

Group Theory in Quantum Mechanics

Lecture 15 (3.12.15)

revised(4.1.15)

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)

D_3 Algebra

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 (“irreps”)

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 $\ell=1-6$

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 $D_3 \supset C_3$

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

P_{A_1} $\kappa_1=1$ D_3 Center
(All-commuting operators)

P_{A_2}

P_{E_1}

$\kappa_1 = i_1 + i_2 + i_3$

$\kappa_2 = r^2 + r$

r

r^2

i_1

i_2

i_3

PE_{xx} PE_{yy}

PE_{xy} PE_{yx}

PE_{11}

PE_{22}

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

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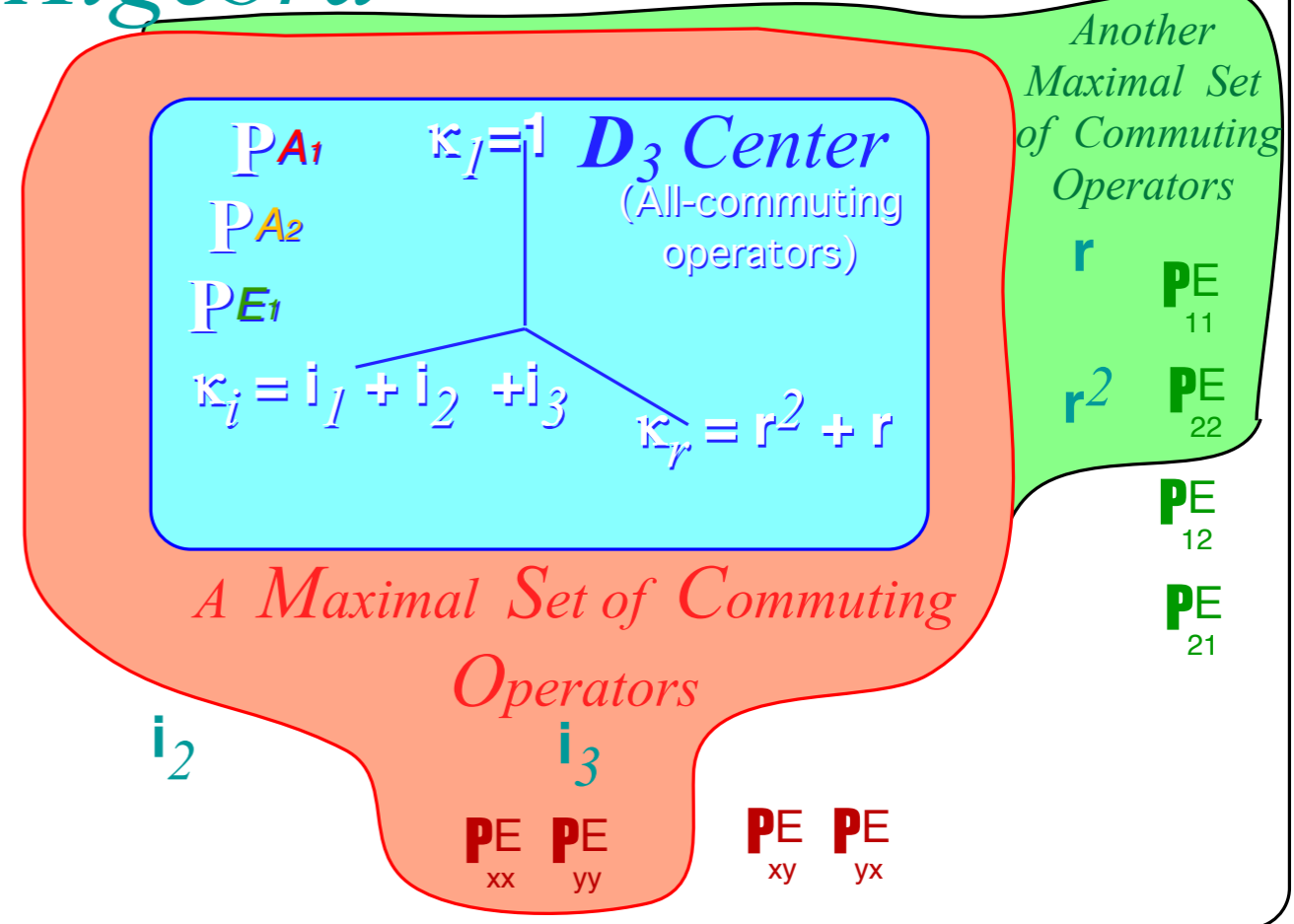
1	r²	r	i₁	i₂	i₃
r	1	r²	i₃	i₁	i₂
r²	r	1	i₂	i₃	i₁
i₁	i₃	i₂	1	r	r²
i₂	i₁	i₃	r²	1	r
i₃	i₂	i₁	r	r²	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
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 g_t

Class-sum κ_k invariance: $g_t \kappa_k = \kappa_k g_t$

D_3 Algebra

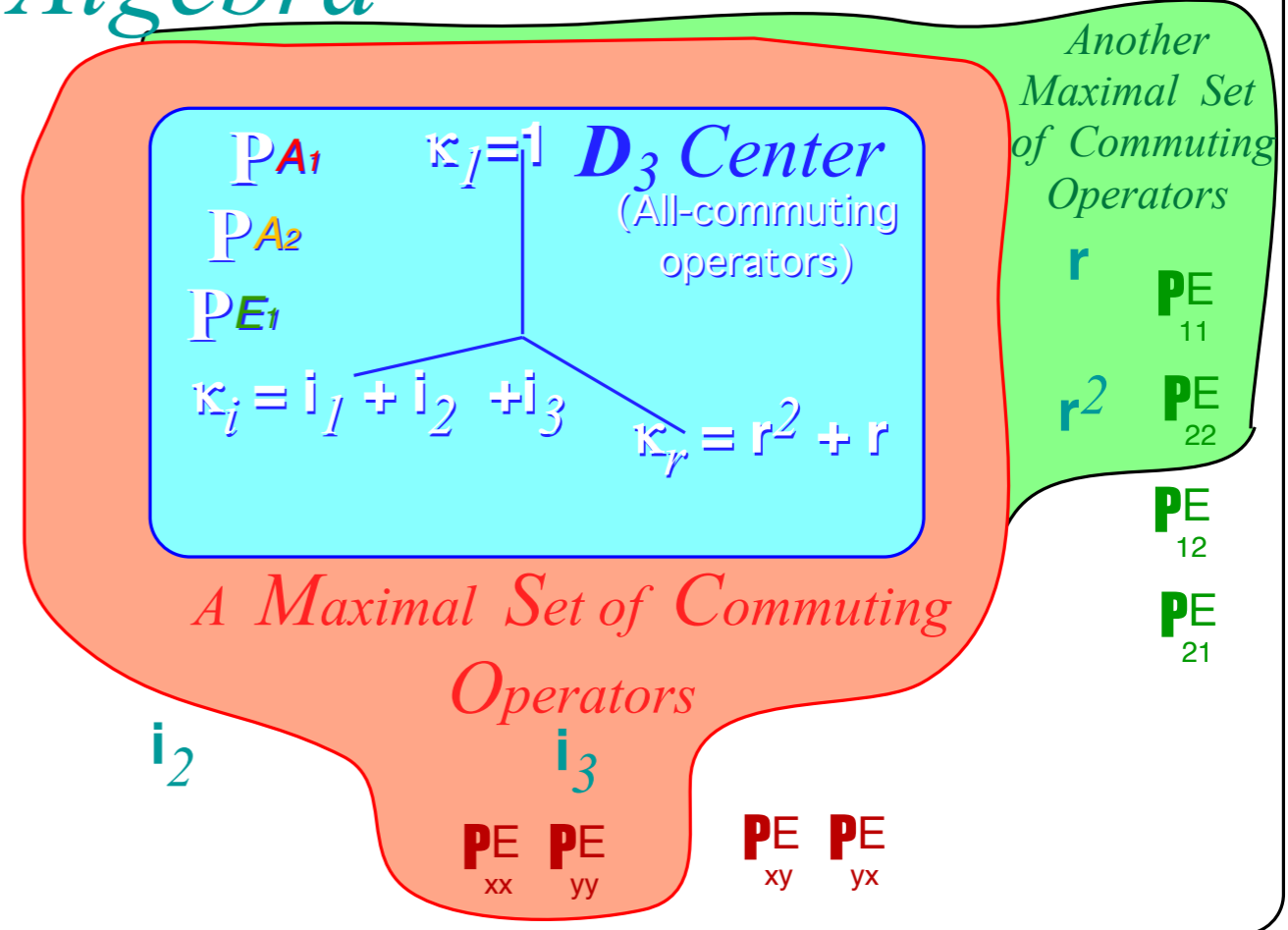


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r²	r	1	i₂	i₃	i₁
i₁	i₃	i₂	1	r	r²
i₂	i₁	i₃	r²	1	r
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$^{\circ}G$ = order of group: ($^{\circ}D_3 = 6$)

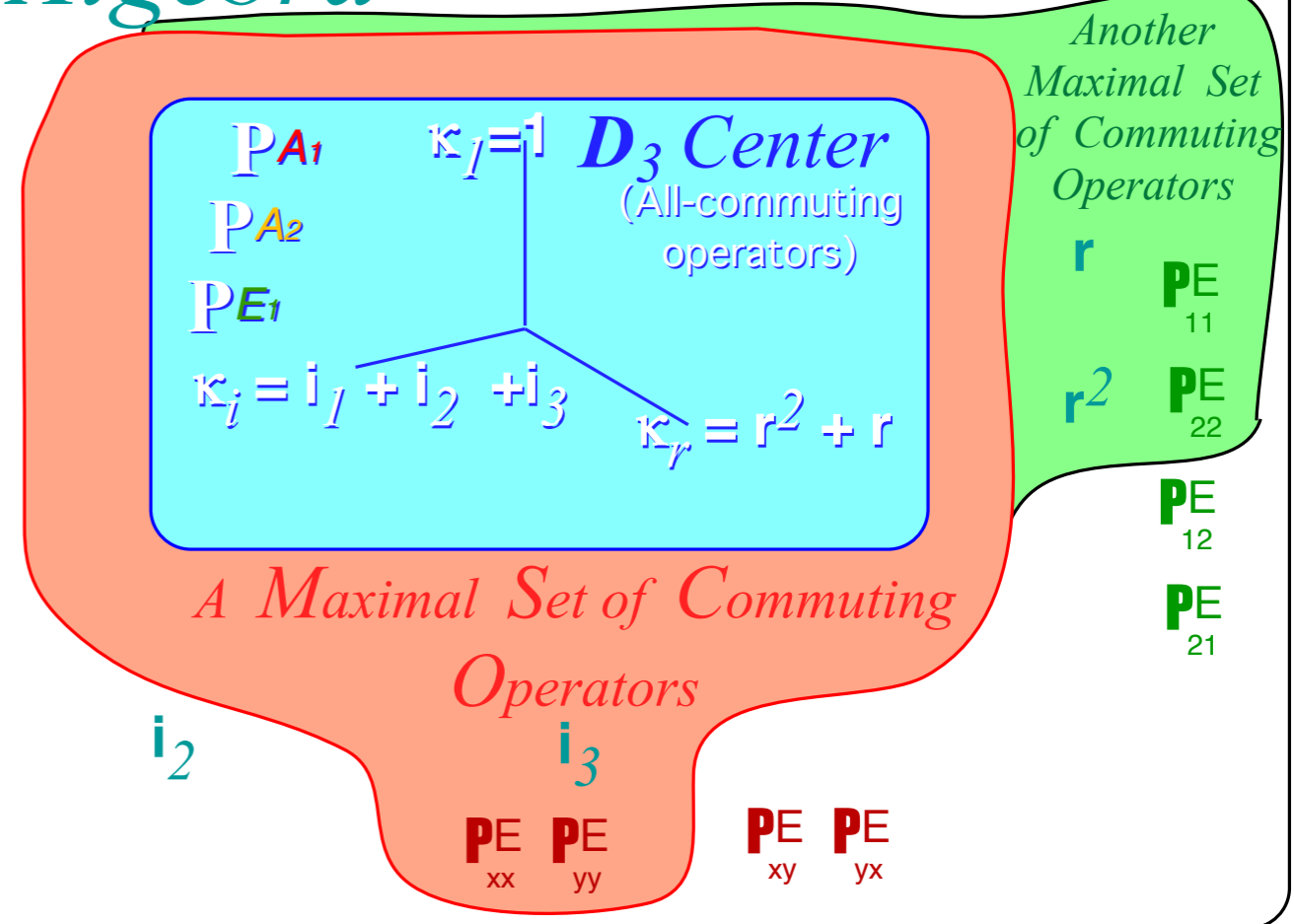
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r	1	r^2	i_3	i_1	i_2
r^2	r	1	i_2	i_3	i_1
i_1	i_3	i_2	1	r	r^2
i_2	i_1	i_3	r^2	1	r
i_3	i_2	i_1	r	r^2	1

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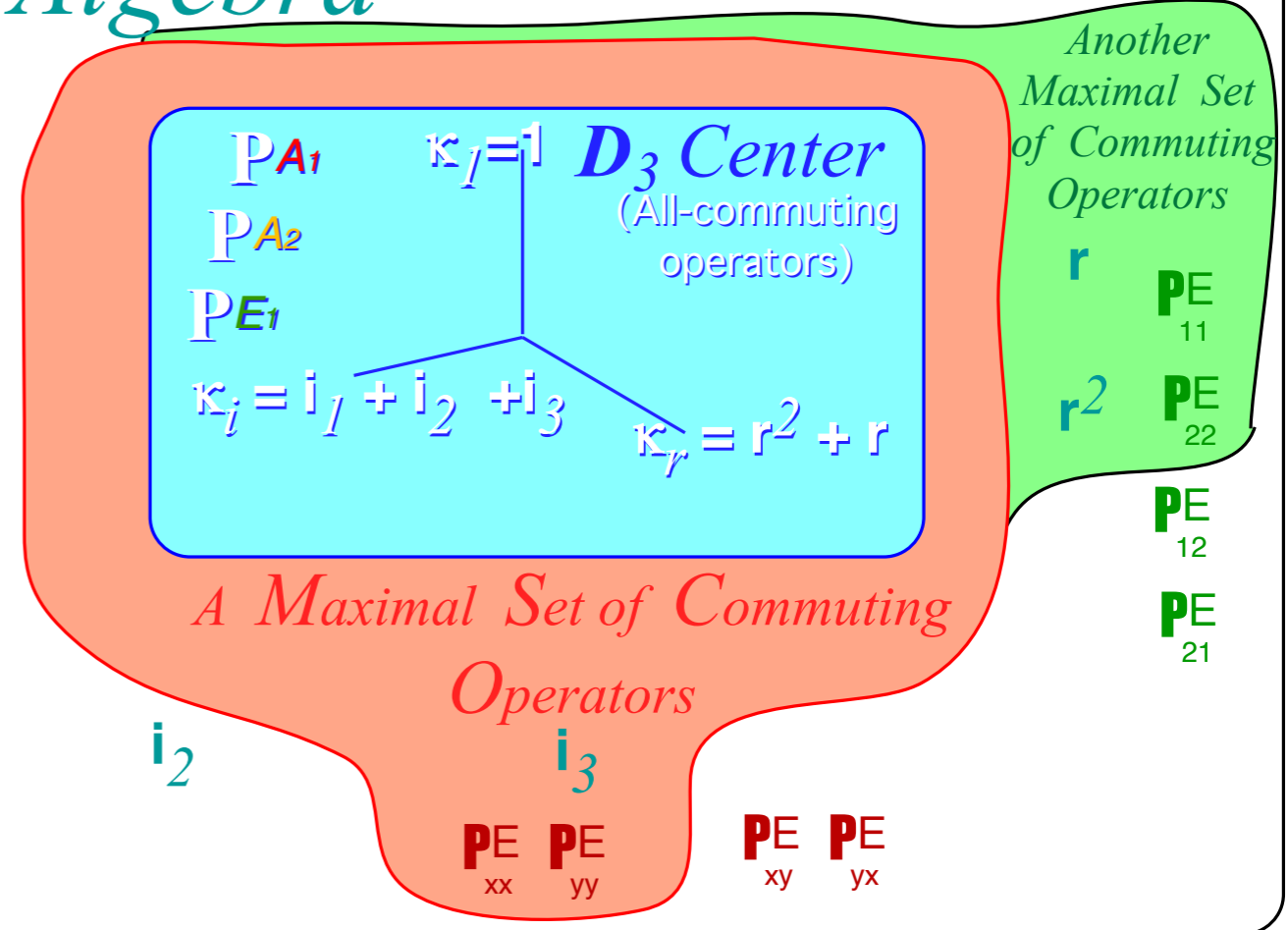
$g_t \kappa_k g_t^{-1} = \kappa_k$ where: $\kappa_k = \sum_{j=1}^{j=^{\circ}\kappa_k} g_j$

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$\circ s_k$ = order of g_k -self-symmetry: ($\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$)

Another Maximal Set of Commuting Operators

- r $P_{E_{11}}$
- r^2 $P_{E_{22}}$
- $P_{E_{12}}$
- $P_{E_{21}}$

A Maximal Set of Commuting Operators

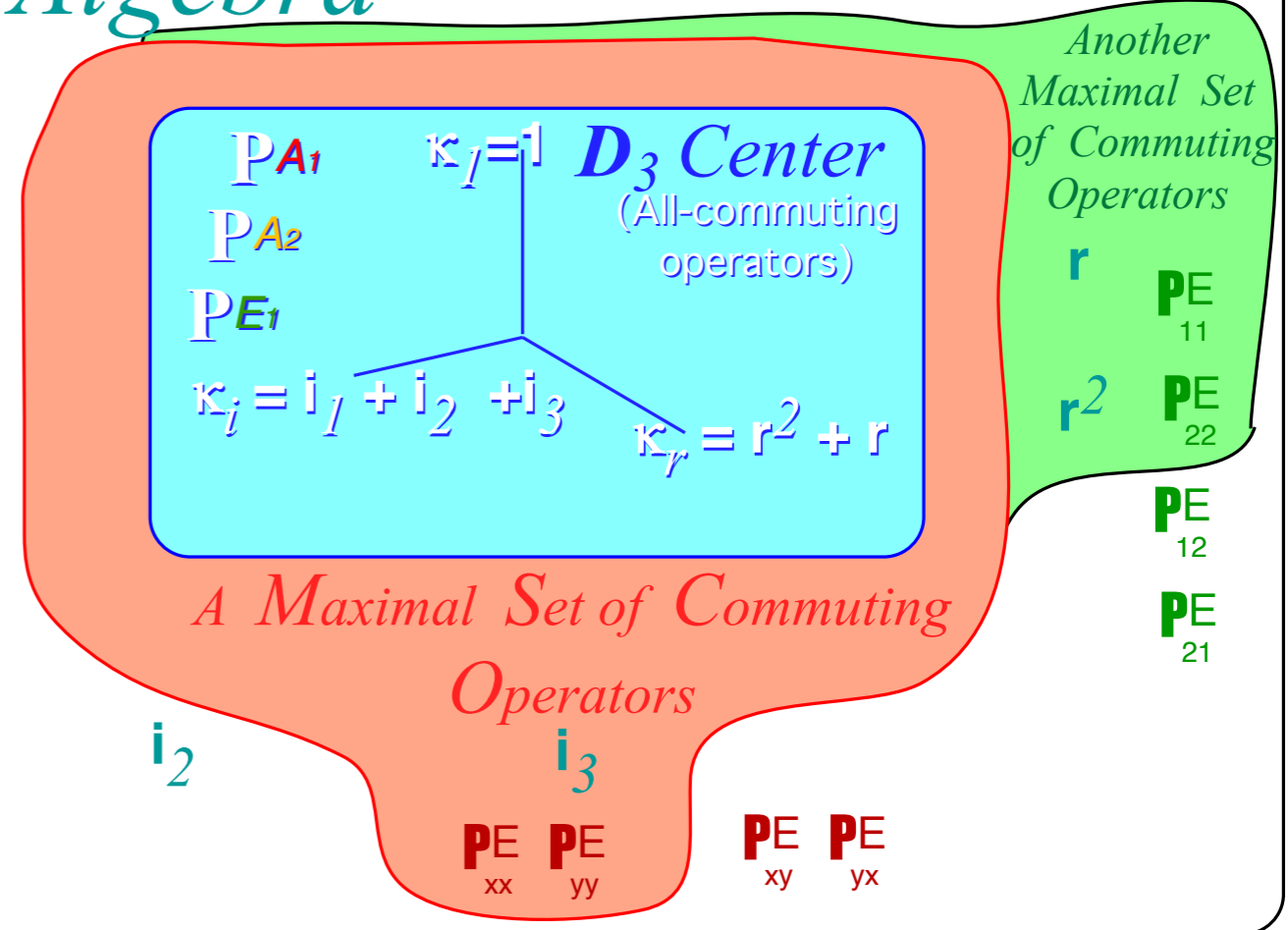
- i_1 $P_{E_{xx}}$
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i ₁	i ₃	i ₂	1	r	r ²
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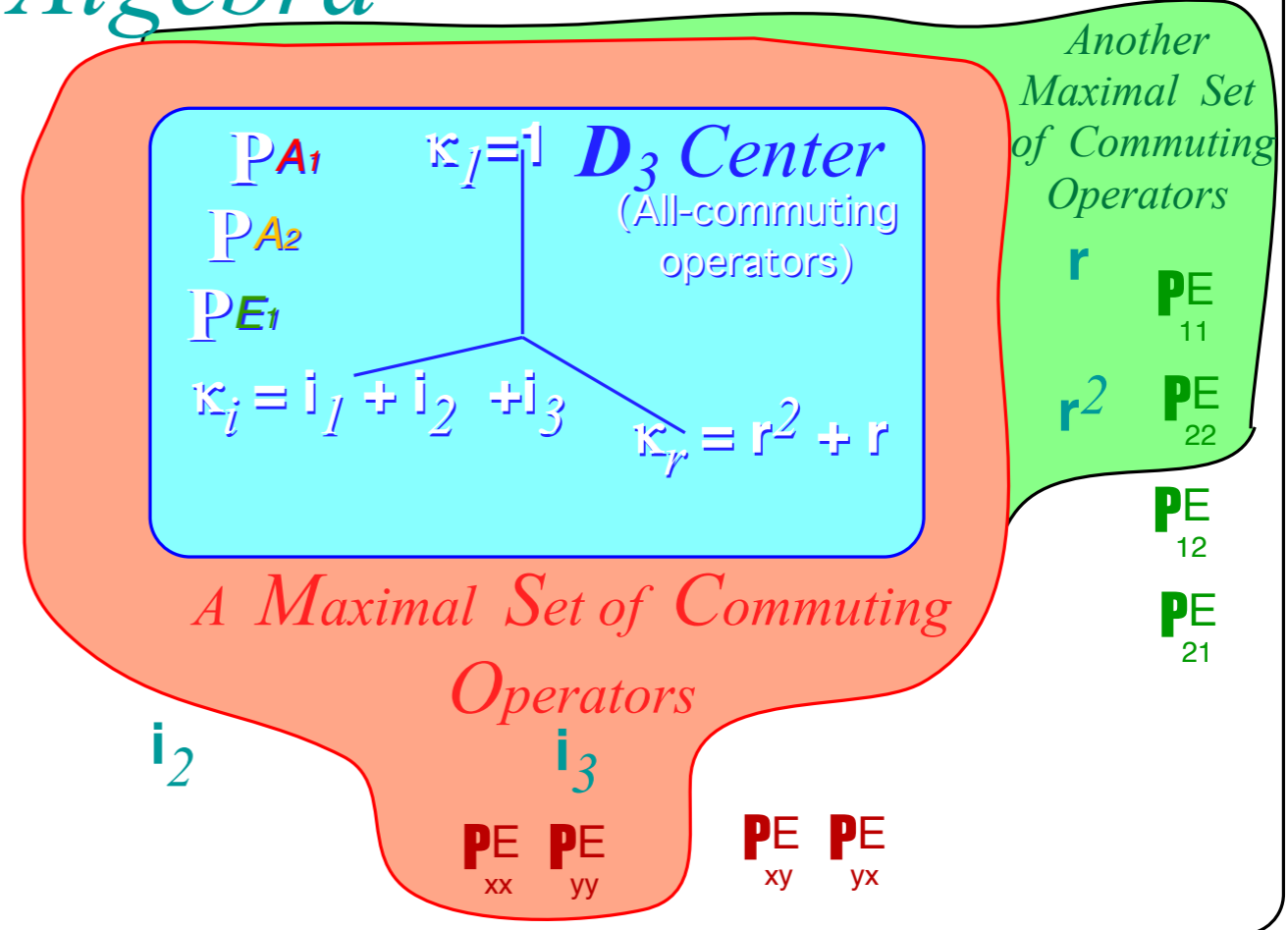
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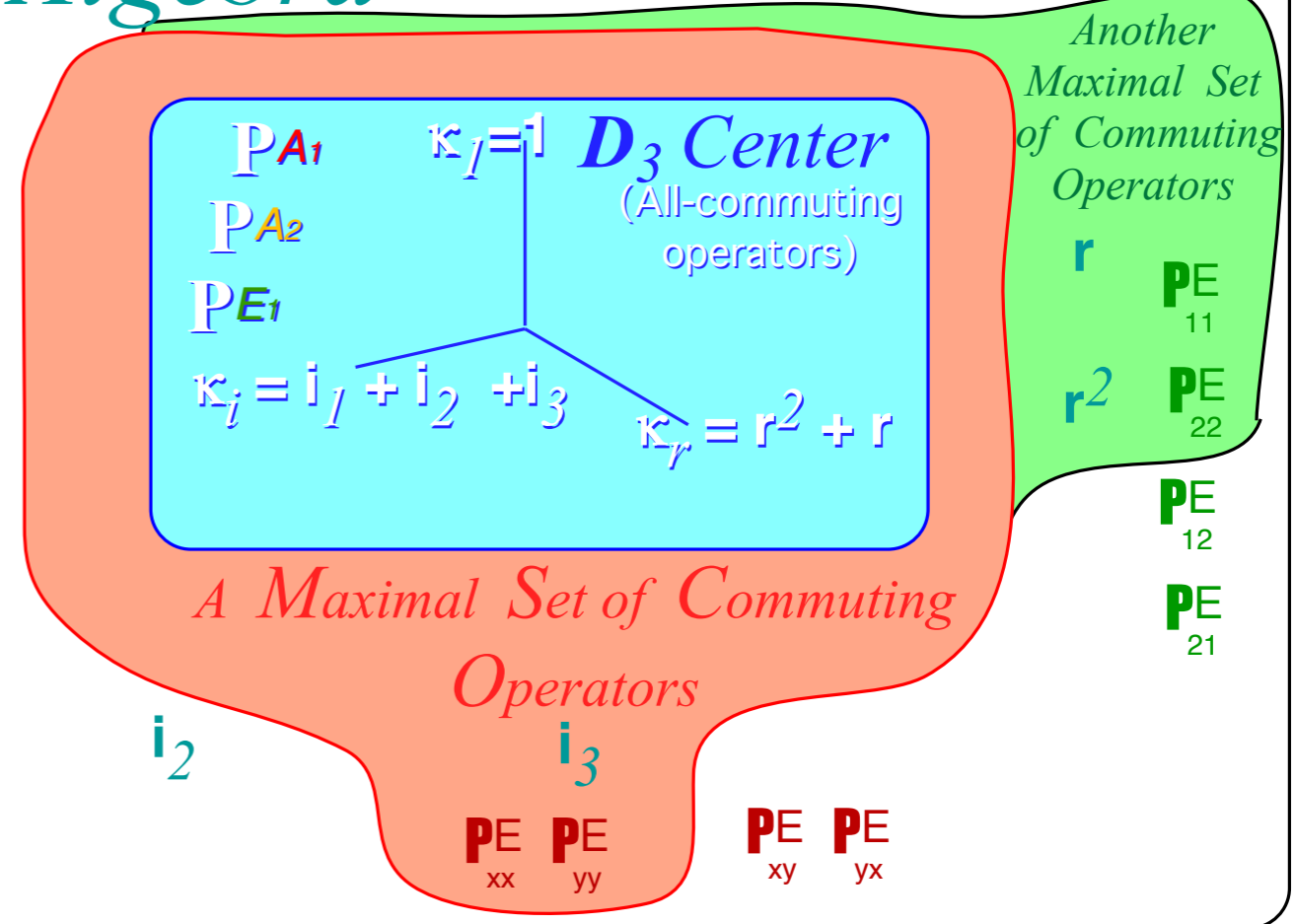
$\circ s_k = \circ G / \circ \kappa_k$ $\circ s_k$ is an integer count of D_3 operators g_s that commute with g_k .

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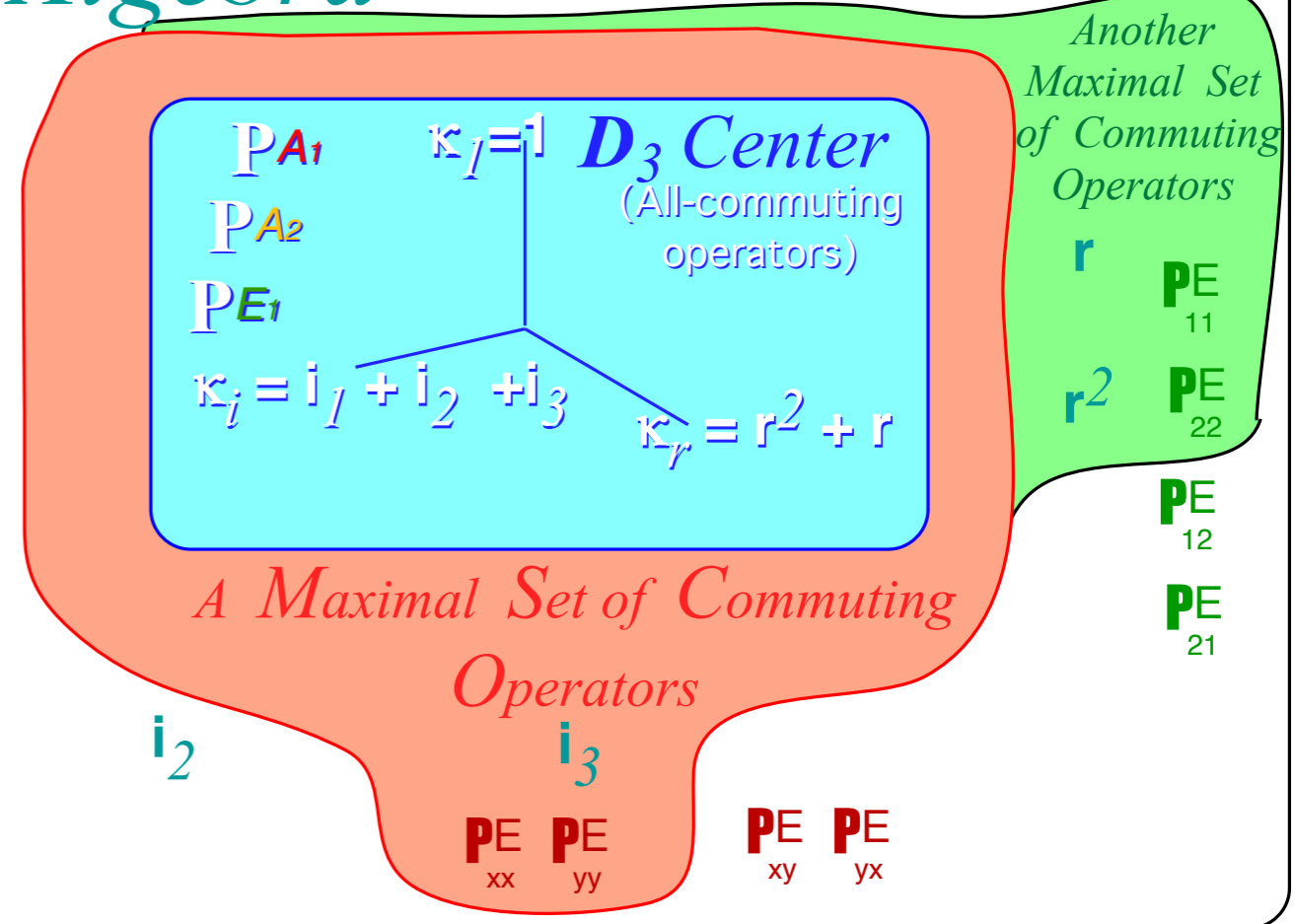
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If an operator g_t transforms g_k into a different element g'_k of its class: $g_t g_k g_t^{-1} = g'_k$, then so does $g_t g_s$. that is: $g_t g_s g_k (g_t g_s)^{-1} = g_t g_s g_k g_s^{-1} g_t^{-1} = g_t g_k g_t^{-1} = g'_k$,

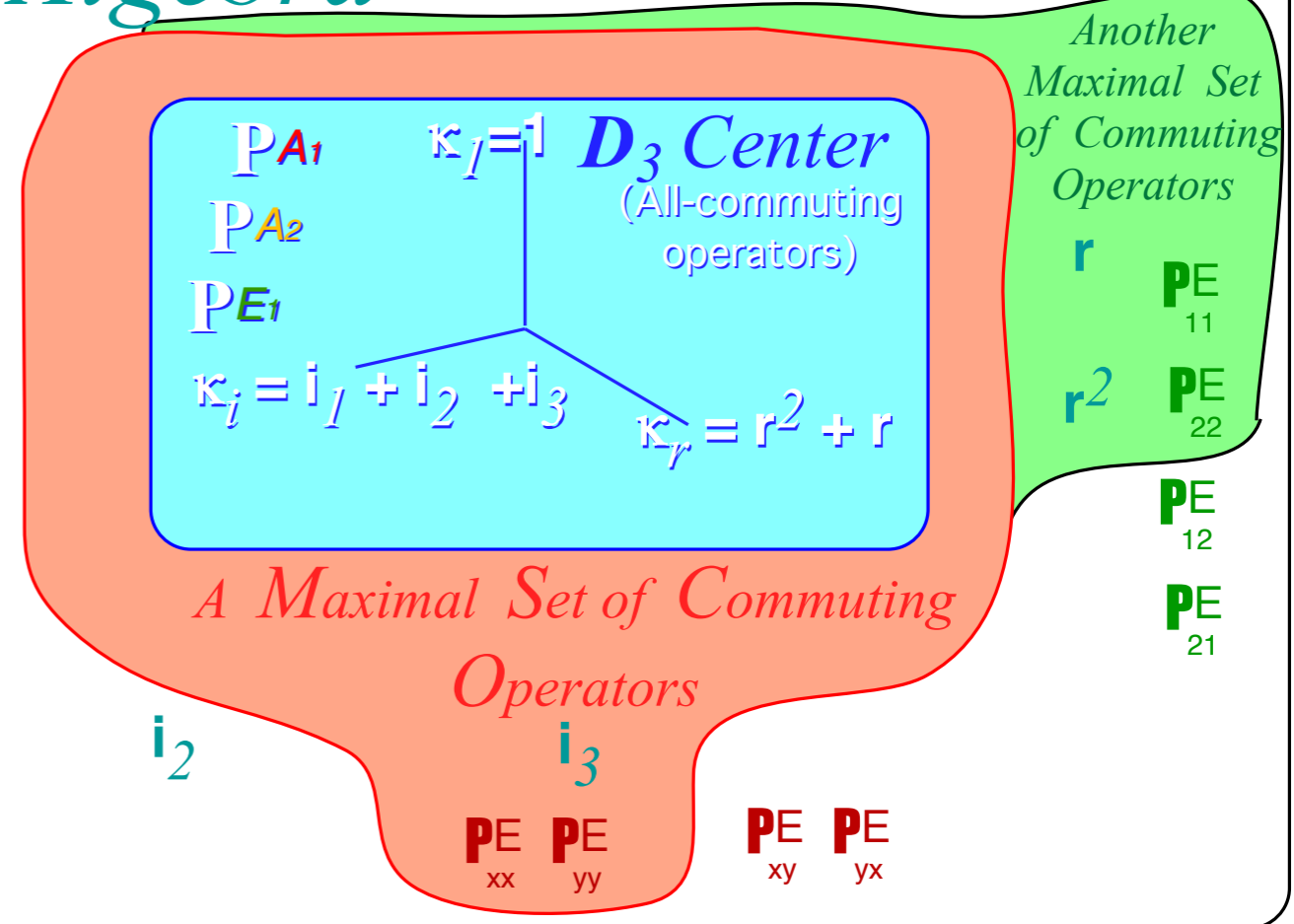
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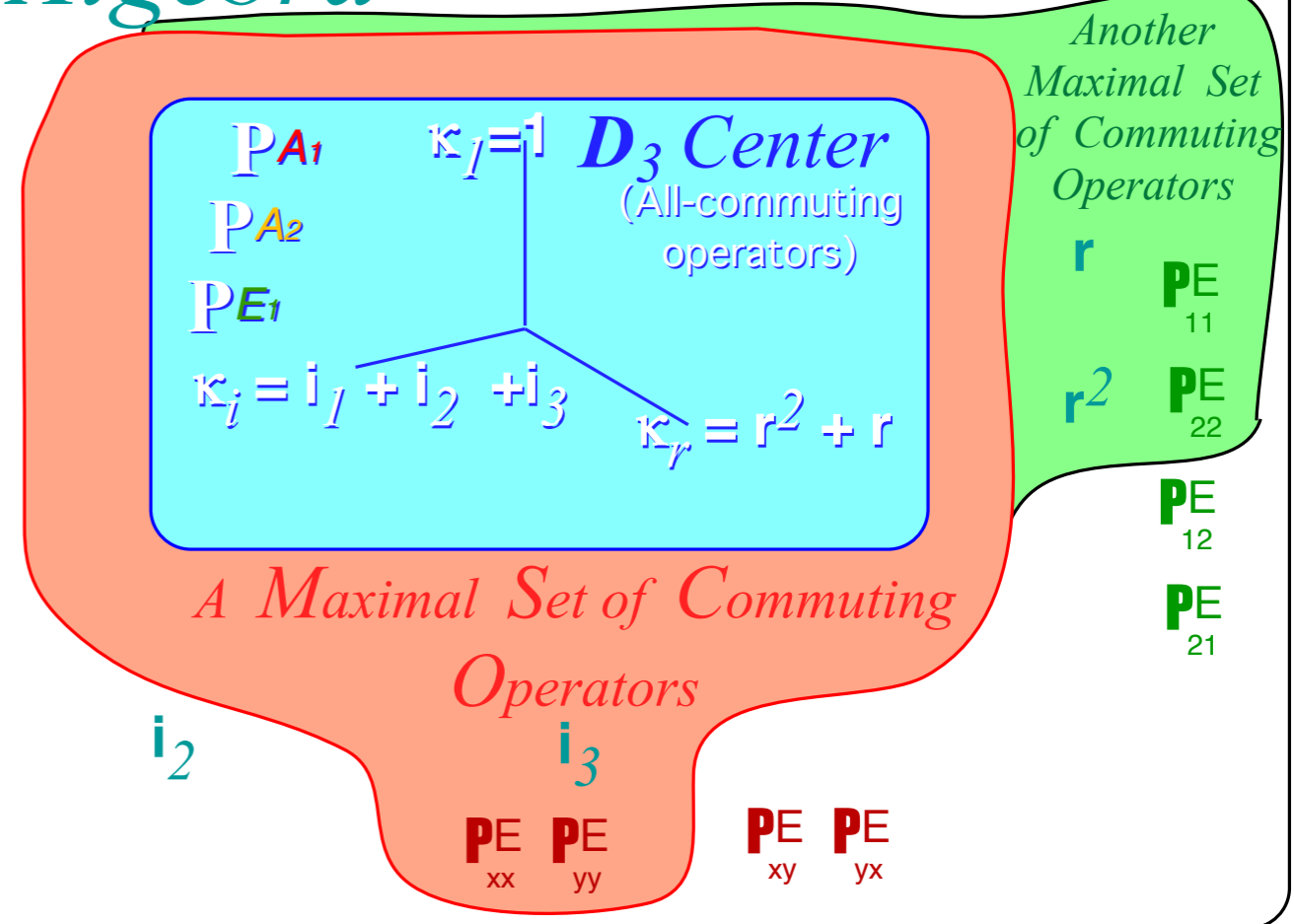
Subgroup $s_k = \{g_0=1, g_1=g_k, g_2, \dots\}$ has $\ell = (\circ \kappa_k - 1)$ **Left Cosets** (one coset for each member of class κ_k).

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

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

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

D_3 Algebra



Class-sum κ_k commutes with all g_t

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

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

$g_t \kappa_k g_t^{-1} = \kappa_k$ where: $\kappa_k = \sum_{j=1}^{\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{\circ G} g_t g_k g_t^{-1}$

$\circ s_k$ = order of g_k -self-symmetry: ($\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$)

$\circ s_k = \circ G / \circ \kappa_k$ $\circ s_k$ is an integer count of D_3 operators g_s that commute with g_k .

These operators g_s form the g_k -self-symmetry group s_k . Each g_s transforms g_k into itself: $g_s g_k g_s^{-1} = g_k$

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that is: $g_t g_s g_k (g_t g_s)^{-1} = g_t g_s g_k g_s^{-1} g_t^{-1} = g_t g_k g_t^{-1} = g'_k$,

Subgroup $s_k = \{g_0=1, g_1=g_k, g_2, \dots\}$ has $\ell = (\circ \kappa_k - 1)$ **Left Cosets** (one coset for each member of class κ_k).

$$\circ \kappa_k \begin{cases} g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\}, \\ g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots \end{cases}$$

$\underbrace{\hspace{10em}}_{\circ s_k}$

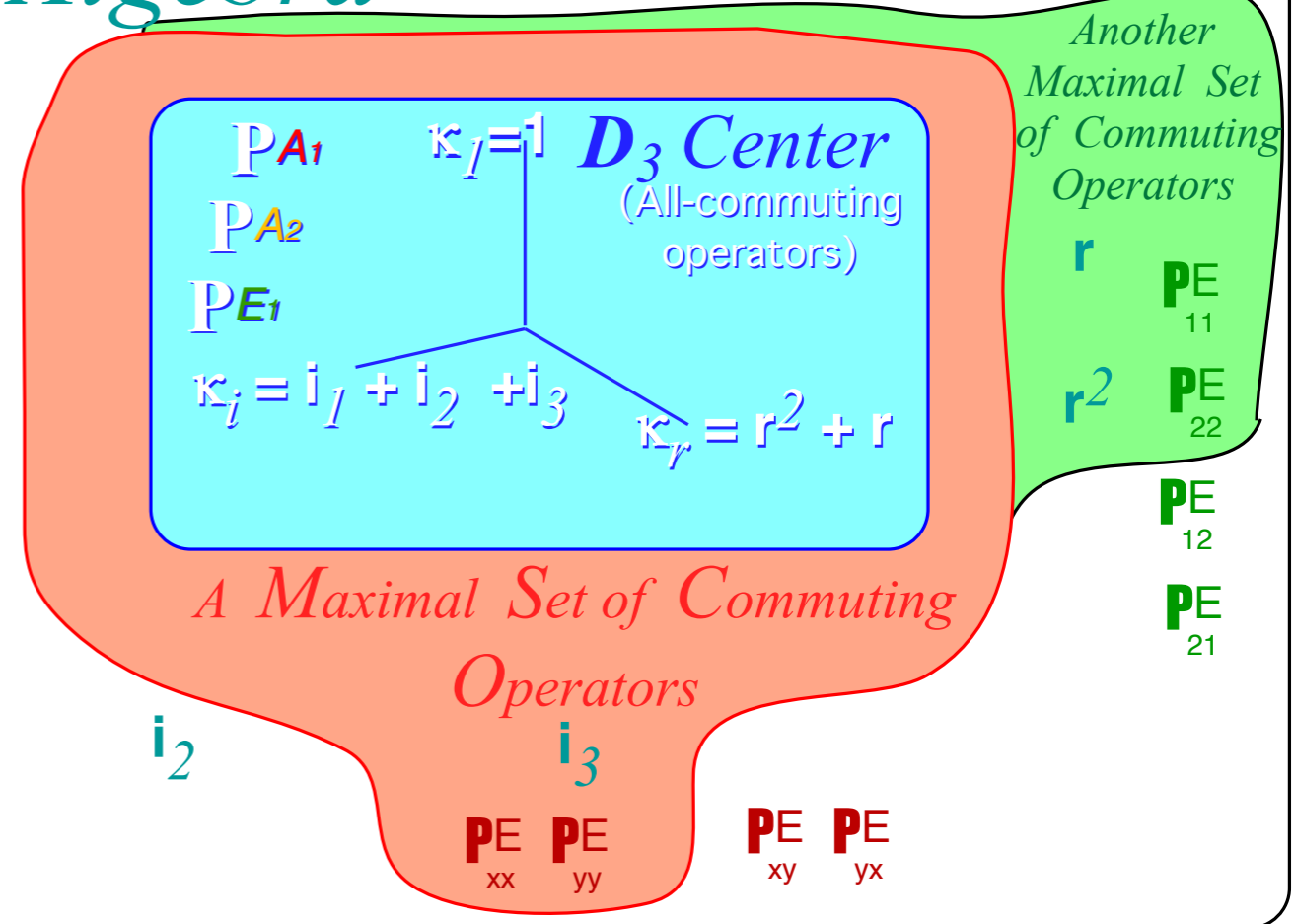
They will divide the group of order $\circ D_3 = \circ \kappa_k \cdot \circ s_k$ evenly into $\circ \kappa_k$ subsets each of order $\circ s_k$.

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

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
κ_i	κ_i	$2\kappa_i$	$3\kappa_1 + 3\kappa_r$

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$$g_t \kappa_k g_t^{-1} = \kappa_k \text{ where: } \kappa_k = \sum_{j=1}^{\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{\circ G} g_t g_k g_t^{-1}$$

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$\circ s_k = \circ G / \circ \kappa_k$ $\circ s_k$ is an integer count of D_3 operators g_s that commute with g_k .

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$$\circ \kappa_k \begin{cases} g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\}, \\ g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots \\ \vdots \end{cases}$$

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

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

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 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 $\ell=1-6$

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*

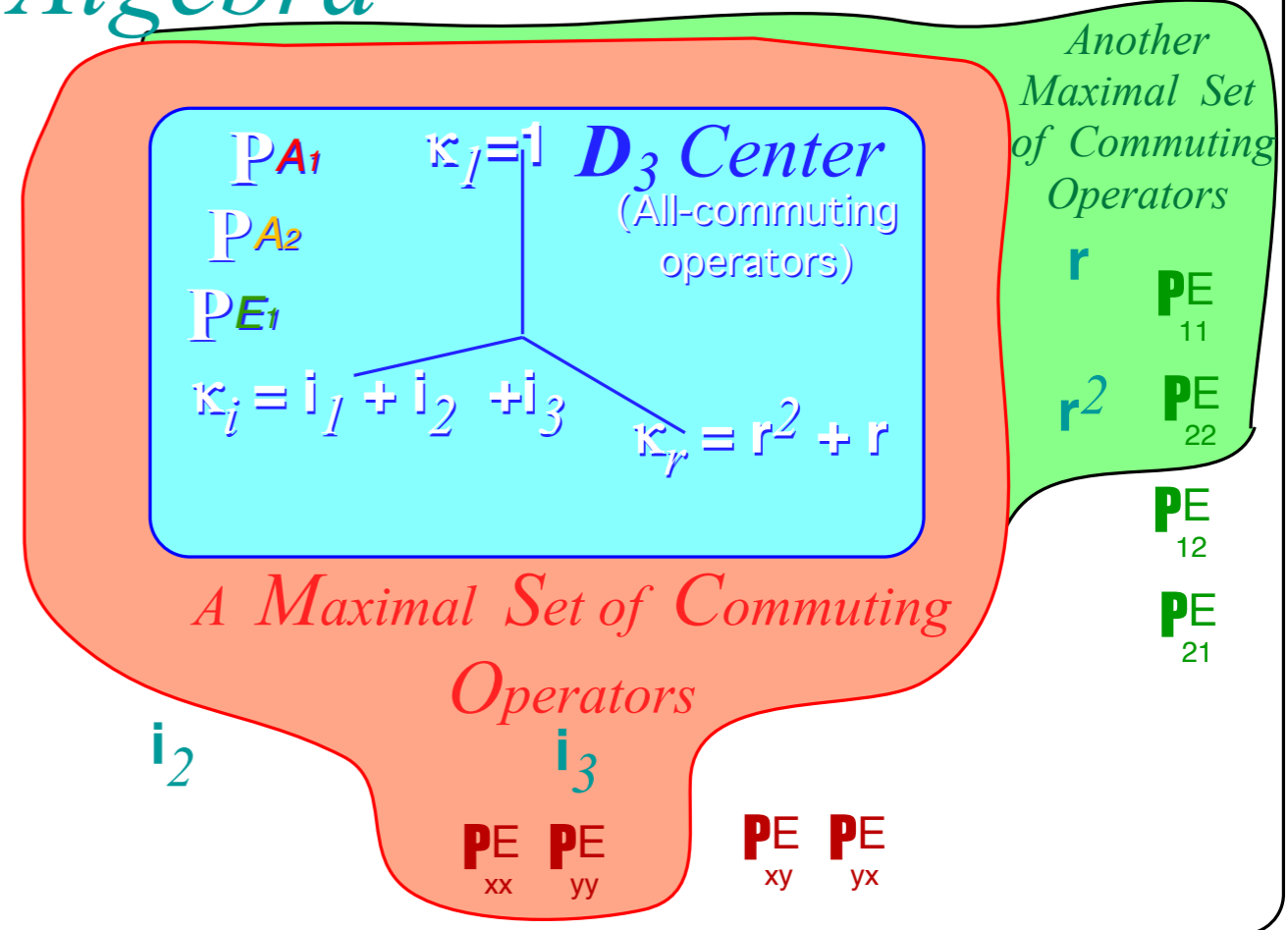
Tunneling modes and spectra for $D_3 \supset C_2$ and $D_3 \supset C_3$ local subgroup chains

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

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

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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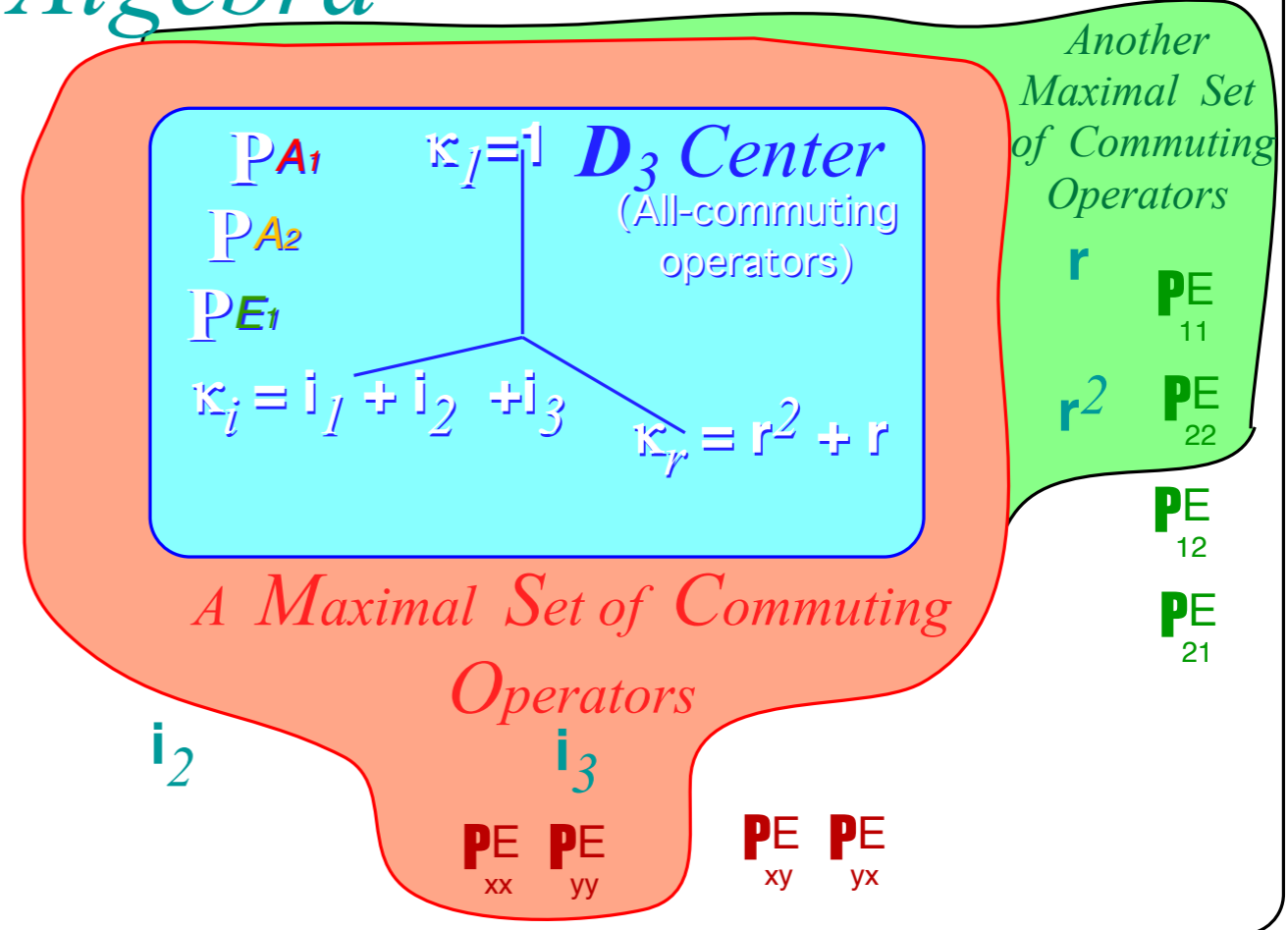
Class minimal equation

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

1	r ²	r	i ₁	i ₂	i ₃
r	1	r ²	i ₃	i ₁	i ₂
r ²	r	1	i ₂	i ₃	i ₁
i ₁	i ₃	i ₂	1	r	r ²
i ₂	i ₁	i ₃	r ²	1	r
i ₃	i ₂	i ₁	r	r ²	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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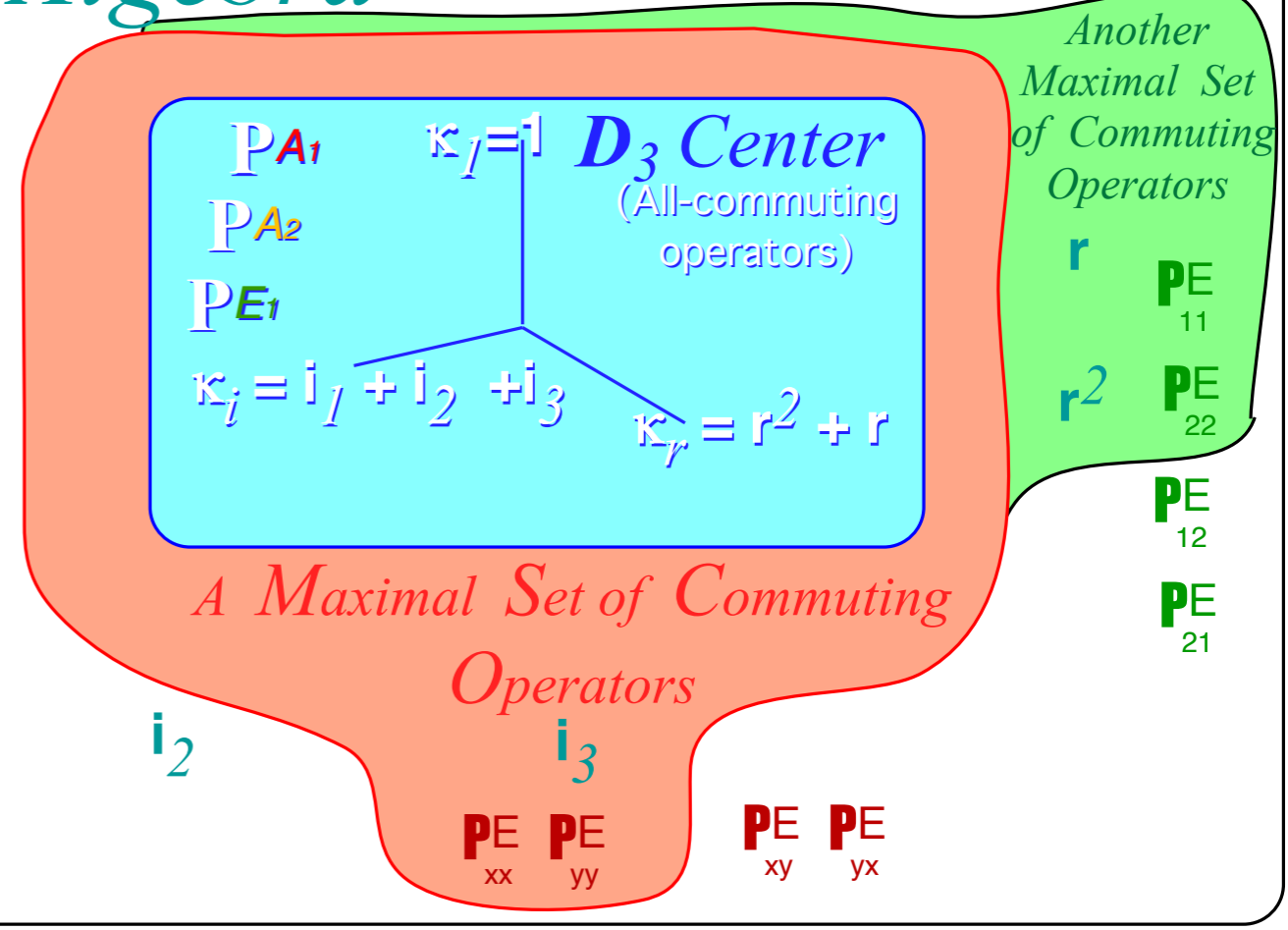
$$\kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot 1$$

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

1	r²	r	i₁	i₂	i₃
r	1	r²	i₃	i₁	i₂
r²	r	1	i₂	i₃	i₁
i₁	i₃	i₂	1	r	r²
i₂	i₁	i₃	r²	1	r
i₃	i₂	i₁	r	r²	1

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i$

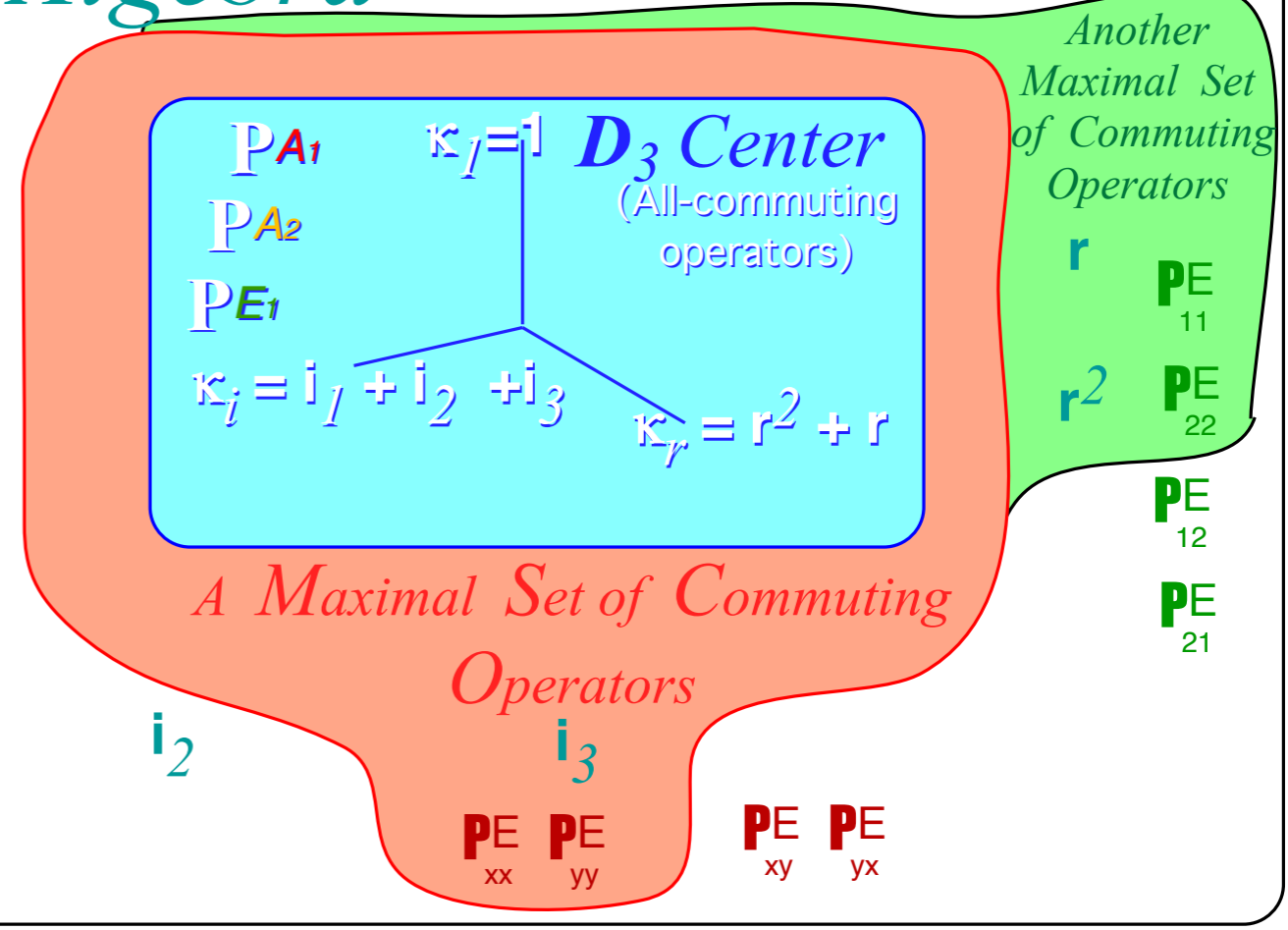
$\kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot 1$

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	$\mathbf{1}$

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

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

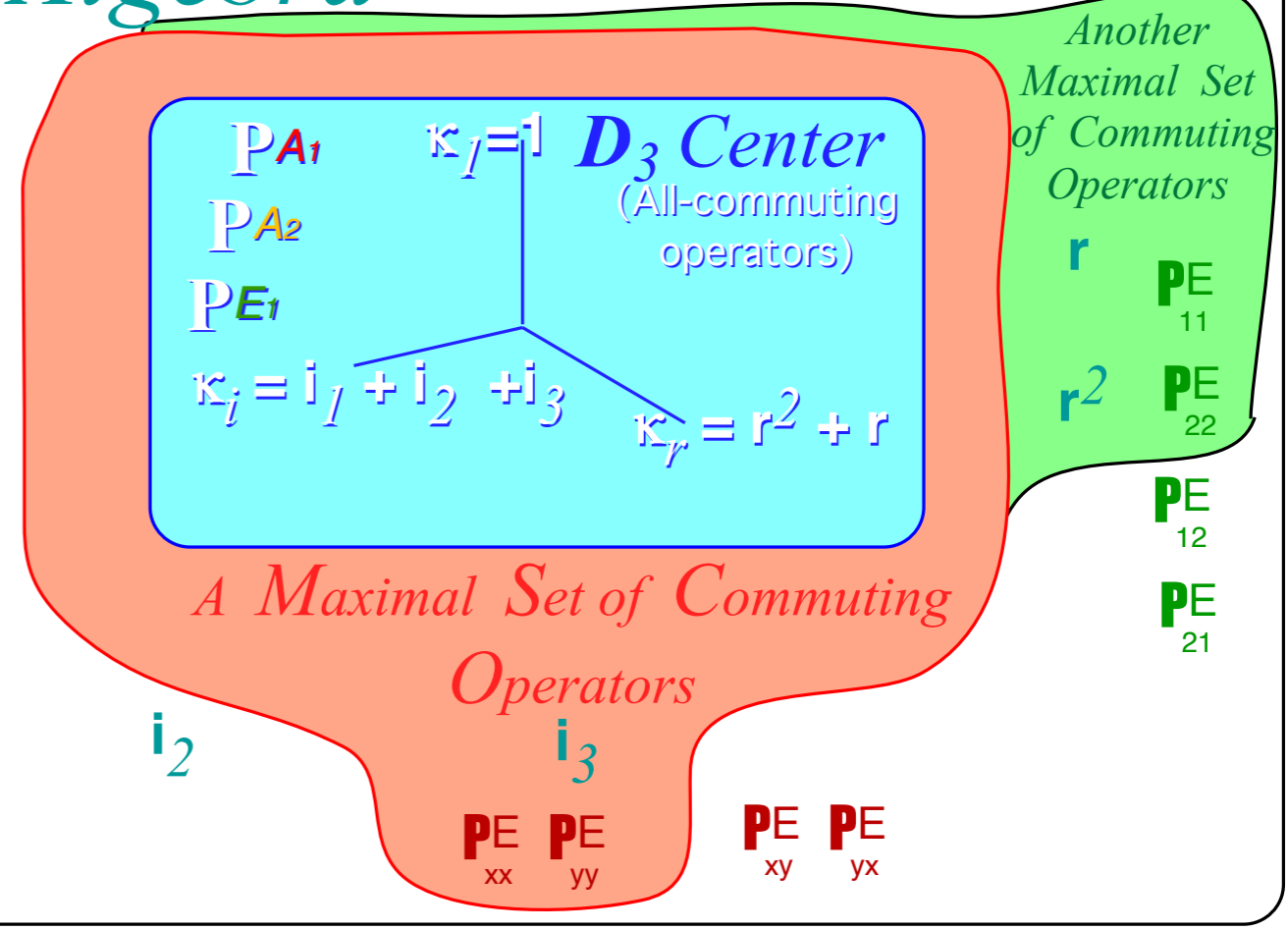
$0 = \kappa_i^3 - 9 \cdot \kappa_i = (\kappa_i - 3 \cdot \mathbf{1})(\kappa_i + 3 \cdot \mathbf{1})(\kappa_i - 0 \cdot \mathbf{1})$

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	$\mathbf{1}$

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

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Class minimal equation

$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \leftarrow \quad \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

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

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

$$\kappa_r = 2 \cdot P^{A_1} + 2 \cdot P^{A_2} - 1 \cdot P^E \quad \leftarrow \quad \kappa_r^2 = \kappa_r + 2 \cdot \mathbf{1} \Rightarrow (\kappa_r - 2 \cdot \mathbf{1})(\kappa_r + \mathbf{1}) = \mathbf{0}$$

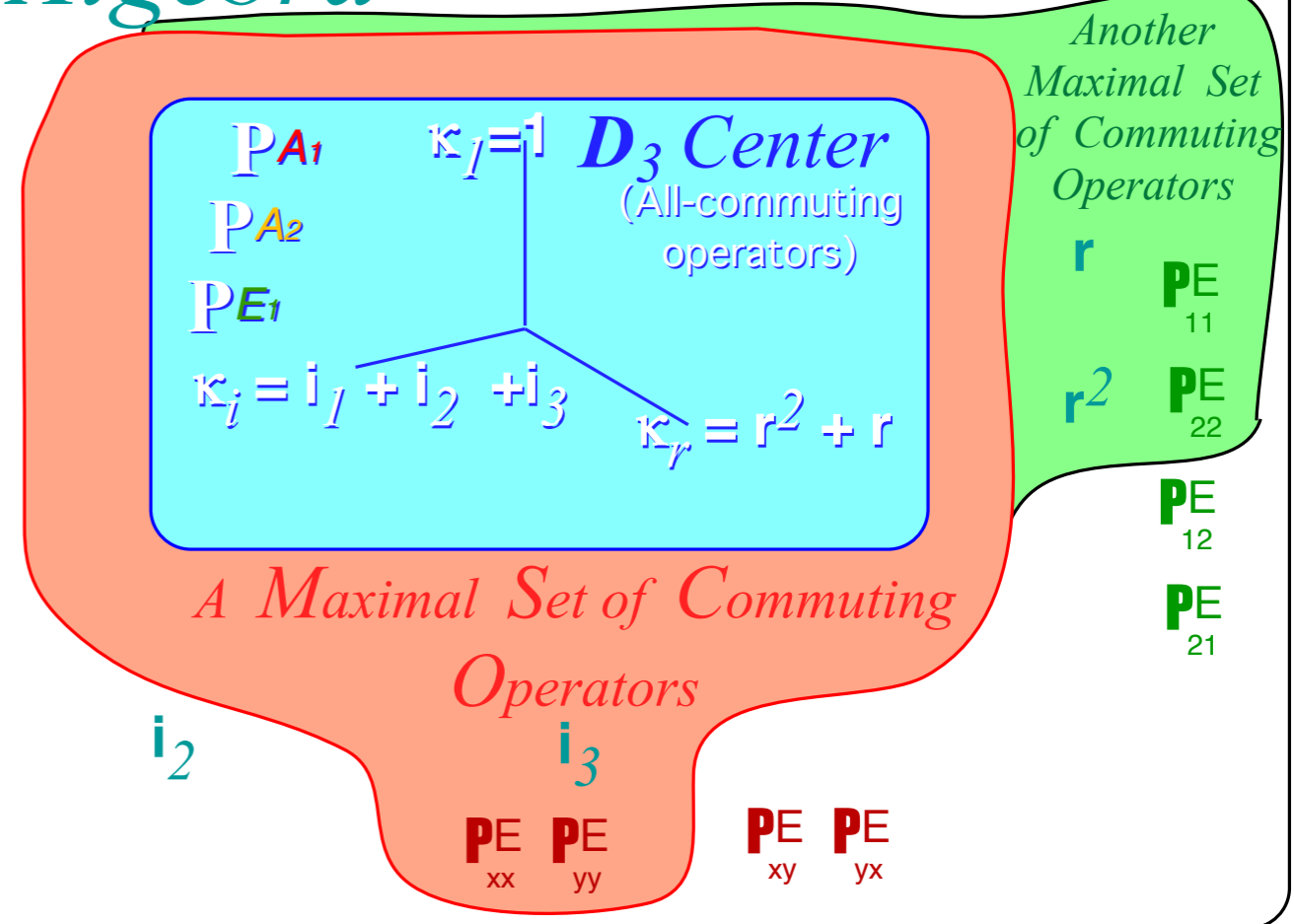
$$\kappa_i = 3 \cdot P^{A_1} - 3 \cdot P^{A_2} + 0 \cdot P^E$$

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	$\mathbf{1}$

	$\kappa_1 = \mathbf{1}$	$\kappa_r = \mathbf{r} + \mathbf{r}^2$	$\kappa_i = \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$
κ_1	κ_1	κ_r	κ_i
κ_r	κ_r	$2\kappa_1 + \kappa_r$	$2\kappa_i$
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$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \leftarrow \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

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

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

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

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

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

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

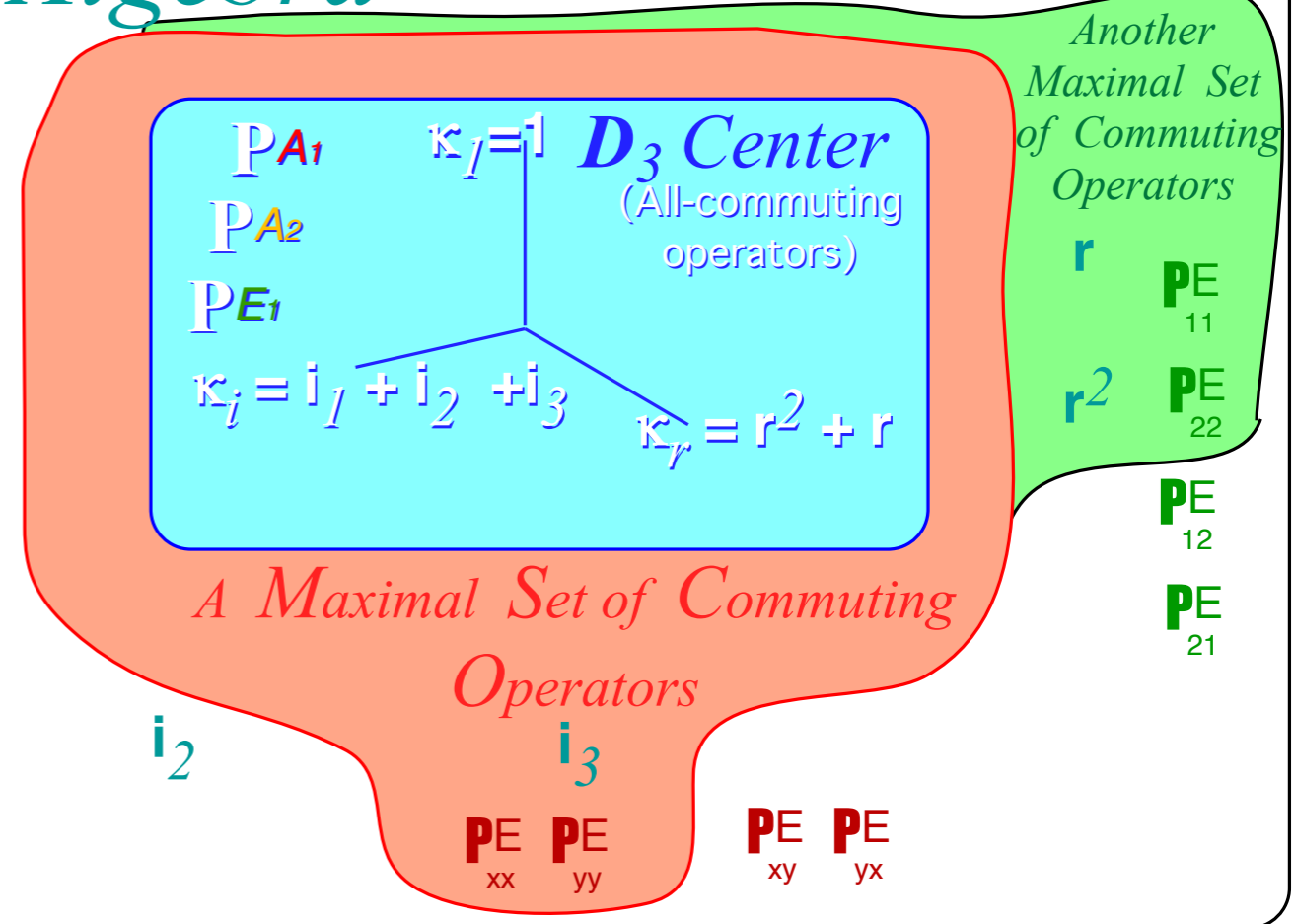
$$\mathbf{P}^E = \frac{(\kappa_i - 3 \cdot \mathbf{1})(\kappa_i + 3 \cdot \mathbf{1})}{(+0 - 3)(+0 + 3)}$$

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$\mathbf{1}$	\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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$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

$$0 = \kappa_i^3 - 9 \cdot \kappa_i = (\kappa_i - 3 \cdot \mathbf{1})(\kappa_i + 3 \cdot \mathbf{1})(\kappa_i - 0 \cdot \mathbf{1}) \quad \text{Class ortho-complete projector relations}$$

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

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

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

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

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

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

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

D_3 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	$\mathbf{1}$

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Class-sum κ_k invariance:

$$\mathbf{g}_t \kappa_k = \kappa_k \mathbf{g}_t$$

${}^\circ G$ = 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

$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \leftarrow \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

$$0 = \kappa_i^3 - 9 \cdot \kappa_i = (\kappa_i - 3 \cdot \mathbf{1})(\kappa_i + 3 \cdot \mathbf{1})(\kappa_i - 0 \cdot \mathbf{1}) \quad \text{Class ortho-complete projector relations}$$

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

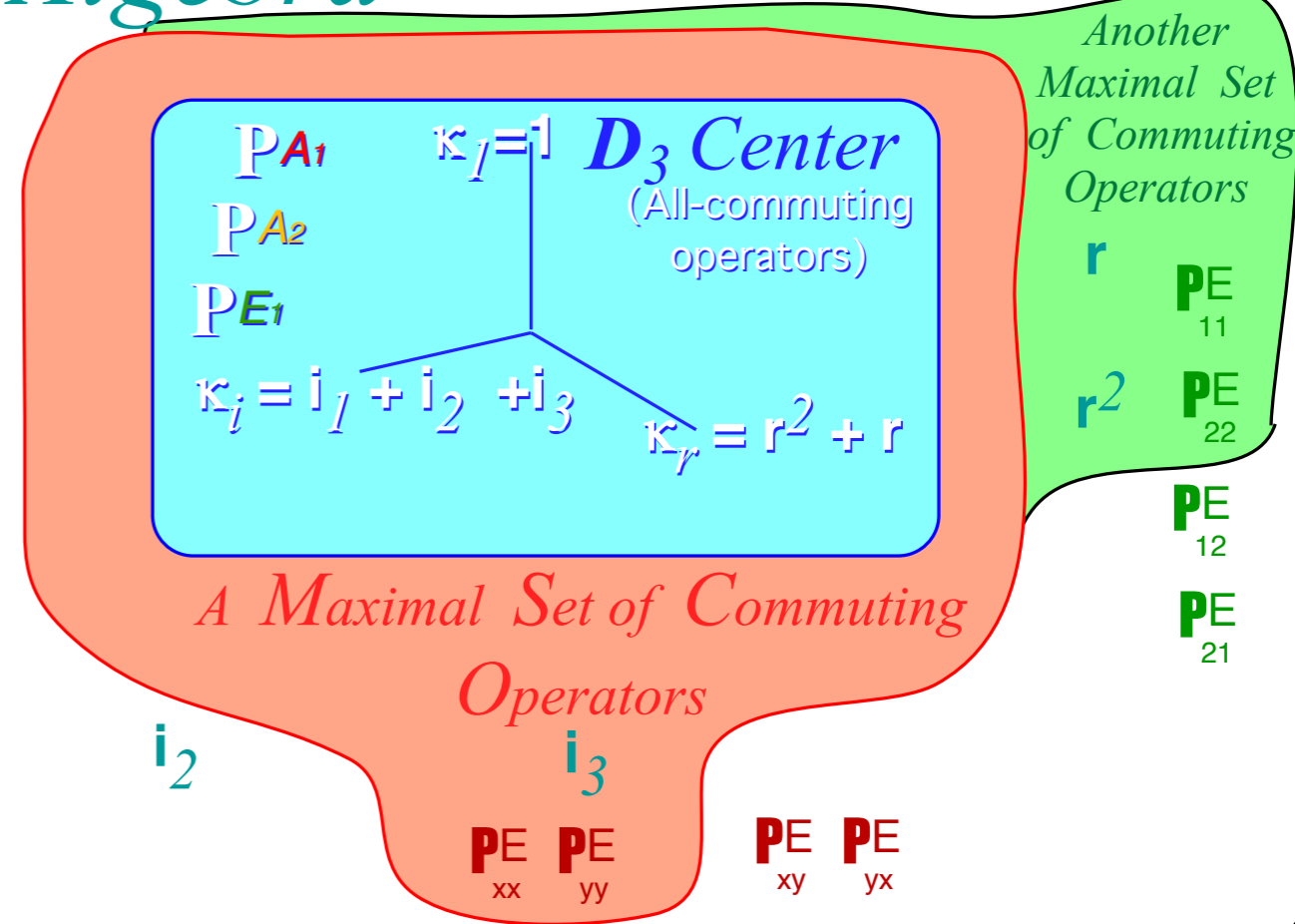
$$\kappa_r = 2 \cdot \mathbf{P}^{A_1} + 2 \cdot \mathbf{P}^{A_2} - 1 \cdot \mathbf{P}^E$$

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

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

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

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



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

$$\mathbf{P}^{(\alpha)} = \frac{\ell^{(\alpha)}}{{}^\circ G} \sum_k \chi_k^{(\alpha)*} \kappa_k$$

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

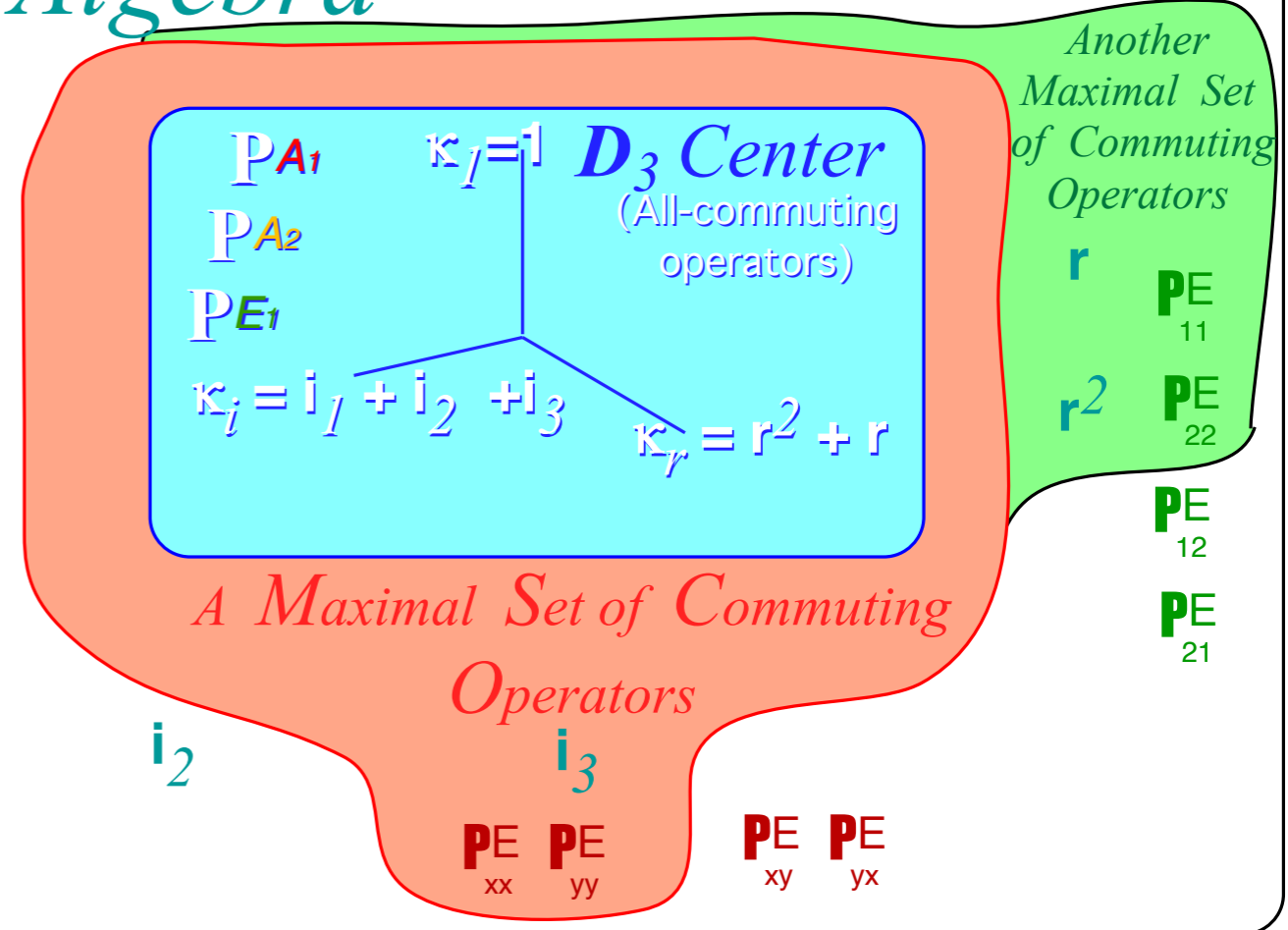
χ_k^α	χ_1^α	χ_r^α	χ_i^α
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	2	-1	0

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

D_3 Algebra

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

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
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 g_t

Class-sum κ_k invariance:

$$g_t \kappa_k = \kappa_k g_t$$

$^{\circ}G$ = 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

$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot 1$$

$$0 = \kappa_i^3 - 9 \cdot \kappa_i = (\kappa_i - 3 \cdot 1)(\kappa_i + 3 \cdot 1)(\kappa_i - 0 \cdot 1) \quad \text{Class ortho-complete projector relations}$$

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

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

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

$$P^{A_1} = (\kappa_1 + \kappa_r + \kappa_i)/6 = (1 + r + r^2 + i_1 + i_2 + i_3)/6$$

$$P^{A_2} = (\kappa_1 + \kappa_r - \kappa_i)/6 = (1 + r + r^2 - i_1 - i_2 - i_3)/6$$

$$P^E = (2\kappa_1 - \kappa_r + 0)/3 = (21 - r - r^2)/3$$

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

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

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

Use $\chi_1^{(\alpha)*} = \ell^{(\alpha)}$ to find κ_1 coefficient

$$P^{(\alpha)} = \frac{(\ell^{(\alpha)})^2}{{}^{\circ}G} \kappa_1 + \dots$$

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: $f^{(a)}(D^{(\alpha)}(G) \downarrow H)$

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D_3 examples for $\ell=1-6$

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

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

$$\begin{array}{c}
 R^G(\mathbf{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{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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}$$

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

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

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

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 traces*

$$\begin{array}{c}
 R^G(\mathbf{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{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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}$$

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

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

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

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

$$\mathbf{P}^E = (2\kappa_1 - \kappa_2 + 0)/3 = (2\mathbf{1} - \mathbf{r} - \mathbf{r}^2 + 0 + 0 + 0)/3 \Rightarrow R(\mathbf{P}^E) = \frac{1}{3} \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 1 \end{pmatrix} \quad \text{Trace} R(\mathbf{P}^E) = 4$$

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

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

$$\begin{array}{c}
 R^G(\mathbf{1}) = \\
 R^G(\mathbf{r}) = \\
 R^G(\mathbf{r}^2) = \\
 R^G(\mathbf{i}_1) = \\
 R^G(\mathbf{i}_2) = \\
 R^G(\mathbf{i}_3) =
 \end{array}
 \begin{array}{c}
 \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}
 \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}
 \end{array}$$

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

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

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

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

$$\begin{array}{c}
 R^G(\mathbf{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{array}{c}
 R^G(\mathbf{r})= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{r}^2)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_1)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_2)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_3)= \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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}$$

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

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

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

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

$$\begin{matrix}
 R^G(\mathbf{1})= & R^G(\mathbf{r})= & R^G(\mathbf{r}^2)= & R^G(\mathbf{i}_1)= & R^G(\mathbf{i}_2)= & R^G(\mathbf{i}_3)= \\
 \begin{matrix} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{matrix} \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}
 \end{matrix}$$

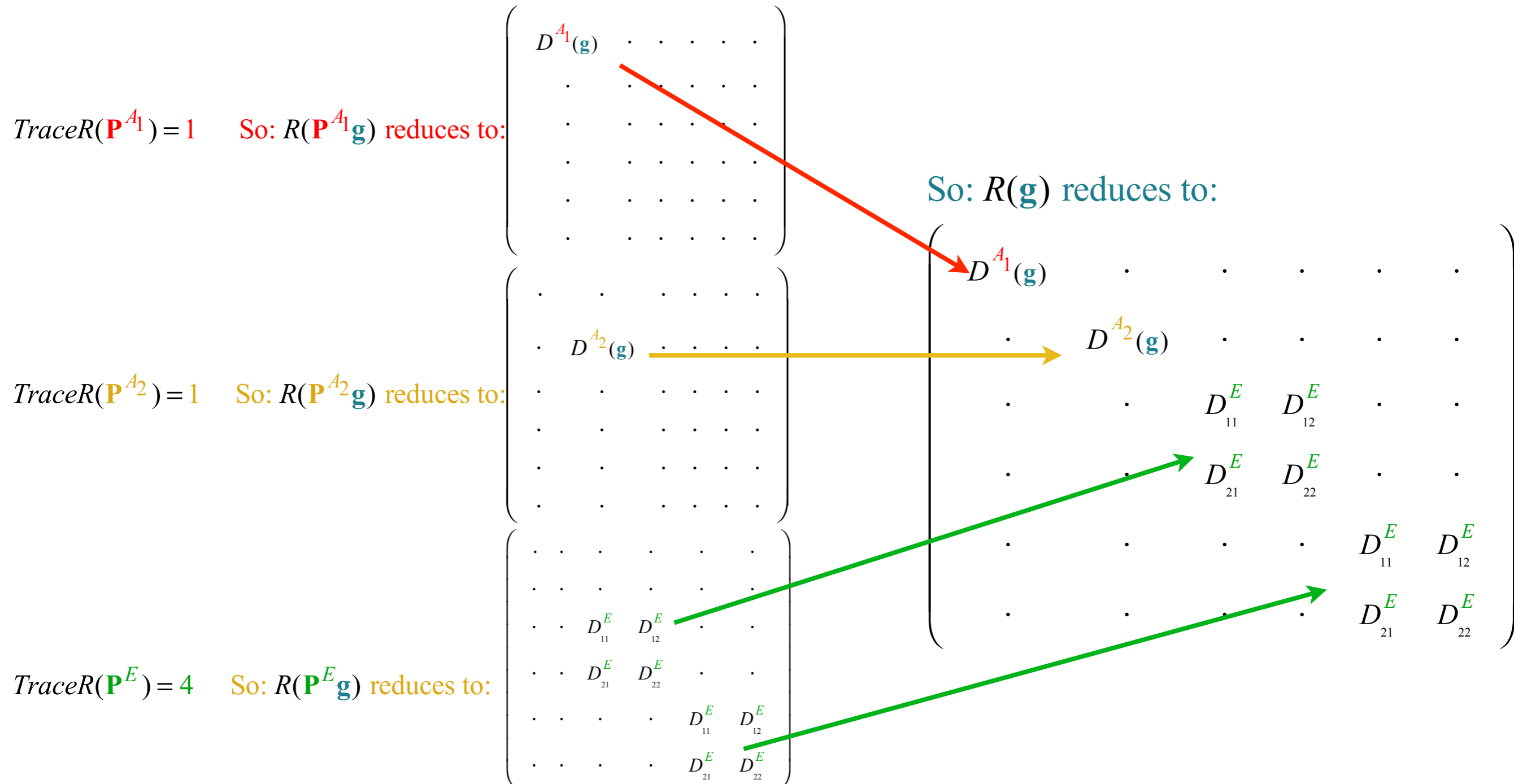
$$R(\mathbf{P}^{A_1}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} /6 \Rightarrow \text{Trace}R(\mathbf{P}^{A_1}) = 1 \quad \text{So: } R(\mathbf{P}^{A_1}\mathbf{g}) \text{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

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

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

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

$$\begin{array}{c}
 R^G(\mathbf{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{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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}$$



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 $\ell=1-6$

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

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

$$\begin{array}{c}
 R^G(\mathbf{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{array}{c}
 R^G(\mathbf{r}) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{r}^2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_1) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_2) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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{array}{c}
 R^G(\mathbf{i}_3) = \\
 \\
 \\
 \\
 \\
 \\
 \end{array}
 \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 E_1

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

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

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

$$\begin{matrix}
 R^G(\mathbf{1}) = & R^G(\mathbf{r}) = & R^G(\mathbf{r}^2) = & R^G(\mathbf{i}_1) = & R^G(\mathbf{i}_2) = & R^G(\mathbf{i}_3) = \\
 \begin{matrix} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{matrix} \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}
 \end{matrix}$$

$\{R^G(\mathbf{g})\}$ 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 E_1

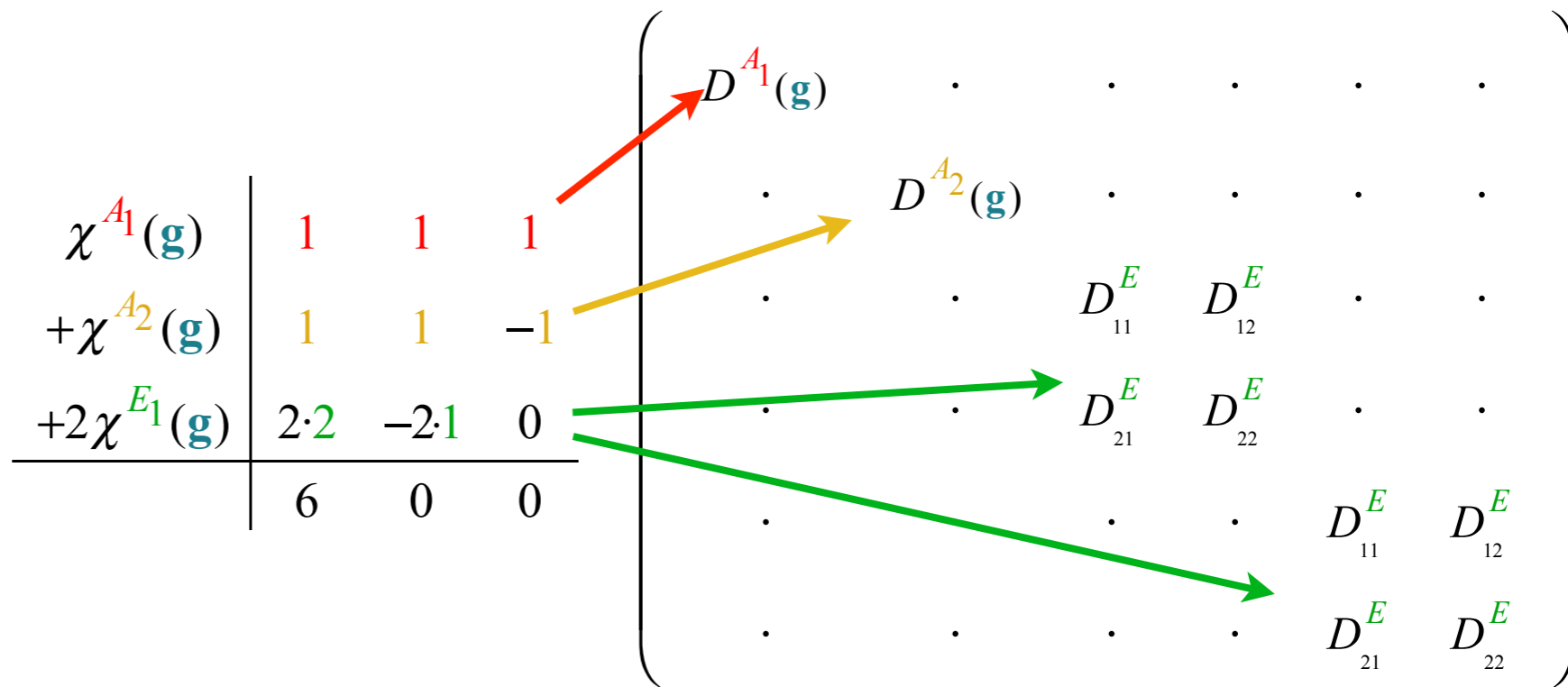
$R(\mathbf{g})$ reduces to:

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

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



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

$$\begin{matrix}
 R^G(\mathbf{1}) = & R^G(\mathbf{r}) = & R^G(\mathbf{r}^2) = & R^G(\mathbf{i}_1) = & R^G(\mathbf{i}_2) = & R^G(\mathbf{i}_3) = \\
 \begin{matrix} 1 \\ r^1 \\ r^2 \\ i_1 \\ i_2 \\ i_3 \end{matrix} \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}
 \end{matrix}$$

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

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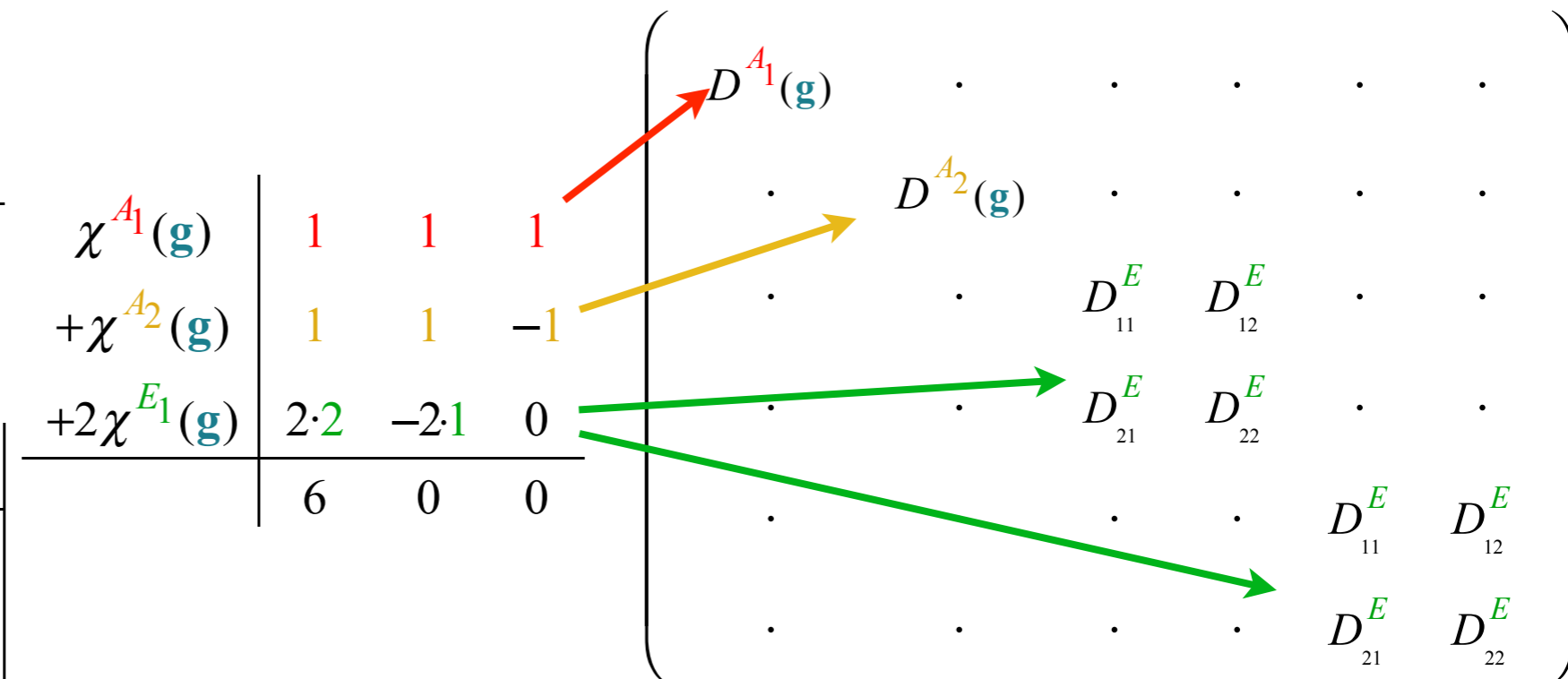
$R(\mathbf{g})$ reduces to:

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

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



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)

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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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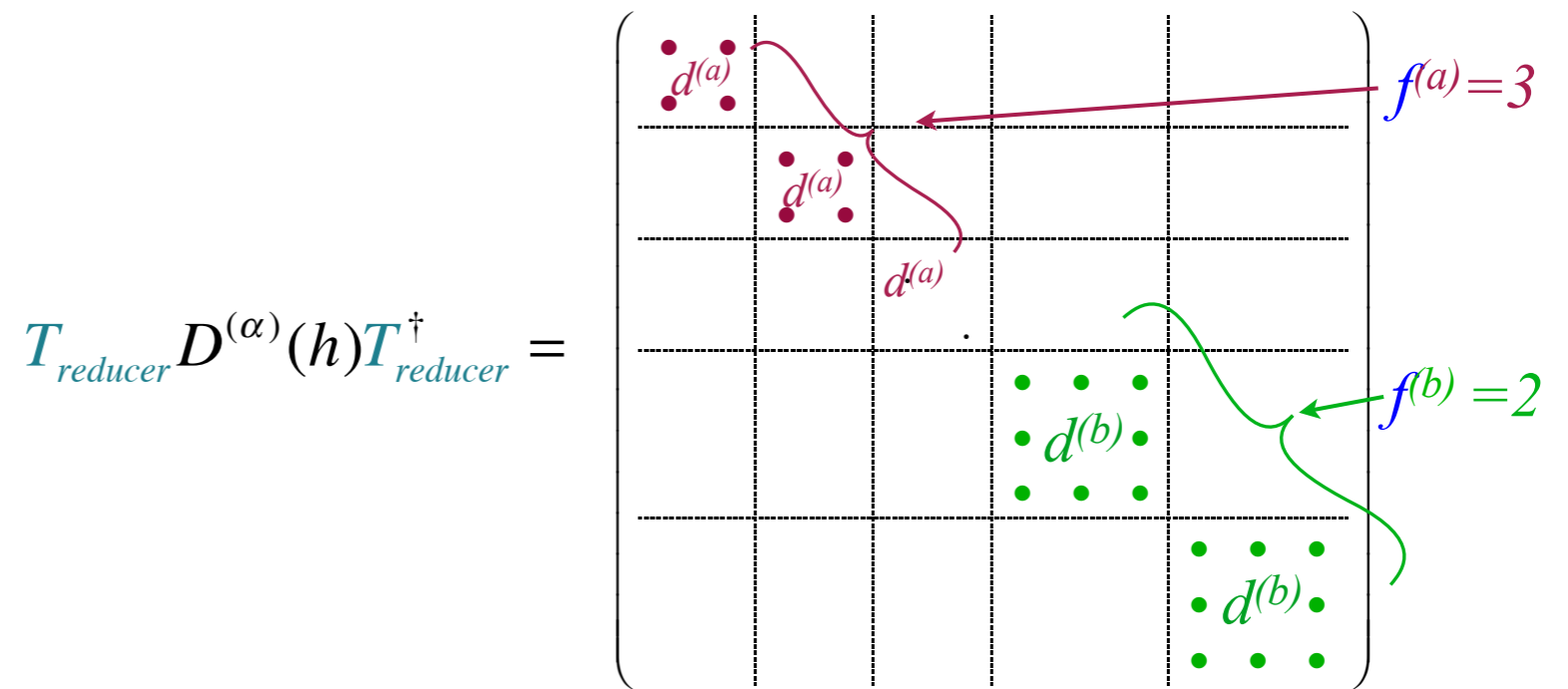


Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G) \downarrow H)$

(irep \equiv irreducible representation)

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

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



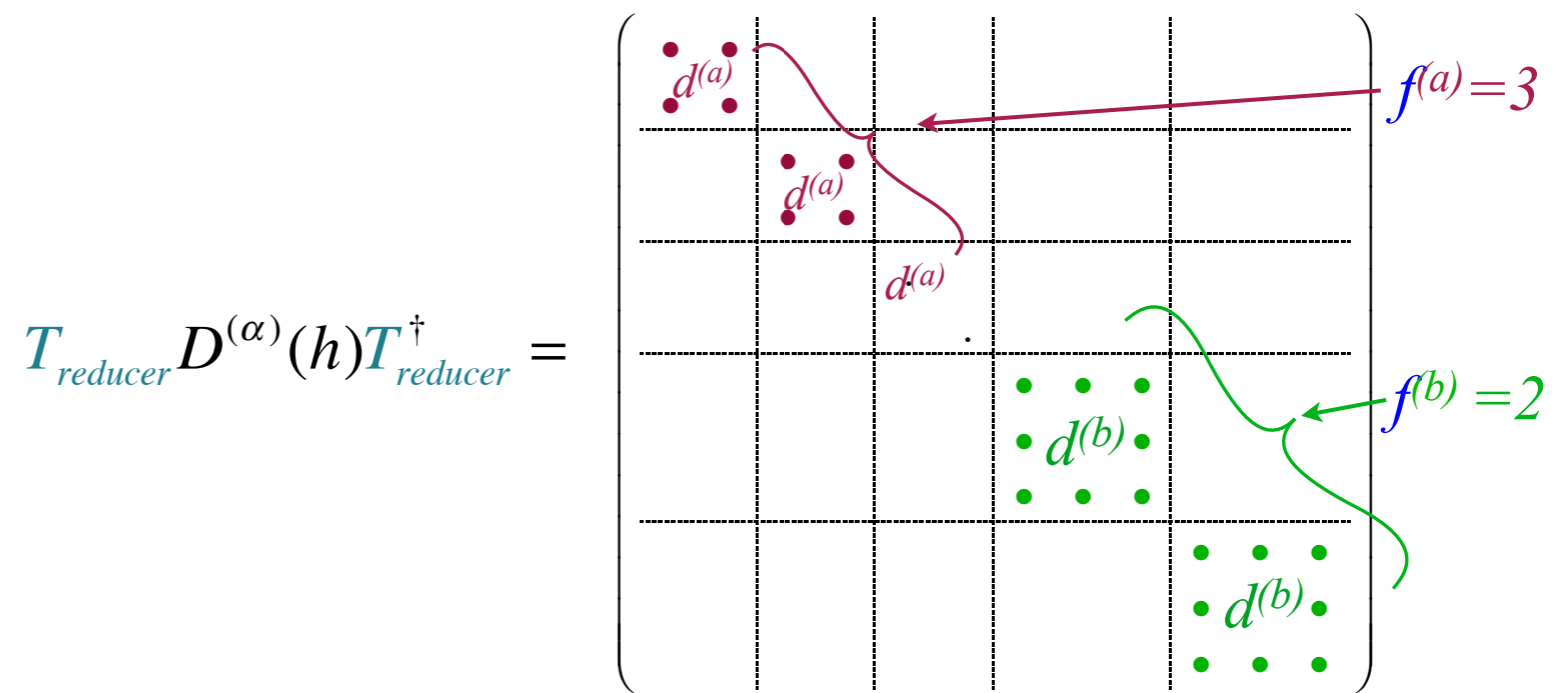
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The following derives formulae for integral $H \subset G$ correlation coefficients $f^{(b)}(D^{(\alpha)}(G) \downarrow H)$

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

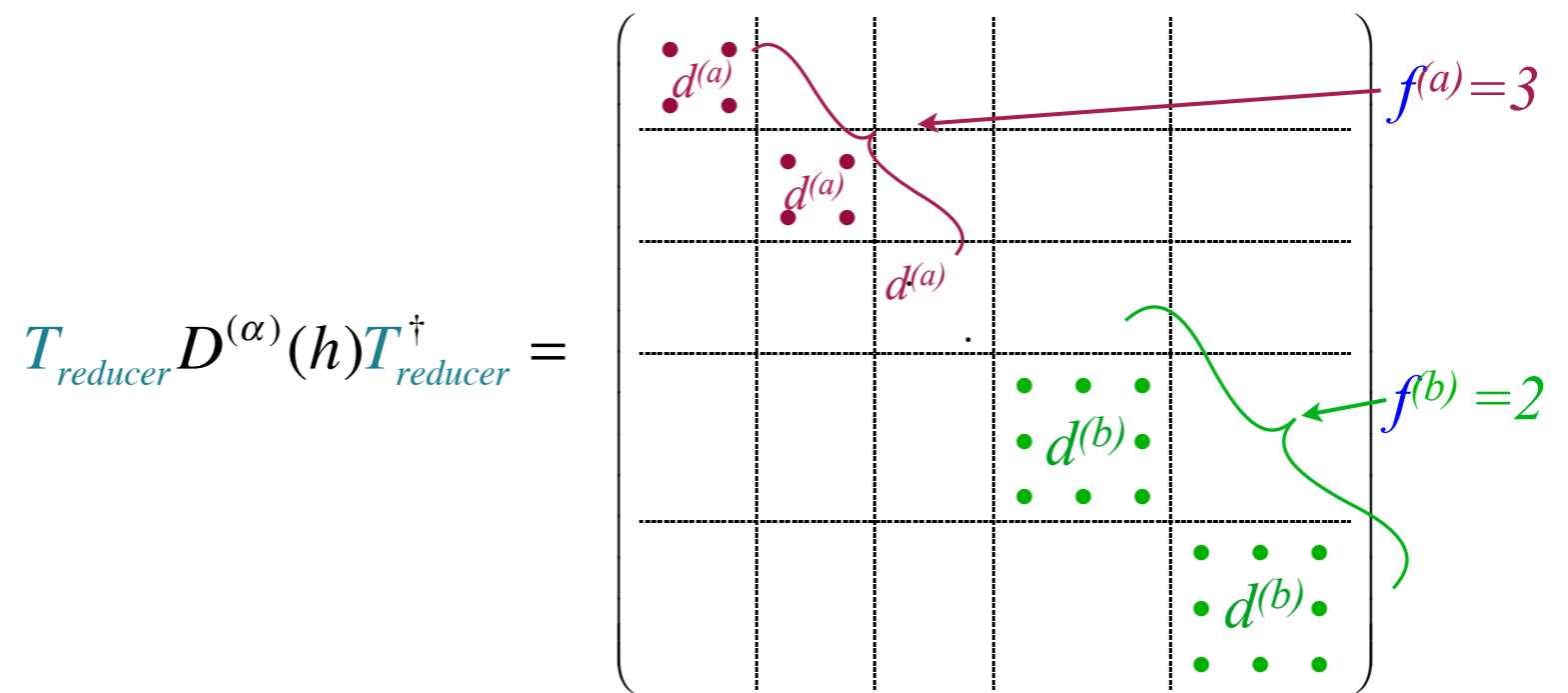
Since each $d^{(b)}(\mathbf{P}^{(b)})$ is $\ell^{(b)}$ -by- $\ell^{(b)}$ unit matrix

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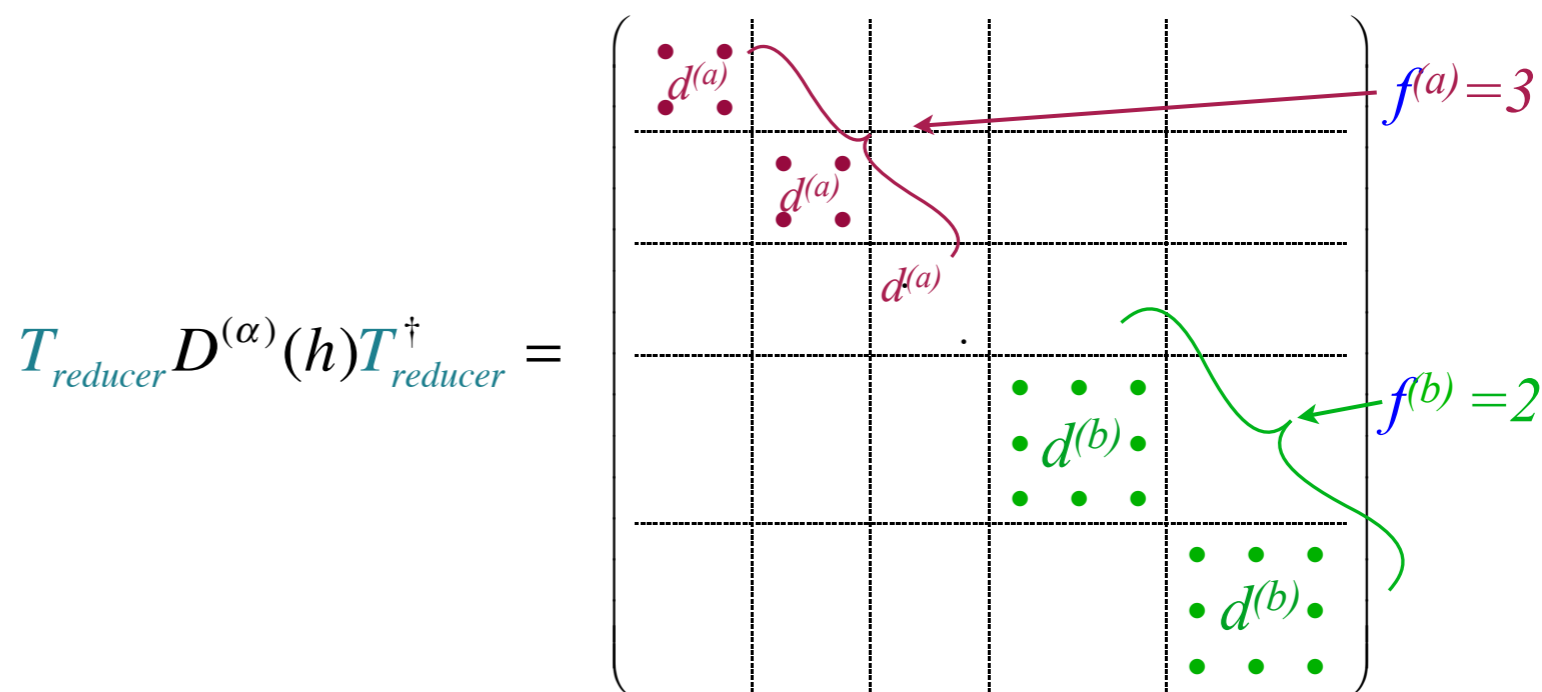
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Class ortho-complete projector relations (p.24)

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

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

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

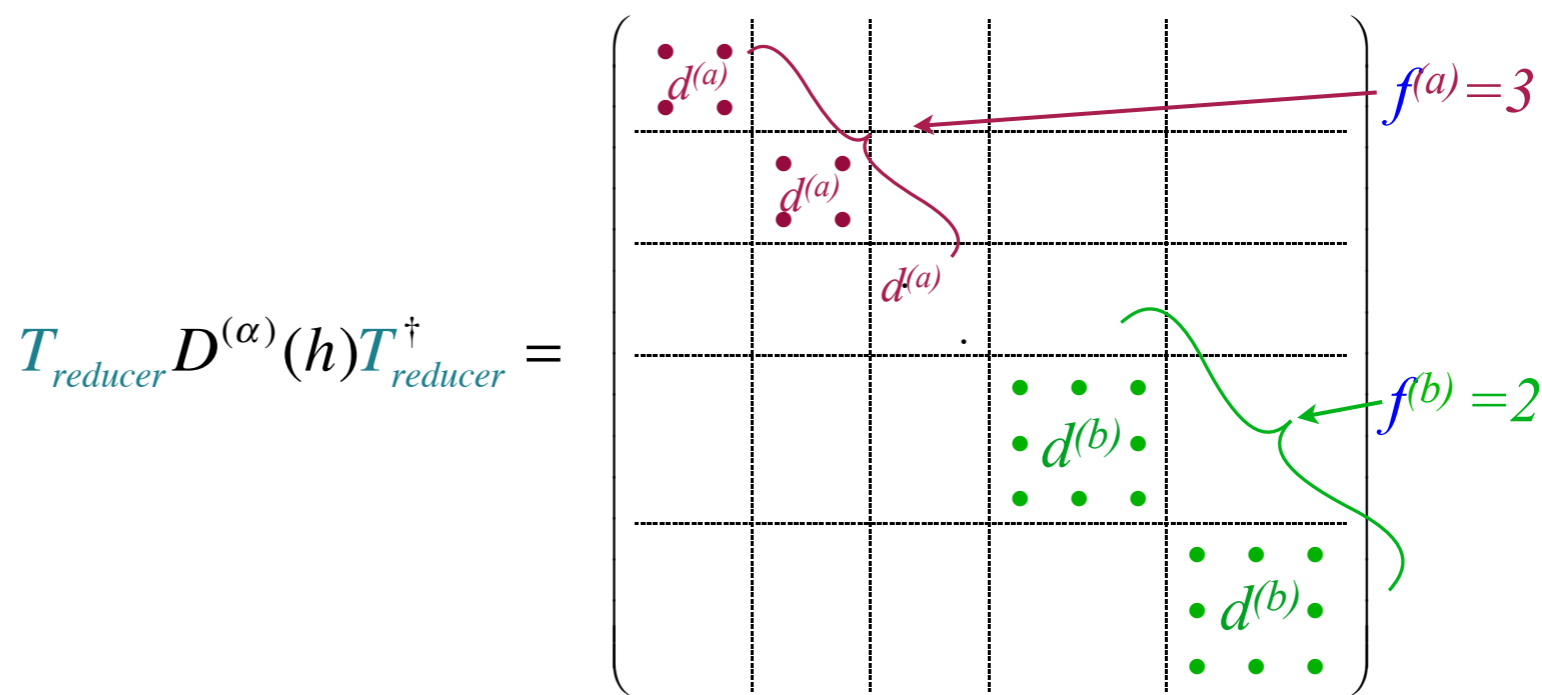
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$$f^{(b)} = \frac{1}{\circ H} \sum_{\substack{\text{classes} \\ \mathbf{\kappa}_k \in H}} \circ \mathbf{\kappa}_k \chi_k^{(b)*} \chi_k^{(\alpha)}$$

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

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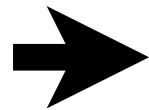
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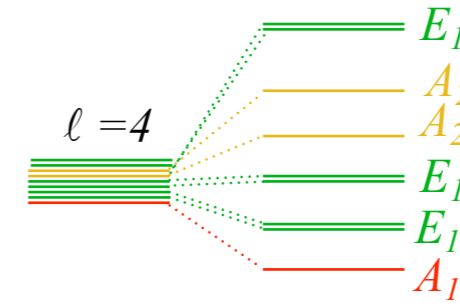


Atomic ℓ -level or $2\ell+1$ -multiplet splitting

Formula from p.44

Example: ($\ell=4$)

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



$\ell=0, s\text{-singlet}$

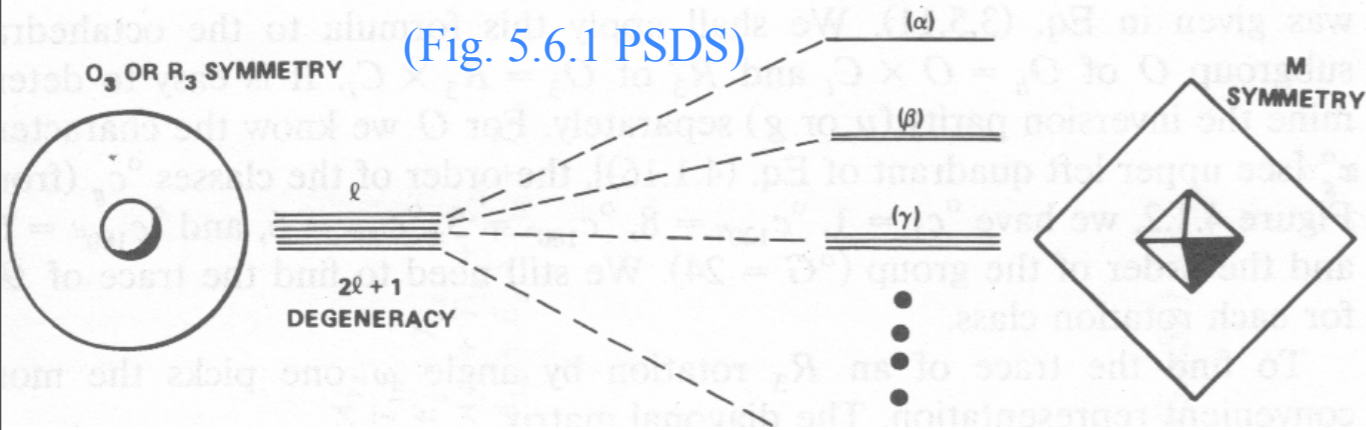
$2\ell+1=1$

$\ell=1, p\text{-triplet}$

$2\ell+1=3$

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

(Fig. 5.6.1 PSDS)

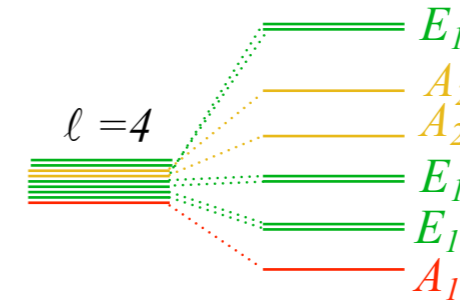


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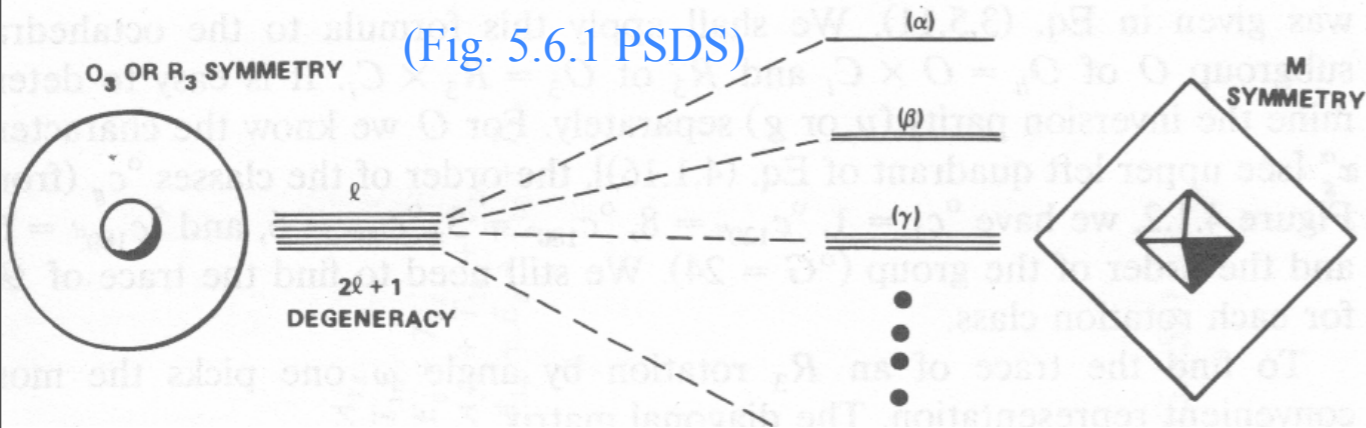
$2\ell+1=3$

$\ell=2$, d -quintet

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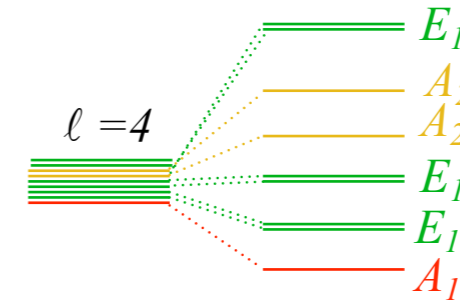


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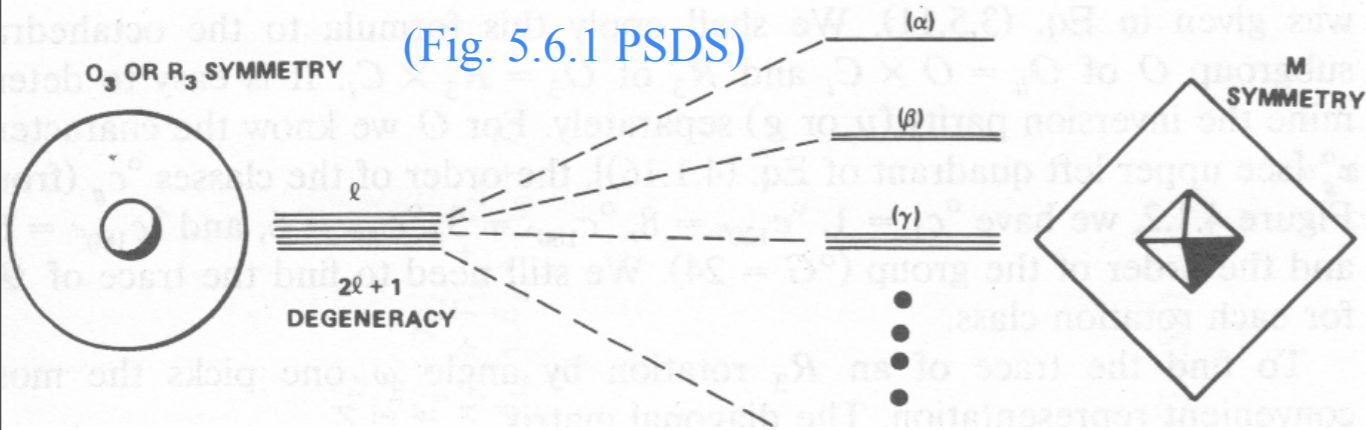
$2\ell+1=5$

$\ell=3$, f -septet

$2\ell+1=7$

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

(Fig. 5.6.1 PSDS)

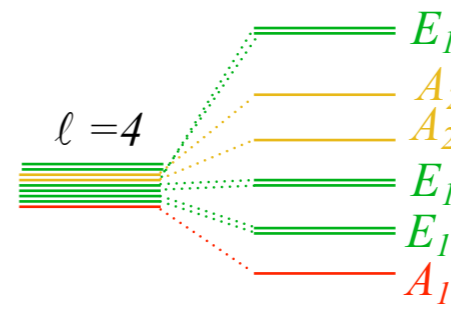


Atomic ℓ -level or $2\ell+1$ -multiplet splitting

Formula from p.44

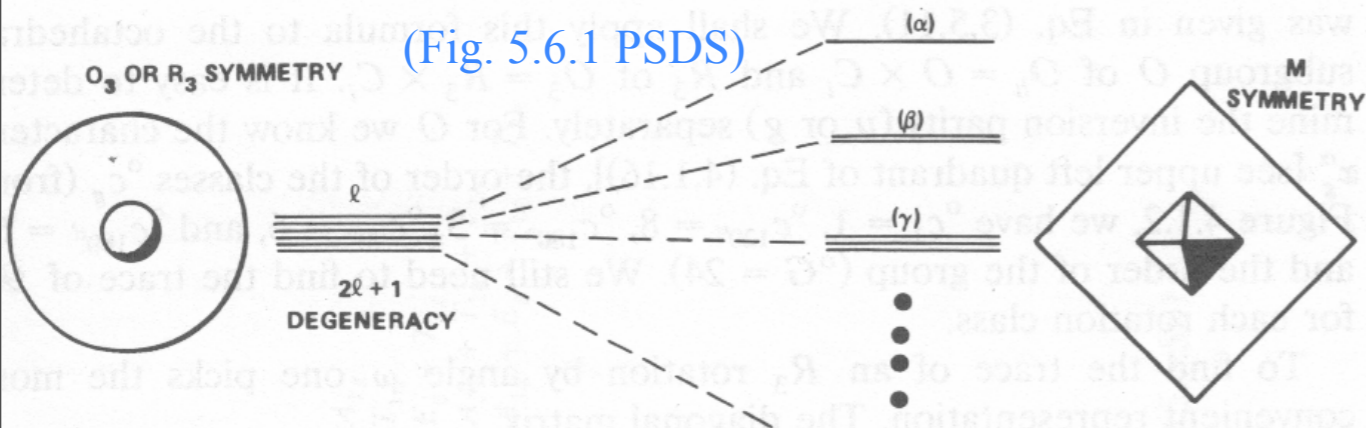
Example: ($\ell=4$)

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



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- $\ell=5, h\text{-}(11)\text{-let}$
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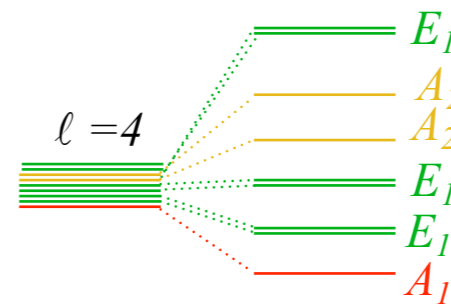


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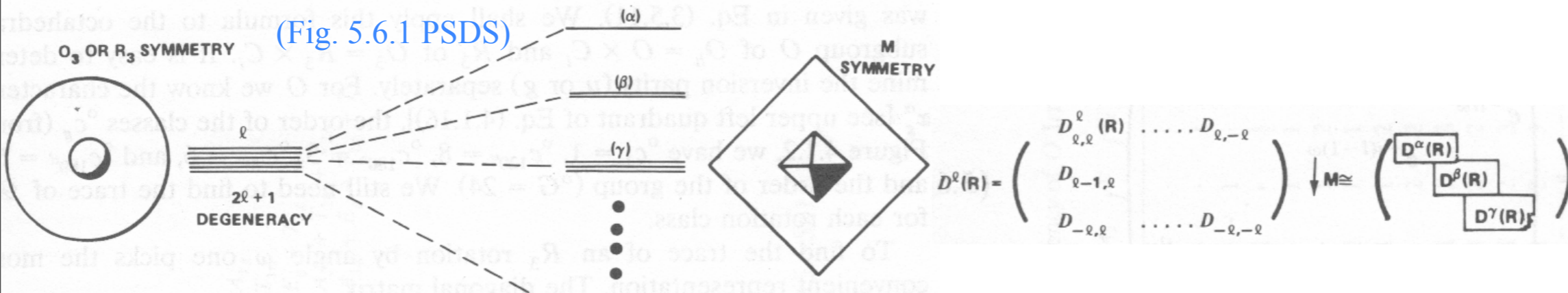
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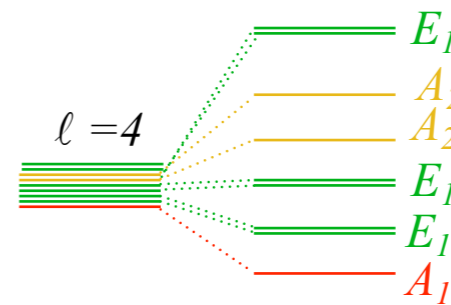
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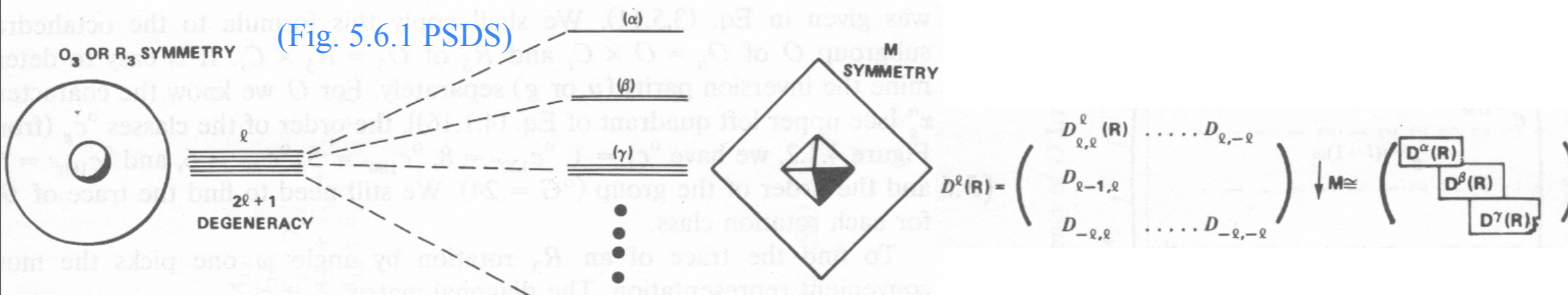
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Crystal-field splitting: $O(3) \supset D_3$ symmetry reduction and $D^\ell \downarrow D_3$ splitting



$U(2)$ characters
from Lecture 12.6 p.134:
(or end of this lecture)

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

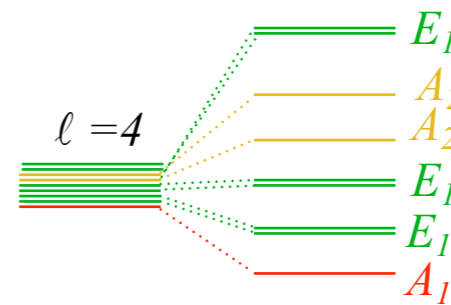
$R(3)$ character
where: $2\ell+1$
is ℓ -orbital dimension

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

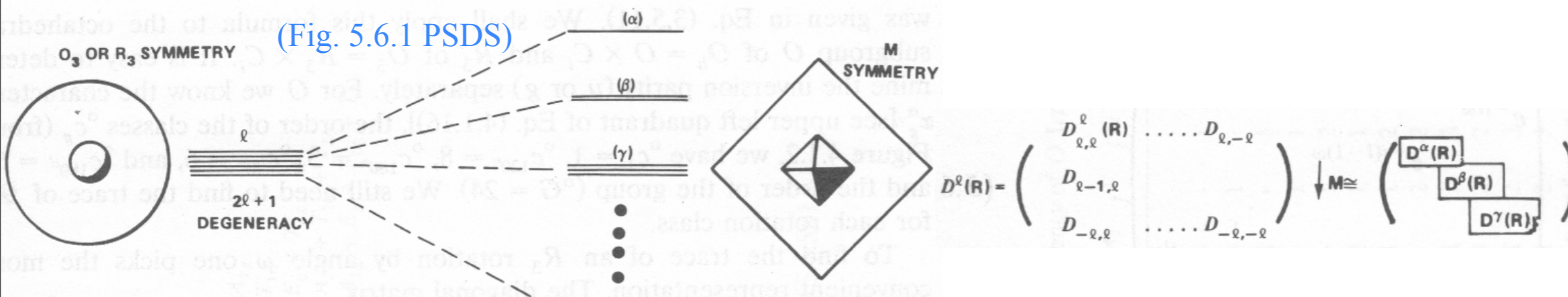
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$\chi^\ell(\Theta)$	$\Theta=0$	$\frac{2\pi}{3}$	π
$\ell=0$	1	1	1
1	3	0	-1
2	5	-1	1
3	7	1	-1
4	9	0	1
5	11	-1	-1
6	13	1	1
7	15	0	-1

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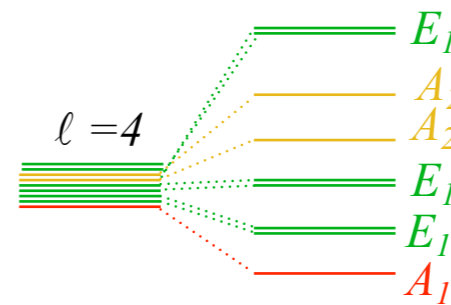
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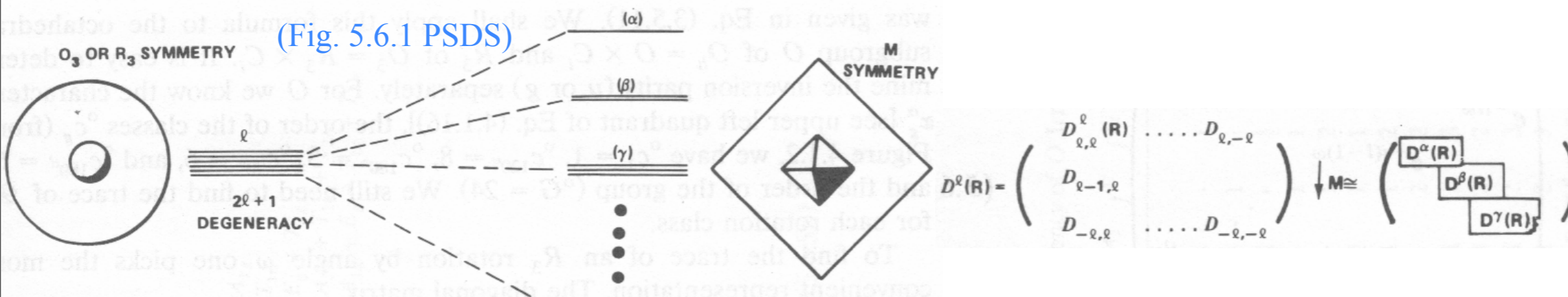
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5	11	-1	-1
6	13	1	1
7	15	0	-1

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

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
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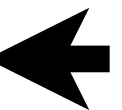
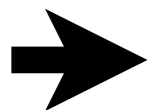
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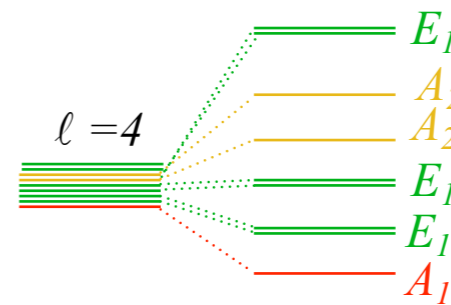


Atomic ℓ -level or $2\ell+1$ -multiplet splitting

Formula from p.44

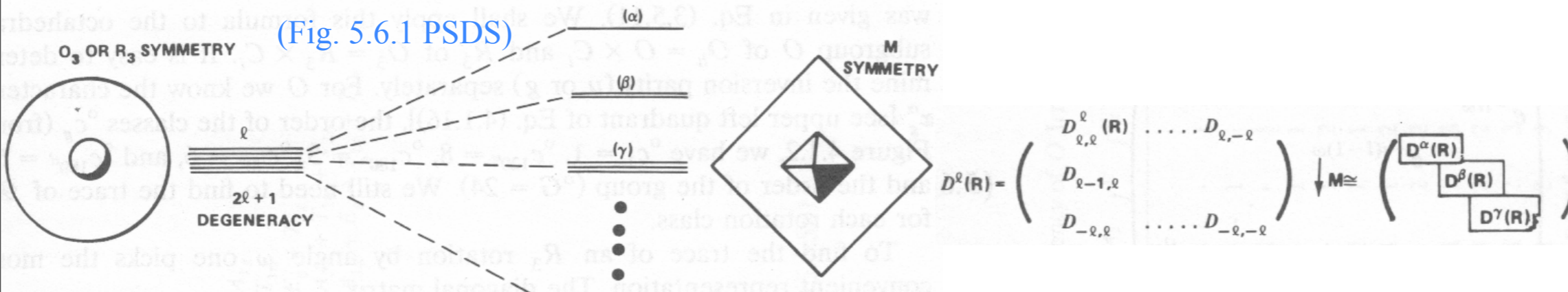
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$$\chi^\ell\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{(2\ell+1)\pi}{n}}{\sin\frac{\pi}{n}}$$

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$R(3)$ 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	$0A_1 \oplus A_2 \oplus E_1$

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

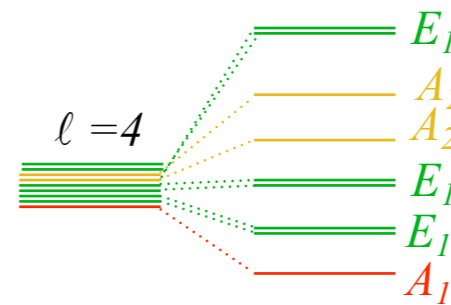
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$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

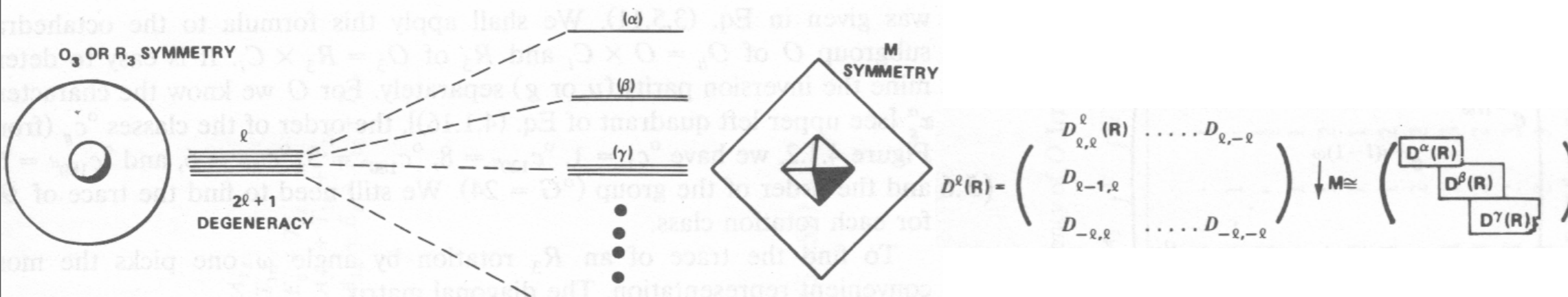
Formula from p.44

Example: ($\ell=4$)

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



- $\ell=0$, 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 12.6 p.134:
(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

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

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

$R(3)$ 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	$0A_1 \oplus A_2 \oplus E_1$

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

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

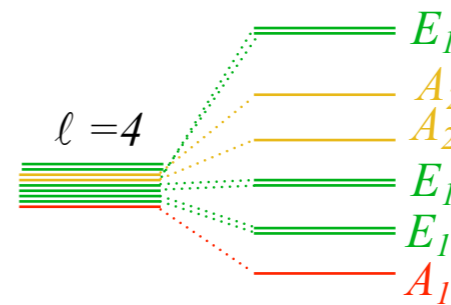
	3	0	-1
$0\chi^{A_1}(\mathbf{g}) =$	0	0	0
$1\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$1\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

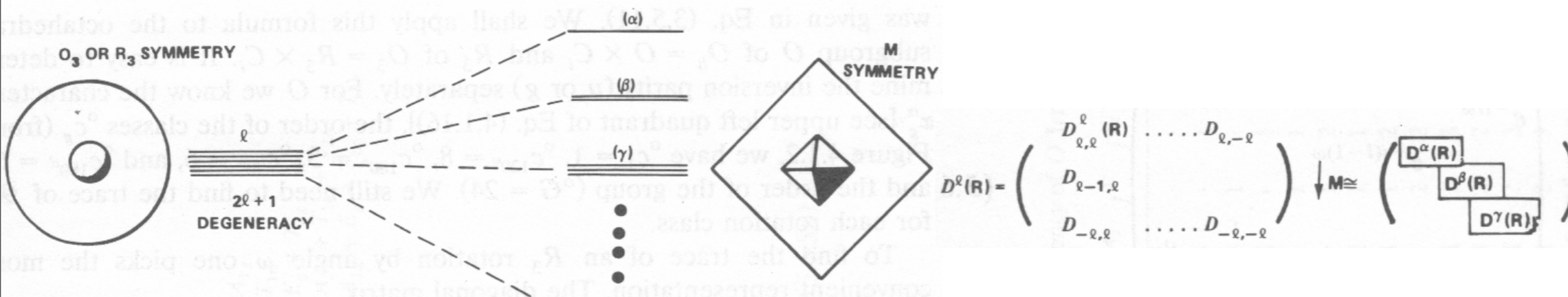
Formula from p.44

Example: ($\ell=4$)

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



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



$U(2)$ characters
from Lecture 12.6 p.134:
(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

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

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

$R(3)$ 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	$1A_1 \oplus 2E_1$

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

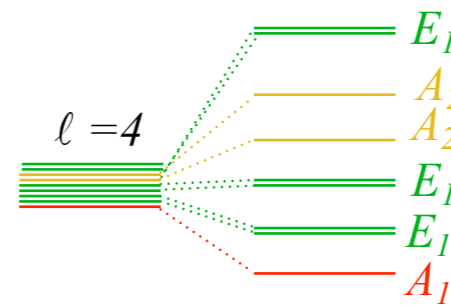
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

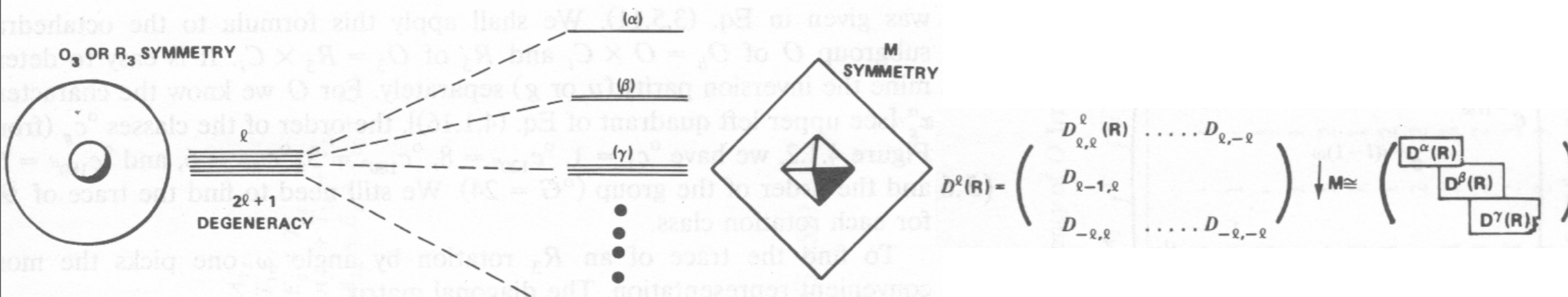
Formula from p.44

Example: ($\ell=4$)

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



- $\ell=0, s$ -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 12.6 p.134:
(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

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

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

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

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

$R(3)$ 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	$1A_1 \oplus 2E_1$

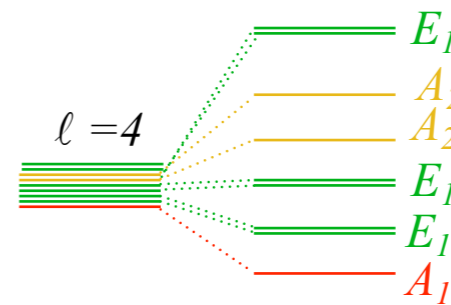
$\chi^{A_1}(\mathbf{g}) =$	5	-1	1
$0\chi^{A_2}(\mathbf{g}) =$	1	1	1
$0\chi^{A_2}(\mathbf{g}) =$	0	0	0
$2\chi^{E_1}(\mathbf{g}) =$	4	-2	0

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

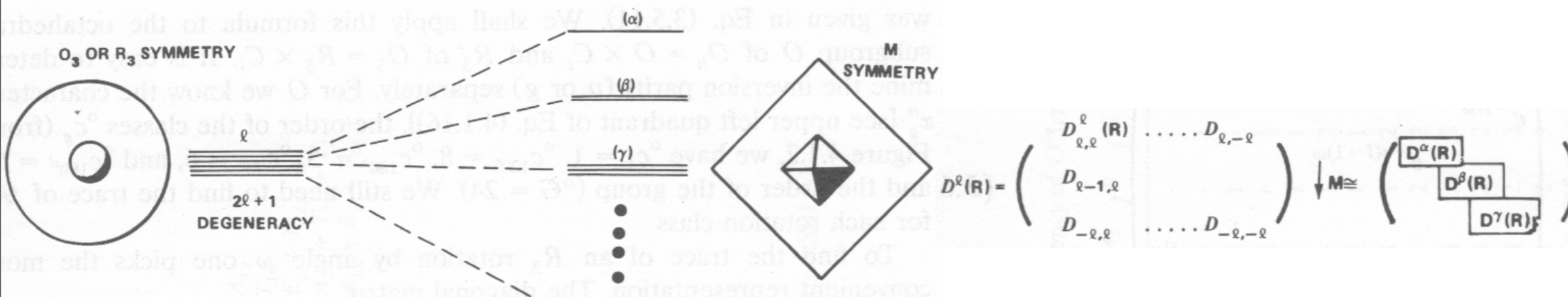
Formula from p.44

Example: ($\ell=4$)

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



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



$U(2)$ characters
from Lecture 12.6 p.134:
(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	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$

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

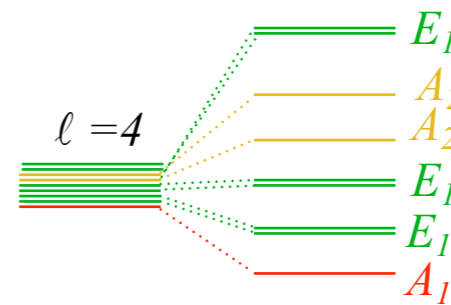
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

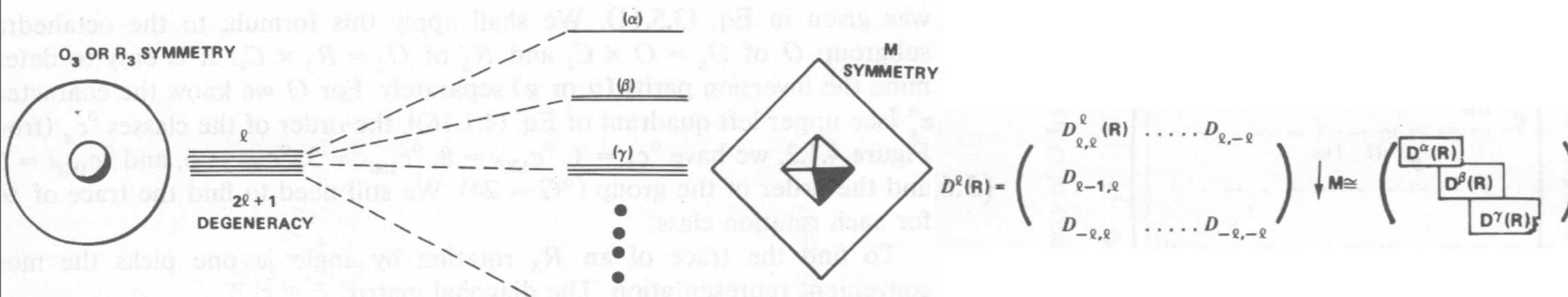
Formula from p.44

Example: ($\ell=4$)

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



- $\ell=0$, 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 12.6 p.134:
(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

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

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

$R(3)$ 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	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
		7	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	

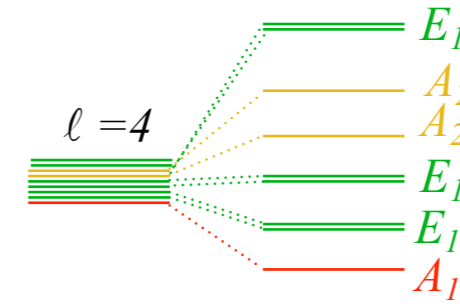
...and D_3 character table from p. 24:

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

Formula from p.44

Example: ($\ell=4$)

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



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

$U(2)$ characters
from Lecture 12.6 p.134:
(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:

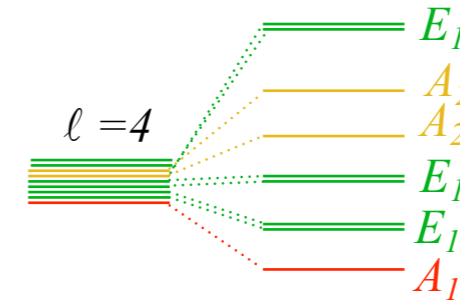
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

$f^{(\alpha)}(\ell)$	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	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	...

Formula from p.44

Example: ($\ell=4$)

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



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

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

$U(2)$ characters
from Lecture 12.6 p.134:
(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:

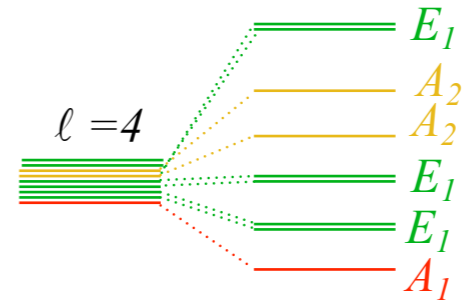
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

$f^{(\alpha)}(\ell)$	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	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	...

Formula from p.44

Example: ($\ell=4$)

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



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

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

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

$U(2)$ characters
from Lecture 12.6 p.134:
(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:

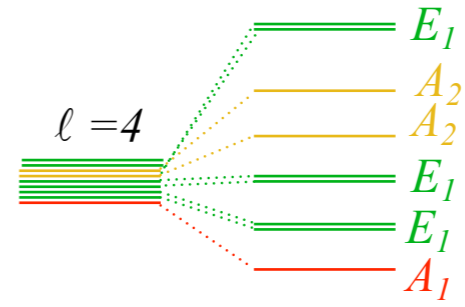
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

Formula from p.44

Example: ($l=4$)

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



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

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

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

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

$U(2)$ characters
from Lecture 12.6 p.134:
(or end of this lecture)

$\chi^l(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$l=0$	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

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

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

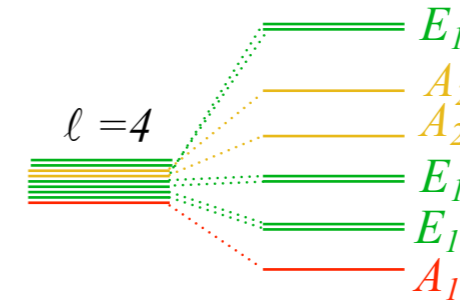
$(\mathfrak{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathfrak{g}) =$	1	1	1
$\chi^{A_2}(\mathfrak{g}) =$	1	1	-1
$\chi^{E_1}(\mathfrak{g}) =$	2	-1	0

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

Formula from p.44

Example: ($l=4$)

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



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

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

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

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

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

$U(2)$ characters
from Lecture 12.6 p.134:
(or end of this lecture)

$\chi^l(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	π
$l=0$	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

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

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

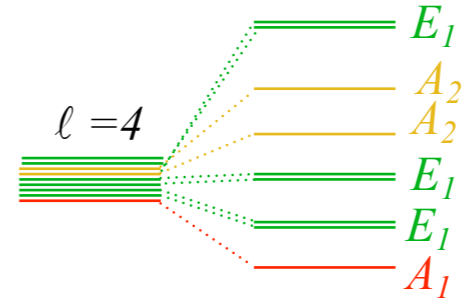
$(\mathfrak{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathfrak{g}) =$	1	1	1
$\chi^{A_2}(\mathfrak{g}) =$	1	1	-1
$\chi^{E_1}(\mathfrak{g}) =$	2	-1	0

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

Formula from p.44

Example: ($\ell=4$)

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



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

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

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

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

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

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

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

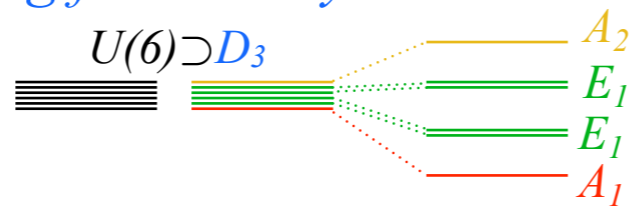
...and D_3 character table from p. 24:

$(\mathfrak{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathfrak{g}) =$	1	1	1
$\chi^{A_2}(\mathfrak{g}) =$	1	1	-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	$0A_1 \oplus A_2 \oplus E_1$
2	1	.	2	$1A_1 \oplus 2E_1$
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: $\ell=6 \mid 13 \ 1 \ 1 \mid = A_1 \mid 1 \ 1 \ 1 \mid \oplus 2R^G \mid 12 \ 0 \ 0 \mid = A_1 \oplus 2[A_1 \oplus A_2 \oplus 2E_1]$ ($\ell=6$ is 1st re-cycling point)

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

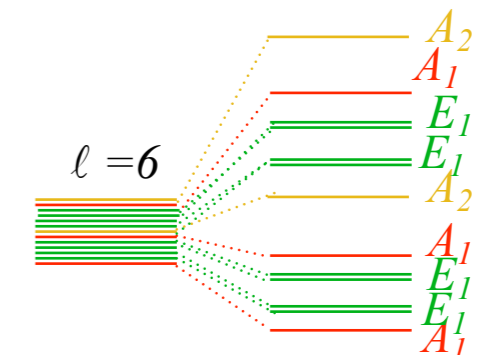
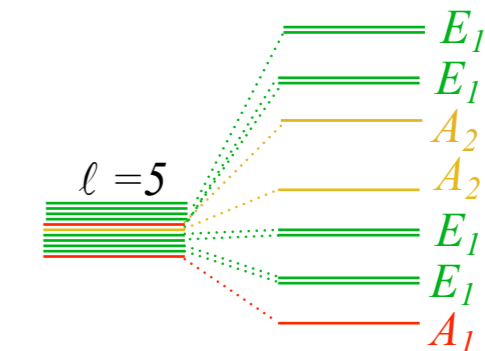
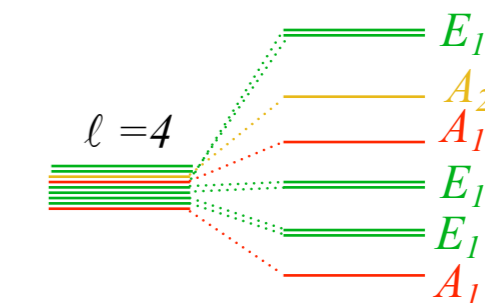
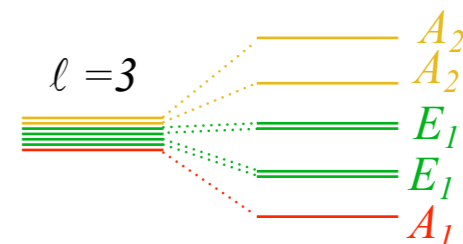
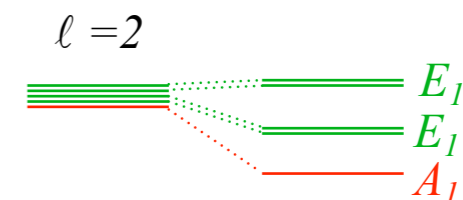
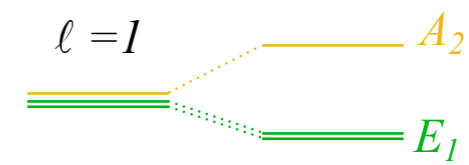


$$R^G(U(6)) \downarrow D_3 = D^{A_1}(\mathfrak{g}) \oplus D^{A_2}(\mathfrak{g}) \oplus 2D^{E_1}(\mathfrak{g})$$

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

$f^{(\alpha)}(\ell)$	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	$1A_1 \oplus 2A_2 \oplus 2E_1$
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	$2A_1 \oplus 3A_2 \oplus 5E_1$

$R(3) \supset D_3$



D_3 character table:

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

Review: Spectral resolution of D_3 Center (Class algebra)

Group theory of equivalence transformations and classes

Lagrange theorems

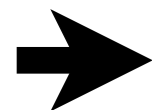
All-commuting class projectors and D_3 -invariant character ortho-completeness

*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 $\ell=1-6$



Group invariant numbers: Centrum, Rank, and Order



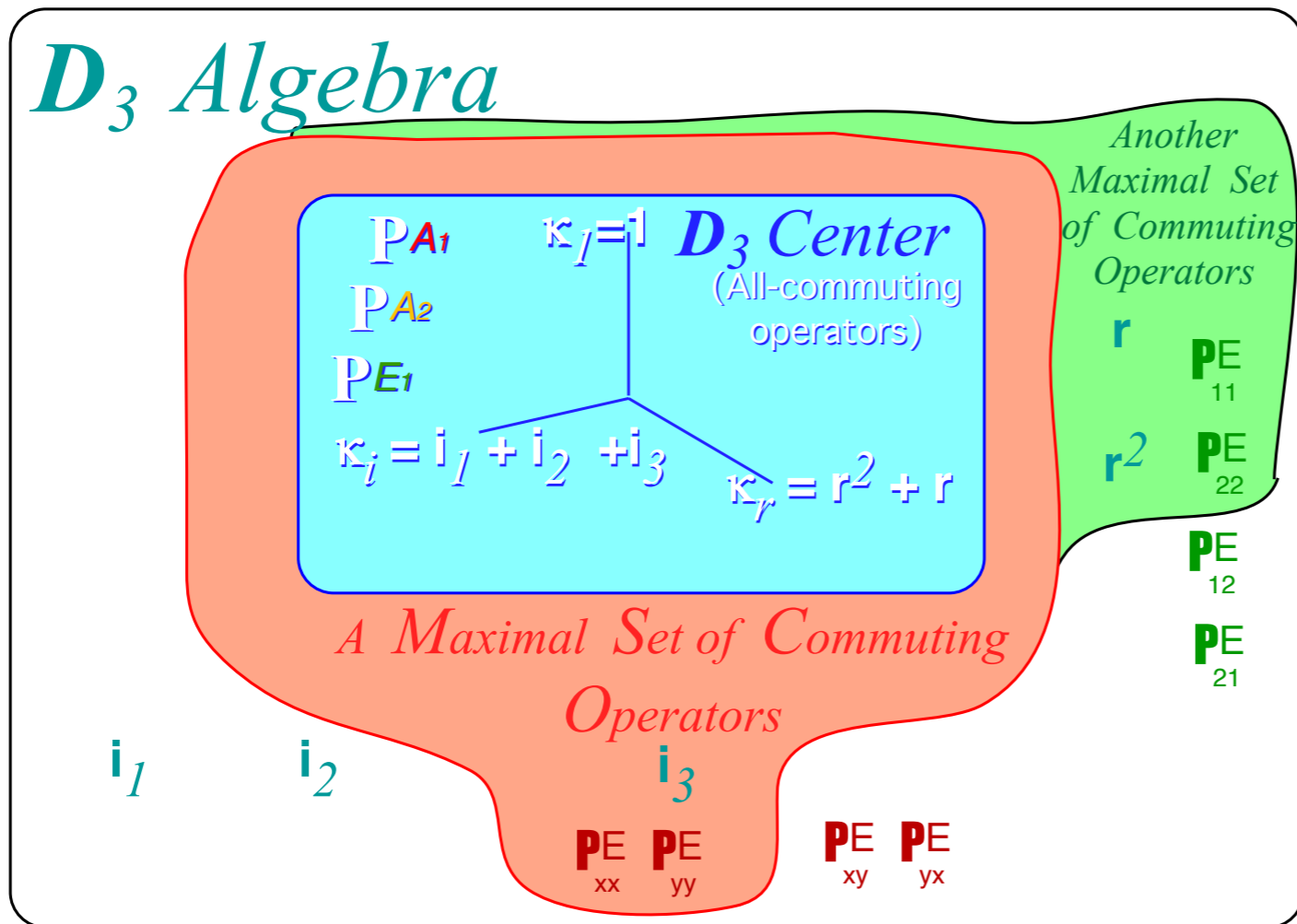
2nd-Stage spectral decompositions of global/local D_3

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

D_3 Algebra



Important invariant numbers or “characters”

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

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

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

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

$$D_3 \quad \kappa = \boxed{1} \quad \boxed{r^1 + r^2} \quad \boxed{i_1 + i_2 + i_3}$$

$$\mathbf{P}^{A_1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

$$\mathbf{P}^E = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 3$$

$$\kappa(D_3) = (1)^0 + (1)^0 + (2)^0 = 3$$

$$\rho(D_3) = (1)^1 + (1)^1 + (2)^1 = 4$$

$$\circ(D_3) = (1)^2 + (1)^2 + (2)^2 = 6$$

Review: Spectral resolution of D_3 Center (Class algebra)

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

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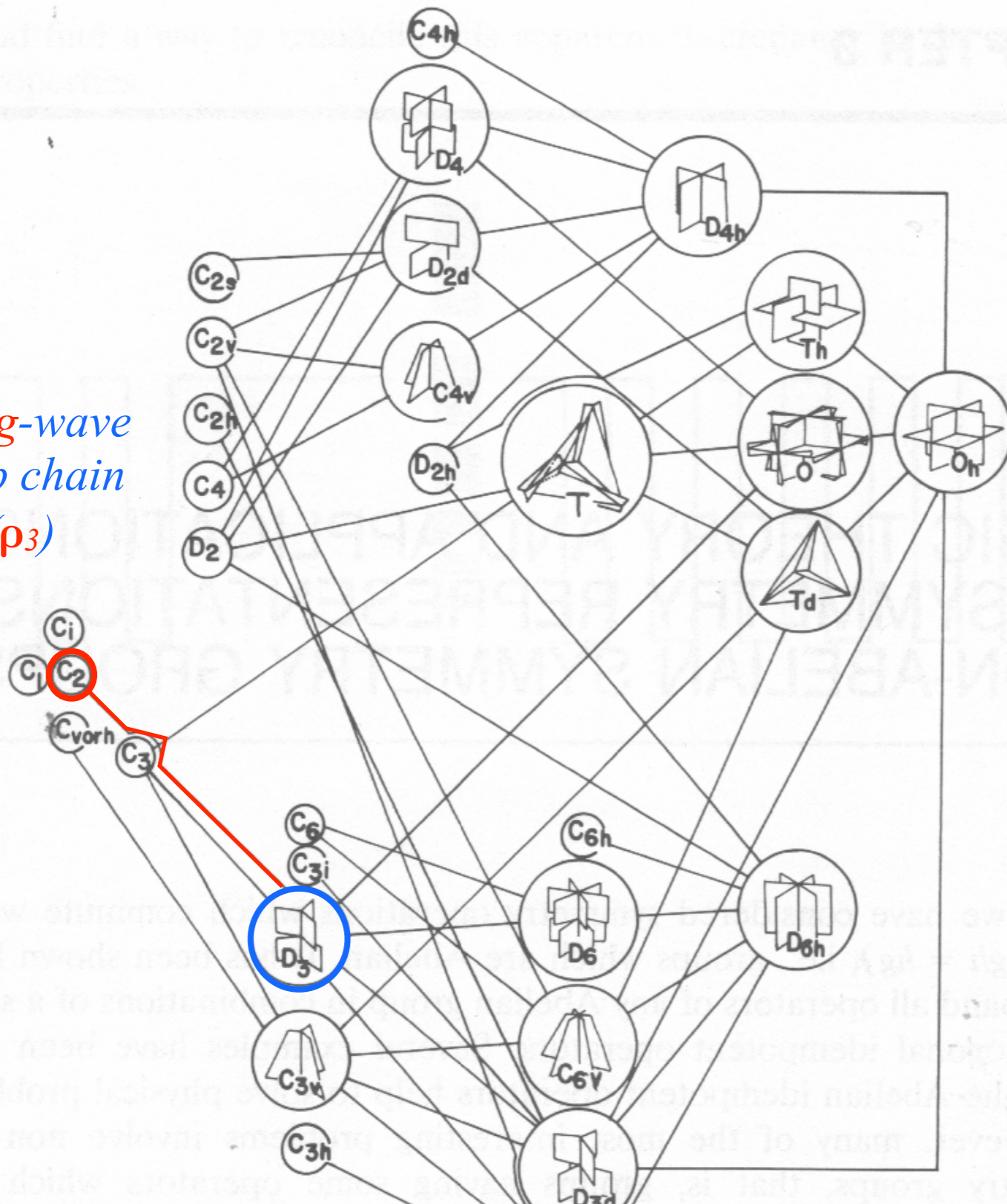
Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

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

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

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



Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

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

$$\mathbf{P}^{A_1} = \begin{array}{ccc|c} 1 & 1 & 1 & /6 \end{array}$$

$$\mathbf{P}^{A_2} = \begin{array}{ccc|c} 1 & 1 & -1 & /6 \end{array}$$

$$\mathbf{P}^E = \begin{array}{ccc|c} 2 & -1 & 0 & /3 \end{array}$$

$$C_2 \quad \kappa = \mathbf{1} \quad \mathbf{i}_3$$

$$p^{0_2} = \begin{array}{cc|c} 1 & 1 & /2 \end{array}$$

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$D_3 \supset C_2$ 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** $\mathbf{P}_{n,n}^{(\alpha)}$

$$D_3 \supset C_2 \quad 0_2 \quad 1_2$$

$$n^{A_1} = \begin{matrix} 1 & \cdot \\ \cdot & 1 \end{matrix}$$

$$n^{A_2} = \begin{matrix} \cdot & 1 \\ 1 & \cdot \end{matrix}$$

$$n^E = \begin{matrix} 1 & 1 \\ 1 & 1 \end{matrix}$$

Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

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$$n^{A_2} = \begin{matrix} \cdot & 1 \\ 1 & \cdot \end{matrix}$$

$$n^E = \begin{matrix} 1 & 1 \\ 1 & 1 \end{matrix}$$

Rank $\rho(D_3) = 4$ implies

there will be exactly 4

“ C_2 -friendly” irep projectors

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

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

Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

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

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

$$\mathbf{P}^{A_1} = \begin{matrix} \mathbf{P}_{0_2 0_2}^{A_1} & \cdot \end{matrix}$$

$$\mathbf{P}^{A_2} = \begin{matrix} \cdot & \mathbf{P}_{1_2 1_2}^{A_2} \end{matrix}$$

$$\mathbf{P}^E = \begin{matrix} \mathbf{P}_{0_2 0_2}^E & \mathbf{P}_{1_2 1_2}^E \end{matrix}$$

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 subgroup(s) $C_2(\mathbf{i})$

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$$\mathbf{P}^E = \begin{matrix} 2 & -1 & 0 \\ /3 \end{matrix}$$

$$C_2 \quad \kappa = \mathbf{1} \quad \mathbf{i}_3$$

$$p^{0_2} = \begin{matrix} 1 & 1 \\ /2 \end{matrix}$$

$$p^{1_2} = \begin{matrix} 1 & -1 \\ /2 \end{matrix}$$

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shows which products of class projector $\mathbf{P}^{(\alpha)}$ with

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

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

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

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

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

$$\mathbf{P}^{A_1} = \begin{matrix} \mathbf{P}_{0_2 0_2}^{A_1} & \cdot \\ \cdot & \mathbf{P}_{1_2 1_2}^{A_2} \end{matrix}$$

$$\mathbf{P}^{A_2} = \begin{matrix} \cdot & \mathbf{P}_{1_2 1_2}^{A_2} \\ \mathbf{P}_{0_2 0_2}^E & \mathbf{P}_{1_2 1_2}^E \end{matrix}$$

$$\mathbf{P}^E = \begin{matrix} \mathbf{P}_{0_2 0_2}^E & \mathbf{P}_{1_2 1_2}^E \end{matrix}$$

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2nd-Stage

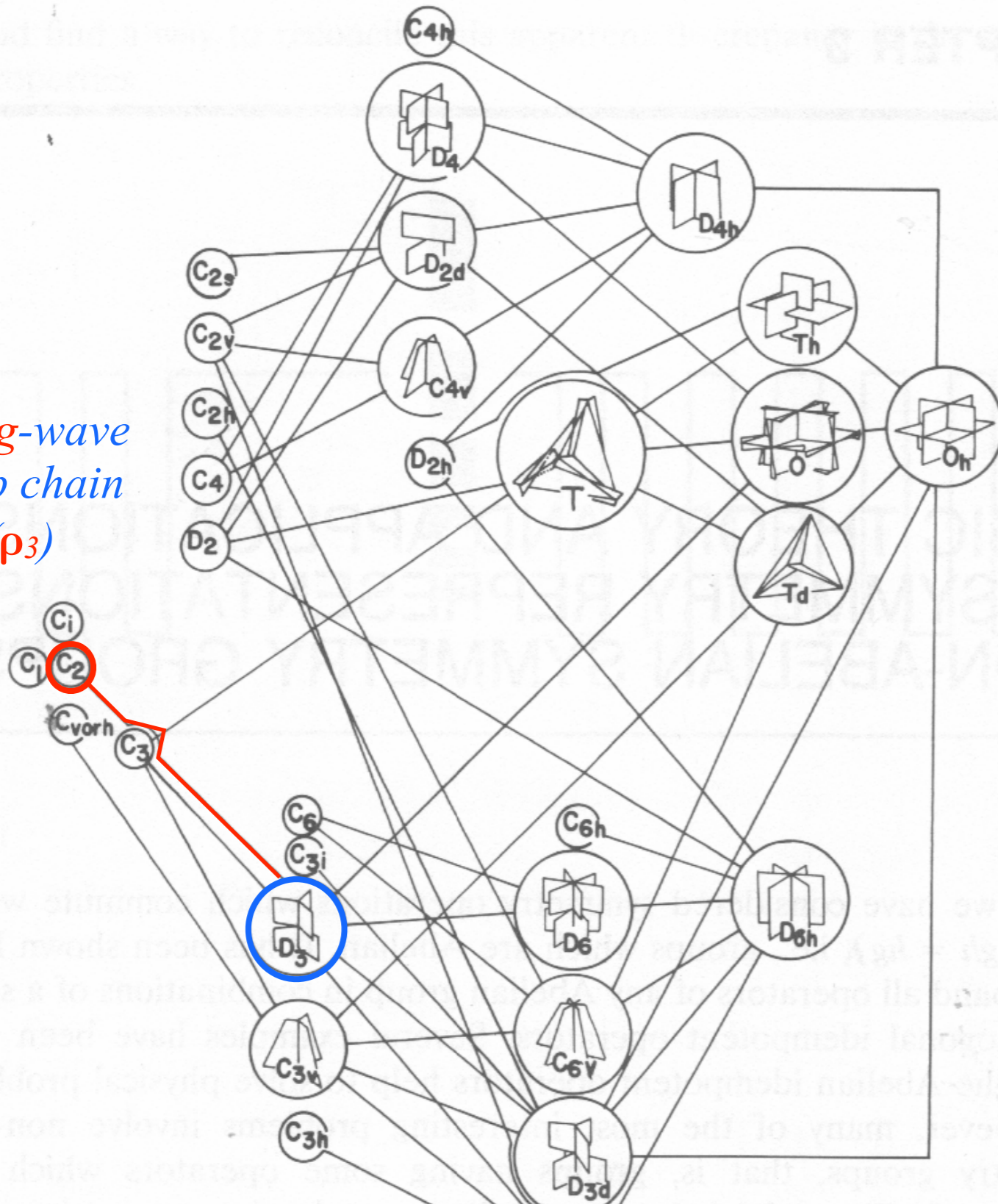
Spectral reduction of non-commutative “Group-table Hamiltonian”

D_3 Example

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

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

Standing-wave
Subgroup chain
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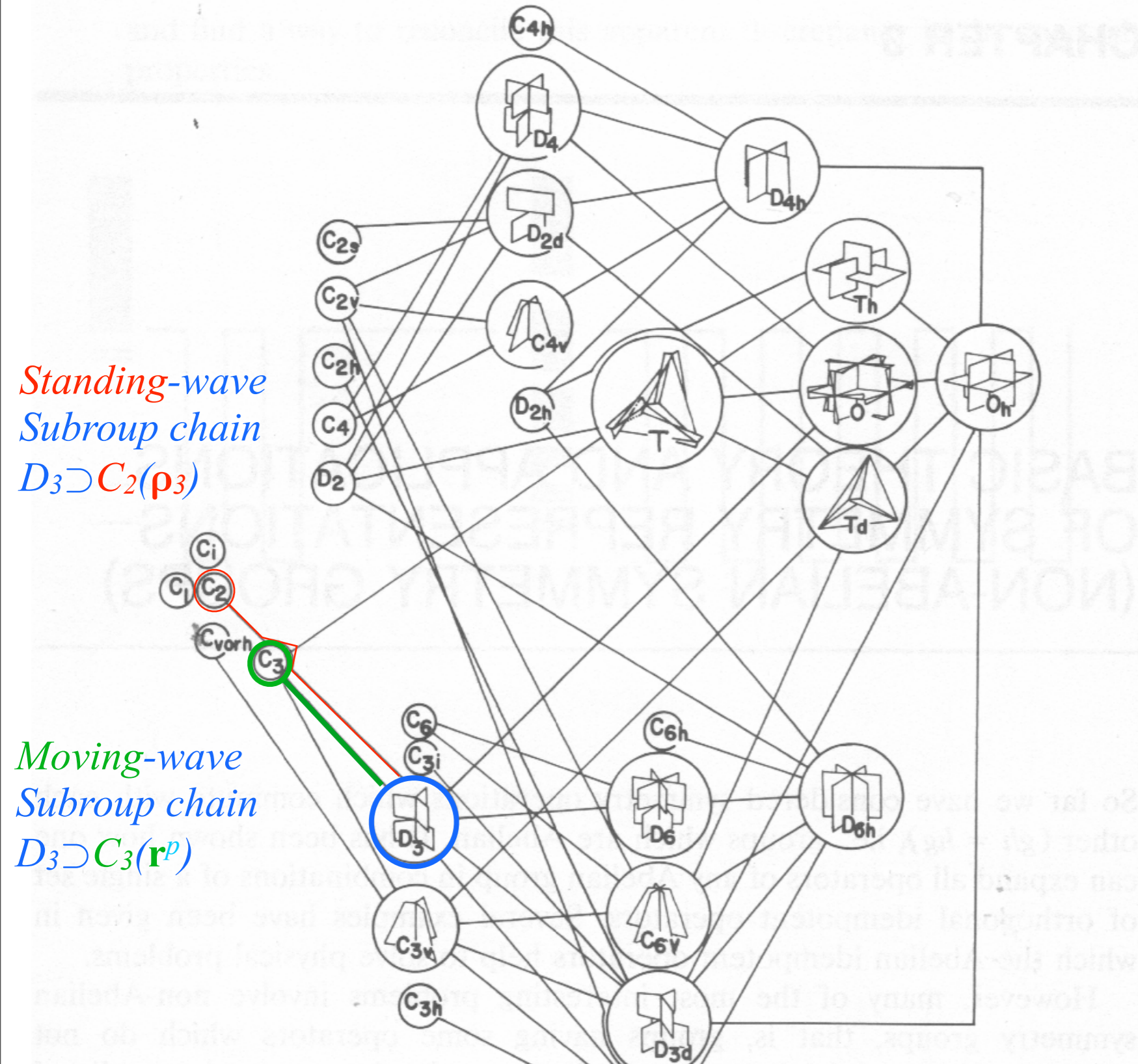
2nd-Stage

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 subgroup(s) $C_2(\mathbf{i})$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)



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 subgroup(s) $C_2(\mathbf{i})$ or ELSE $C_3(\mathbf{r})$ (C_2 and C_3 don't commute)

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

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

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

$$\mathbf{P}^{A_1} = \begin{bmatrix} \mathbf{P}^{A_1} & \cdot & \cdot \\ \cdot & \mathbf{P}_{0_3 0_3}^{A_1} & \cdot \\ \cdot & \cdot & \mathbf{P}_{0_3 0_3}^{A_2} \end{bmatrix}$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & \mathbf{P}_{0_3 0_3}^{A_2} & \cdot \\ \cdot & \cdot & \mathbf{P}_{0_3 0_3}^{A_1} \end{bmatrix}$$

$$\mathbf{P}^E = \begin{bmatrix} \cdot & \mathbf{P}_{1_3 1_3}^E & \mathbf{P}_{2_3 2_3}^E \\ \mathbf{P}_{1_3 1_3}^E & \cdot & \cdot \\ \mathbf{P}_{2_3 2_3}^E & \cdot & \cdot \end{bmatrix}$$

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

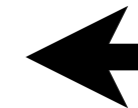
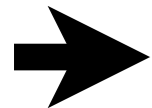
D_3 examples for $\ell=1-6$

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 $D_3 \supset C_3$

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-Stage

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

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

$$\begin{aligned} \mathbf{P}_{0_2 0_2}^{A_1} &= \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (1 + \mathbf{i}_3) / 2 = \left(\begin{array}{ccc} 1 & \mathbf{r}^1 + \mathbf{r}^2 & \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3 \end{array} \right) / 6 \\ \mathbf{P}_{1_2 1_2}^{A_2} &= \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (1 - \mathbf{i}_3) / 2 = \left(\begin{array}{ccc} 1 & \mathbf{r}^1 + \mathbf{r}^2 & -\mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3 \end{array} \right) / 6 \\ \mathbf{P}_{0_2 0_2}^E &= \mathbf{P}^E p^{0_2} = \mathbf{P}^E (1 + \mathbf{i}_3) / 2 = \left(\begin{array}{ccc} 2 & 1 - \mathbf{r}^1 - \mathbf{r}^2 & -\mathbf{i}_1 - \mathbf{i}_2 + 2\mathbf{i}_3 \end{array} \right) / 6 \\ \mathbf{P}_{1_2 1_2}^E &= \mathbf{P}^E p^{1_2} = \mathbf{P}^E (1 - \mathbf{i}_3) / 2 = \left(\begin{array}{ccc} 2 & 1 - \mathbf{r}^1 - \mathbf{r}^2 & \mathbf{i}_1 + \mathbf{i}_2 - 2\mathbf{i}_3 \end{array} \right) / 6 \end{aligned}$$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{0_2 0_2}^E + \mathbf{P}_{1_2 1_2}^E$
class κ_i splits into $\kappa_{i_{12}}$ and κ_{i_3}

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

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

$$D_3 \quad \kappa = \begin{array}{|c|c|c|} \hline 1 & \mathbf{r}^1 + \mathbf{r}^2 & \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3 \\ \hline \end{array}$$

$$\begin{aligned} \mathbf{P}^{A_1} &= \begin{array}{|c|c|c|} \hline 1 & 1 & 1 \\ \hline \end{array} / 6 \\ \mathbf{P}^{A_2} &= \begin{array}{|c|c|c|} \hline 1 & 1 & -1 \\ \hline \end{array} / 6 \\ \mathbf{P}^E &= \begin{array}{|c|c|c|} \hline 2 & -1 & 0 \\ \hline \end{array} / 3 \end{aligned}$$

$$\begin{aligned} \mathbf{P}_{0_3 0_3}^{A_1} &= \mathbf{P}^{A_1} p^{0_3} = \mathbf{P}^{A_1} (1 + \mathbf{r}^1 + \mathbf{r}^2) / 3 = \left(\begin{array}{ccc} 1 & \mathbf{r}^1 + \mathbf{r}^2 & \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3 \end{array} \right) / 6 \\ \mathbf{P}_{0_3 0_3}^{A_2} &= \mathbf{P}^{A_2} p^{0_3} = \mathbf{P}^{A_2} (1 + \mathbf{r}^1 + \mathbf{r}^2) / 3 = \left(\begin{array}{ccc} 1 & \mathbf{r}^1 + \mathbf{r}^2 & -\mathbf{i}_1 - \mathbf{i}_2 - \mathbf{i}_3 \end{array} \right) / 6 \\ \mathbf{P}_{1_3 1_3}^E &= \mathbf{P}^E p^{1_3} = \mathbf{P}^E (1 + \varepsilon \mathbf{r}^1 + \varepsilon^* \mathbf{r}^2) / 3 = \left(\begin{array}{ccc} 1 & \varepsilon \mathbf{r}^1 + \varepsilon^* \mathbf{r}^2 & \end{array} \right) / 3 \\ \mathbf{P}_{2_3 2_3}^E &= \mathbf{P}^E p^{2_3} = \mathbf{P}^E (1 + \varepsilon^* \mathbf{r}^1 + \varepsilon \mathbf{r}^2) / 3 = \left(\begin{array}{ccc} 1 & \varepsilon^* \mathbf{r}^1 + \varepsilon \mathbf{r}^2 & \end{array} \right) / 3 \end{aligned}$$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{1_3 1_3}^E + \mathbf{P}_{2_3 2_3}^E$
class κ_r splits into κ_{r_1} and κ_{r_2}

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

2nd-Stage

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

Rank $\rho(D_3)=4$
idempotents

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

$$\mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (1+i_3)/2 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6$$

$$\mathbf{P}_{1_2 1_2}^{A_2} = \mathbf{P}^{A_2} p^{1_2} = \mathbf{P}^{A_2} (1-i_3)/2 = (1 + r^1 + r^2 - i_1 - i_2 - i_3)/6$$

$$\mathbf{P}_{0_2 0_2}^E = \mathbf{P}^E p^{0_2} = \mathbf{P}^E (1+i_3)/2 = (2 - r^1 - r^2 - i_1 - i_2 + 2i_3)/6$$

$$\mathbf{P}_{1_2 1_2}^E = \mathbf{P}^E p^{1_2} = \mathbf{P}^E (1-i_3)/2 = (2 - r^1 - r^2 + i_1 + i_2 - 2i_3)/6$$

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{0_2 0_2}^E + \mathbf{P}_{1_2 1_2}^E$
class κ_i splits into $\kappa_{i_{12}}$ and κ_{i_3}

4 different idempotent

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

$$\mathbf{P}_{0_3 0_3}^{A_1} = \mathbf{P}^{A_1} p^{0_3} = \mathbf{P}^{A_1} (1+r^1+r^2)/3 = (1 + r^1 + r^2 + i_1 + i_2 + i_3)/6$$

$$\mathbf{P}_{0_3 0_3}^{A_2} = \mathbf{P}^{A_2} p^{0_3} = \mathbf{P}^{A_2} (1+r^1+r^2)/3 = (1 + r^1 + r^2 - i_1 - i_2 - i_3)/6$$

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

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

\mathbf{P}^E splits into $\mathbf{P}^E = \mathbf{P}_{1_3 1_3}^E + \mathbf{P}_{2_3 2_3}^E$
class κ_r splits into κ_{r_1} and κ_{r_2}

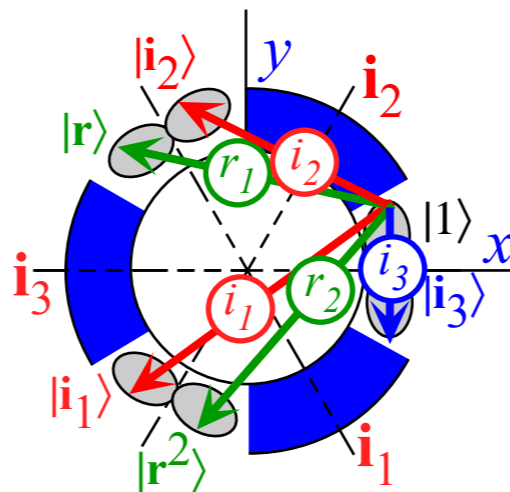
Centrum $\kappa(D_3)=3$
idempotents
 $\mathbf{P}^{(\alpha)}$

$$D_3 \kappa = \begin{bmatrix} 1 & r^1+r^2 & i_1+i_2+i_3 \\ \mathbf{P}^{A_1} = & 1 & 1 & 1 & /6 \\ \mathbf{P}^{A_2} = & 1 & 1 & -1 & /6 \\ \mathbf{P}^E = & 2 & -1 & 0 & /3 \end{bmatrix}$$

$r=r_2$ must equal r_1
 $i=i_2$ must equal i_1

For Local $D_3 \supset C_2(i_3)$ symmetry

i_3 is free parameter



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

$i=i_1=i_2=i_3$

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

r_1 and r_2 are free

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*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



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

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

$$\mathbf{P}^{A_1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

$$\mathbf{P}^{A_2} = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 6$$

$$\mathbf{P}^E = \begin{bmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{bmatrix} / 3$$

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

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

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

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

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

$$\mathbf{P}^{A_1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} / 6$$

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$$\mathbf{P}^E = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 2 & -1 & 0 \end{pmatrix} / 3$$

Rank $\rho(D_3)=4$
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$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} \mathbf{p}^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

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

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

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

3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

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

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

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

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

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

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

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3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

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$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = \mathbf{P}_{x,x}^{A_1} \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^{A_1} + 0 + 0 + 0$$

$$+ 0 + \mathbf{P}_{y,y}^{A_2} \cdot \mathbf{g} \cdot \mathbf{P}_{y,y}^{A_2} + 0 + 0$$

where:

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

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

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

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

$$+ 0 + 0 + \mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^E + \mathbf{P}_{x,x}^E \cdot \mathbf{g} \cdot \mathbf{P}_{y,y}^E$$

$$+ 0 + 0 + \mathbf{P}_{y,y}^E \cdot \mathbf{g} \cdot \mathbf{P}_{x,x}^E + \mathbf{P}_{y,y}^E \cdot \mathbf{g} \cdot \mathbf{P}_{y,y}^E$$

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

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

Need to Define

6 Irreducible

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

Order $^\circ(D_3) = 6$

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

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

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

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

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3rd and Final Step:

Spectral resolution of ALL 6 of D_3 :

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

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

$$\mathbf{g} = \mathbf{1} \cdot \mathbf{g} \cdot \mathbf{1} = D^{A_1} (\mathbf{g}) \mathbf{P}_{x,x}^{A_1} + 0 + 0 + 0$$

$$+ 0 + D^{A_2} (\mathbf{g}) \mathbf{P}_{y,y}^{A_2} + 0 + 0$$

where:

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

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Need to Define

6 Irreducible

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

Order $^\circ(D_3) = 6$

Centrum $\kappa(D_3)=3$
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$$D_3 \kappa = \mathbf{1} \quad \mathbf{r}^1 + \mathbf{r}^2 \quad \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3$$

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Rank $\rho(D_3)=4$
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where:

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

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

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

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

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

Global (LAB) symmetry

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

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

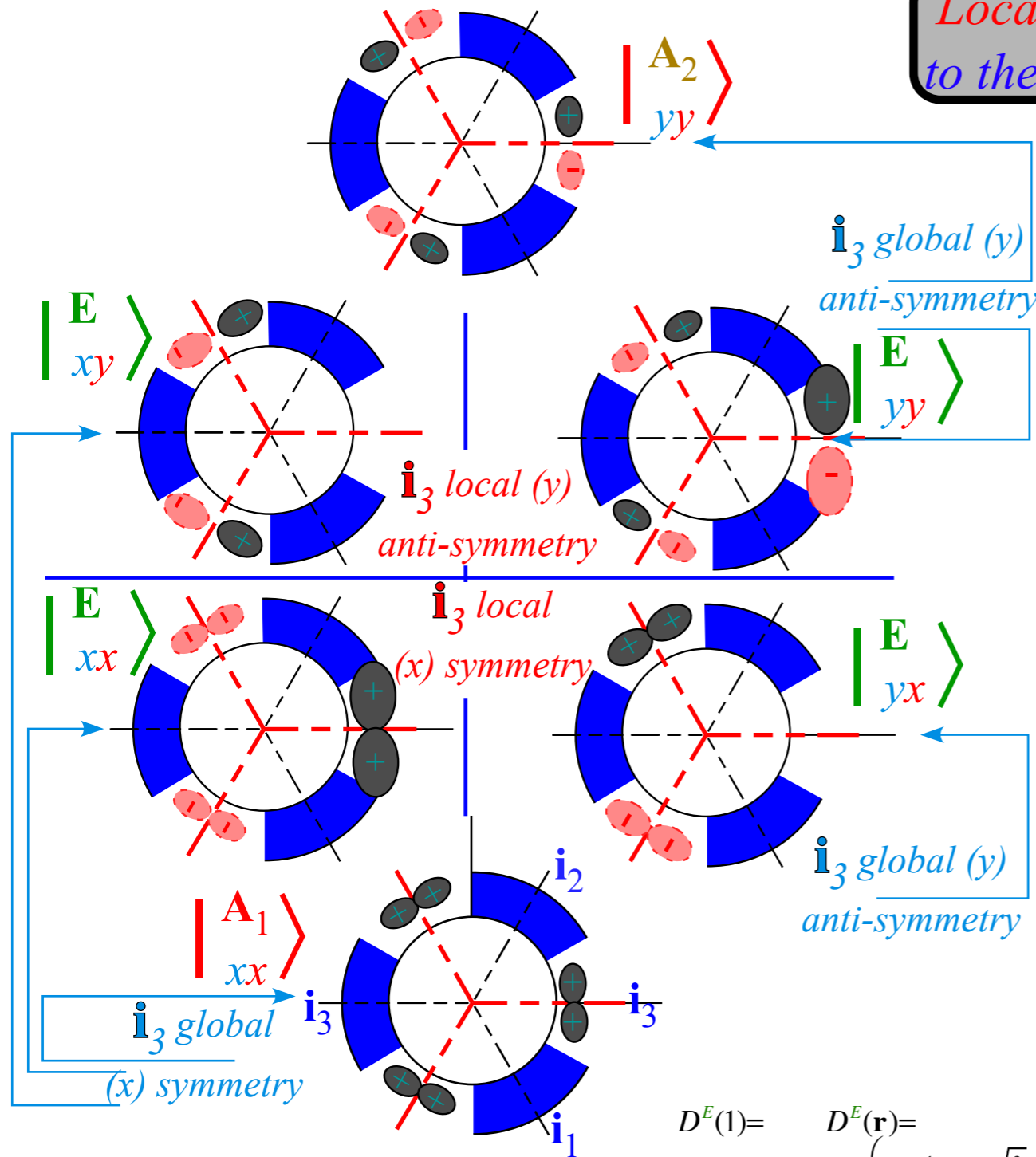
$$|_{eb}^{(m)} \rangle = \mathbf{P}_{eb}^{(m)} |1\rangle$$

Local (BOD) symmetry

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

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

Here the "Mock-Mach" is being applied!



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

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

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

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

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

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

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

$$D^E(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

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

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

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

$$D^E(\mathbf{i}_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

external LAB

internal BOD

symmetry label-e

symmetry label-b

GLOBAL

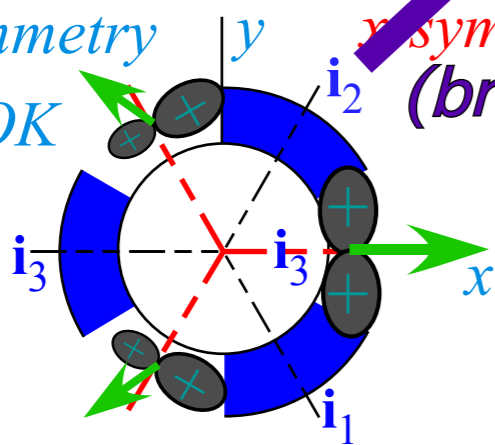
LOCAL

GLOBAL

$(i_3) = 0_2$

x-symmetry

\mathbf{i}_3 OK



~~LOCAL~~

~~$(i_3) = 0_2$~~

~~x-symmetry~~

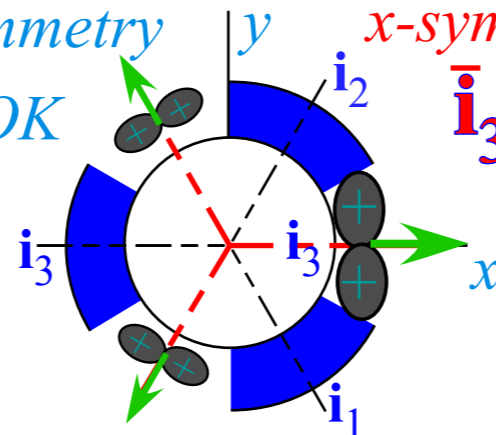
~~(broken $\bar{\mathbf{i}}_3$)~~

GLOBAL

$(i_3) = 0_2$

x-symmetry

\mathbf{i}_3 OK



LOCAL

$(i_3) = 0_2$

x-symmetry

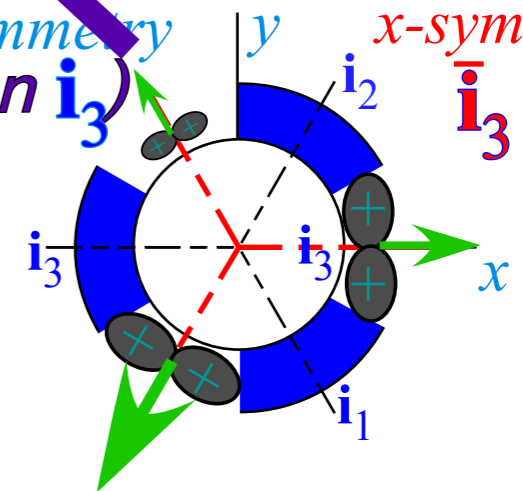
$\bar{\mathbf{i}}_3$ OK

~~GLOBAL~~

~~$(i_3) = 0_2$~~

~~x-symmetry~~

~~(broken \mathbf{i}_3)~~



LOCAL

$(i_3) = 0_2$

x-symmetry

$\bar{\mathbf{i}}_3$ OK

$$\mathbf{P}_{mn}^{(\mu)} = \frac{\ell(\mu)}{|\mathcal{G}|} \sum_{\mathbf{g}} D_{mn}^{(\mu)}(\mathbf{g})^* \mathbf{g}$$

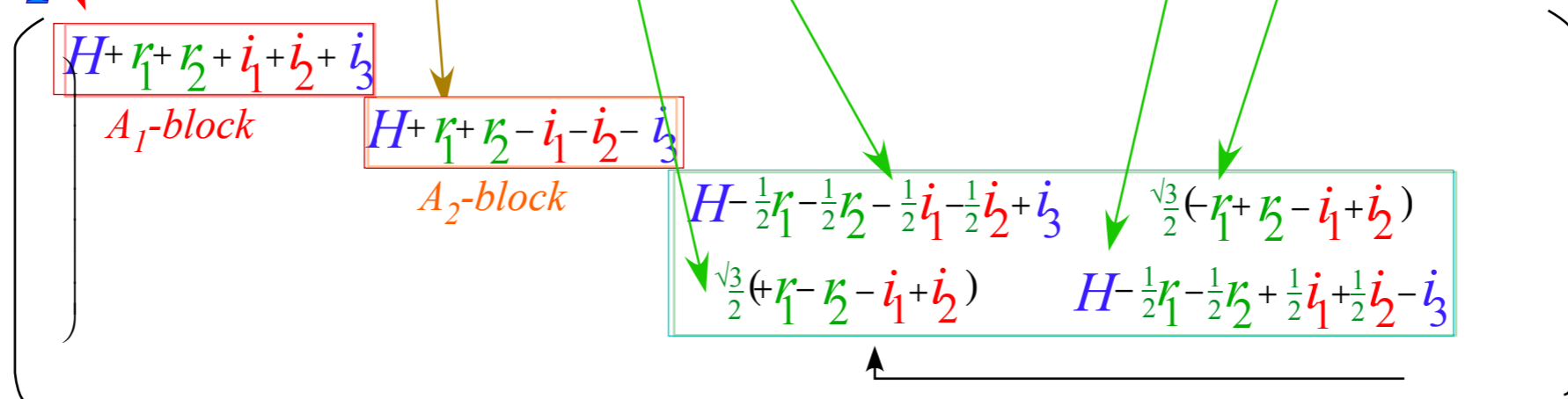
Spectral Efficiency: Same $D(a)_{mn}$ projectors give a lot!

$$\begin{array}{l} \mathbf{P}_{x,x}^{A_1} = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(1 \ 1 \ 1 \ 1 \ 1 \ 1)/6} \\ \mathbf{P}_{y,y}^{A_2} = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(1 \ 1 \ 1 \ -1 \ -1 \ -1)/6} \end{array}$$

$$\begin{array}{l} \mathbf{P}_{x,x}^E = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(2 \ -1 \ -1 \ -1 \ -1 \ +2)/6} \\ \mathbf{P}_{y,x}^E = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(0 \ 1 \ -1 \ -1 \ +1 \ 0)/\sqrt{3}/2} \end{array}$$

$$\begin{array}{l} \mathbf{P}_{x,y}^E = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(0 \ -1 \ 1 \ -1 \ +1 \ 0)/\sqrt{3}/2} \\ \mathbf{P}_{y,y}^E = \frac{1 \ r^1 \ r^2 \ i_1 \ i_2 \ i_3}{(2 \ -1 \ -1 \ +1 \ +1 \ -2)/6} \end{array}$$

- Eigenstates (shown before)
- Complete Hamiltonian



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

$$\begin{array}{l} r_1 = r_2 = r_1^* = r, \quad i_1 = i_2 = i_1^* = i \\ \text{gives: } A_1\text{-level: } H + 2r + 2i + i_3 \\ A_1\text{-level: } H + 2r - 2i - i_3 \\ E_x\text{-level: } H - r - i + i_3 \\ E_y\text{-level: } H - r + i - i_3 \end{array}$$

Global (LAB) symmetry

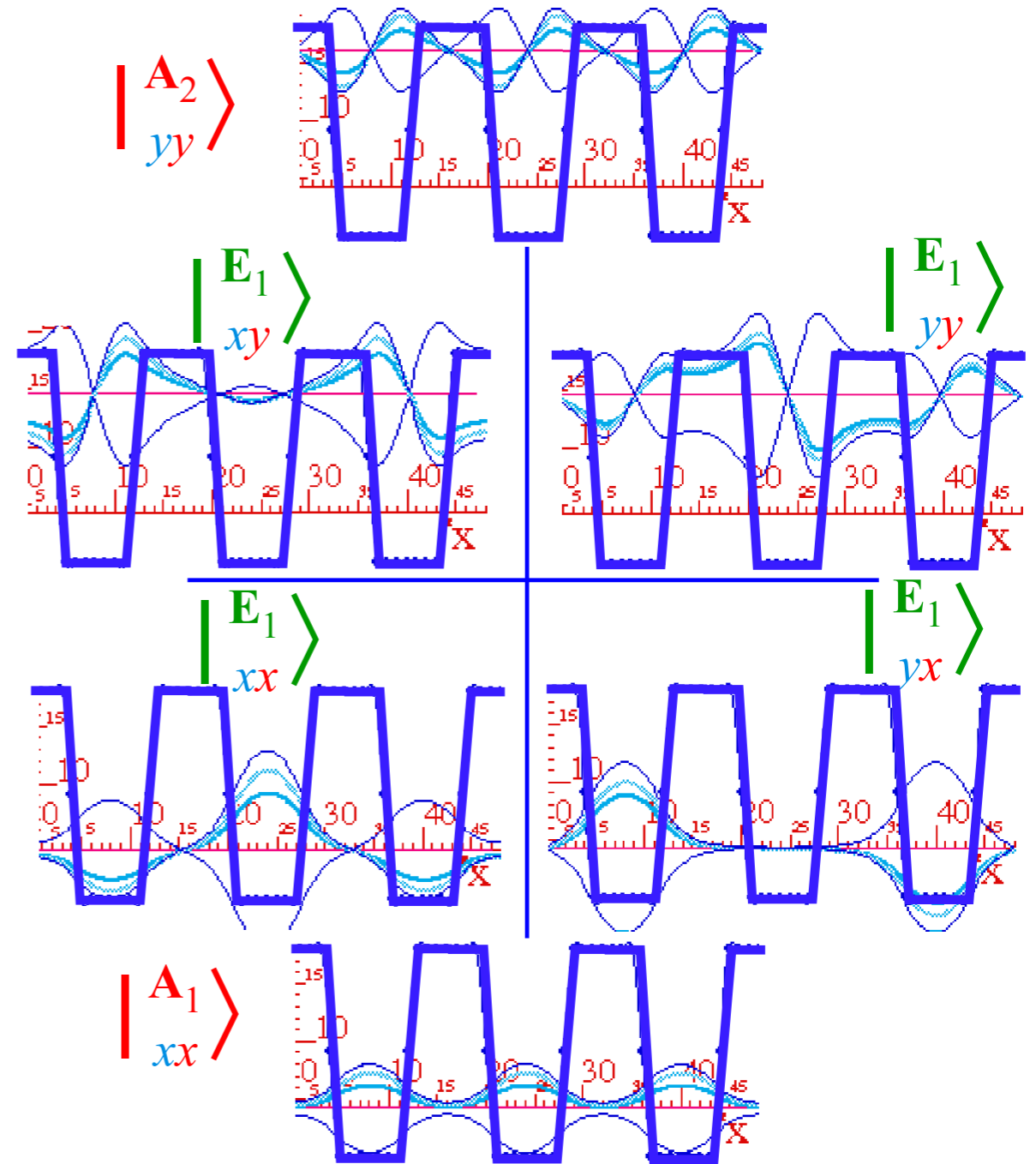
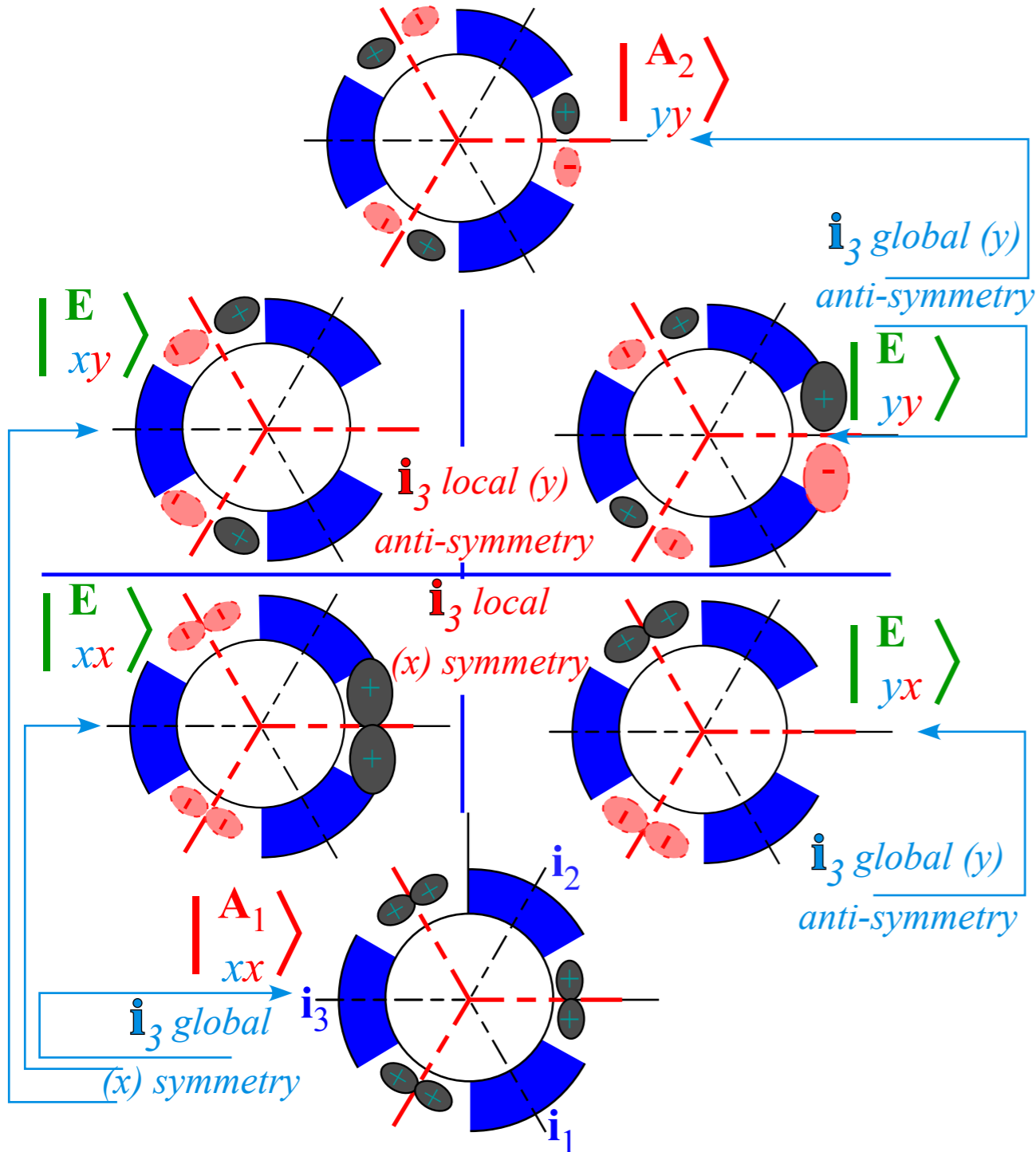
$D_3 > C_2$ i_3 projector states

Local (BOD) symmetry

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

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

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

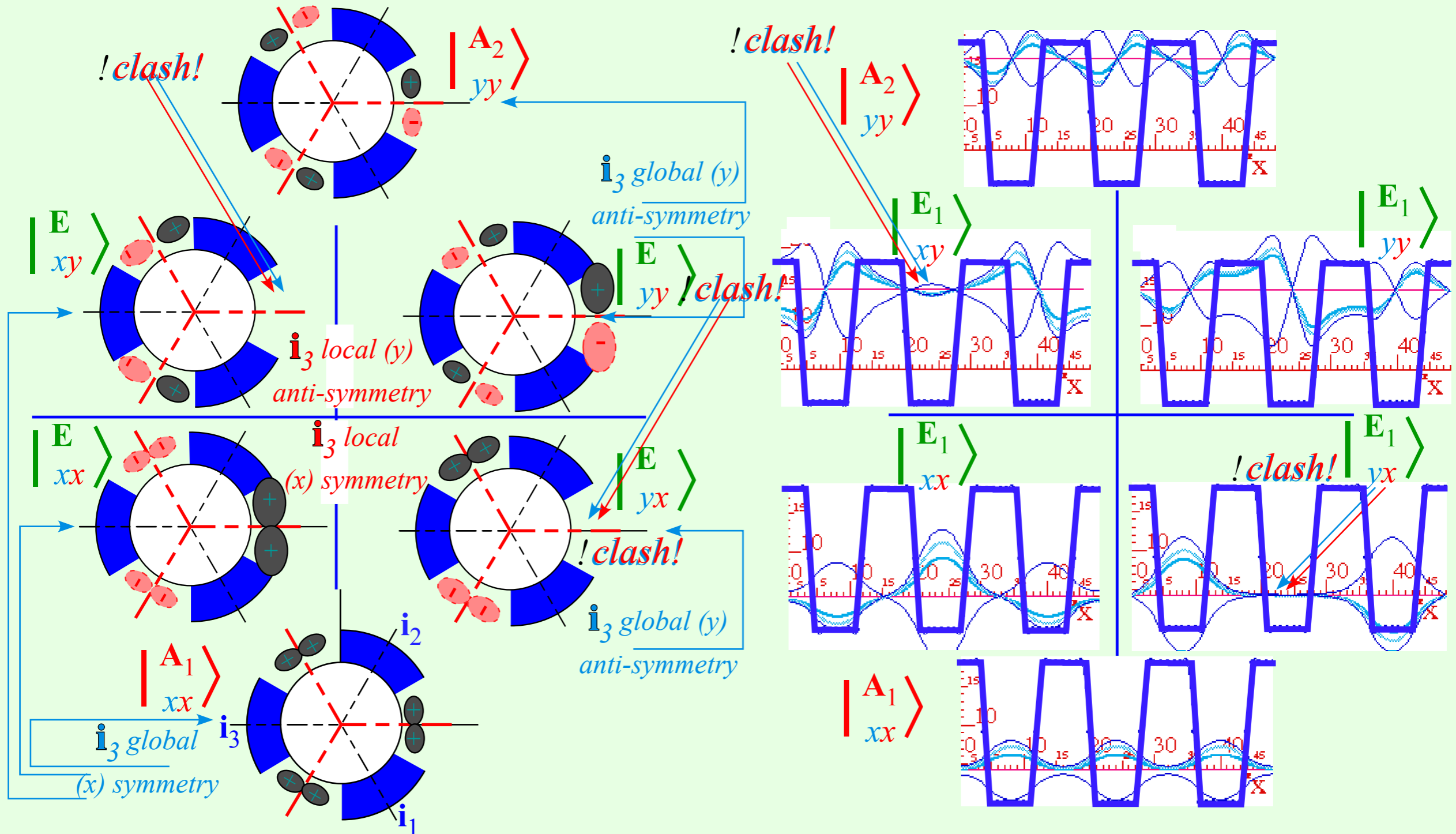


$$D^{A_1}(\mathbf{g}) = +I, D^{A_2}(\mathbf{r}^p) = +I, D^{A_2}(\mathbf{i}_q) = -I$$

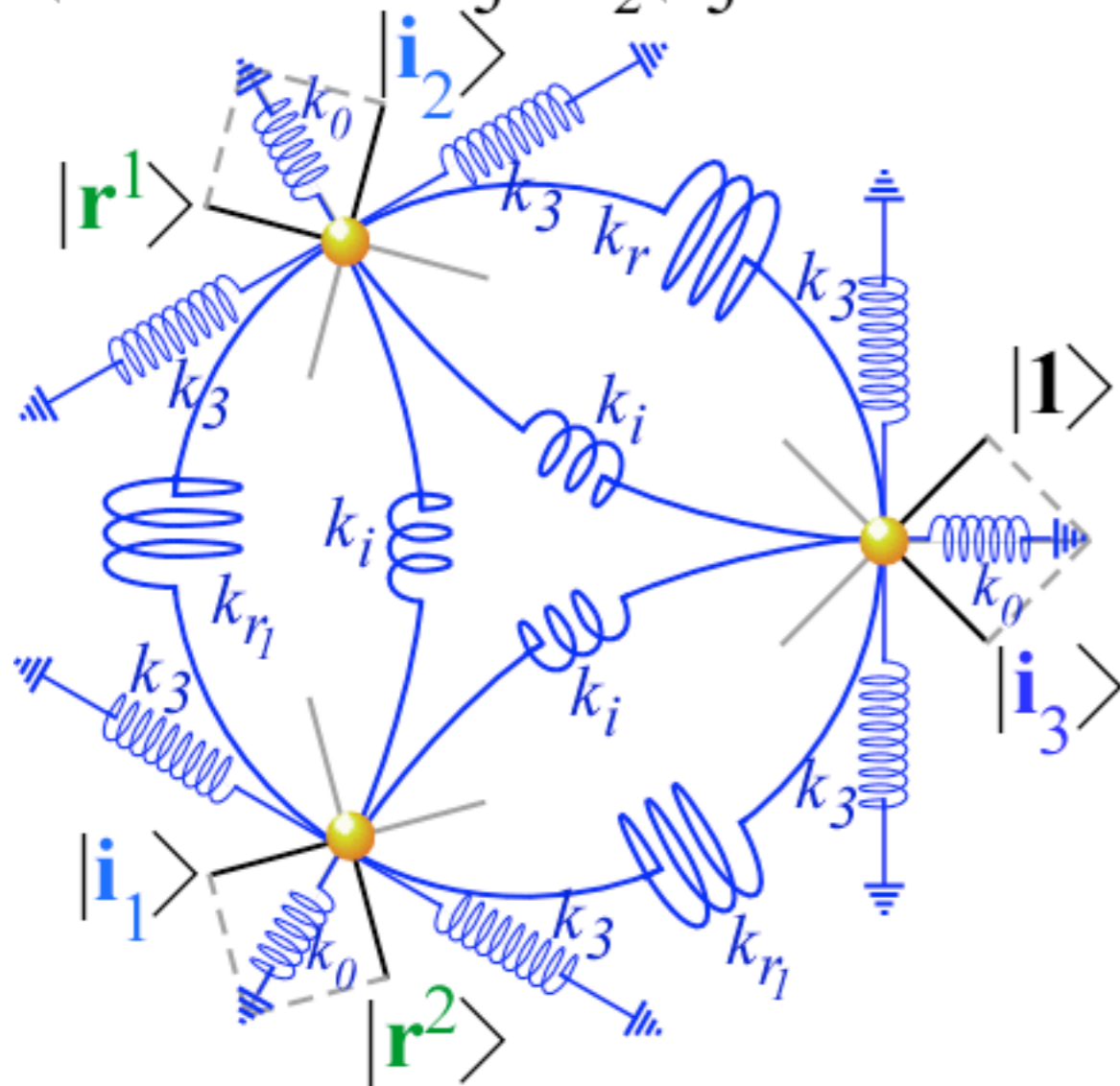
$$D^E(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, D^E(\mathbf{r}) = \begin{pmatrix} -\frac{1}{2} & -\sqrt{\frac{3}{4}} \\ \sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix}, D^E(\mathbf{r}^2) = \begin{pmatrix} -\frac{1}{2} & \sqrt{\frac{3}{4}} \\ -\sqrt{\frac{3}{4}} & -\frac{1}{2} \end{pmatrix},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

When there is no there, there...

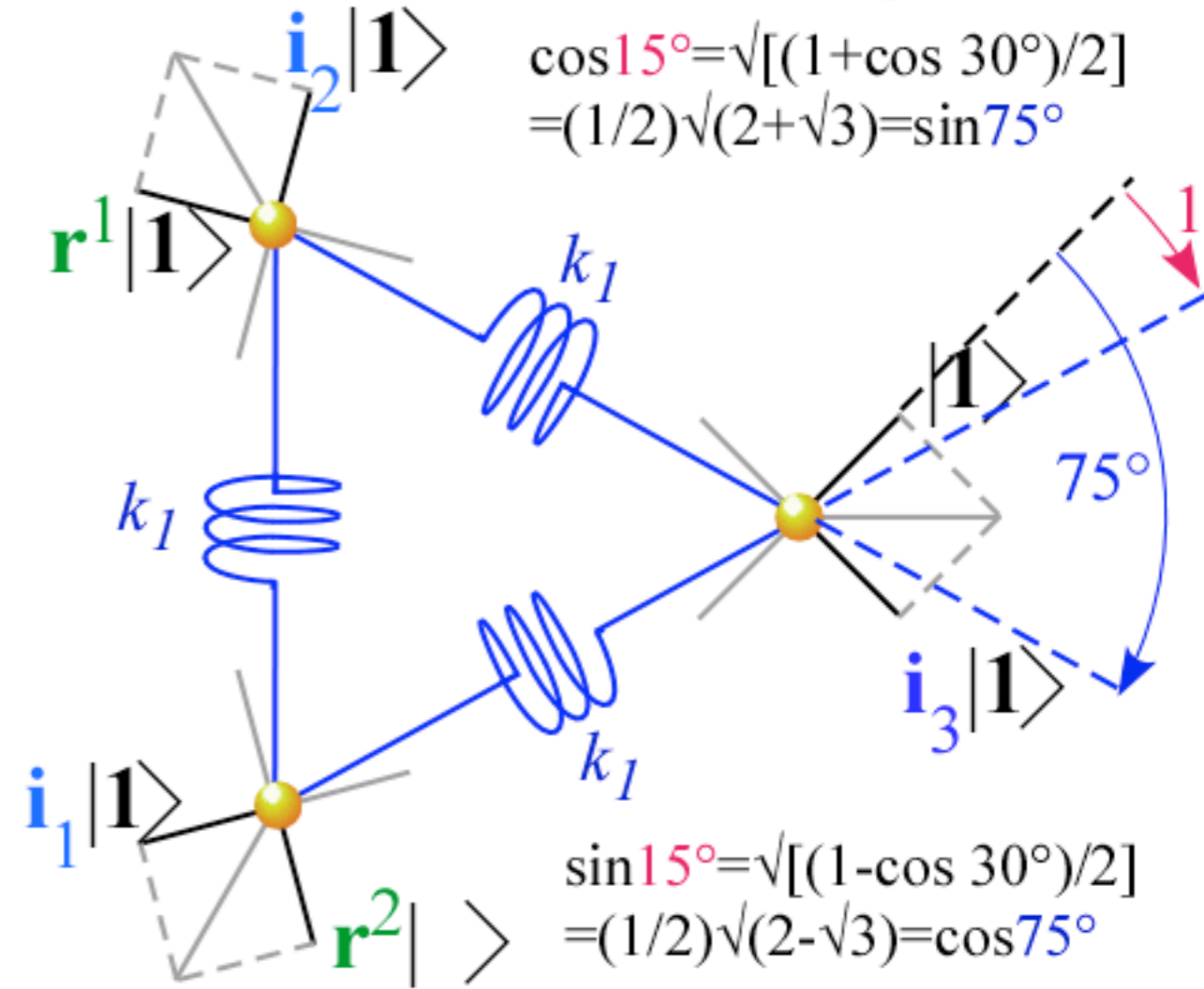
Nobody Home
where **LOCAL**
and **GLOBAL**

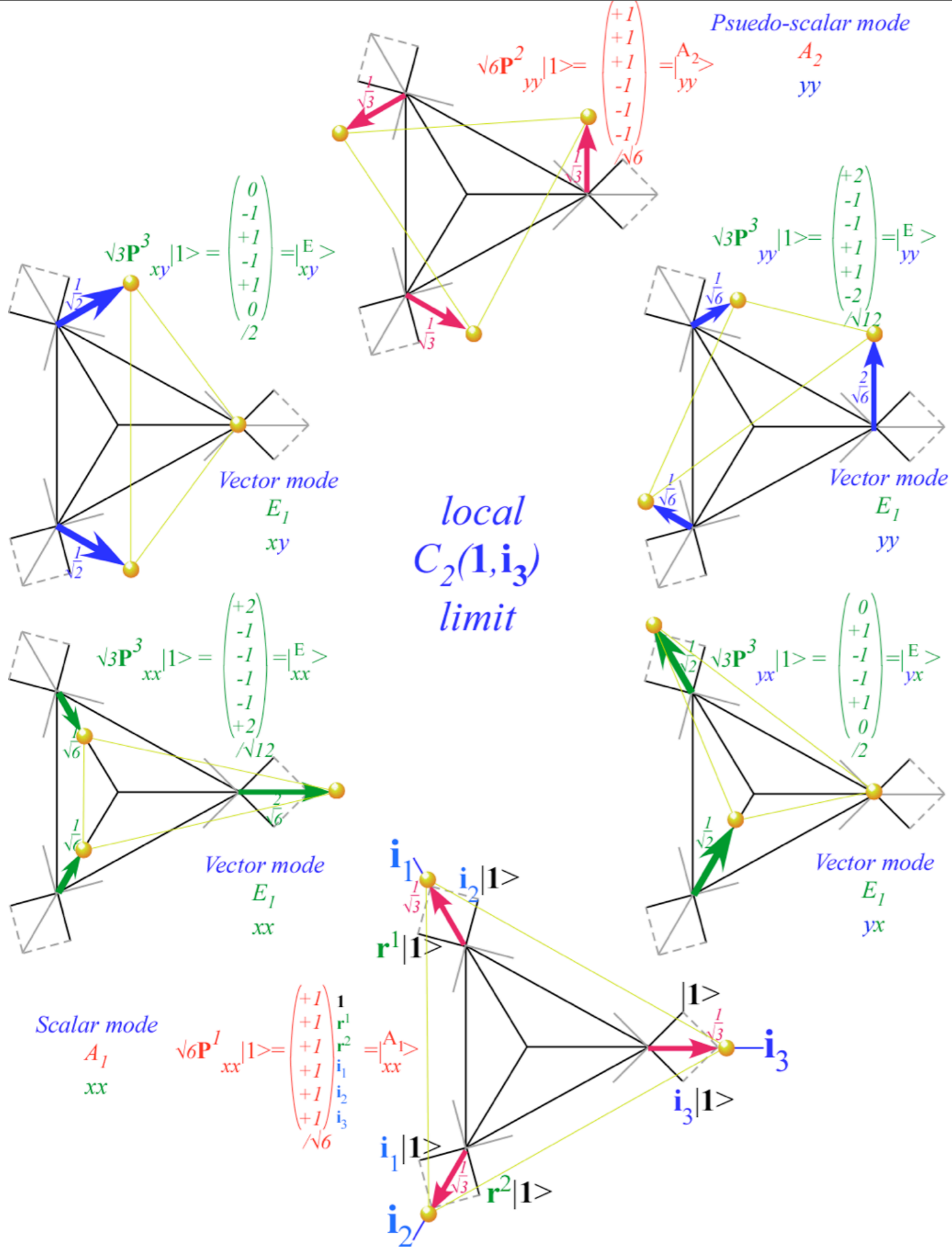


(a) Local $D_3 \supset C_2(i_3)$ model

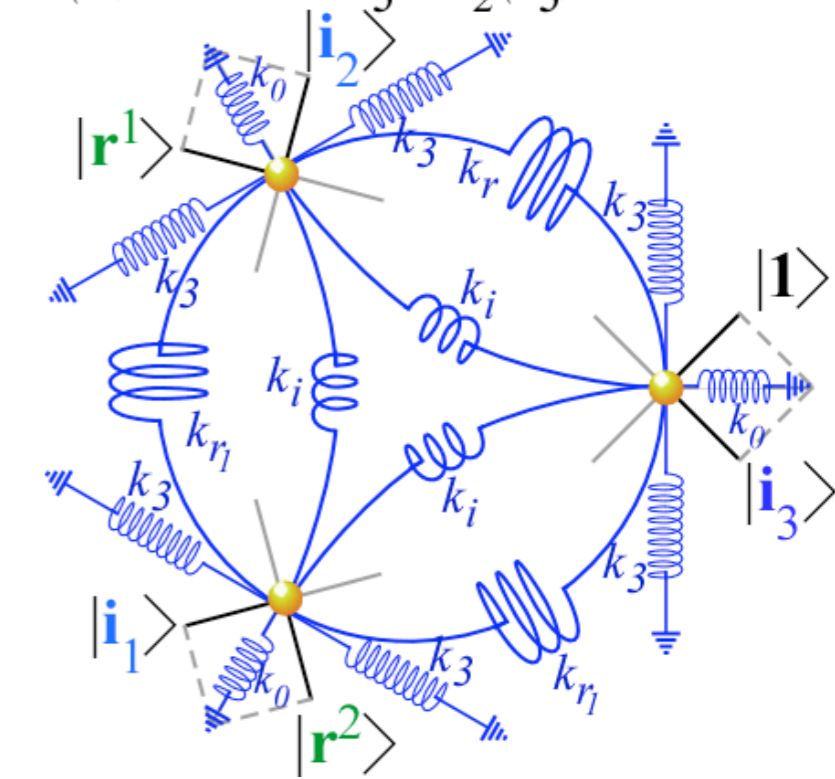


(b) Mixed local symmetry D_3 model





(a) Local $D_3 \supset C_2(i_3)$ model



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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor- $j=1/2$)

$$\chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector- $j=1$)

Excerpts from Lecture 12.6 page 126-136

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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\Theta/2)$ for $m \geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2} \quad \text{(spinor-j=1/2)}$$

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \dots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \dots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

Excerpts from Lecture 12.6 page 126-136

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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta/2} & \cdot \\ \cdot & e^{+i\theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\Theta/2)$ for $m \geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2} \quad \text{\textit{(spinor-j=1/2)}}$$

$$\chi^0(\Theta) = e^{-i\Theta \cdot 0} = 1 \quad \text{\textit{(scalar-j=0)}}$$

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \dots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^1(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta \quad \text{\textit{(vector-j=1)}}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \dots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^2(\Theta) = e^{-i2\Theta} + \dots + e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos2\Theta \quad \text{\textit{(tensor-j=2)}}$$

Excerpts from Lecture 12.6 page 126-136

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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta/2} & \cdot \\ \cdot & e^{+i\Theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\Theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\Theta/2)$ for $m \geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2} \quad \text{(spinor-j=1/2)}$$

$$\chi^0(\Theta) = e^{-i\Theta \cdot 0} = 1 \quad \text{(scalar-j=0)}$$

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \dots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^1(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta \quad \text{(vector-j=1)}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \dots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^2(\Theta) = e^{-i2\Theta} + \dots + e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos2\Theta \quad \text{(tensor-j=2)}$$

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

~~$$\chi^j(\Theta) = \text{Trace} D^{(j)}(\Theta) = e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)} + e^{+i\Theta j}$$~~

~~$$\chi^j(\Theta)e^{-i\Theta} = e^{-i\Theta(j+1)} + e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)}$$~~

Subtracting gives:

$$\chi^j(\Theta)(1 - e^{-i\Theta}) = -e^{-i\Theta(j+1)} + e^{+i\Theta j}$$

Excerpts from Lecture 12.6 page 126-136

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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta/2} & \cdot \\ \cdot & e^{+i\Theta/2} \end{pmatrix} \quad \chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\Theta} \end{pmatrix}$$

(spinor-j=1/2) *(vector-j=1)*

$\chi^j(\Theta)$ involves a sum of $2\cos(m\Theta/2)$ for $m \geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2} \quad \text{(spinor-j=1/2)} \quad \chi^0(\Theta) = e^{-i\Theta \cdot 0} = 1 \quad \text{(scalar-j=0)}$$

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \dots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} \quad \chi^1(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta \quad \text{(vector-j=1)}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \dots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2} \quad \chi^2(\Theta) = e^{-i2\Theta} + \dots + e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos2\Theta \quad \text{(tensor-j=2)}$$

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

~~$$\chi^j(\Theta) = \text{Trace} D^{(j)}(\Theta) = e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)} + e^{+i\Theta j}$$~~

~~$$\chi^j(\Theta)e^{-i\Theta} = e^{-i\Theta(j+1)} + e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)}$$~~

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 12.6 page 126-136

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 $m=\{-j, -j+1, \dots, j-1, j\}$.

$$\chi^{1/2}(\Theta) = \text{trace} D^{1/2}(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta/2} & \cdot \\ \cdot & e^{+i\Theta/2} \end{pmatrix}$$

(spinor-j=1/2)

$$\chi^1(\Theta) = \text{trace} D^1(\Theta) = \text{trace} \begin{pmatrix} e^{-i\Theta} & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & e^{-i\Theta} \end{pmatrix}$$

(vector-j=1)

$\chi^j(\Theta)$ involves a sum of $2\cos(m\Theta/2)$ for $m \geq 0$ up to $m=j$.

$$\chi^{1/2}(\Theta) = e^{-i\frac{\Theta}{2}} + e^{i\frac{\Theta}{2}} = 2\cos\frac{\Theta}{2} \quad \text{(spinor-j=1/2)}$$

$$\chi^0(\Theta) = e^{-i\Theta \cdot 0} = 1 \quad \text{(scalar-j=0)}$$

$$\chi^{3/2}(\Theta) = e^{-i\frac{3\Theta}{2}} + \dots + e^{i\frac{3\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2}$$

$$\chi^1(\Theta) = e^{-i\Theta} + 1 + e^{i\Theta} = 1 + 2\cos\Theta \quad \text{(vector-j=1)}$$

$$\chi^{5/2}(\Theta) = e^{-i\frac{5\Theta}{2}} + \dots + e^{i\frac{5\Theta}{2}} = 2\cos\frac{\Theta}{2} + 2\cos\frac{3\Theta}{2} + 2\cos\frac{5\Theta}{2}$$

$$\chi^2(\Theta) = e^{-i2\Theta} + \dots + e^{i2\Theta} = 1 + 2\cos\Theta + 2\cos2\Theta \quad \text{(tensor-j=2)}$$

$\chi^j(\Theta)$ is a geometric series with ratio $e^{i\Theta}$ between each successive term.

~~$$\chi^j(\Theta) = \text{Trace} D^{(j)}(\Theta) = e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)} + e^{+i\Theta j}$$~~

~~$$\chi^j(\Theta)e^{-i\Theta} = e^{-i\Theta(j+1)} + e^{-i\Theta j} + e^{-i\Theta(j-1)} + e^{-i\Theta(j-2)} + \dots + e^{+i\Theta(j-2)} + e^{+i\Theta(j-1)}$$~~

Subtracting/dividing gives $\chi^j(\Theta)$ formula.

$$\chi^j(\Theta) = \frac{e^{+i\Theta j} - e^{-i\Theta(j+1)}}{1 - e^{-i\Theta}} = \frac{e^{+i\Theta(j+\frac{1}{2})} - e^{-i\Theta(j+\frac{1}{2})}}{e^{+i\frac{\Theta}{2}} - e^{-i\frac{\Theta}{2}}} = \frac{\sin\Theta(j+\frac{1}{2})}{\sin\frac{\Theta}{2}}$$

For C_n angle $\Theta=2\pi/n$ this χ^j has a lot of geometric significance.

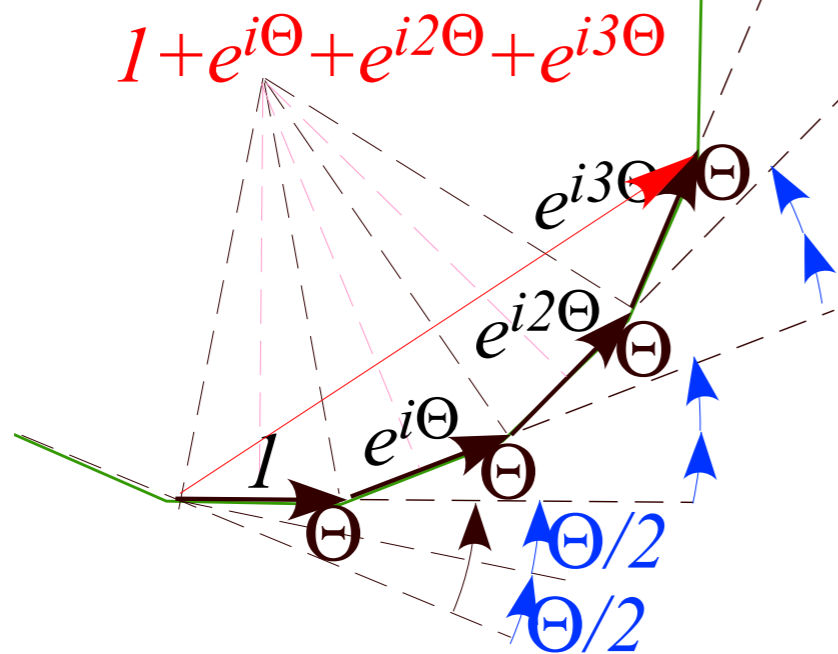
$$\chi^j\left(\frac{2\pi}{n}\right) = \frac{\sin\frac{\pi}{n}(2j+1)}{\sin\frac{\pi}{n}} = \frac{\sin\frac{\pi\ell^j}{n}}{\sin\frac{\pi}{n}}$$

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 12.6
page 136

$(j)^{th}$ n -gon segments

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

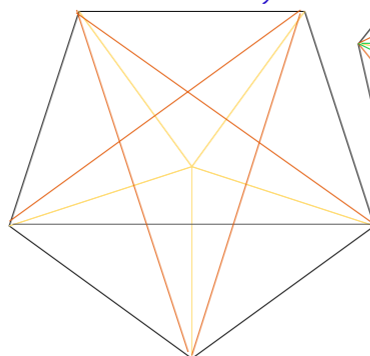
$$\ell^j = 2j+1$$

$$n = 7$$

$$\ell^j = 1, 2, 3$$

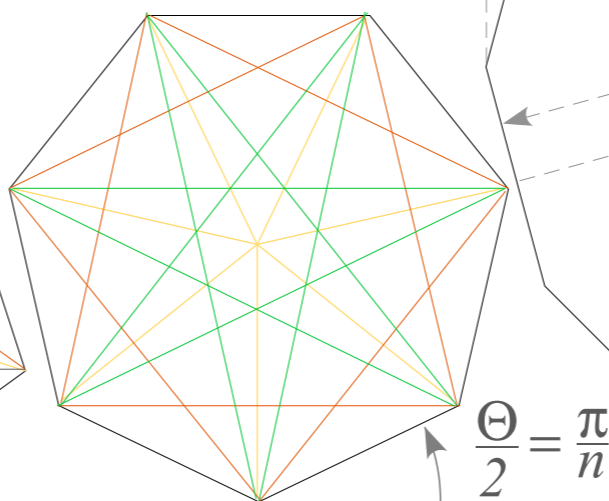
$$n = 5$$

$$\ell^j = 1, 2$$



$$\chi^0(2\pi/5) = 1$$

$$\chi^{1/2}(2\pi/5) = 1.618... \\ = (1 + \sqrt{5})/2 =$$

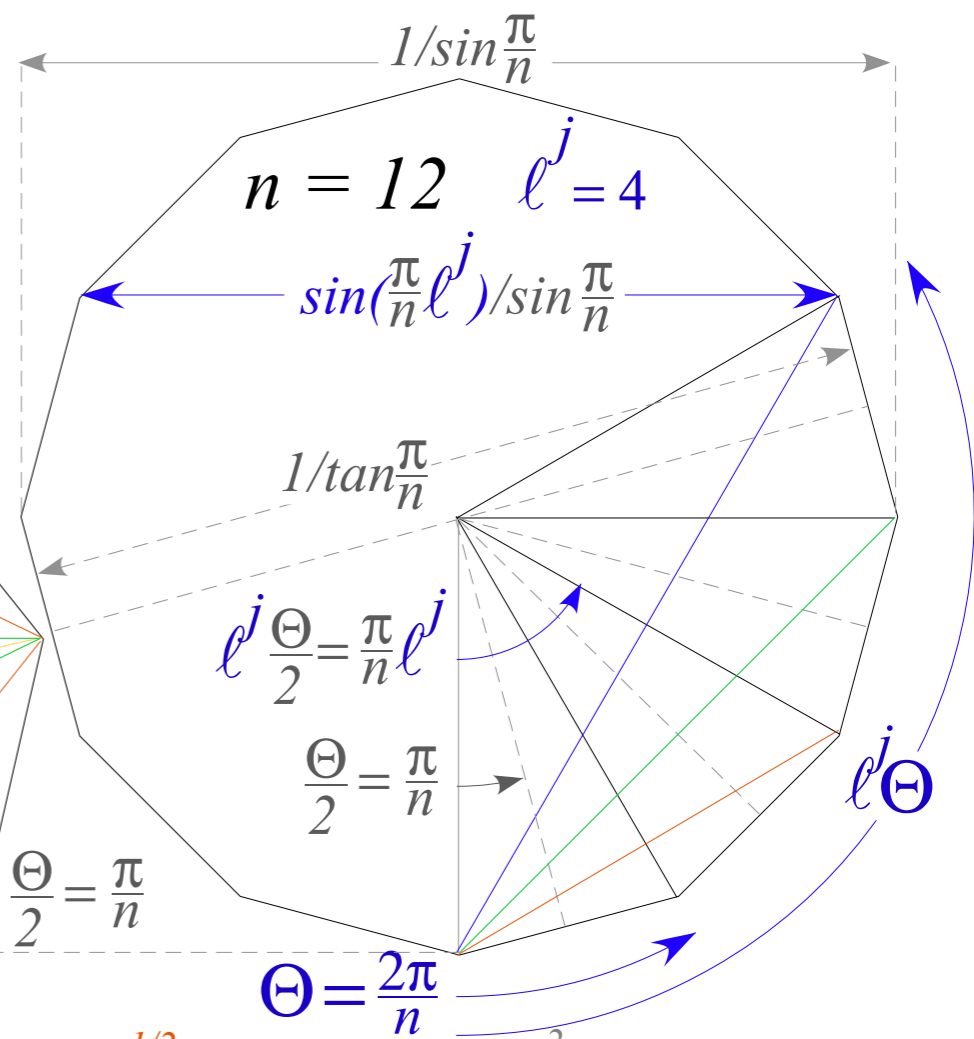


$$\chi^0(2\pi/7) = 1$$

$$\chi^{1/2}(2\pi/7) = 1.802...$$

$$\chi^1(2\pi/7) = 2.247...$$

$$\chi^{3/2}(2\pi/7) = 2.247...$$



$$\Theta = \frac{2\pi}{n}$$

$$\chi^{1/2}(2\pi/12) = 1.932...$$

$$\chi^1(2\pi/12) = 2.732...$$

$$\chi^{3/2}(2\pi/12) = 3.346...$$

$$\chi^2(2\pi/12) = 3.732...$$

$$\chi^{5/2}(2\pi/12) = 3.864...$$

$$\chi^3(2\pi/12) = 3.732...$$