

# Group Theory in Quantum Mechanics

## Lecture 14 (3.14.13)

### 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 )

*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 characters*

*Character ortho-completeness*

*Group invariant numbers: Centrum, Rank, and Order*

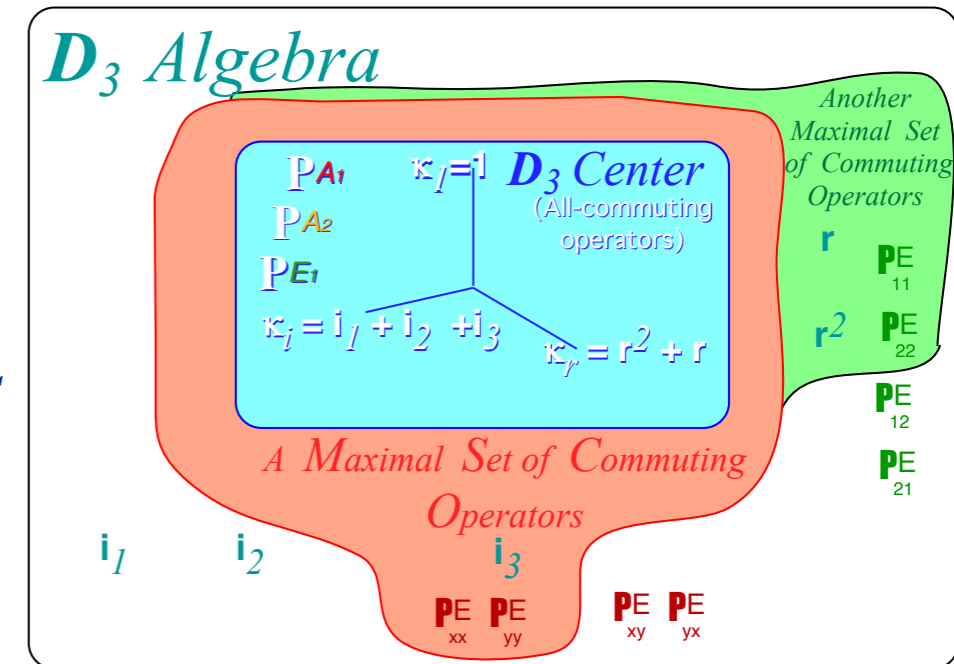
*2nd-Stage spectral decompositions of global/local  $D_3$*

*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*



(Fig. 15.2.1 QTCA)

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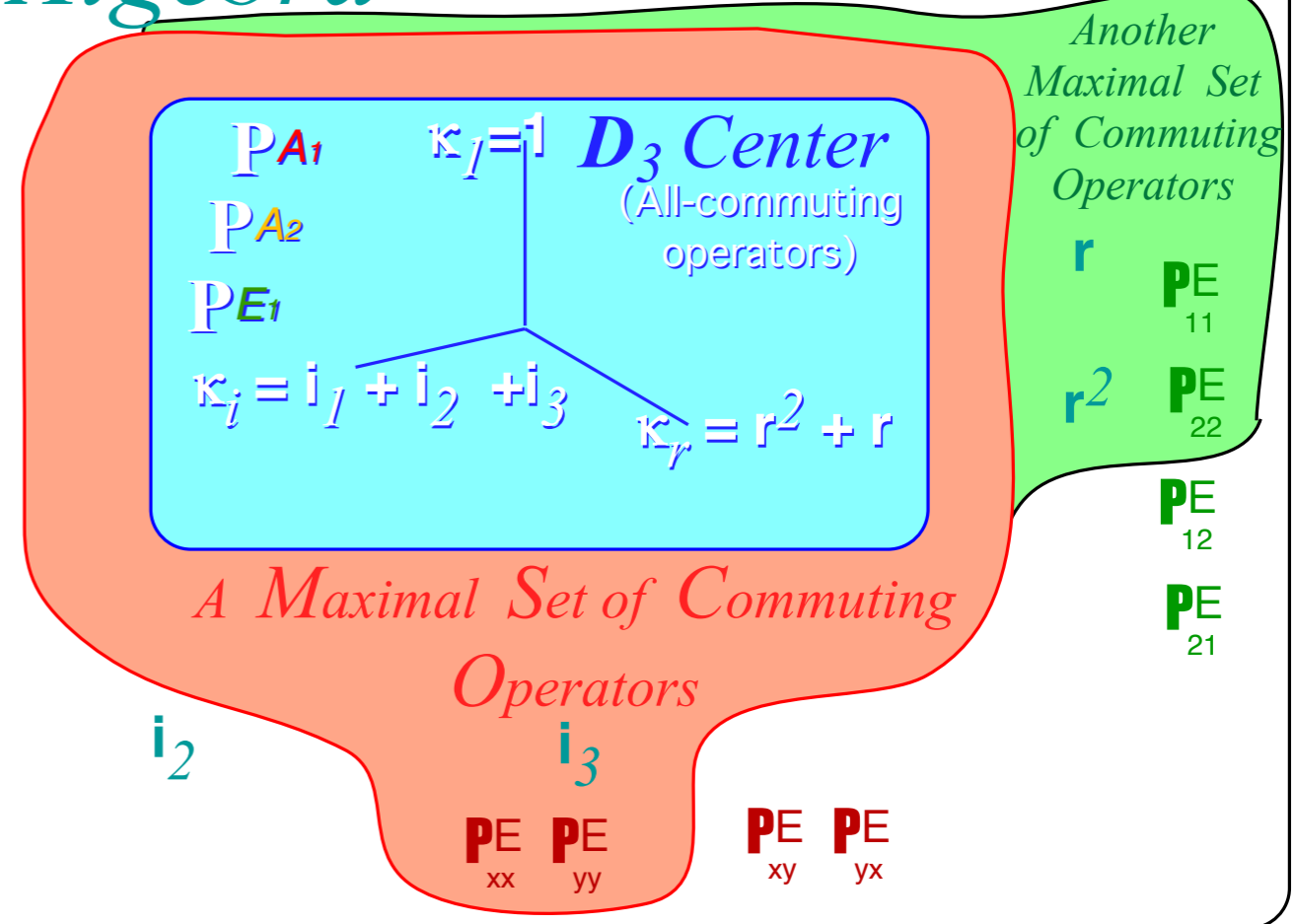
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<b>1</b>	<b>r<sup>2</sup></b>	<b>r</b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>
<b>r</b>	<b>1</b>	<b>r<sup>2</sup></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>
<b>r<sup>2</sup></b>	<b>r</b>	<b>1</b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>
<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>1</b>	<b>r</b>	<b>r<sup>2</sup></b>
<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>r<sup>2</sup></b>	<b>1</b>	<b>r</b>
<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>r</b>	<b>r<sup>2</sup></b>	<b>1</b>

	$\kappa_1 = 1$	$\kappa_r = r + r^2$	$\kappa_i = i_1 + i_2 + i_3$
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# $D_3$ Algebra



Class-sum  $\kappa_k$  commutes with all  $g_t$

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

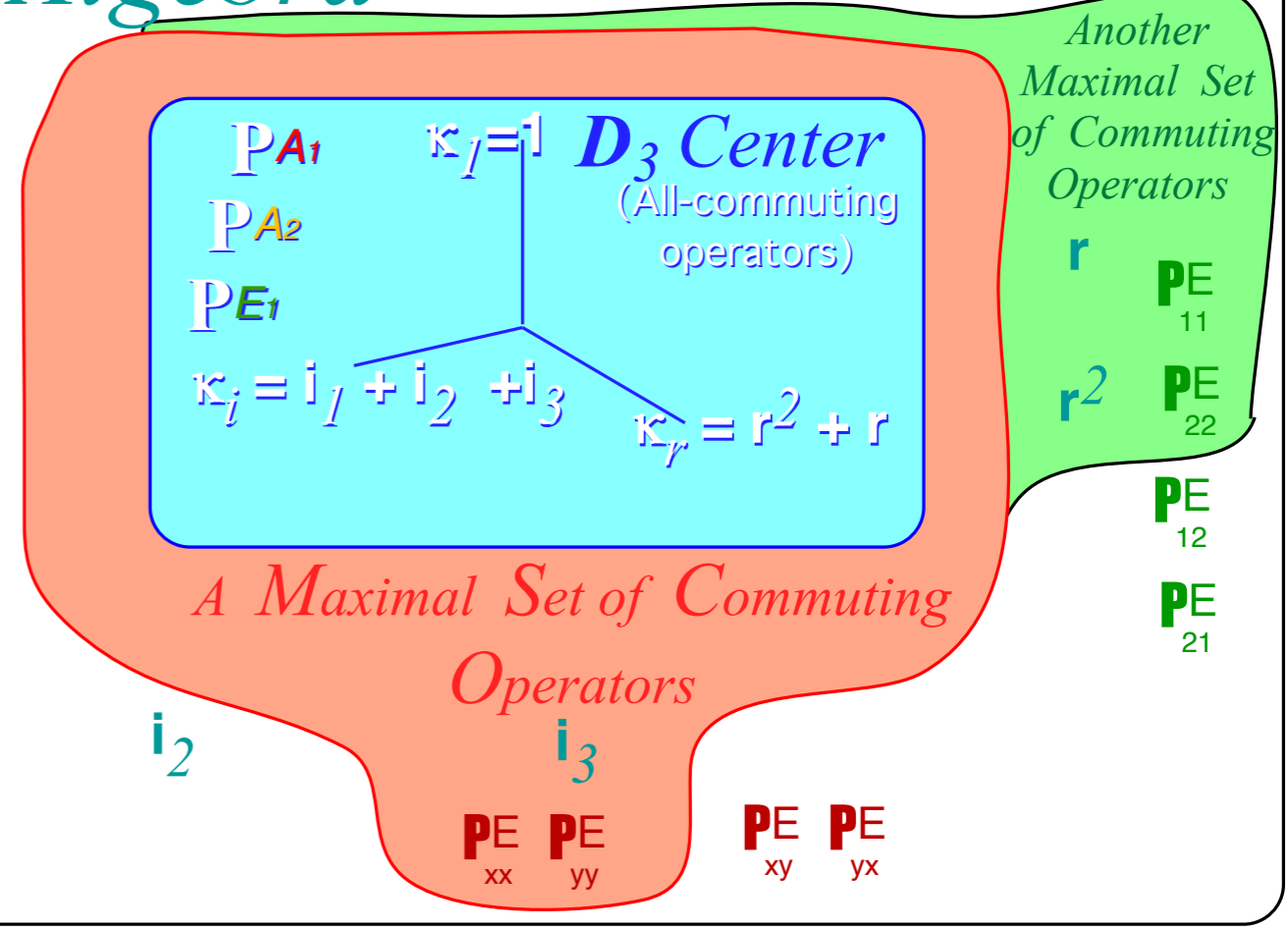
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1	$r^2$	$r$	$i_1$	$i_2$	$i_3$
$r$	1	$r^2$	$i_3$	$i_1$	$i_2$
$r^2$	$r$	1	$i_2$	$i_3$	$i_1$
$i_1$	$i_3$	$i_2$	1	$r$	$r^2$
$i_2$	$i_1$	$i_3$	$r^2$	1	$r$
$i_3$	$i_2$	$i_1$	$r$	$r^2$	1

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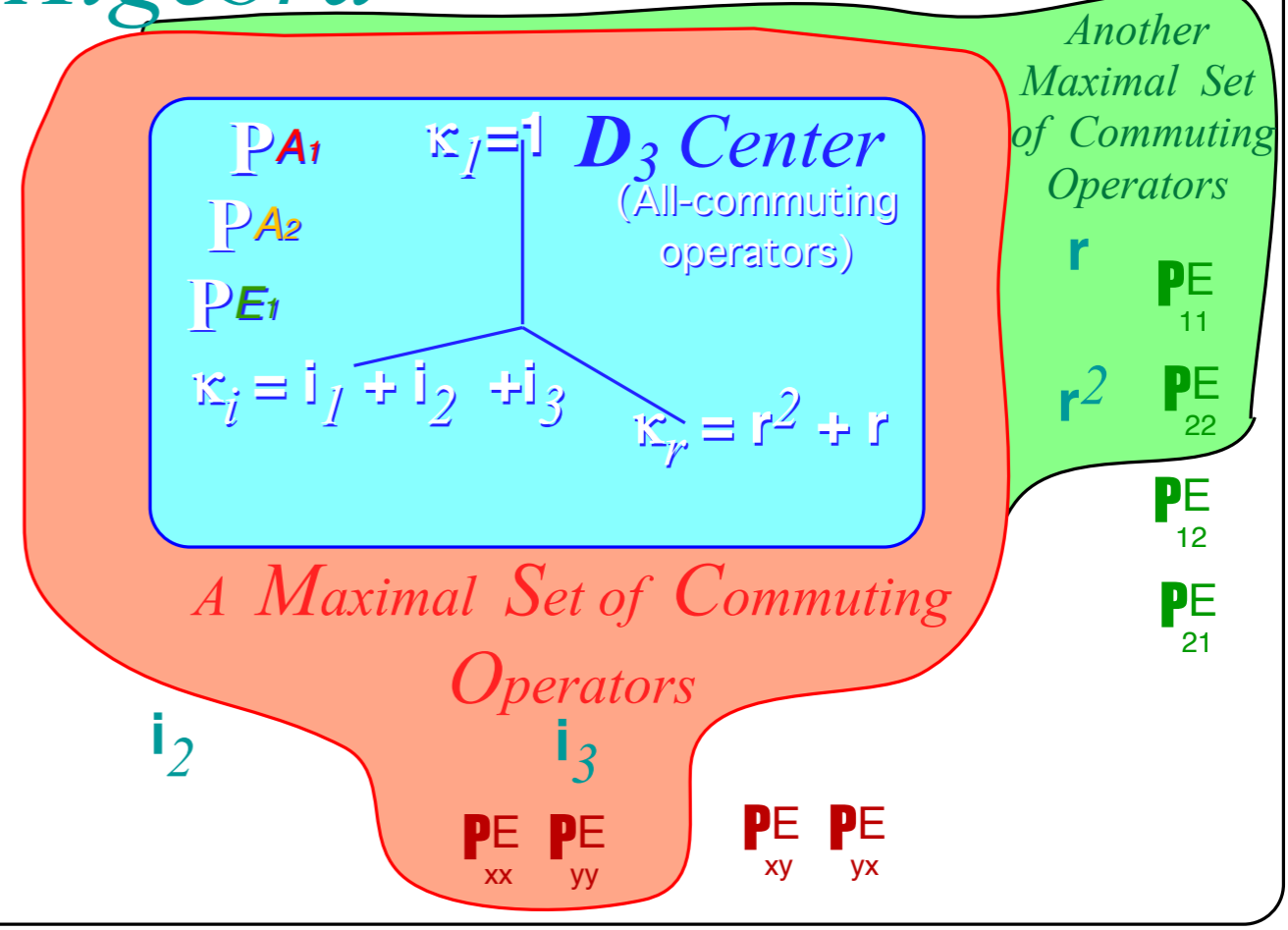
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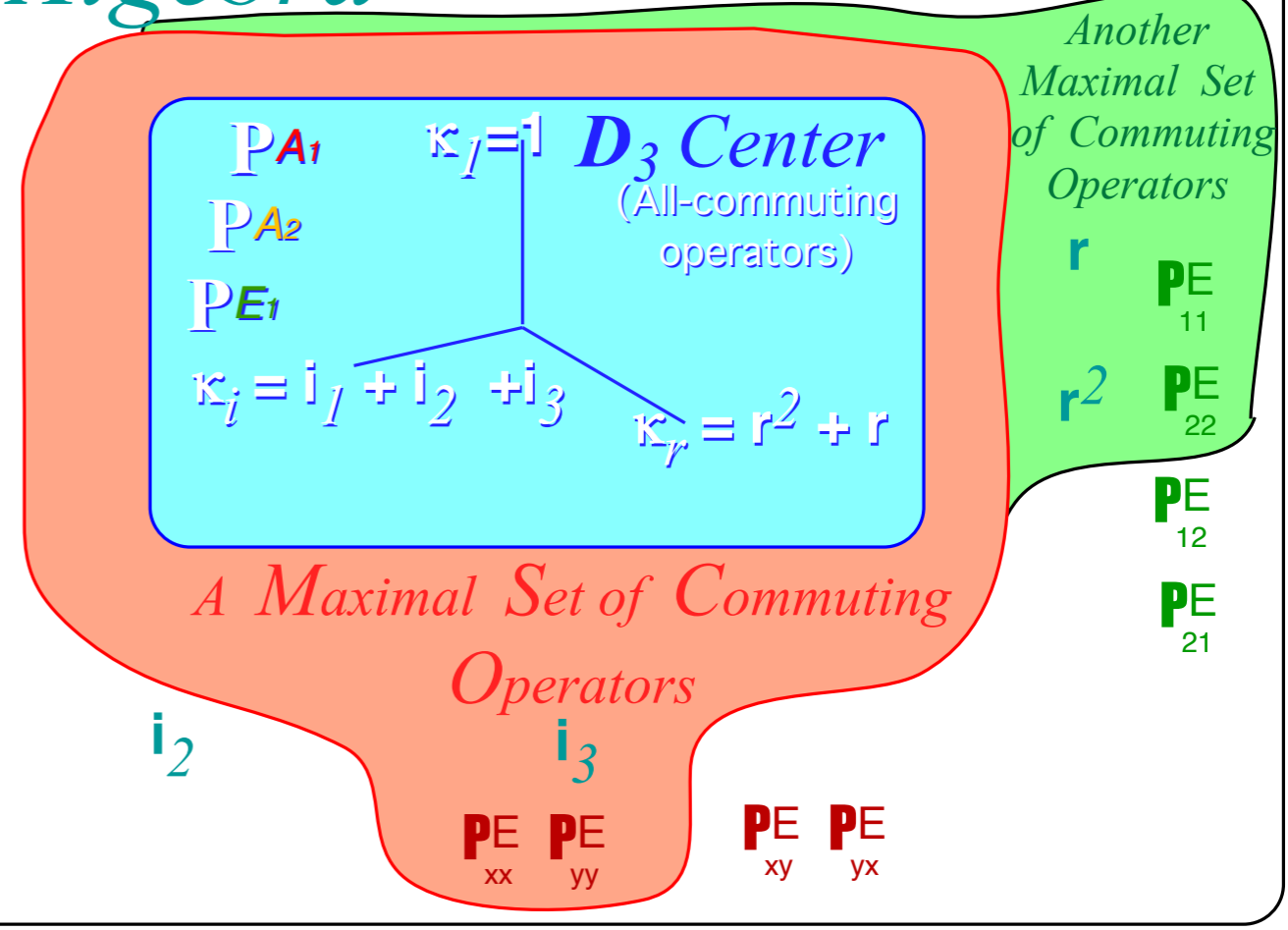
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<b>r</b>	<b>1</b>	<b>r<sup>2</sup></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>
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<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>1</b>	<b>r</b>	<b>r<sup>2</sup></b>
<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>r<sup>2</sup></b>	<b>1</b>	<b>r</b>
<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>r</b>	<b>r<sup>2</sup></b>	<b>1</b>

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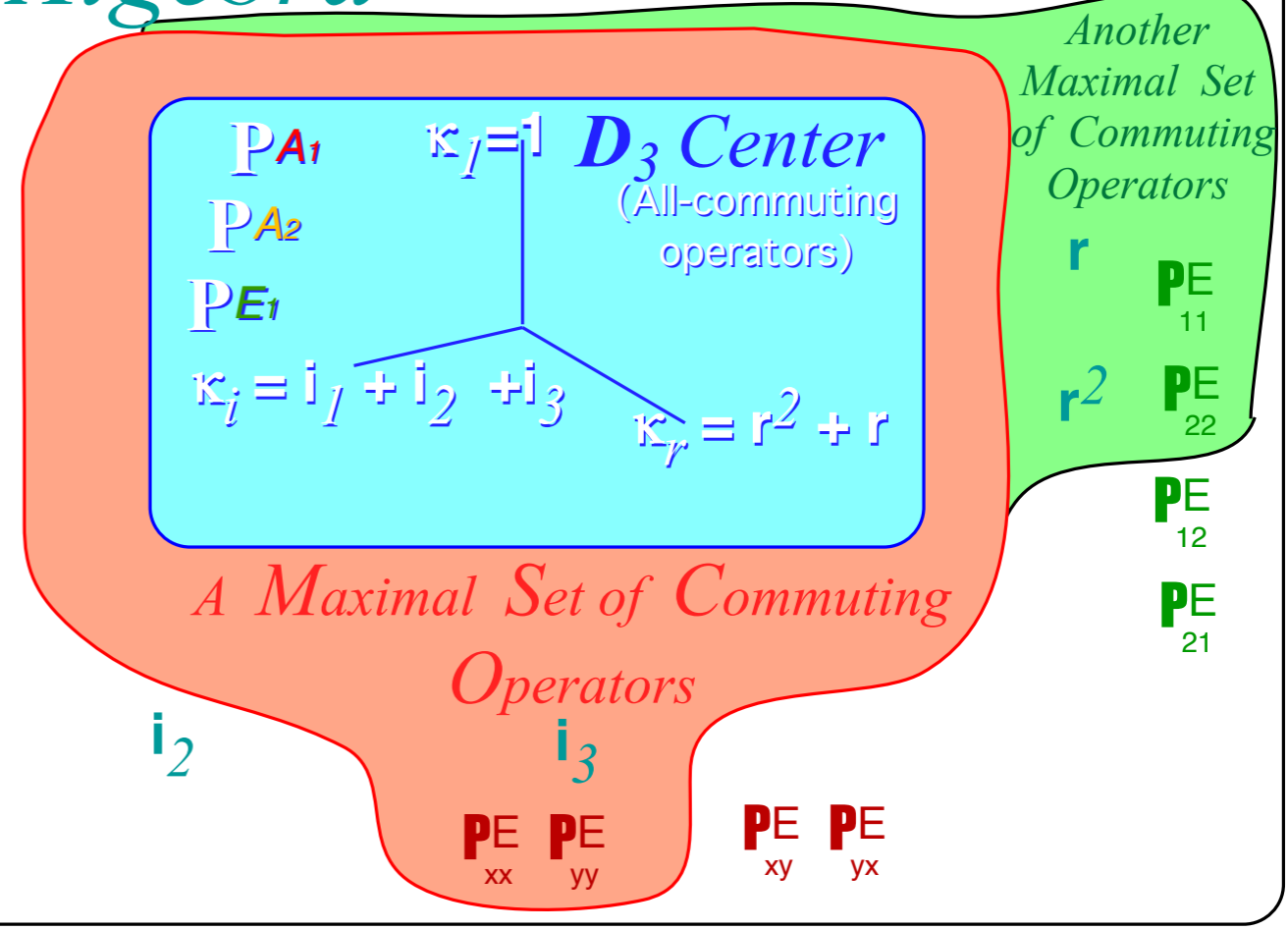
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<b>r</b>	<b>1</b>	<b>r<sup>2</sup></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>
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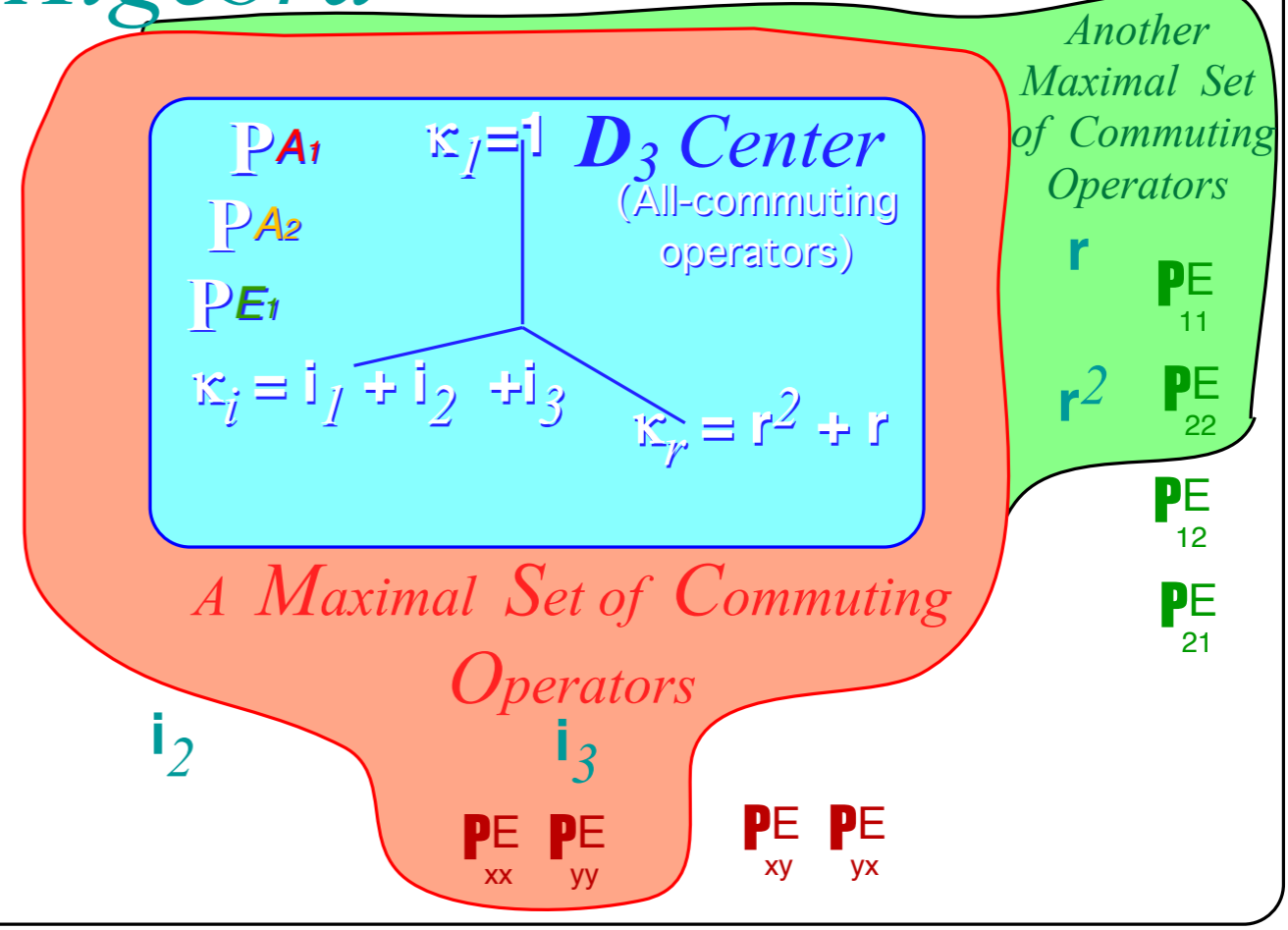
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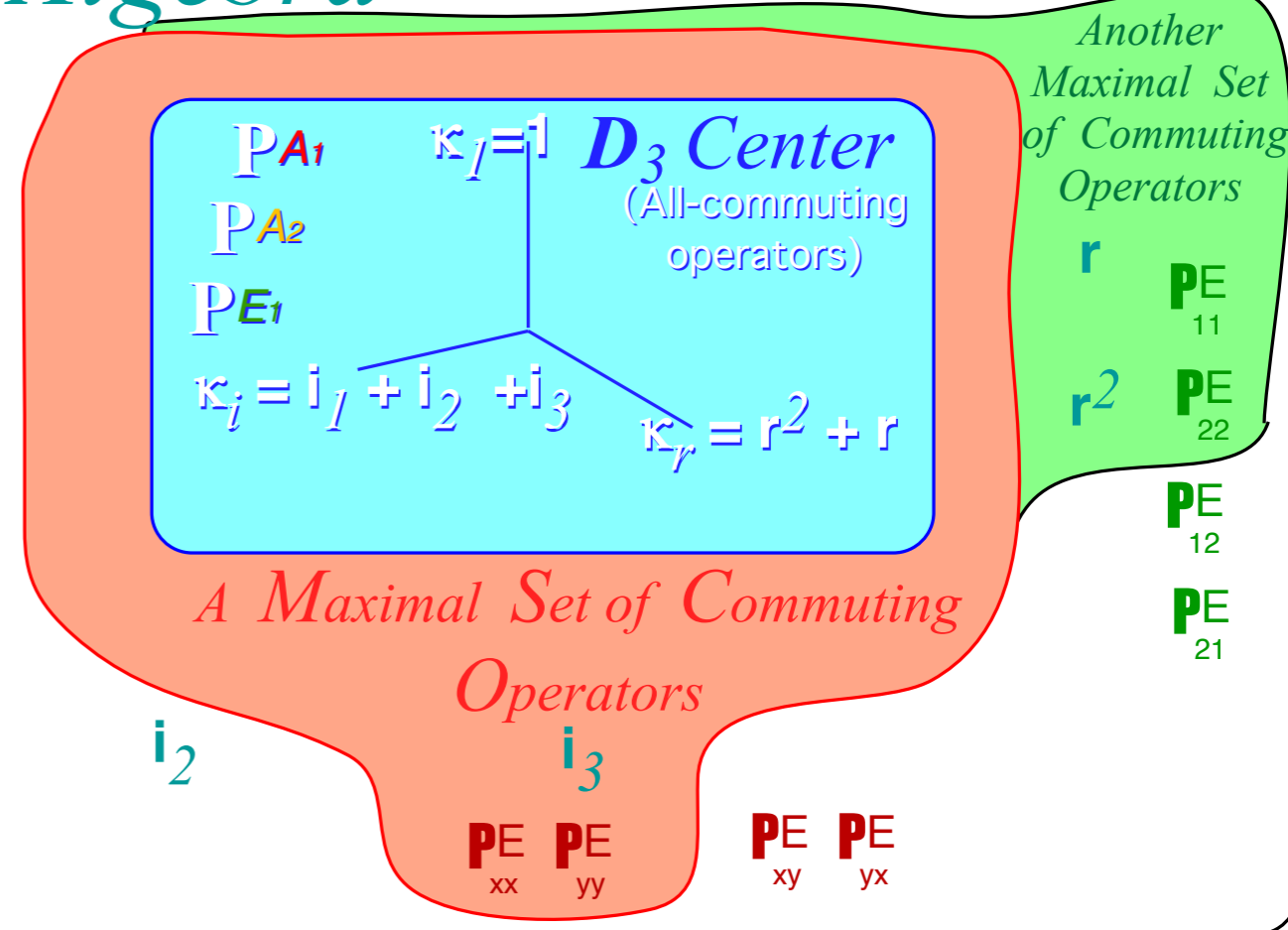
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⋮

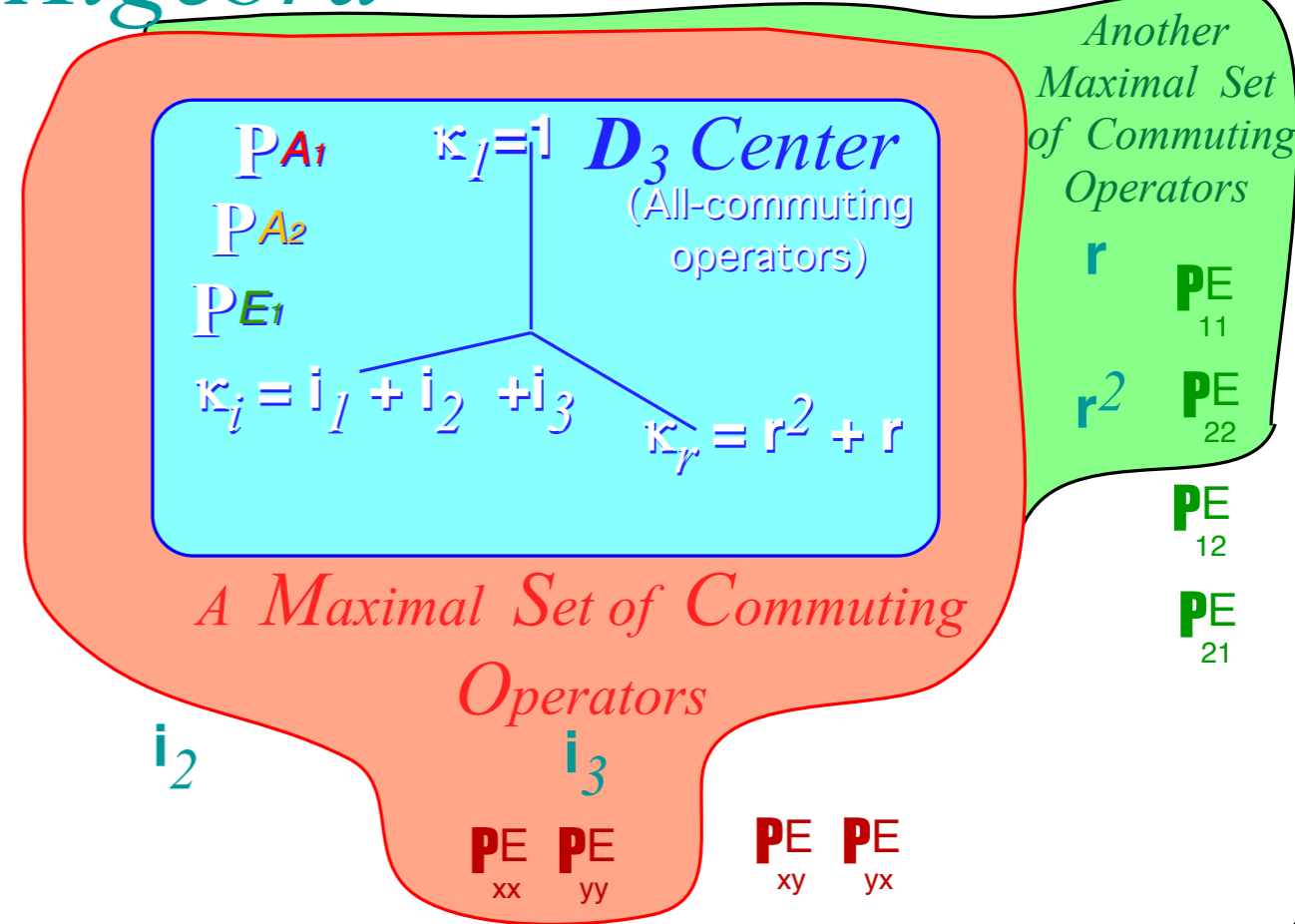
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Subgroup  $s_k = \{g_0=1, g_1=g_k, g_2, \dots\}$  has  $\ell = (\circ \kappa_k - 1)$  Left Cosets (one coset for each member of class  $\kappa_k$ ).

$g_l s_k = g_l \{g_0=1, g_1=g_k, g_2, \dots\},$

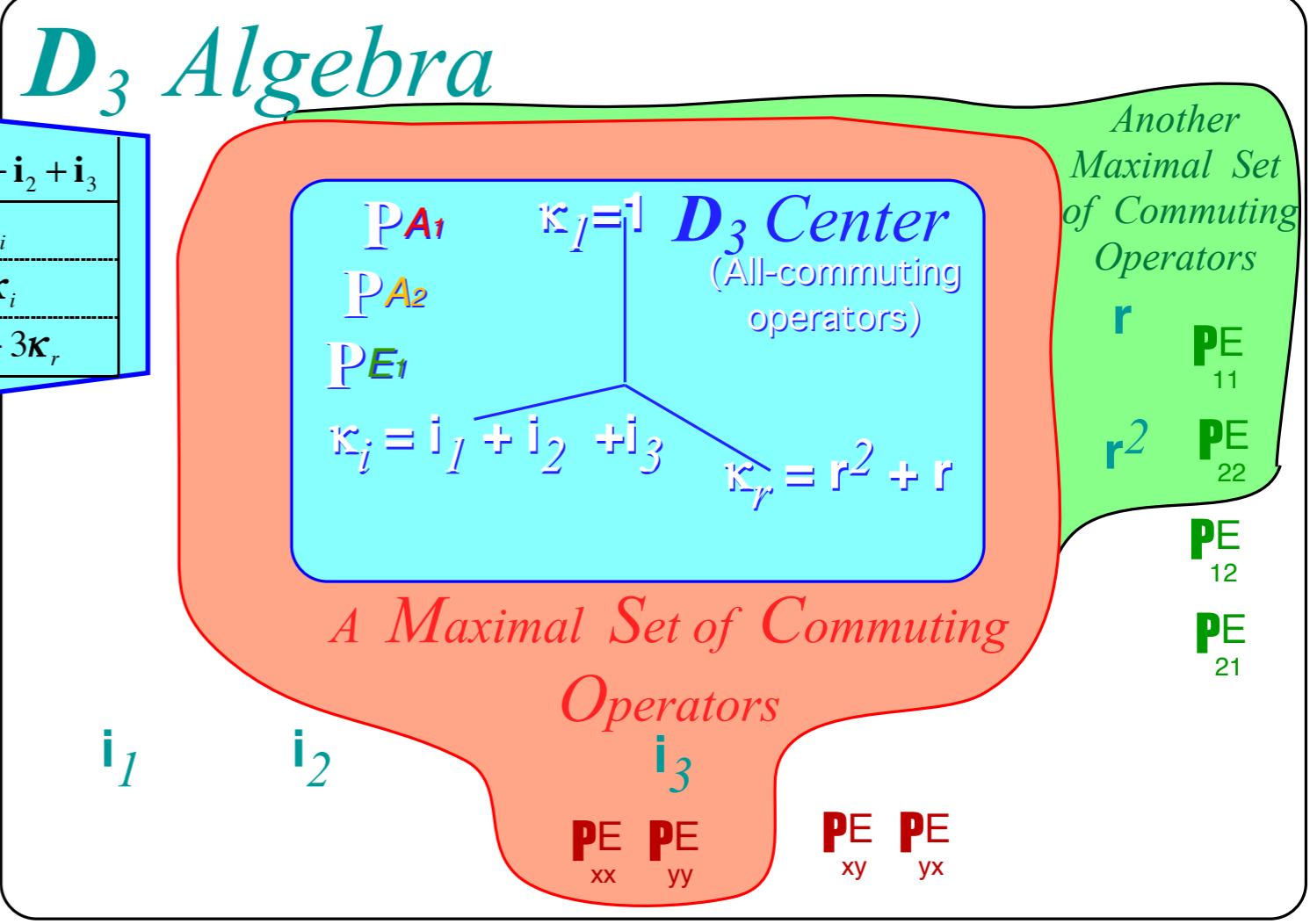
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- $g_t \kappa_k g_t^{-1} = \kappa_k$  where:  $\kappa_k = \sum_{j=1}^{\circ \kappa_k} g_j = \frac{1}{\circ s_k} \sum_{t=1}^{\circ G} g_t g_k g_t^{-1}$
- $\circ s_k =$  order of  $g_k$ -self-symmetry: ( $\circ s_1 = 6, \circ s_r = 3, \circ s_i = 2$ )
- $\circ s_k = \circ G / \circ \kappa_k$   $\circ s_k$  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:  $g_s g_k g_s^{-1} = g_k$

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

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  $\kappa_k$ ).

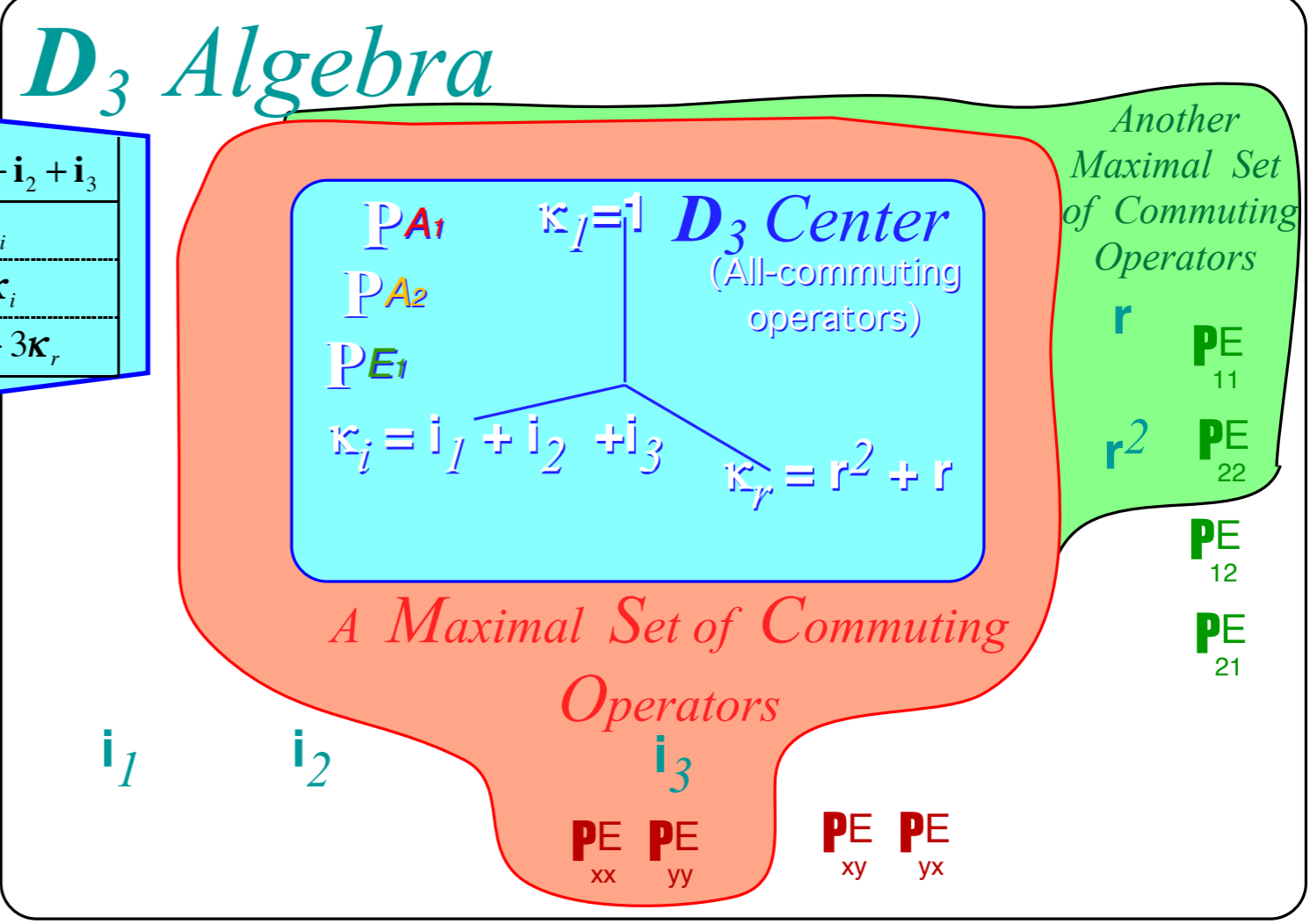
- $g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\}$ ,
- $g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots$
- $\vdots$
- $g_\ell s_k = g_\ell \{g_0=1, g_1=g_k, g_2, \dots\}$

Review: Spectral resolution of  $D_3$  Center (Class 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

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



Class-sum  $\kappa_k$  commutes with all  $g_t$

- Class-sum  $\kappa_k$  invariance:  $g_t \kappa_k = \kappa_k g_t$
- $\circ G =$  order of group: ( $\circ D_3 = 6$ )
- $\circ \kappa_k =$  order of class  $\kappa_k$ : ( $\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$ )
- $g_t \kappa_k g_t^{-1} = \kappa_k$  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:  $g_s g_k g_s^{-1} = g_k$

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

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  $\kappa_k$ ).

$$g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\},$$

$$g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots$$

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  $\circ s_k$ .

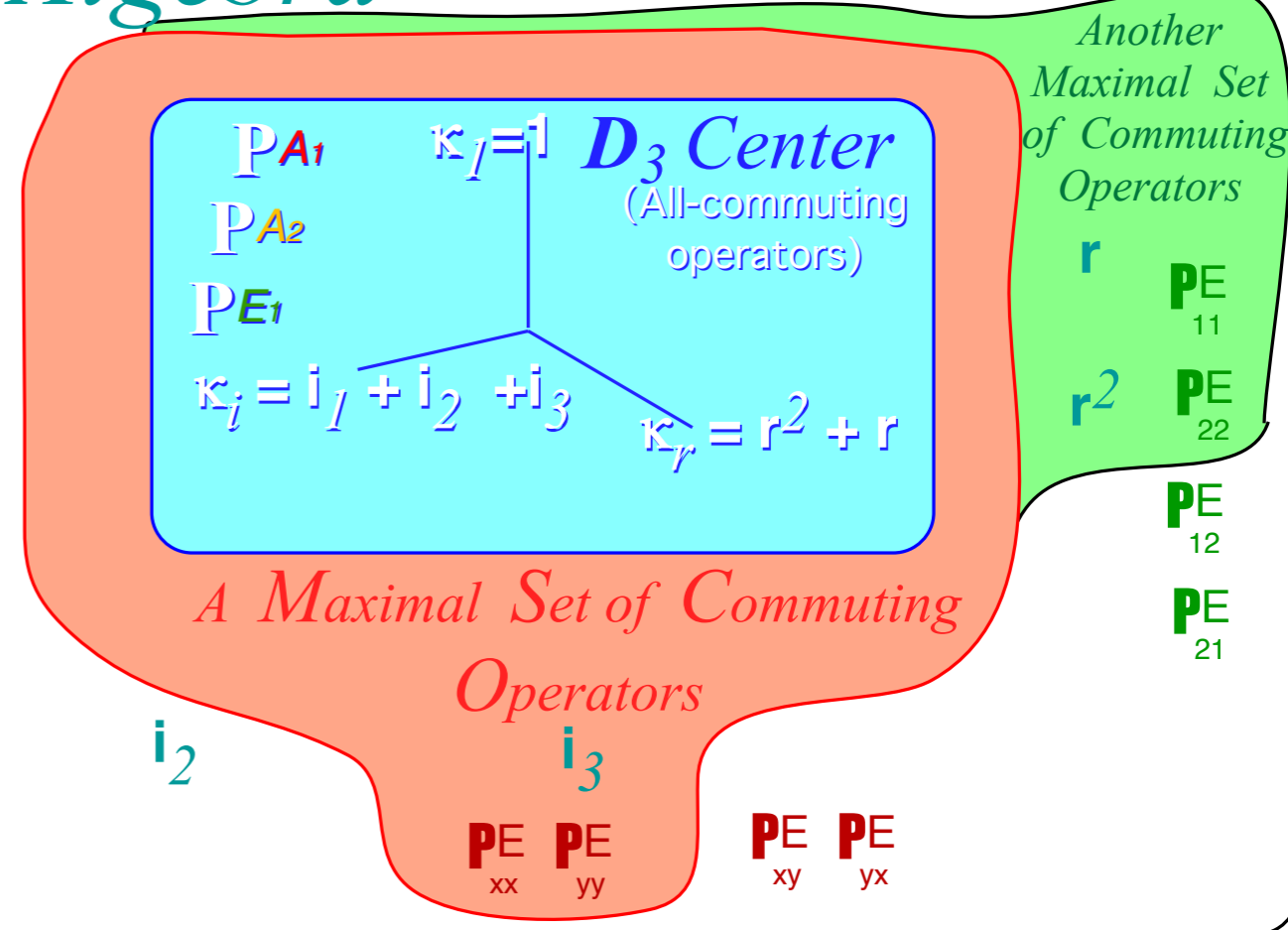
Review: Spectral resolution of  $D_3$  Center (Class algebra)

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

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

# $D_3$ Algebra



Class-sum  $\kappa_k$  commutes with all  $g_t$

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

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

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

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

$\circ s_k$  = 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:  $g_s g_k g_s^{-1} = g_k$

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

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  $\kappa_k$ ).

$$g_1 s_k = g_1 \{g_0=1, g_1=g_k, g_2, \dots\},$$

$$g_2 s_k = g_2 \{g_0=1, g_1=g_k, g_2, \dots\}, \dots$$

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 characters* 

*Character ortho-completeness*

*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*

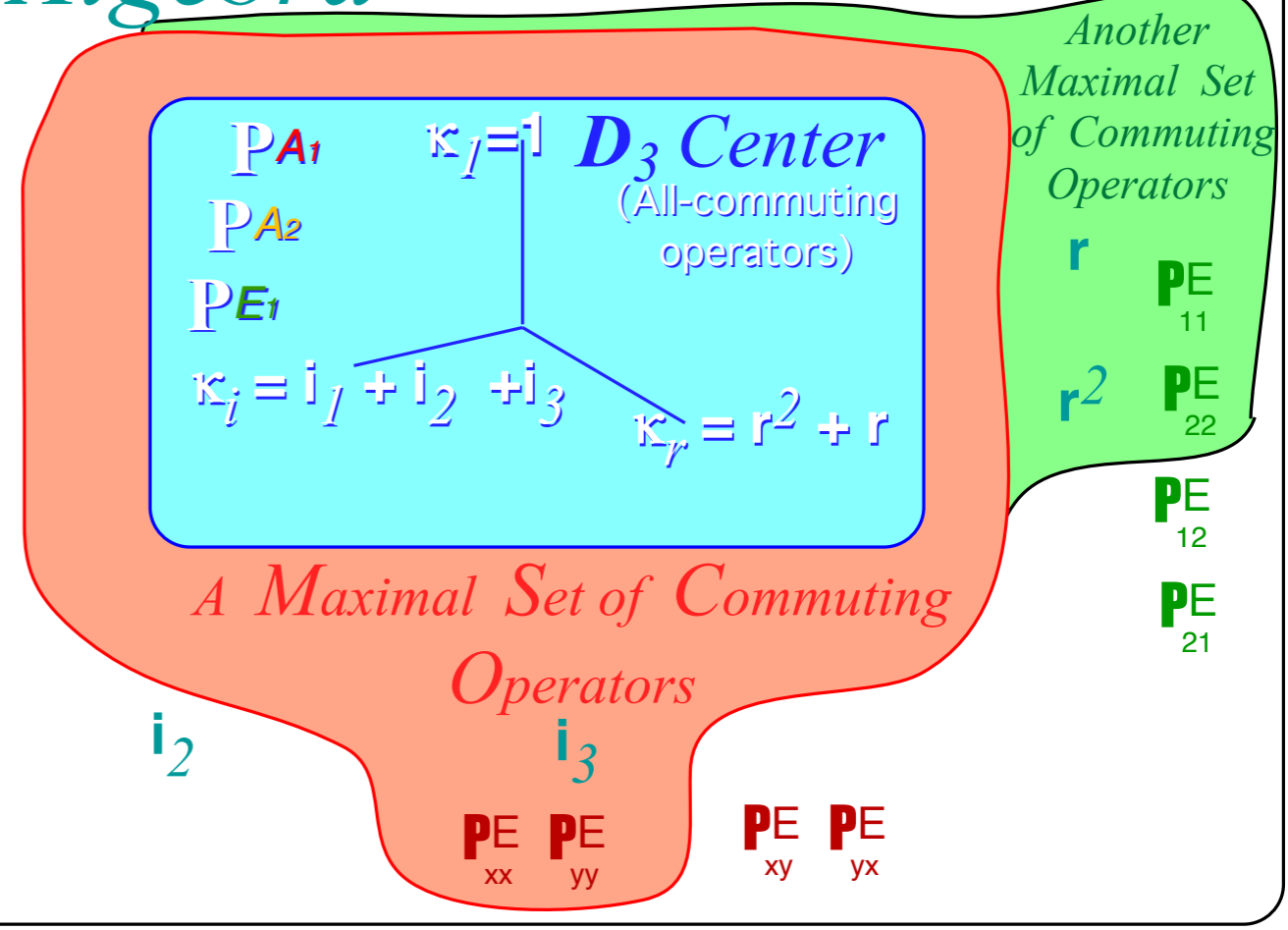
Review: Spectral resolution of  $D_3$  Center (Class algebra)

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

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

# $D_3$ Algebra



Class-sum  $\kappa_k$  commutes with all  $g_t$

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

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

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

Class minimal equation



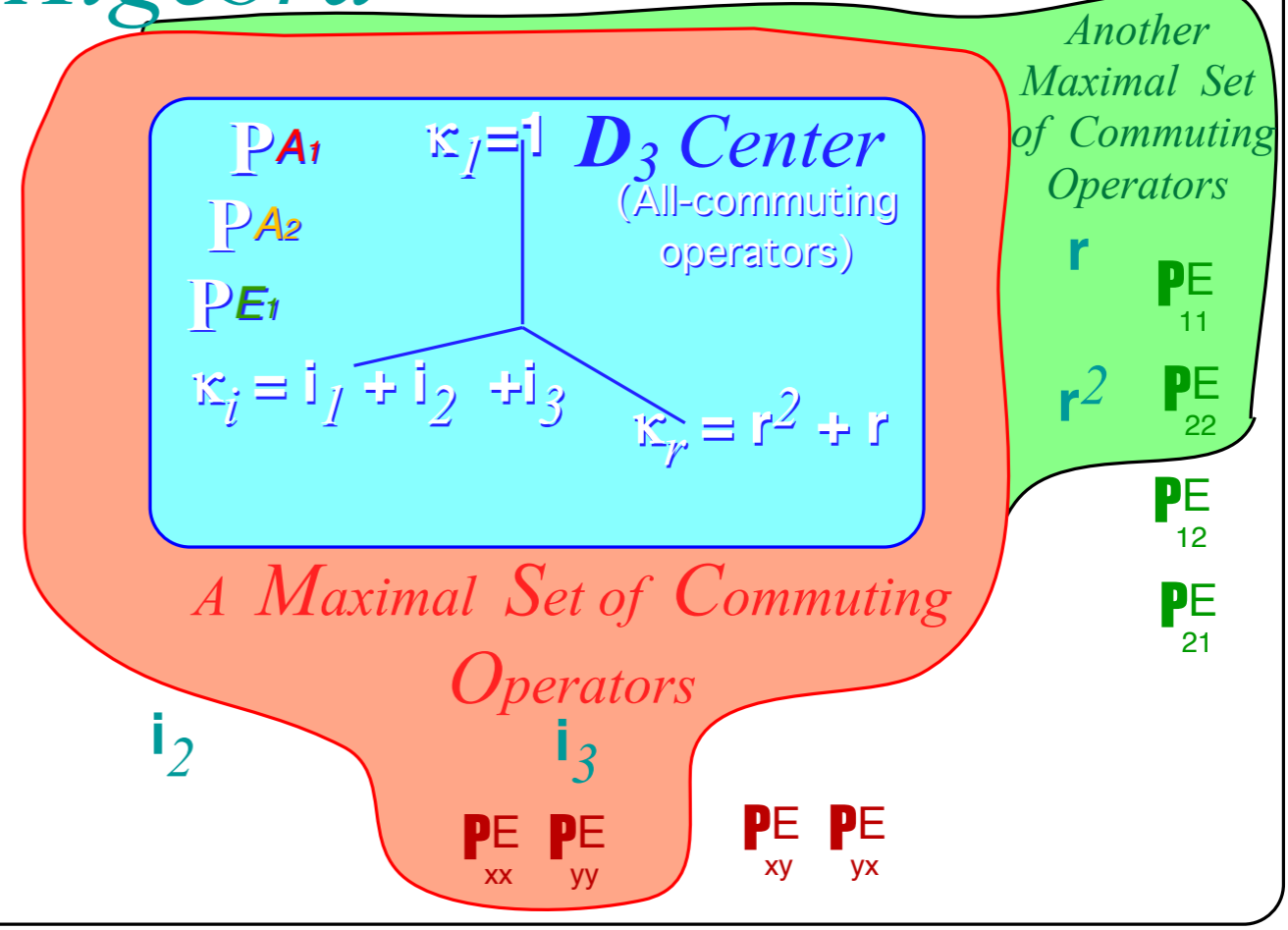
Review: Spectral resolution of  $D_3$  Center (Class algebra)

<b>1</b>	<b>r<sup>2</sup></b>	<b>r</b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>
<b>r</b>	<b>1</b>	<b>r<sup>2</sup></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>
<b>r<sup>2</sup></b>	<b>r</b>	<b>1</b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>
<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>1</b>	<b>r</b>	<b>r<sup>2</sup></b>
<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>r<sup>2</sup></b>	<b>1</b>	<b>r</b>
<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>r</b>	<b>r<sup>2</sup></b>	<b>1</b>

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

# $D_3$ Algebra



Class-sum  $\kappa_k$  commutes with all  $g_t$

Class-sum  $\kappa_k$  invariance:

$$g_t \kappa_k = \kappa_k g_t$$

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

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

Class minimal equation

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

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

# $D_3$ Algebra

<b>1</b>	<b>r<sup>2</sup></b>	<b>r</b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>
<b>r</b>	<b>1</b>	<b>r<sup>2</sup></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>2</sub></b>
<b>r<sup>2</sup></b>	<b>r</b>	<b>1</b>	<b>i<sub>2</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>1</sub></b>
<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>1</b>	<b>r</b>	<b>r<sup>2</sup></b>
<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>i<sub>3</sub></b>	<b>r<sup>2</sup></b>	<b>1</b>	<b>r</b>
<b>i<sub>3</sub></b>	<b>i<sub>2</sub></b>	<b>i<sub>1</sub></b>	<b>r</b>	<b>r<sup>2</sup></b>	<b>1</b>

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

Class-sum  $\kappa_k$  commutes with all  $g_t$

Class-sum  $\kappa_k$  invariance:

$$g_t \kappa_k = \kappa_k g_t$$

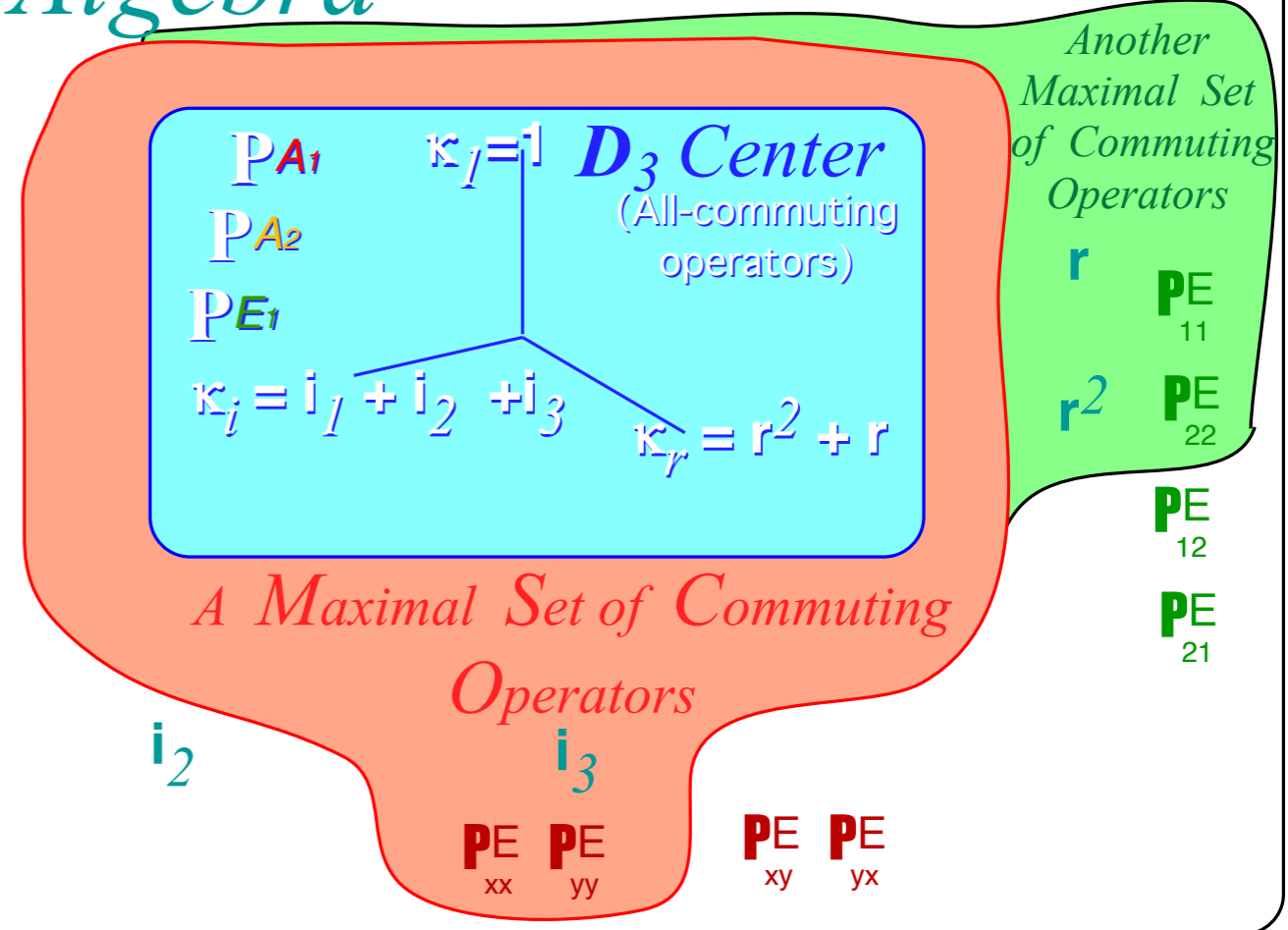
$^{\circ}G$  = order of group: ( $^{\circ}D_3 = 6$ )

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

Class minimal equation

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

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



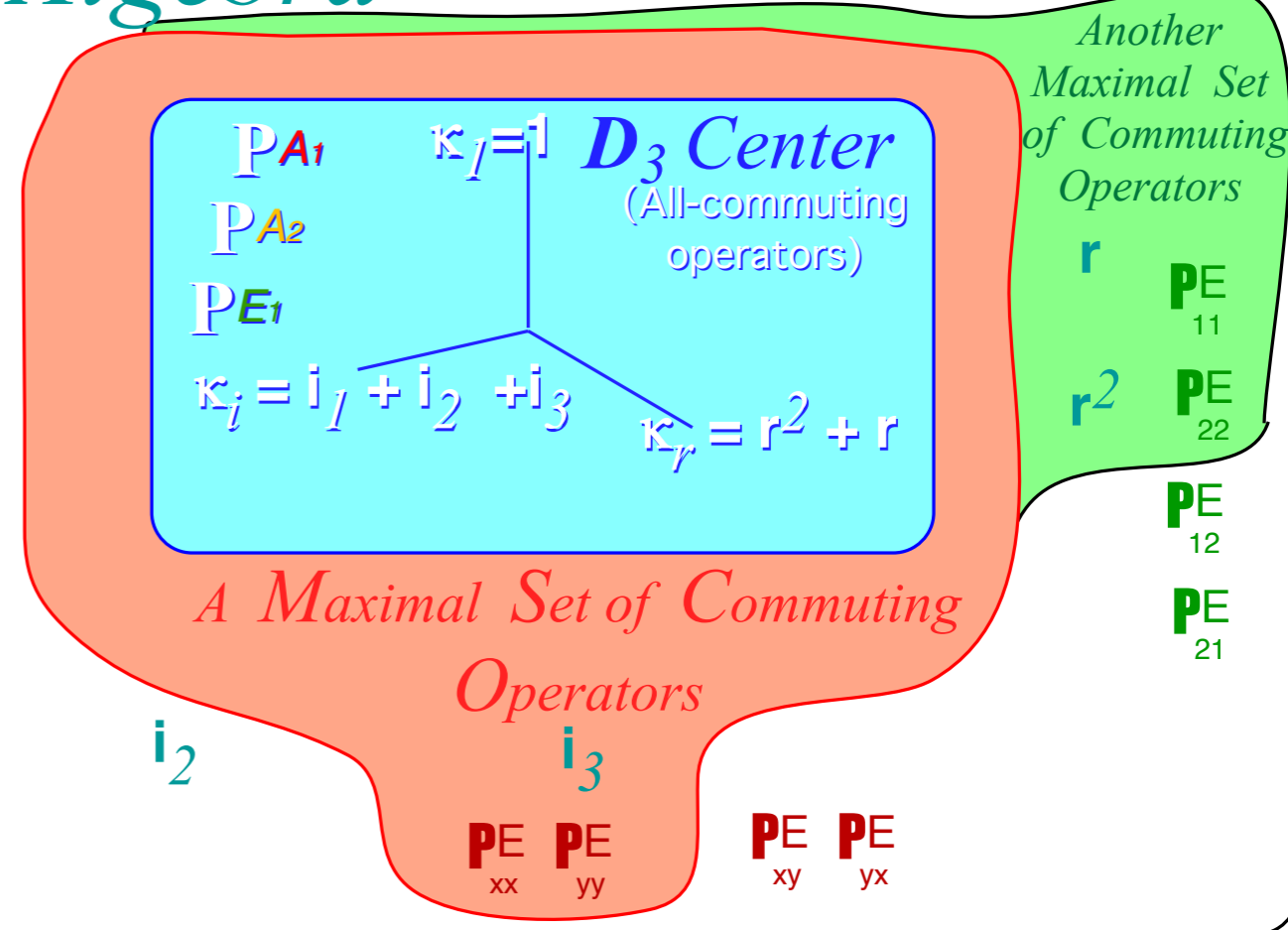
Review: Spectral resolution of  $D_3$  Center (Class algebra)

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

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

# $D_3$ Algebra



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

Class-sum  $\kappa_k$  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  $\kappa_k$ : ( ${}^\circ \kappa_1 = 1, {}^\circ \kappa_r = 2, {}^\circ \kappa_i = 3$ )

Class minimal equation

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

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

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

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

# $D_3$ Algebra

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

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

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

Class-sum  $\kappa_k$  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  $\kappa_k$ : ( ${}^\circ \kappa_1 = 1, {}^\circ \kappa_r = 2, {}^\circ \kappa_i = 3$ )

Class minimal equation

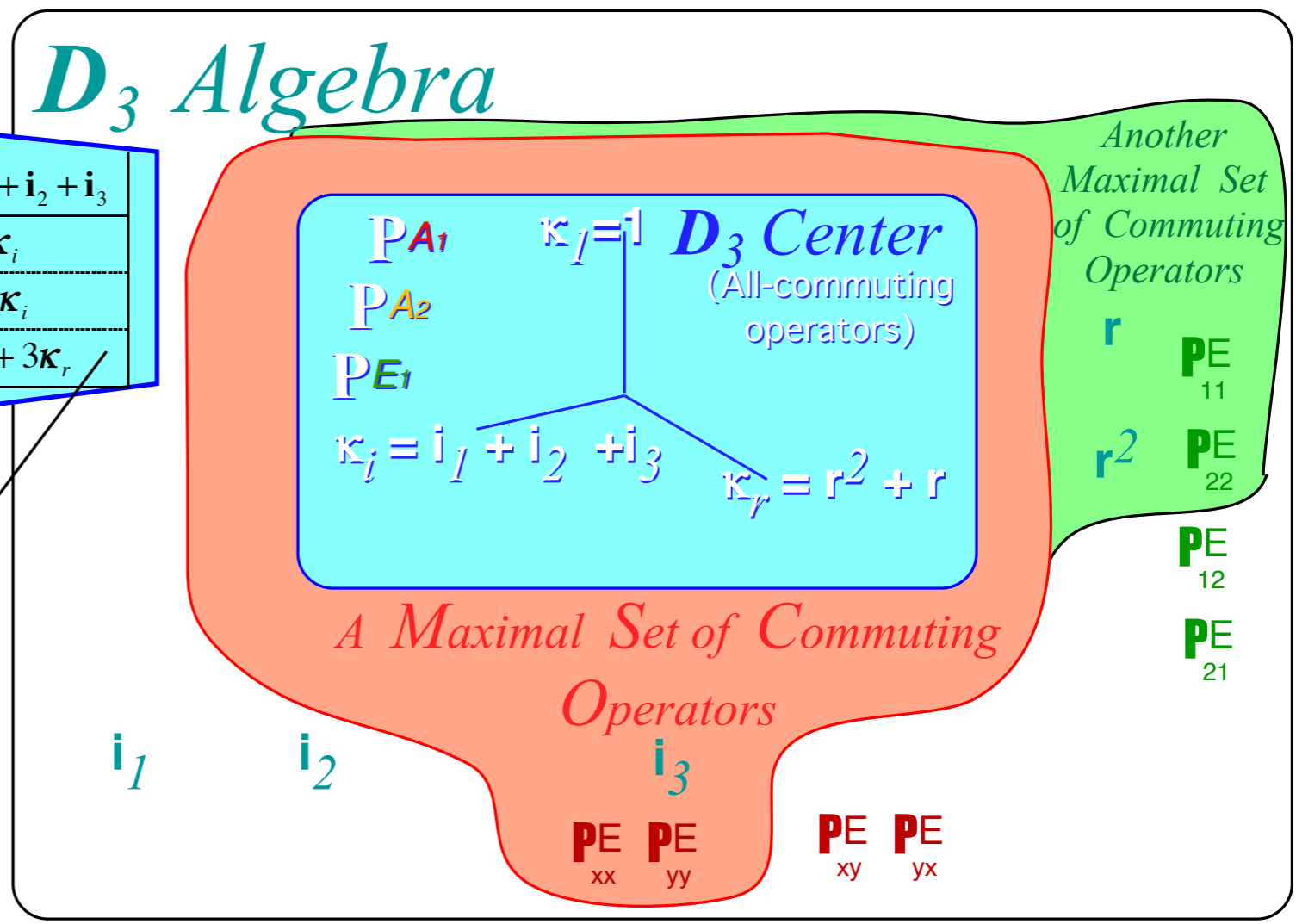
$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \leftarrow \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

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

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

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

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



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

# $D_3$ Algebra

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

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

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

Class-sum  $\kappa_k$  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  $\kappa_k$ : ( $^{\circ}\kappa_1 = 1, ^{\circ}\kappa_r = 2, ^{\circ}\kappa_i = 3$ )

Class minimal equation

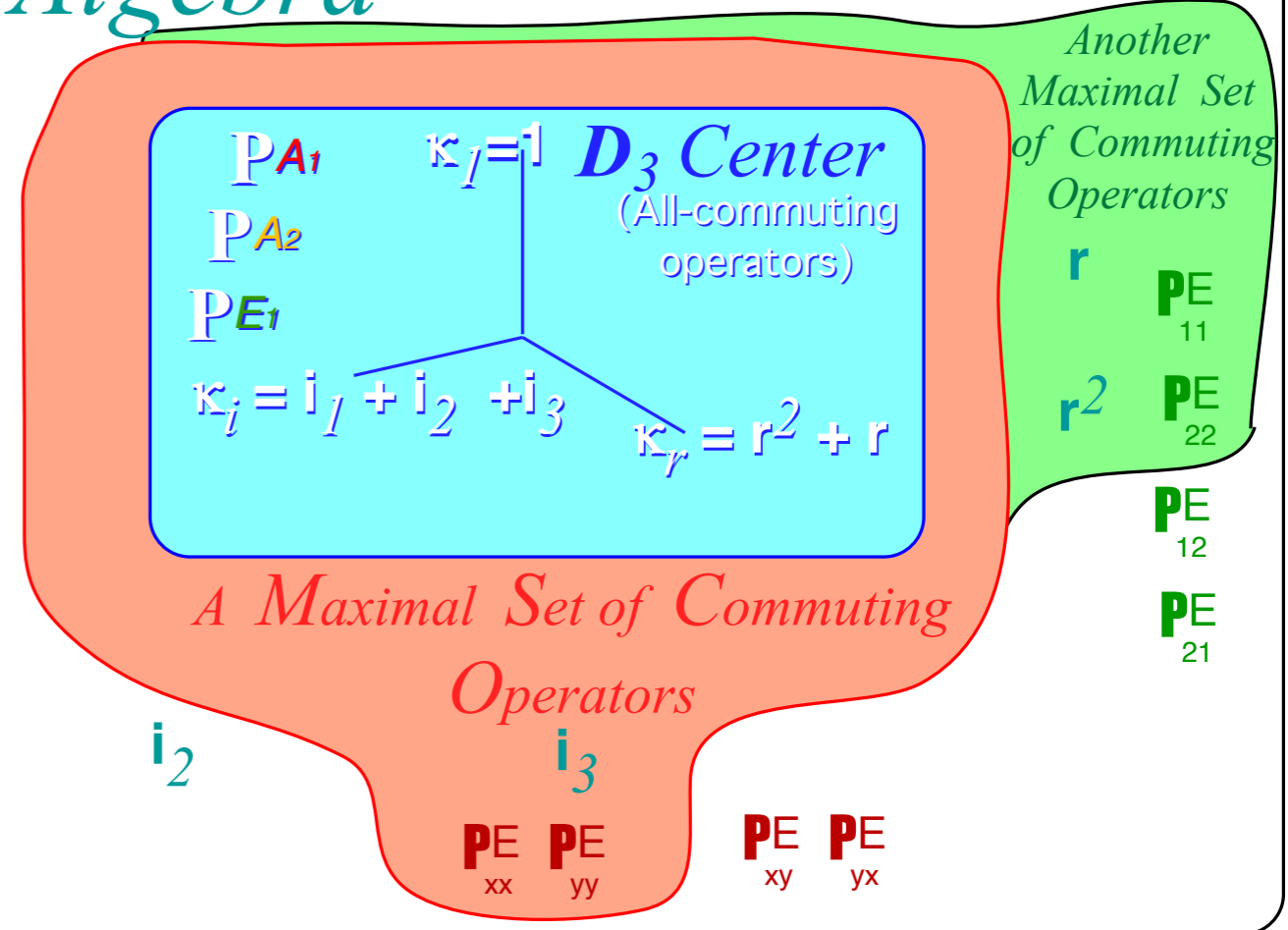
$$\kappa_i^3 = 3 \cdot \kappa_r \kappa_i + 3 \cdot \kappa_i = 9 \cdot \kappa_i \quad \leftarrow \kappa_i^2 = 3 \cdot \kappa_r + 3 \cdot \mathbf{1}$$

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

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

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

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



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

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

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

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

# $D_3$ Algebra

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

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

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

Class-sum  $\kappa_k$  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  $\kappa_k$ : ( ${}^\circ \kappa_1 = 1, {}^\circ \kappa_r = 2, {}^\circ \kappa_i = 3$ )

Class minimal equation

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

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

Class ortho-complete projector relations

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

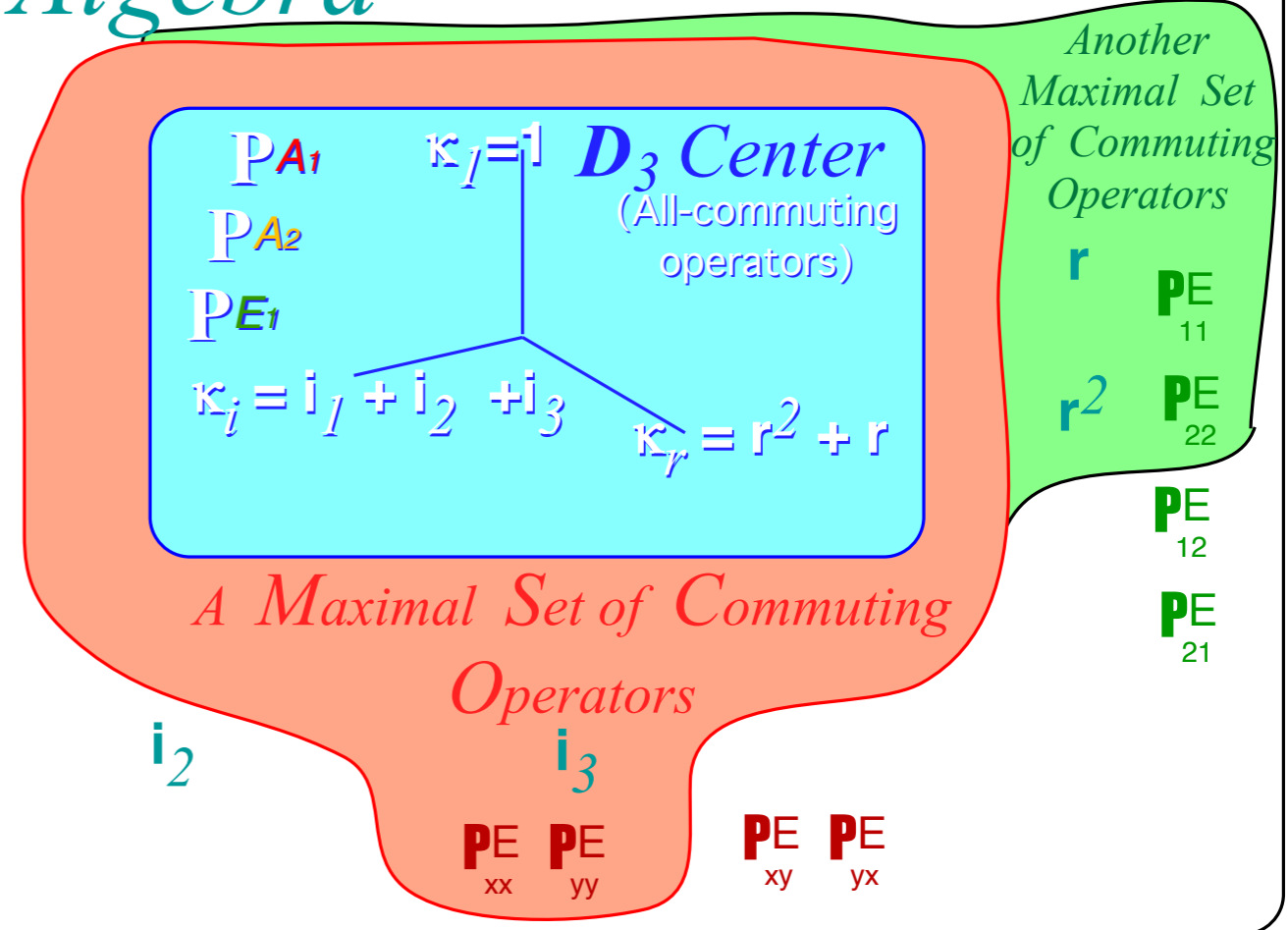
$$\kappa_r = 2 \cdot \mathbf{P}^{A_1} - 2 \cdot \mathbf{P}^{A_2} - 1 \cdot \mathbf{P}^E$$

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

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

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

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



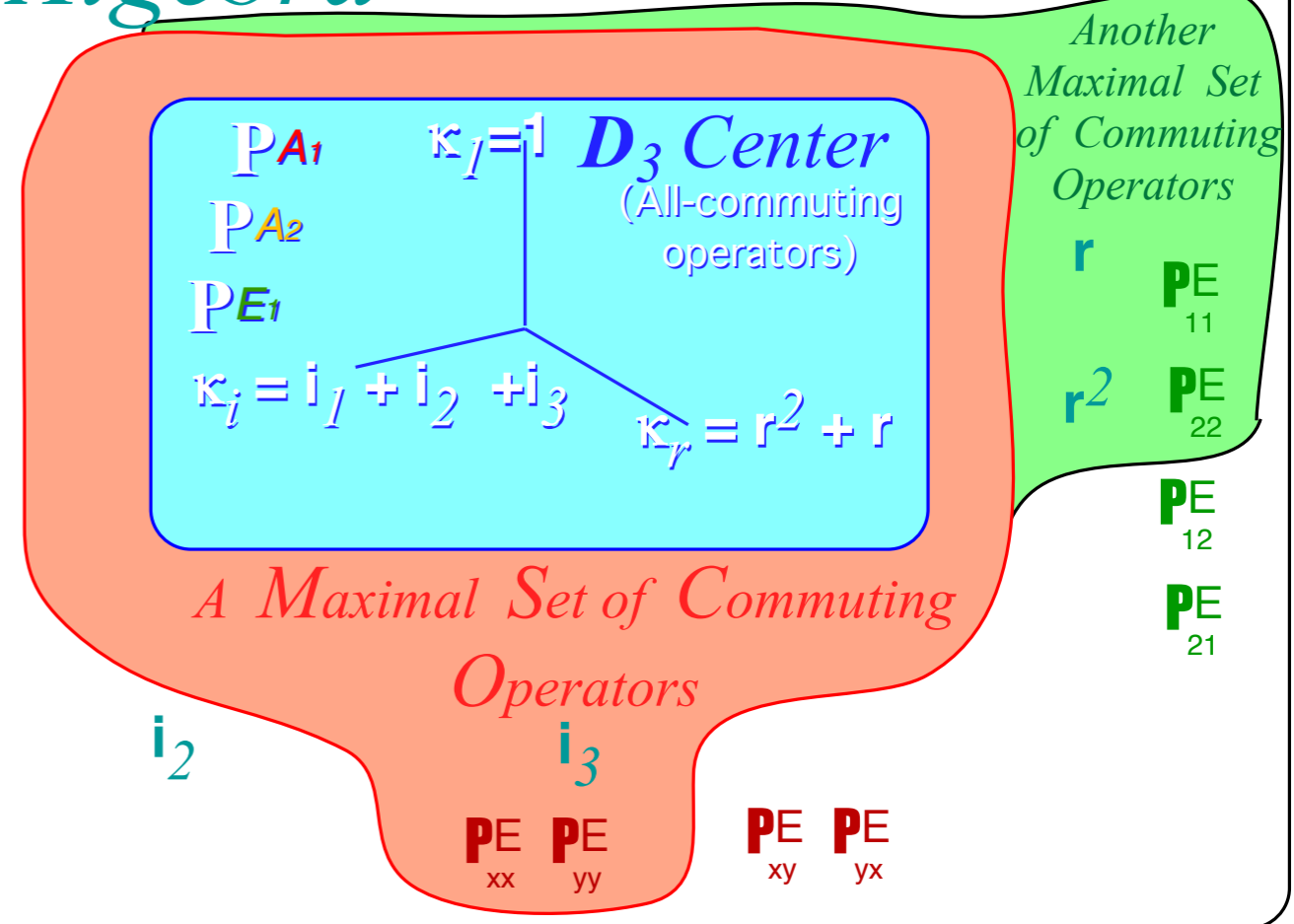
Review: Spectral resolution of  $D_3$  Center (Class algebra)

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

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

# $D_3$ Algebra



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

Class-sum  $\kappa_k$  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  $\kappa_k$ : ( $\circ \kappa_1 = 1, \circ \kappa_r = 2, \circ \kappa_i = 3$ )

Class minimal equation

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

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

Class ortho-complete projector and character relations

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

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

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

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

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

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

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

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

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

$\chi_k^\alpha$	$\chi_1^\alpha$	$\chi_r^\alpha$	$\chi_i^\alpha$
$\alpha = A_1$	1	1	1
$\alpha = A_2$	1	1	-1
$\alpha = E$	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*

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

*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*

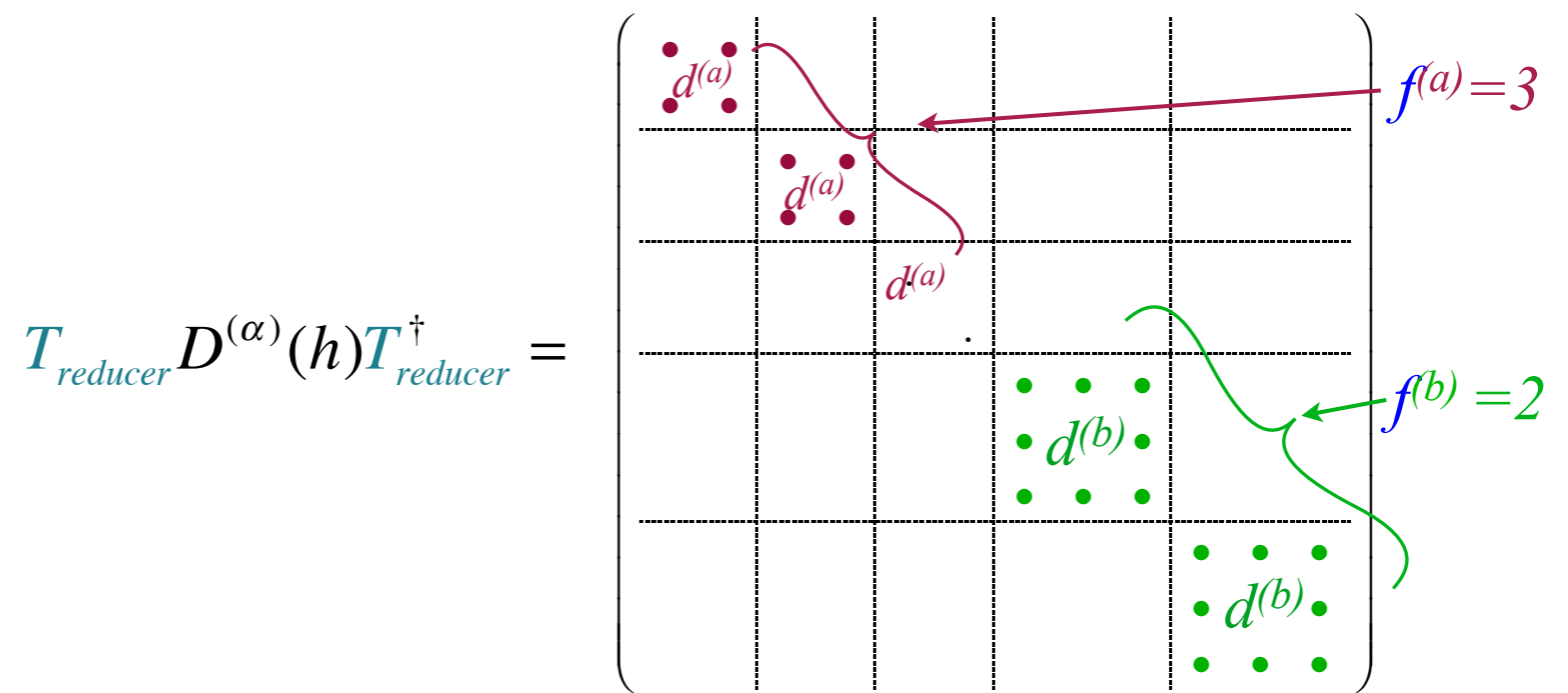


# Subgroup splitting and correlation frequency formula: $f^{(a)}(D^{(\alpha)}(G) \downarrow H)$

(irep  $\equiv$  irreducible representation)

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

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



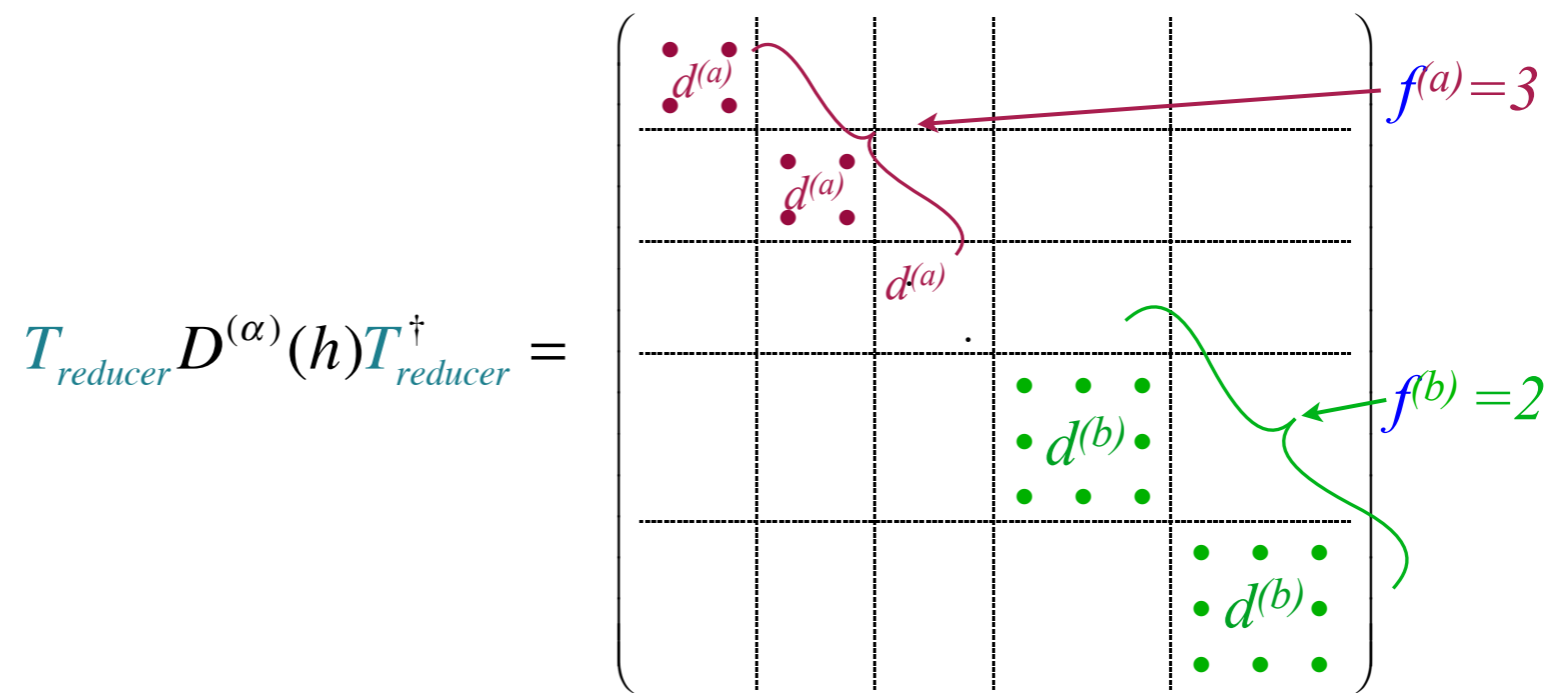
The following derives formulae for integral  $H \subset G$  correlation coefficients  $f^{(a)}(D^{(\alpha)}(G) \downarrow H)$

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

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

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



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

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

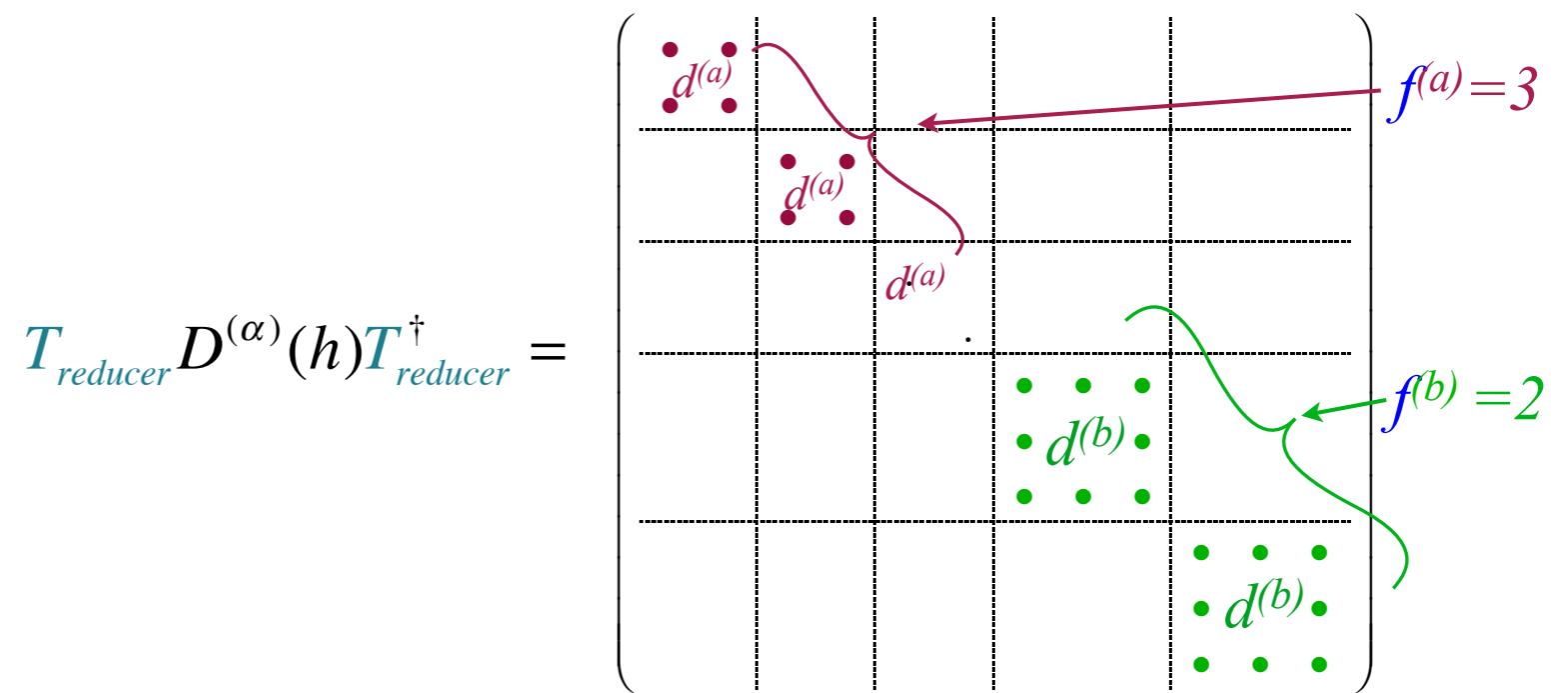
Since each  $d^{(b)}(\mathbf{P}^{(b)})$  is  $\ell^{(b)}$ -by- $\ell^{(b)}$  unit matrix

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

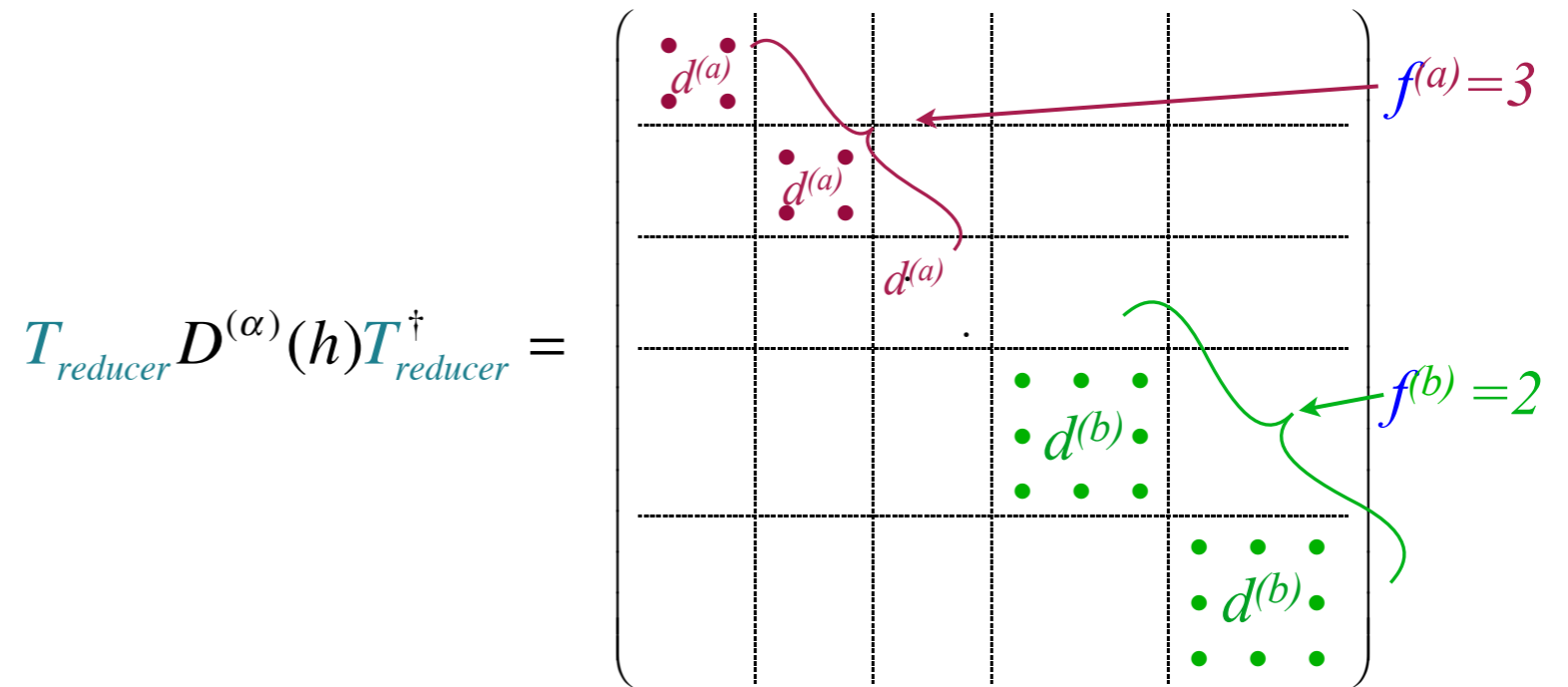
$$f^{(b)} = \frac{1}{\ell^{(b)}} \text{Trace} D^{(\alpha)}(\mathbf{P}^{(b)})$$

# 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  $d^{(a)}(H)$

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



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

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

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

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

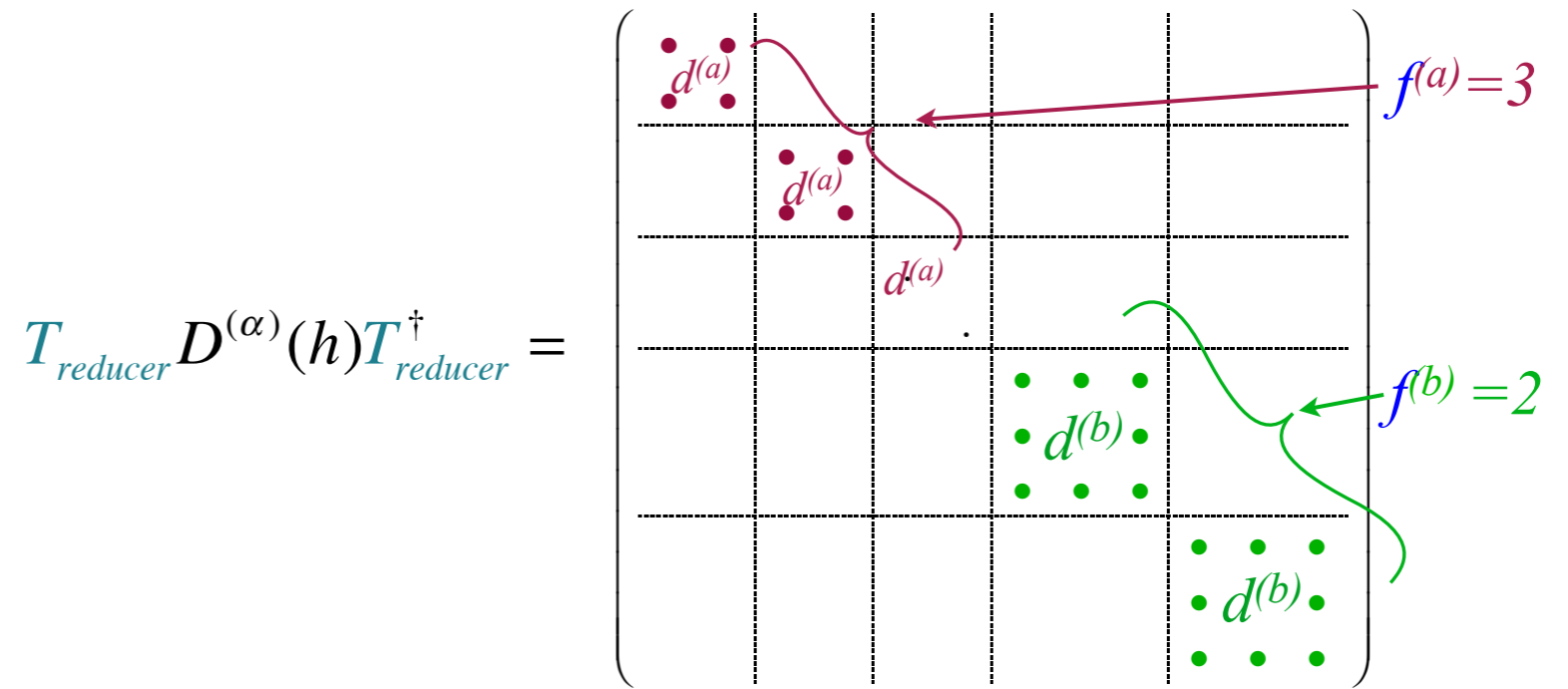
$$\mathbf{P}^{(b)} = \frac{\ell^{(b)}}{\circ H} \sum_{k \in H} \chi_k^{(b)*} \mathbf{\kappa}_k$$

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

(irep  $\equiv$  irreducible representation)

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

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

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

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

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

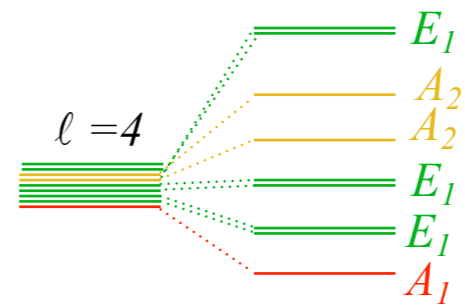
$$\mathbf{P}^{(\alpha)} = \frac{\ell^{(\alpha)}}{\circ G} \sum_{\mathbf{\kappa} \in G} \chi_{\mathbf{\kappa}}^{(\alpha)*} \mathbf{\kappa}_{\mathbf{\kappa}}$$

$$\mathbf{P}^{(b)} = \frac{\ell^{(b)}}{\circ H} \sum_{\mathbf{\kappa} \in H} \chi_{\mathbf{\kappa}}^{(b)*} \mathbf{\kappa}_{\mathbf{\kappa}}$$

# From end of Lecture 13

Example to use:

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



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

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

...and  $D_3$  character table:

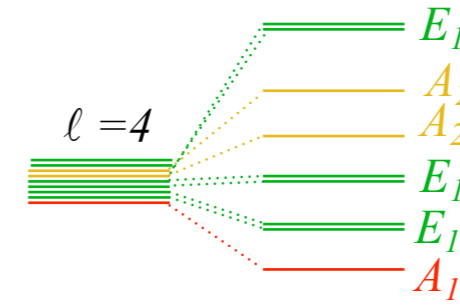
$(\mathbf{g}) =$	$\{\mathbf{1}\}$	$\{\mathbf{r}^1, \mathbf{r}^2\}$	$\{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
$\chi^{A_2}(\mathbf{g}) =$	1	1	-1
$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

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

# From end of Lecture 13

Example to use:

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



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

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

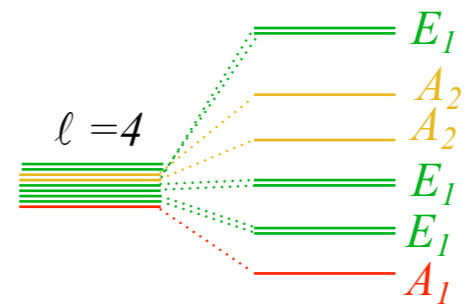
$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
$\chi^{A_1}(\mathbf{g}) =$	1	1	1
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$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

$f^{(\alpha)}(l)$	$f^{A_1}$	$f^{A_2}$	$f^{E_1}$	
$l = 0$	1	.	.	$1A_1$
1	.	1	1	$0A_1 \oplus A_2 \oplus E_1$
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# From end of Lecture 13

Example to use:

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



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

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

$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	$\pi$
$\ell = 0$	1	1	1
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$\chi^{E_1}(\mathbf{g}) =$	2	-1	0

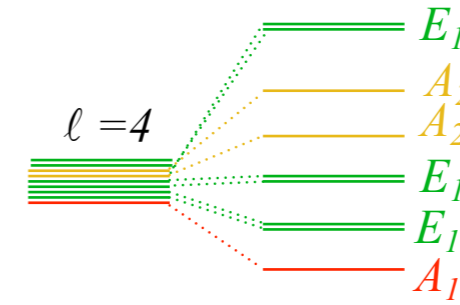
$f^{(\alpha)}(\ell)$	$f^{A_1}$	$f^{A_2}$	$f^{E_1}$	
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3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	$1A_1 \oplus 2A_2 \oplus 3E_1$
5	2	1	3	$2A_1 \oplus A_2 \oplus 3E_1$
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7	2	3	5	$2A_1 \oplus 3A_2 \oplus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



# From end of Lecture 13

Example to use:

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



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

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

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

$\chi^\ell(\Theta)$	$\Theta = 0$	$\frac{2\pi}{3}$	$\pi$
$\ell = 0$	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:

$(\mathbf{g}) =$	$\{1\}$	$\{r^1, r^2\}$	$\{i_1, i_2, i_3\}$
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$\chi^{A_2}(\mathbf{g}) =$	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	.	.	$1A_1$
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2	1	.	2	$1A_1 \oplus 2E_1$
3	1	2	2	$1A_1 \oplus 2A_2 \oplus 2E_1$
4	1	2	3	$1A_1 \oplus 2A_2 \oplus 3E_1$
5	2	1	3	$2A_1 \oplus A_2 \oplus 3E_1$
6	3	2	4	$3A_1 \oplus 2A_2 \oplus 4E_1$
7	2	3	5	$2A_1 \oplus 3A_2 \oplus 5E_1$

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

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**→** *Group invariant numbers: Centrum, Rank, and Order* **←**

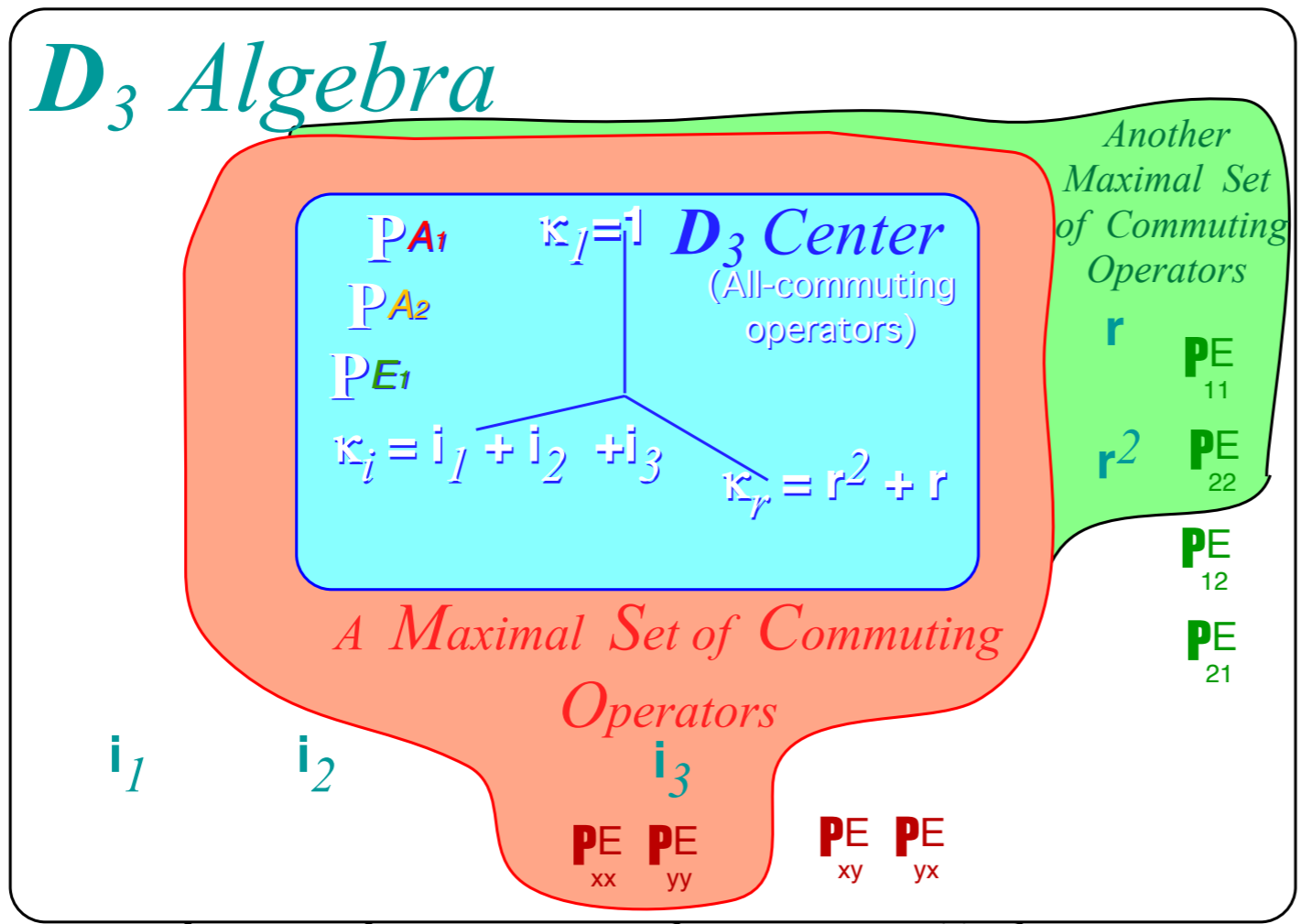
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# $D_3$ Algebra



## 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

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

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

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

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

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

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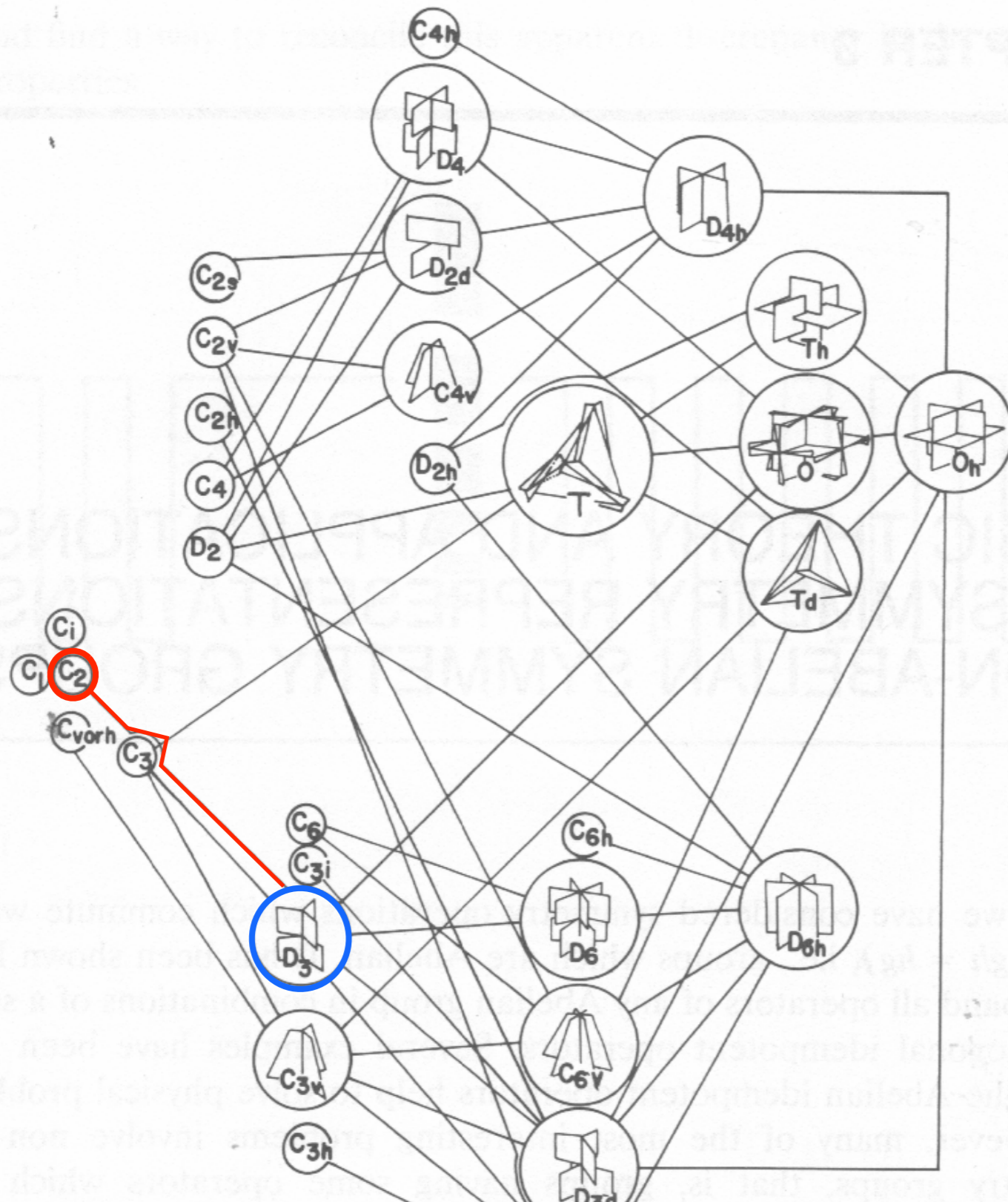


# Spectral reduction of non-commutative “Group-table Hamiltonian”

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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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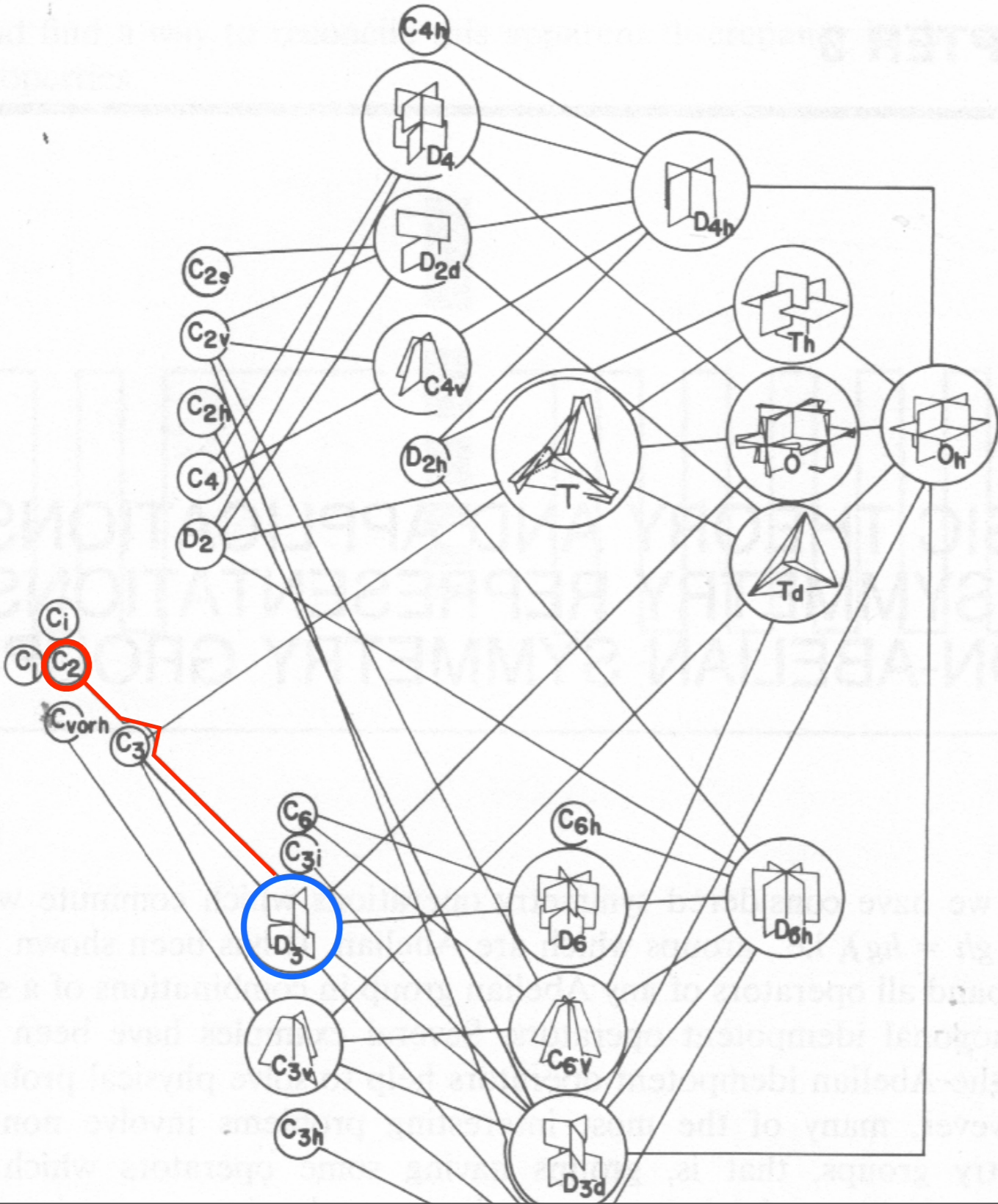


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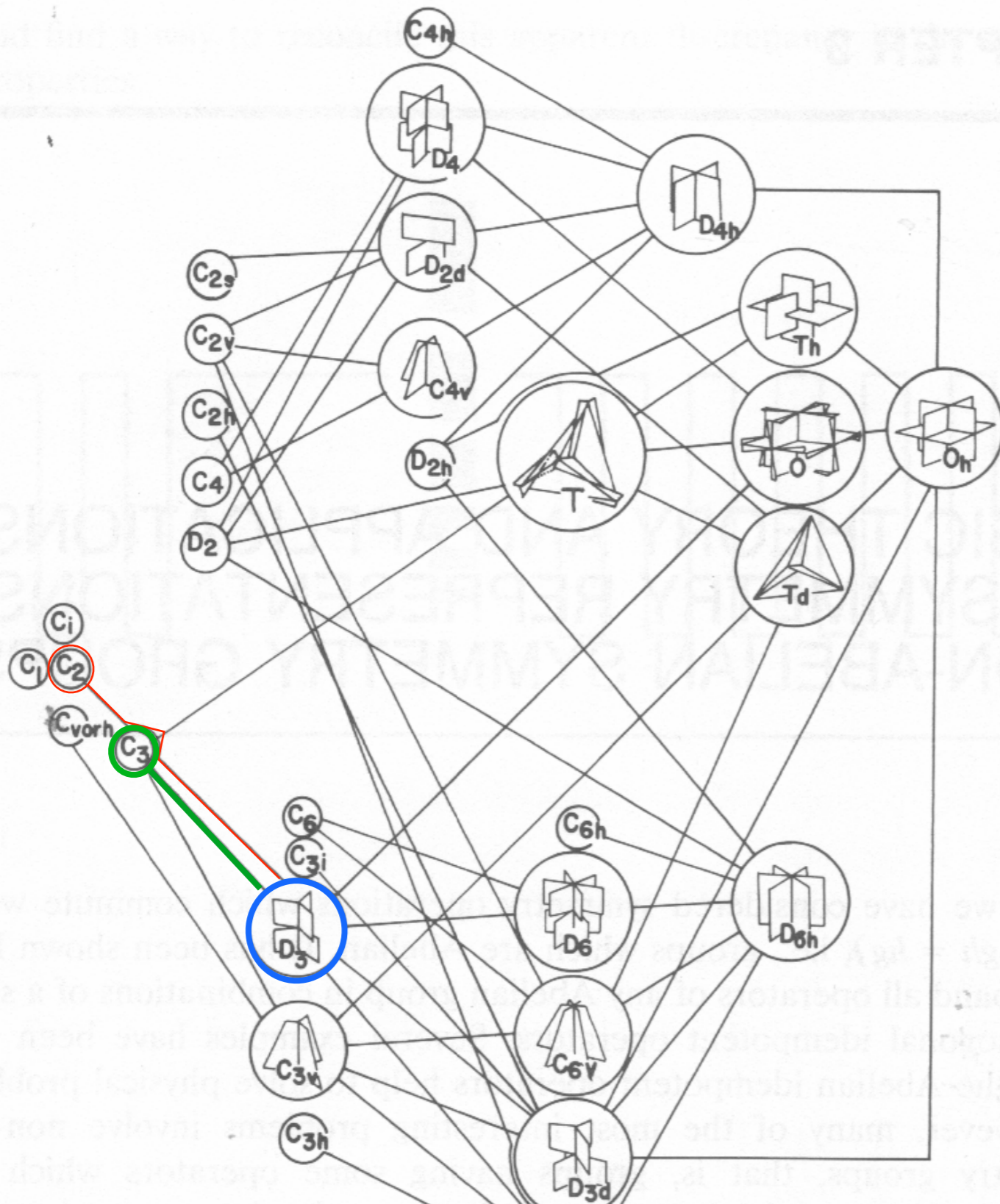


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Let:

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

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Same for Correlation table:  $D_3 \supset C_3 \quad 0_3 \quad 1_3 \quad 2_3$

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

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

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

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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

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there will be exactly 4

“ $C_2$ -friendly” irep projectors

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

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

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*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*

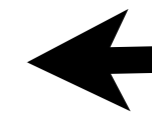
*Subgroup splitting and correlation frequency formula:  $f^{(a)}(D^{(\alpha)}(G) \downarrow H)$*

*Group invariant numbers: Centrum, Rank, and Order*

*2nd-Stage spectral decompositions of global/local  $D_3$*

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

 *Splitting classes*



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

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

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

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

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

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

$$D_3 \kappa = \begin{pmatrix} 1 & r^1 + r^2 & i_1 + i_2 + i_3 \end{pmatrix}$$

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

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

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

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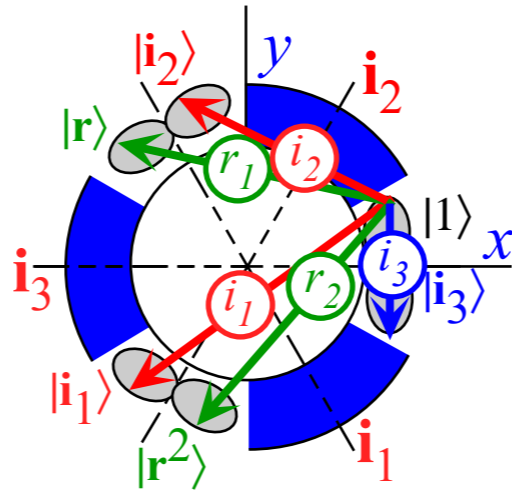
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$r=r_2$  must equal  $r_1$   
 $i=i_2$  must equal  $i_1$

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

$i_3$  is free parameter



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

4 different idempotent

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

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

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

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

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

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

class  $\kappa_r$  splits into  $\kappa_{r_1}$  and  $\kappa_{r_2}$

$i=i_1=i_2=i_3$

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

$r_1$  and  $r_2$  are free

$$D_3 \kappa = \begin{bmatrix} 1 & r^1+r^2 & i_1+i_2+i_3 \end{bmatrix}$$

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

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

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

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

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

*Group invariant numbers: Centrum, Rank, and Order*

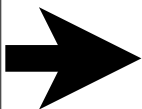
*2nd-Stage spectral decompositions of global/local  $D_3$*

*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*



Centrum  $\kappa(D_3)=3$   
 idempotents  
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Rank  $\rho(D_3)=4$   
 idempotents  
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$$\mathbf{P}_{x,x}^{A_1} = \mathbf{P}_{0_2 0_2}^{A_1} = \mathbf{P}^{A_1} p^{0_2} = \mathbf{P}^{A_1} (\mathbf{1} + \mathbf{i}_3) / 2 = (\mathbf{1} + \mathbf{r}^1 + \mathbf{r}^2 + \mathbf{i}_1 + \mathbf{i}_2 + \mathbf{i}_3) / 6$$

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

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*3rd and Final Step:*  
*Spectral resolution of ALL 6 of  $D_3$  :*

Centrum  $\kappa(D_3)=3$   
 idempotents  
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3rd and Final Step:

Spectral resolution of ALL 6 of  $D_3$  :

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idempotents  
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3rd and Final Step:

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

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Order  $^0(D_3)=6$   
projectors  
 $\mathbf{P}_{m,n}^{(\alpha)}$

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Order  $^0(D_3)=6$   
projectors  
 $\mathbf{P}_{m,n}^{(\alpha)}$

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

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

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

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

Centrum  $\kappa(D_3)=3$   
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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

$$\mathbf{g} = \sum_m \sum_e \sum_b D_{eb}^{(m)}(\mathbf{g}) \mathbf{P}_{eb}^{(m)}$$

$$\mathbf{P}_{eb}^{(m)} = (\text{norm}) \sum_{\mathbf{g}} D_{eb}^{(m)*}(\mathbf{g}) \mathbf{g}$$

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

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

Global (LAB) symmetry

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

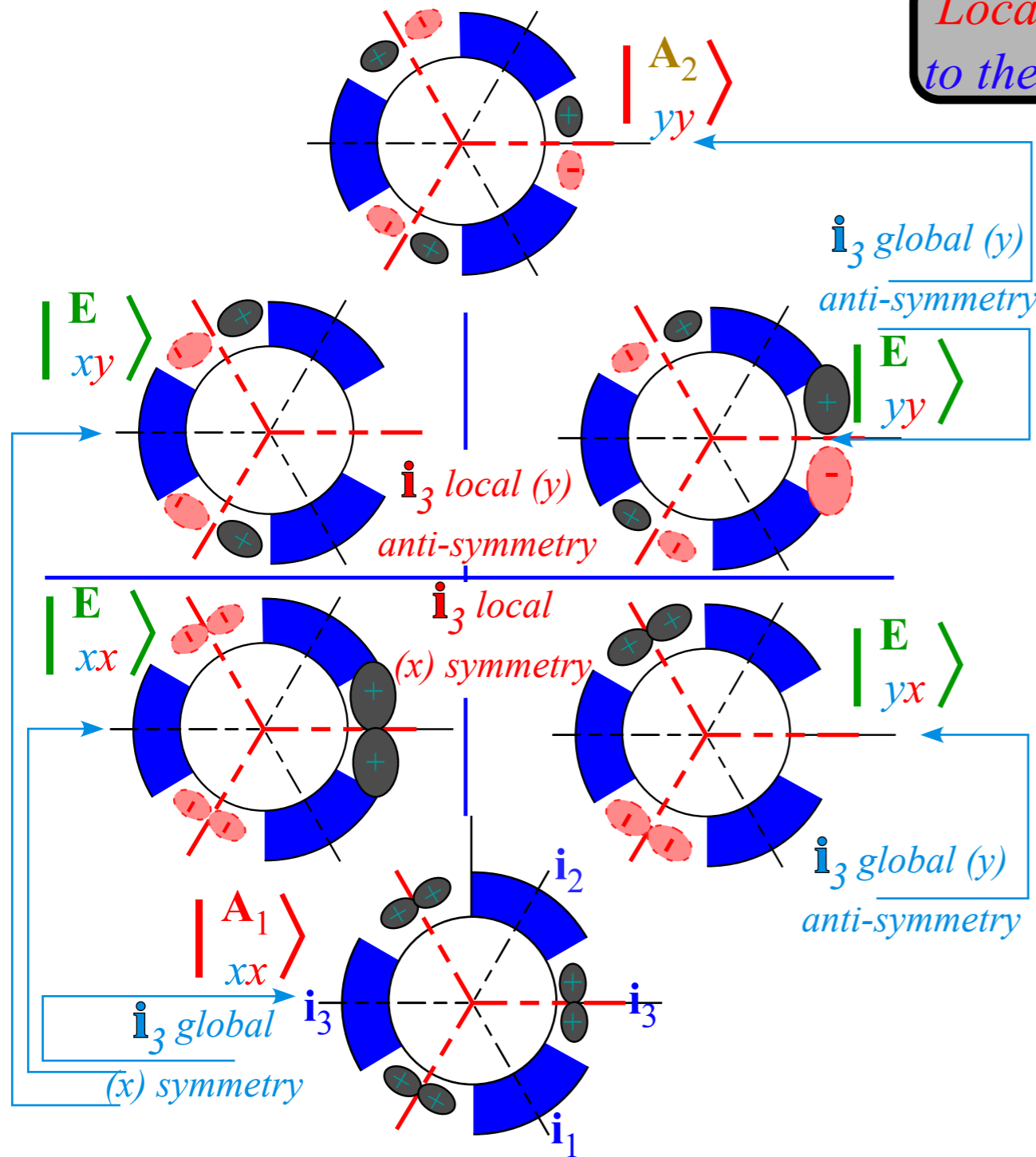
$D_3 > C_2$   $\mathbf{i}_3$  projector states

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

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  $\mathbf{g}^\dagger$



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

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

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

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

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

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

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

external LAB

internal BOD

symmetry label-e

symmetry label-b

GLOBAL

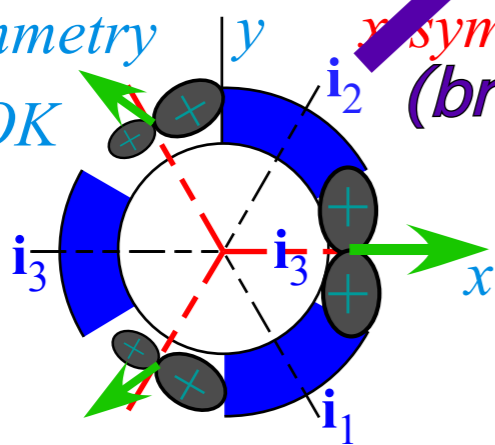
LOCAL

GLOBAL

$(i_3) = 0_2$

x-symmetry

$\mathbf{i}_3$  OK



~~LOCAL~~

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

~~x-symmetry~~

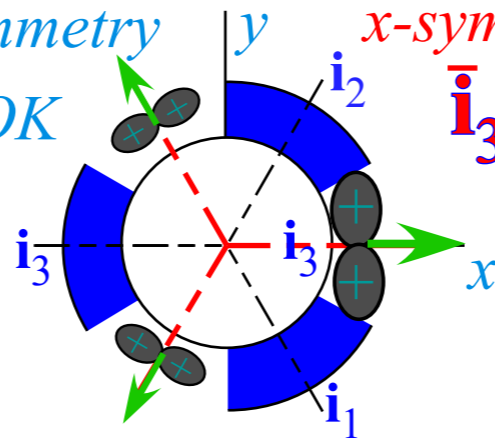
~~(broken  $\bar{\mathbf{i}}_3$ )~~

GLOBAL

$(i_3) = 0_2$

x-symmetry

$\mathbf{i}_3$  OK



LOCAL

$(i_3) = 0_2$

x-symmetry

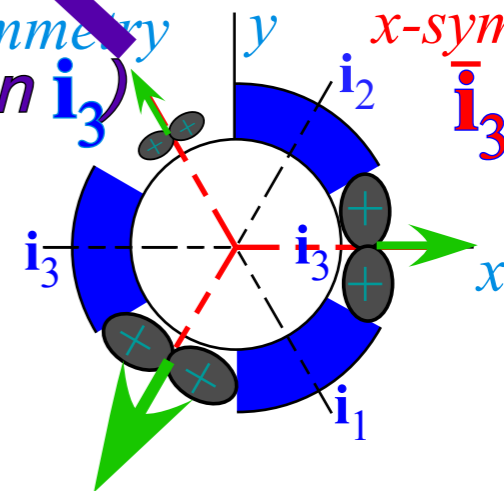
$\bar{\mathbf{i}}_3$  OK

~~GLOBAL~~

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

~~x-symmetry~~

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



LOCAL

$(i_3) = 0_2$

x-symmetry

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

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

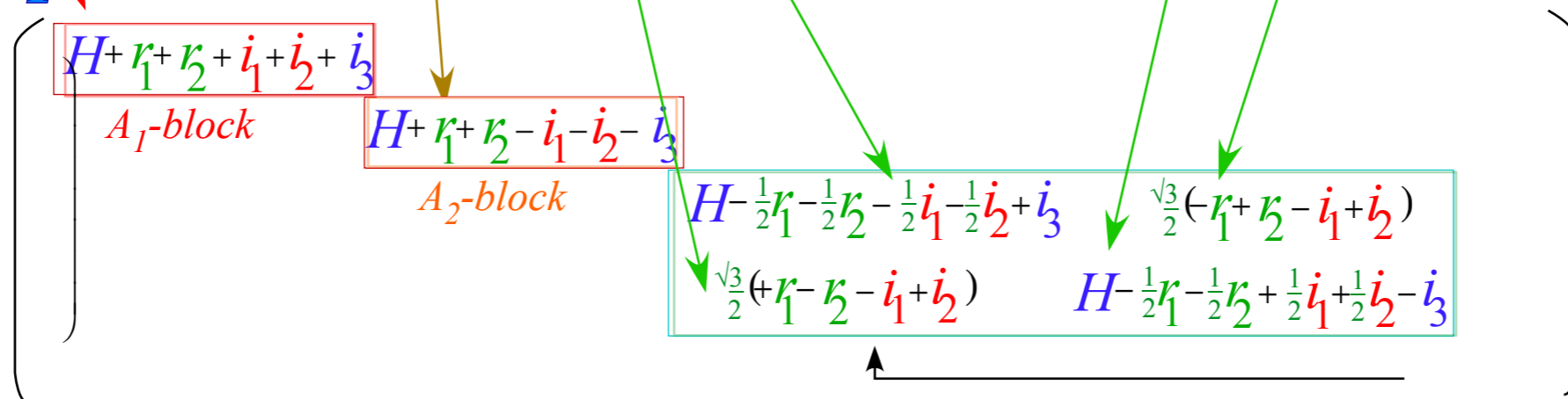
*Spectral Efficiency: Same  $D(a)_{mn}$  projectors give a lot!*

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

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

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

- *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

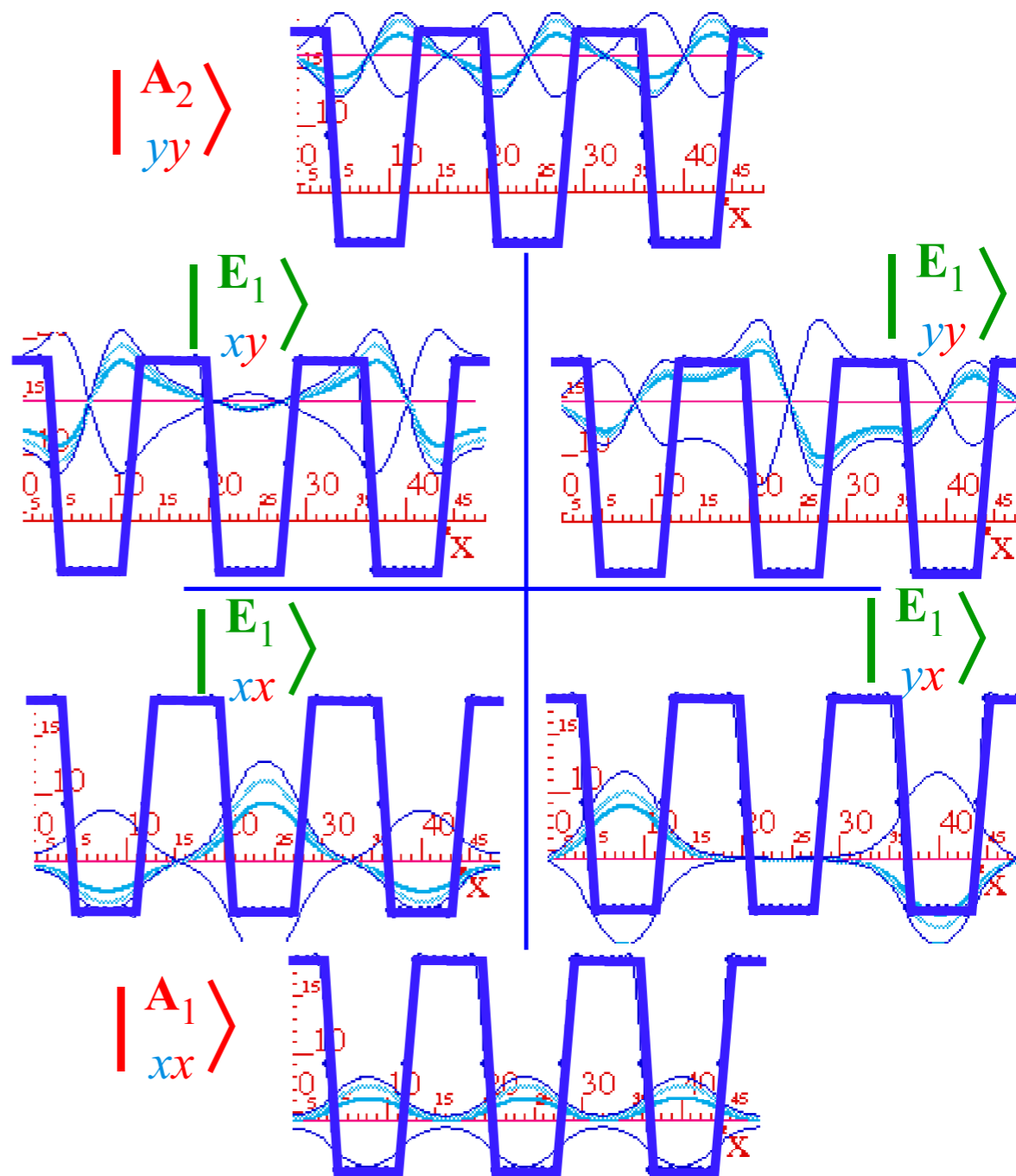
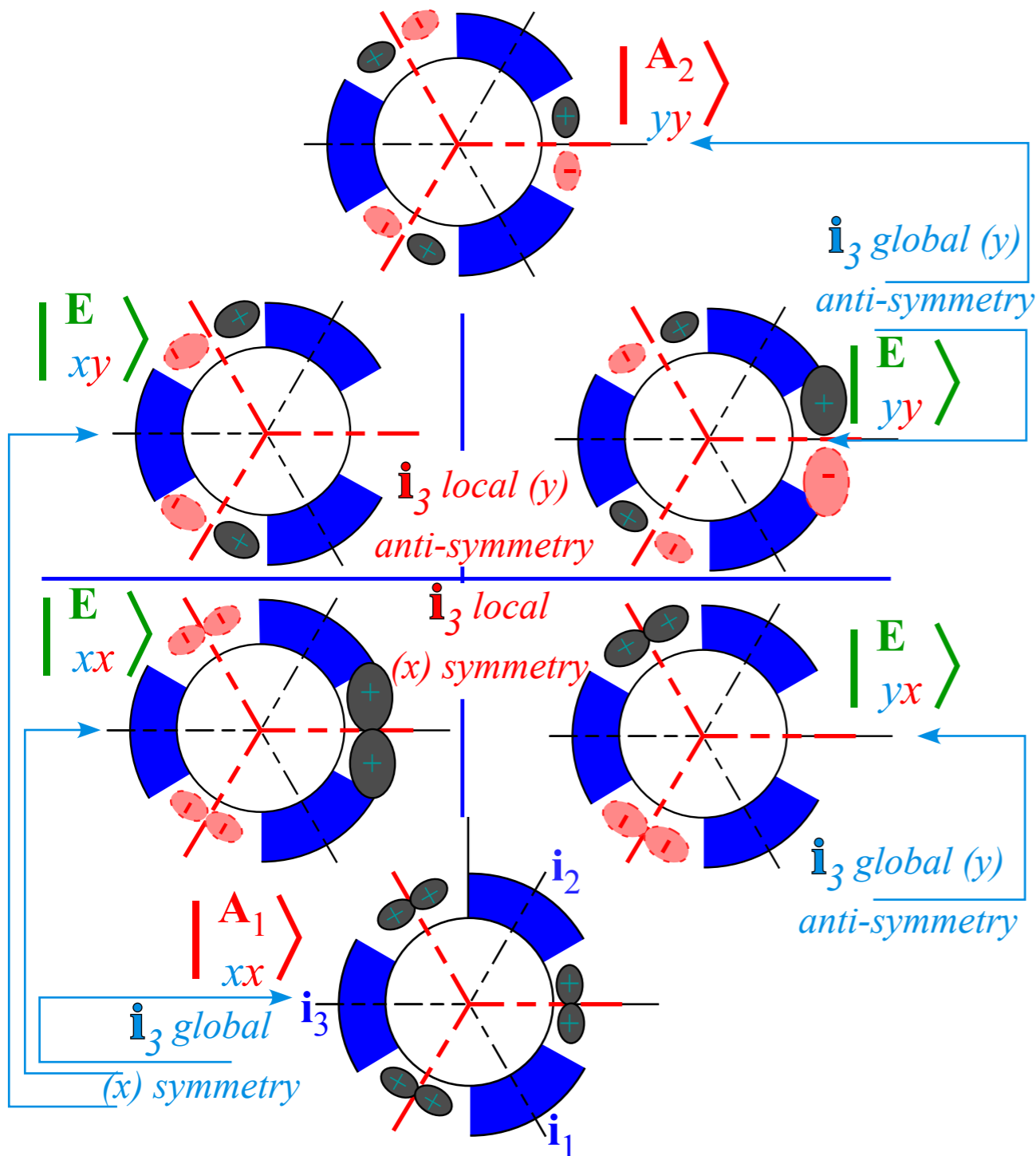
$D_3 > C_2$   $i_3$  projector states

Local (BOD) symmetry

$$i_3 |_{eb}^{(m)} \rangle = i_3 P_{eb}^{(m)} |1\rangle = (-1)^e |^{(m)} \rangle$$

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

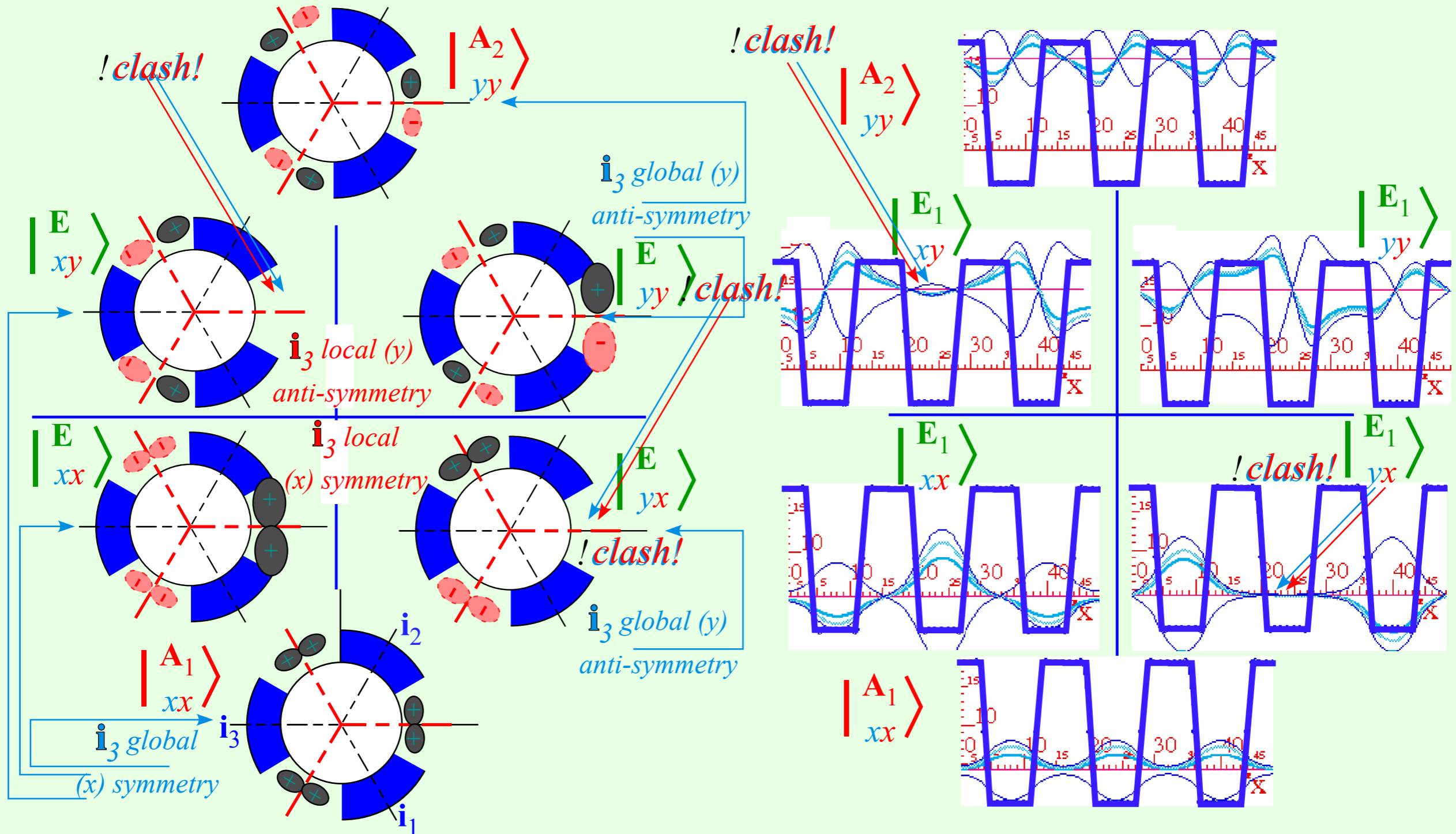
$$\bar{i}_3 |_{eb}^{(m)} \rangle = \bar{i}_3 P_{eb}^{(m)} |1\rangle = P_{eb}^{(m)} \bar{i}_3 |1\rangle = P_{eb}^{(m)} i_3^\dagger |1\rangle = (-1)^b |^{(m)} \rangle$$



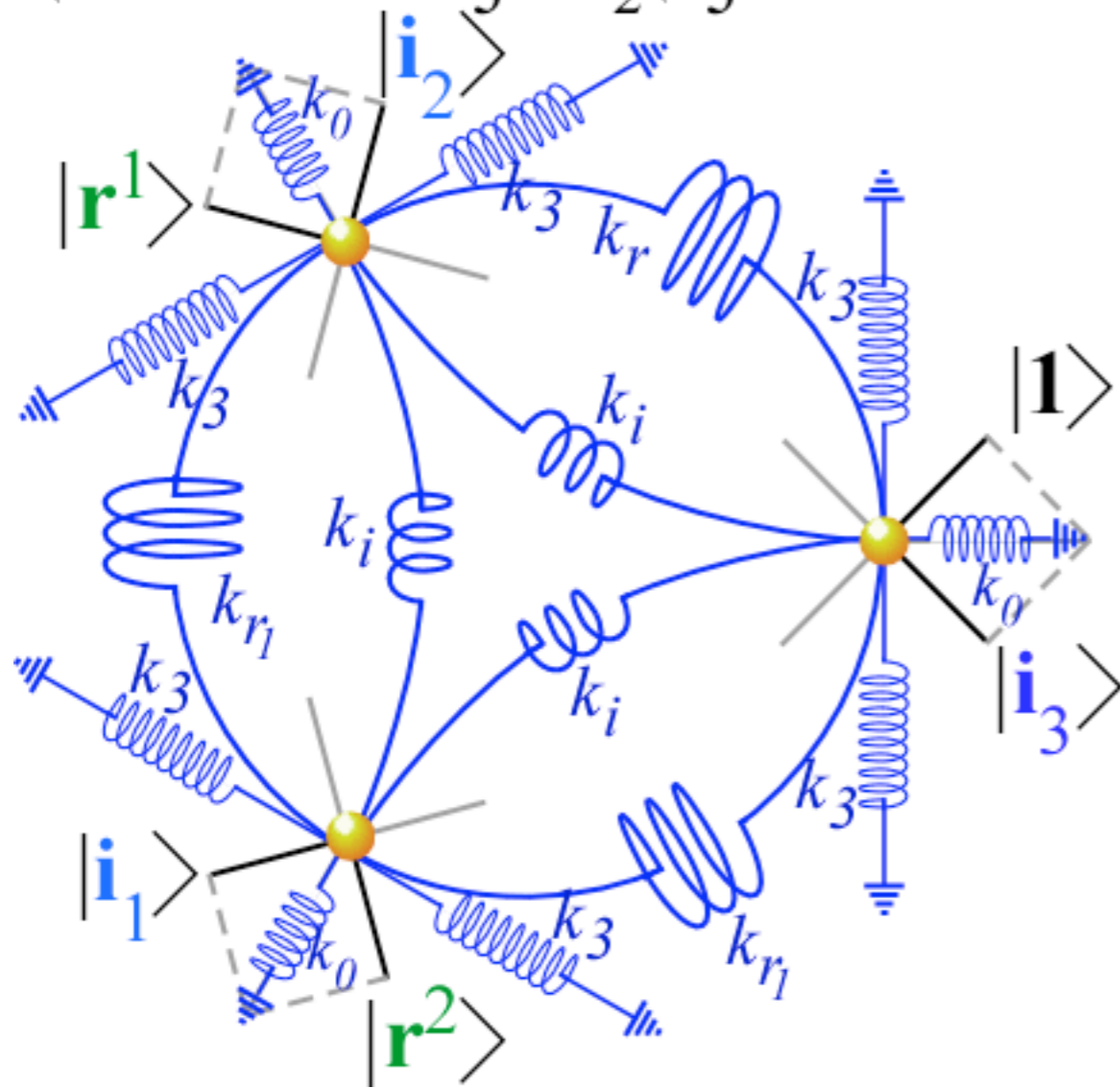


# When there is no there, there...

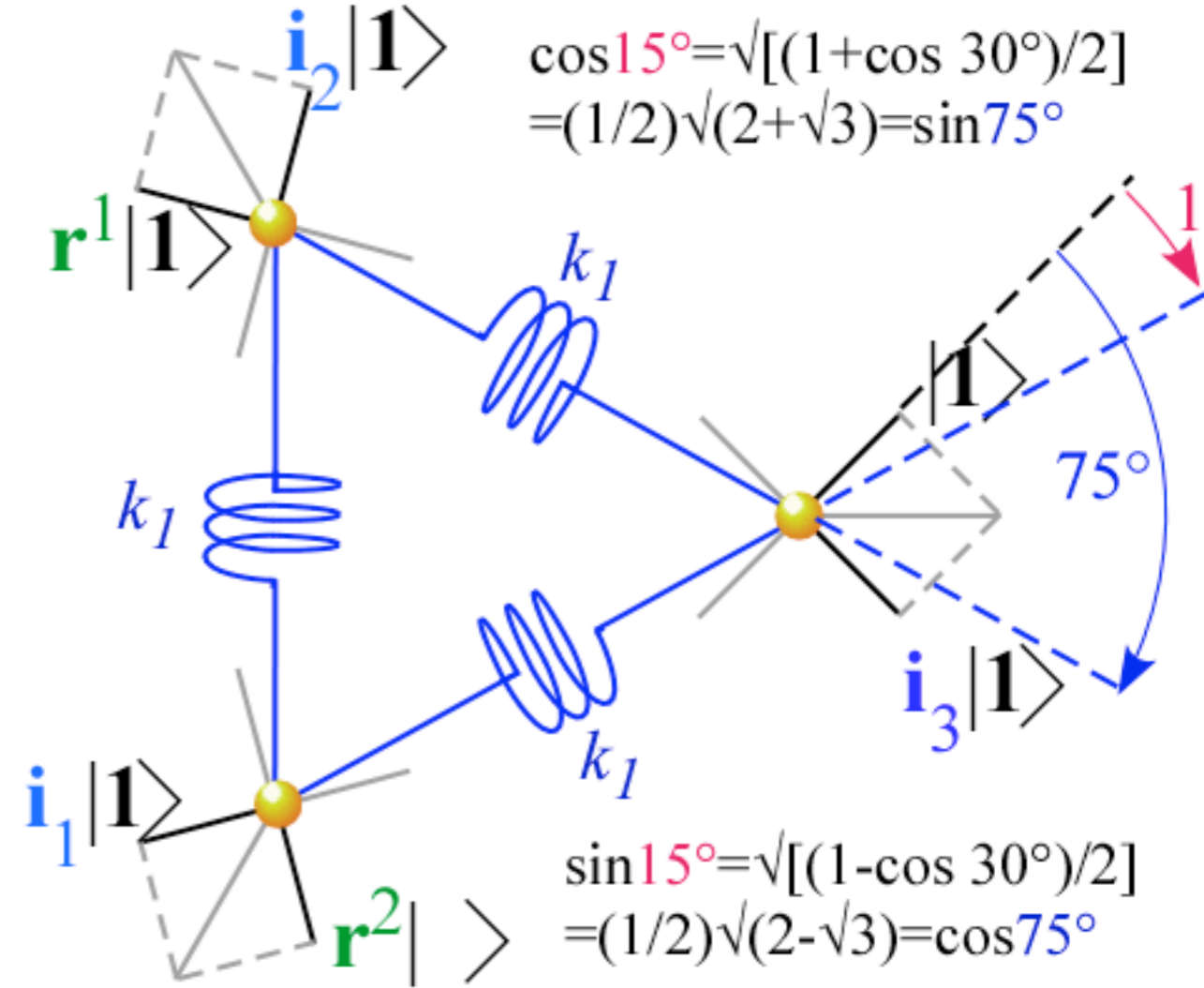
Nobody Home  
where *LOCAL*  
and *GLOBAL*

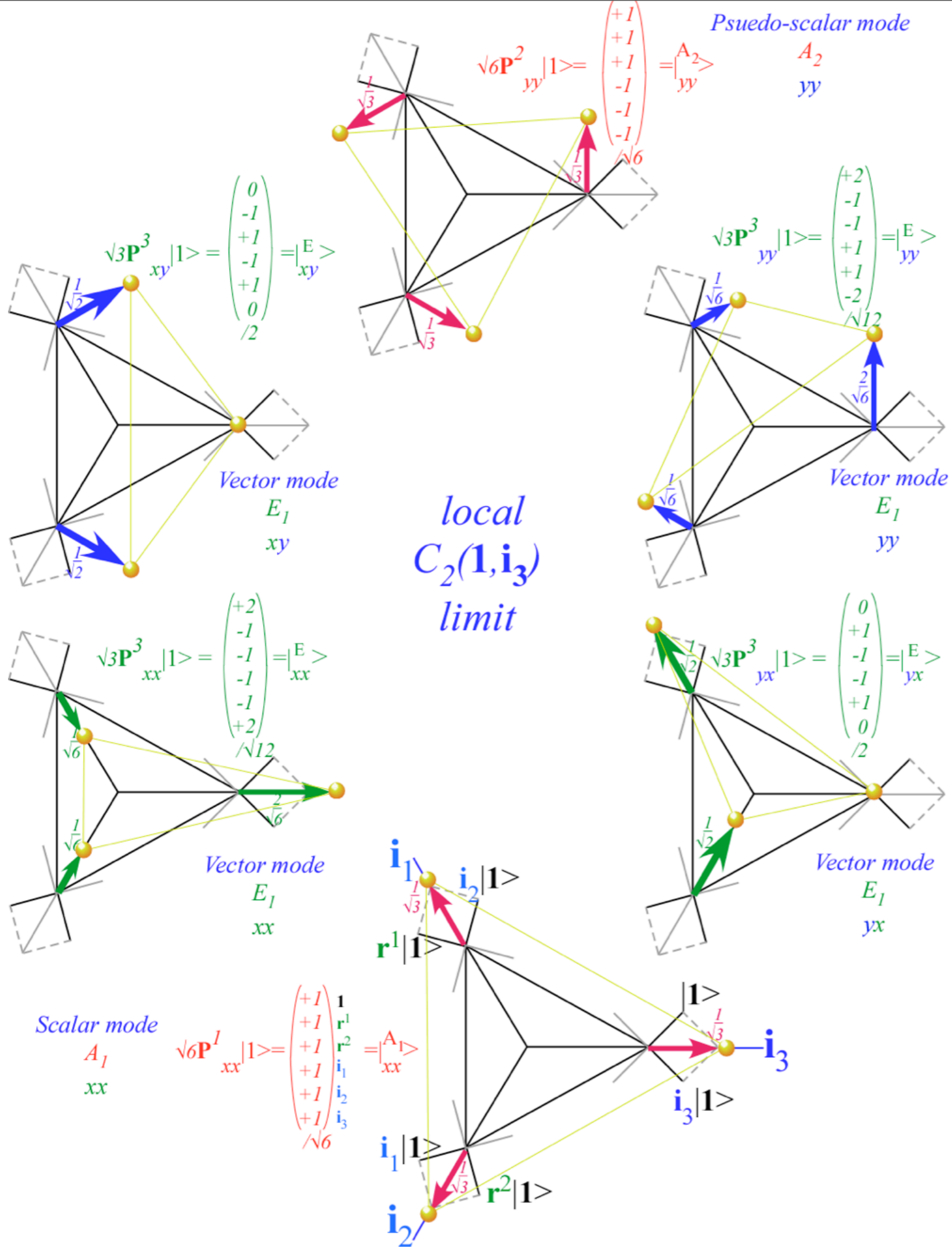


(a) Local  $D_3 \supset C_2(i_3)$  model



(b) Mixed local symmetry  $D_3$  model





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

