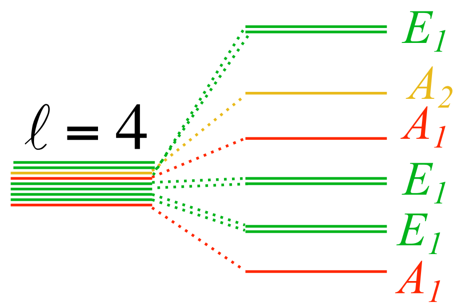
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	2	1	3	$\oplus 1A_2 \oplus 3E_1$

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^\circ D_3}\sum_{\substack{classes\\ \kappa_k \in D_3}} {}^\circ\kappa_k \chi_k^{(b)*}\chi_k^{(\ell)}$$



ℓ=4, g-nonet
2ℓ+1=9

$$f^{(E_1)} = \frac{1}{{}^\circ D_3}\sum_{\substack{classes\\ \kappa_k \in D_3}} {}^\circ\kappa_k \chi_k^{(E_1)*}\chi_k^{(\ell=4)} = \frac{1}{{}^\circ D_3}\left({}^\circ\kappa_{0^\circ}\chi_{0^\circ}^{(E_1)*}\chi_{0^\circ}^{(\ell=4)} + {}^\circ\kappa_{120^\circ}\chi_{120^\circ}^{(E_1)*}\chi_{120^\circ}^{(\ell=4)} + {}^\circ\kappa_{180^\circ}\chi_{180^\circ}^{(E_1)*}\chi_{180^\circ}^{(\ell=4)}\right)$$

$$= \frac{1}{6}\left(1\cdot 2^*\cdot 9 \quad + \quad 2\cdot -1^*\cdot 0 \quad + \quad 3\cdot 0^*\cdot 1\right)$$

$$f^{(E_1)} = 3$$

$$f^{(A_2)} = \frac{1}{6}\left(1\cdot 1^*\cdot 9 \quad + \quad 2\cdot 1^*\cdot 0 \quad + \quad 3\cdot -1^*\cdot 1\right) = 1$$

$$f^{(A_1)} = \frac{1}{6}\left(1\cdot 1^*\cdot 9 \quad + \quad 2\cdot 1^*\cdot 0 \quad + \quad 3\cdot 1^*\cdot 1\right) = 2$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^\ell(\Theta) = \frac{\sin(\ell+\frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1\oplus A_2\oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1\oplus 2A_2\oplus 2E_1$
4	2	1	3	$2A_1\oplus 1A_2\oplus 3E_1$

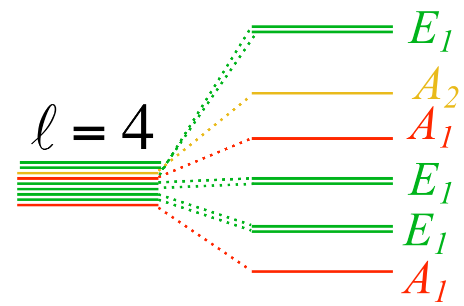
...and *D₃* character table from p. 24:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

Formula from p.44

Example: (ℓ=4)

$$f^{(b)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(b)*} \chi_k^{(\ell)}$$



ℓ=4, g-nonet
$2\ell+1=9$

$$f^{(E_1)} = \frac{1}{{}^{\circ}D_3} \sum_{\substack{classes\\ \kappa_k \in D_3}} {}^{\circ}\kappa_k \chi_k^{(E_1)*} \chi_k^{(\ell=4)} = \frac{1}{{}^{\circ}D_3}\left({}^{\circ}\kappa_{0^\circ}\chi_{0^\circ}^{(E_1)*}\chi_{0^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{120^\circ}\chi_{120^\circ}^{(E_1)*}\chi_{120^\circ}^{(\ell=4)} + {}^{\circ}\kappa_{180^\circ}\chi_{180^\circ}^{(E_1)*}\chi_{180^\circ}^{(\ell=4)} \right)$$

$$= \frac{1}{6}\left(1\cdot 2^* \cdot 9 \quad + \quad 2\cdot -1^* \cdot 0 \quad + \quad 3 \cdot 0^* \cdot 1 \right)$$

$$f^{(E_1)} = 3$$

$$f^{(A_2)} = \frac{1}{6}\left(1\cdot 1^* \cdot 9 \quad + \quad 2\cdot 1^* \cdot 0 \quad + \quad 3 \cdot -1^* \cdot 1 \right) = 1$$

$$f^{(A_1)} = \frac{1}{6}\left(1\cdot 1^* \cdot 9 \quad + \quad 2\cdot 1^* \cdot 0 \quad + \quad 3 \cdot 1^* \cdot 1 \right) = 2$$

U(2) characters
from Lecture 14.5 p.93:
(or end of this lecture)

$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$\ell = 0$	1	1	1
1	3	0	−1
2	5	−1	1
3	7	1	−1
4	9	0	1
5	11	−1	−1
6	13	1	1
7	15	0	−1

$$\chi^\ell(\Theta) = \frac{\sin(\ell + \frac{1}{2})\Theta}{\sin\frac{\Theta}{2}}$$

...and D_3 character table from p. 24:

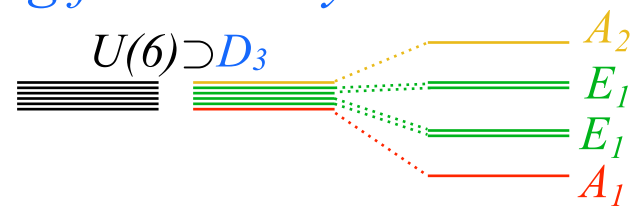
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1,\mathbf{r}^2\}$	$\{\mathbf{i}_1,\mathbf{i}_2,\mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	−1
$\chi^{E_1}(\mathbf{g}) =$	2	−1	0

$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	2	1	3	$2A_1 \oplus 1A_2 \oplus 3E_1$
5	1	2	4	$1A_1 \oplus 2A_2 \oplus 4E_1$
6	3	2	4	$3A_1 \oplus 2A_2 \oplus 4E_1$
7	2	3	5	$2A_1 \oplus 3A_2 \oplus 5E_1$

$$Note: \quad \ell=6 \left| 13 \quad 1 \quad 1 \right| = A_1 \left| 1 \quad 1 \quad 1 \right| \oplus 2R^G \left| 12 \quad 0 \quad 0 \right| = A_1 \oplus 2[A_1 \oplus A_2 \oplus 2E_1]$$

(ℓ=6 is 1st re-cycling point)

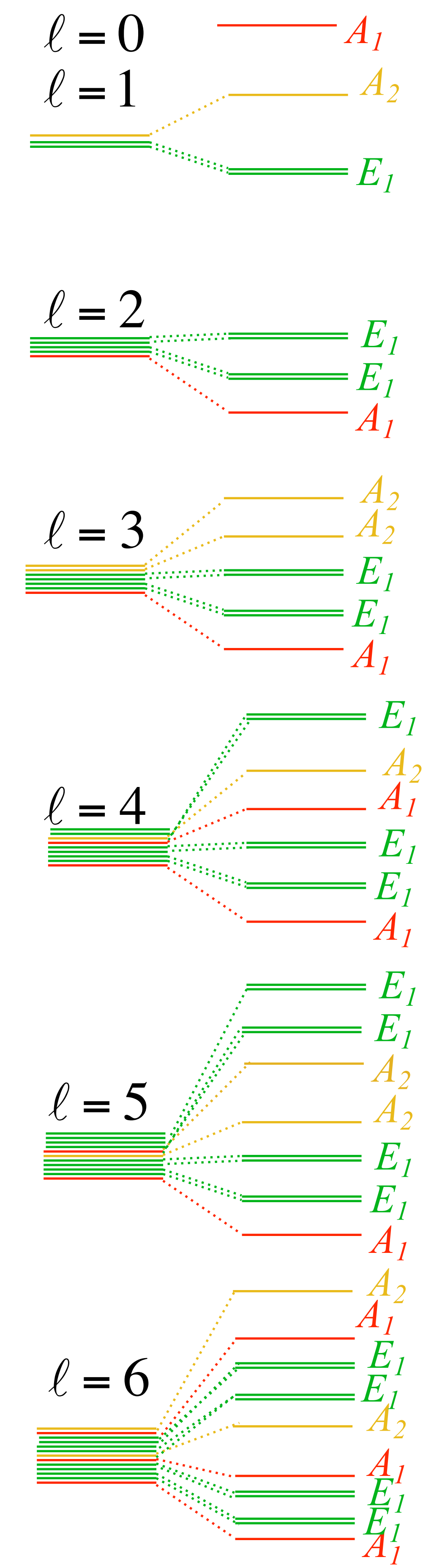
Spectral splitting in symmetry breaking foretold by character analysis (on p. 38)



$R^G(U(6))\downarrow D_3 = D^{A_1}(\mathbf{g}) \oplus D^{A_2}(\mathbf{g}) \oplus 2D^{E_1}(\mathbf{g})$

Crystal-field splitting: O(3)⊃D₃ symmetry reduction and $D^\ell\downarrow D_3$ splitting

R(3)⊃D3



$f^{(\alpha)}(\ell)$	f^{A_1}	f^{A_2}	f^{E_1}	
$\ell = 0$	1	·	·	$1A_1$
1	·	1	1	$0A_1 \oplus A_2 \oplus E_1$
2	1	·	2	$1A_1 \quad \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	2	1	3	$2A_1 \oplus 1A_2 \oplus 3E_1$
5	1	2	4	$1A_1 \oplus 2A_2 \oplus 4E_1$
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7	2	3	5	$2A_1 \oplus 3A_2 \oplus 5E_1$

D_3 character table:

$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

*Spectral resolution to **irreducible representations** (or "**irreps**") foretold by **characters** or traces*

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for ℓ=1-6

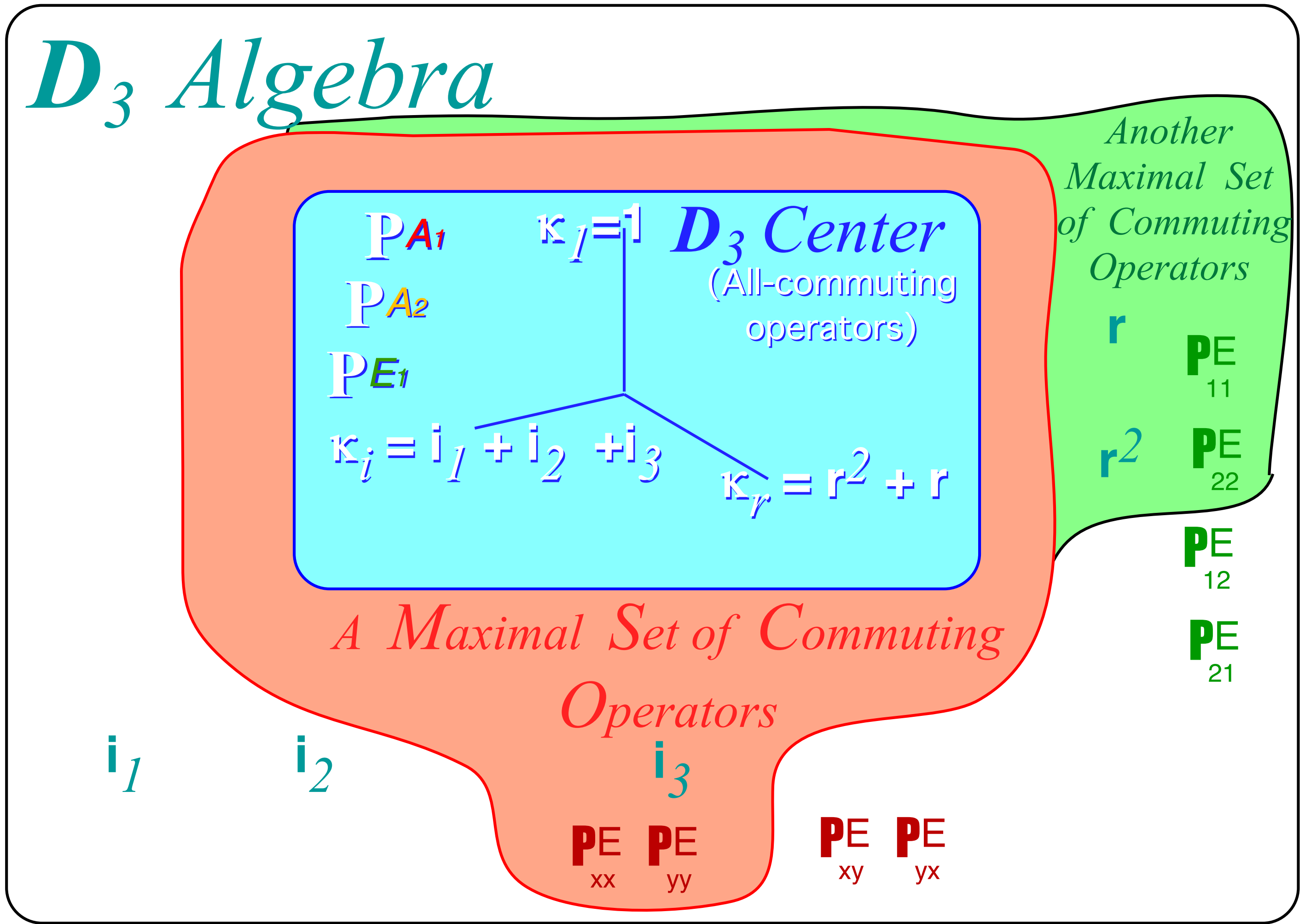
Group invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$

*3rd-stage spectral resolution to **irreducible representations** (ireps) and Hamiltonian eigensolutions*

Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains



Important invariant numbers or "characters"

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

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

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

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

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

$$\kappa(D_3)=(1)^0+(1)^0+(2)^0=3$$
$$\rho(D_3)=(1)^1+(1)^1+(2)^1=4$$
$$^\circ(D_3)=(1)^2+(1)^2+(2)^2=6$$

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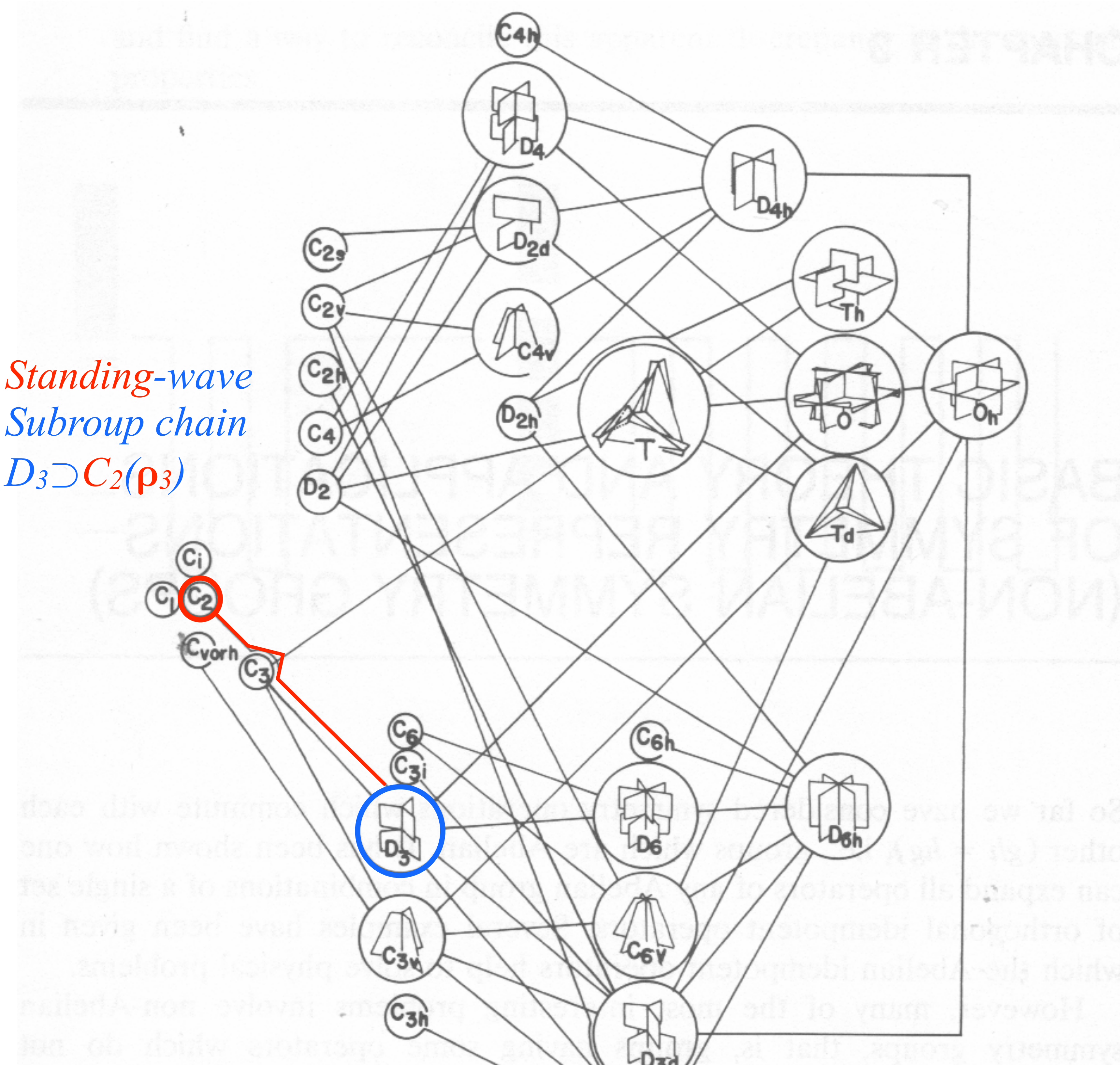
Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

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

Correlate D_3 characters with its subgoup(s) C_2(i)

Standing-wave
Subroup chain
$D_3 \supset C_2(\rho_3)$



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) $C_2(\mathbf{i})$

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

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

D_3 Example

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Correlate D_3 characters with its subgoup(s) $C_2(\mathbf{i})$

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

$D_3 \supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1 = p^{0_2} + p^{1_2}$ will make IRREDUCIBLE $\mathbf{P}^{(\alpha)}_{n,n}$

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

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

D_3 Example

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$n^{E}=$	1	1

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$$\mathbf{P}^{(\alpha)}1 = \mathbf{P}^{(\alpha)}(p^{0_2} + p^{1_2})$$
$$= \mathbf{P}^{(\alpha)}_{0_2 0_2} + \mathbf{P}^{(\alpha)}_{1_2 1_2}$$

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

D_3 Example

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$n^{A_2}=$	·	1
$n^{E}=$	1	1

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$$= \mathbf{P}^{(\alpha)}_{0_2 0_2} + \mathbf{P}^{(\alpha)}_{1_2 1_2}$$

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

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

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

D_3 Example

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$$\mathbf{P}^{(\alpha)}1 = \mathbf{P}^{(\alpha)}(p^{0_2} + p^{1_2})$$
$$= \mathbf{P}^{(\alpha)}_{0_2 0_2} + \mathbf{P}^{(\alpha)}_{1_2 1_2}$$

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

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

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

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

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

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

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

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2nd-Stage

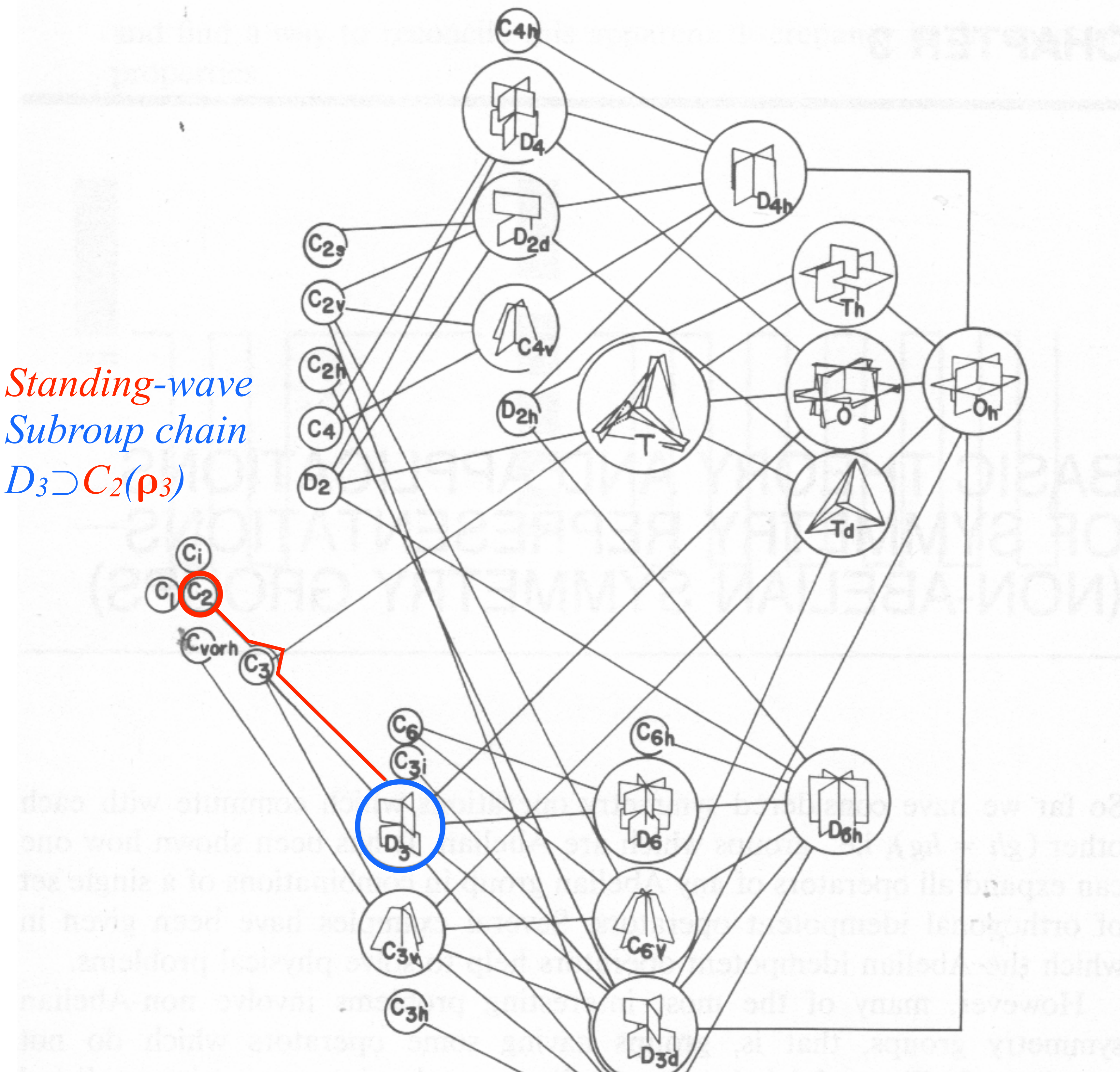
Spectral reduction of non-commutative "Group-table Hamiltonian"

D_3 Example

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

Correlate D_3 characters with its subgoup(s) C_2(i)

Standing-wave Subroup chain $D_3 \supset C_2(\rho_3)$



2nd-Stage

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

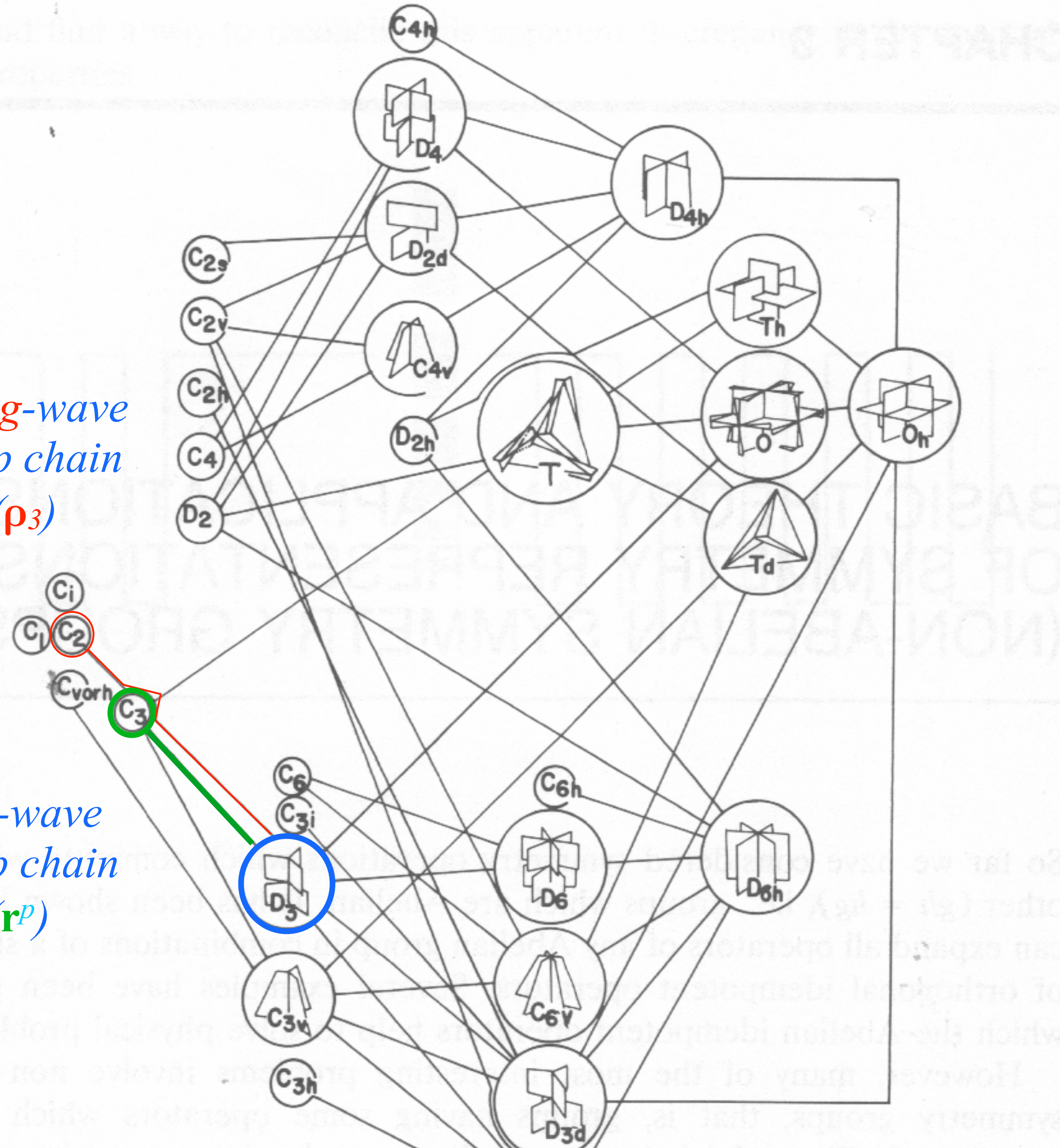
D_3 Example

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

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

Standing-wave Subroup chain $D_3 \supset C_2(\rho_3)$

Moving-wave Subroup chain $D_3 \supset C_3(\mathbf{r}^p)$



2nd-Stage

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)

$$\begin{array}{c|ccc|c} D_3\ \kappa= & \mathbf{1} & \mathbf{r}^1+\mathbf{r}^2 & \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3 & \\ \mathbf{P}^{A_1}= & 1 & 1 & 1 & /6 \\ \mathbf{P}^{A_2}= & 1 & 1 & -1 & /6 \\ \mathbf{P}^{E}= & 2 & -1 & 0 & /3 \end{array}$$

$$\begin{array}{c|cc|c} C_2\ \kappa= & \mathbf{1} & \mathbf{i}_3 & \\ p^{0_2}= & 1 & 1 & /2 \\ p^{1_2}= & 1 & -1 & /2 \end{array}$$

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

$$\begin{array}{c|ccc|c} C_3\ \kappa= & \mathbf{1} & \mathbf{r}^1 & \mathbf{r}^2 & \\ p^{0_3}= & 1 & 1 & 1 & /3 \\ p^{1_3}= & 1 & \varepsilon & \varepsilon^* & /3 \\ p^{2_3}= & 2 & \varepsilon^* & \varepsilon & /3 \end{array}$$

*$D_3\supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1=p^{0_2}+p^{1_2}$ will make **IRREDUCIBLE** $\mathbf{P}^{(\alpha)}_{n,n}$*

$$\begin{array}{c|cc} D_3\supset C_2 & 0_2 & 1_2 \\ n^{A_1}= & 1 & \cdot \\ n^{A_2}= & \cdot & 1 \\ n^{E}= & 1 & 1 \end{array}$$

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$$\mathbf{P}^{(\alpha)}1=\mathbf{P}^{(\alpha)}(p^{0_2}+p^{1_2})$$
$$=\mathbf{P}^{(\alpha)}_{0_20_2}+\mathbf{P}^{(\alpha)}_{1_21_2}$$

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

$$\begin{array}{c|cc} \mathbf{P}^{A_1}= & \mathbf{P}^{A_1}_{0_20_2} & \cdot \\ \mathbf{P}^{A_2}= & \cdot & \mathbf{P}^{A_2}_{1_21_2} \\ \mathbf{P}^{E}= & \mathbf{P}^{E}_{0_20_2} & \mathbf{P}^{E}_{1_21_2} \end{array}$$

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

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

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

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

2nd-Stage

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

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

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

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

$D_3 \supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1 = p^{0_2} + p^{1_2}$ will make **IRREDUCIBLE** $\mathbf{P}^{(\alpha)}_{n,n}$

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

Same for Correlation table:

$D_3 \supset C_3$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$$\mathbf{P}^{(\alpha)}1 = \mathbf{P}^{(\alpha)}(p^{0_2} + p^{1_2}) = \mathbf{P}^{(\alpha)}_{0_2 0_2} + \mathbf{P}^{(\alpha)}_{1_2 1_2}$$

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

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

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

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

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

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

2nd-Stage

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)

$$\begin{array}{c|ccc|c} D_3\ \kappa= & \mathbf{1} & \mathbf{r}^1+\mathbf{r}^2 & \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3 & \\ \hline \mathbf{P}^{A_1}= & 1 & 1 & 1 & /6 \\ \mathbf{P}^{A_2}= & 1 & 1 & -1 & /6 \\ \mathbf{P}^{E}= & 2 & -1 & 0 & /3 \end{array}$$

$$\begin{array}{c|cc|c} C_2\ \kappa= & \mathbf{1} & \mathbf{i}_3 & \\ \hline p^{0_2}= & 1 & 1 & /2 \\ p^{1_2}= & 1 & -1 & /2 \end{array}$$

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

$$\begin{array}{c|ccc|c} C_3\ \kappa= & \mathbf{1} & \mathbf{r}^1 & \mathbf{r}^2 & \\ \hline p^{0_3}= & 1 & 1 & 1 & /3 \\ p^{1_3}= & 1 & \varepsilon & \varepsilon^* & /3 \\ p^{2_3}= & 1 & \varepsilon^* & \varepsilon & /3 \end{array}$$

$D_3 \supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1 = p^{0_2} + p^{1_2}$ will make IRREDUCIBLE $\mathbf{P}^{(\alpha)}_{n,n}$

$$\begin{array}{c|cc} D_3\supset C_2 & 0_2 & 1_2 \\ \hline n^{A_1}= & 1 & \cdot \\ n^{A_2}= & \cdot & 1 \\ n^{E}= & 1 & 1 \end{array}$$

Same for Correlation table:

$$\begin{array}{c|ccc} D_3\supset C_3 & 0_3 & 1_3 & 2_3 \\ \hline n^{A_1}= & 1 & \cdot & \cdot \\ n^{A_2}= & 1 & \cdot & \cdot \\ n^{E}= & \cdot & 1 & 1 \end{array}$$

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$$\mathbf{P}^{(\alpha)}1 = \mathbf{P}^{(\alpha)}(p^{0_2}+p^{1_2}) = \mathbf{P}^{(\alpha)}_{0_20_2} + \mathbf{P}^{(\alpha)}_{1_21_2}$$

$$\begin{array}{c|cc} & 1 = p^{0_2} & + p^{1_2} \\ \hline \mathbf{P}^{A_1}= & \mathbf{P}^{A_1}_{0_20_2} & \cdot \\ \mathbf{P}^{A_2}= & \cdot & \mathbf{P}^{A_2}_{1_21_2} \\ \mathbf{P}^{E}= & \mathbf{P}^{E}_{0_20_2} & \mathbf{P}^{E}_{1_21_2} \end{array}$$

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_3-friendly" irreducible projectors

$$\mathbf{P}^{(\alpha)}1 = \mathbf{P}^{(\alpha)}(p^{0_3}+p^{1_3}+p^{2_3}) = \mathbf{P}^{(\alpha)}_{0_20_2} + \mathbf{P}^{(\alpha)}_{1_31_3} + \mathbf{P}^{(\alpha)}_{2_32_3}$$

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

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

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2nd-Stage

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

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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

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

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
$p^{2_3}=$	1	ε^*	ε	/3

$D_3\supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1=p^{0_2}+p^{1_2}$ will make IRREDUCIBLE $\mathbf{P}^{(\alpha)}_{n,n}$

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

Same for Correlation table:

$D_3\supset C_3$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$$\mathbf{P}^{(\alpha)}1=\mathbf{P}^{(\alpha)}(p^{0_2}+p^{1_2})$$
$$=\mathbf{P}^{(\alpha)}_{0_20_2}+\mathbf{P}^{(\alpha)}_{1_21_2}$$

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

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

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

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

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

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

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

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

2nd-Stage

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
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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

Let:

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

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
$p^{2_3}=$	1	ε^*	ε	/3

*$D_3\supset C_2$ Correlation table shows which products of class projector $\mathbf{P}^{(\alpha)}$ with C_2-unit $1=p^{0_2}+p^{1_2}$ will make **IRREDUCIBLE** $\mathbf{P}^{(\alpha)}_{n,n}$*

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

Same for *Correlation table:*

$D_3\supset C_3$	0_3	1_3	2_3
$n^{A_1}=$	1	·	·
$n^{A_2}=$	1	·	·
$n^{E}=$	·	1	1

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_2-friendly" irep projectors

$\mathbf{P}^{(\alpha)}1=\mathbf{P}^{(\alpha)}(p^{0_2}+p^{1_2})$

$=\mathbf{P}^{(\alpha)}_{0_20_2}+\mathbf{P}^{(\alpha)}_{1_21_2}$

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

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

Rank $\rho(D_3)=4$ implies there will be exactly 4 "C_3-friendly" irreducible projectors

$\mathbf{P}^{(\alpha)}1=\mathbf{P}^{(\alpha)}(p^{0_3}+p^{1_3}+p^{2_3})$

$=\mathbf{P}^{(\alpha)}_{0_20_2}+\mathbf{P}^{(\alpha)}_{1_31_3}+\mathbf{P}^{(\alpha)}_{2_32_3}$

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

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

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

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

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

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

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

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

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

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

Review:Spectral resolution of ***D_3 Center*** *(Class algebra)*

Group theory of equivalence transformations and classes

Lagrange theorems

All-commuting class projectors and D_3-invariant character ortho-completeness

Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G)\downarrow H)$

Atomic ℓ-level or $2\ell+1$-multiplet splitting

D_3 examples for ℓ=1-6

Group invariant numbers: Centrum, Rank, and Order

2nd-Stage spectral decompositions of global/local D_3

Splitting class projectors using subgroup chains $D_3 \supset C_2$ and $D_3 \supset C_3$

Splitting classes

3rd-stage spectral resolution to ***irreducible representations*** *(ireps) and Hamiltonian eigensolutions*

Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

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

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

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

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

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

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

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

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

$\mathbf{P}^E$ *splits into* $\mathbf{P}^E=\mathbf{P}^E_{0_20_2}+\mathbf{P}^E_{1_21_2}$, *class* $\kappa_\mathbf{i}$ *splits into* $\kappa_{\mathbf{i}_{12}}$ *and* $\kappa_{\mathbf{i}_3}$

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

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

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

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

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

$\mathbf{P}^E$ *splits into* $\mathbf{P}^E=\mathbf{P}^E_{1_31_3}+\mathbf{P}^E_{2_32_3}$, *class* $\kappa_\mathbf{r}$ *splits into* $\kappa_{\mathbf{r}^1}$ *and* $\kappa_{\mathbf{r}^2}$

Compare ahead to Lect.17 p. 12

2nd-Stage

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

D_3 $\kappa =$	$\mathbf{1}$	$\mathbf{r}^1+\mathbf{r}^2$	$\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3$	
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Rank $\rho(D_3)=4$ idempotents $\mathbf{P}^{(\alpha)}$

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

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

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

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

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

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

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

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

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

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

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

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

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

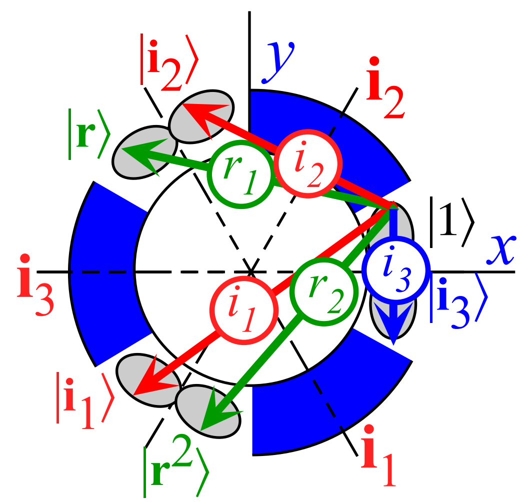
class $\kappa_{\mathbf{r}}$ splits into $\kappa_{\mathbf{r}^1}$ and $\kappa_{\mathbf{r}^2}$

$r=r_2$ must equal r_1

$i=i_2$ must equal i_1

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

i_3 is free parameter



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

$i=i_1=i_2=i_3$

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

r_1 and r_2 are free

*Review: Spectral resolution of **D_3 Center** (Class algebra)*

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

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

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

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

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

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

3rd and Final Step:
Spectral resolution of ALL 6 of D3 :

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

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

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

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

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

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

3rd and Final Step:
Spectral resolution of ALL 6 of D3 :

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

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

Compare ahead to Lect.17 p.14

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

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

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

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

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

3rd and Final Step:
Spectral resolution of ALL 6 of D3 :

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

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

$$\begin{aligned}\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}=\mathbf{P}^{A_1}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}_{x,x} &+ 0 + 0 + 0\\ +\,0 &+ \mathbf{P}^{A_2}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}_{y,y} + 0 + 0\\ +\,0 &+ 0 + \mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}\\ +\,0 &+ 0 + \mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}\end{aligned}$$

$\mathbf{P}^{\mu}_{mn}$ **g**-*expansion*
in Lect.17 p. 35-51

Compare ahead to Lect.17 p.14-18

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

$$\mathbf{P}^{A_1}_{x,x}=\mathbf{P}^{A_1}_{0_20_2}=\mathbf{P}^{A_1}\mathbf{p}^{0_2}=\mathbf{P}^{A_1}(\mathbf{1}+\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3)/6$$
$$\mathbf{P}^{A_2}_{y,y}=\mathbf{P}^{A_2}_{1_21_2}=\mathbf{P}^{A_2}\mathbf{p}^{1_2}=\mathbf{P}^{A_2}(\mathbf{1}-\mathbf{i}_3)/2=(\mathbf{1}+\mathbf{r}^1+\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2-\mathbf{i}_3)/6$$
$$\mathbf{P}^{E}_{x,x}=\mathbf{P}^{E}_{0_20_2}=\mathbf{P}^{E}\mathbf{p}^{0_2}=\mathbf{P}^{E}(\mathbf{1}+\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2-\mathbf{i}_1-\mathbf{i}_2+2\mathbf{i}_3)/6$$
$$\mathbf{P}^{E}_{y,y}=\mathbf{P}^{E}_{1_21_2}=\mathbf{P}^{E}\mathbf{p}^{1_2}=\mathbf{P}^{E}(\mathbf{1}-\mathbf{i}_3)/2=(2\mathbf{1}-\mathbf{r}^1-\mathbf{r}^2+\mathbf{i}_1+\mathbf{i}_2-2\mathbf{i}_3)/6$$

3rd and Final Step:

Spectral resolution of ALL 6 of D3 :

The old ‘g-equals-1-times-g-times-1’ Trick

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

$$\begin{aligned}\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}=\mathbf{P}^{A_1}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}_{x,x}&+0+0+0\\ &+0+\mathbf{P}^{A_2}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}_{y,y}+0+0\\ &+0+0+\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}\\ &+0+0+\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}+\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}\end{aligned}$$

where:

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

Need to Define 6 Irreducible Projectors $\mathbf{P}^{(\alpha)}_{m,n}$

Order $°(D_3)=6$

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

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

$$\begin{aligned}\mathbf{g}=\mathbf{1}\cdot\mathbf{g}\cdot\mathbf{1}=\;& D^{A_1}(\mathbf{g})\mathbf{P}^{A_1}_{x,x} + 0 + 0 + 0\\ &+ 0 + D^{A_2}(\mathbf{g})\mathbf{P}^{A_2}_{y,y} + 0 + 0\\ &+ 0 + 0 + D^{E}_{x,x}(\mathbf{g})\mathbf{P}^{E}_{x,x} + D^{E}_{x,y}(\mathbf{g})\mathbf{P}^{E}_{x,y}\\ &+ 0 + 0 + D^{E}_{y,x}(\mathbf{g})\mathbf{P}^{E}_{y,x} + D^{E}_{y,y}(\mathbf{g})\mathbf{P}^{E}_{y,y}\end{aligned}$$

where:

$$\mathbf{P}^{A_1}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}_{x,x}=D^{A_1}(\mathbf{g})\mathbf{P}^{A_1}_{x,x}$$

$$\mathbf{P}^{A_2}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}_{y,y}=D^{A_2}(\mathbf{g})\mathbf{P}^{A_2}_{y,y}$$

$$\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}=D^{E}_{x,x}(\mathbf{g})\mathbf{P}^{E}_{x,x}\qquad \mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}=D^{E}_{x,y}(\mathbf{g})\mathbf{P}^{E}_{x,y}$$

$$\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}=D^{E}_{y,x}(\mathbf{g})\mathbf{P}^{E}_{y,x}\qquad \mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}=D^{E}_{y,y}(\mathbf{g})\mathbf{P}^{E}_{y,y}$$

Need to Define 6 Irreducible Projectors $\mathbf{P}^{(\alpha)}_{m,n}$

Order $°(D_3)=6$

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

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

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D3 :

The old ‘g-equals-1-times-g-times-1’ Trick

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

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

where:

$$\mathbf{P}^{A_1}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{A_1}_{x,x}=D^{A_1}(\mathbf{g})\mathbf{P}^{A_1}_{x,x}$$

$$\mathbf{P}^{A_2}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{A_2}_{y,y}=D^{A_2}(\mathbf{g})\mathbf{P}^{A_2}_{y,y}$$

$$\mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}=D^{E}_{x,x}(\mathbf{g})\mathbf{P}^{E}_{x,x} \qquad \mathbf{P}^{E}_{x,x}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}=D^{E}_{x,y}(\mathbf{g})\mathbf{P}^{E}_{x,y}$$

$$\mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{x,x}=D^{E}_{y,x}(\mathbf{g})\mathbf{P}^{E}_{y,x} \qquad \mathbf{P}^{E}_{y,y}\cdot\mathbf{g}\cdot\mathbf{P}^{E}_{y,y}=D^{E}_{y,y}(\mathbf{g})\mathbf{P}^{E}_{y,y}$$

Need to Define 6 Irreducible Projectors $\mathbf{P}^{(\alpha)}_{m,n}$

Order $°(D_3)=6$

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

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

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

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

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

3rd and Final Step:
Spectral resolution of ALL 6 of D3 :

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

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

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

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

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

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

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

Compare ahead to Lect.17 p.18-21

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

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

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

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 :

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

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

The old '$\mathbf{g}$-equals-$\mathbf{1}$-times-$\mathbf{g}$-times-$\mathbf{1}$' Trick

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

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

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

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

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

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

Compare ahead to Lect.17 p.18-21

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

$$\begin{array}{l|ccc|l} D_3\ \kappa= & \mathbf{1} & \mathbf{r}^1+\mathbf{r}^2 & \mathbf{i}_1+\mathbf{i}_2+\mathbf{i}_3 & \\ \hline \mathbf{P}^{A_1}= & 1 & 1 & 1 & /6 \\ \mathbf{P}^{A_2}= & 1 & 1 & -1 & /6 \\ \mathbf{P}^{E}= & 2 & -1 & 0 & /3 \end{array}$$

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

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

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D3 :

The old ‘g-equals-1-times-g-times-1’ Trick

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

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

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

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

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

$$\begin{array}{l|cccccc|l} & \mathbf{1} & \mathbf{r}^1 & \mathbf{r}^2 & \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 & \\ \hline \mathbf{P}^{A_1}_{x,x}= & (1 & 1 & 1 & 1 & 1 & 1) & /6 \\ \mathbf{P}^{A_2}_{y,y}= & (1 & 1 & 1 & -1 & -1 & -1) & /6 \end{array}$$

$$\begin{array}{l|cccccc|l} & \mathbf{1} & \mathbf{r}^1 & \mathbf{r}^2 & \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 & \\ \hline \mathbf{P}^{E}_{x,x}= & (2 & -1 & -1 & -1 & -1 & +2) & /6 \\ \mathbf{P}^{E}_{y,x}= & (0 & 1 & -1 & -1 & +1 & 0) & /\sqrt{3}/2 \end{array}$$

$$\begin{array}{l|cccccc|l} & \mathbf{1} & \mathbf{r}^1 & \mathbf{r}^2 & \mathbf{i}_1 & \mathbf{i}_2 & \mathbf{i}_3 & \\ \hline \mathbf{P}^{E}_{x,y}= & (0 & -1 & 1 & -1 & +1 & 0) & /\sqrt{3}/2 \\ \mathbf{P}^{E}_{y,y}= & (2 & -1 & -1 & +1 & +1 & -2) & /6 \end{array}$$

where D_3 *irreducible representations* are: $D^{A_1}(\mathbf{g})=+1,\quad D^{A_2}(\mathbf{g})=\pm 1,$

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

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

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

Global (LAB) symmetry

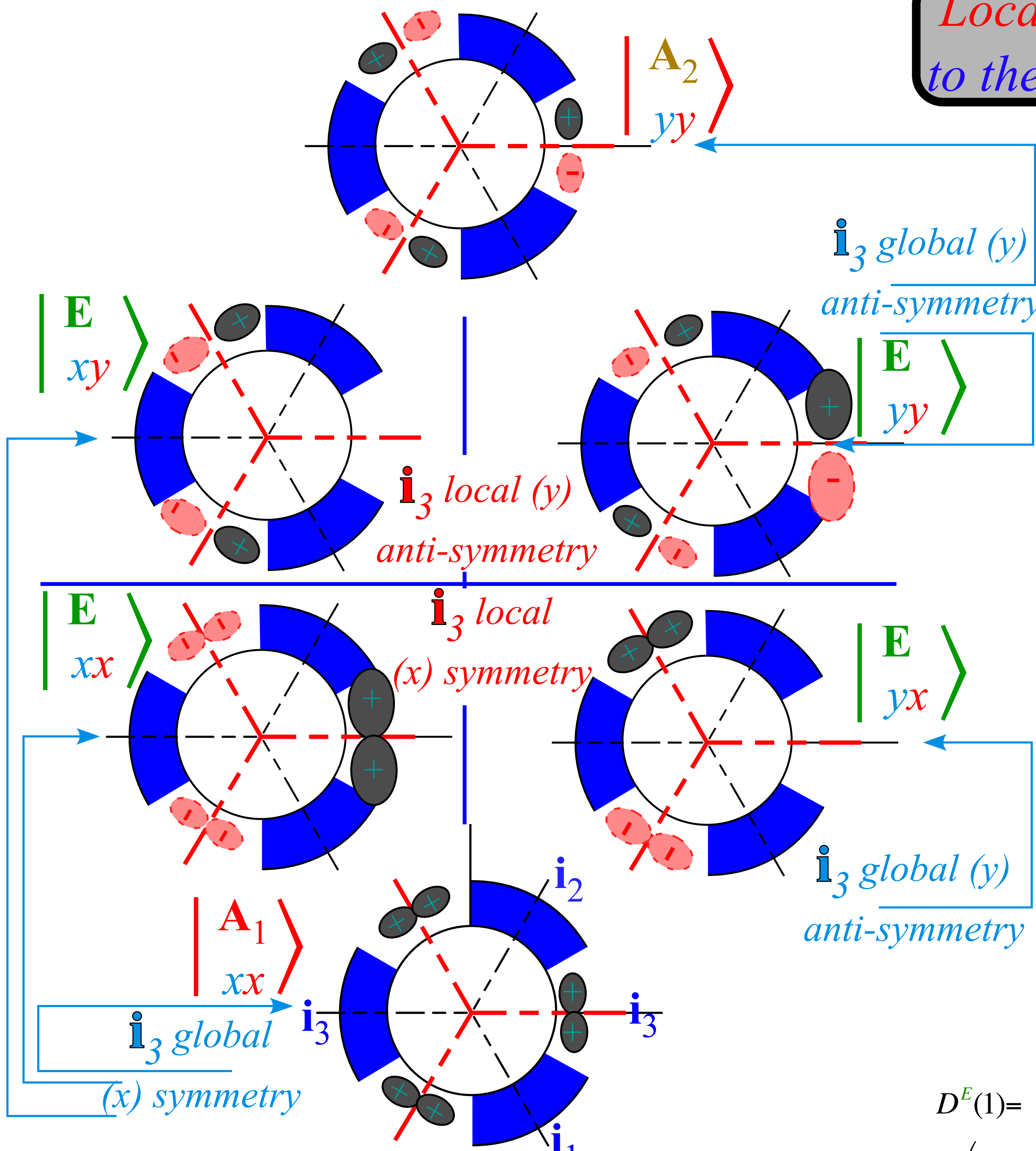
$$\mathbf{i}_3\left|{}^{(m)}_{eb}\right\rangle = \mathbf{i}_3\mathbf{P}^{(m)}_{eb}\left|1\right\rangle = (-1)^e\left|{}^{(m)}\right\rangle$$

Local (BOD) symmetry

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

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

Here the "Mock-Mach" is being applied!



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

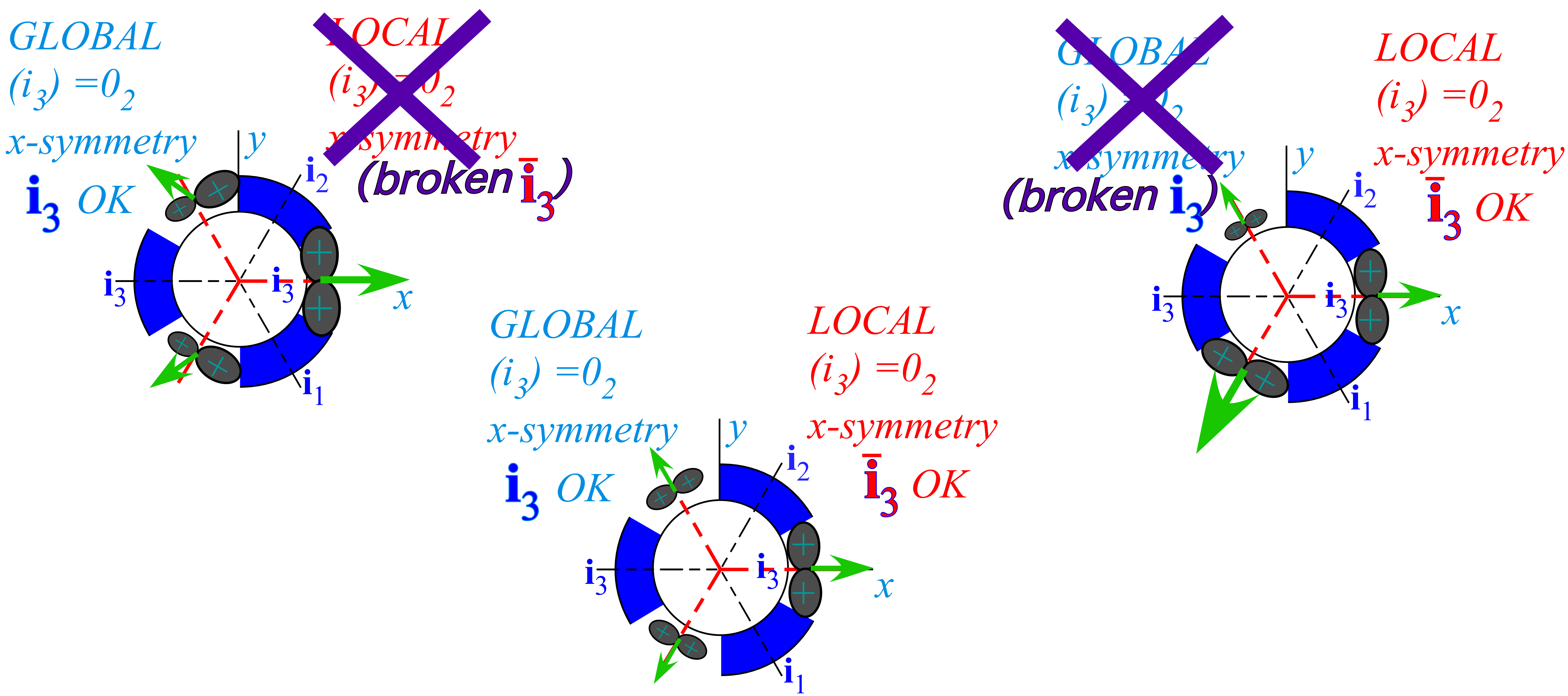
Ket norm factors detailed in Lect.17 p.23-30

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

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

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

external LAB	*internal BOD*
symmety label-e	*symmety label-b*
GLOBAL	*LOCAL*



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

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

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

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

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

- *Eigenstates (shown before)*
- *Complete Hamiltonian*

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

A_1-block *A_2-block*

- *Local symmetery eigenvalue formulae* (Local Symmetry=> off-diagonal=0)

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

gives:

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

A_2-level: $H+2r-2i-i_3$

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

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

Rigorous Global vs Local Calculus begins on p.90 of Lecture 17. Matrix forms on p. 125-129 and p. 130-146.

$\mathbf{P}^{\mu}{}_{mn}$ **g**-*expansion in Lect.17 p. 35-51*

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

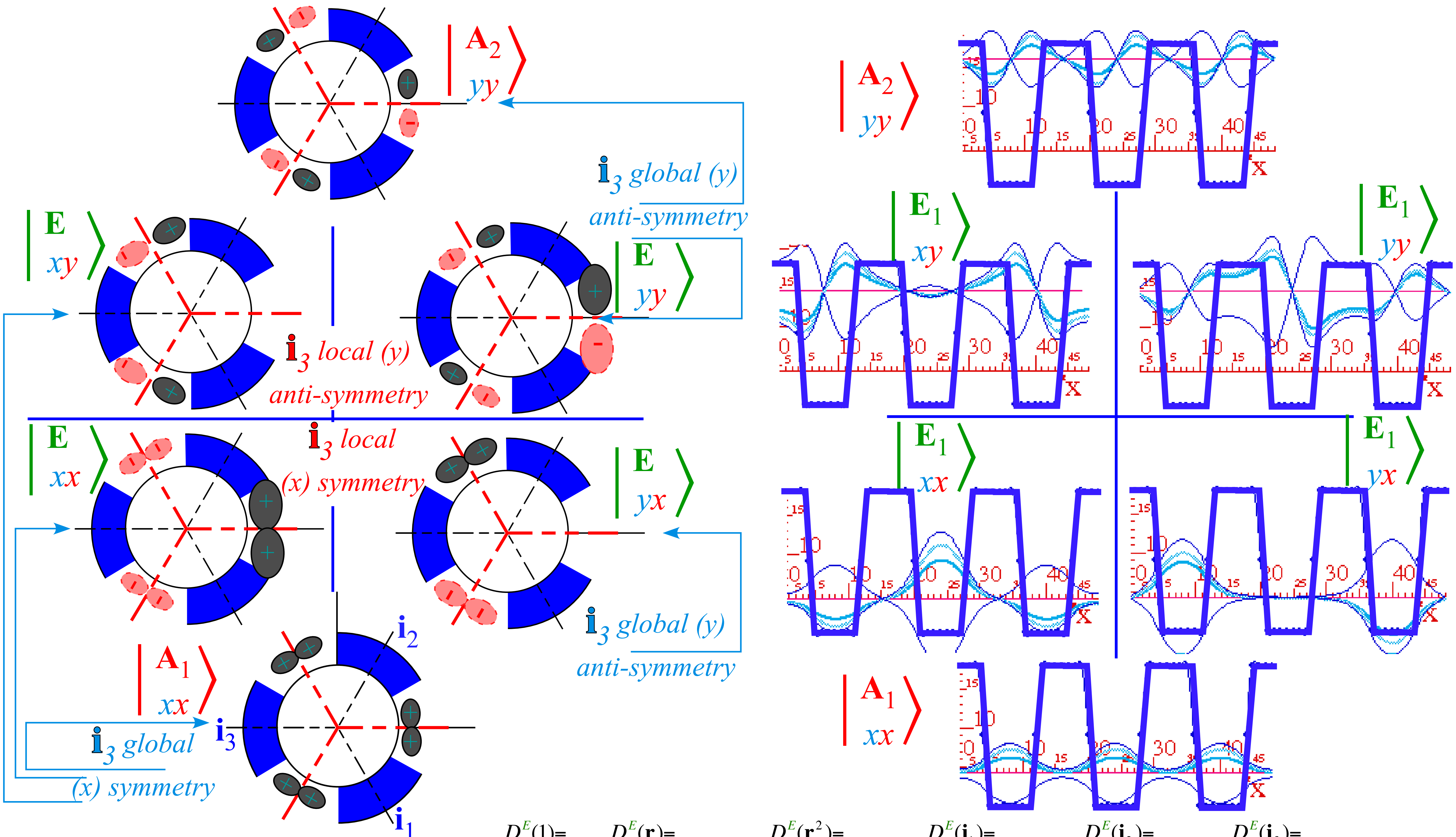
$$\left|{}^{(m)}_{eb}\right\rangle = \mathbf{P}^{(m)}_{eb}\left|1\right\rangle$$

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

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

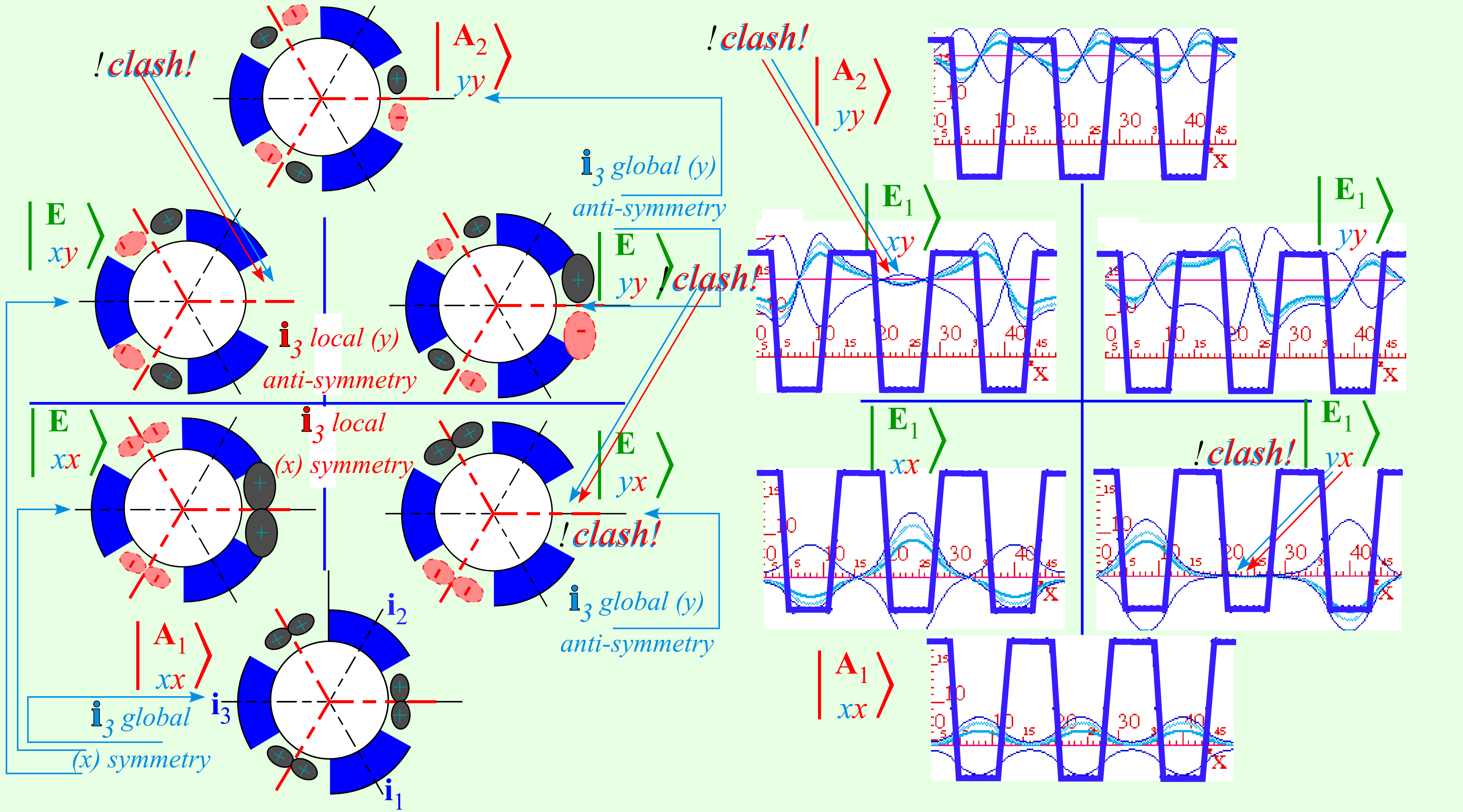


$D^{A_1}(\mathbf{g}) = +1,\ D^{A_2}(\mathbf{r}^p) = +1,\ D^{A_2}(\mathbf{i}_q) = -1$

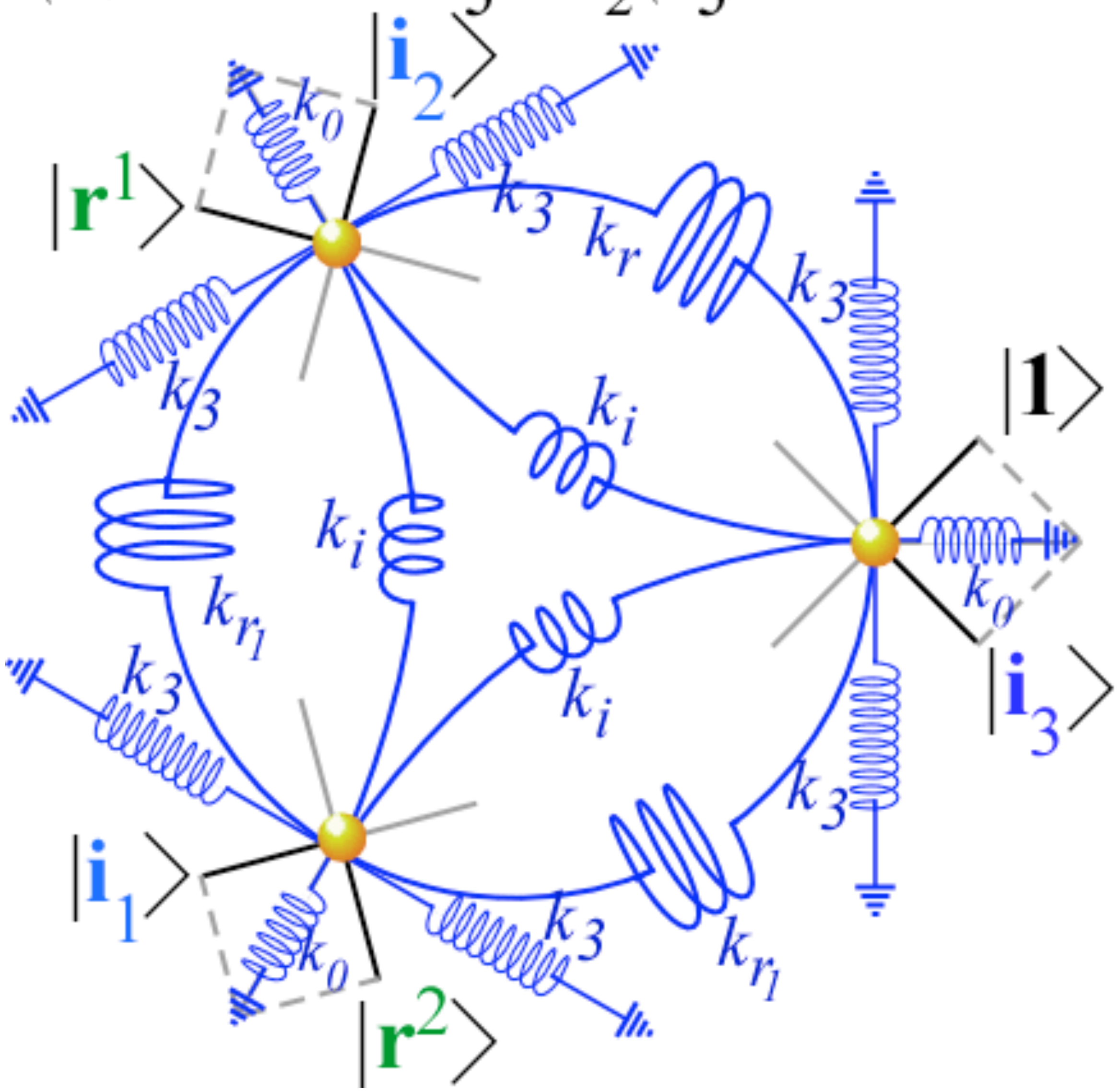
$D^E(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $D^E(\mathbf{r}) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$ $D^E(\mathbf{r}^2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}$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

When there is no there, there...

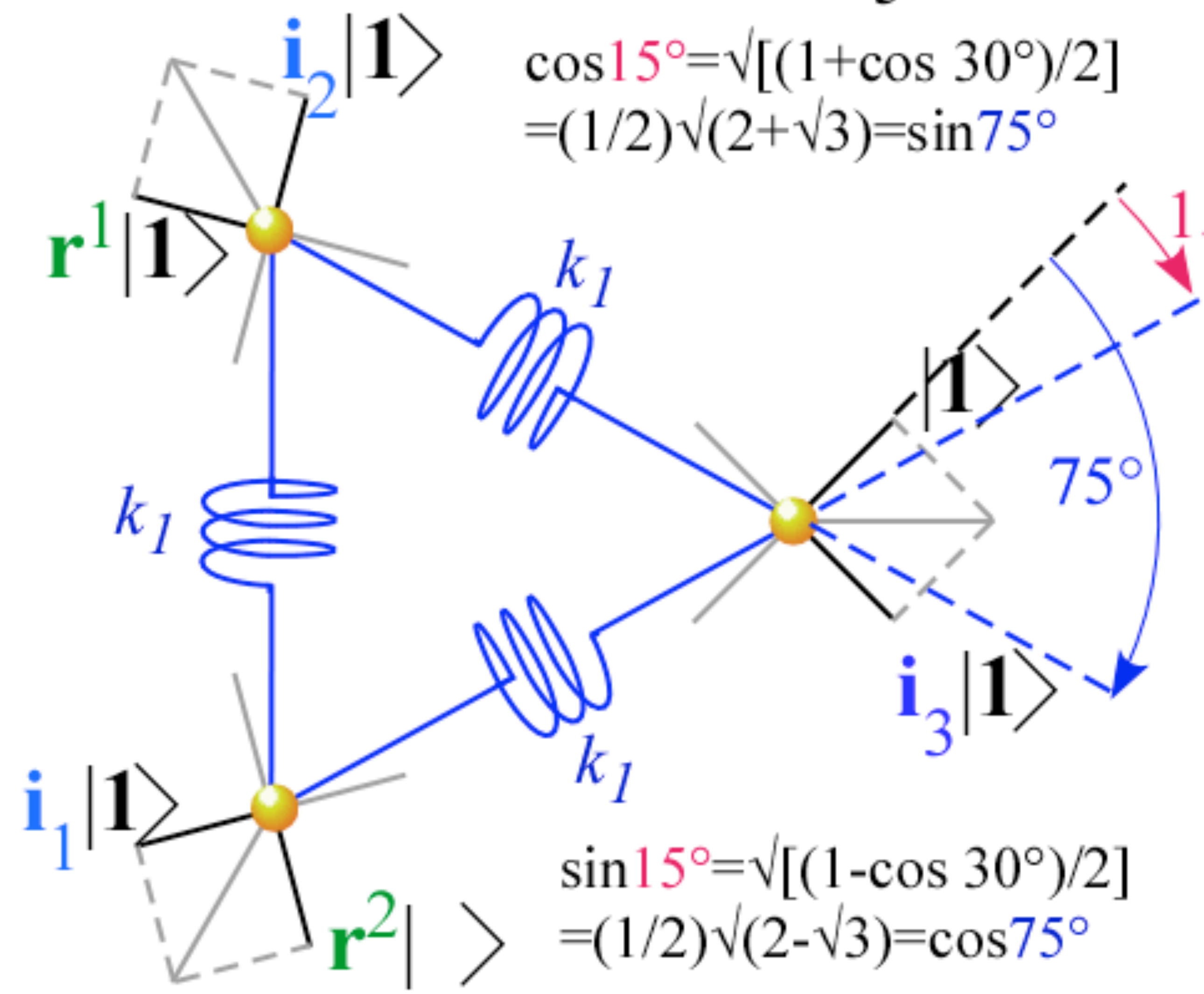
Nobody Home
where LOCAL
and GLOBAL



(a) *Local* $D_3 \supset C_2(i_3)$ *model*



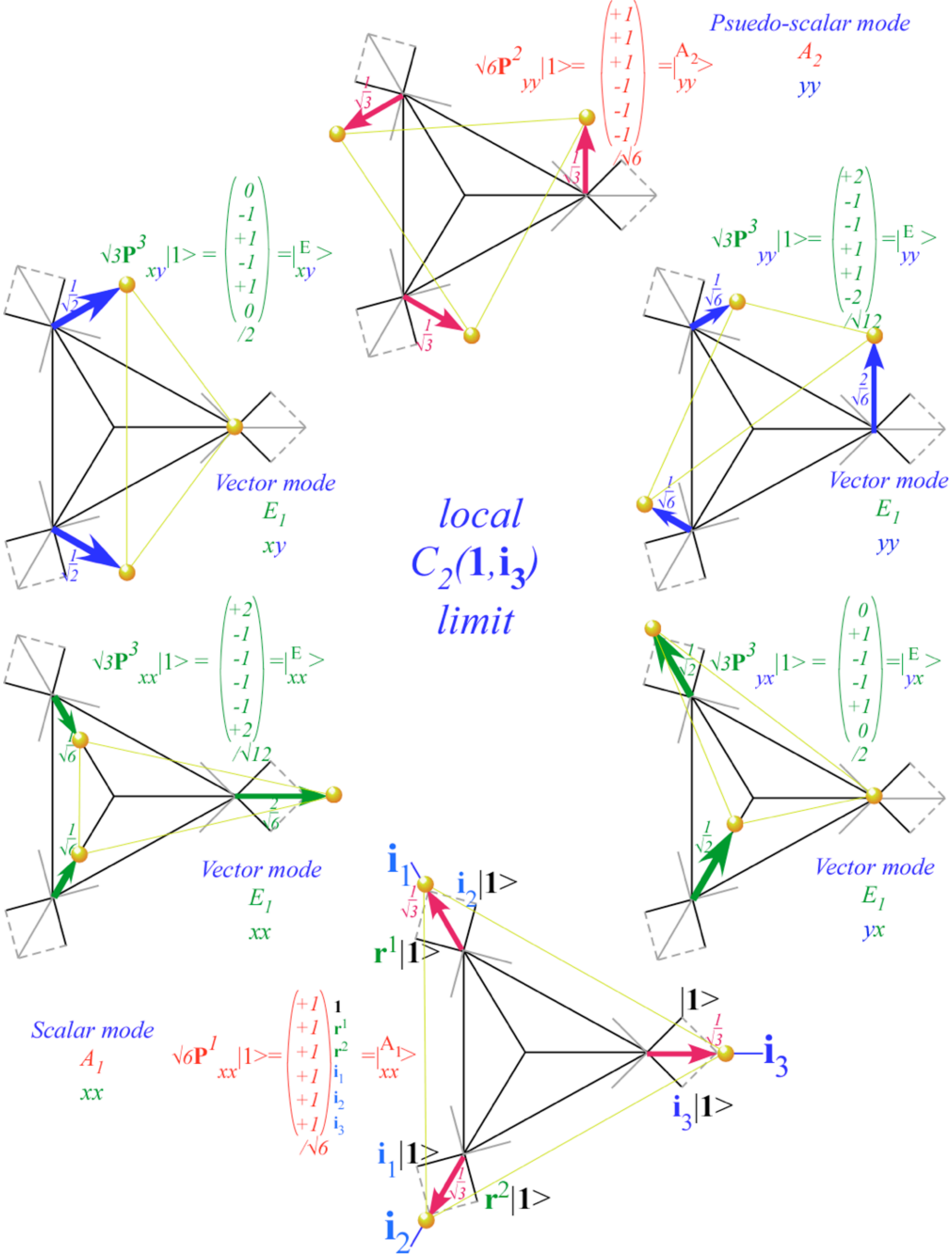
(b) *Mixed local symmetry* D_3 *model*



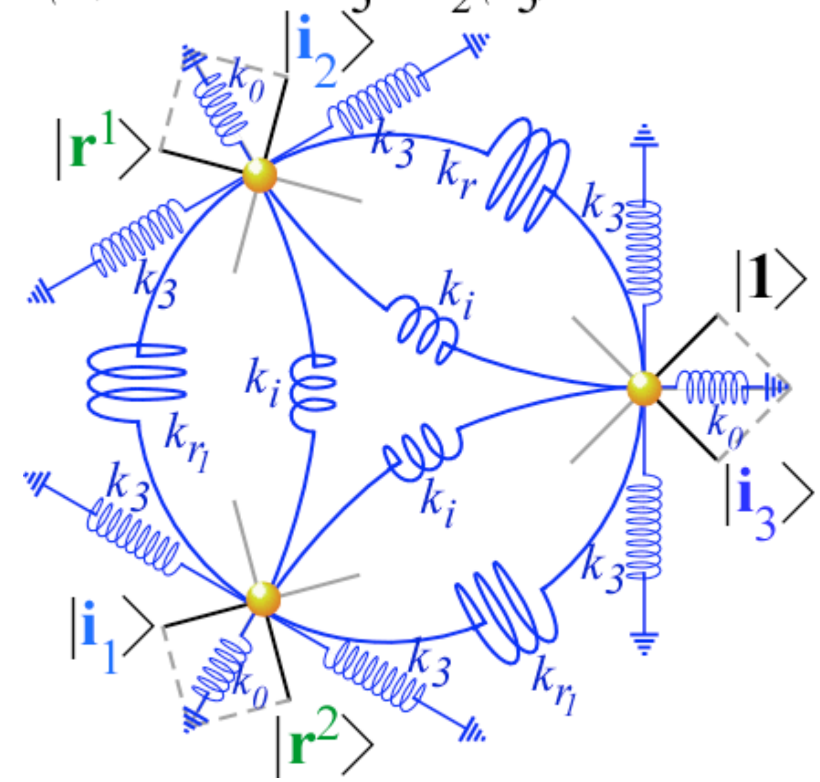
See p. 12-45 of Lecture 18

MolVibes Web Application: http://www.uark.edu/ua/modphys/markup/MolVibesWeb.html

MolVibes Web Simulation
3 Atom with C3v symmetry



(a) Local $D_3 \supset C_2(i_3)$ model



See p. 12-45 of Lecture 18

MolVibes Web Simulation
3 Atom with C3v symmetry

Polygonal geometry of $U(2)\supset C_N$ character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$

is an ($\ell^j=2j+1$)-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = trace D^{1/2}(\Theta) = trace\begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^{1}(\Theta) = trace D^{1}(\Theta) = trace\begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

Excerpts from Lecture 13 page 135-146 (also Lecture 14.5 p. 93-104)

Polygonal geometry of $U(2)\supset C_N$ character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$

is an $(\ell^j=2j+1)$-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = trace D^{1/2}(\Theta) = trace\begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^{1}(\Theta) = trace D^{1}(\Theta) = trace\begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\,\Theta/2)$ for $m\geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} \qquad = 2\cos\frac{\Theta}{2}$$ (spinor-j=1/2)

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \ldots \qquad + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \ldots \qquad + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

Excerpts from Lecture 13 page 135-146

Polygonal geometry of $U(2)\supset C_N$ character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$
is an ($\ell^j=2j+1$)-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = trace D^{1/2}(\Theta) = trace\begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$
(spinor-j=1/2)

$$\chi^{1}(\Theta) = trace D^{1}(\Theta) = trace\begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$
(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\,\Theta/2)$ for $m\geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} \qquad = 2\cos\frac{\Theta}{2}$$
(spinor-j=1/2)

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \ldots \qquad + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \ldots \qquad + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^{0}(\Theta) = e^{-i\Theta\cdot 0} \qquad = 1$$
(scalar-j=0)

$$\chi^{1}(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} \quad = 1 + 2\cos\Theta$$
(vector-j=1)

$$\chi^{2}(\Theta) = e^{-i2\Theta} + \ldots e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos 2\Theta$$
(tensor-j=2)

Excerpts from Lecture 13 page 135-146

Polygonal geometry of U(2)⊃C$_N$ character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$

is an ($\ell^j=2j+1$)-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = trace D^{1/2}(\Theta) = trace \begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^{1}(\Theta) = trace D^{1}(\Theta) = trace \begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\,\Theta/2)$ for $m\geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2}$$

(spinor-j=1/2)

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \ldots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \ldots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^{0}(\Theta) = e^{-i\Theta\cdot 0} = 1$$

(scalar-j=0)

$$\chi^{1}(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta$$

(vector-j=1)

$$\chi^{2}(\Theta) = e^{-i2\Theta} + \ldots e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos 2\Theta$$

(tensor-j=2)

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

$$\chi^j(\Theta) = Trace D^{(j)}(\Theta) = e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \ldots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)} + e^{+i\Theta j}$$

$$\chi^j(\Theta)e^{-i\Theta} = e^{-i\Theta(j+1)} + e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \ldots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)}$$

Subtracting gives:

$$\chi^j(\Theta)(1-e^{-i\Theta}) = -e^{-i\Theta(j+1)} + e^{+i\Theta j}$$

Excerpts from Lecture 13 page 135-146

Polygonal geometry of U(2)⊃C_N character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$
is an ($\ell^j=2j+1$)-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta)=traceD^{1/2}(\Theta)=trace\begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2}\end{pmatrix}$$
(spinor-j=1/2)

$$\chi^{1}(\Theta)=traceD^{1}(\Theta)=trace\begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta}\end{pmatrix}$$
(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\,\Theta/2)$ for $m\geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta)=e^{-i\frac{\Theta}{2}}+e^{i\frac{\Theta}{2}} =2\cos\frac{\Theta}{2}$$
(spinor-j=1/2)

$$\chi^{3/2}(\Theta)=e^{-i\frac{3\Theta}{2}}+\ldots +e^{i\frac{3\Theta}{2}}=2\cos\frac{\Theta}{2}+2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta)=e^{-i\frac{5\Theta}{2}}+\ldots +e^{i\frac{5\Theta}{2}}=2\cos\frac{\Theta}{2}+2\cos\frac{3\Theta}{2}+2\cos\frac{5\Theta}{2}$$

$$\chi^{0}(\Theta)=e^{-i\Theta\cdot 0}=1$$
(scalar-j=0)

$$\chi^{1}(\Theta)=e^{-i\Theta}+1+e^{i\Theta}=1+2\cos\Theta$$
(vector-j=1)

$$\chi^{2}(\Theta)=e^{-i2\Theta}+\ldots e^{i2\Theta}=1+2\cos\Theta+2\cos 2\Theta$$
(tensor-j=2)

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

$$\chi^j(\Theta)=TraceD^{(j)}(\Theta)=\cancel{e^{-i\Theta j}}+e^{-i\Theta(j-1)}+e^{-i\Theta(j-2)}+\ldots+e^{+i\Theta(j-2)}+e^{+i\Theta(j-1)}+e^{+i\Theta j}$$

$$\chi^j(\Theta)e^{-i\Theta}=e^{-i\Theta(j+1)}+e^{-i\Theta j}+e^{-i\Theta(j-1)}+e^{-i\Theta(j-2)}+\ldots+e^{+i\Theta(j-2)}+e^{+i\Theta(j-1)}$$

Subtracting/dividing gives $\chi^j(\Theta)$ formula.

$$\chi^j(\Theta)=\frac{e^{+i\Theta j}-e^{-i\Theta(j+1)}}{1-e^{-i\Theta}}=\frac{e^{+i\Theta(j+\frac{1}{2})}-e^{-i\Theta(j+\frac{1}{2})}}{e^{+i\frac{\Theta}{2}}-e^{-i\frac{\Theta}{2}}}=\frac{\sin\Theta(j+\frac{1}{2})}{\sin\frac{\Theta}{2}}$$

Excerpts from Lecture 13 page 135-146

Polygonal geometry of U(2)⊃C_N character spectral function

Trace-character $\chi^j(\Theta)$ of U(2) rotation by C_n angle $\Theta=2\pi/n$

is an ($\ell^j=2j+1$)-term sum of $e^{-im\Theta}$ over allowed m-quanta $m=\{-j, -j+1, \ldots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = traceD^{1/2}(\Theta) = trace\begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^{1}(\Theta) = traceD^{1}(\Theta) = trace\begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\,\Theta/2)$ for $m\geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2}$$ *(spinor-j=1/2)*

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \ldots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \ldots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^{0}(\Theta) = e^{-i\Theta\cdot 0} = 1$$ *(scalar-j=0)*

$$\chi^{1}(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta$$ *(vector-j=1)*

$$\chi^{2}(\Theta) = e^{-i2\Theta} + \ldots e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos 2\Theta$$ *(tensor-j=2)*

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

$$\chi^j(\Theta) = TraceD^{(j)}(\Theta) = \cancel{e^{-i\Theta j}} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \ldots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)} + e^{+i\Theta j}$$

$$\chi^j(\Theta)e^{-i\Theta} = e^{-i\Theta(j+1)} + \cancel{e^{-i\Theta j}} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \ldots + e^{+i\Theta(j-2)} + \cancel{e^{+i\Theta(j-1)}}$$

Subtracting/dividing gives $\chi^j(\Theta)$ formula.

$$\chi^j(\Theta) = \frac{e^{+i\Theta j} - e^{-i\Theta(j+1)}}{1-e^{-i\Theta}} = \frac{e^{+i\Theta(j+\frac{1}{2})} - e^{-i\Theta(j+\frac{1}{2})}}{e^{+i\frac{\Theta}{2}} - e^{-i\frac{\Theta}{2}}} = \frac{\sin\Theta(j+\frac{1}{2})}{\sin\frac{\Theta}{2}}$$

For C_n angle $\Theta=2\pi/n$ this χ^j has a lot of geometric significance.

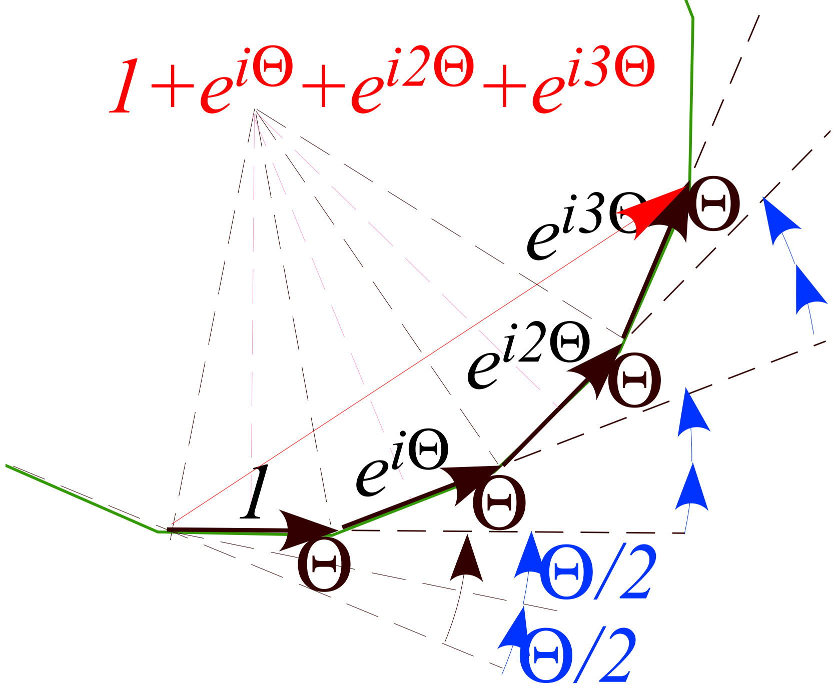
$$\boxed{\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}}$$

Character Spectral Function
where: $\ell^j=2j+1$
is U(2) irrep dimension

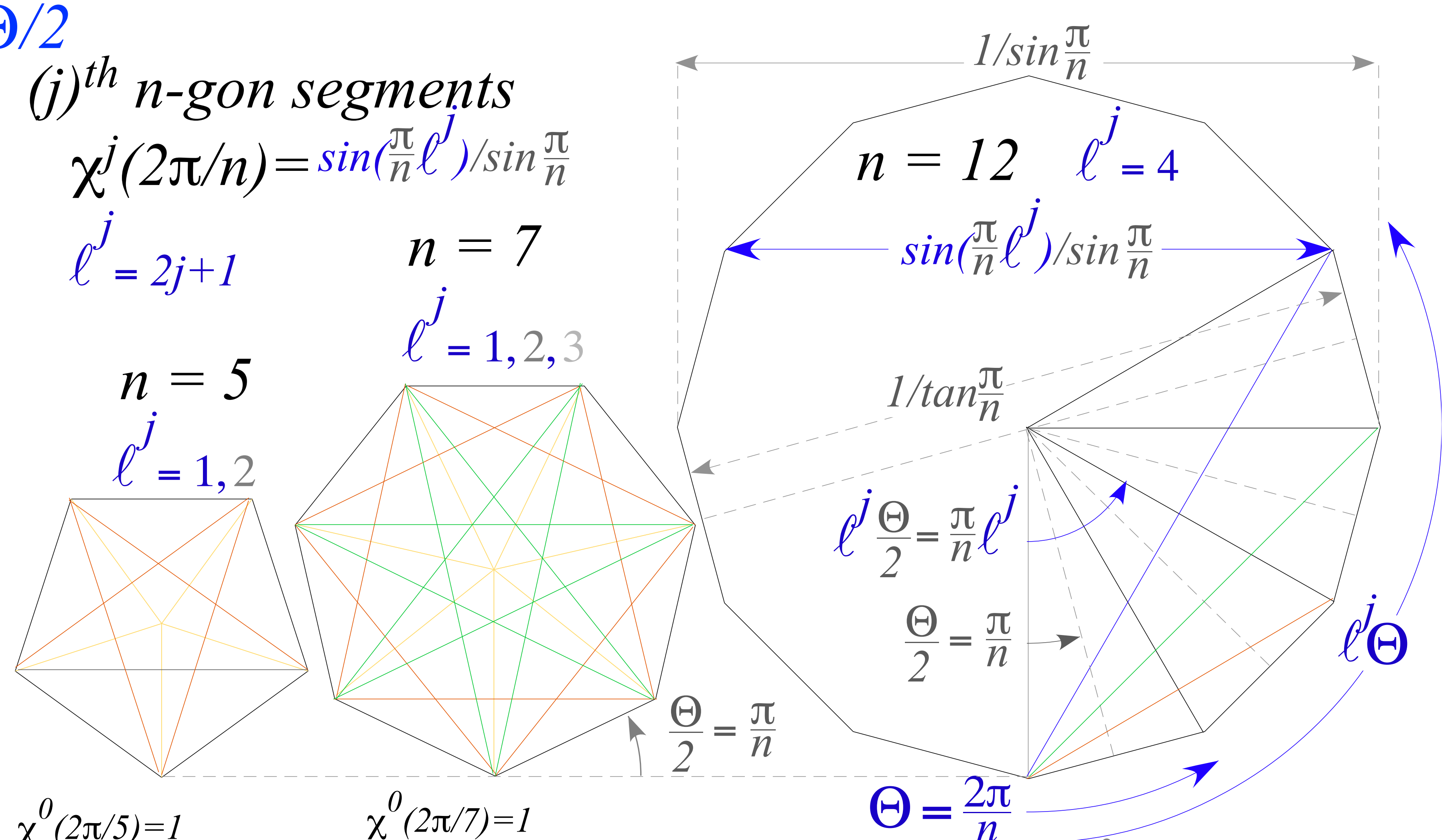
Polygonal geometry of $U(2)\supset C_N$ character spectral function

$$\chi^j\left(\frac{2\pi}{n}\right)=\frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}}=\frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

Character Spectral Function
where: $\ell^j=2j+1$
is U(2) irrep dimension



Excerpts from
Lecture 14.5
page 93-103



$\chi^0(2\pi/5)=1$
$\chi^{1/2}(2\pi/5)=1.618...$
$=(1+\sqrt{5})/2=$

$\chi^0(2\pi/7)=1$
$\chi^{1/2}(2\pi/7)=1.802...$
$\chi^{1}(2\pi/7)=2.247...$
$\chi^{3/2}(2\pi/7)=2.247...$

$\chi^{1/2}(2\pi/12)=1.932...$
$\chi^{1}(2\pi/12)=2.732...$
$\chi^{3/2}(2\pi/12)=3.346...$

$\chi^{2}(2\pi/12)=3.732...$
$\chi^{5/2}(2\pi/12)=3.864...$
$\chi^{3}(2\pi/12)=3.732...$