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Condensed Matter Theory Group
Paul Scherrer Institute

Introduction to group theory and the classification of [superconducting] states

European School on Superconductivity and Magnetism in Quantum Materials
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PAUL SCHERRER INSTITUT
PSI

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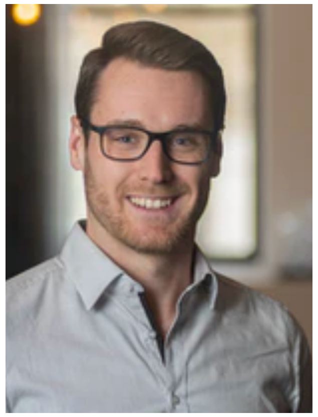
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Outline

Brief introduction to group theory concepts:

Group ⇒ Conjugacy Classes ⇒ Group Representation
⇒ Character ⇒ Irreducible Representations

Crystallographic Point Groups:

⇒ SC order parameter classification [Sigrist-Ueda]
⇒ Conventional/unconventional
⇒ Nematic/Chiral

Beyond the Sigrist-Ueda Classification:

⇒ Multiple internal DOFs (orbitals/layers/sublattices)
⇒ Nonsymmorphic symmetries

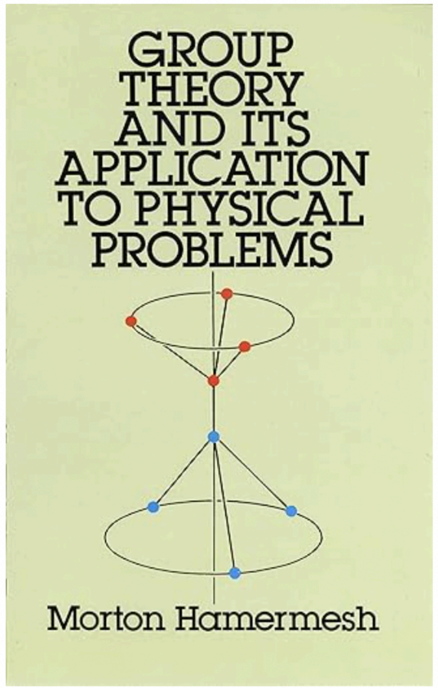
Introduction to Group Theory

Bibliography

M. Hamermesh, *Group Theory and its Application to Physical Problems*, Addison-Wesley (1962);

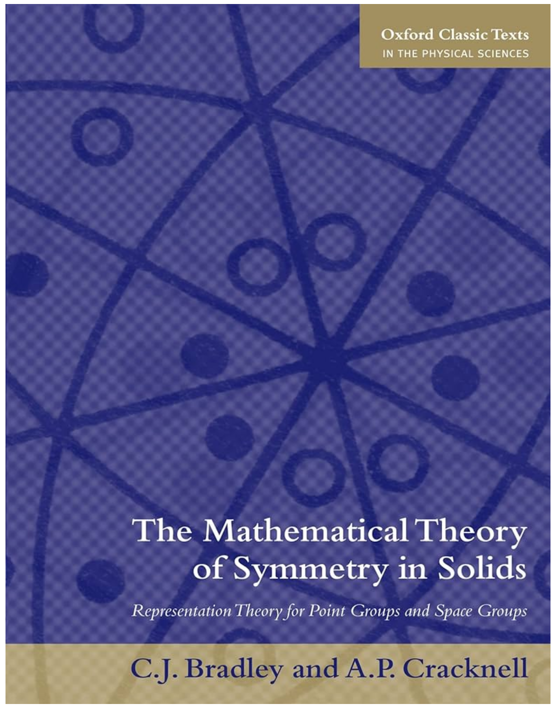
C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups*, Claredon Press (1972);

M.S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory Application to the Physics of Condensed Matter*, Springer (2008).



GROUP THEORY AND ITS APPLICATION TO PHYSICAL PROBLEMS

Morton Hamermesh

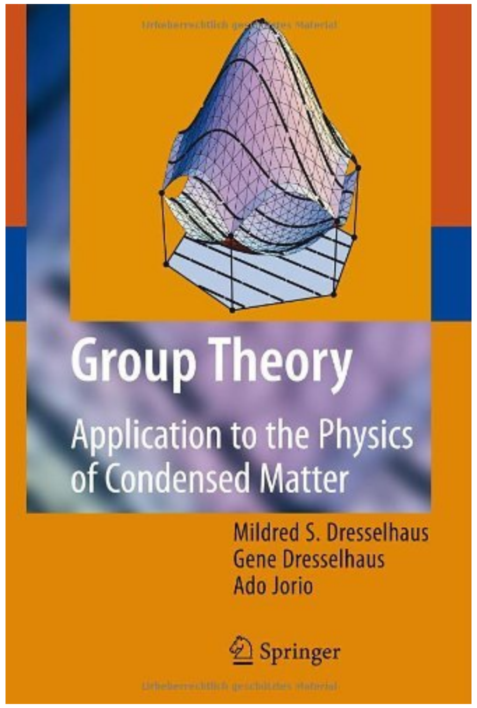


Oxford Classic Texts
IN THE PHYSICAL SCIENCES

The Mathematical Theory of Symmetry in Solids

Representation Theory for Point Groups and Space Groups

C.J. Bradley and A.P. Cracknell



Group Theory

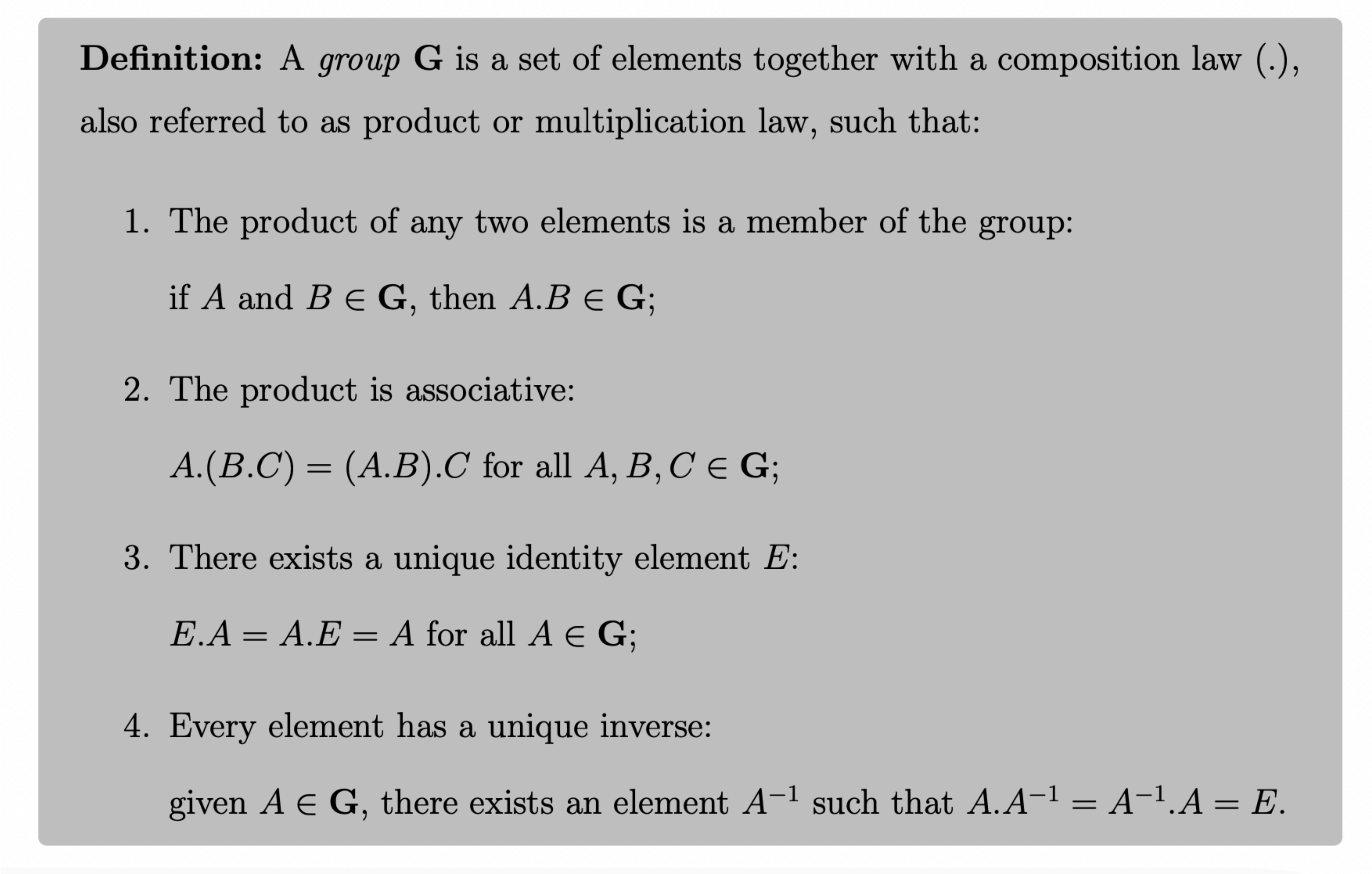
Application to the Physics of Condensed Matter

Mildred S. Dresselhaus
Gene Dresselhaus
Ado Jorio

Springer

What is a group?

What is a group?



Definition: A *group* $\mathbf{G}$ is a set of elements together with a composition law (.), also referred to as product or multiplication law, such that:

1. The product of any two elements is a member of the group:

   if A and $B \in \mathbf{G}$, then $A.B \in \mathbf{G}$;

2. The product is associative:

   $A.(B.C) = (A.B).C$ for all $A, B, C \in \mathbf{G}$;

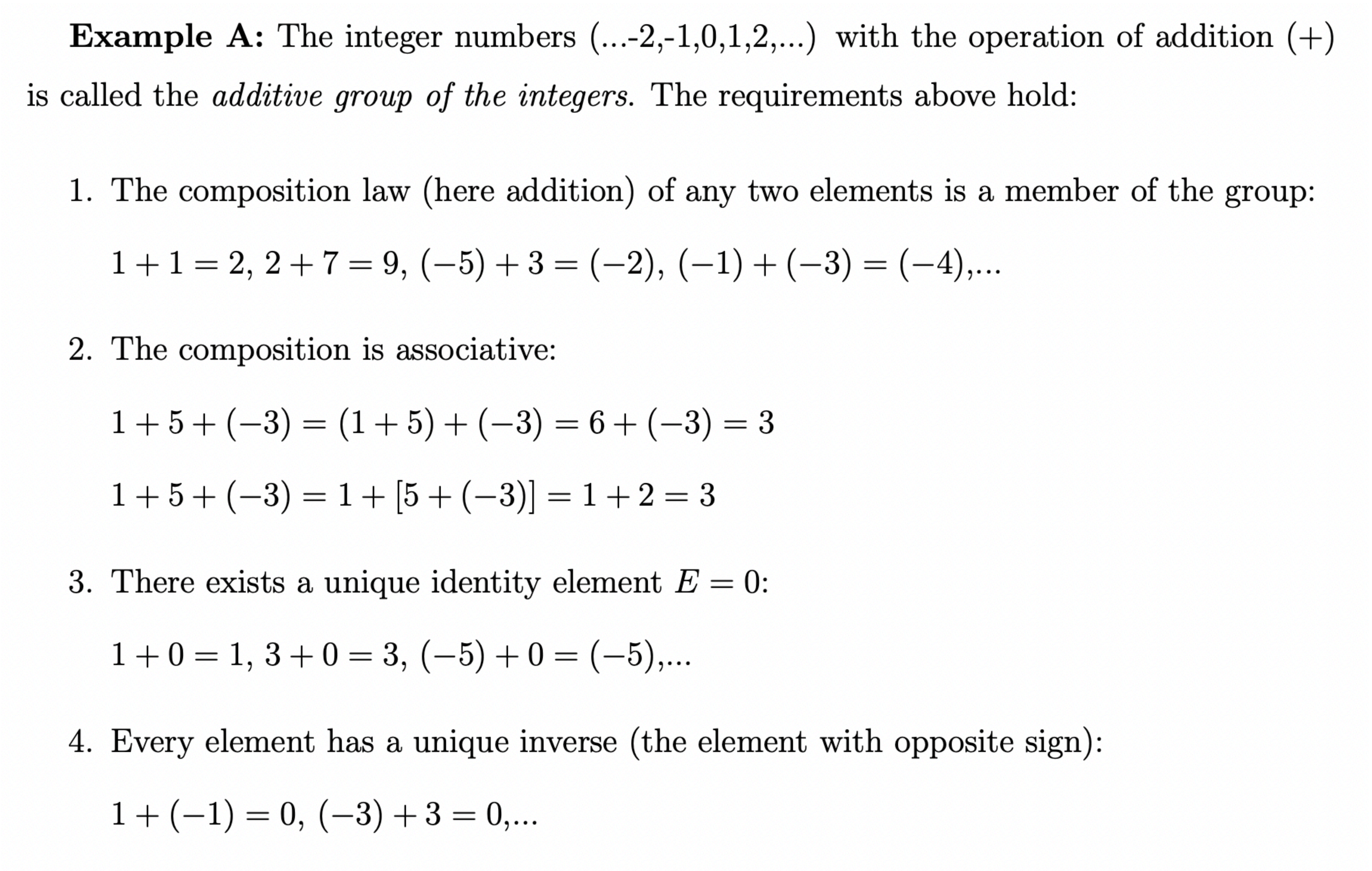
3. There exists a unique identity element E:

   $E.A = A.E = A$ for all $A \in \mathbf{G}$;

4. Every element has a unique inverse:

   given $A \in \mathbf{G}$, there exists an element A^{-1} such that $A.A^{-1} = A^{-1}.A = E$.

Additive Group of the Integers



Example A: The integer numbers (...-2,-1,0,1,2,...) with the operation of addition (+) is called the *additive group of the integers.* The requirements above hold:

1. The composition law (here addition) of any two elements is a member of the group:

   $1+1=2,\ 2+7=9,\ (-5)+3=(-2),\ (-1)+(-3)=(-4)$,...

2. The composition is associative:

   $1+5+(-3)=(1+5)+(-3)=6+(-3)=3$

   $1+5+(-3)=1+[5+(-3)]=1+2=3$

3. There exists a unique identity element $E=0$:

   $1+0=1,\ 3+0=3,\ (-5)+0=(-5)$,...

4. Every element has a unique inverse (the element with opposite sign):

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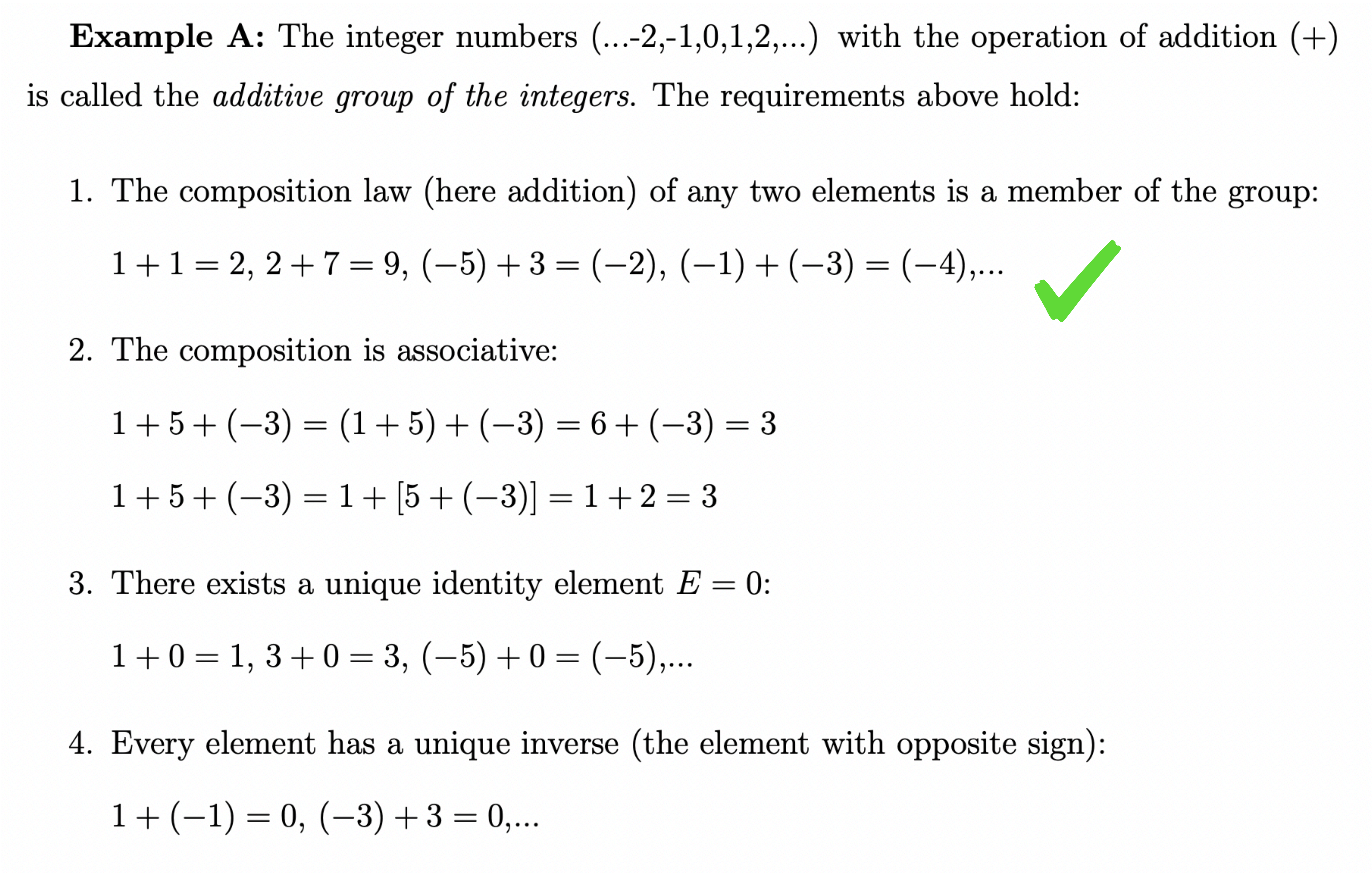

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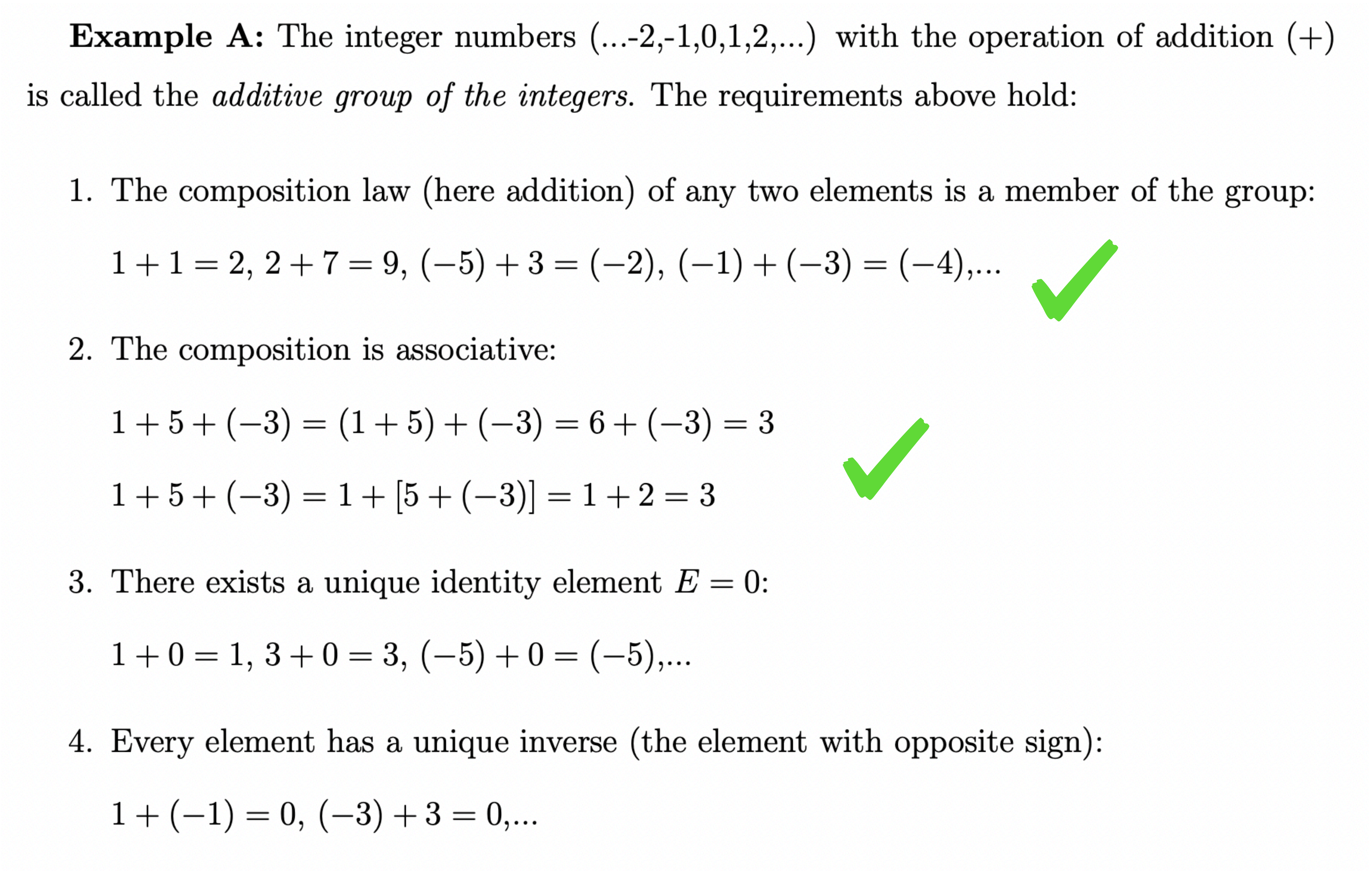

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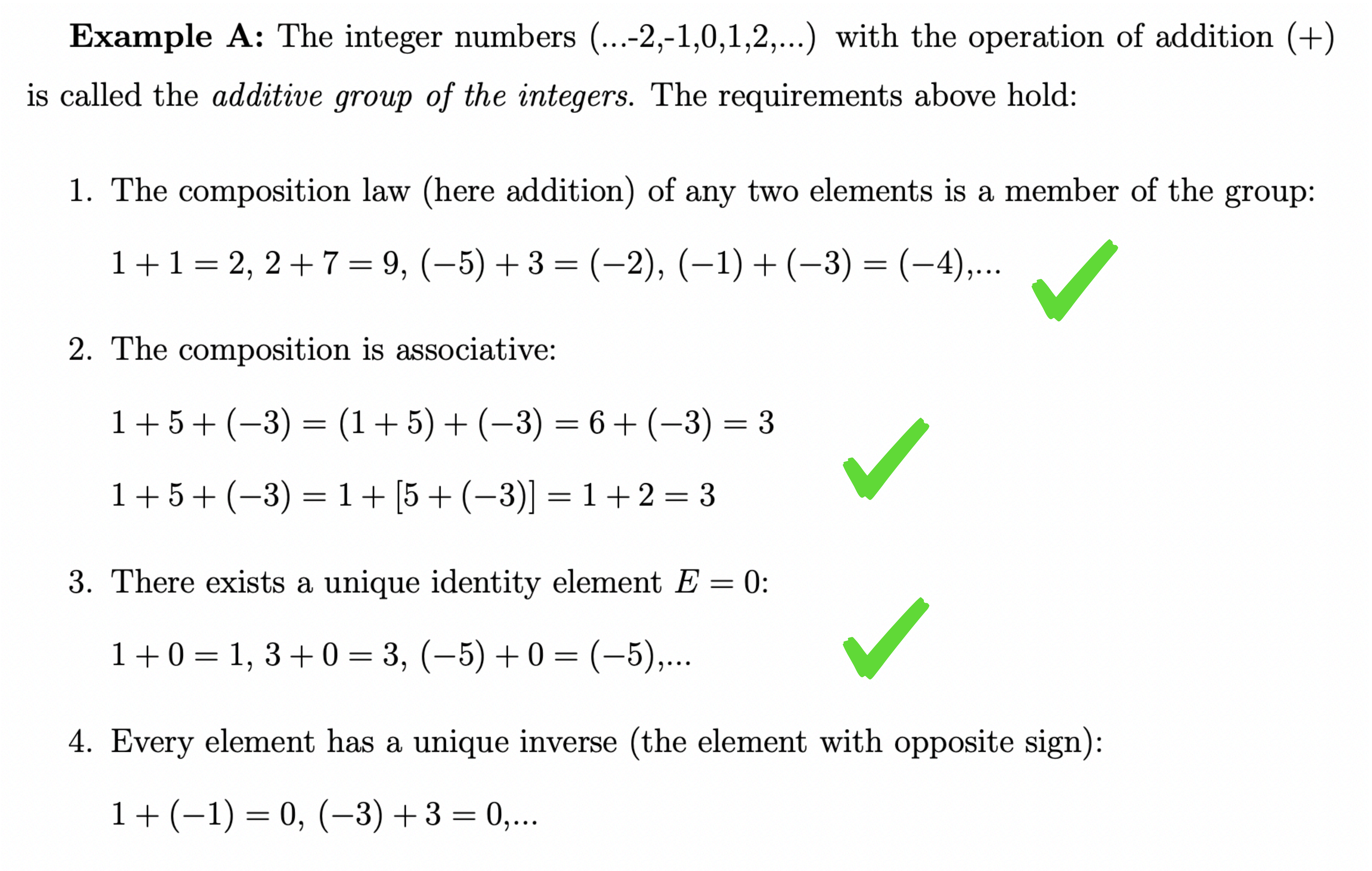

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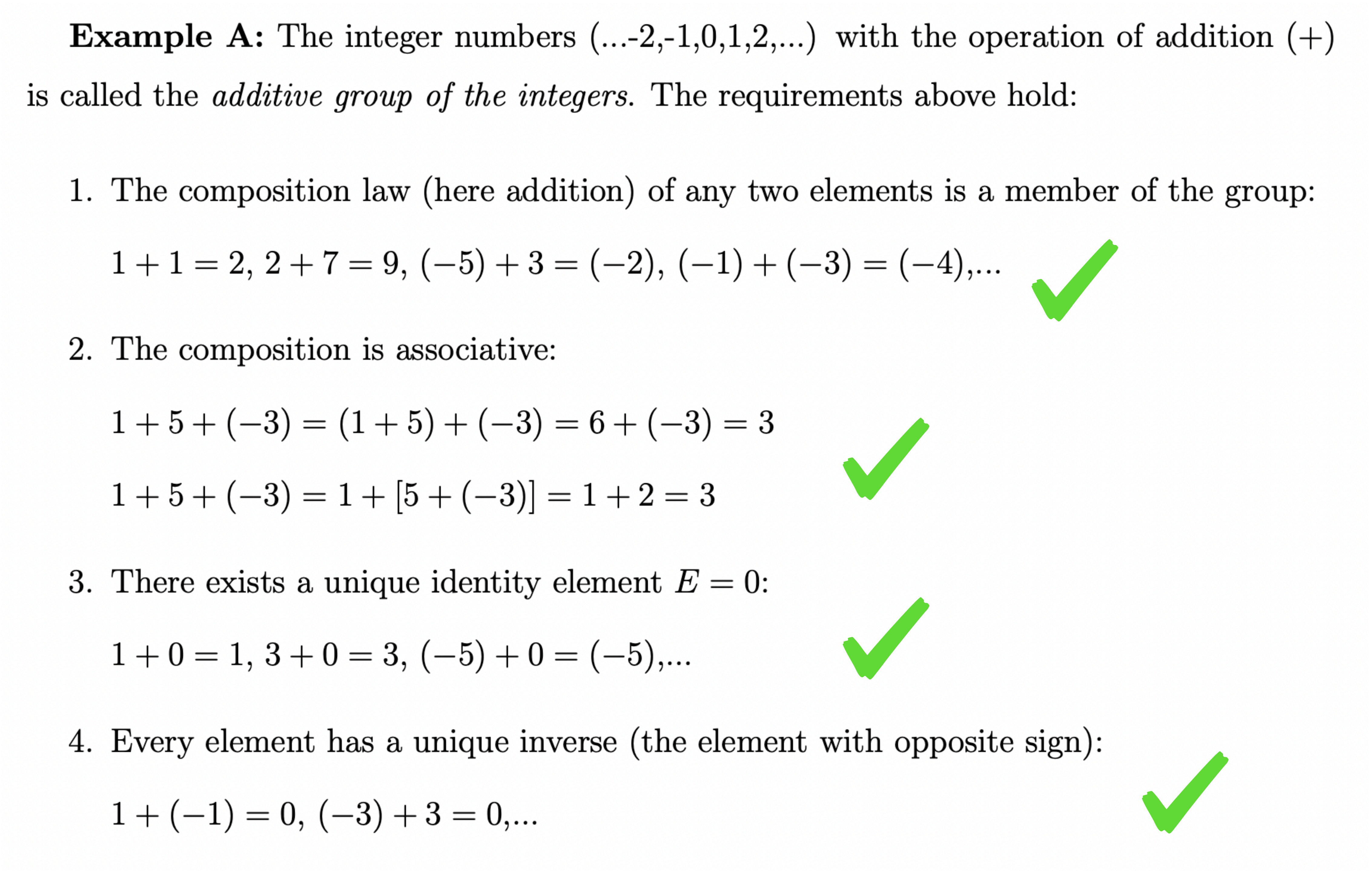

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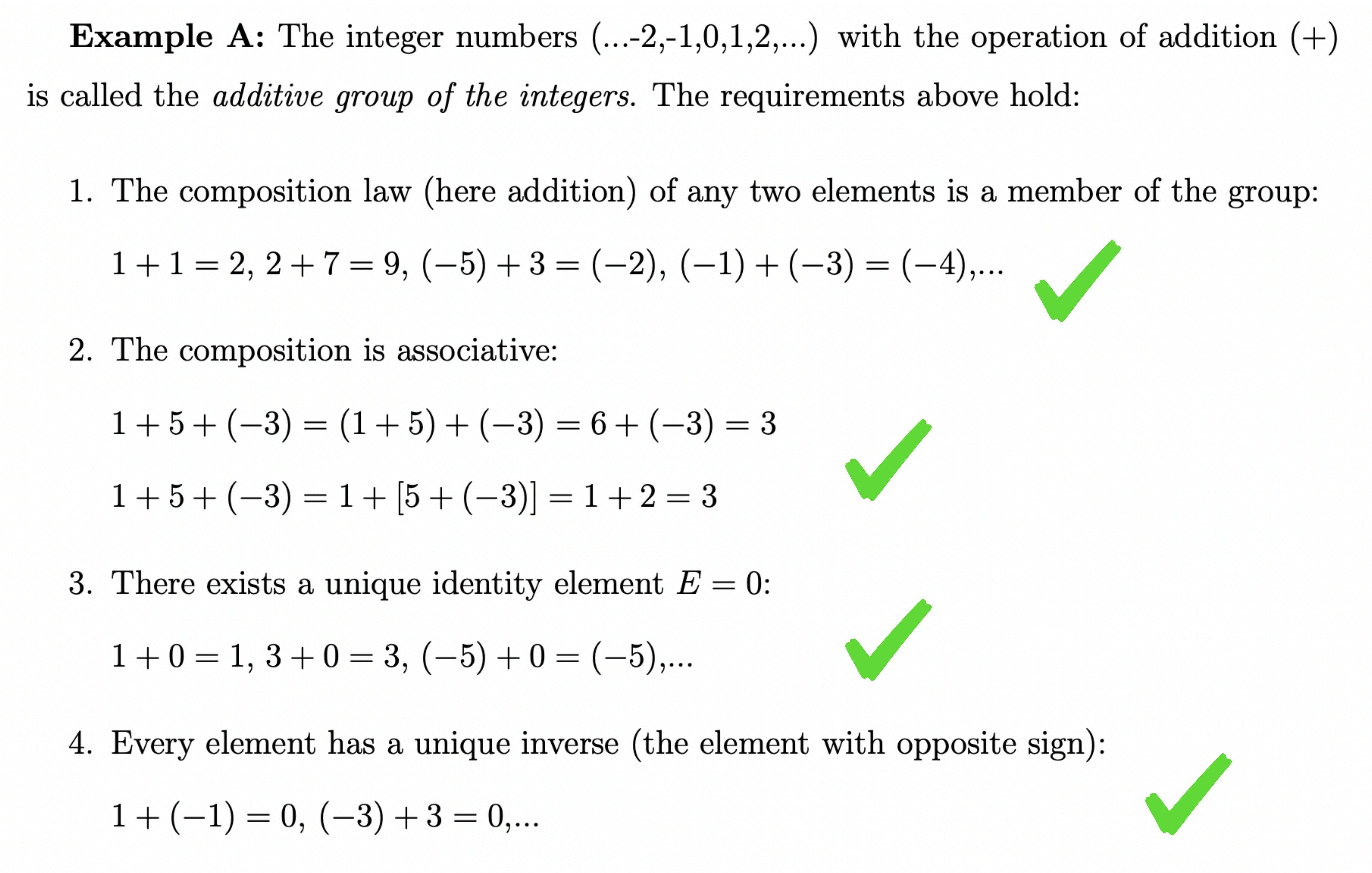

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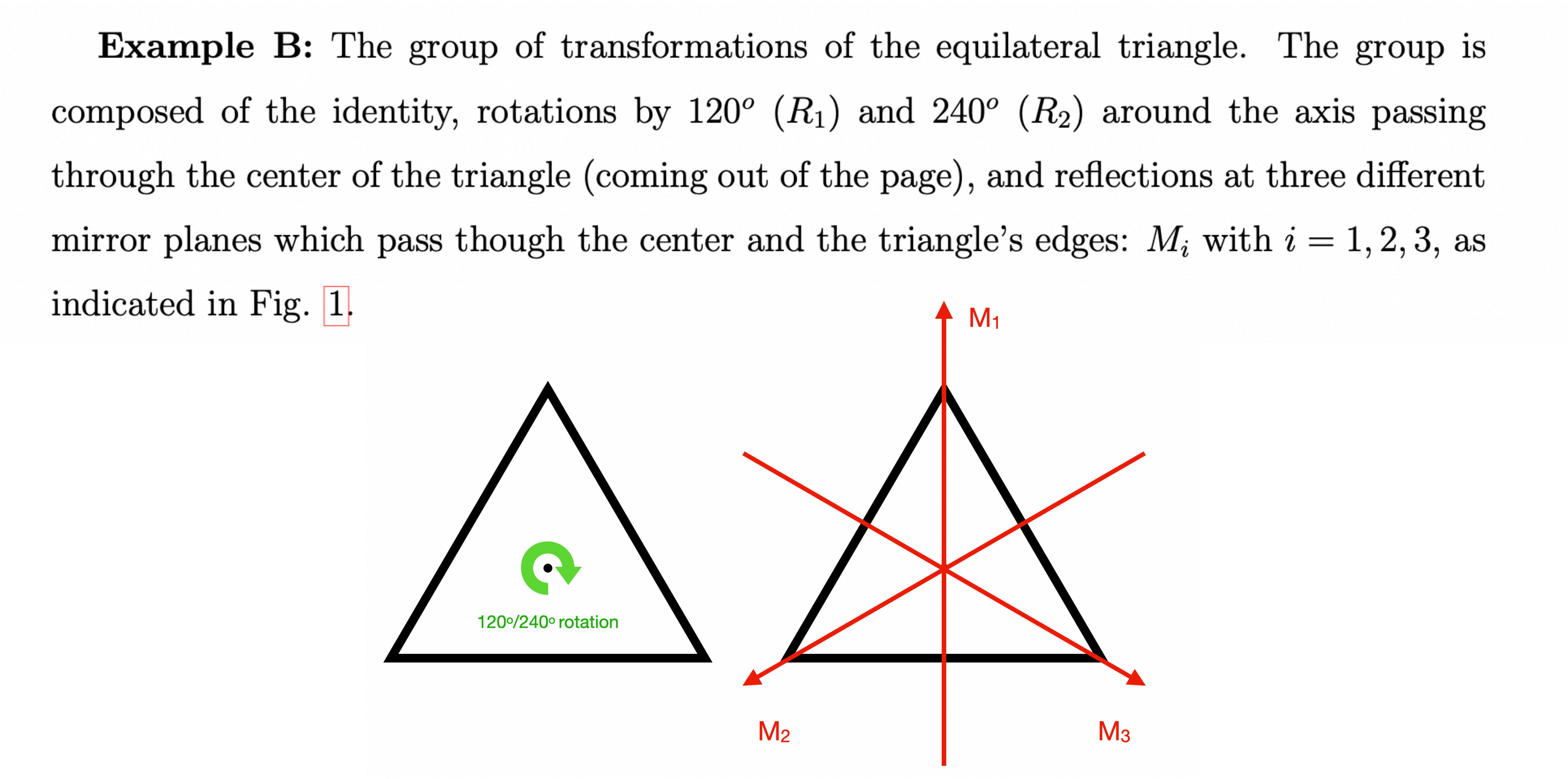
Order of the group: number of elements in the group
[The additive group of the integers is infinite]

Group of Symmetries of the Equilateral Triangle



Example B: The group of transformations of the equilateral triangle. The group is composed of the identity, rotations by 120^o (R_1) and 240^o (R_2) around the axis passing through the center of the triangle (coming out of the page), and reflections at three different mirror planes which pass though the center and the triangle's edges: M_i with $i = 1, 2, 3$, as indicated in Fig. 1.

Group of Symmetries of the Equilateral Triangle

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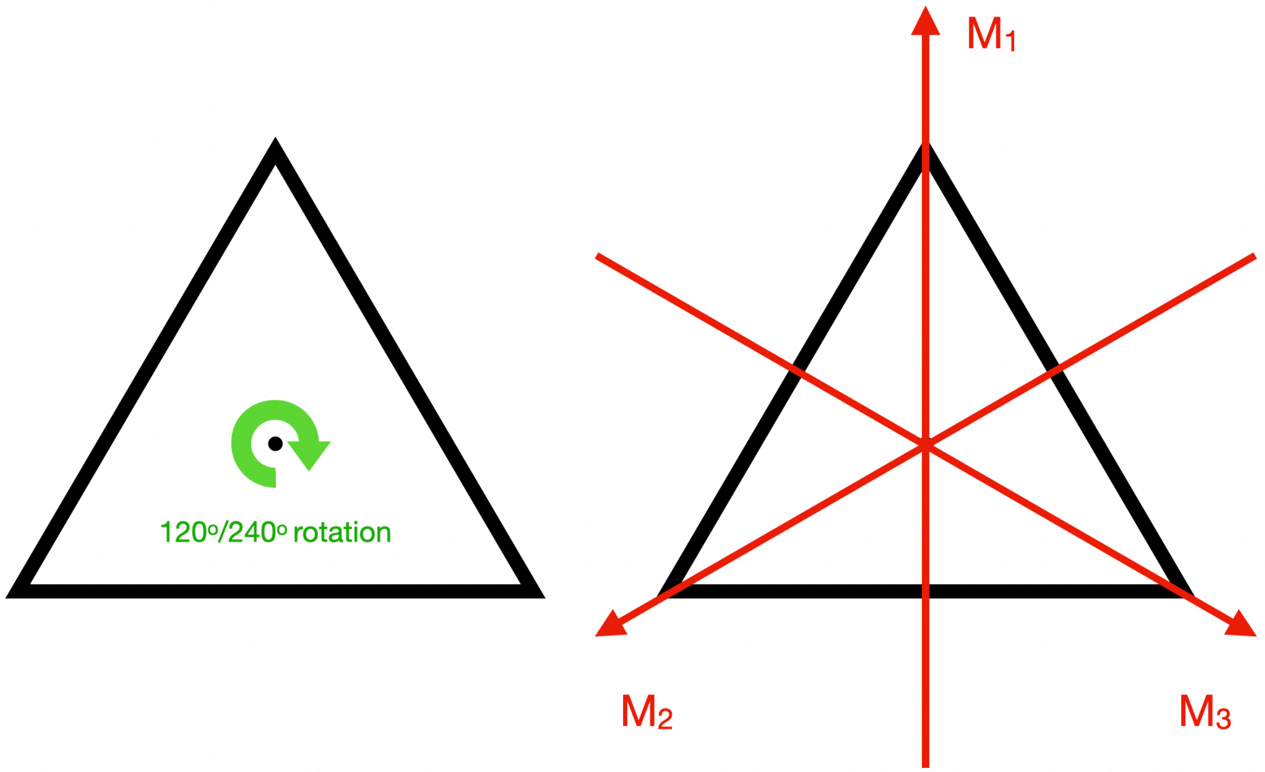


six operations in the group: $E, R_1, R_2, M_1, M_2, M_3$.

Order of the group: number of elements in the group
[The group of symmetries of the equilateral triangle has order 6]

Group of Symmetries of the Equilateral Triangle

1. The "product" (here the composition) of any two elements is a member of the group

Convention: Apply first the right most operation.

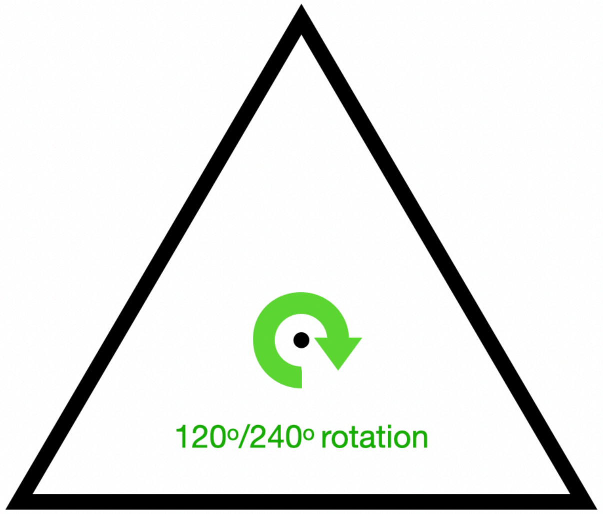
For the rotations:

$$R_1.R_1 = R_2$$

$$R_1.R_2 = E$$

$$R_2.R_1 = E$$

$$R_2.R_2 = R_1$$



rotations by 120^o (R_1) and 240^o (R_2)

Convention: Clockwise rotations

Group of Symmetries of the Equilateral Triangle

1. The "product" (here the composition) of any two elements is a member of the group

Convention: Apply first the right most operation.

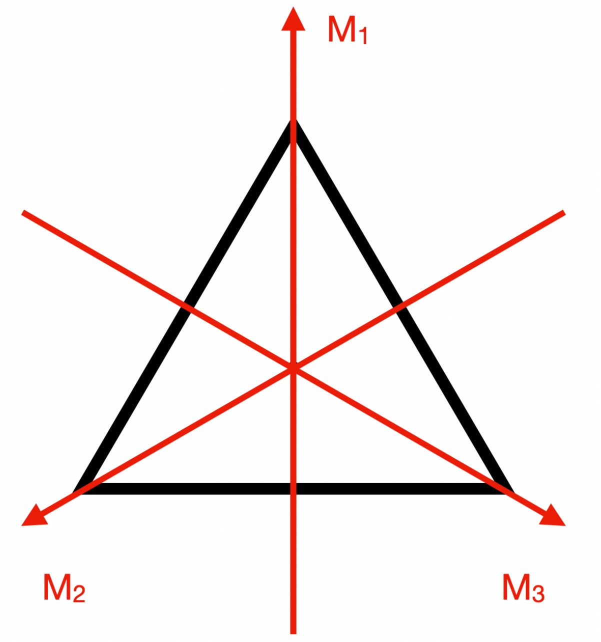
For the mirror operations

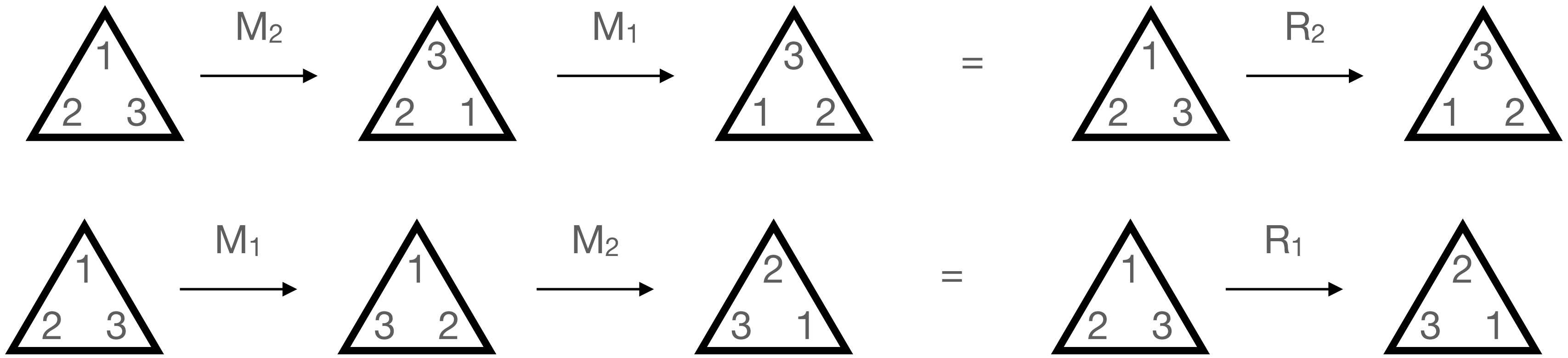
$$M_i.M_i = E \text{ for } i = 1, 2, 3$$

$$M_1.M_2 = R_2$$

$$M_2.M_1 = R_1$$

...





(you can check the remaining combinations)

Group of Symmetries of the Equilateral Triangle

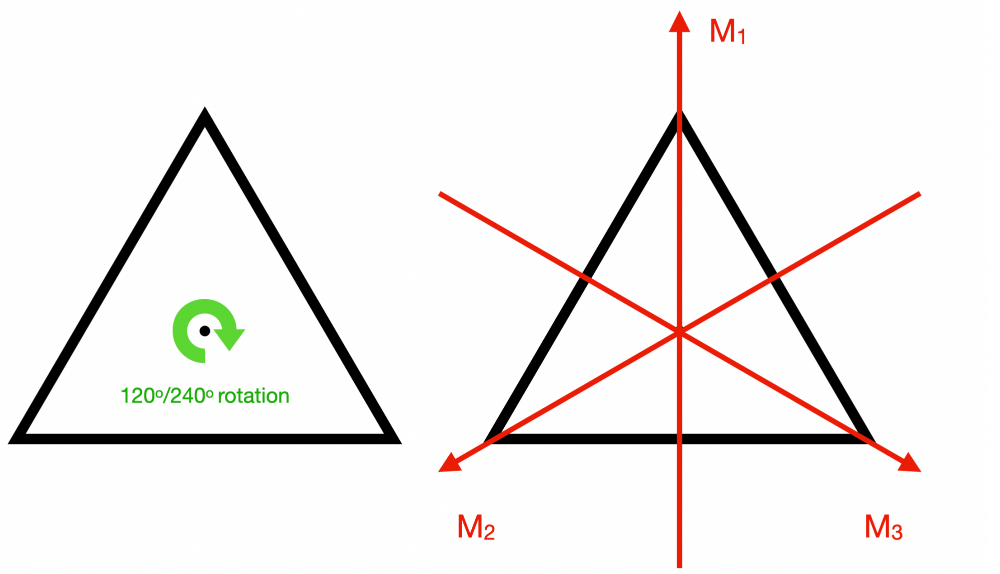
1. The "product" (here the composition) of any two elements is a member of the group (note that the right most operation is the one to be applied first):

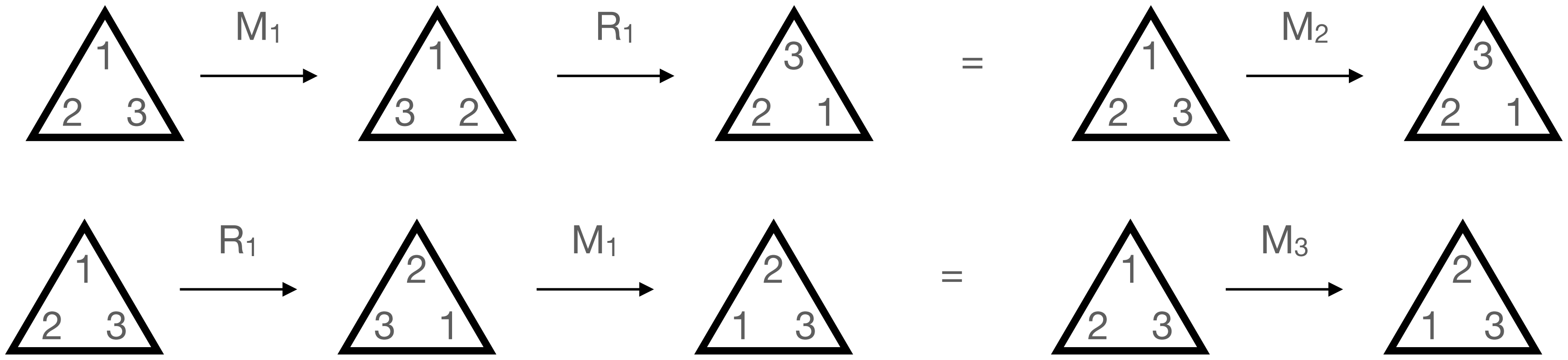
Mixing rotations and mirror operations

$$R_1.M_1 = M_2$$

$$M_1.R_1 = M_3$$

$$\dots$$





(you can check the remaining combinations)

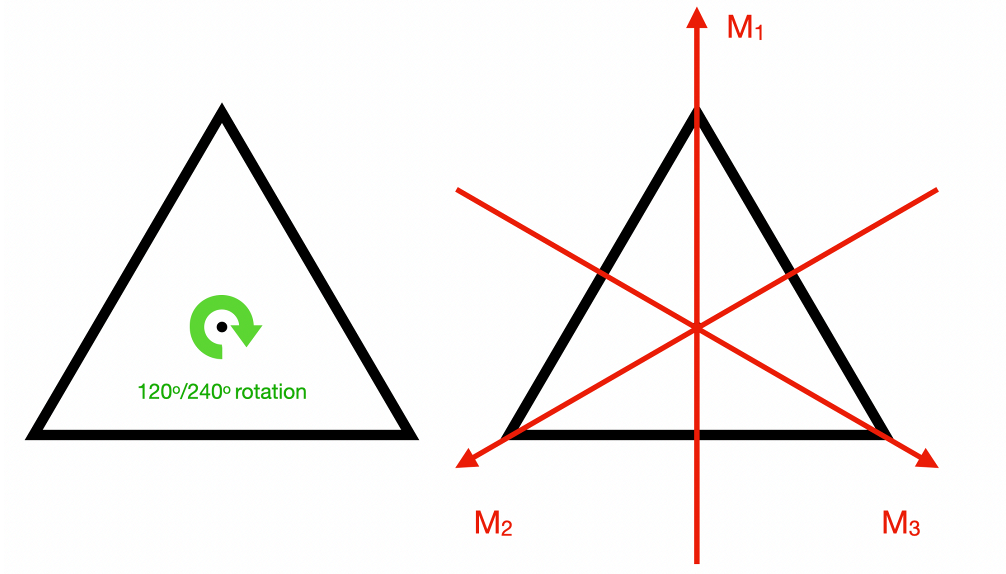
Group of Symmetries of the Equilateral Triangle

1. The product of any two elements is a member of the group:

   if A and $B \in \mathbf{G}$, then $A.B \in \mathbf{G}$;

There is a total of 36 pairs of operations to be checked. You can check that all combinations result in one of the six operations in the group: $E, R_1, R_2, M_1, M_2, M_3$.

Multiplication Table



	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
$\mathbf{E}$	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

Group of Symmetries of the Equilateral Triangle

1. The product of any two elements is a member of the group:

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✓

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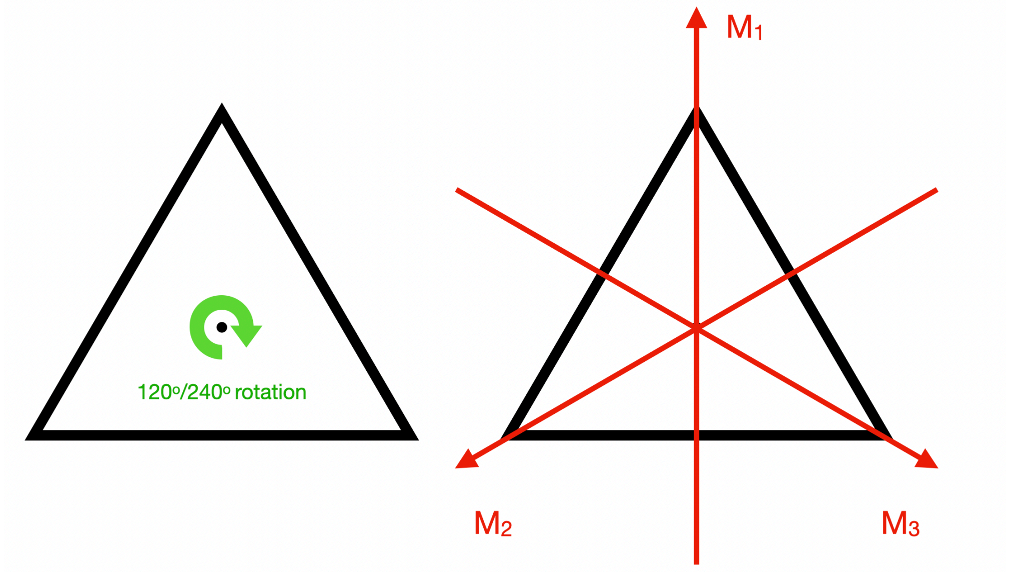

	E	**$\mathbf{R_1}$**	**$\mathbf{R_2}$**	**$\mathbf{M_1}$**	**$\mathbf{M_2}$**	**$\mathbf{M_3}$**
E	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

Group of Symmetries of the Equilateral Triangle

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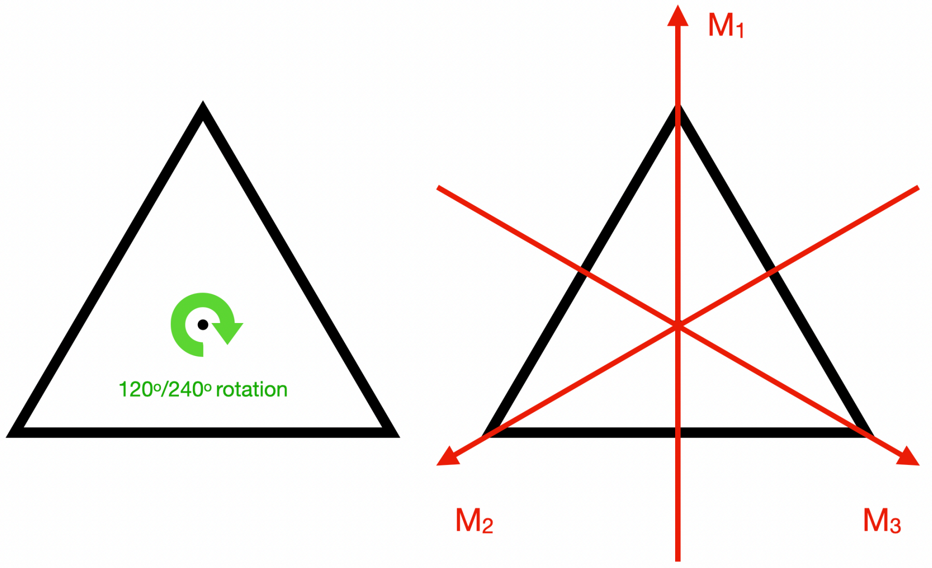

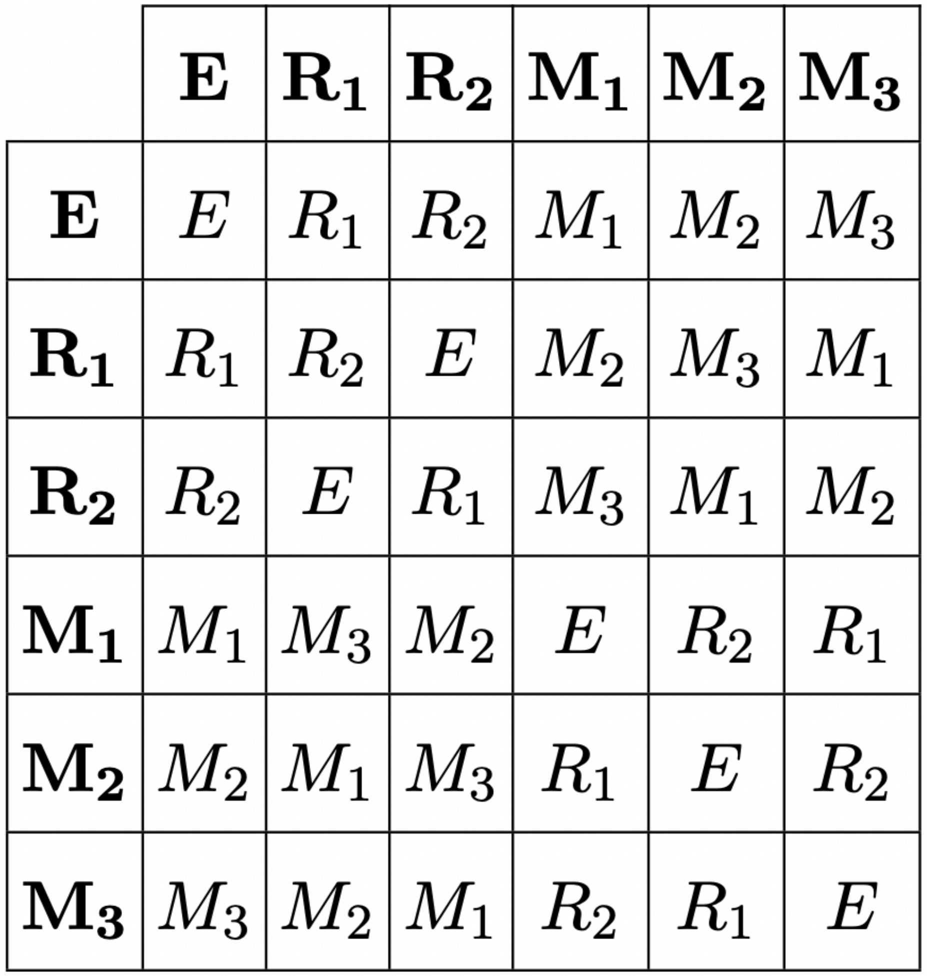

	E	**R₁**	**R₂**	**M₁**	**M₂**	**M₃**
E	E	R_1	R_2	M_1	M_2	M_3
R₁	R_1	R_2	E	M_2	M_3	M_1
R₂	R_2	E	R_1	M_3	M_1	M_2
M₁	M_1	M_3	M_2	E	R_2	R_1
M₂	M_2	M_1	M_3	R_1	E	R_2
M₃	M_3	M_2	M_1	R_2	R_1	E

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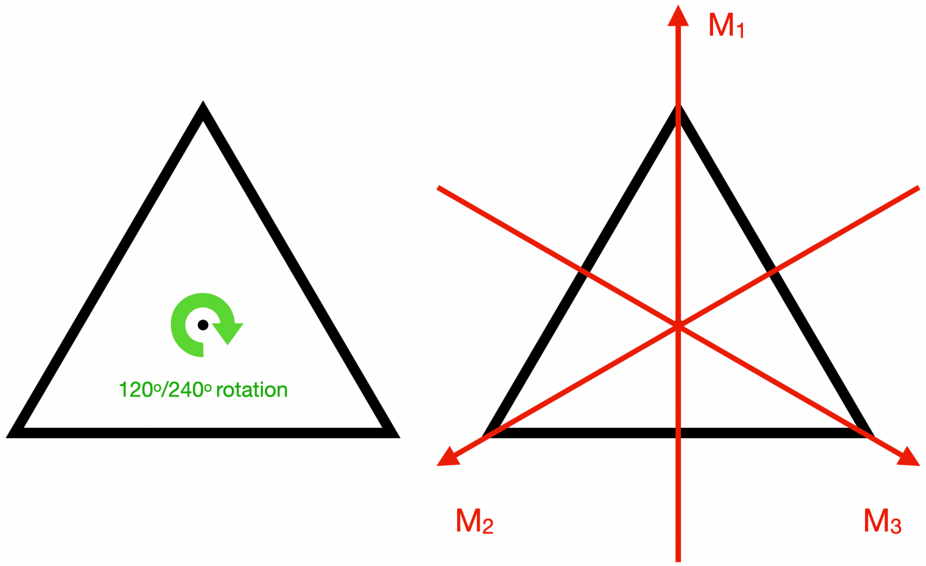

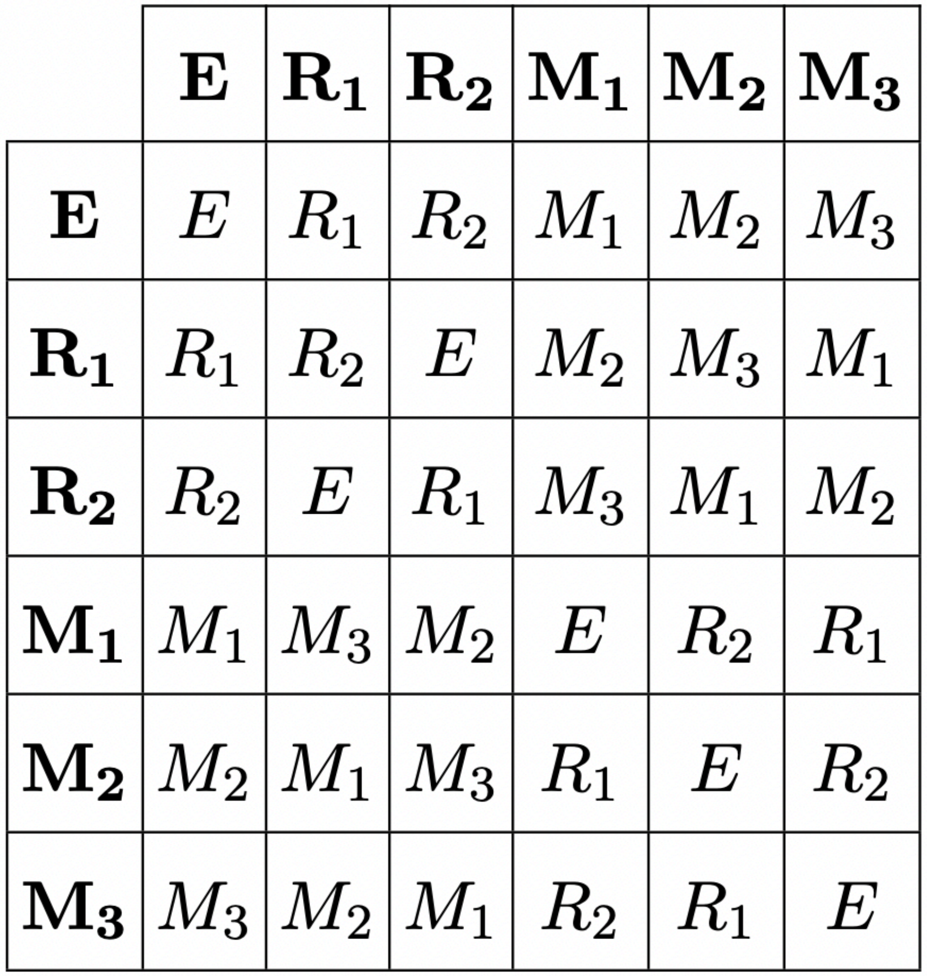

	E	**R₁**	**R₂**	**M₁**	**M₂**	**M₃**
E	E	R_1	R_2	M_1	M_2	M_3
R₁	R_1	R_2	E	M_2	M_3	M_1
R₂	R_2	E	R_1	M_3	M_1	M_2
M₁	M_1	M_3	M_2	E	R_2	R_1
M₂	M_2	M_1	M_3	R_1	E	R_2
M₃	M_3	M_2	M_1	R_2	R_1	E

Homework!

✓

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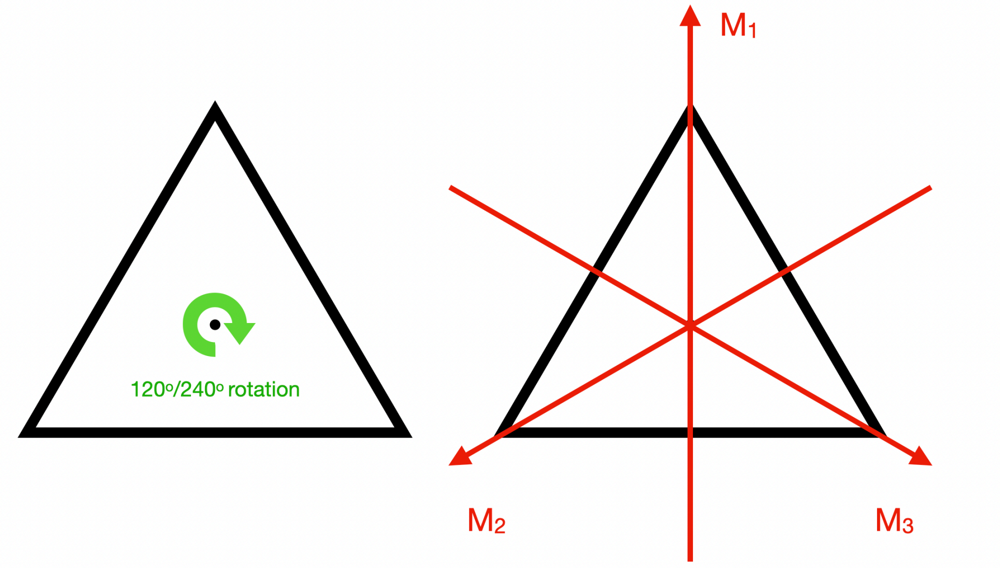

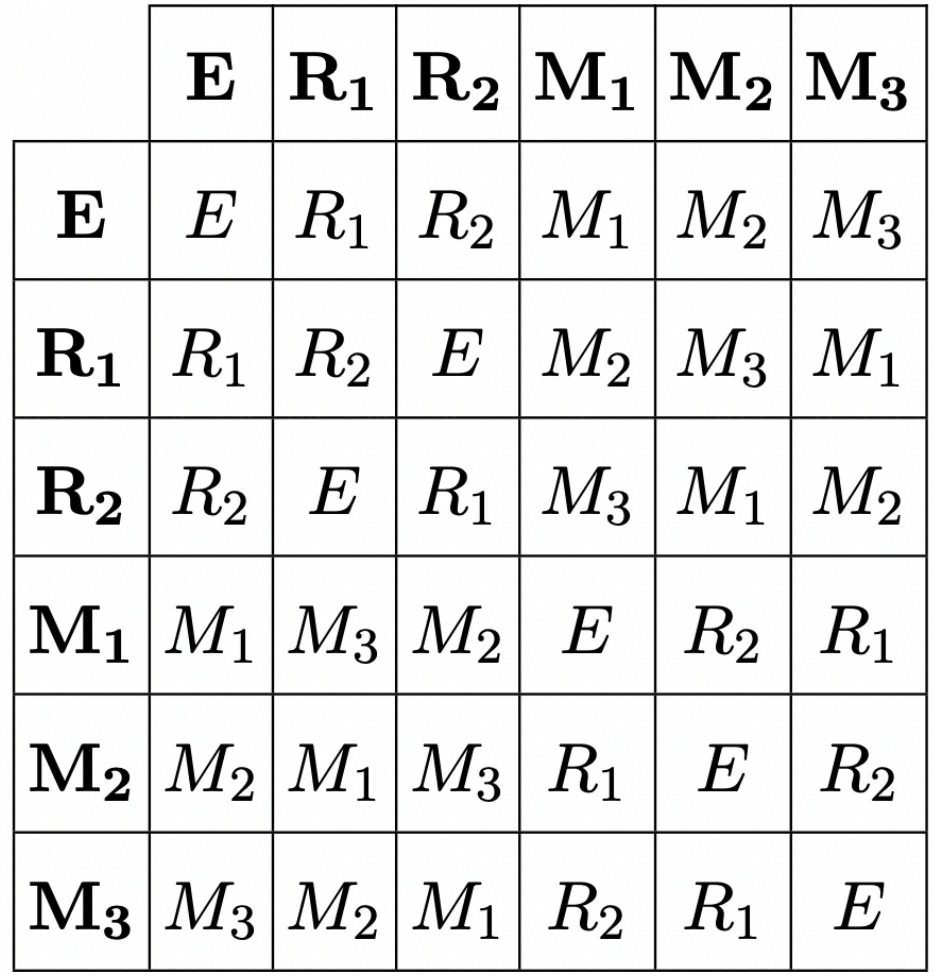

	E	**R₁**	**R₂**	**M₁**	**M₂**	**M₃**
E	E	R_1	R_2	M_1	M_2	M_3
R₁	R_1	R_2	E	M_2	M_3	M_1
R₂	R_2	E	R_1	M_3	M_1	M_2
M₁	M_1	M_3	M_2	E	R_2	R_1
M₂	M_2	M_1	M_3	R_1	E	R_2
M₃	M_3	M_2	M_1	R_2	R_1	E

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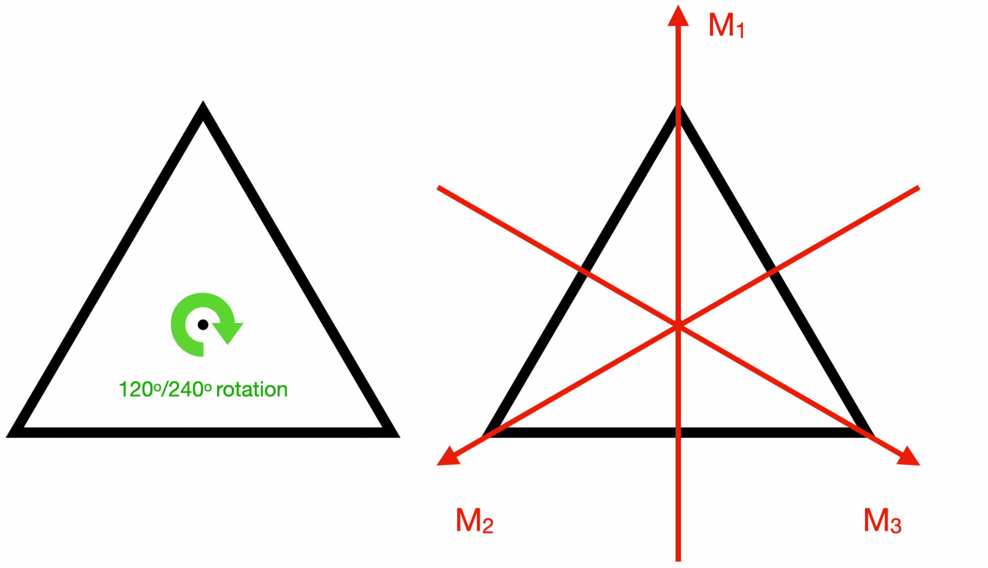

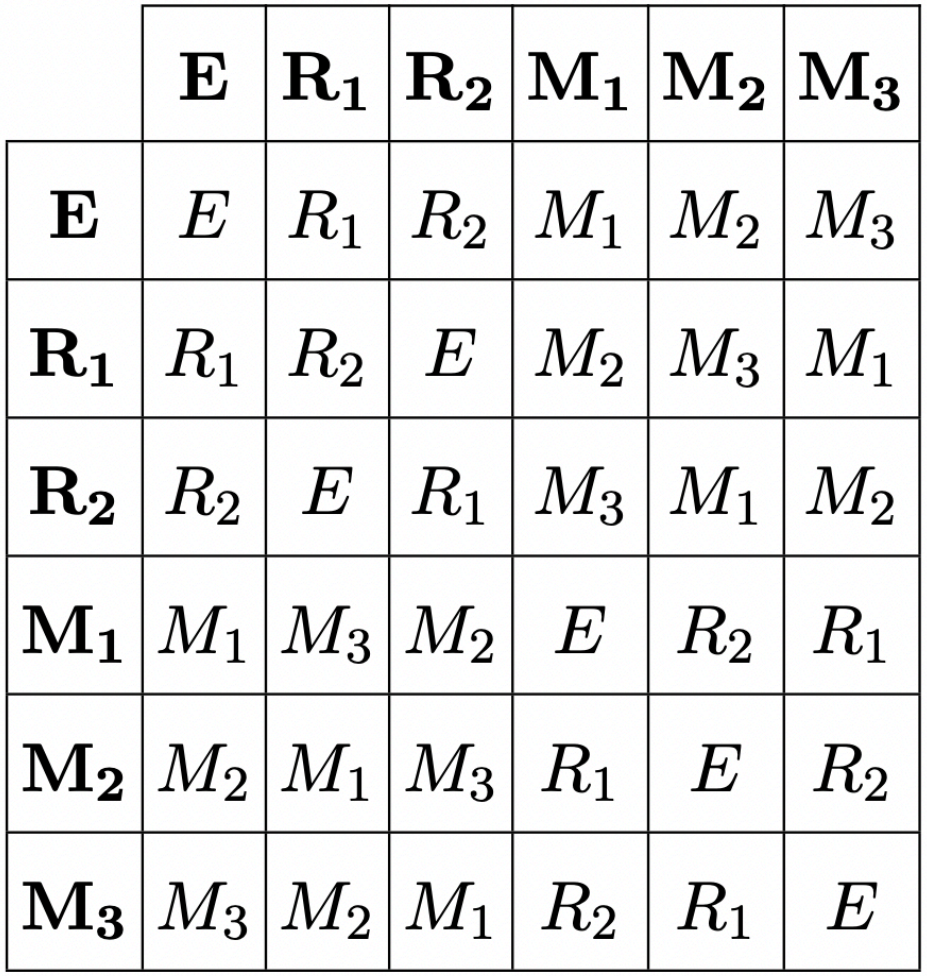

	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
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$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
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Homework!

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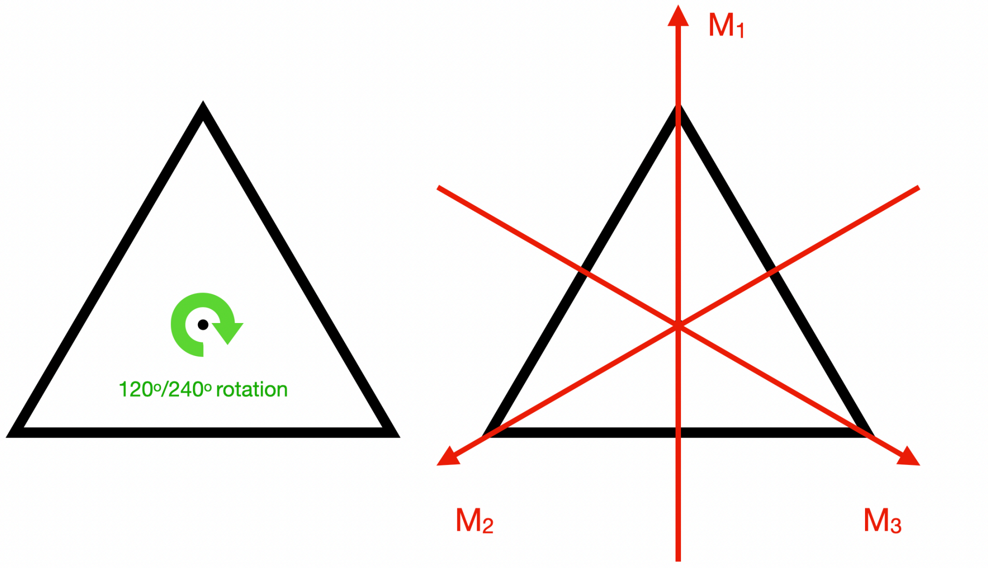
Group of Symmetries of the Equilateral Triangle

Multiplication Table



	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
$\mathbf{E}$	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

Homework!

✓ 2. The product is associative:

$A.(B.C) = (A.B).C$ for all $A, B, C \in \mathbf{G}$;

✓ 3. There exists a unique identity element E:

$E.A = A.E = A$ for all $A \in \mathbf{G}$;

✓ 4. Every element has a unique inverse:

given $A \in \mathbf{G}$, there exists an element A^{-1} such that $A.A^{-1} = A^{-1}.A = E$.

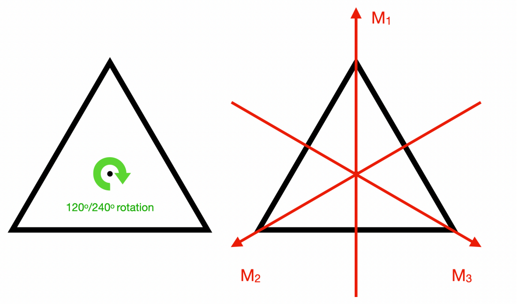
C_{3v} point group

[isomorphic to S_3]

Conjugate Elements

Conjugate Elements: Two elements G_1 and G_2 are said to be conjugate if there exists an element G in $\mathbf{G}$ such that $G_1 = GG_2G^{-1}$;

Conjugate Elements



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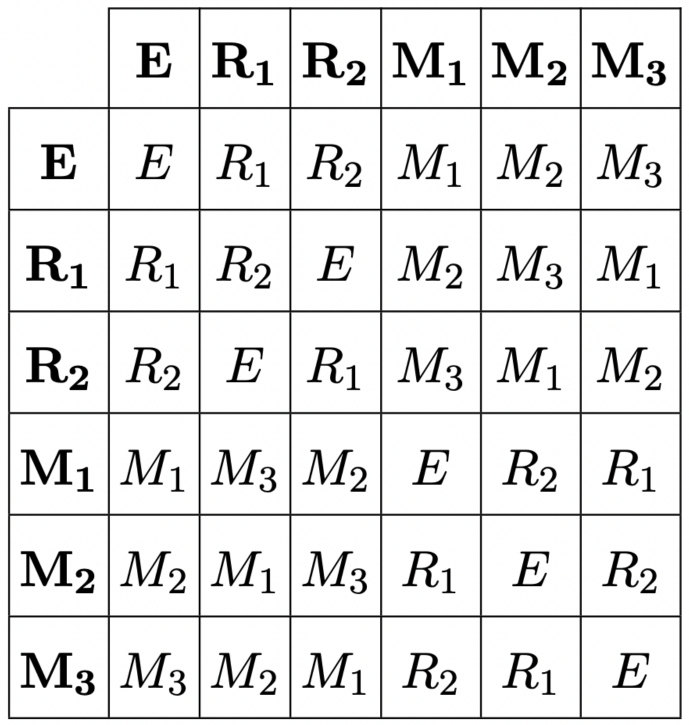
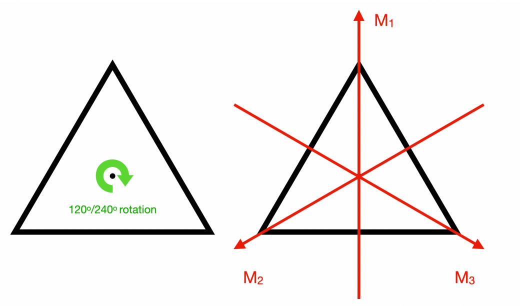
Group of Symmetries of the Equilateral triangle



	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
$\mathbf{E}$	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

Conjugate Elements



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Group of Symmetries of the Equilateral triangle

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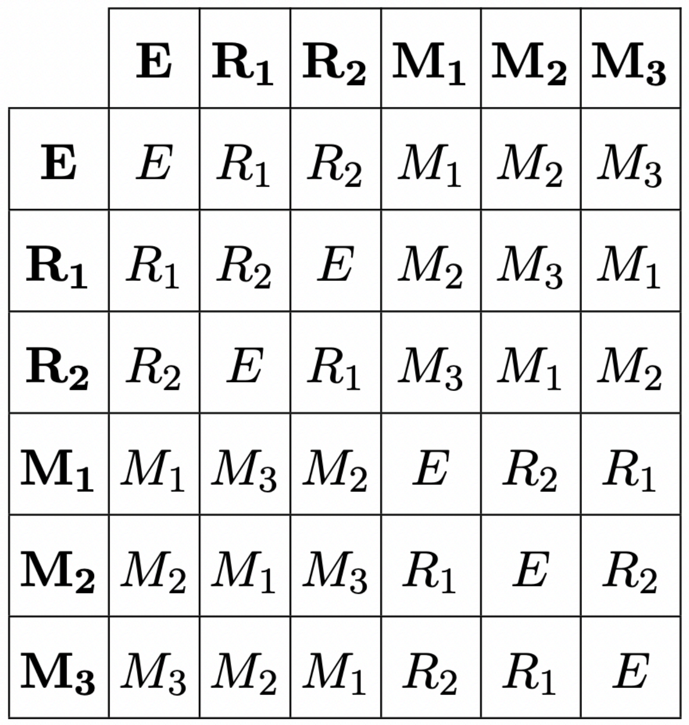
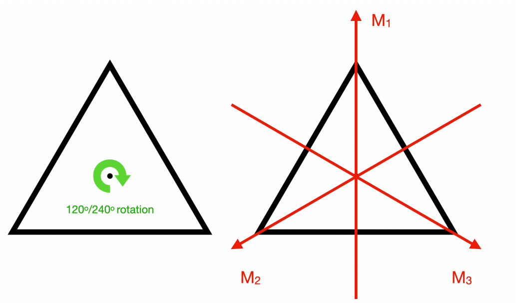
E is not conjugate to any other element



	E	**R₁**	**R₂**	**M₁**	**M₂**	**M₃**
E	E	R_1	R_2	M_1	M_2	M_3
R₁	R_1	R_2	E	M_2	M_3	M_1
R₂	R_2	E	R_1	M_3	M_1	M_2
M₁	M_1	M_3	M_2	E	R_2	R_1
M₂	M_2	M_1	M_3	R_1	E	R_2
M₃	M_3	M_2	M_1	R_2	R_1	E

Conjugate Elements



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Group of Symmetries of the Equilateral triangle

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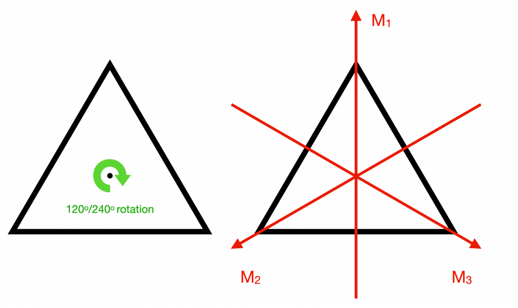
II) Rotations: $M_i.R_1.M_i^{-1} = M_i.R_1M_i = R_2$

Rotations are conjugate to each other

	E	**R₁**	**R₂**	**M₁**	**M₂**	**M₃**
E	E	R_1	R_2	M_1	M_2	M_3
R₁	R_1	R_2	E	M_2	M_3	M_1
R₂	R_2	E	R_1	M_3	M_1	M_2
M₁	M_1	M_3	M_2	E	R_2	R_1
M₂	M_2	M_1	M_3	R_1	E	R_2
M₃	M_3	M_2	M_1	R_2	R_1	E

Conjugate Elements



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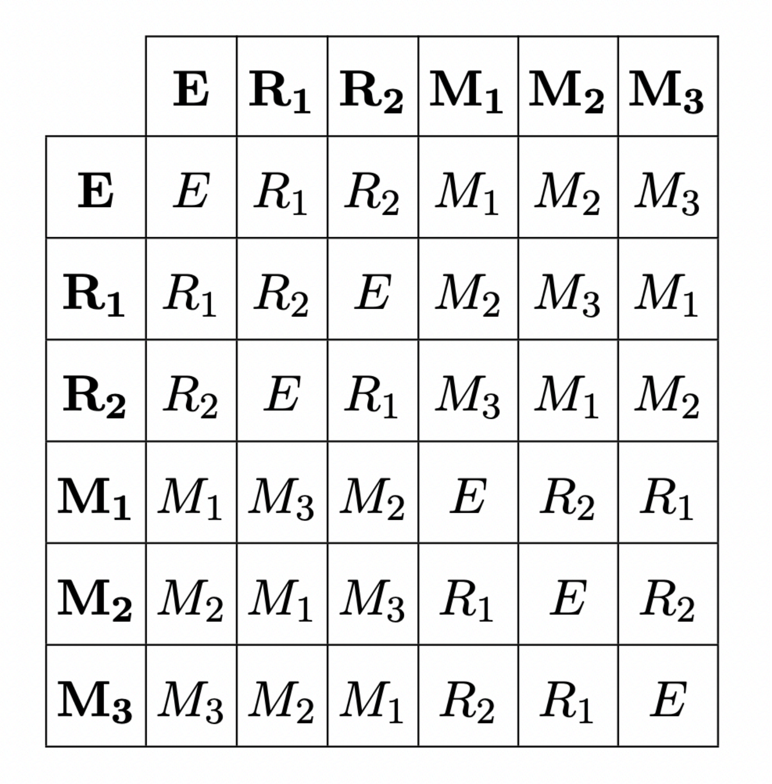
Rotations are conjugate to each other

III) Reflections: $R_1.M_a.R_1^{-1} = R_1.M_a.R_2 = M_b$

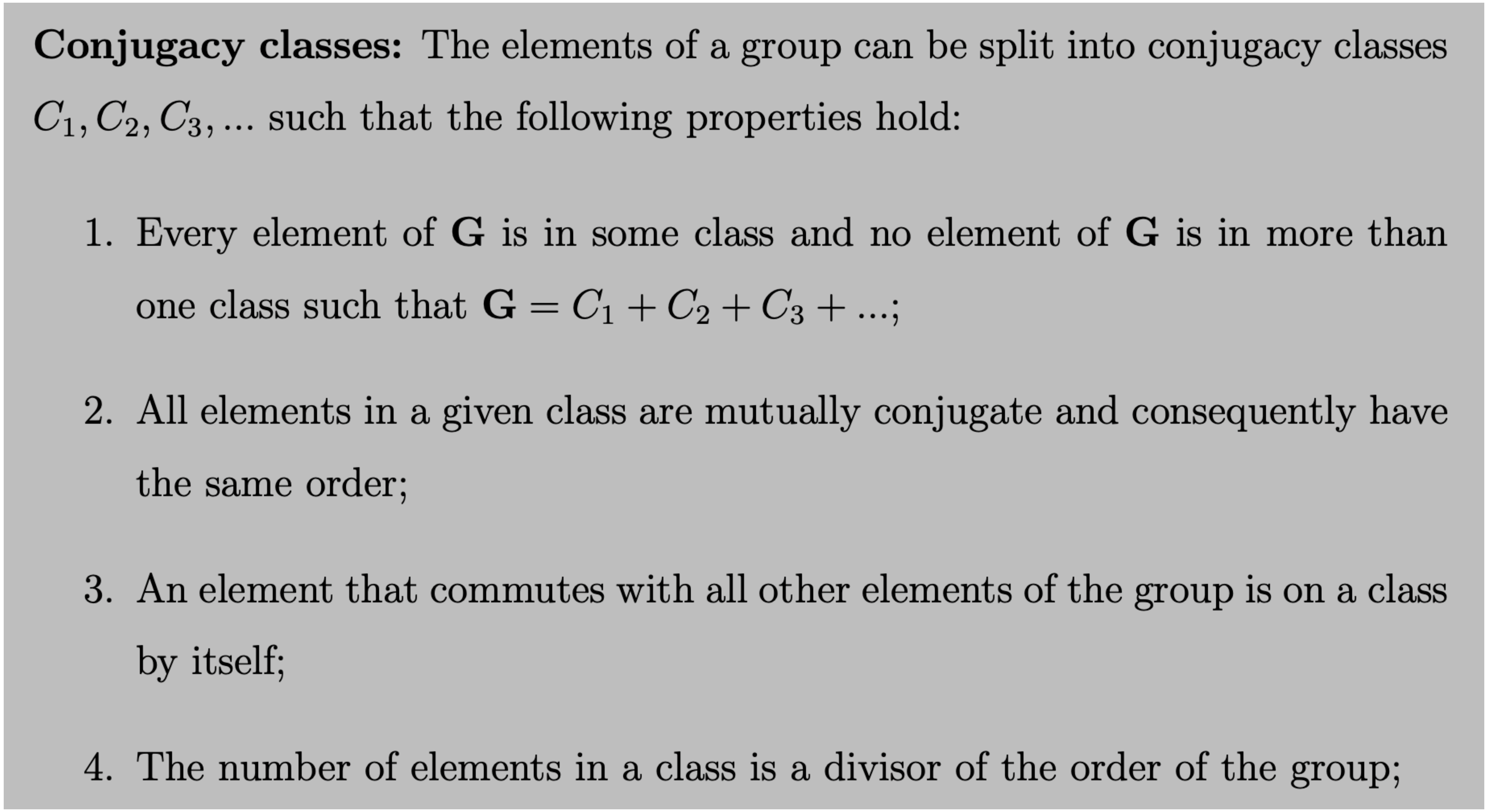
$a = \{1, 2, 3\}$ and $b = \{3, 1, 2\}$

Reflections are conjugate among themselves



	E	**R_1**	**R_2**	**M_1**	**M_2**	**M_3**
E	E	R_1	R_2	M_1	M_2	M_3
R_1	R_1	R_2	E	M_2	M_3	M_1
R_2	R_2	E	R_1	M_3	M_1	M_2
M_1	M_1	M_3	M_2	E	R_2	R_1
M_2	M_2	M_1	M_3	R_1	E	R_2
M_3	M_3	M_2	M_1	R_2	R_1	E

Conjugacy Classes



Conjugacy classes: The elements of a group can be split into conjugacy classes $C_1, C_2, C_3, ...$ such that the following properties hold:

1. Every element of **G** is in some class and no element of **G** is in more than one class such that $\mathbf{G} = C_1 + C_2 + C_3 + ...$;
2. All elements in a given class are mutually conjugate and consequently have the same order;
3. An element that commutes with all other elements of the group is on a class by itself;
4. The number of elements in a class is a divisor of the order of the group;

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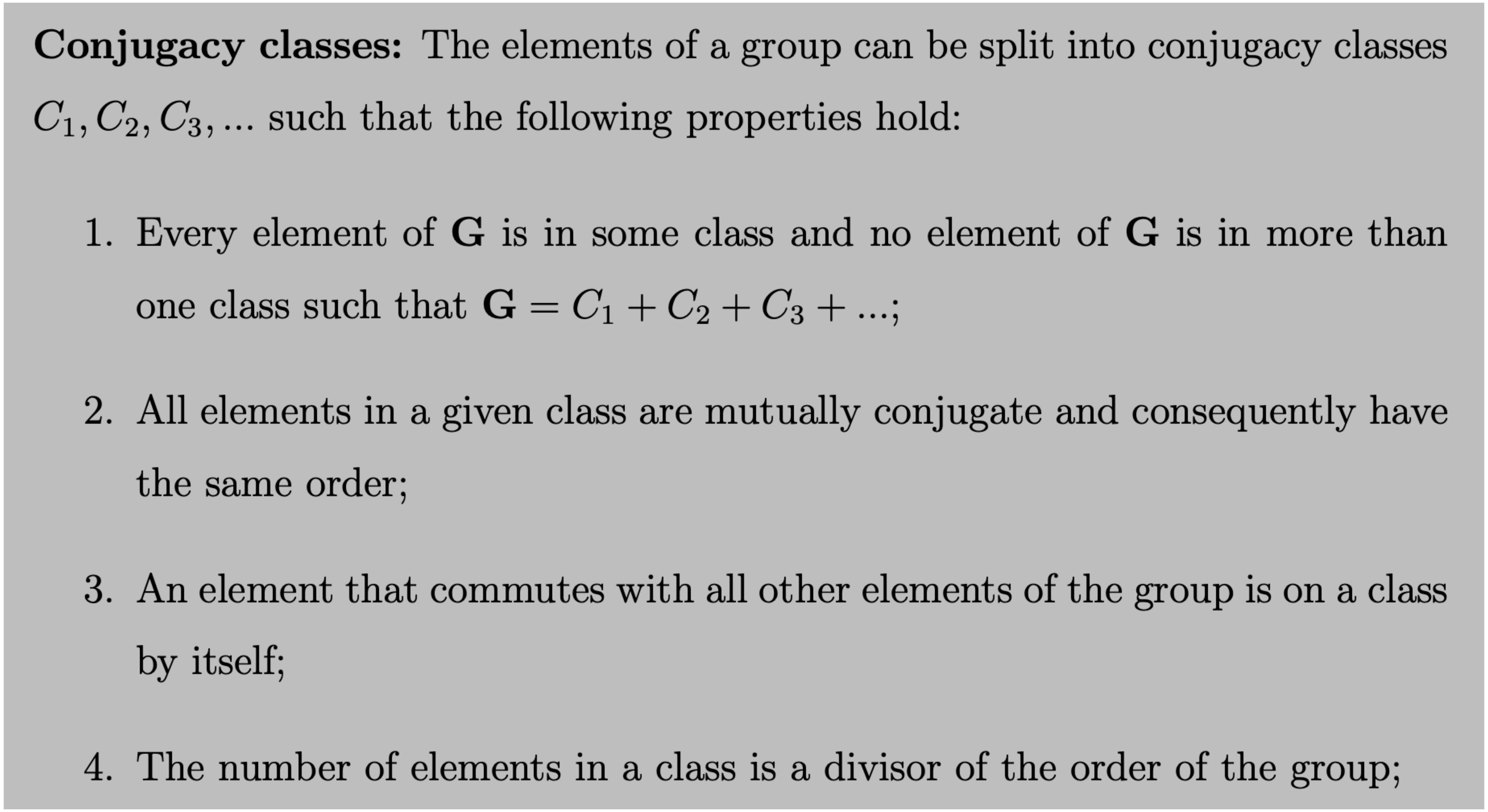

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Order of an element: the number of times the element needs to be applied to be equal to the identity.

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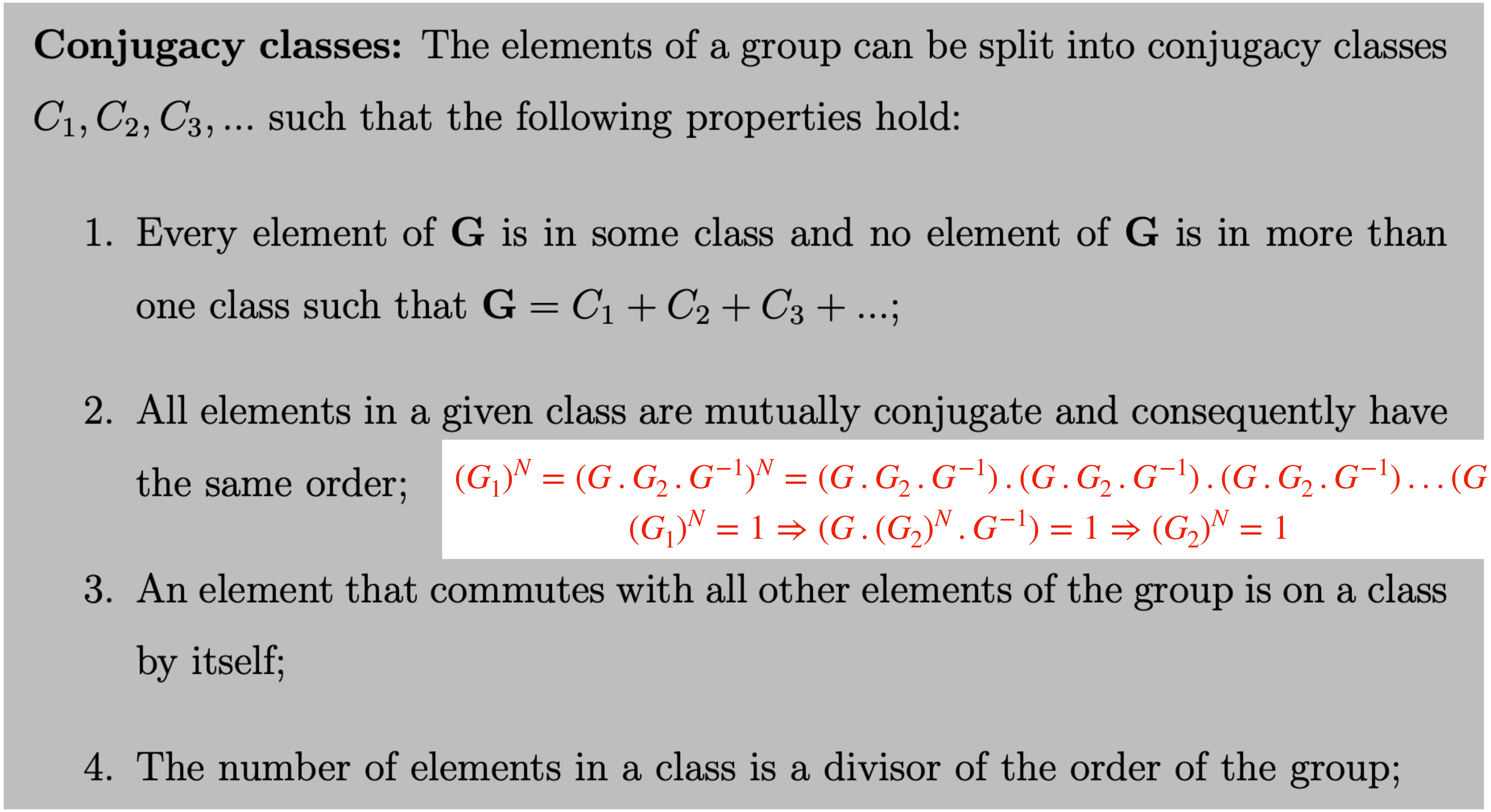

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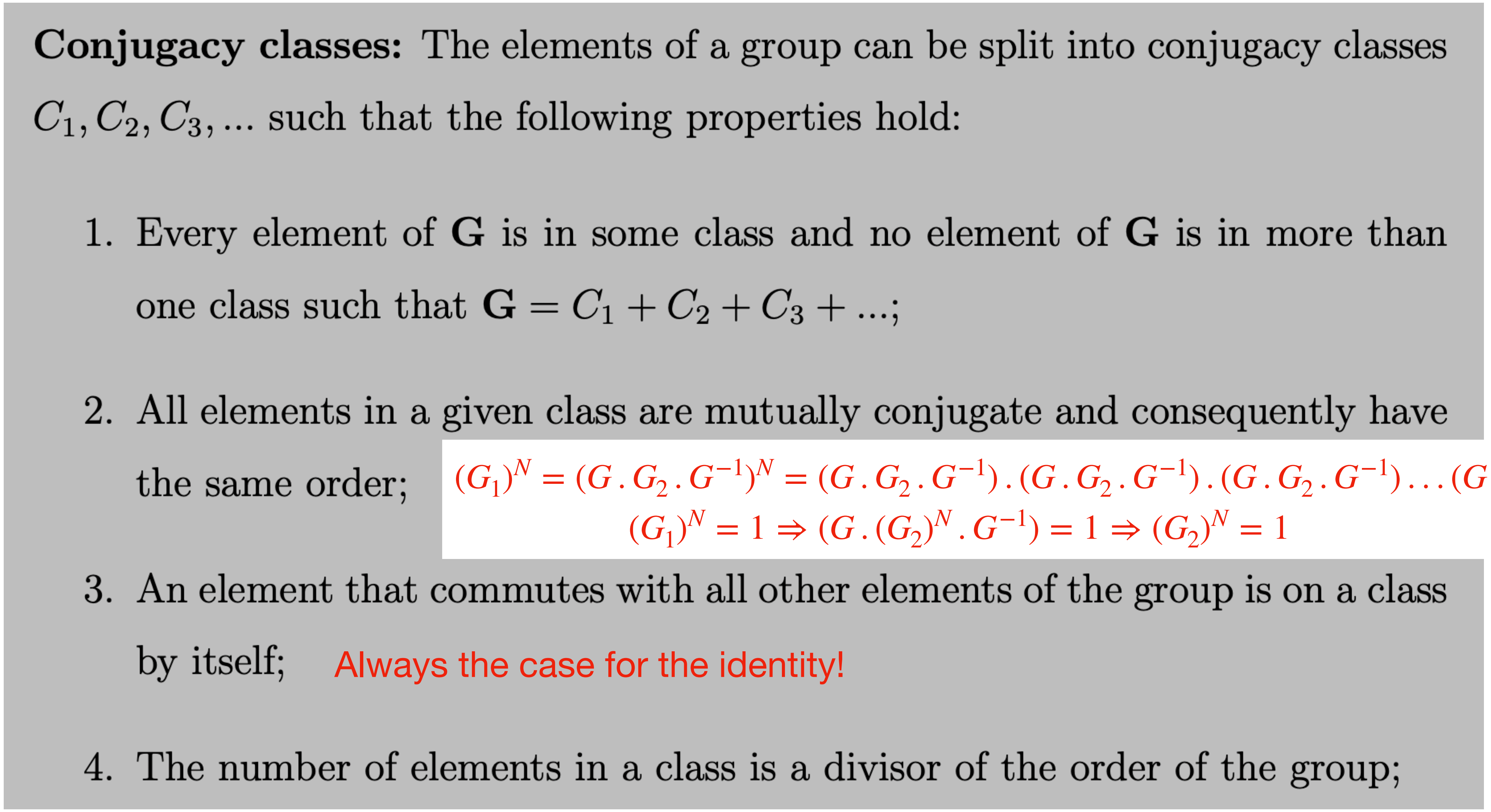

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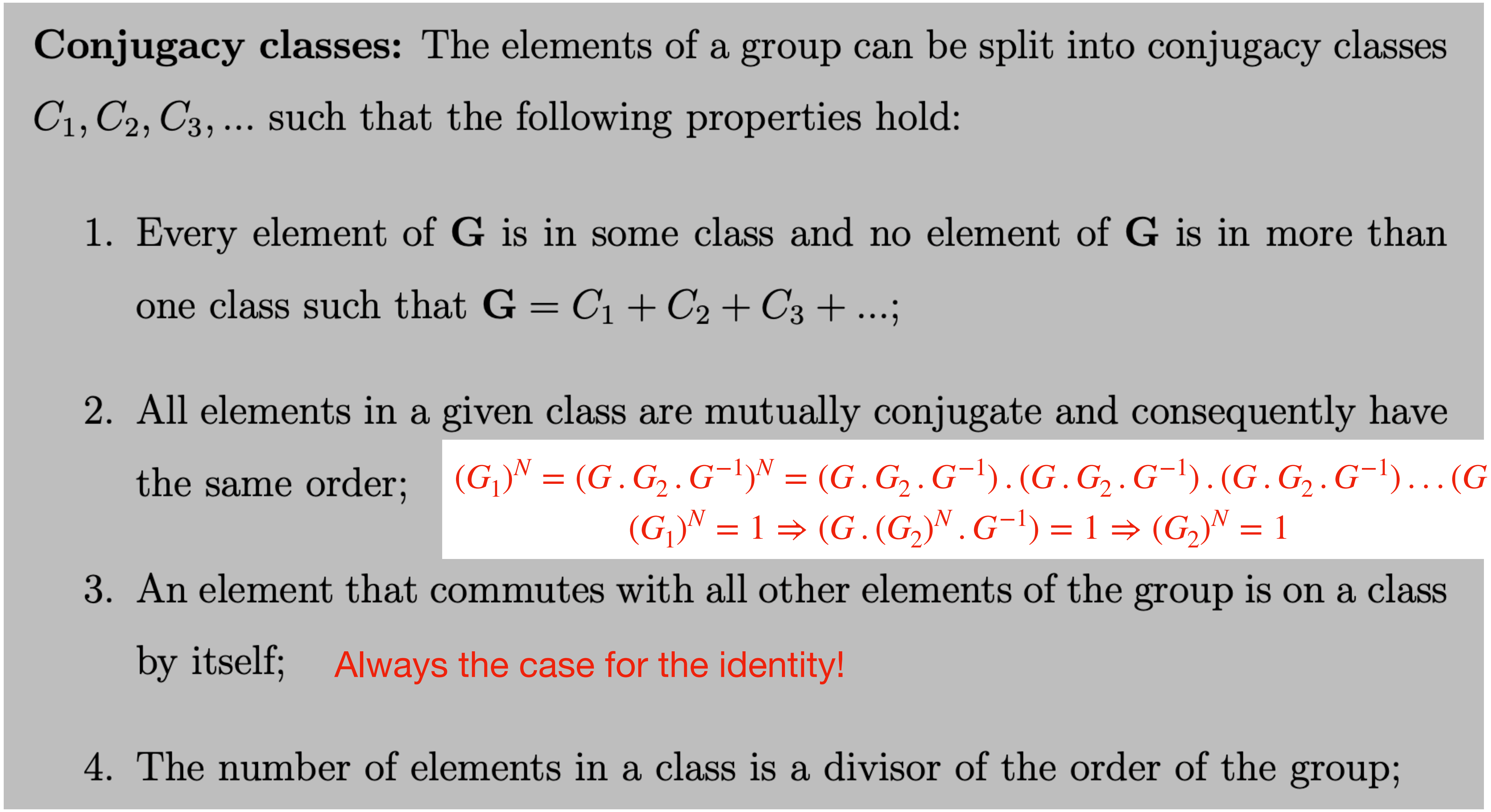

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Always the case for the identity!

$$C_1 = \{E\}$$

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$C_1 = \{E\}$ 1 element/order 1

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✓

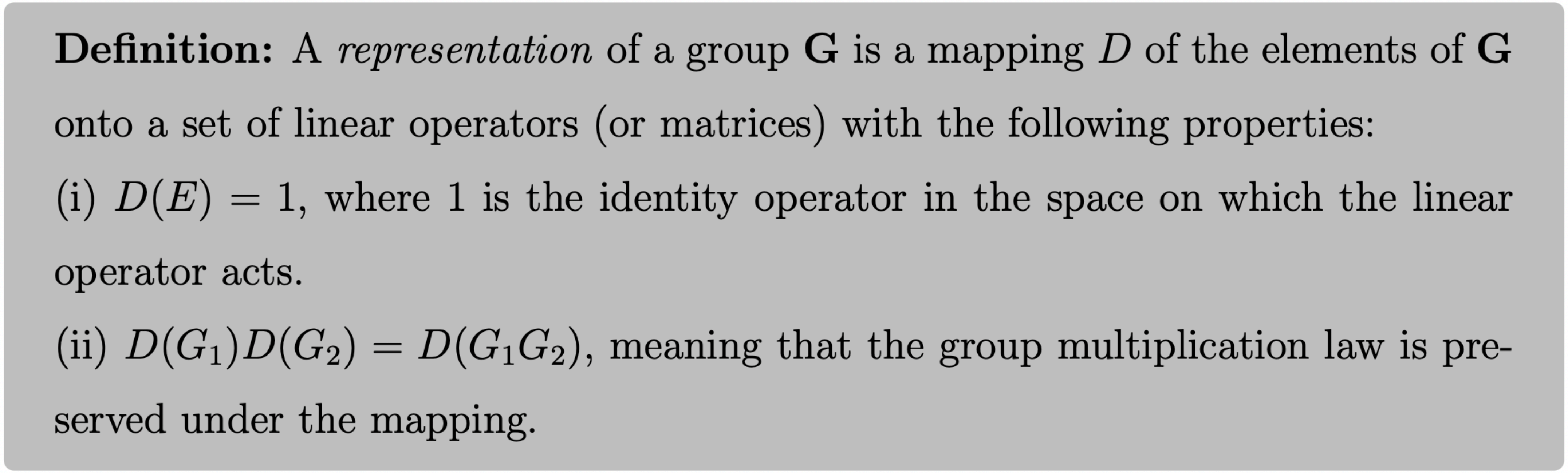
Group Representation

Definition: A *representation* of a group $\mathbf{G}$ is a mapping D of the elements of $\mathbf{G}$ onto a set of linear operators (or matrices) with the following properties:

(i) $D(E) = 1$, where 1 is the identity operator in the space on which the linear operator acts.

(ii) $D(G_1)D(G_2) = D(G_1G_2)$, meaning that the group multiplication law is preserved under the mapping.

Group Representation



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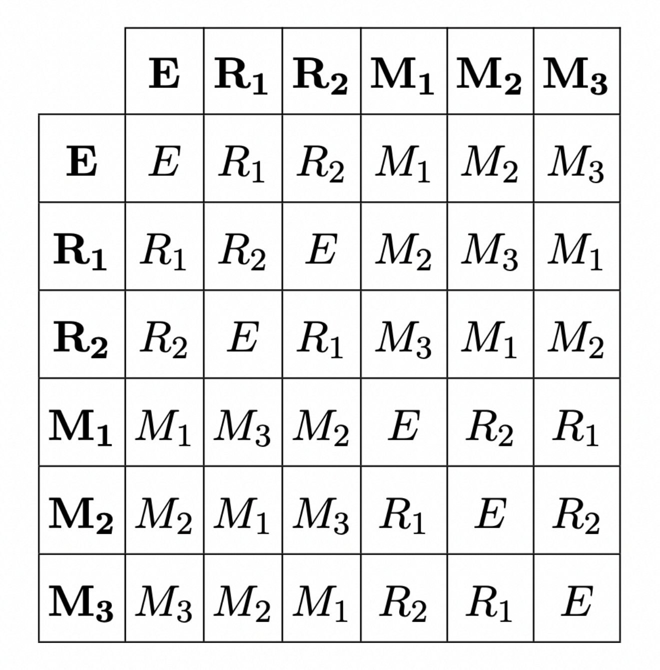

	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
$\mathbf{E}$	E	R_1	R_2	M_1	M_2	M_3
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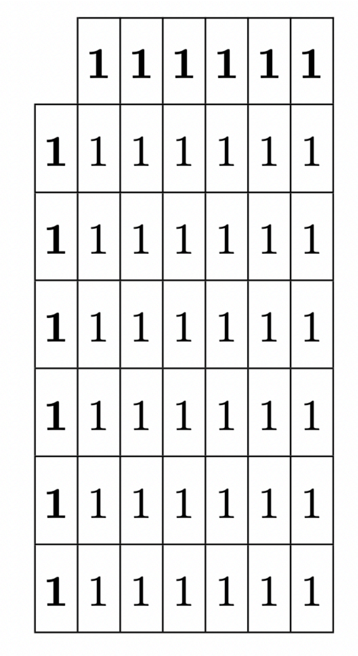
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

→



	1	**1**	**1**	**1**	**1**	**1**
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
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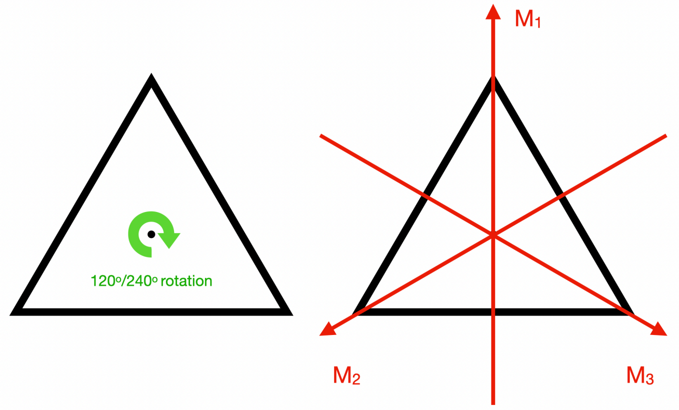
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

	1	**1**	**1**	**1**	**1**	**1**
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1
1	1	1	1	1	1	1

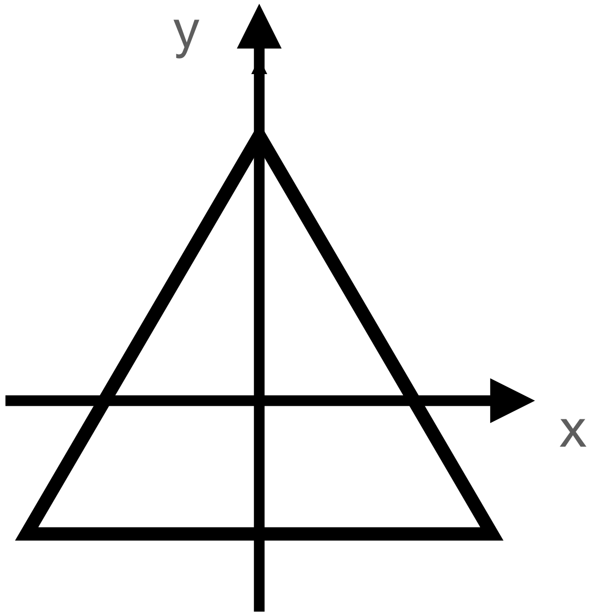
Ok, but what about non-trivial representations?

Group Representation



Group of Symmetries of the Equilateral triangle

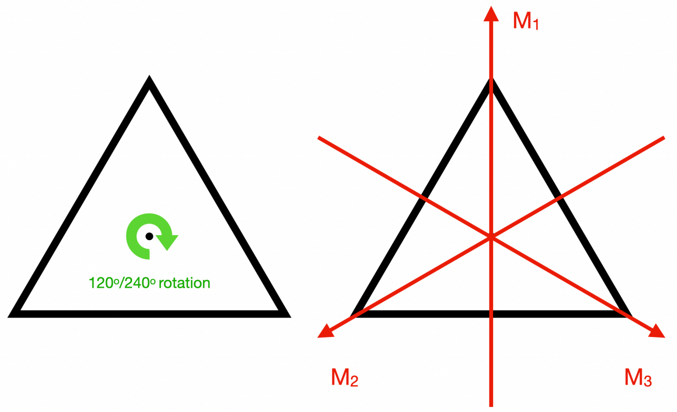
Thinking of transformations acting on the coordinates (x,y,z):



$$R_1 = \begin{pmatrix} -1/2 & +\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$M_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Group Representation



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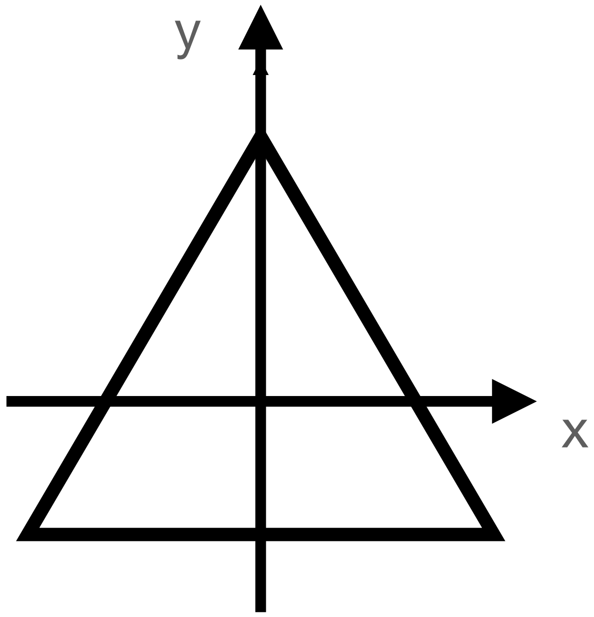

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	E	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
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$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
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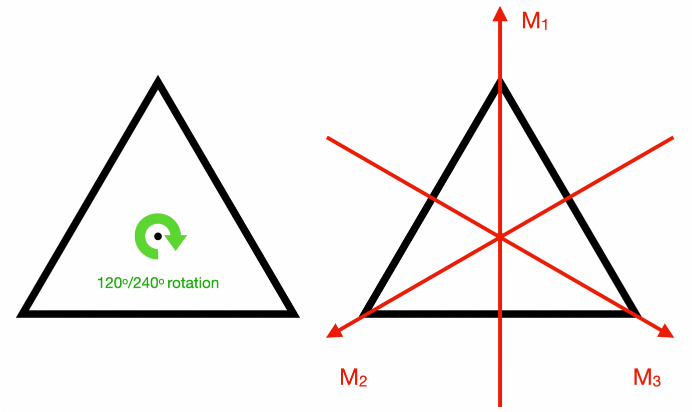
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

You can check if matrices reproduce the structure of the group

Group Representation



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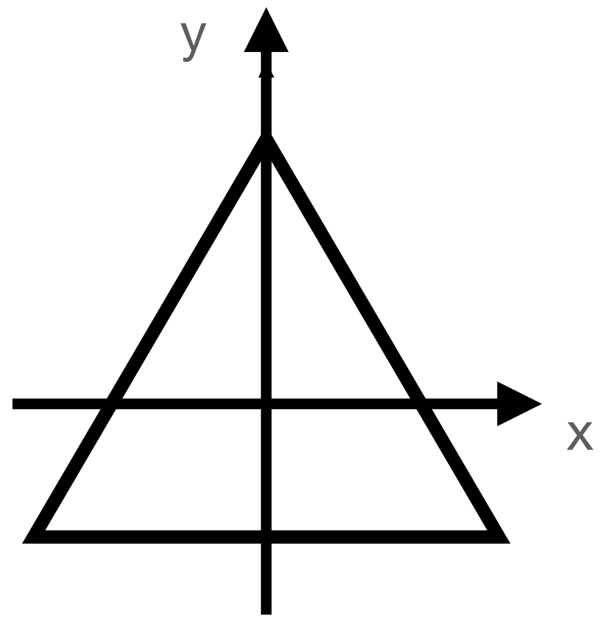

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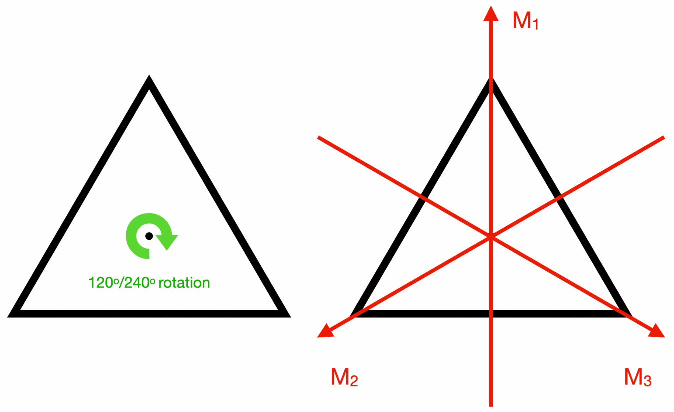
	E	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
E	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

You can check if matrices reproduce the structure of the group

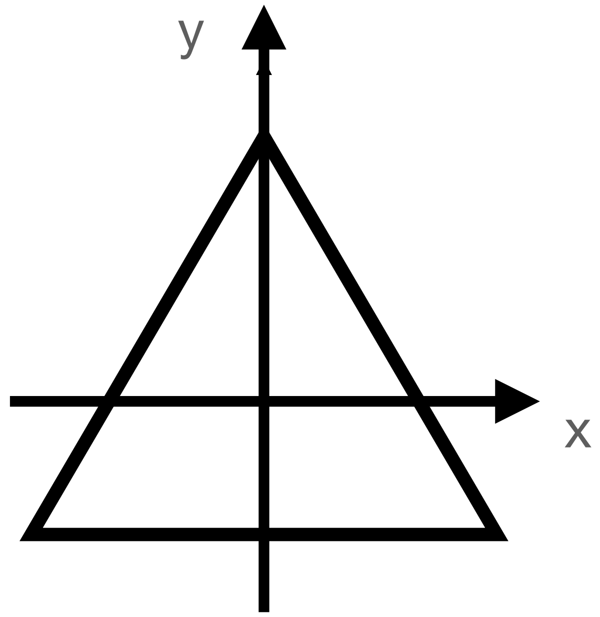
Dimension of the representation: the dimension of the space on which it acts

Group Representation



Group of Symmetries of the Equilateral triangle

Thinking of transformations acting on the coordinates (x,y,z):



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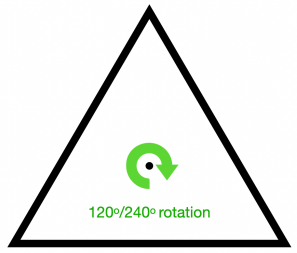
	$\mathbf{E}$	$\mathbf{R_1}$	$\mathbf{R_2}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$
$\mathbf{E}$	E	R_1	R_2	M_1	M_2	M_3
$\mathbf{R_1}$	R_1	R_2	E	M_2	M_3	M_1
$\mathbf{R_2}$	R_2	E	R_1	M_3	M_1	M_2
$\mathbf{M_1}$	M_1	M_3	M_2	E	R_2	R_1
$\mathbf{M_2}$	M_2	M_1	M_3	R_1	E	R_2
$\mathbf{M_3}$	M_3	M_2	M_1	R_2	R_1	E

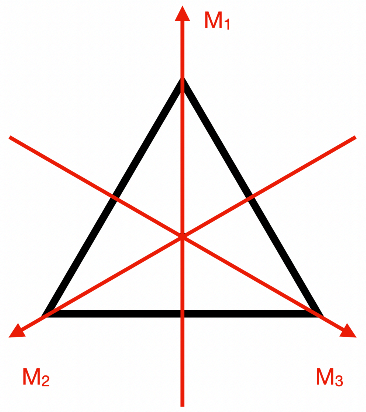
You can check if matrices reproduce the structure of the group

Dimension of the representation: the dimension of the space on which it acts

Generators of the group: the minimal set of operations out of which the entire group can be derived [not unique]

Group Representation





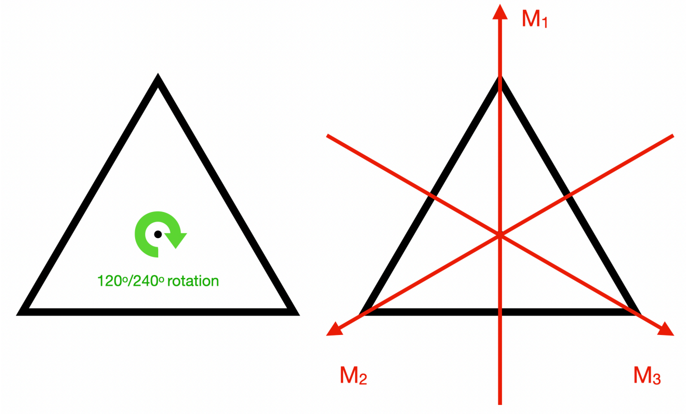
Group of Symmetries of the Equilateral triangle

Thinking of transformations acting on the coordinates (x,y,z):

$$R_1 = \left(\begin{array}{cc|c} -1/2 & +\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \qquad M_1 = \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$$

Note: The z-component never mix with the x- and y-components. This means we can divide the space in {x,y} and {z} and treat them independently. In this case we say the representation is **reducible**.

Group Representation



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Two-dimensional irreducible representation

$$D_1(R_1) = \begin{pmatrix} -1/2 & +\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$D_1(M_1) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

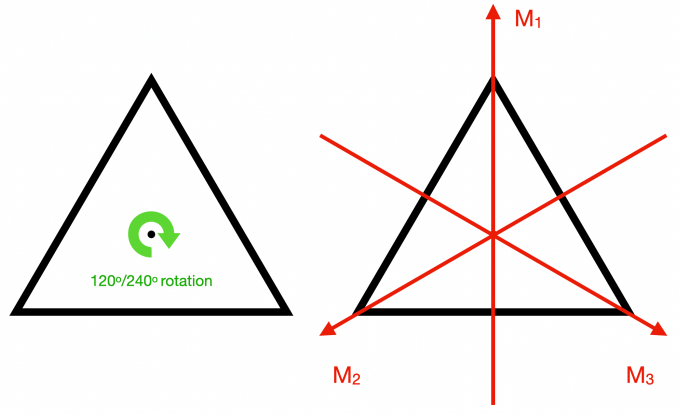
One-dimensional irreducible representation

$$D_2(R_1) = 1$$

$$D_2(M_1) = 1$$

[Trivial representation]

Group Representation



Group of Symmetries of the Equilateral triangle

Two-dimensional irreducible representation

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One-dimensional [trivial] irreducible representation

$$D_2(R_1) = 1$$

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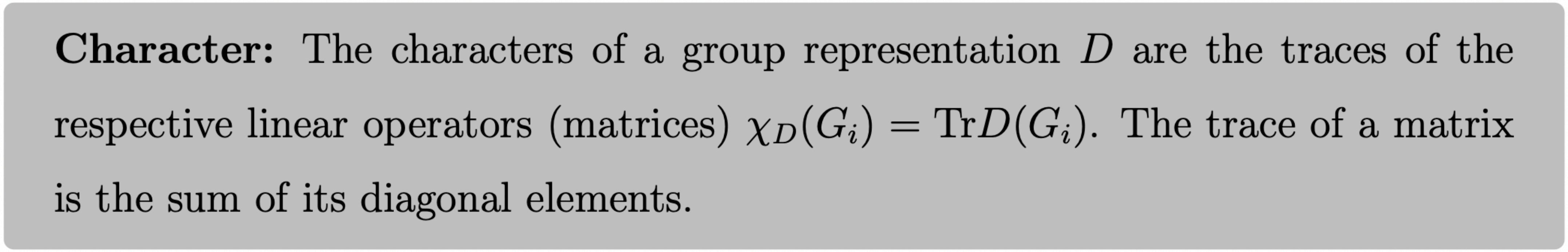
Question: How can we know that we have identified all the representations?

Character

Character: The characters of a group representation D are the traces of the respective linear operators (matrices) $\chi_D(G_i) = \mathrm{Tr} D(G_i)$. The trace of a matrix is the sum of its diagonal elements.

Character



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Conjugate elements have the same character: $G.G_1.G^{-1} = G_2$

$$\chi(G_2) = \chi(G.G_1.G^{-1}) = \chi(G^{-1}.G.G_1) = \chi(G_1)$$

[cyclic property of the trace]

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[cyclic property of the trace]

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Trivial irrep	1	1	1
Non-trivial irrep	2	-1	0

$$D_1(R_1) = \begin{pmatrix} -1/2 & +\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$$

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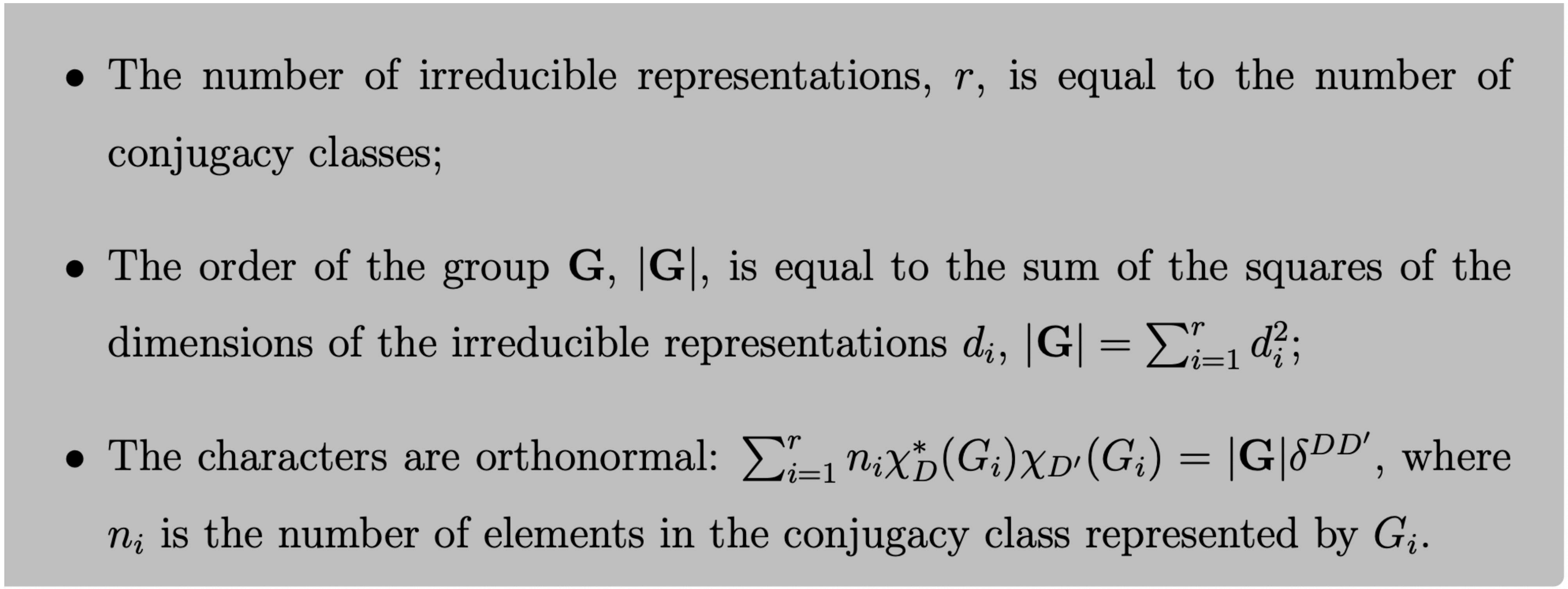
Question: Have identified all the representations?

Character Table and Irreducible Representations

The characters and representations are connected by the following properties:



- The number of irreducible representations, r, is equal to the number of conjugacy classes;
- The order of the group $\mathbf{G}$, $|\mathbf{G}|$, is equal to the sum of the squares of the dimensions of the irreducible representations d_i, $|\mathbf{G}| = \sum_{i=1}^{r} d_i^2$;
- The characters are orthonormal: $\sum_{i=1}^{r} n_i \chi_D^*(G_i)\chi_{D'}(G_i) = |\mathbf{G}|\delta^{DD'}$, where n_i is the number of elements in the conjugacy class represented by G_i.

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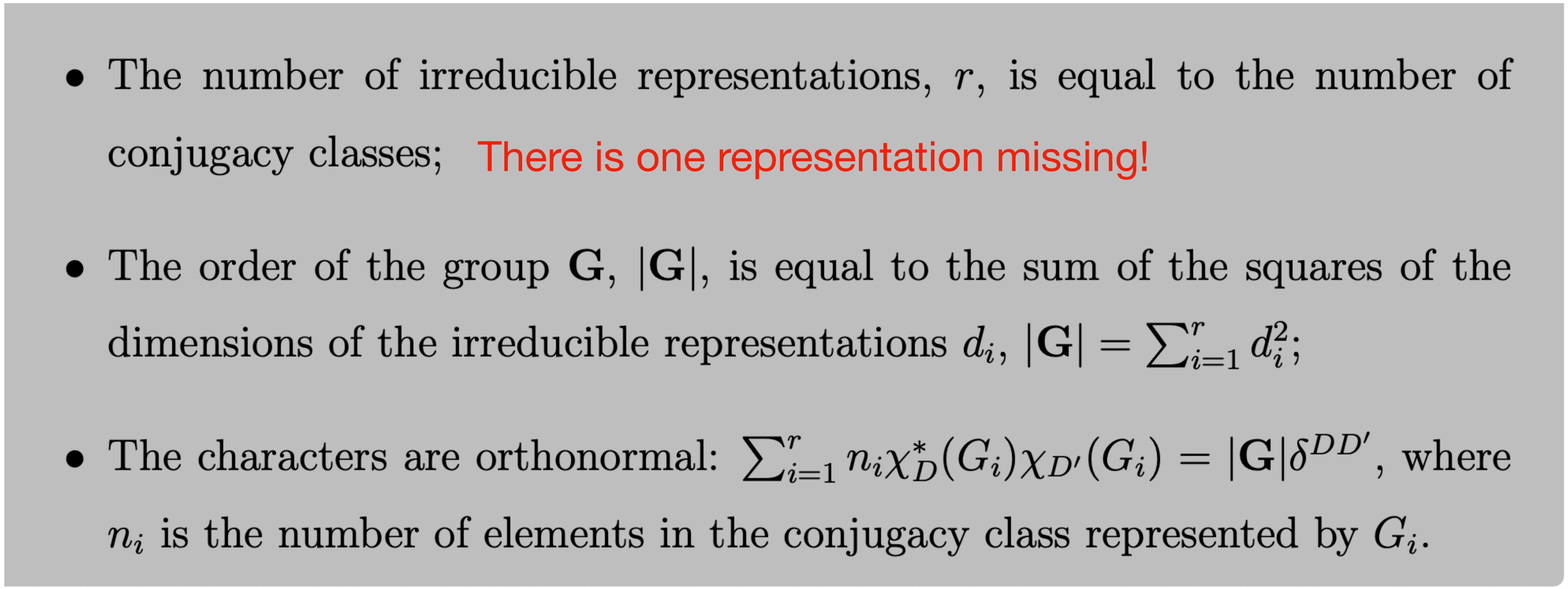

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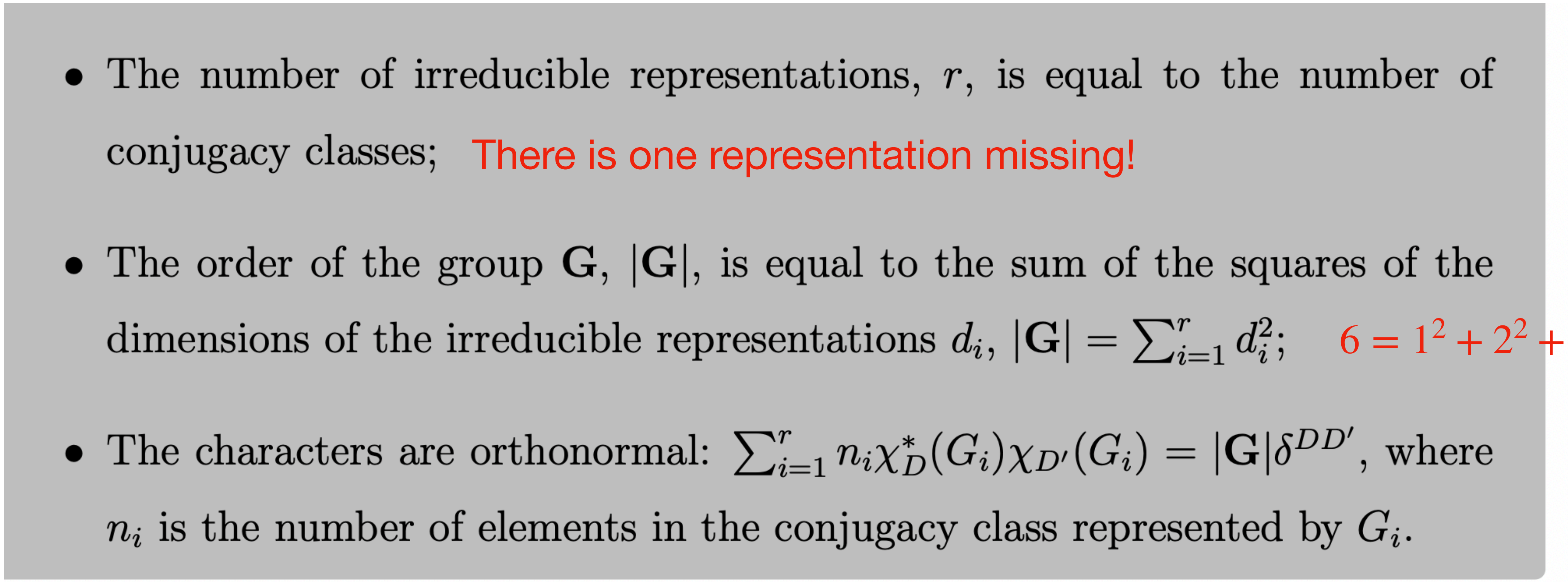

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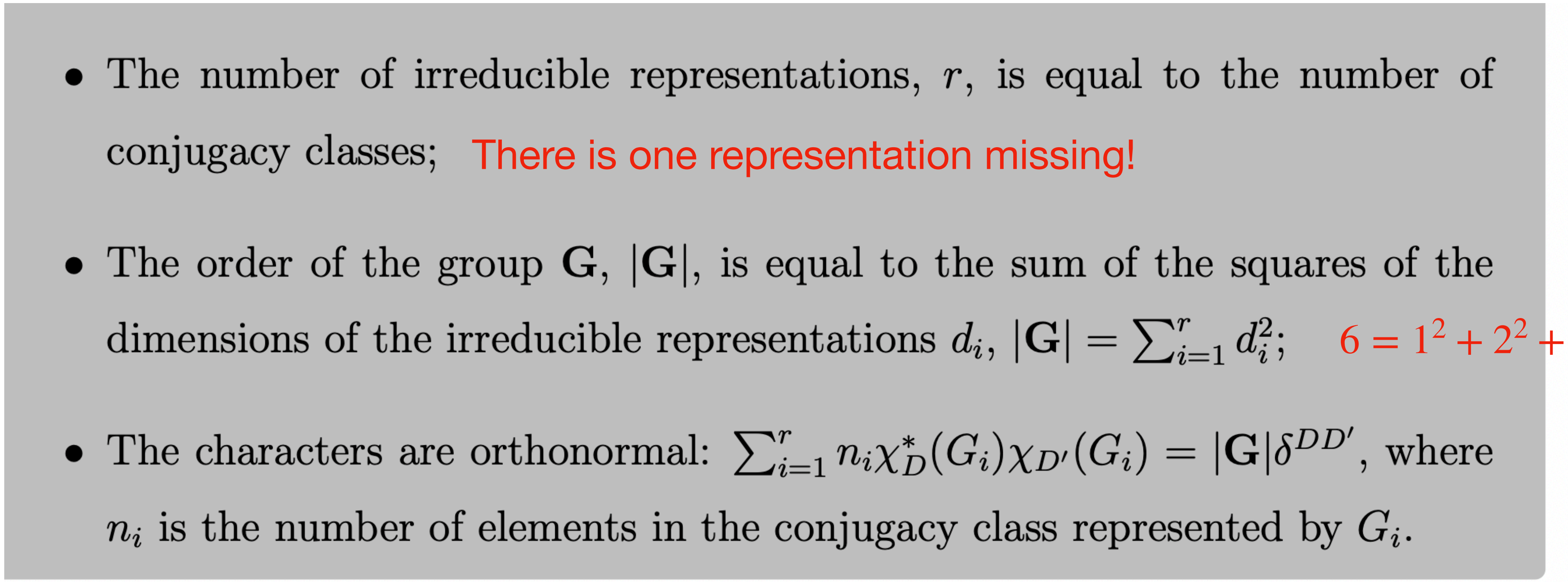

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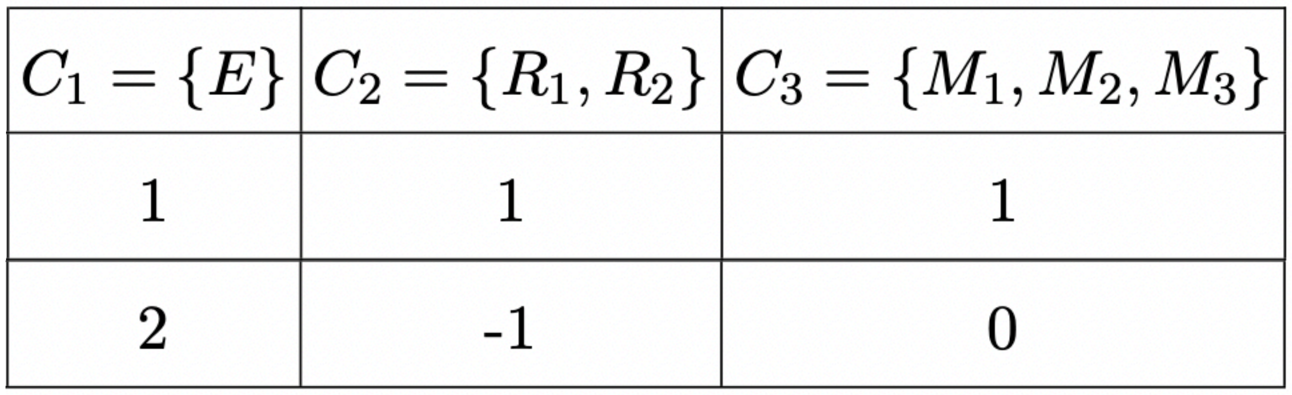

	$C_1 = \{E\}$	$C_2 = \{R_1, R_2\}$	$C_3 = \{M_1, M_2, M_3\}$
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Non-trivial irrep	2	-1	0

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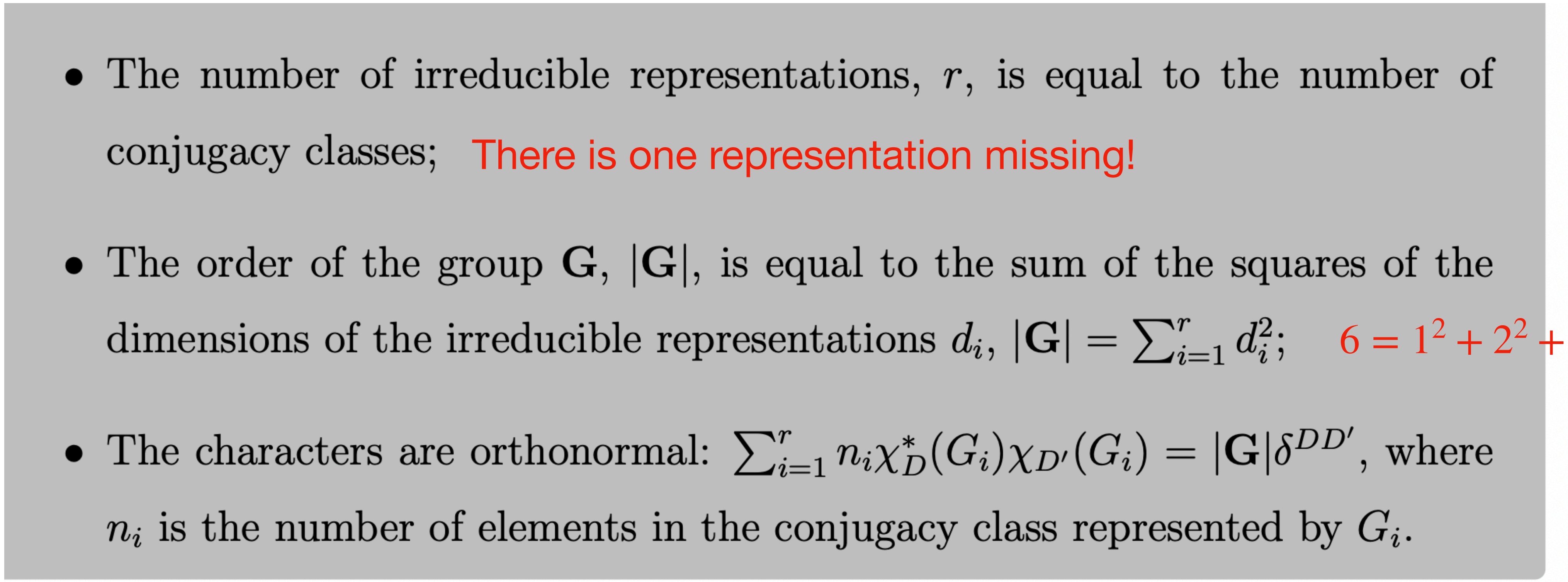

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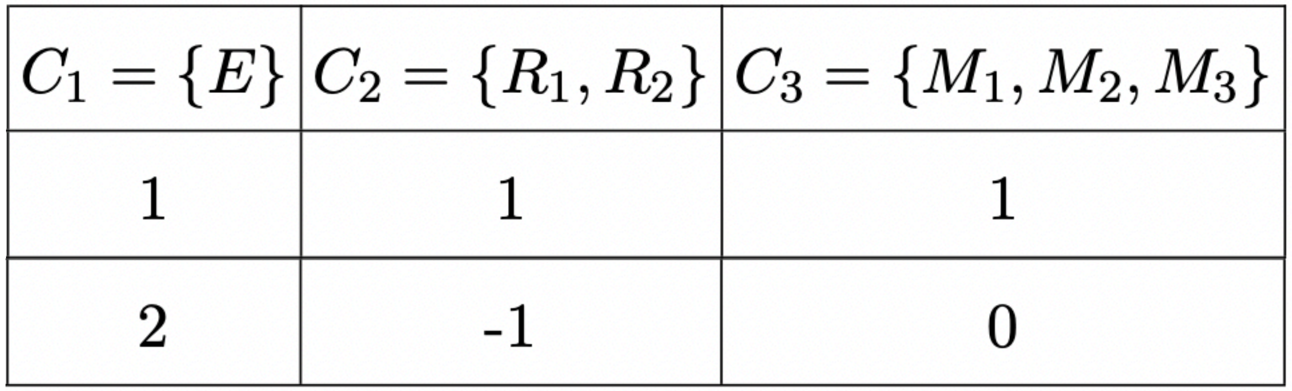

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	1		

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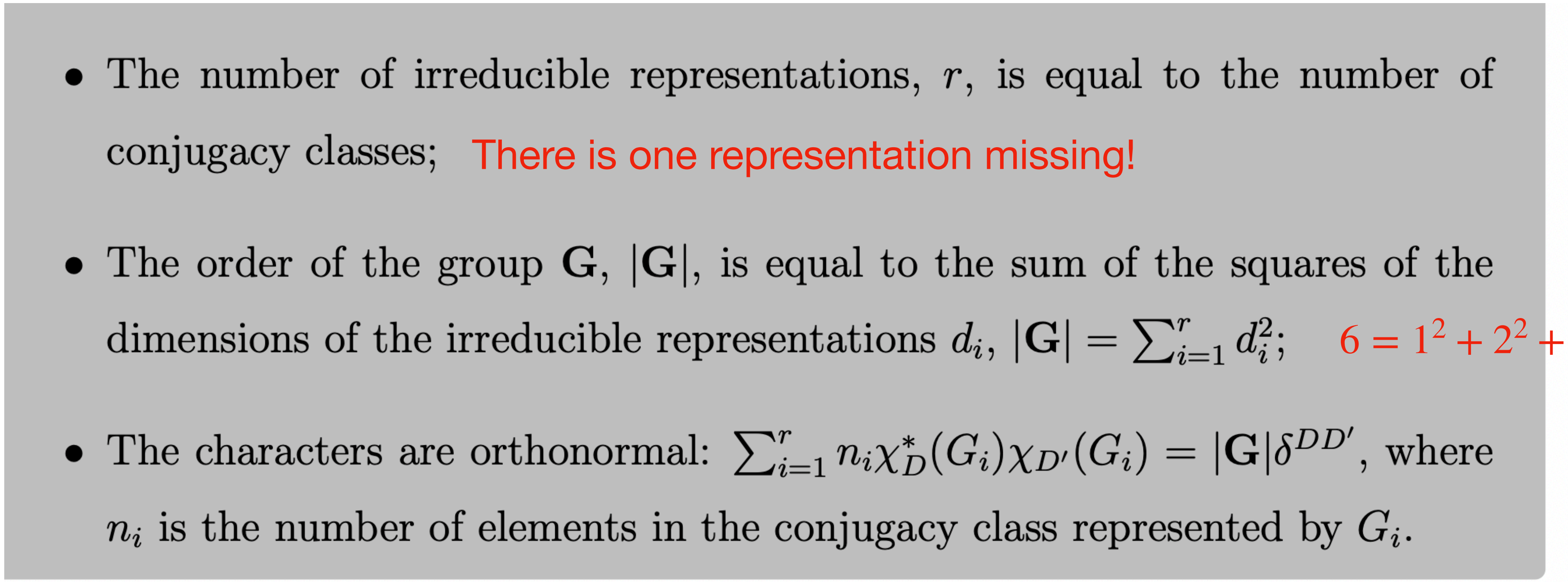

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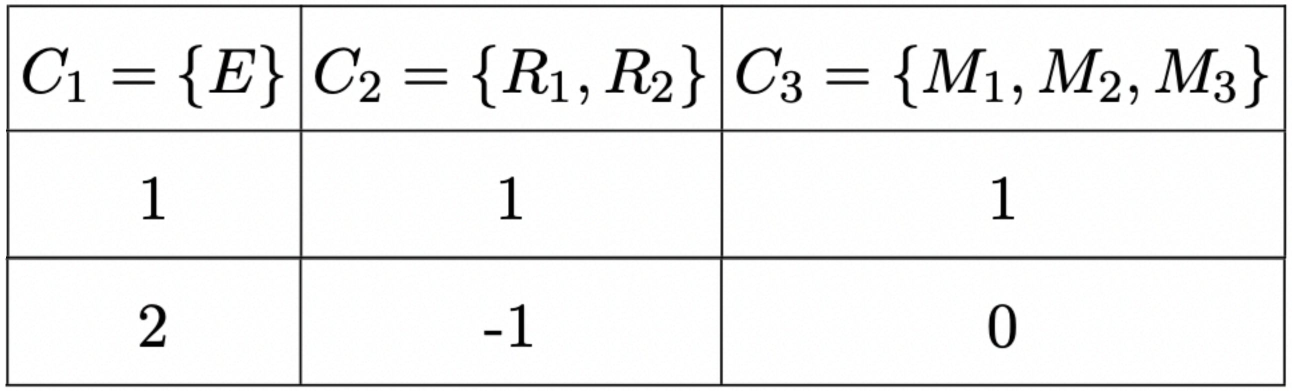

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	1	A	B

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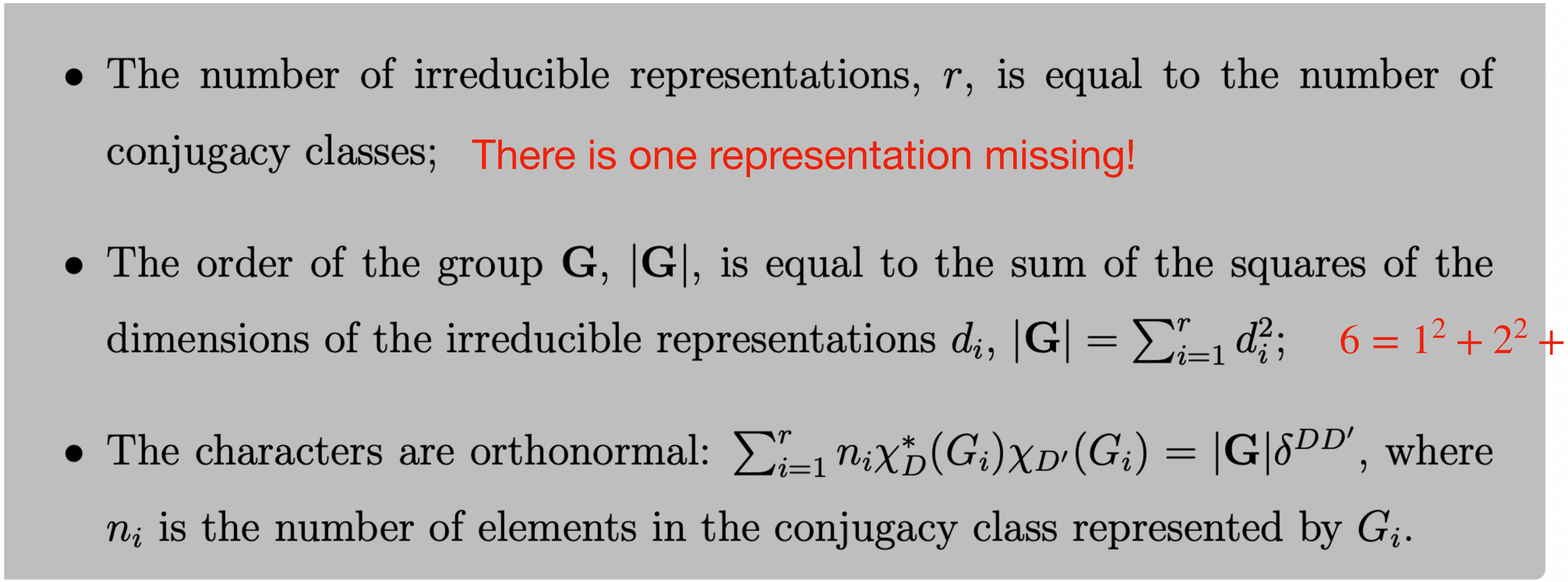

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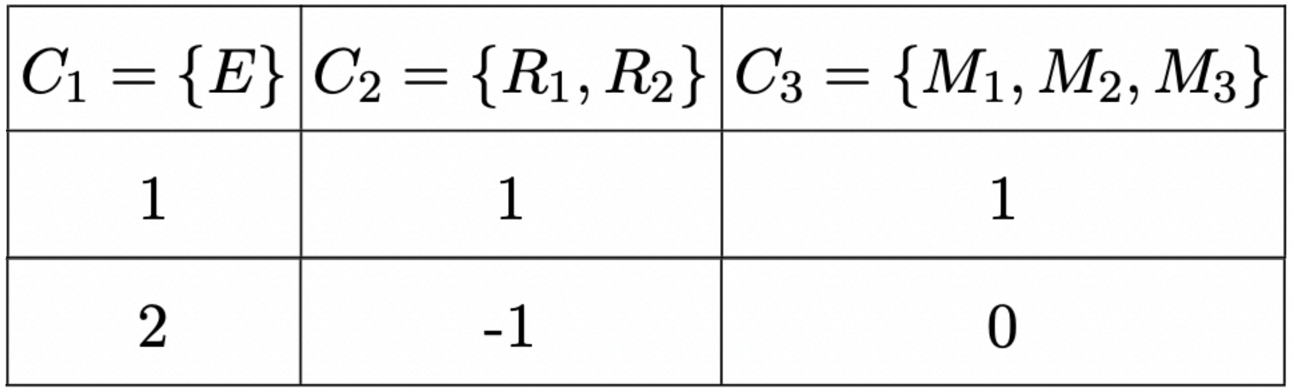

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$$(1).1.1 + (2)1.A + (3).1.B = 0$$
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Character Table and Irreducible Representations

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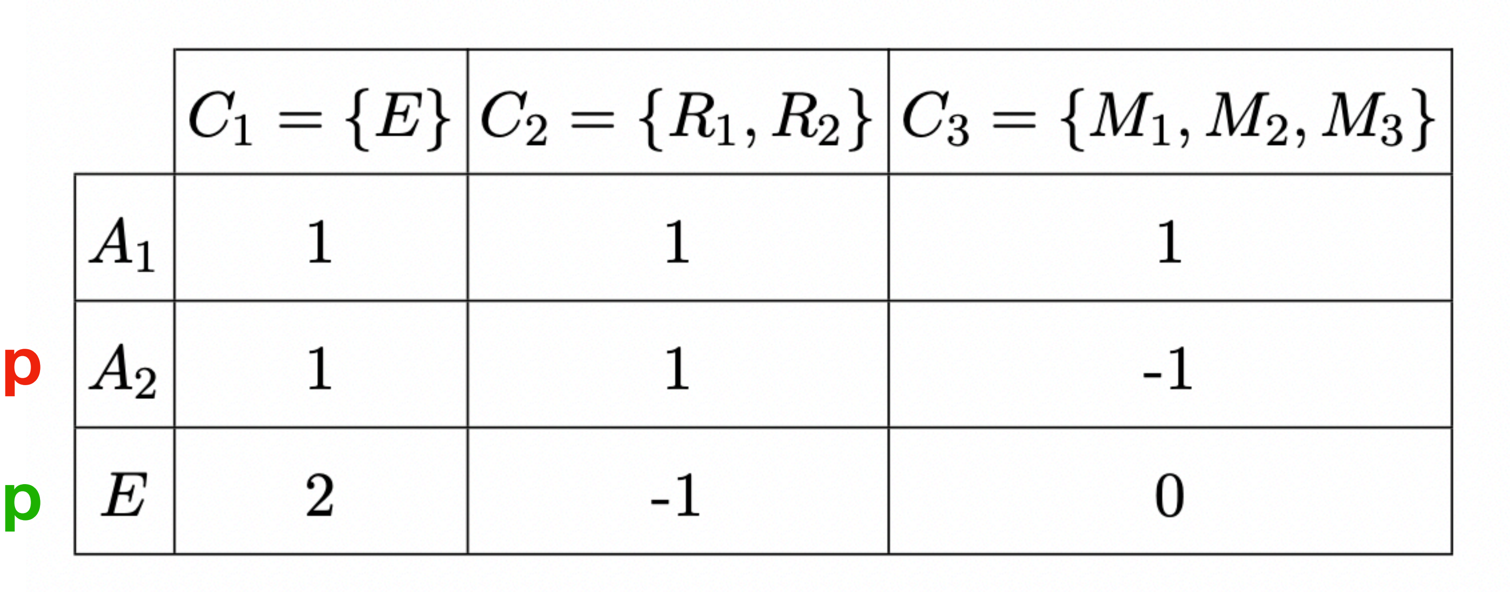
Character Table and Irreducible Representations

Trivial irrep

Non-trivial irrep

Non-trivial irrep



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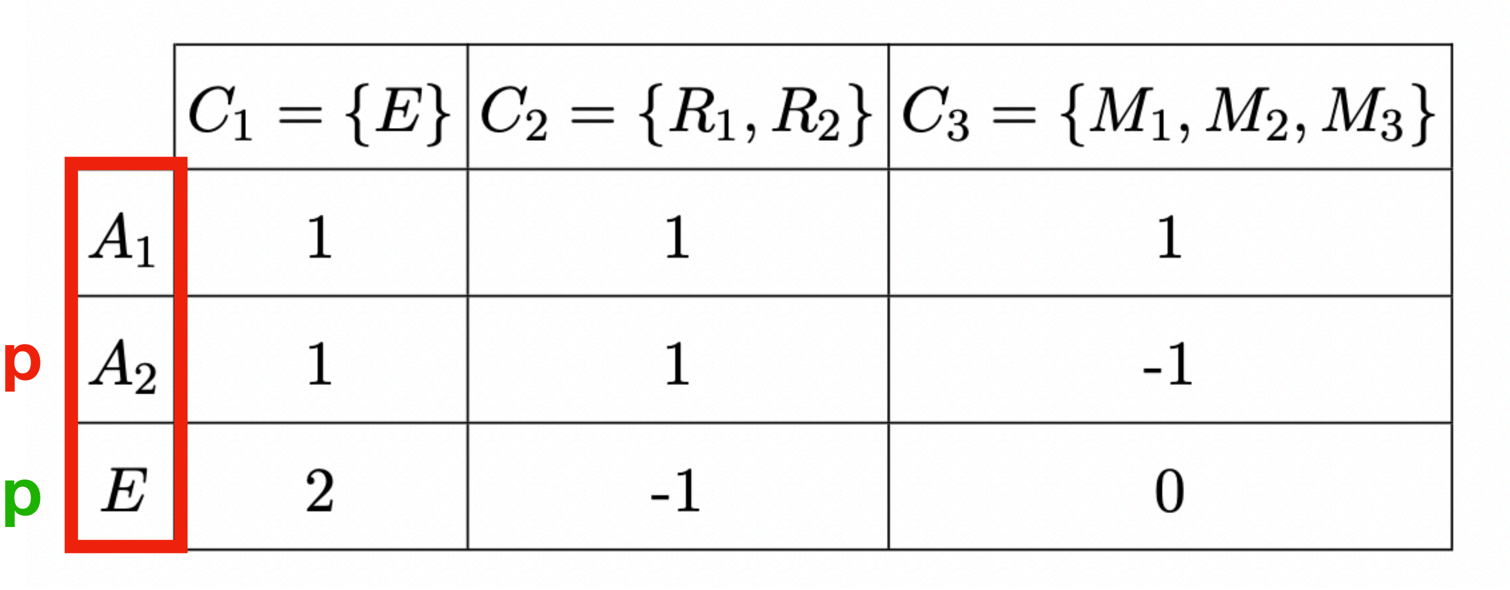
Character Table and Irreducible Representations



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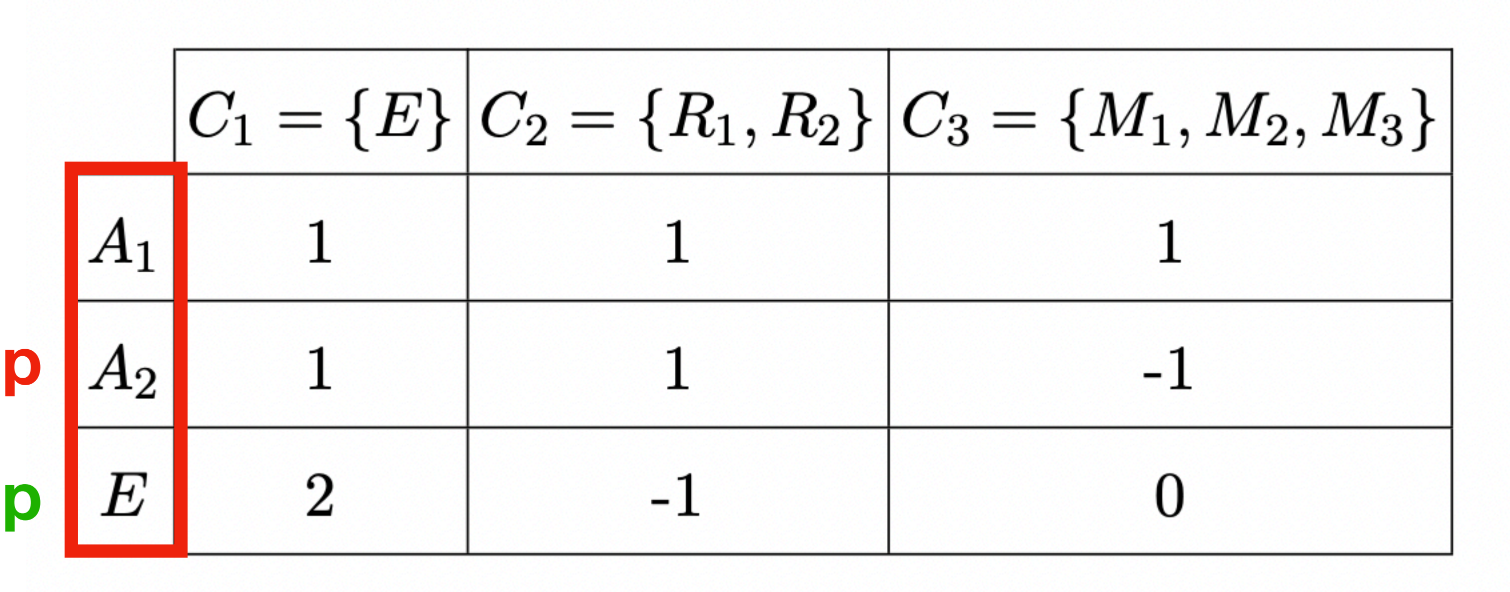
Character Table and Irreducible Representations



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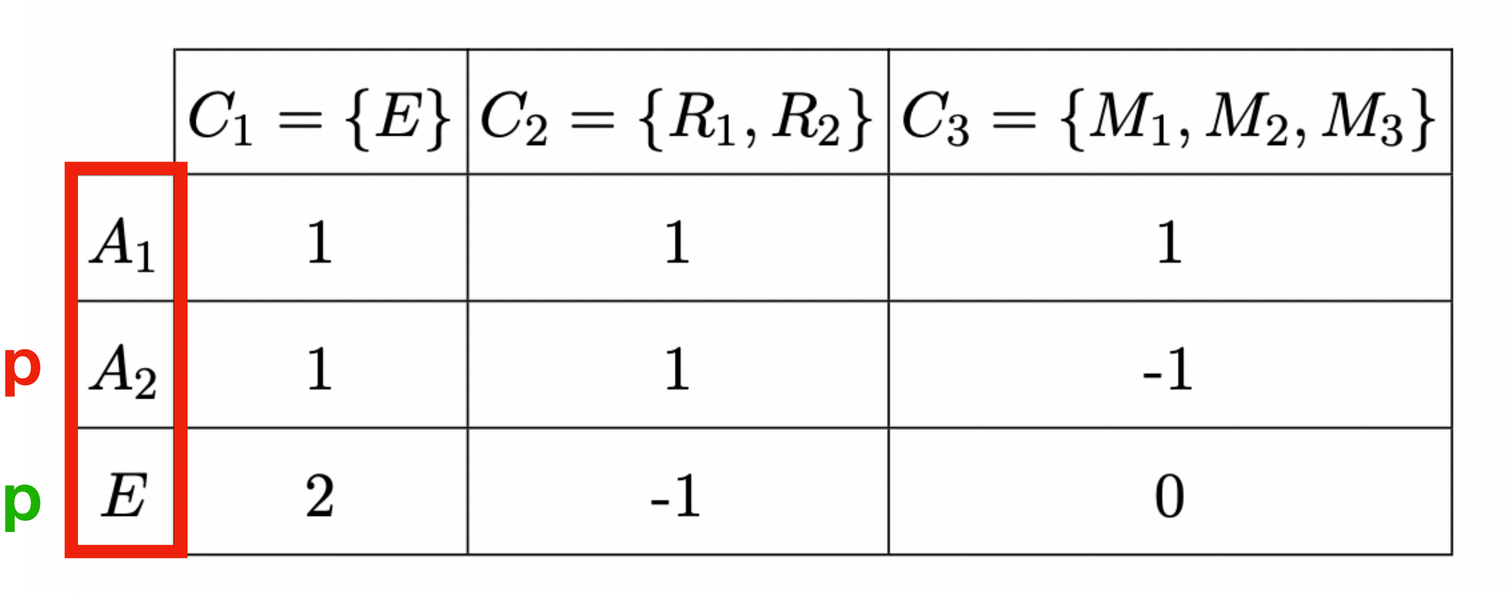
Note that these properties can in principle be derived directly from the group structure, without thinking about any geometric realisation of the transformations!

Character Table and Irreducible Representations



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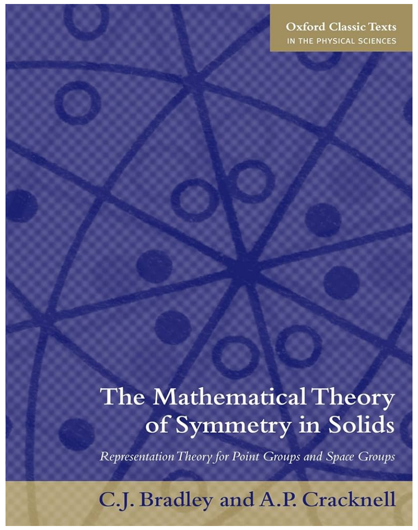


These are can be found in

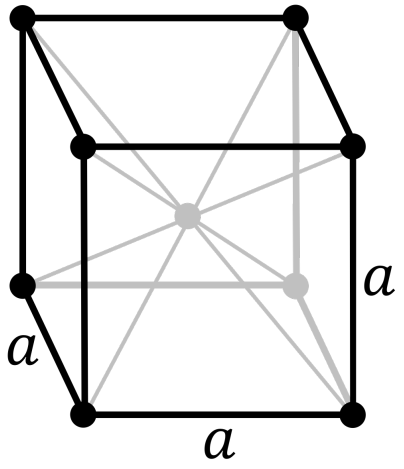
- Bradley and Cracknell
- Bilbao crystallographic server
- …

bilbao crystallographic server

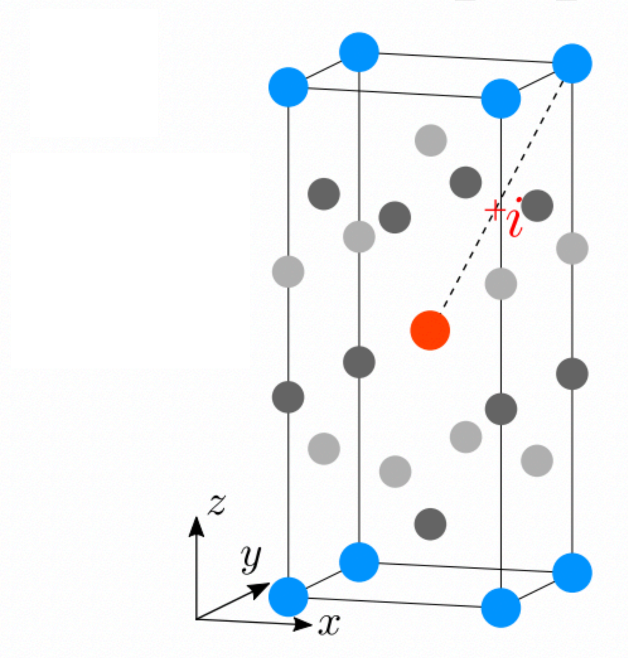
Crystallographic Groups

SC and other ordered phases emerge in…

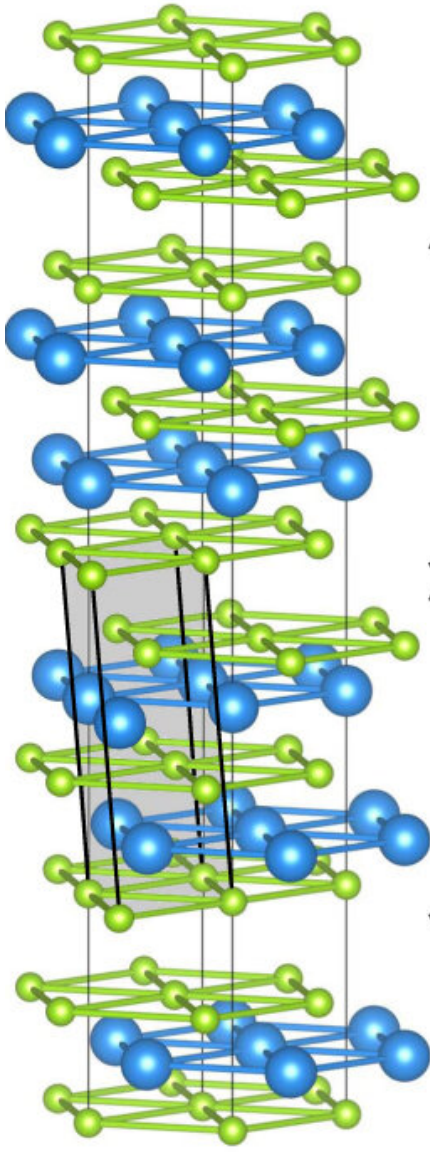
[Im-3m]
Elemental Niobium



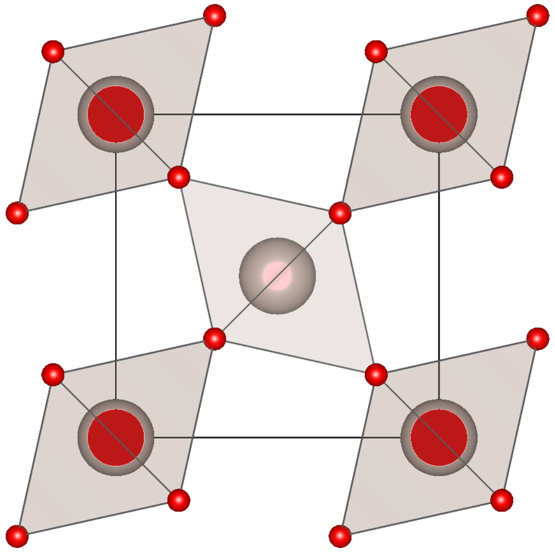
[P4/nmm]
$CeRh_2As_2$



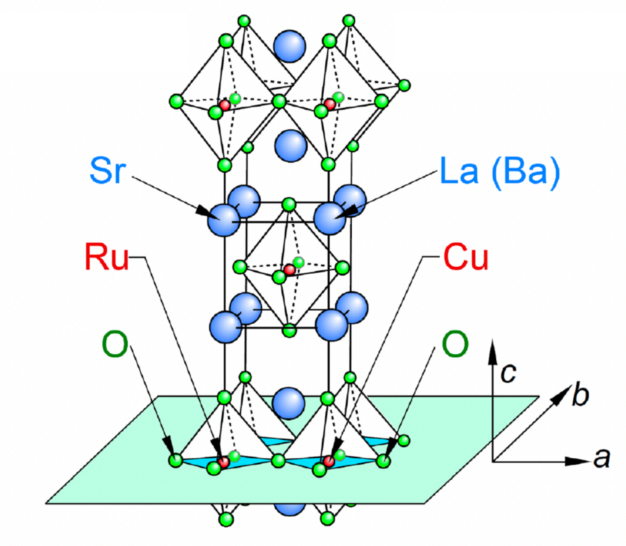
[R-3m]
Bi_2Se_3



[$P4_2$/mnm]
RuO_2

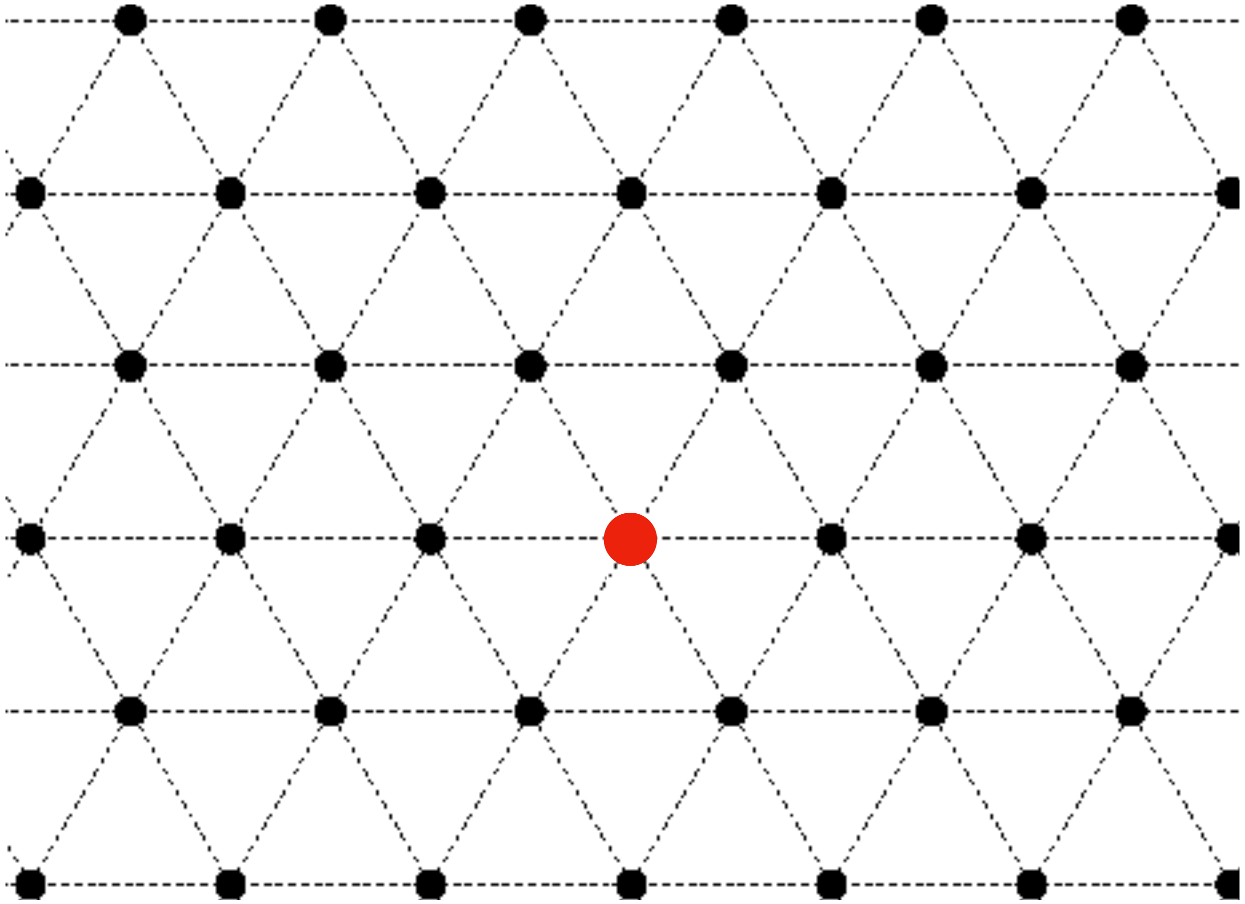


[I4/mmm]
Sr_2RuO_4



…and many others…

From the triangle to the triangular lattice



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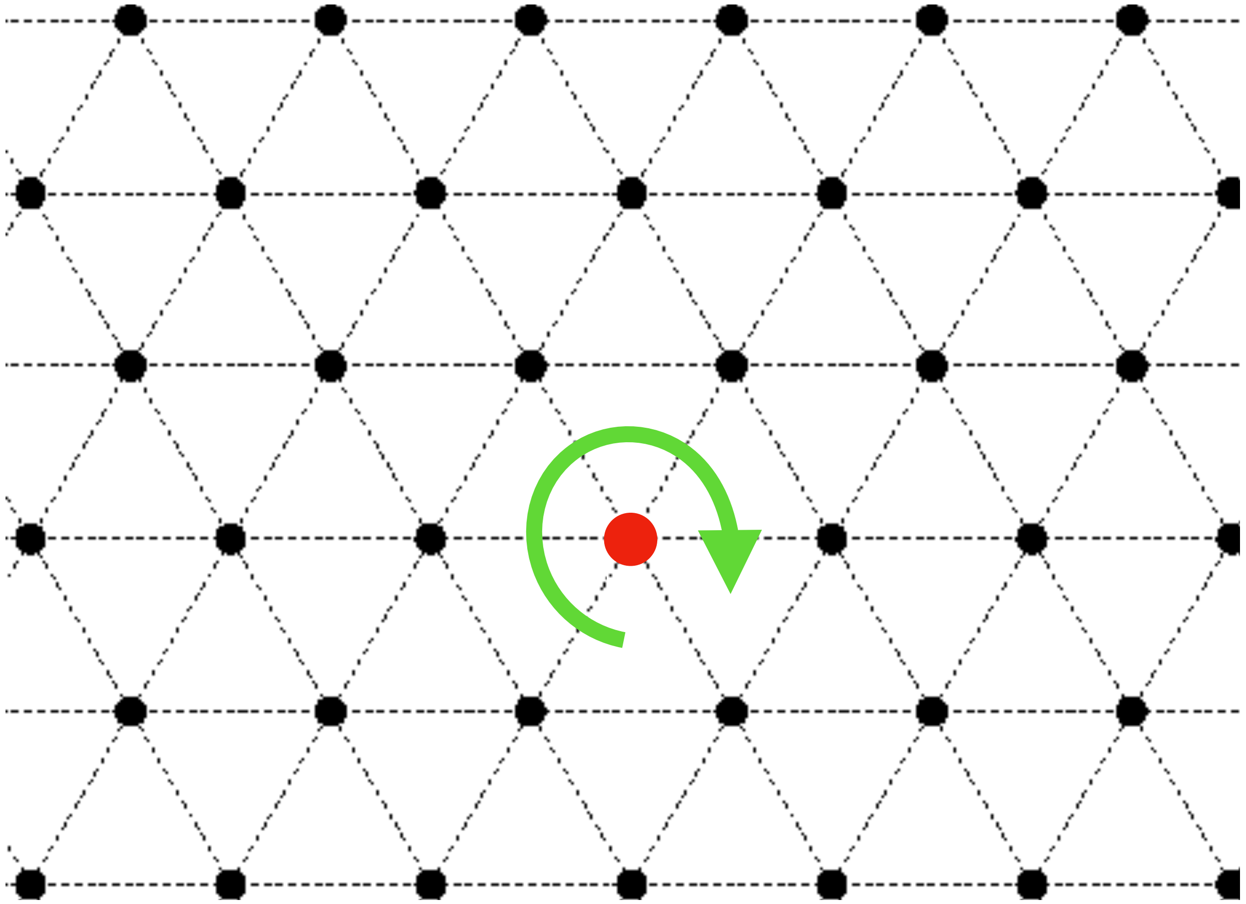
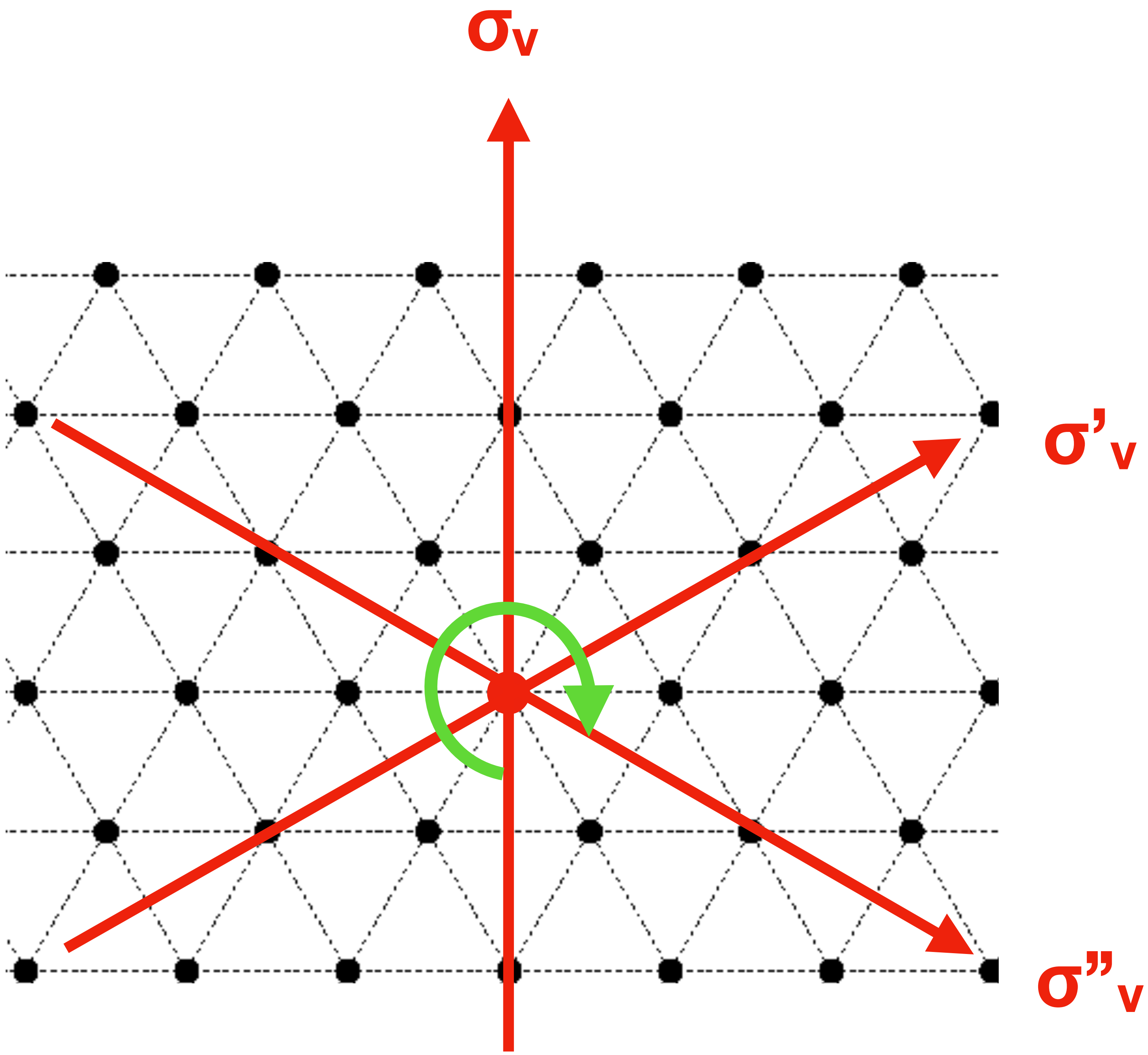


E, R[60^o], R[120^o], R[180^o], R[240^o], R[300^o]

$=C_6$ $=C_3$ $=C_2$ $=C_3^{-1}$ $=C_6^{-1}$

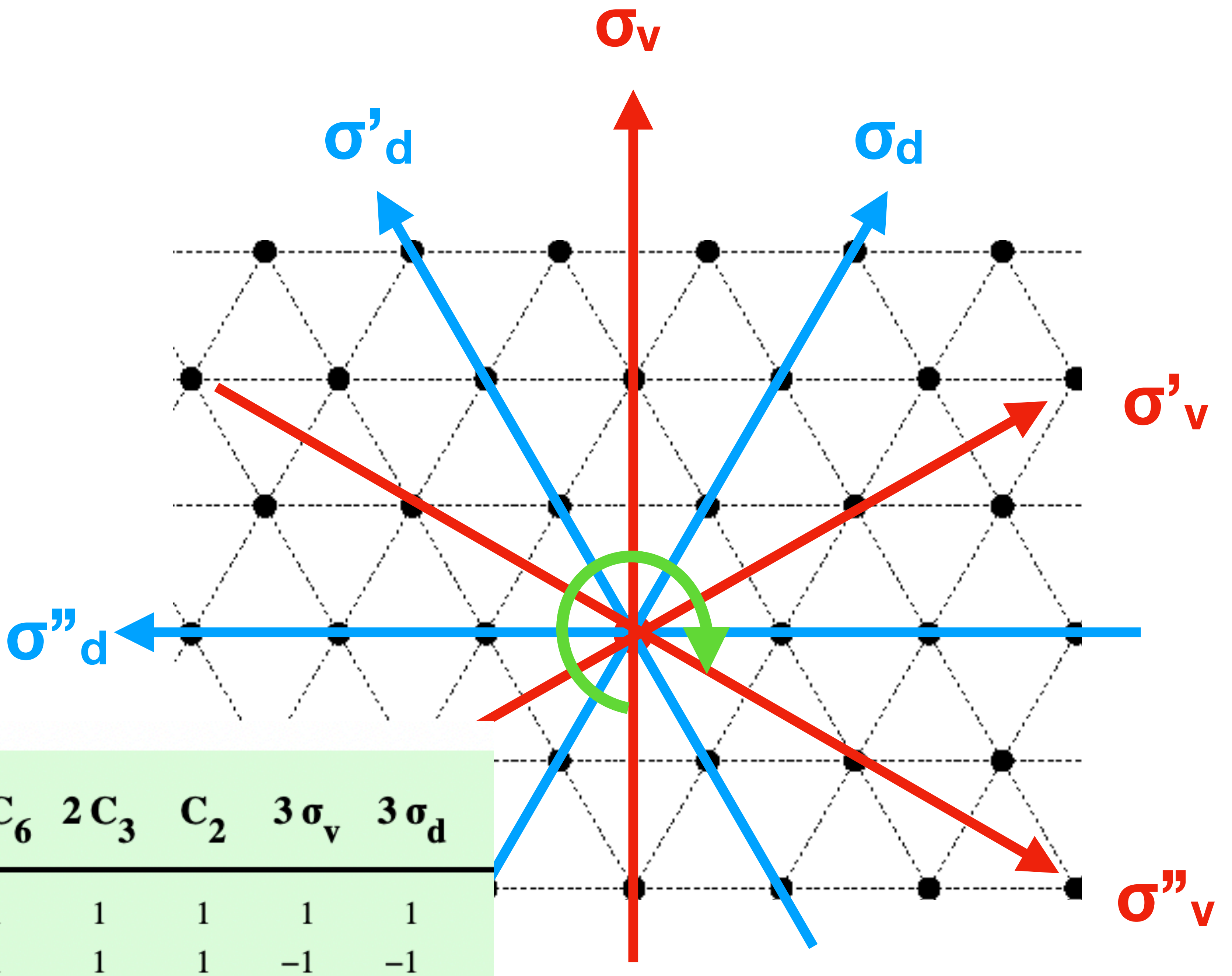
From the triangle to the triangular lattice



E, $R[60^o]$, $R[120^o]$, $R[180^o]$, $R[240^o]$, $R[300^o]$

$=C_6$ $=C_3$ $=C_2$ $=C_3^{-1}$ $=C_6^{-1}$

From the triangle to the triangular lattice

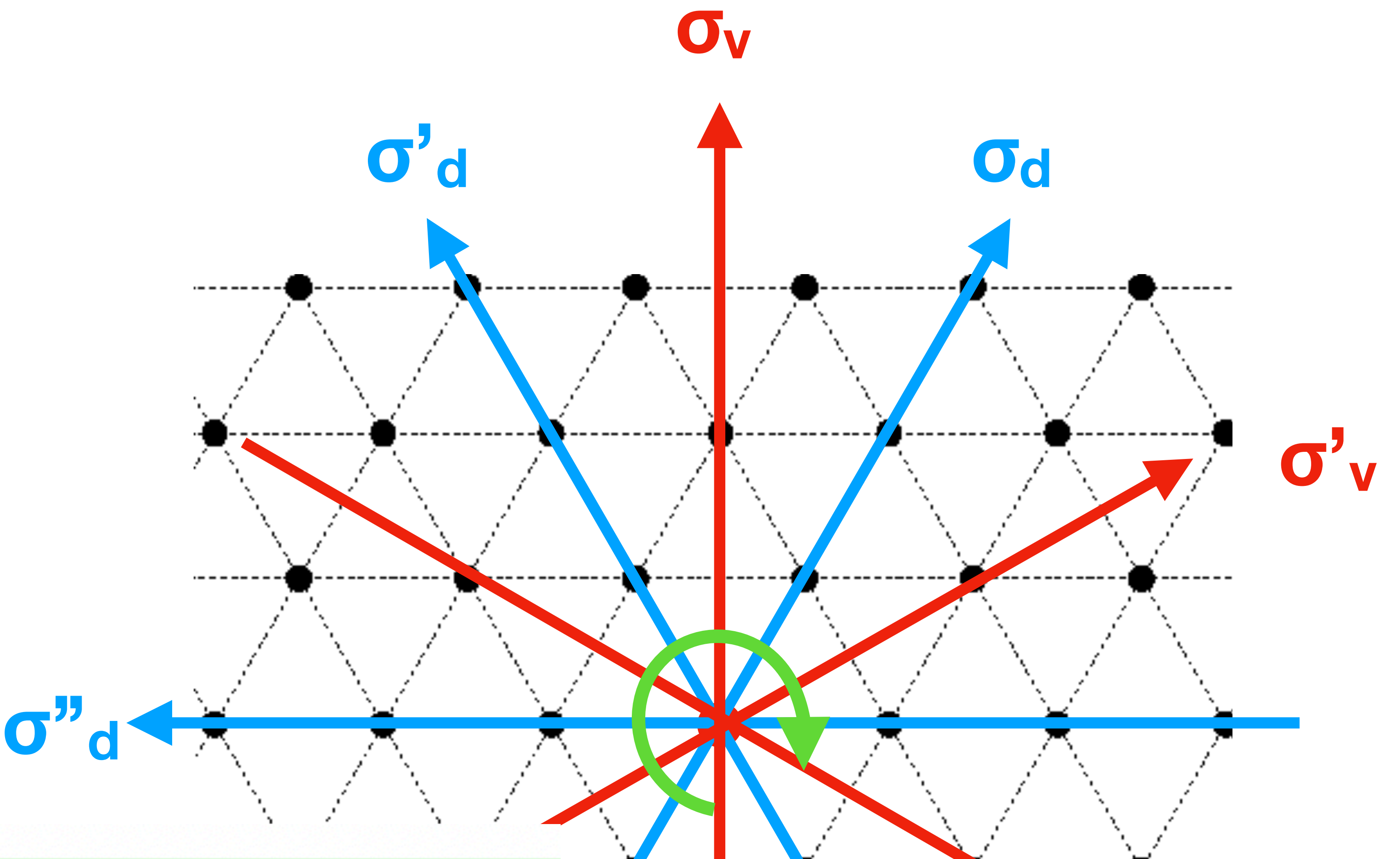


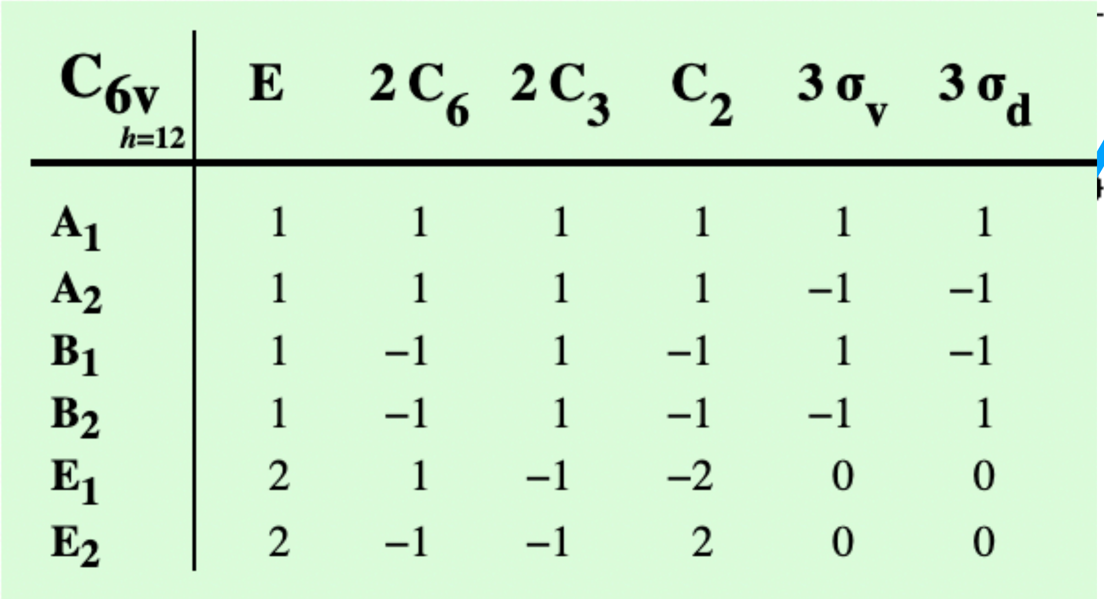
C_{6v} $h=12$	E	$2\,C_6$	$2\,C_3$	C_2	$3\,\sigma_v$	$3\,\sigma_d$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	−1	−1
B_1	1	−1	1	−1	1	−1
B_2	1	−1	1	−1	−1	1
E_1	2	1	−1	−2	0	0
E_2	2	−1	−1	2	0	0

E, R[60°], R[120°], R[180°], R[240°], R[300°]

$=C_6$ $=C_3$ $=C_2$ $=C_3^{-1}$ $=C_6^{-1}$

From the triangle to the triangular lattice





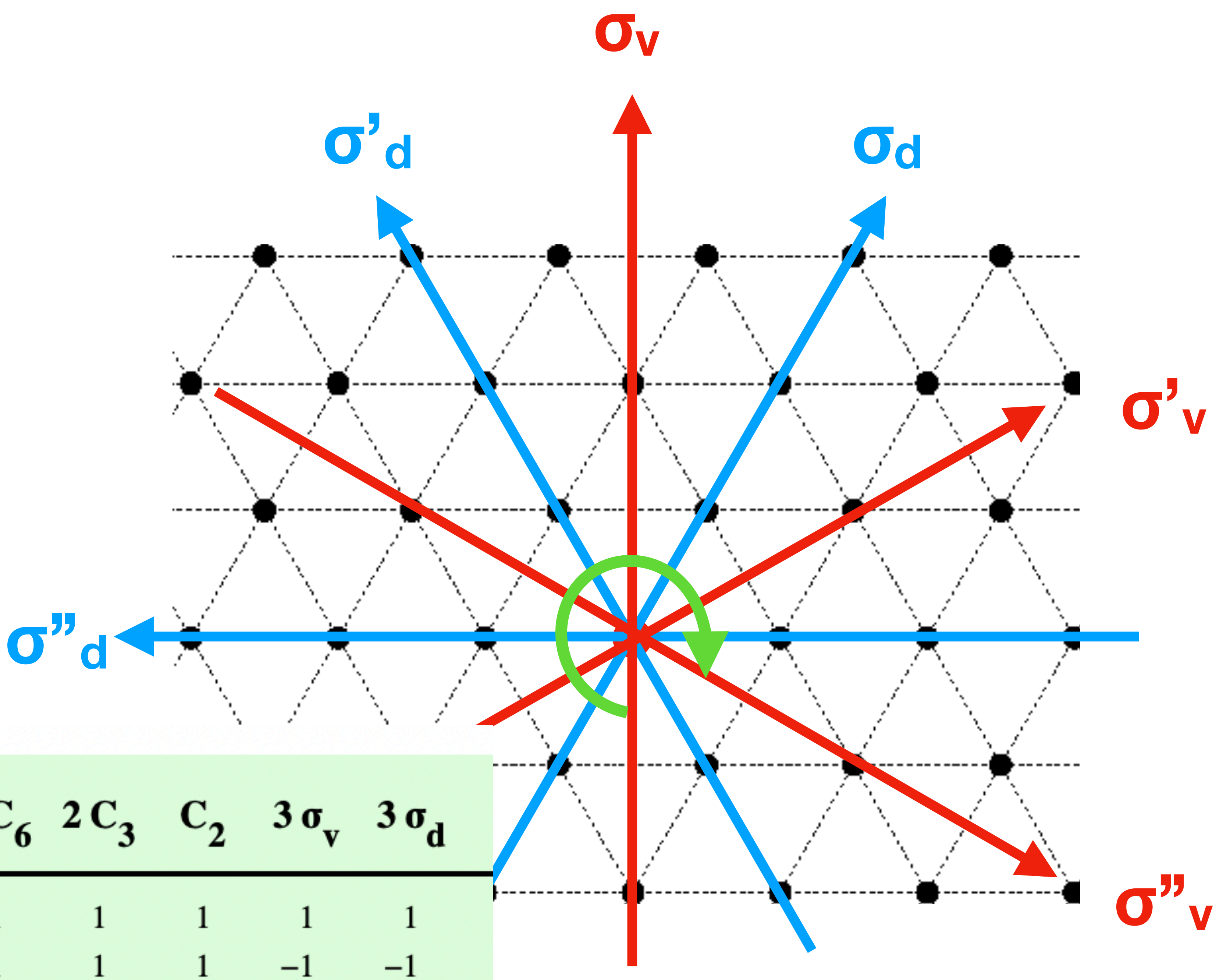
C_{6v} $h=12$	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	−1	−1
B_1	1	−1	1	−1	1	−1
B_2	1	−1	1	−1	−1	1
E_1	2	1	−1	−2	0	0
E_2	2	−1	−1	2	0	0

E, R[60°], R[120°], R[180°], R[240°], R[300°]

$=C_6$ $=C_3$ $=C_2$ $=C_3^{-1}$ $=C_6^{-1}$

[12 elements in 6 classes]

From the triangle to the triangular lattice



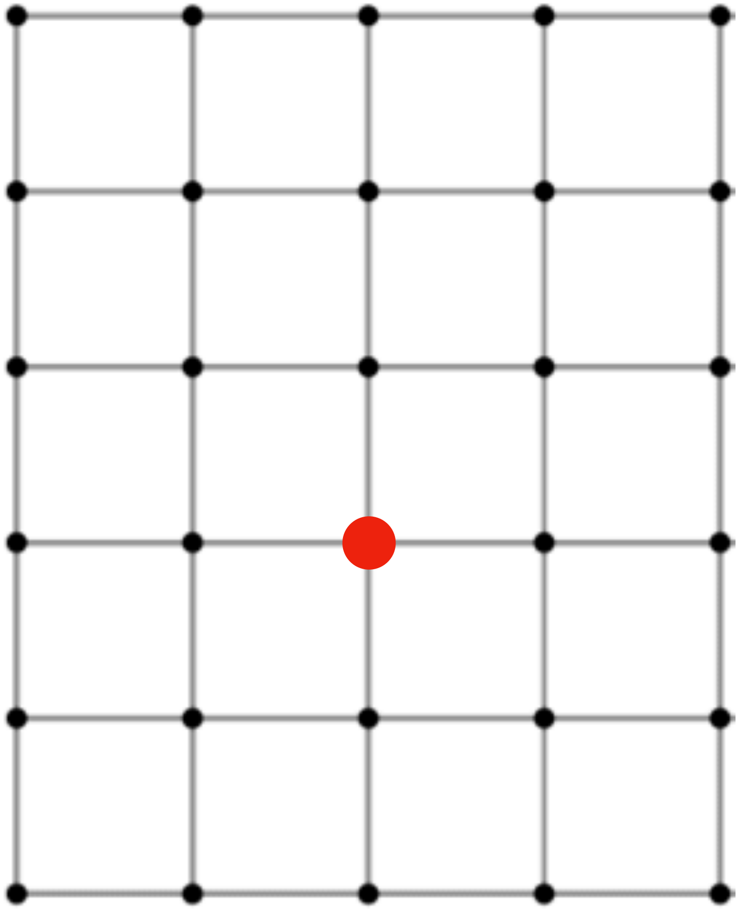
C_{6v} $h=12$	E	$2C_6$	$2C_3$	C_2	$3\sigma_v$	$3\sigma_d$
A_1	1	1	1	1	1	1
A_2	1	1	1	1	–1	–1
B_1	1	–1	1	–1	1	–1
B_2	1	–1	1	–1	–1	1
E_1	2	1	–1	–2	0	0
E_2	2	–1	–1	2	0	0

E, R[60°], R[120°], R[180°], R[240°], R[300°]

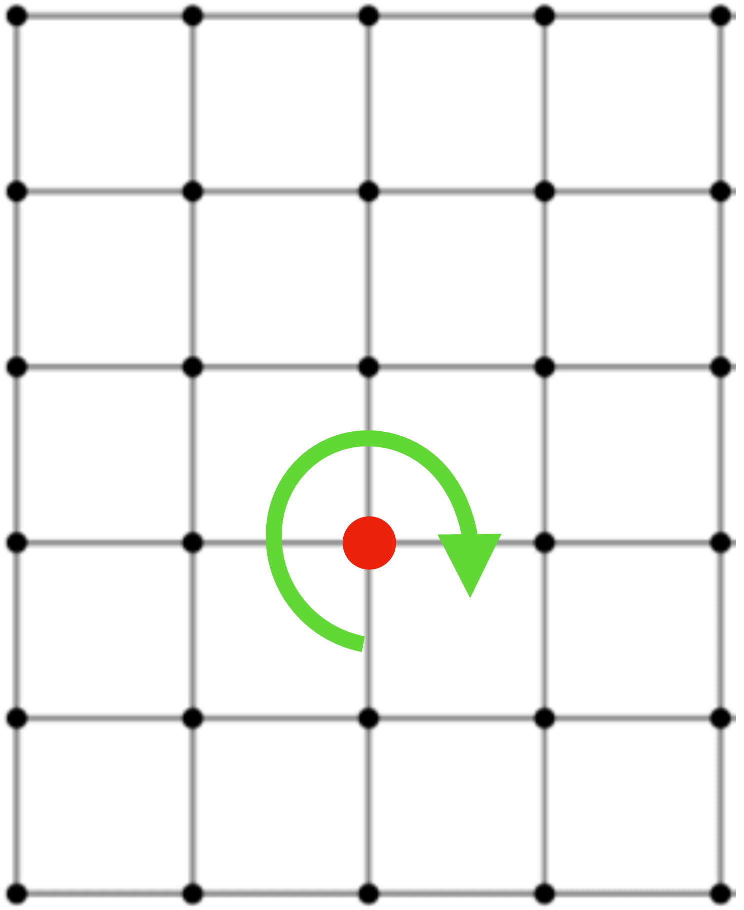
$=C_6$ $=C_3$ $=C_2$ $=C_3^{-1}$ $=C_6^{-1}$

[12 elements in 6 classes]

Symmetries of the square lattice



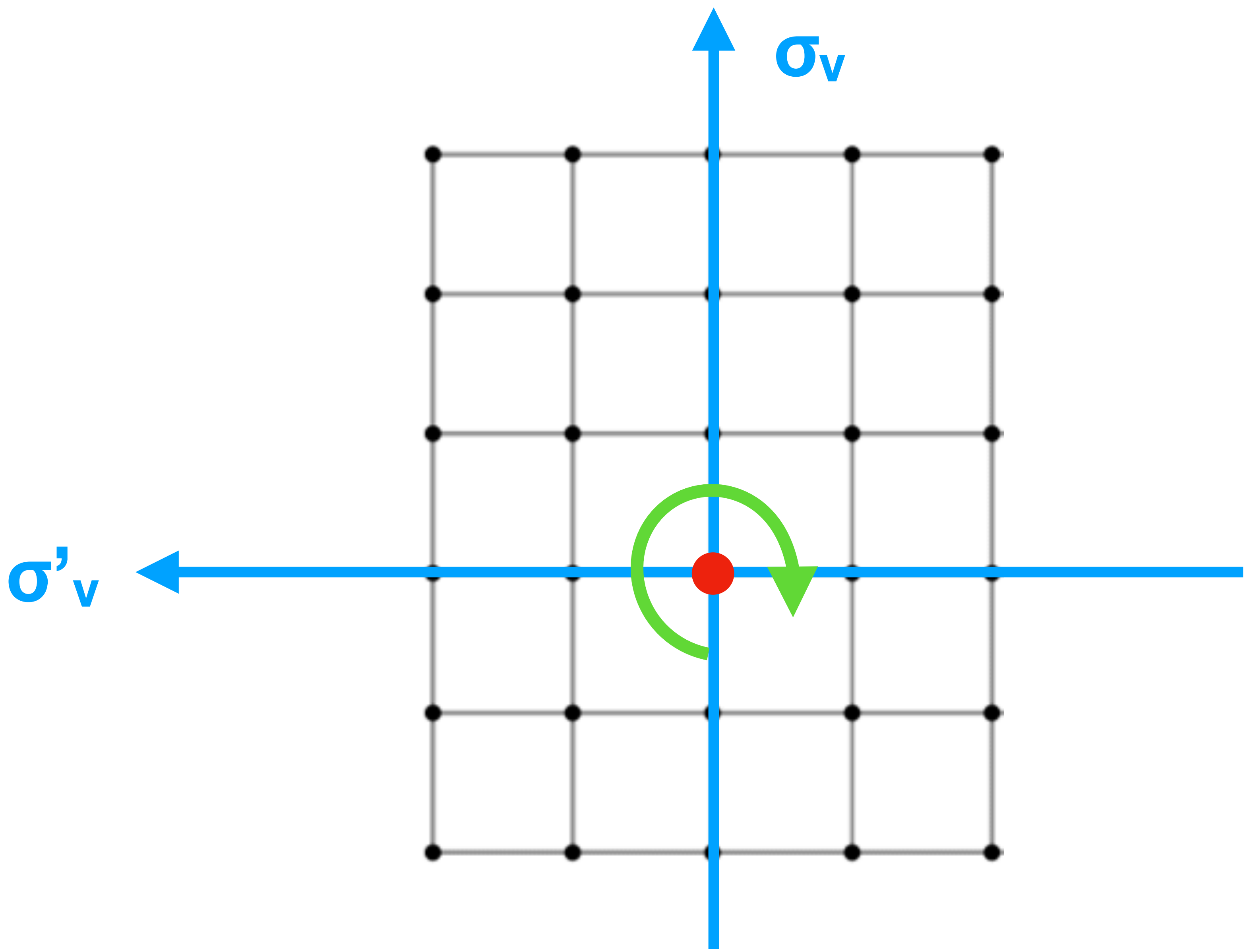
Symmetries of the square lattice



$E, R[90^{o}], R[180^{o}], R[270^{o}]$

$=C_4$ $=C_2$

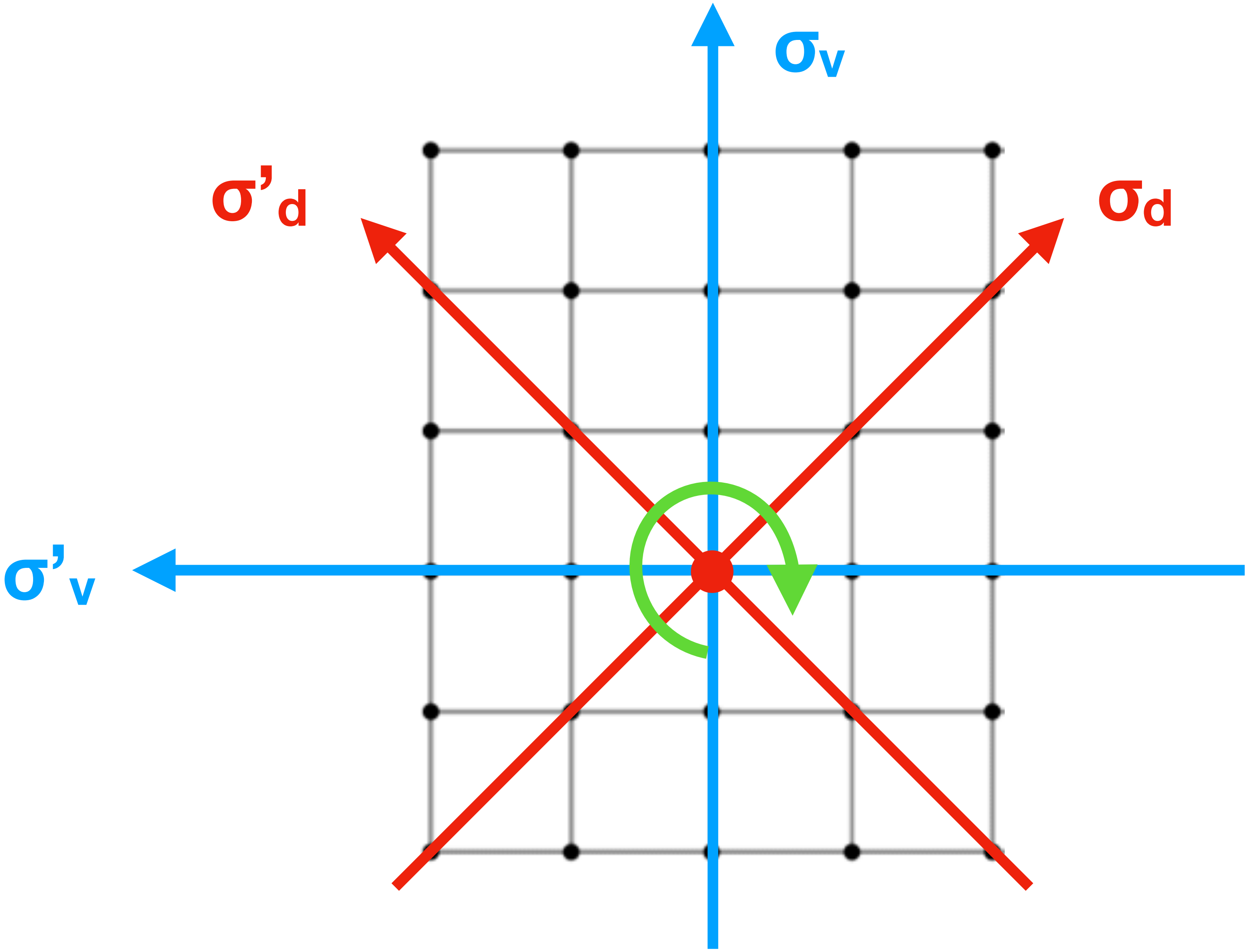
Symmetries of the square lattice



E, R[90°], R[180°], R[270°]

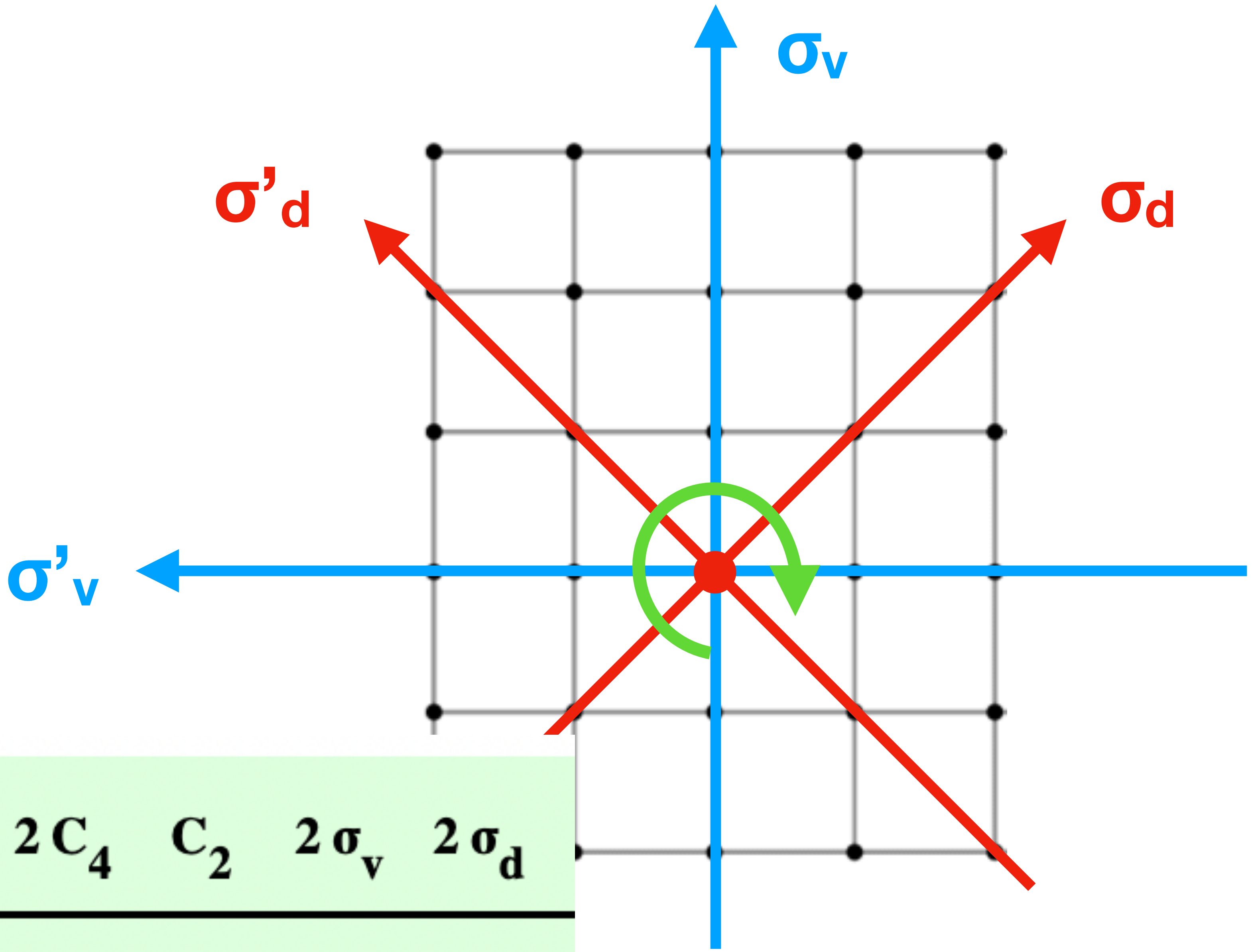
$=C_4$ $=C_2$

Symmetries of the square lattice



E, R[90^o], R[180^o], R[270^o]
=C_4 =C_2

Symmetries of the square lattice

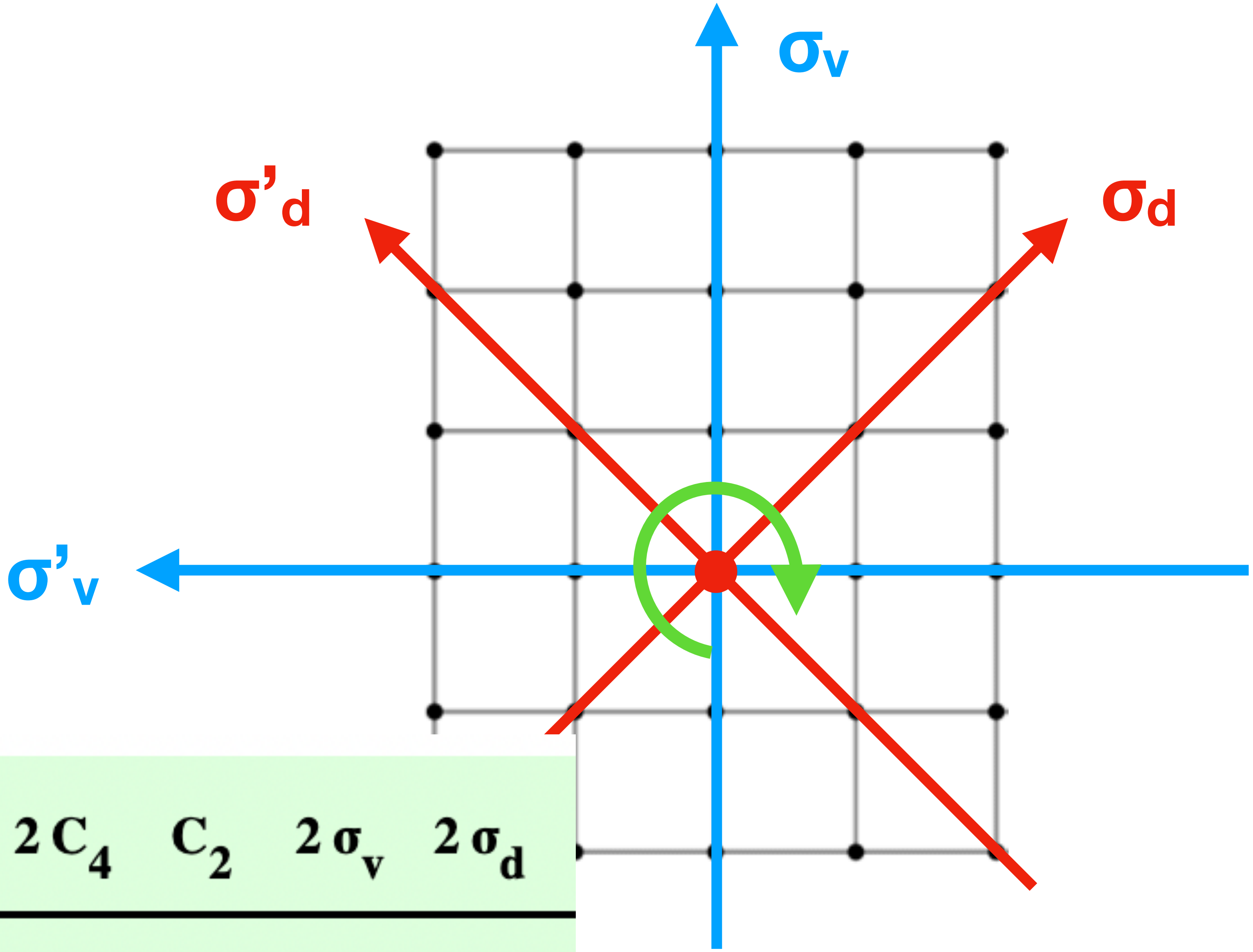


C_{4v} $h=8$	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

E, R[90°], R[180°], R[270°]
$=C_4$ $=C_2$

[8 elements in 5 classes]

Symmetries of the square lattice



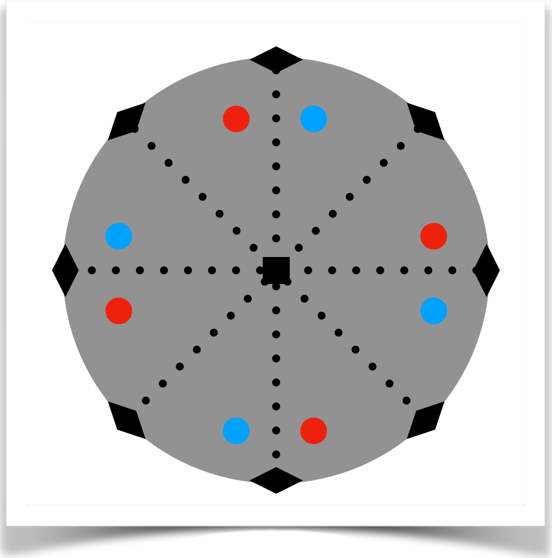
C_{4v} $h=8$	E	2 C_4	C_2	2 σ_v	2 σ_d
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

E, R[90°], R[180°], R[270°]

$=C_4$ $=C_2$

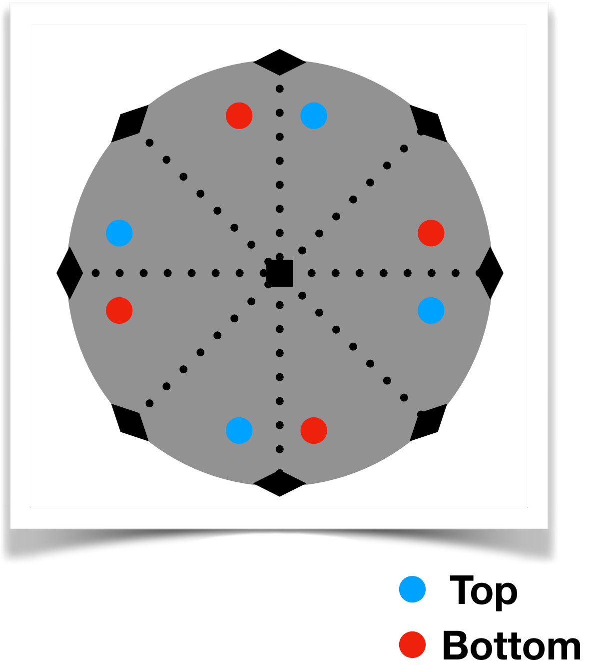
[8 elements in 5 classes]

D_4 [dihedral] point group

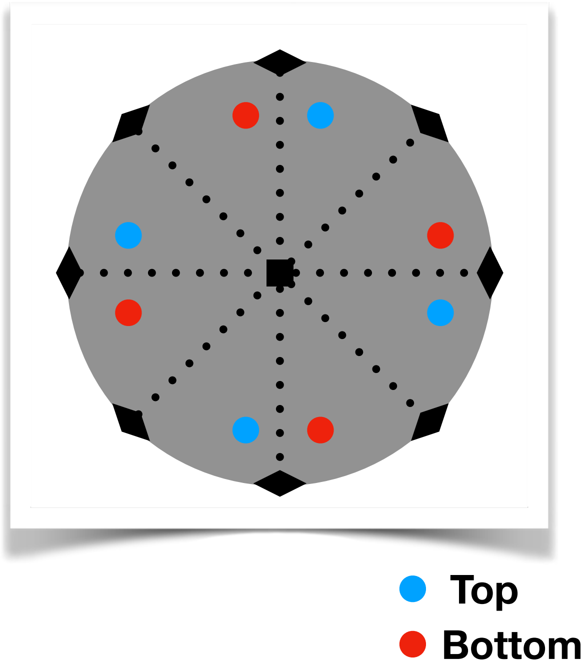


● Top
● Bottom

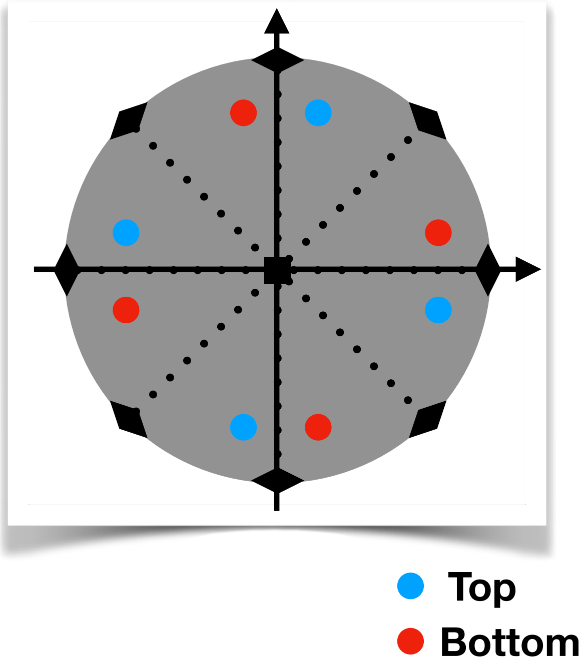
D_4 [dihedral] point group



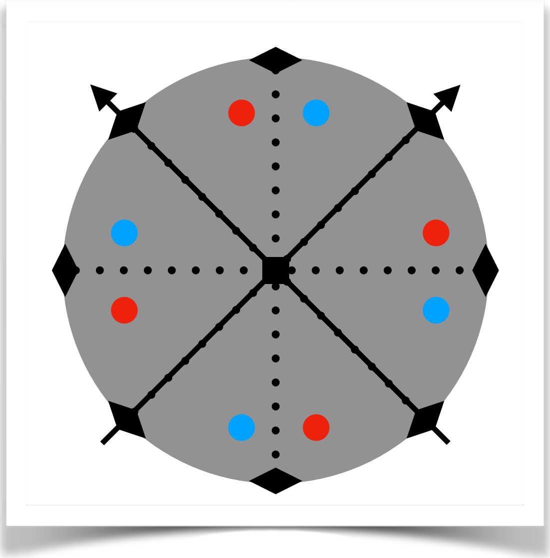
D$_4$ [dihedral] point group



D_4 [dihedral] point group



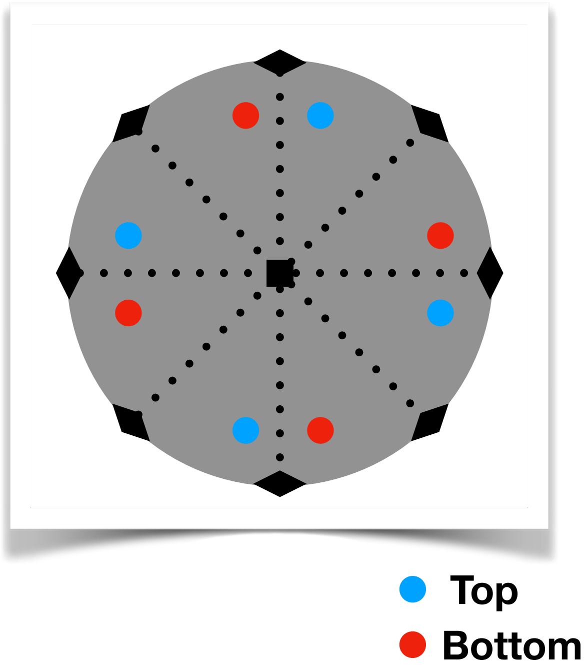
D_4 [dihedral] point group



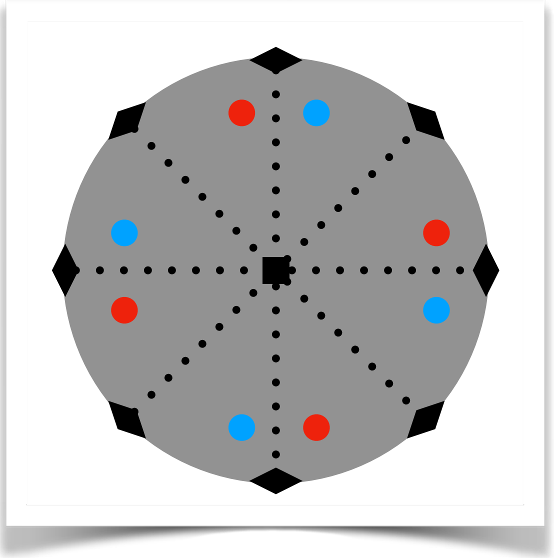
● Top

● Bottom

D_4 [dihedral] point group



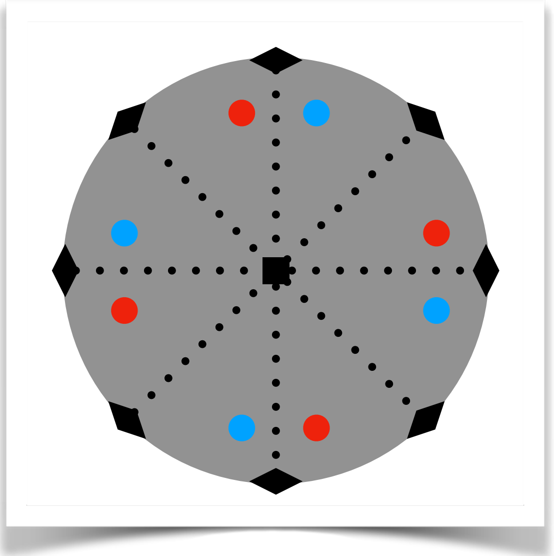
D4 [dihedral] point group



Character table and irreducible representations (Irrep)

E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$

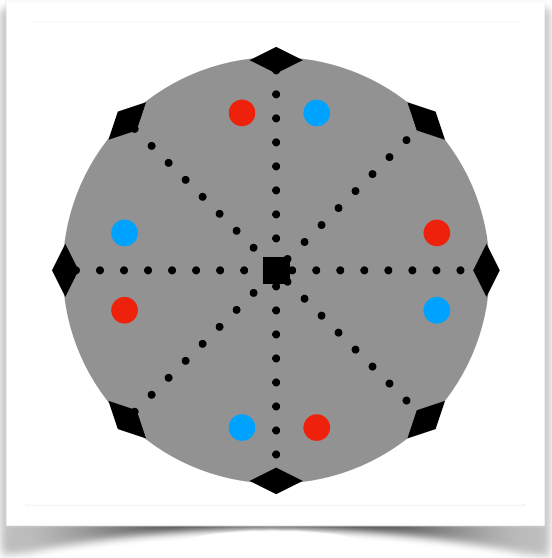
D_4 [dihedral] point group



Character table and irreducible representations (Irrep)

$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	$+1$	-1	-1
B_1	$+1$	-1	$+1$	$+1$	-1
B_2	$+1$	-1	$+1$	-1	$+1$
E	$+2$	0	-2	0	0

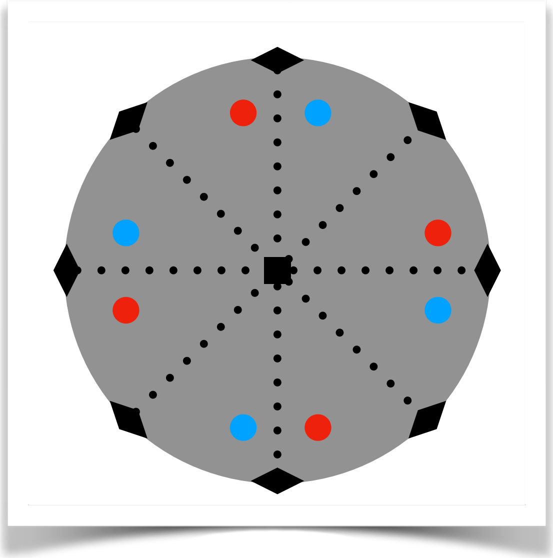
D₄ [dihedral] point group



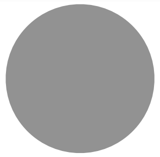
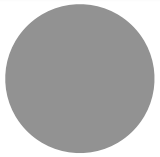
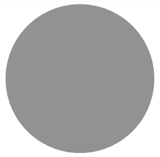
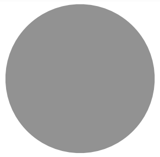
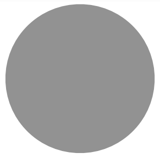
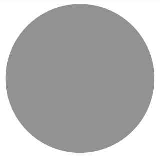
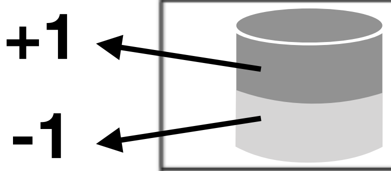
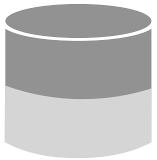
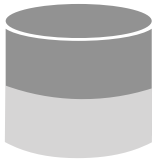
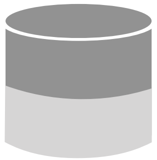
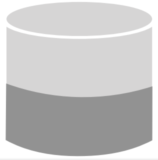
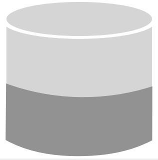
Character table and irreducible representations (Irrep)

$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
● A_1	● $+1$	● $+1$	● $+1$	● $+1$	● $+1$
A_2	$+1$	$+1$	$+1$	-1	-1
B_1	$+1$	-1	$+1$	$+1$	-1
B_2	$+1$	-1	$+1$	-1	$+1$
E	$+2$	0	-2	0	0

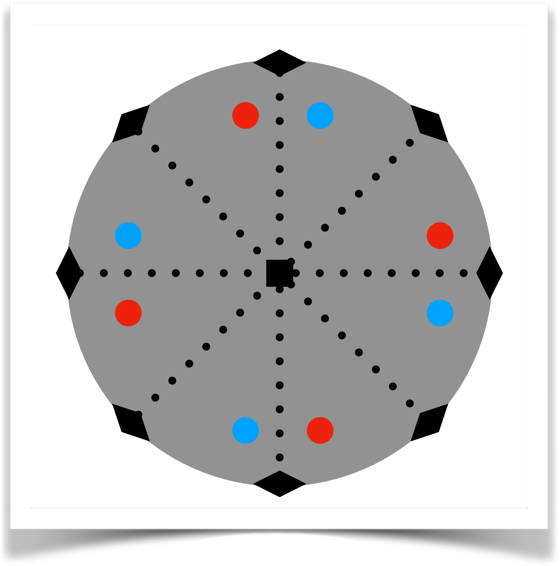
D_4 [dihedral] point group



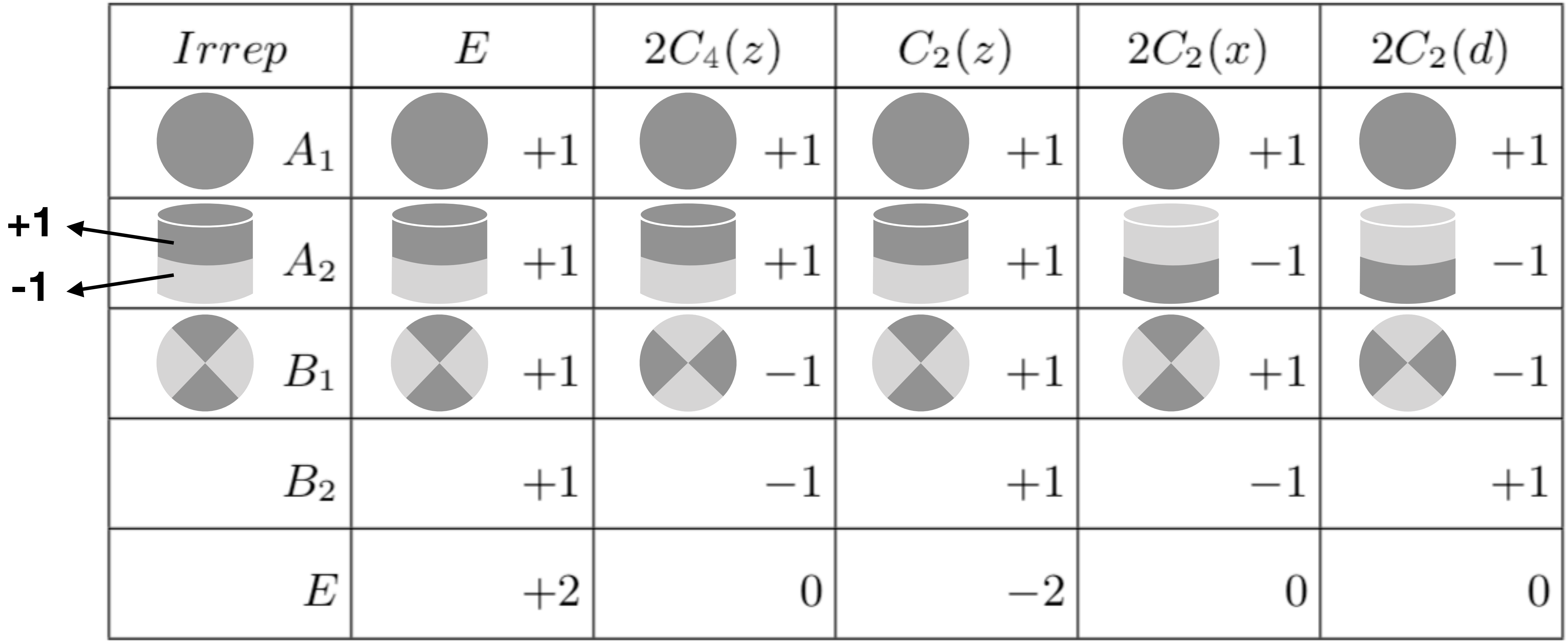
Character table and irreducible representations (Irrep)

$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
 A_1	 $+1$	 $+1$	 $+1$	 $+1$	 $+1$
 A_2	 $+1$	 $+1$	 $+1$	 -1	 -1
B_1	$+1$	-1	$+1$	$+1$	-1
B_2	$+1$	-1	$+1$	-1	$+1$
E	$+2$	0	-2	0	0

D_4 [dihedral] point group

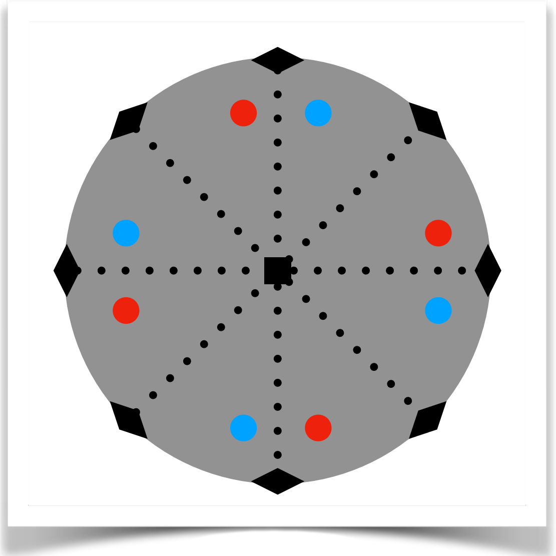


Character table and irreducible representations (Irrep)

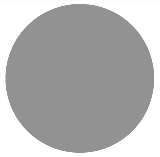
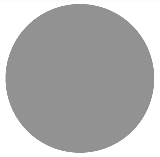
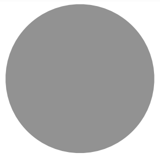
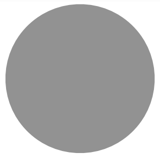
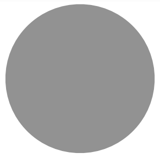
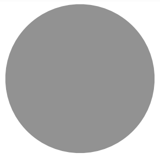
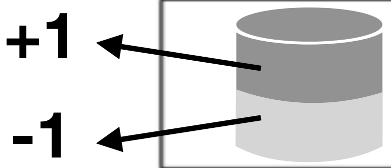
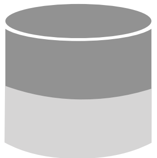
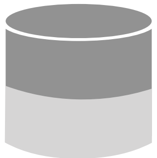
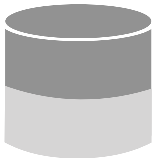
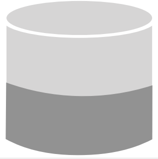
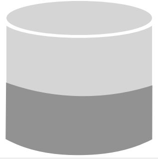
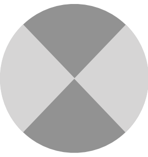
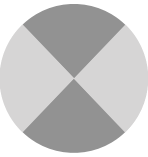
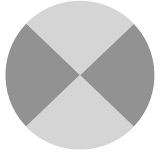
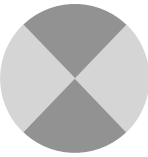
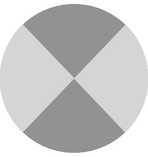
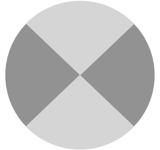
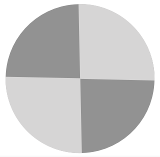
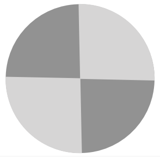
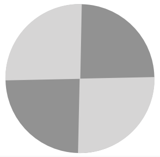
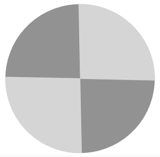
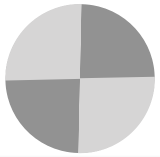
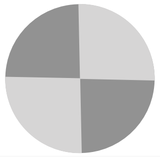


$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	$+1$	-1	-1
B_1	$+1$	-1	$+1$	$+1$	-1
B_2	$+1$	-1	$+1$	-1	$+1$
E	$+2$	0	-2	0	0

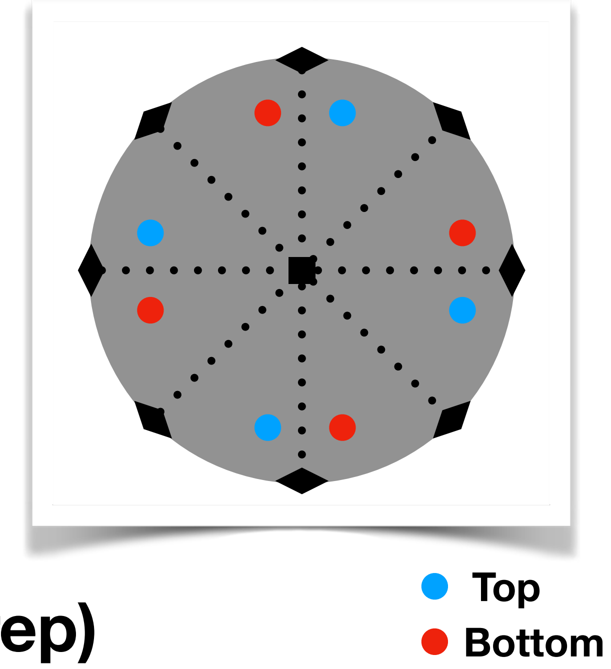
D_4 [dihedral] point group



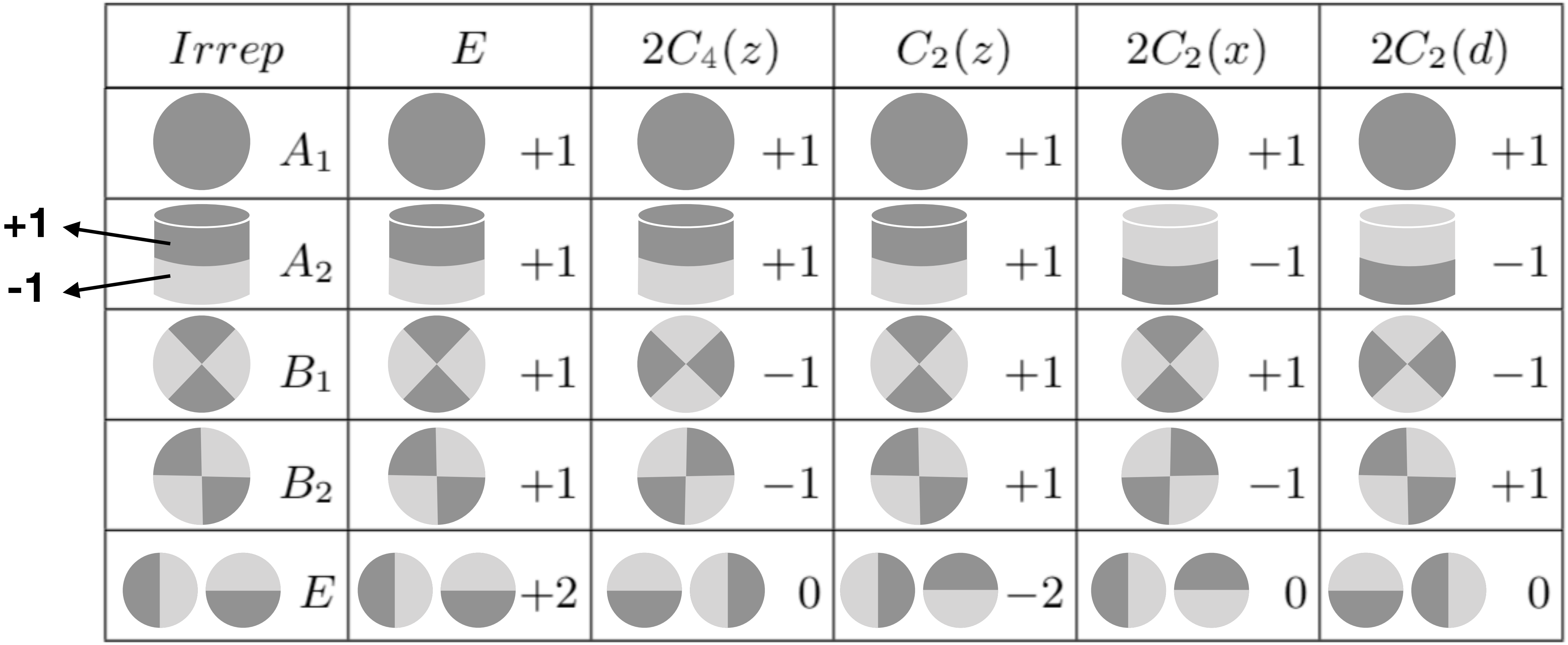
Character table and irreducible representations (Irrep)

$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
 A_1	 $+1$	 $+1$	 $+1$	 $+1$	 $+1$
 A_2	 $+1$	 $+1$	 $+1$	 -1	 -1
 B_1	 $+1$	 -1	 $+1$	 $+1$	 -1
 B_2	 $+1$	 -1	 $+1$	 -1	 $+1$
E	$+2$	0	-2	0	0

D_4 [dihedral] point group

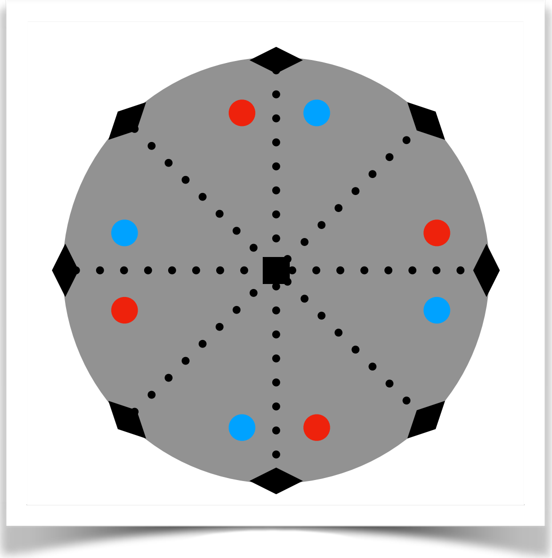


Character table and irreducible representations (Irrep)

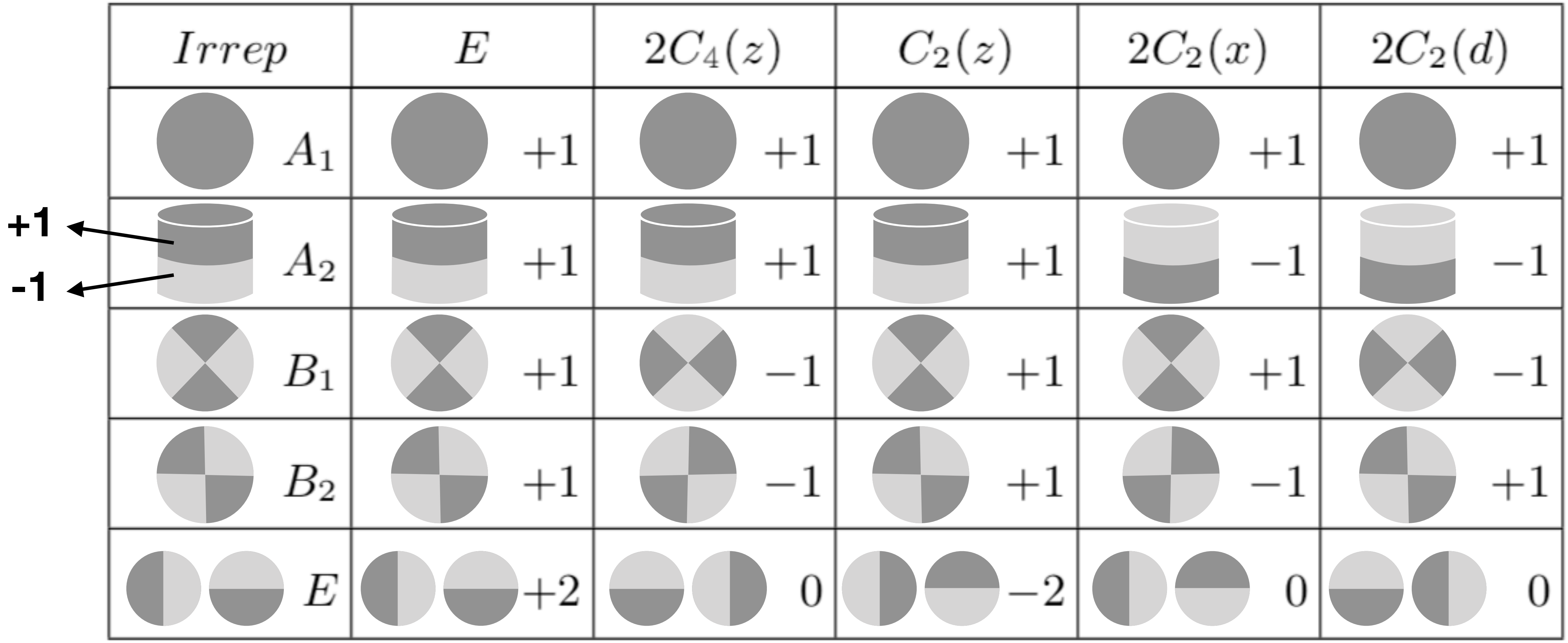


$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$
A_1	$+1$	$+1$	$+1$	$+1$	$+1$
A_2	$+1$	$+1$	$+1$	-1	-1
B_1	$+1$	-1	$+1$	$+1$	-1
B_2	$+1$	-1	$+1$	-1	$+1$
E	$+2$	0	-2	0	0

D_4 [dihedral] point group



Character table and irreducible representations (Irrep)



$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$	
A_1	$+1$	$+1$	$+1$	$+1$	$+1$	**~cte**
A_2	$+1$	$+1$	$+1$	-1	-1	**~z**
B_1	$+1$	-1	$+1$	$+1$	-1	**~x^2-y^2**
B_2	$+1$	-1	$+1$	-1	$+1$	**~xy**
E	$+2$	0	-2	0	0	**~{x,y}**

Basis functions

Crystallographic Point Groups

[There are 32 crystallographic point groups in 3D]

Crystal family	Crystal system	Hermann-Mauguin		Shubnikov[1]	Schoenflies	Orbifold	Coxeter	Order
		(full)	(short)					
Triclinic		1	1	1	C_1	11	$[\ ]^+$	1
		$\bar{1}$	$\bar{1}$	$\tilde{2}$	$C_i = S_2$	×	$[2^+,2^+]$	2
Monoclinic		2	2	2	C_2	22	$[2]^+$	2
		m	m	m	$C_s = C_{1h}$	*	[ ]	2
		$\frac{2}{m}$	2/m	$2 : m$	C_{2h}	2*	$[2,2^+]$	4
Orthorhombic		222	222	$2 : 2$	$D_2 = V$	222	$[2,2]^+$	4
		mm2	mm2	$2 \cdot m$	C_{2v}	*22	[2]	4
		$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	mmm	$m \cdot 2 : m$	$D_{2h} = V_h$	*222	[2,2]	8
Tetragonal		4	4	4	C_4	44	$[4]^+$	4
		$\bar{4}$	$\bar{4}$	$\tilde{4}$	S_4	2×	$[2^+,4^+]$	4
		$\frac{4}{m}$	4/m	$4 : m$	C_{4h}	4*	$[2,4^+]$	8
		422	422	$4 : 2$	D_4	422	$[4,2]^+$	8
		4mm	4mm	$4 \cdot m$	C_{4v}	*44	[4]	8
		$\bar{4}$2m	$\bar{4}$2m	$\tilde{4} \cdot m$	$D_{2d} = V_d$	2*2	$[2^+,4]$	8
		$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	4/mmm	$m \cdot 4 : m$	D_{4h}	*422	[4,2]	16
Hexagonal	Trigonal	3	3	3	C_3	33	$[3]^+$	3
		$\bar{3}$	$\bar{3}$	$\tilde{6}$	$C_{3i} = S_6$	3×	$[2^+,6^+]$	6
		32	32	$3 : 2$	D_3	322	$[3,2]^+$	6
		3m	3m	$3 \cdot m$	C_{3v}	*33	[3]	6
		$\bar{3}\frac{2}{m}$	$\bar{3}$m	$\tilde{6} \cdot m$	D_{3d}	2*3	$[2^+,6]$	12
	Hexagonal	6	6	6	C_6	66	$[6]^+$	6
		$\bar{6}$	$\bar{6}$	$3 : m$	C_{3h}	3*	$[2,3^+]$	6
		$\frac{6}{m}$	6/m	$6 : m$	C_{6h}	6*	$[2,6^+]$	12
		622	622	$6 : 2$	D_6	622	$[6,2]^+$	12
		6mm	6mm	$6 \cdot m$	C_{6v}	*66	[6]	12
		$\bar{6}$m2	$\bar{6}$m2	$m \cdot 3 : m$	D_{3h}	*322	[3,2]	12
		$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	6/mmm	$m \cdot 6 : m$	D_{6h}	*622	[6,2]	24
Cubic		23	23	$3/2$	T	332	$[3,3]^+$	12
		$\frac{2}{m}\bar{3}$	m$\bar{3}$	$\tilde{6}/2$	T_h	3*2	$[3^+,4]$	24
		432	432	$3/4$	O	432	$[4,3]^+$	24
		$\bar{4}$3m	$\bar{4}$3m	$3/\tilde{4}$	T_d	*332	[3,3]	24
		$\frac{4}{m}\bar{3}\frac{2}{m}$	m$\bar{3}$m	$\tilde{6}/4$	O_h	*432	[4,3]	48

C_n: n-fold rotation

C_{nh}: C_n + ⊥ mirror

C_{nv}: C_n + n || mirrors

S_n: n-fold rotation-reflection

D_n: n-fold rotations + n 2-fold ⊥ rotations

D_{nh}: D_n + ⊥ mirror

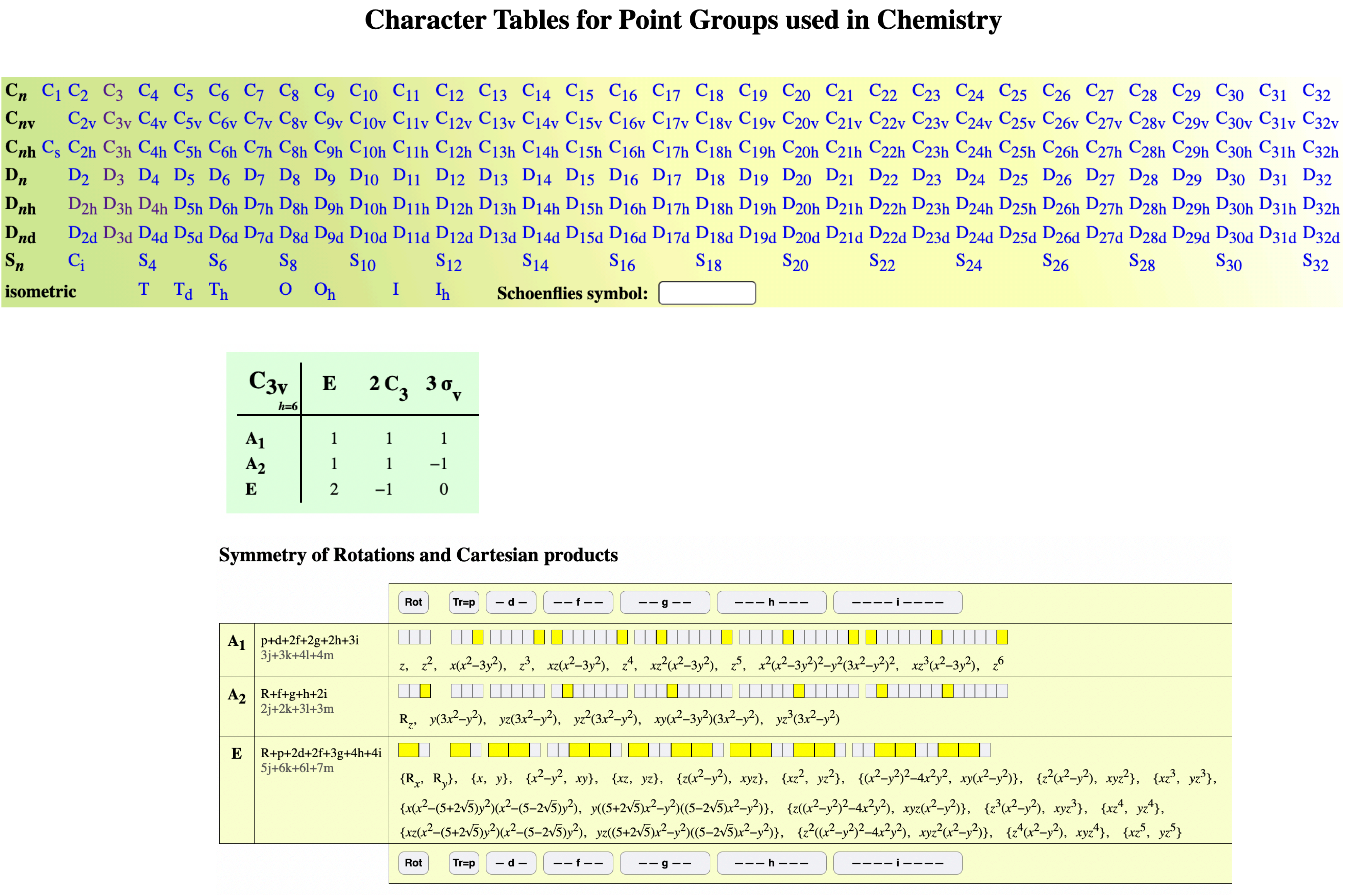
D_{nd}: D_n + n || mirror

T: Tetrahedron

[h: with inversion, d: with improper rotations]

O: Octahedron [h: with inversion]

https://en.wikipedia.org/wiki/Crystallographic_point_group



Character Tables for Point Groups used in Chemistry

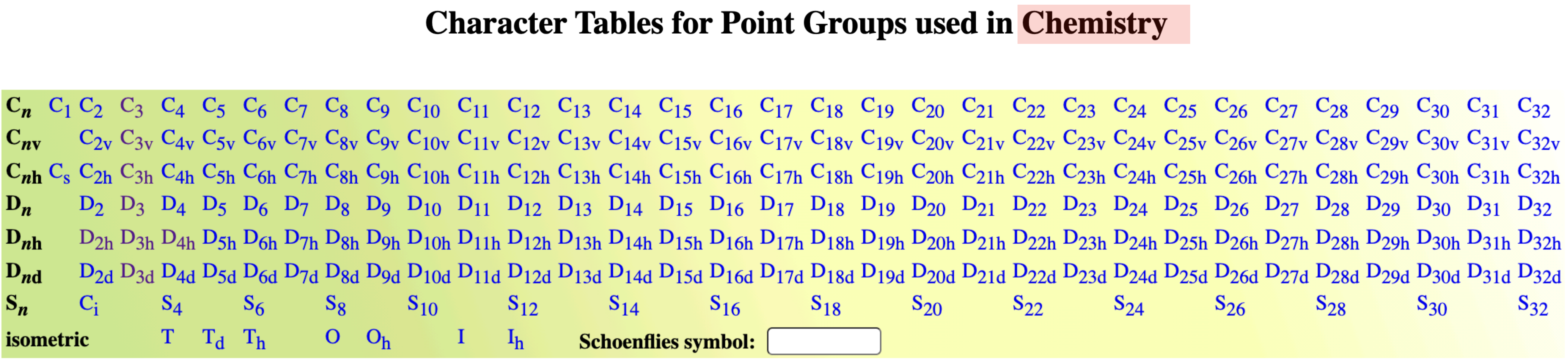
C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}	C_{26}	C_{27}	C_{28}	C_{29}	C_{30}	C_{31}	C_{32}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}	C_{21v}	C_{22v}	C_{23v}	C_{24v}	C_{25v}	C_{26v}	C_{27v}	C_{28v}	C_{29v}	C_{30v}	C_{31v}	C_{32v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}	C_{21h}	C_{22h}	C_{23h}	C_{24h}	C_{25h}	C_{26h}	C_{27h}	C_{28h}	C_{29h}	C_{30h}	C_{31h}	C_{32h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}	D_{21}	D_{22}	D_{23}	D_{24}	D_{25}	D_{26}	D_{27}	D_{28}	D_{29}	D_{30}	D_{31}	D_{32}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}	D_{21h}	D_{22h}	D_{23h}	D_{24h}	D_{25h}	D_{26h}	D_{27h}	D_{28h}	D_{29h}	D_{30h}	D_{31h}	D_{32h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}	D_{21d}	D_{22d}	D_{23d}	D_{24d}	D_{25d}	D_{26d}	D_{27d}	D_{28d}	D_{29d}	D_{30d}	D_{31d}	D_{32d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}		S_{22}		S_{24}		S_{26}		S_{28}		S_{30}		S_{32}
isometric				T	T_d	T_h		O	O_h		I	I_h		**Schoenflies symbol:**																		

C_{3v} $h=6$	E	$2\,C_3$	$3\,\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

Symmetry of Rotations and Cartesian products

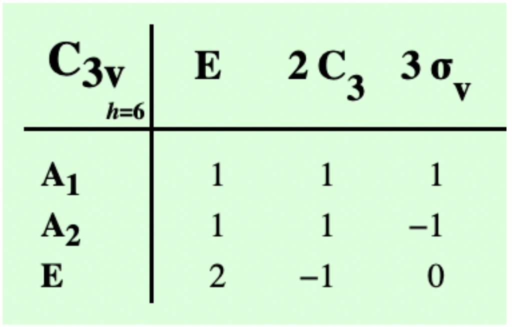
		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –
A_1	p+d+2f+2g+2h+3i 3j+3k+4l+4m	☐☐☐ ☐☐🟨 ☐☐☐☐🟨 🟨☐☐☐☐☐🟨 ☐☐🟨☐☐☐☐☐🟨 ☐☐☐☐🟨☐☐☐☐☐🟨 🟨☐☐☐☐☐🟨☐☐☐☐☐🟨 z, z^2, $x(x^2-3y^2)$, z^3, $xz(x^2-3y^2)$, z^4, $xz^2(x^2-3y^2)$, z^5, $x^2(x^2-3y^2)^2-y^2(3x^2-y^2)^2$, $xz^3(x^2-3y^2)$, z^6
A_2	R+f+g+h+2i 2j+2k+3l+3m	☐☐🟨 ☐☐☐ ☐☐☐☐☐ ☐🟨☐☐☐☐☐ ☐☐☐🟨☐☐☐☐☐ ☐☐☐☐☐🟨☐☐☐☐☐ ☐🟨☐☐☐☐☐🟨☐☐☐☐☐ R_z, $y(3x^2-y^2)$, $yz(3x^2-y^2)$, $yz^2(3x^2-y^2)$, $xy(x^2-3y^2)(3x^2-y^2)$, $yz^3(3x^2-y^2)$
E	R+p+2d+2f+3g+4h+4i 5j+6k+6l+7m	🟨🟨☐ 🟨🟨☐ 🟨🟨🟨🟨☐ ☐☐🟨🟨🟨🟨☐ 🟨🟨☐☐🟨🟨🟨🟨☐ 🟨🟨🟨🟨☐☐🟨🟨🟨🟨☐ ☐☐🟨🟨🟨🟨☐☐🟨🟨🟨🟨☐ $\{R_x,\ R_y\}$, $\{x,\ y\}$, $\{x^2-y^2,\ xy\}$, $\{xz,\ yz\}$, $\{z(x^2-y^2),\ xyz\}$, $\{xz^2,\ yz^2\}$, $\{(x^2-y^2)^2-4x^2y^2,\ xy(x^2-y^2)\}$, $\{z^2(x^2-y^2),\ xyz^2\}$, $\{xz^3,\ yz^3\}$, $\{x(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2),\ y((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{z((x^2-y^2)^2-4x^2y^2),\ xyz(x^2-y^2)\}$, $\{z^3(x^2-y^2),\ xyz^3\}$, $\{xz^4,\ yz^4\}$, $\{xz(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2),\ yz((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{z^2((x^2-y^2)^2-4x^2y^2),\ xyz^2(x^2-y^2)\}$, $\{z^4(x^2-y^2),\ xyz^4\}$, $\{xz^5,\ yz^5\}$
		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –

http://gernot-katzers-spice-pages.com/character_tables/



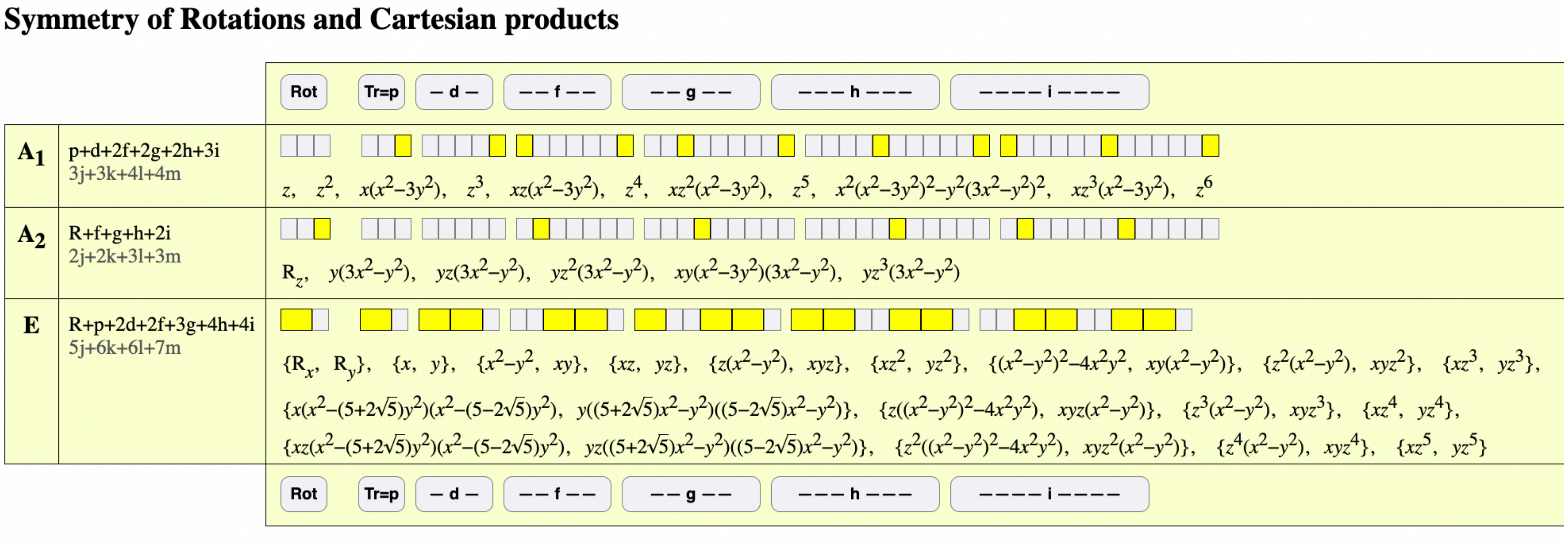
Character Tables for Point Groups used in Chemistry

C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}	C_{21}	C_{22}	C_{23}	C_{24}	C_{25}	C_{26}	C_{27}	C_{28}	C_{29}	C_{30}	C_{31}	C_{32}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}	C_{21v}	C_{22v}	C_{23v}	C_{24v}	C_{25v}	C_{26v}	C_{27v}	C_{28v}	C_{29v}	C_{30v}	C_{31v}	C_{32v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}	C_{21h}	C_{22h}	C_{23h}	C_{24h}	C_{25h}	C_{26h}	C_{27h}	C_{28h}	C_{29h}	C_{30h}	C_{31h}	C_{32h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}	D_{21}	D_{22}	D_{23}	D_{24}	D_{25}	D_{26}	D_{27}	D_{28}	D_{29}	D_{30}	D_{31}	D_{32}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}	D_{21h}	D_{22h}	D_{23h}	D_{24h}	D_{25h}	D_{26h}	D_{27h}	D_{28h}	D_{29h}	D_{30h}	D_{31h}	D_{32h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}	D_{21d}	D_{22d}	D_{23d}	D_{24d}	D_{25d}	D_{26d}	D_{27d}	D_{28d}	D_{29d}	D_{30d}	D_{31d}	D_{32d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}		S_{22}		S_{24}		S_{26}		S_{28}		S_{30}		S_{32}
isometric				T	T_d	T_h		O	O_h		I	I_h	**Schoenflies symbol:**																			



C_{3v} *h=6*	E	$2\,C_3$	$3\,\sigma_v$
A_1	1	1	1
A_2	1	1	−1
E	2	−1	0

Note: For crystallographic point groups only (32) groups with rotation axes of order n=1,2,3,4,6 are allowed!



Symmetry of Rotations and Cartesian products

		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –
A_1	p+d+2f+2g+2h+3i 3j+3k+4l+4m	z, z^2, $x(x^2-3y^2)$, z^3, $xz(x^2-3y^2)$, z^4, $xz^2(x^2-3y^2)$, z^5, $x^2(x^2-3y^2)^2-y^2(3x^2-y^2)^2$, $xz^3(x^2-3y^2)$, z^6
A_2	R+f+g+h+2i 2j+2k+3l+3m	R_z, $y(3x^2-y^2)$, $yz(3x^2-y^2)$, $yz^2(3x^2-y^2)$, $xy(x^2-3y^2)(3x^2-y^2)$, $yz^3(3x^2-y^2)$
E	R+p+2d+2f+3g+4h+4i 5j+6k+6l+7m	$\{R_x, R_y\}$, $\{x, y\}$, $\{x^2-y^2, xy\}$, $\{xz, yz\}$, $\{z(x^2-y^2), xyz\}$, $\{xz^2, yz^2\}$, $\{(x^2-y^2)^2-4x^2y^2, xy(x^2-y^2)\}$, $\{z^2(x^2-y^2), xyz^2\}$, $\{xz^3, yz^3\}$, $\{x(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), y((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{z((x^2-y^2)^2-4x^2y^2), xyz(x^2-y^2)\}$, $\{z^3(x^2-y^2), xyz^3\}$, $\{xz^4, yz^4\}$, $\{xz(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), yz((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{z^2((x^2-y^2)^2-4x^2y^2), xyz^2(x^2-y^2)\}$, $\{z^4(x^2-y^2), xyz^4\}$, $\{xz^5, yz^5\}$
		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –

http://gernot-katzers-spice-pages.com/character_tables/

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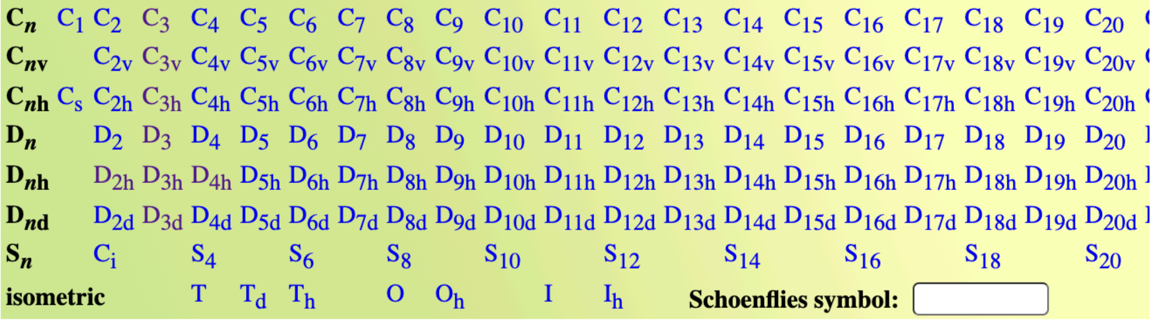

$\mathbf{C}_{\boldsymbol{n}}$	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}
$\mathbf{C}_{\boldsymbol{n}\mathbf{v}}$		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}
$\mathbf{C}_{\boldsymbol{n}\mathbf{h}}$	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}
$\mathbf{D}_{\boldsymbol{n}}$		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}
$\mathbf{D}_{\boldsymbol{n}\mathbf{h}}$		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}
$\mathbf{D}_{\boldsymbol{n}\mathbf{d}}$		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}
$\mathbf{S}_{\boldsymbol{n}}$		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}
isometric				T	T_d	T_h		O	O_h		I	I_h		**Schoenflies symbol:**						

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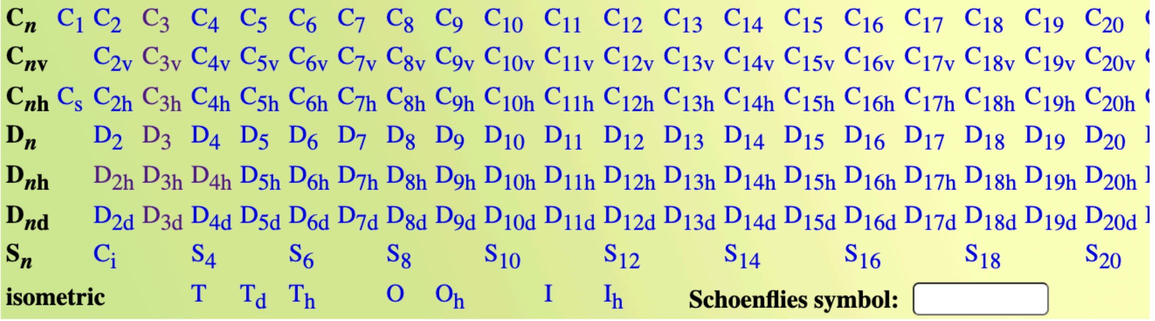

C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}
isometric				T	T_d	T_h		O	O_h		I	I_h		**Schoenflies symbol:**			☐			

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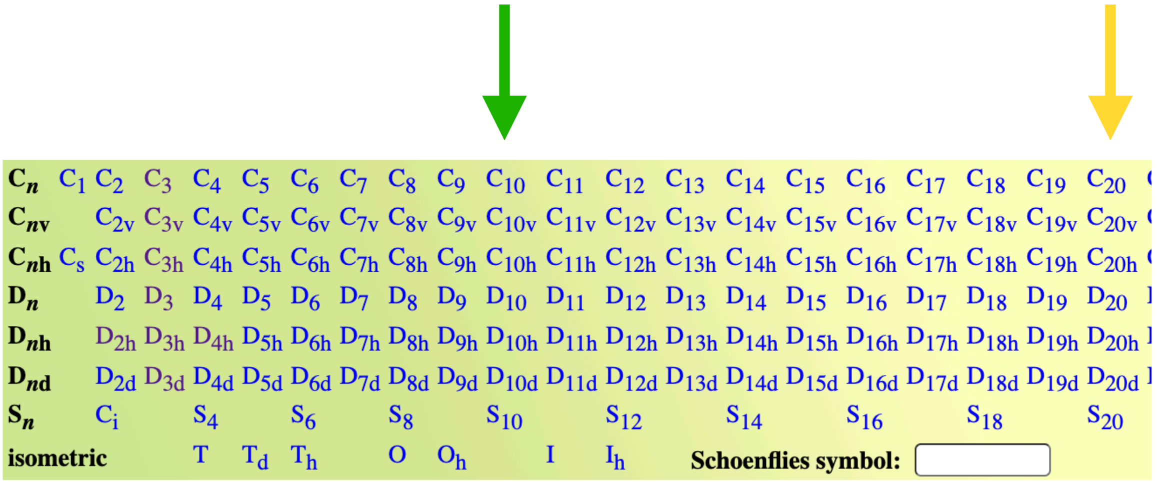

C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}
isometric				T	T_d	T_h		O	O_h		I	I_h		**Schoenflies symbol:**						

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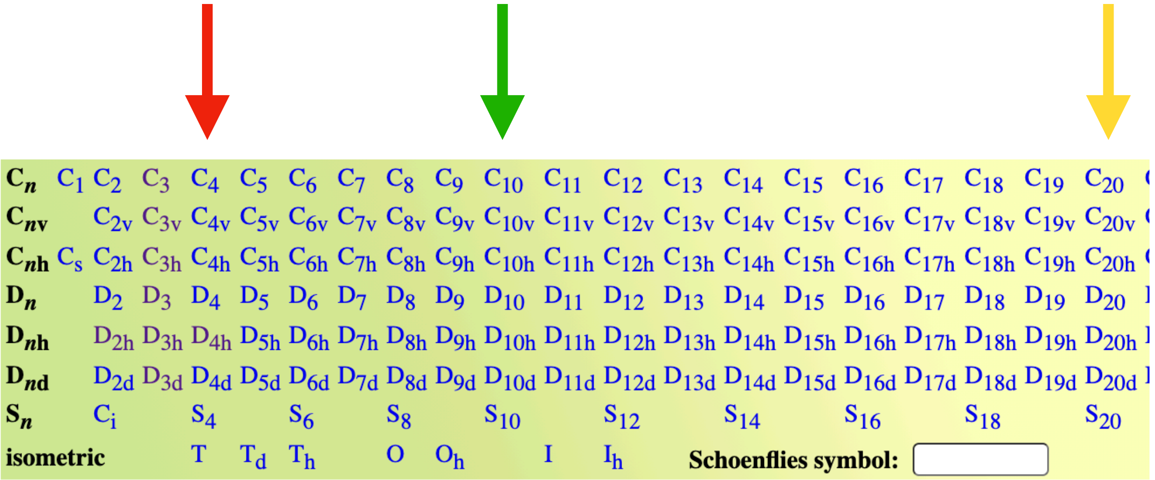

C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}
isometric				T	T_d	T_h		O	O_h		I	I_h	**Schoenflies symbol:**							

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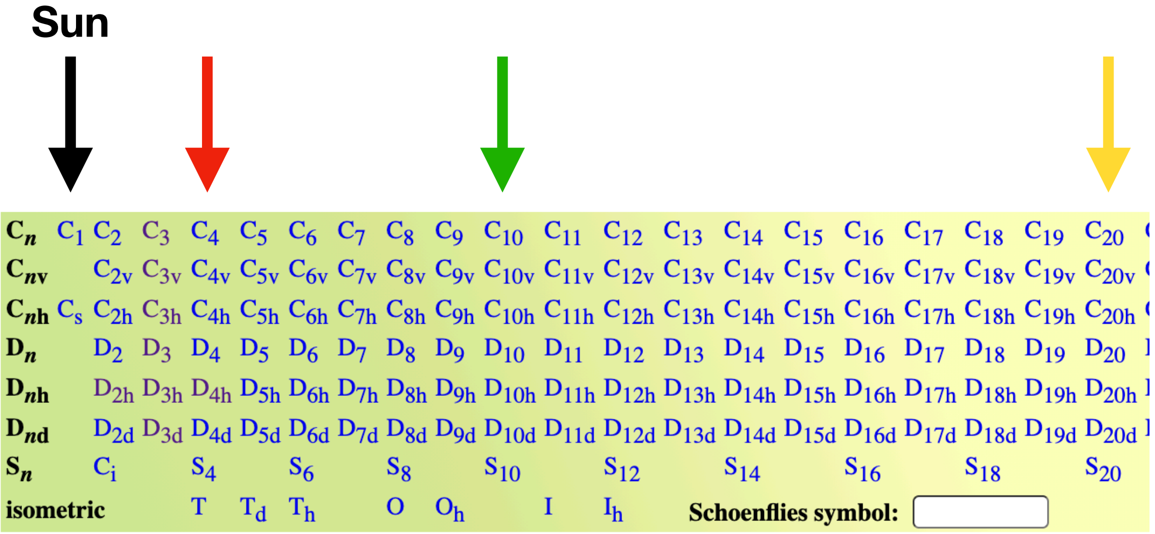

C_n	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	C_{15}	C_{16}	C_{17}	C_{18}	C_{19}	C_{20}
C_{nv}		C_{2v}	C_{3v}	C_{4v}	C_{5v}	C_{6v}	C_{7v}	C_{8v}	C_{9v}	C_{10v}	C_{11v}	C_{12v}	C_{13v}	C_{14v}	C_{15v}	C_{16v}	C_{17v}	C_{18v}	C_{19v}	C_{20v}
C_{nh}	C_s	C_{2h}	C_{3h}	C_{4h}	C_{5h}	C_{6h}	C_{7h}	C_{8h}	C_{9h}	C_{10h}	C_{11h}	C_{12h}	C_{13h}	C_{14h}	C_{15h}	C_{16h}	C_{17h}	C_{18h}	C_{19h}	C_{20h}
D_n		D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}	D_{11}	D_{12}	D_{13}	D_{14}	D_{15}	D_{16}	D_{17}	D_{18}	D_{19}	D_{20}
D_{nh}		D_{2h}	D_{3h}	D_{4h}	D_{5h}	D_{6h}	D_{7h}	D_{8h}	D_{9h}	D_{10h}	D_{11h}	D_{12h}	D_{13h}	D_{14h}	D_{15h}	D_{16h}	D_{17h}	D_{18h}	D_{19h}	D_{20h}
D_{nd}		D_{2d}	D_{3d}	D_{4d}	D_{5d}	D_{6d}	D_{7d}	D_{8d}	D_{9d}	D_{10d}	D_{11d}	D_{12d}	D_{13d}	D_{14d}	D_{15d}	D_{16d}	D_{17d}	D_{18d}	D_{19d}	D_{20d}
S_n		C_i		S_4		S_6		S_8		S_{10}		S_{12}		S_{14}		S_{16}		S_{18}		S_{20}
isometric				T	T_d	T_h		O	O_h		I	I_h		**Schoenflies symbol:**						

What does this all have to do with SC order parameters?

Review of basic symmetries of the order parameter

From fermionic anti-symmetry: $\hat{\Delta}(\mathbf{k}) = -\,\hat{\Delta}^T(-\mathbf{k})$

$$\Delta_{\alpha\beta}(\mathbf{k}) \sim \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle$$

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If inversion is a symmetry: $P\hat{\Delta}(\mathbf{k})P^{-1} = \hat{\Delta}(-\mathbf{k}) = \pm\,\Delta(\mathbf{k})$

[Assumption: does not modify the internal DOFs]

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[Assumption: does not modify the internal DOFs]

Two decoupled sectors of SC order parameters:

$$\hat{\Delta}_E(\mathbf{k}) = -\,\hat{\Delta}_E^T(-\mathbf{k}) = -\,\hat{\Delta}_E^T(\mathbf{k})$$

$$\dashrightarrow\ (i\sigma_2)$$

$\sim |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

Spin Singlet

Even Parity

$$\hat{\Delta}_O(\mathbf{k}) = -\,\hat{\Delta}_O^T(-\mathbf{k}) = \hat{\Delta}_O^T(\mathbf{k})$$

$$\dashrightarrow\ \sigma_3 \propto \sigma_1(i\sigma_2)$$

$$\dashrightarrow\ \sigma_0 \propto \sigma_2(i\sigma_2)$$

$$\dashrightarrow\ \sigma_1 \propto \sigma_3(i\sigma_2)$$

$\sim |\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle$

$\sim |\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$

$\sim |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$

Spin triplet

Odd Parity

Review of basic symmetries of the order parameter

From fermionic anti-symmetry: $\hat{\Delta}(\mathbf{k}) = -\,\hat{\Delta}^T(-\mathbf{k})$

$$\Delta_{\alpha\beta}(\mathbf{k}) \sim \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle$$

For a generic symmetry G:

$$D(G)\hat{\Delta}(\mathbf{k})D(G)^{-1} = \hat{\Delta}[D_{3D}^{-1}(G)\mathbf{k}] = \pm\,\Delta(\mathbf{k})$$

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Can classify the order parameter according to its properties under a given symmetry operation (as even/odd in analogy to the parity)

Preserves Symmetry

Breaks Symmetry

Review of basic symmetries of the order parameter

From fermionic anti-symmetry: $\hat{\Delta}(\mathbf{k}) = -\,\hat{\Delta}^T(-\mathbf{k})$

$$\Delta_{\alpha\beta}(\mathbf{k}) \sim \langle c_{-\mathbf{k}\alpha} c_{\mathbf{k}\beta} \rangle$$

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$$D(G)\hat{\Delta}(\mathbf{k})D(G)^{-1} = \hat{\Delta}[D_{3D}^{-1}(G)\mathbf{k}] = \pm\,\Delta(\mathbf{k})$$

Can classify the order parameter according to its properties under a given symmetry operation (as even/odd in analogy to the parity)

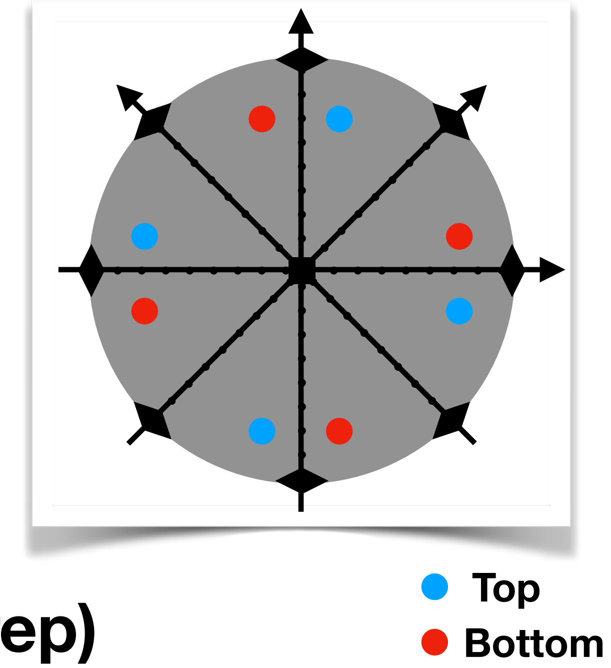
Preserves Symmetry

Breaks Symmetry

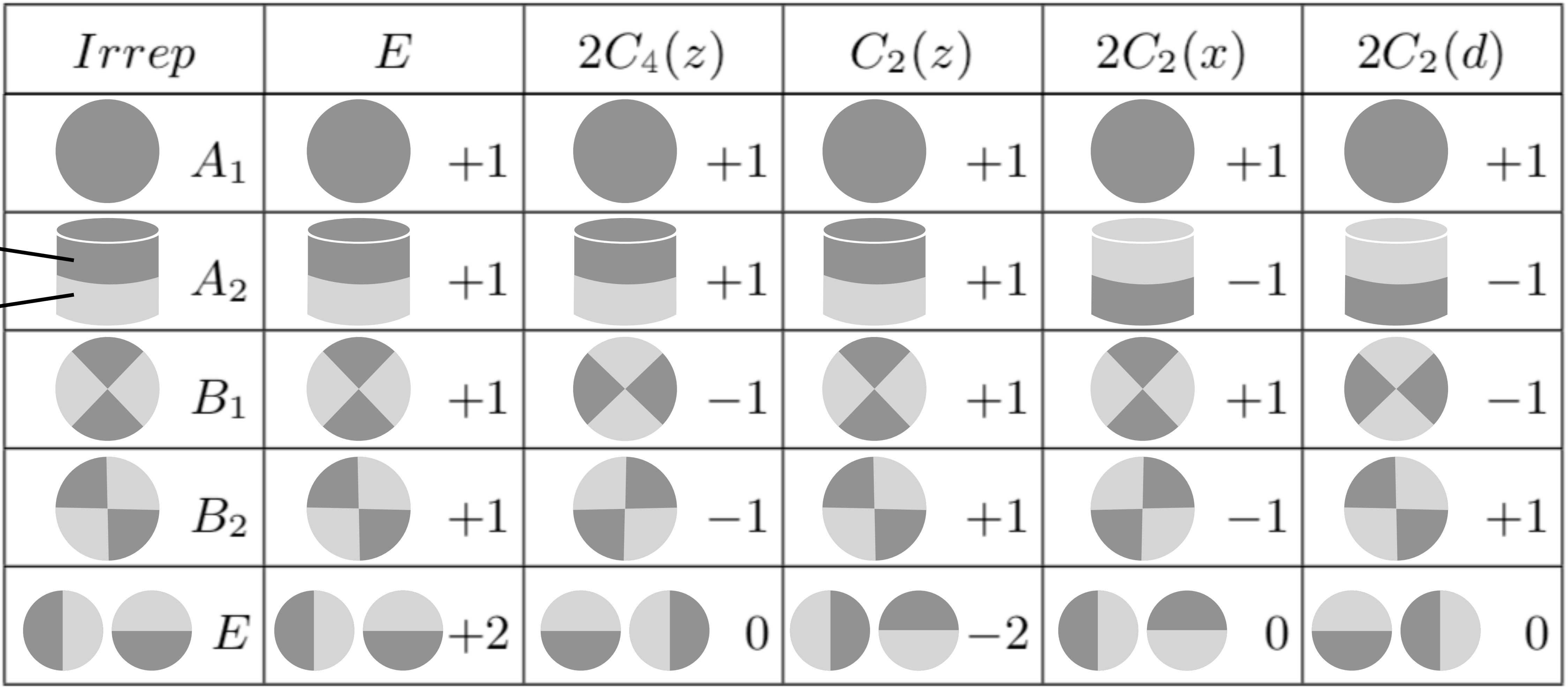
Note: Now there can be multiple symmetry operations present!

[Irreducible representations are now useful!]

D_4 [dihedral] point group



Character table and irreducible representations (Irrep)

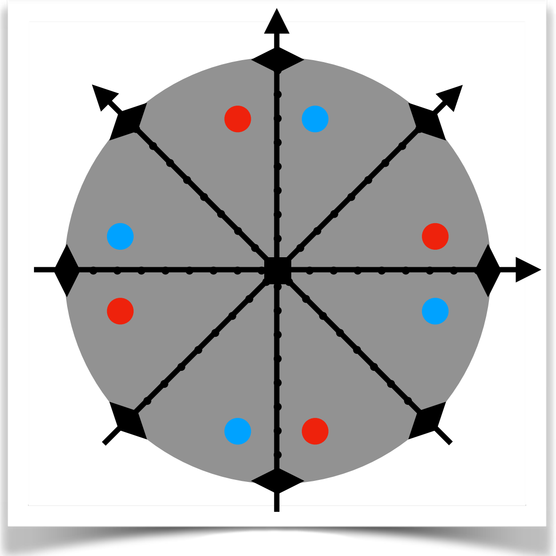


+1

-1

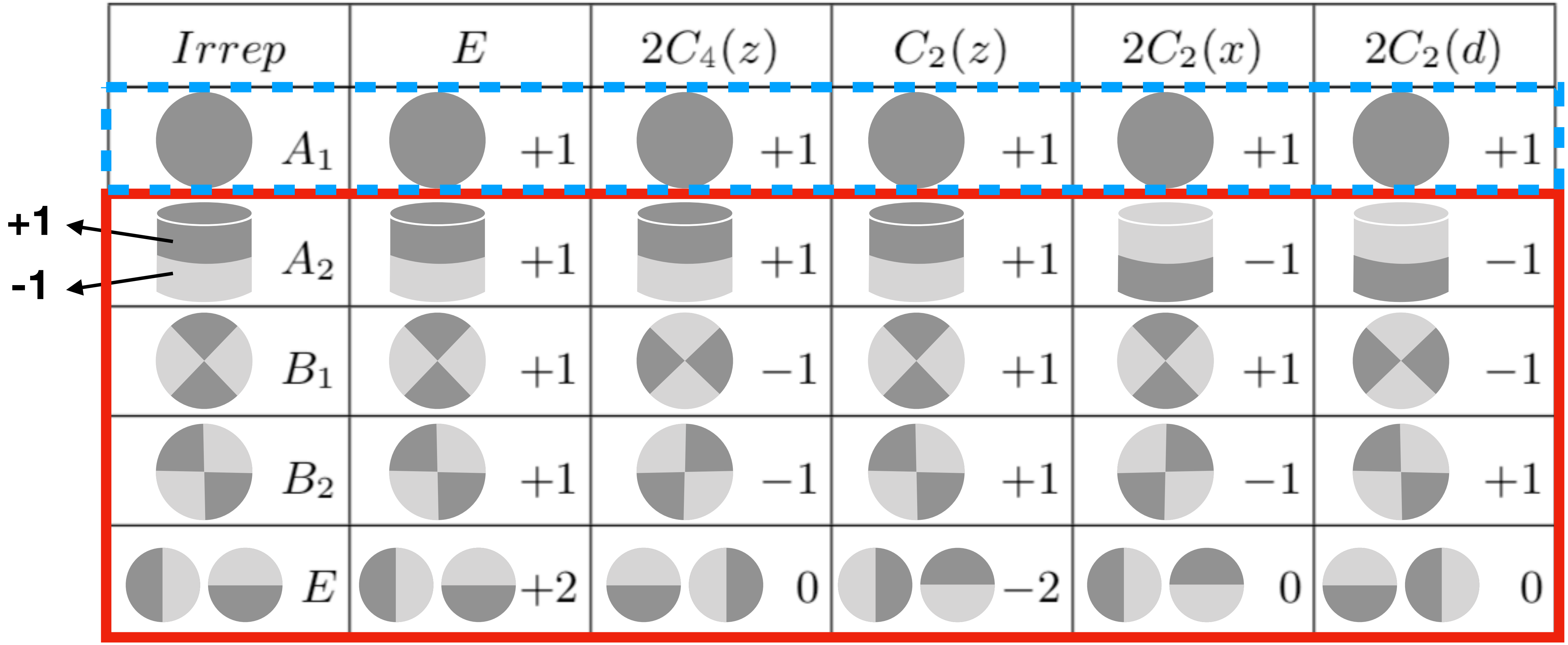
$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$	Basis functions
A_1	$+1$	$+1$	$+1$	$+1$	$+1$	~cte
A_2	$+1$	$+1$	$+1$	-1	-1	~z
B_1	$+1$	-1	$+1$	$+1$	-1	~x^2-y^2
B_2	$+1$	-1	$+1$	-1	$+1$	~xy
E	$+2$	0	-2	0	0	~{x,y}

D_4 [dihedral] point group



● Top
● Bottom

Character table and irreducible representations (Irrep)



$Irrep$	E	$2C_4(z)$	$C_2(z)$	$2C_2(x)$	$2C_2(d)$	
A_1	$+1$	$+1$	$+1$	$+1$	$+1$	~cte
A_2	$+1$	$+1$	$+1$	-1	-1	~z
B_1	$+1$	-1	$+1$	$+1$	-1	~x^2-y^2
B_2	$+1$	-1	$+1$	-1	$+1$	~xy
E	$+2$	0	-2	0	0	~{x,y}

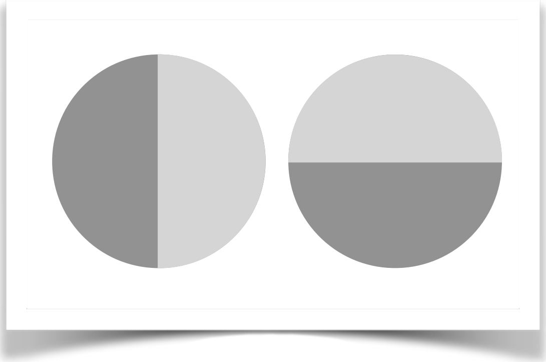
Unconventional SC: (almost always) Nodal gap structure!

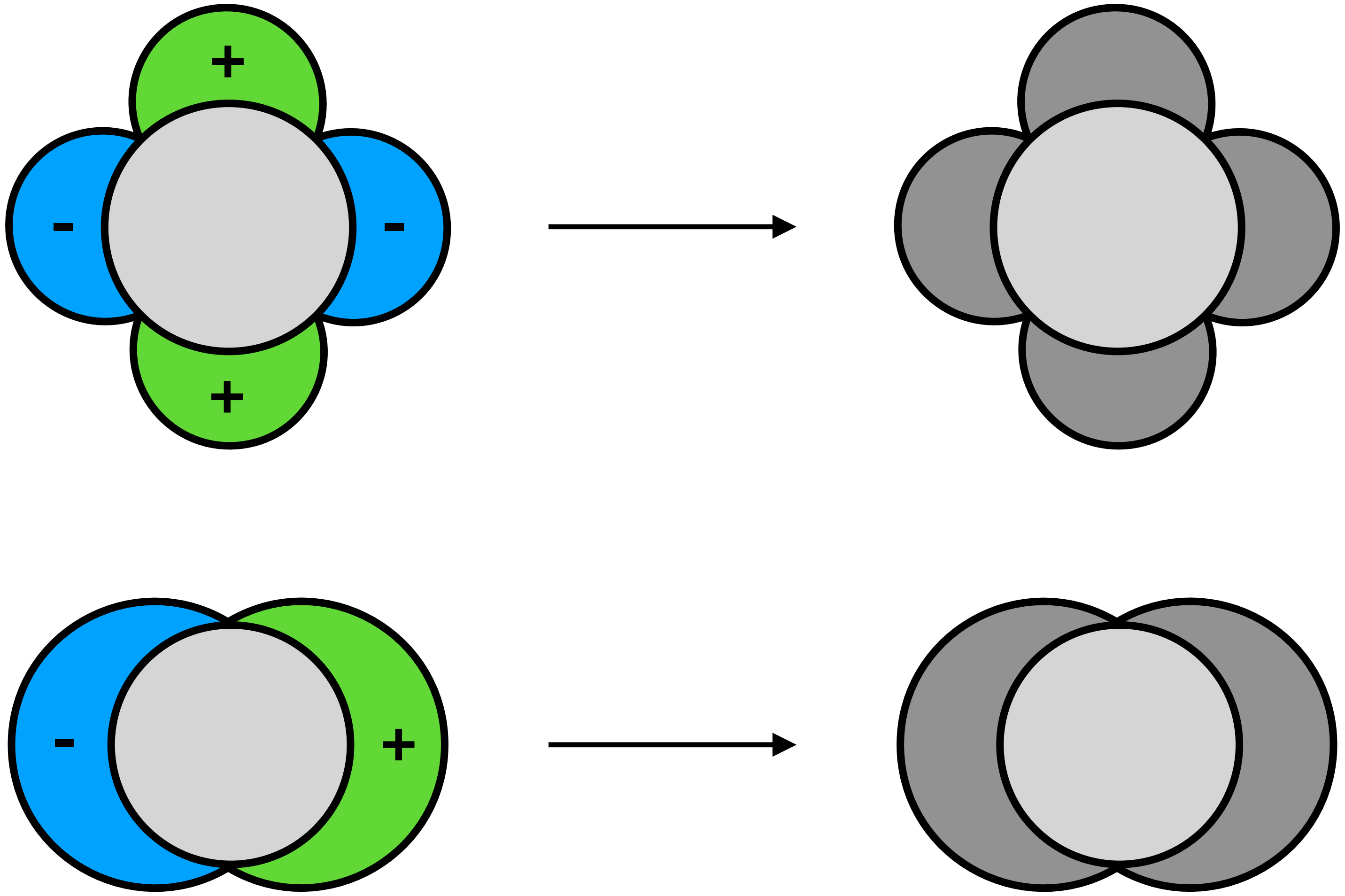
Conventional SC: (almost always) Fully gapped!

Basis functions

Unconventional Superconductors

Special scenario I: 2D Irrep and Nematicity





Gap **Gap amplitude**

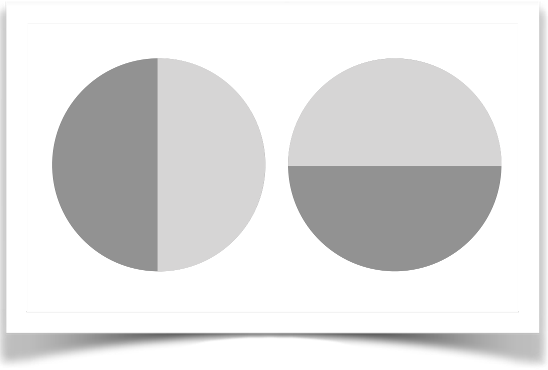
1D Irrep

…preserves the point group symmetry.

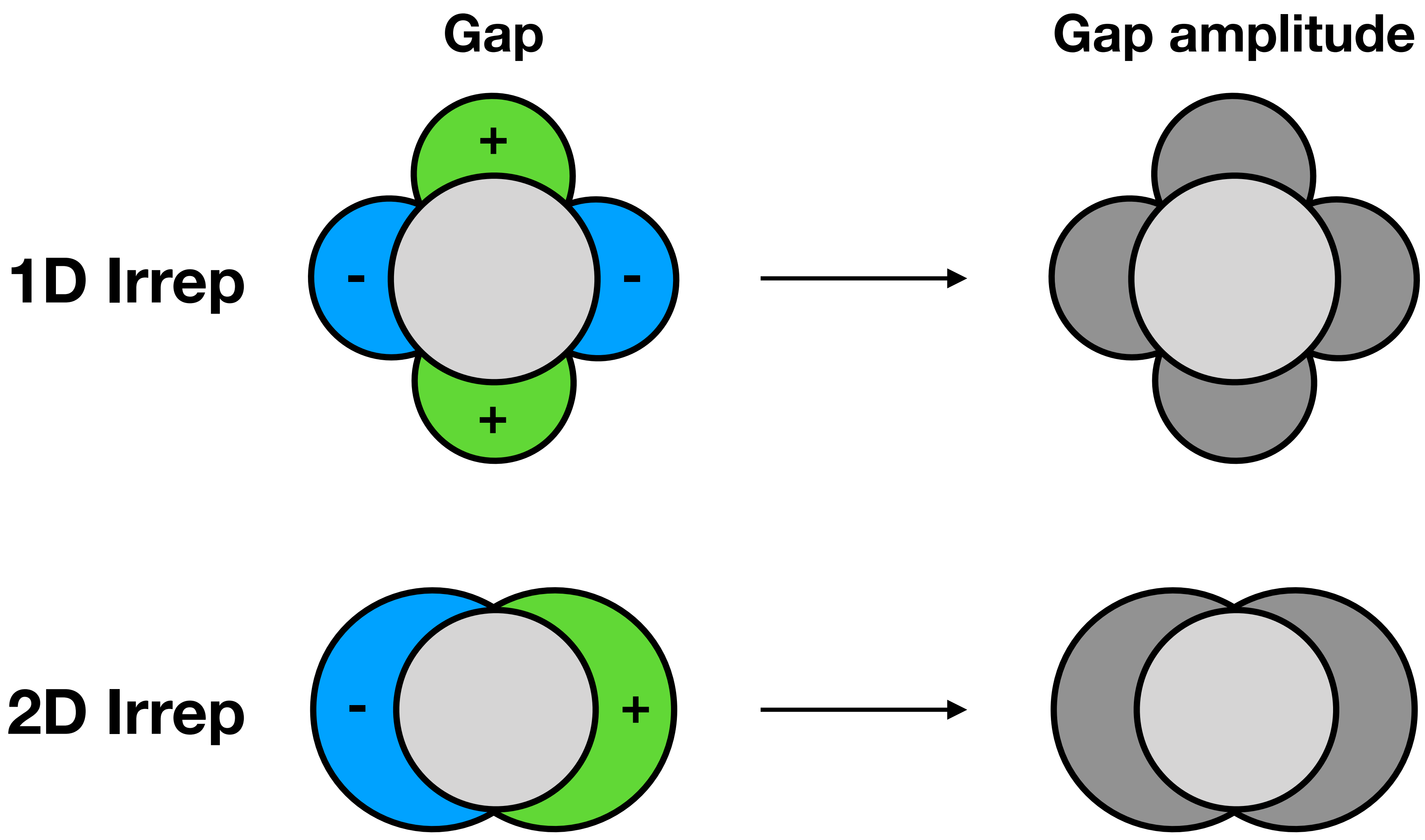
2D Irrep

…breaks the point group symmetry.

Unconventional Superconductors



Special scenario I: 2D Irrep and Nematicity

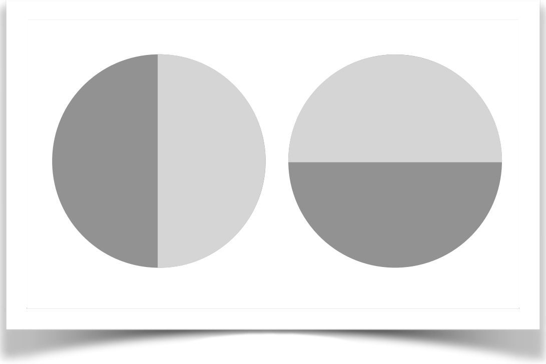


…preserves the point group symmetry.

[NEMATIC SC]

…breaks the point group symmetry.

Unconventional Superconductors



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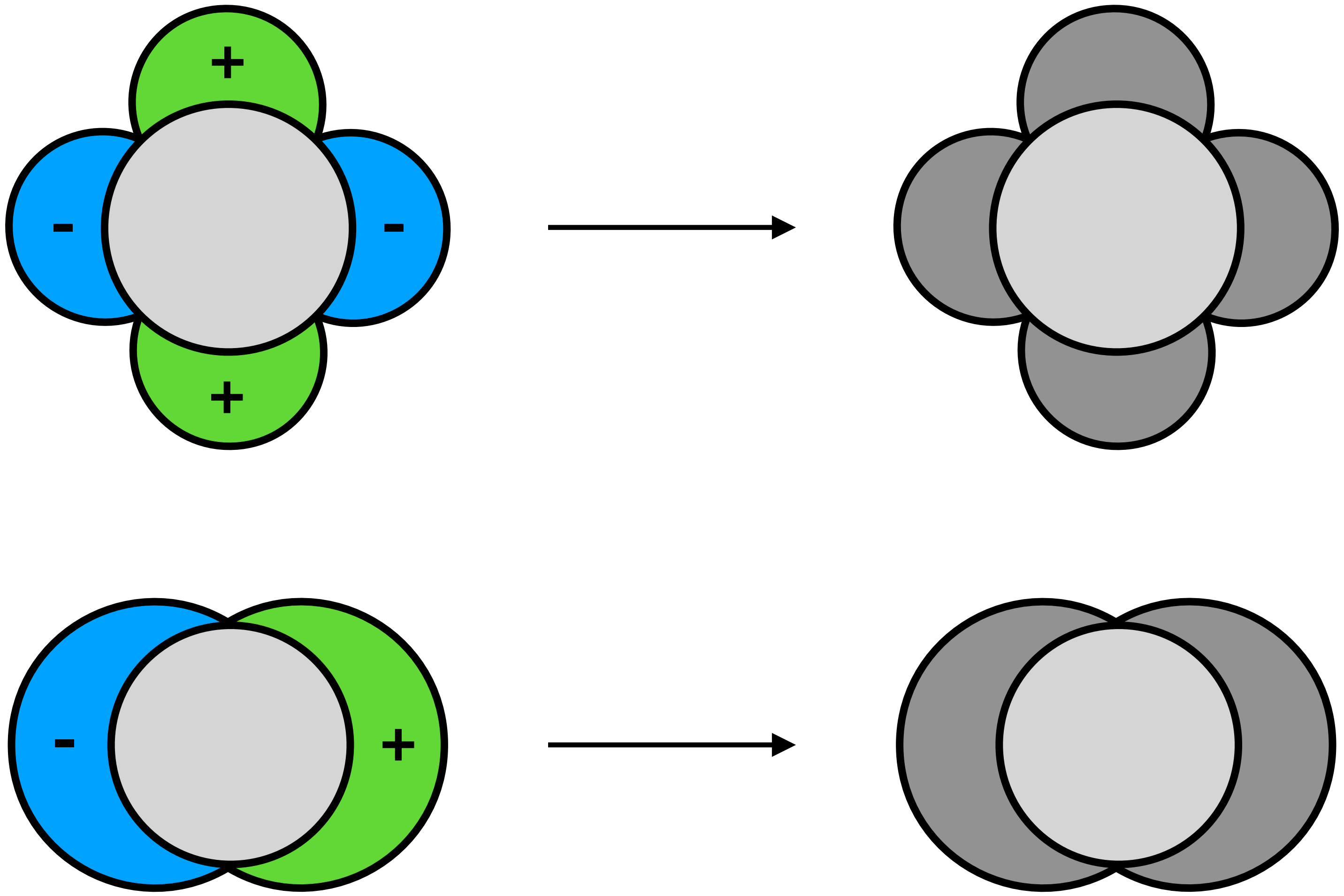


Gap

Gap amplitude

1D Irrep

...preserves the point group symmetry.

2D Irrep

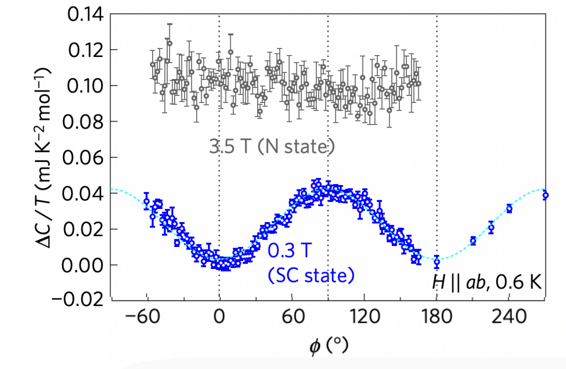
[NEMATIC SC]

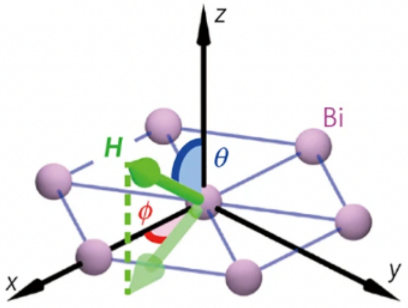
...breaks the point group symmetry.

What are the observable consequences?

- Distinct anisotropy in C/T and H_{c2}
- Associated lattice deformations

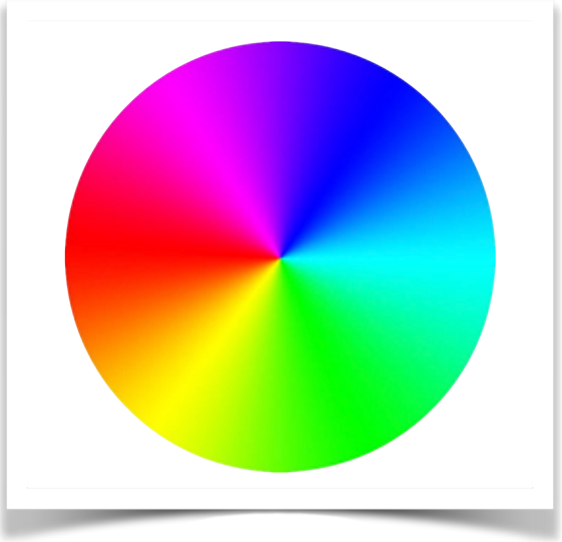
$Cu_xBi_2Se_3$





S. Yonezawa et al., Nature Physics **13**, 123 (2017)

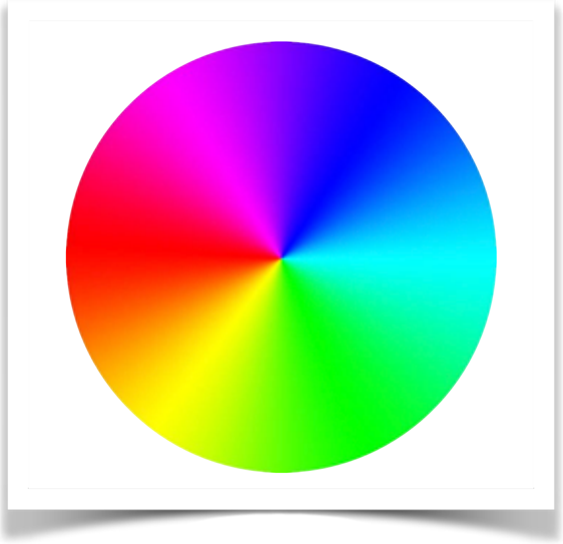
Unconventional Superconductors



Special scenario II: 2D Irrep and TRSB

A complex superposition of the two components in a 2D irrep usually lifts the nodes (generally more stable):

Unconventional Superconductors



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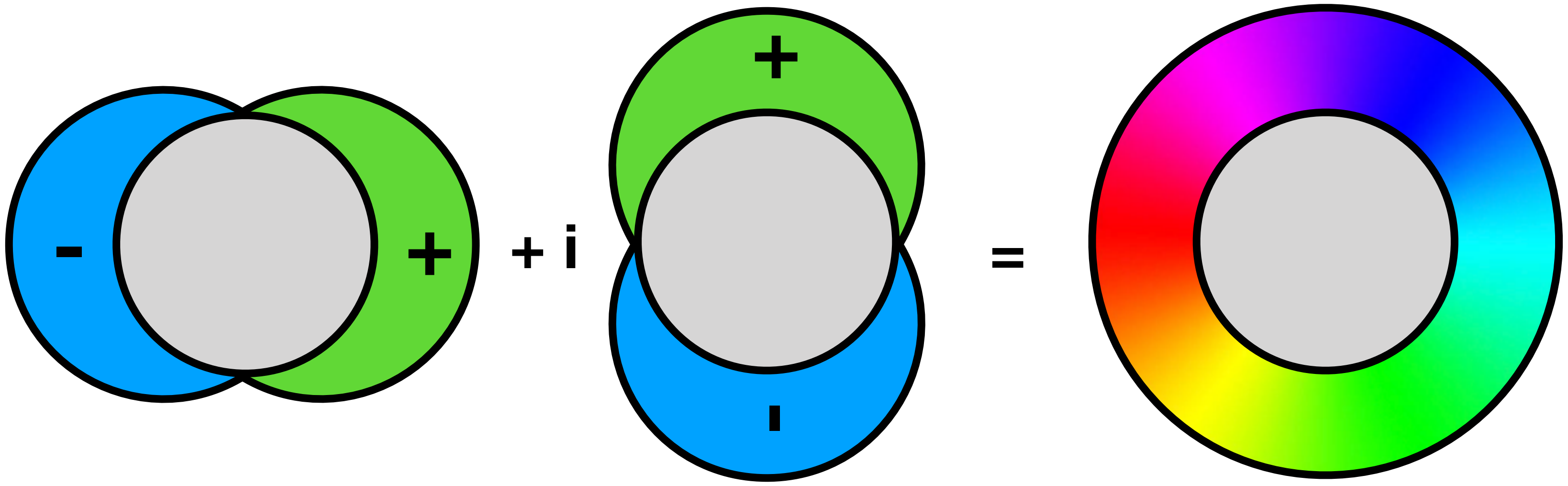
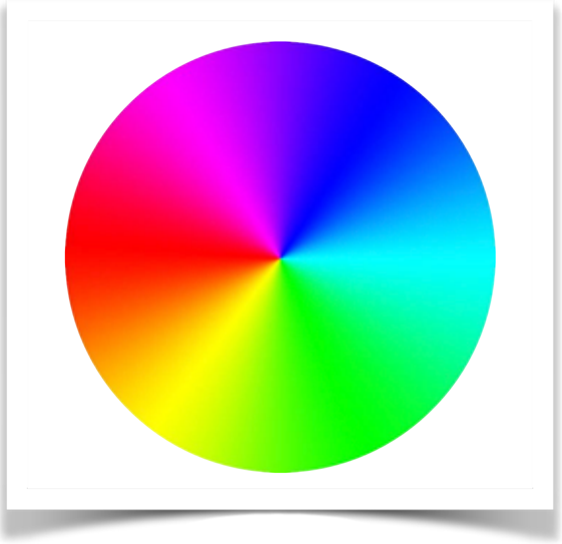


Unconventional Superconductors



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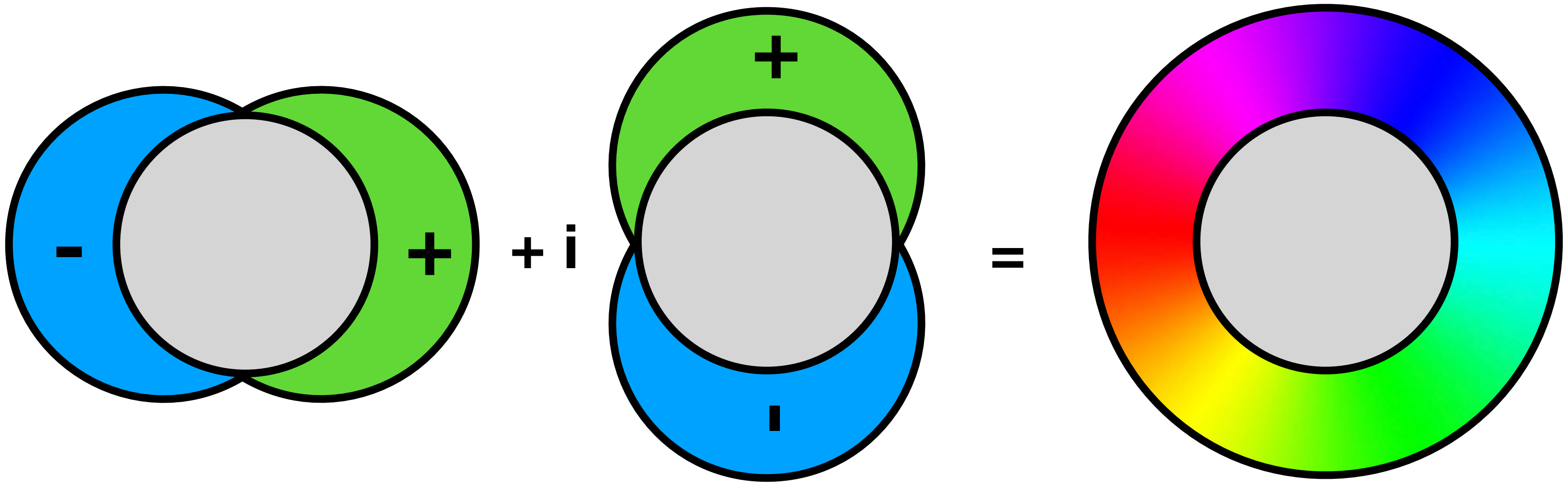


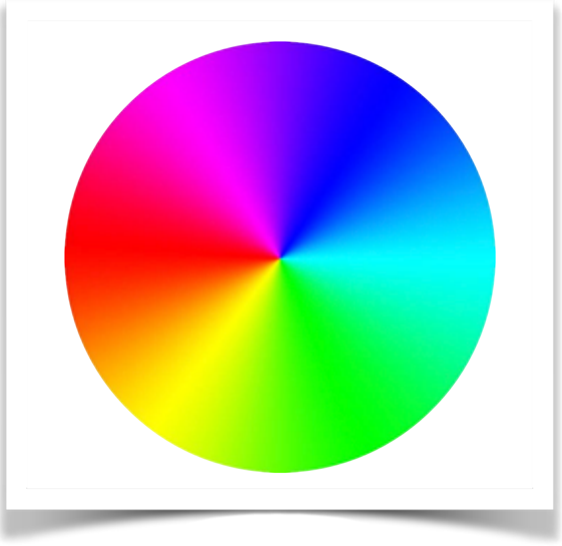
[CHIRAL SC]

$$\Delta(\mathbf{k}) \sim k_x \pm i k_y$$

$$|\,\Delta(\mathbf{k})\,| \sim k_x^2 + k_y^2$$

Note: Isotropic Gap, but certainly unconventional!

Unconventional Superconductors



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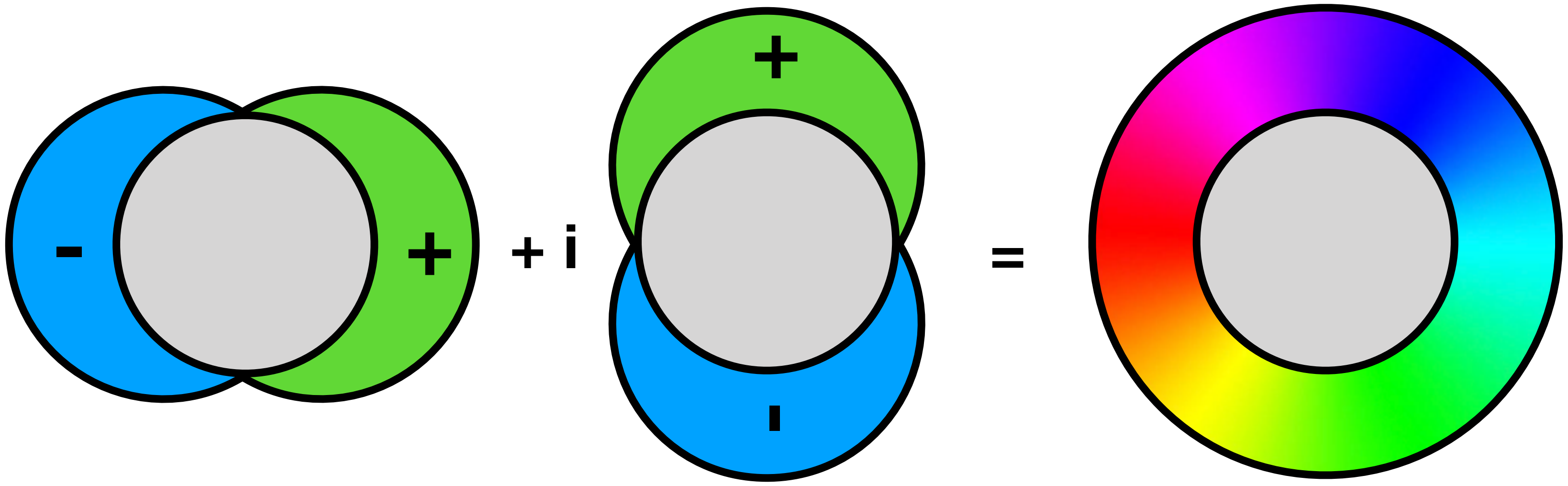

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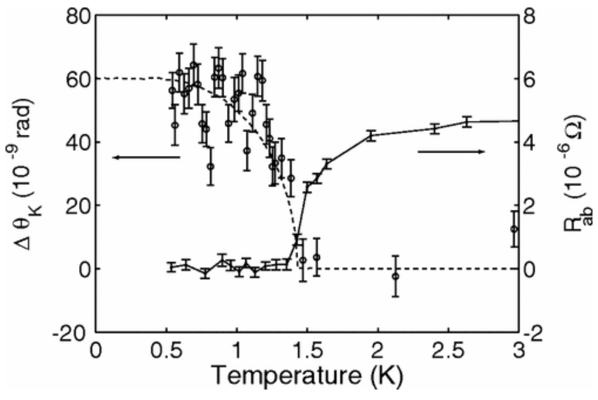
What are the observable consequences?

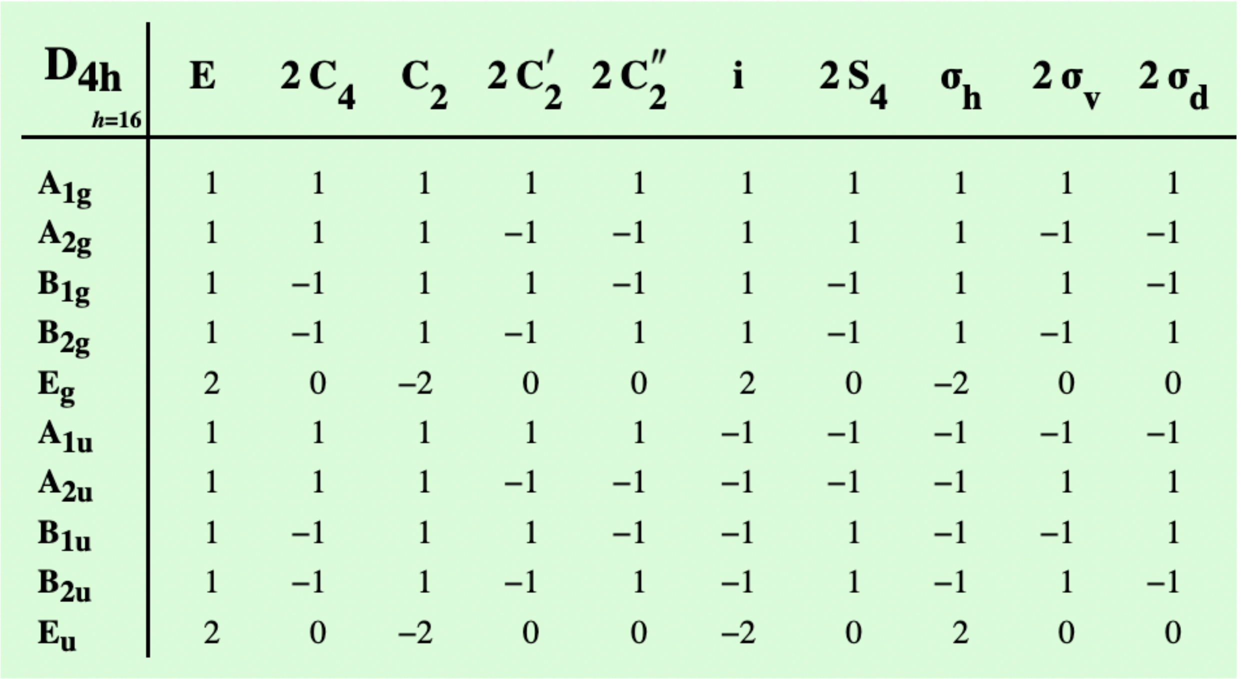
- **Polar Kerr Effect**
- **Muon Spin Relaxation**

Sr_2RuO_4

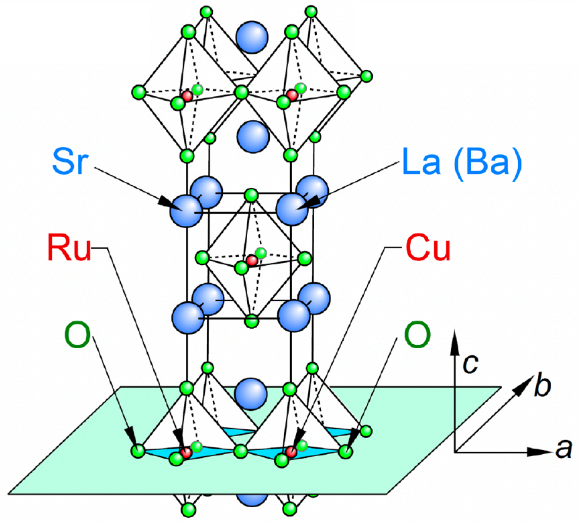


J. Xia et al., Phys. Rev. Lett. **97**, 167002 (2006)

$D_{4h} = D_4$ + inversion



D_{4h} $h=16$	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1
E_g	2	0	−2	0	0	2	0	−2	0	0
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1
E_u	2	0	−2	0	0	−2	0	2	0	0



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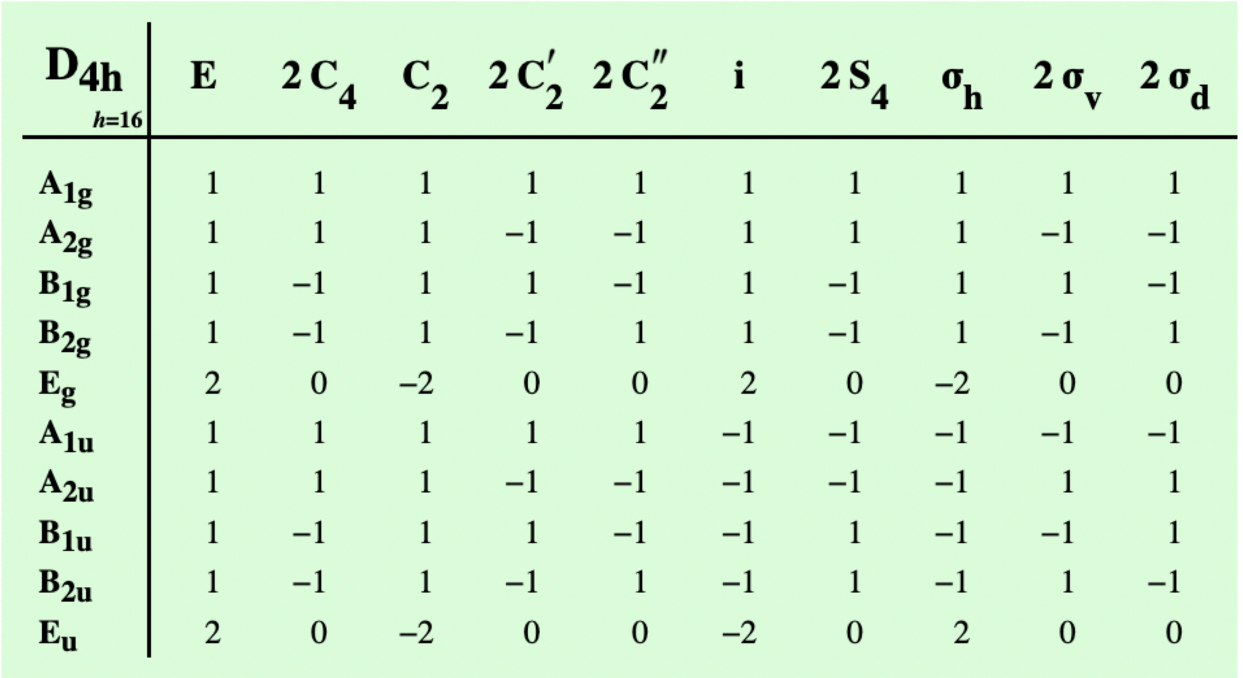
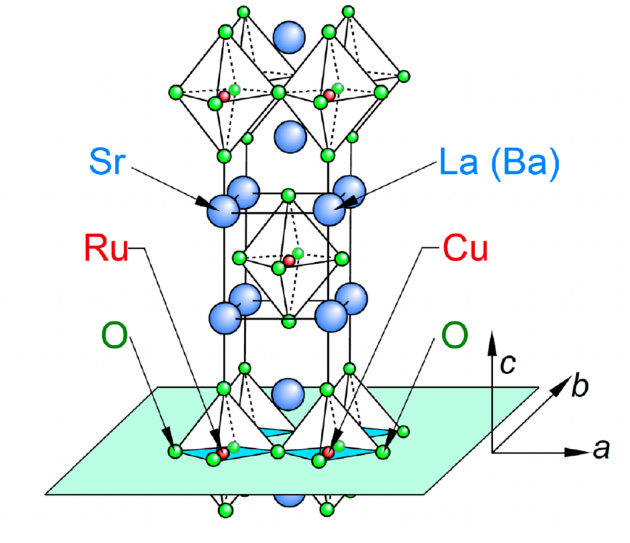
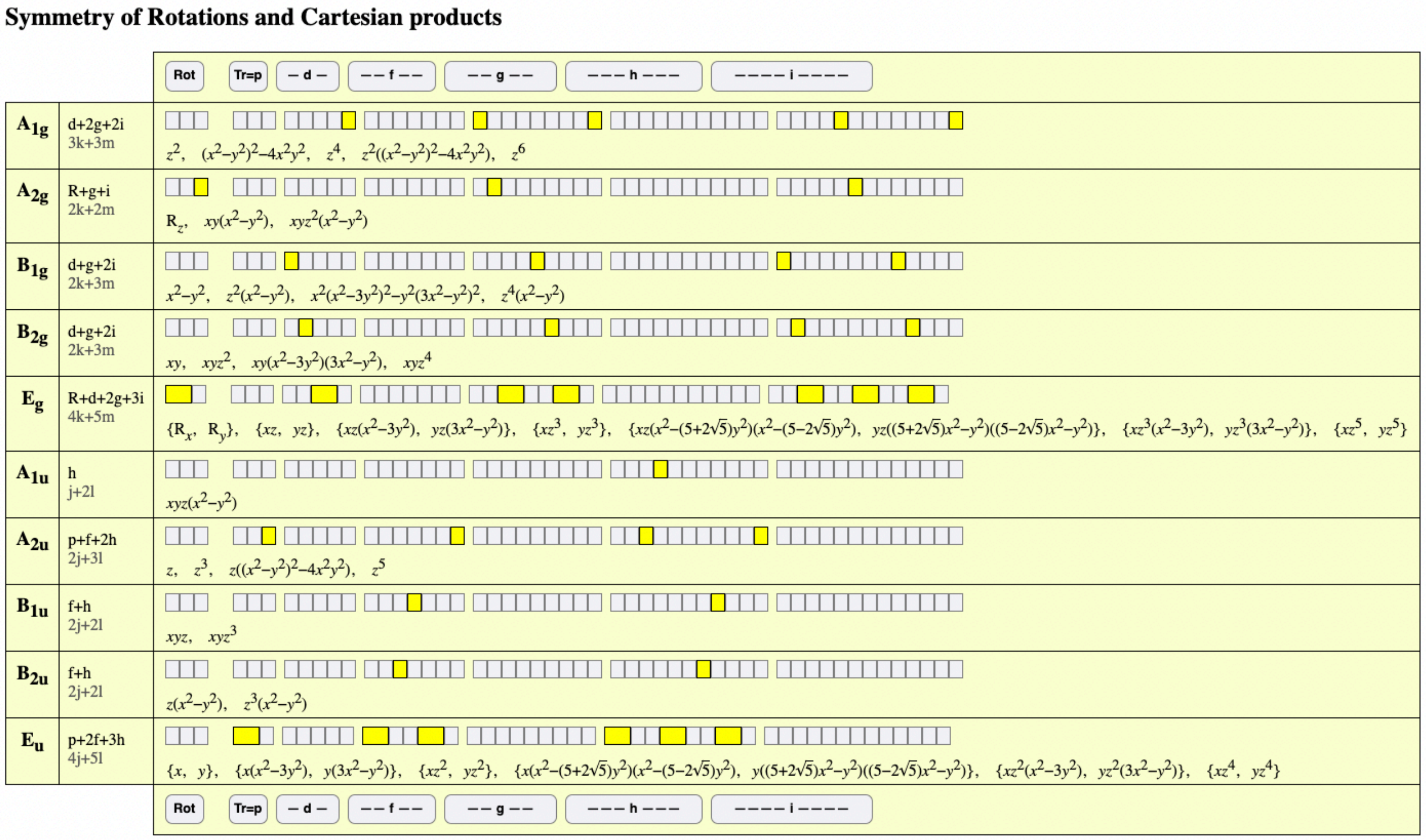


D_{4h} $h=16$	E	$2C_4$	C_2	$2C_2'$	$2C_2''$	i	$2S_4$	σ_h	$2\sigma_v$	$2\sigma_d$
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1
E_g	2	0	−2	0	0	2	0	−2	0	0
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1
E_u	2	0	−2	0	0	−2	0	2	0	0

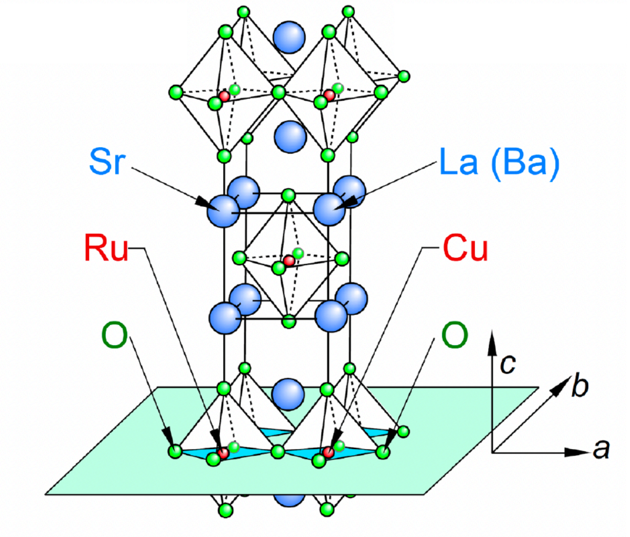


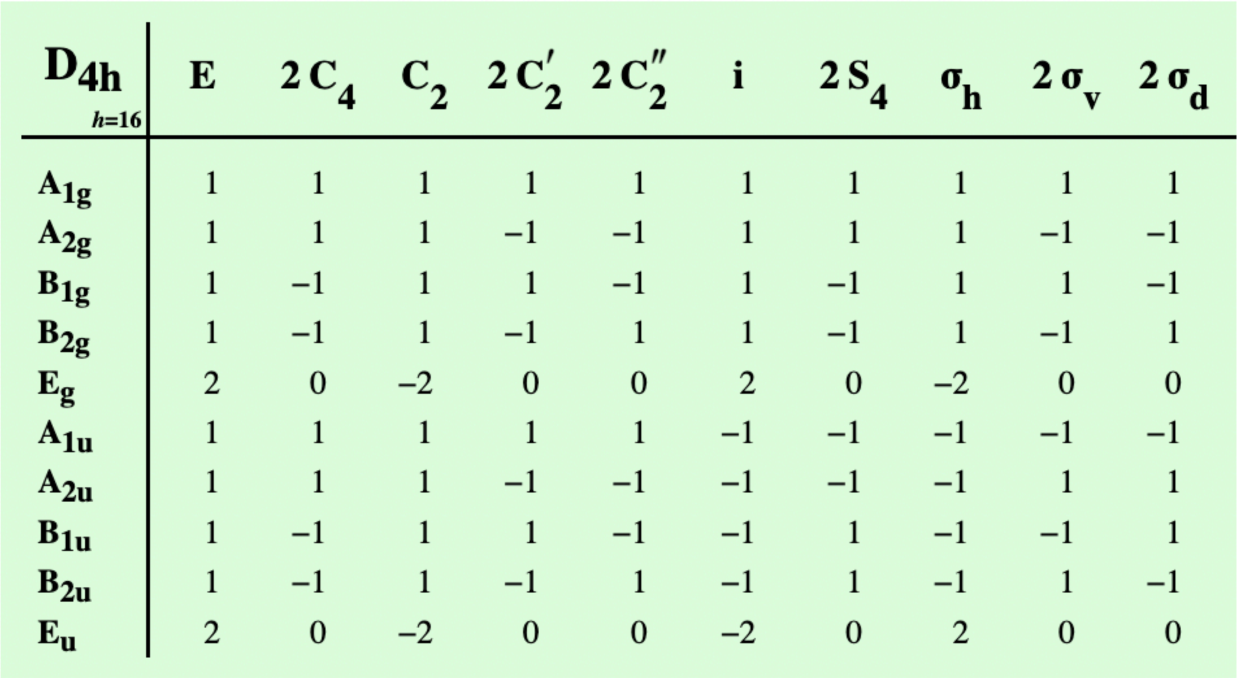


Symmetry of Rotations and Cartesian products

		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –
A_{1g}	d+2g+2i 3k+3m	z^2, $(x^2-y^2)^2-4x^2y^2$, z^4, $z^2((x^2-y^2)^2-4x^2y^2)$, z^6
A_{2g}	R+g+i 2k+2m	R_z, $xy(x^2-y^2)$, $xyz^2(x^2-y^2)$
B_{1g}	d+g+2i 2k+3m	x^2-y^2, $z^2(x^2-y^2)$, $x^2(x^2-3y^2)^2-y^2(3x^2-y^2)^2$, $z^4(x^2-y^2)$
B_{2g}	d+g+2i 2k+3m	xy, xyz^2, $xy(x^2-3y^2)(3x^2-y^2)$, xyz^4
E_g	R+d+2g+3i 4k+5m	$\{R_x, R_y\}$, $\{xz, yz\}$, $\{xz(x^2-3y^2), yz(3x^2-y^2)\}$, $\{xz^3, yz^3\}$, $\{xz(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), yz((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{xz^3(x^2-3y^2), yz^3(3x^2-y^2)\}$, $\{xz^5, yz^5\}$
A_{1u}	h j+2l	$xyz(x^2-y^2)$
A_{2u}	p+f+2h 2j+3l	z, z^3, $z((x^2-y^2)^2-4x^2y^2)$, z^5
B_{1u}	f+h 2j+2l	xyz, xyz^3
B_{2u}	f+h 2j+2l	$z(x^2-y^2)$, $z^3(x^2-y^2)$
E_u	p+2f+3h 4j+5l	$\{x, y\}$, $\{x(x^2-3y^2), y(3x^2-y^2)\}$, $\{xz^2, yz^2\}$, $\{x(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), y((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{xz^2(x^2-3y^2), yz^2(3x^2-y^2)\}$, $\{xz^4, yz^4\}$
		Rot Tr=p – d – – – f – – – – g – – – – – h – – – – – – – i – – – –

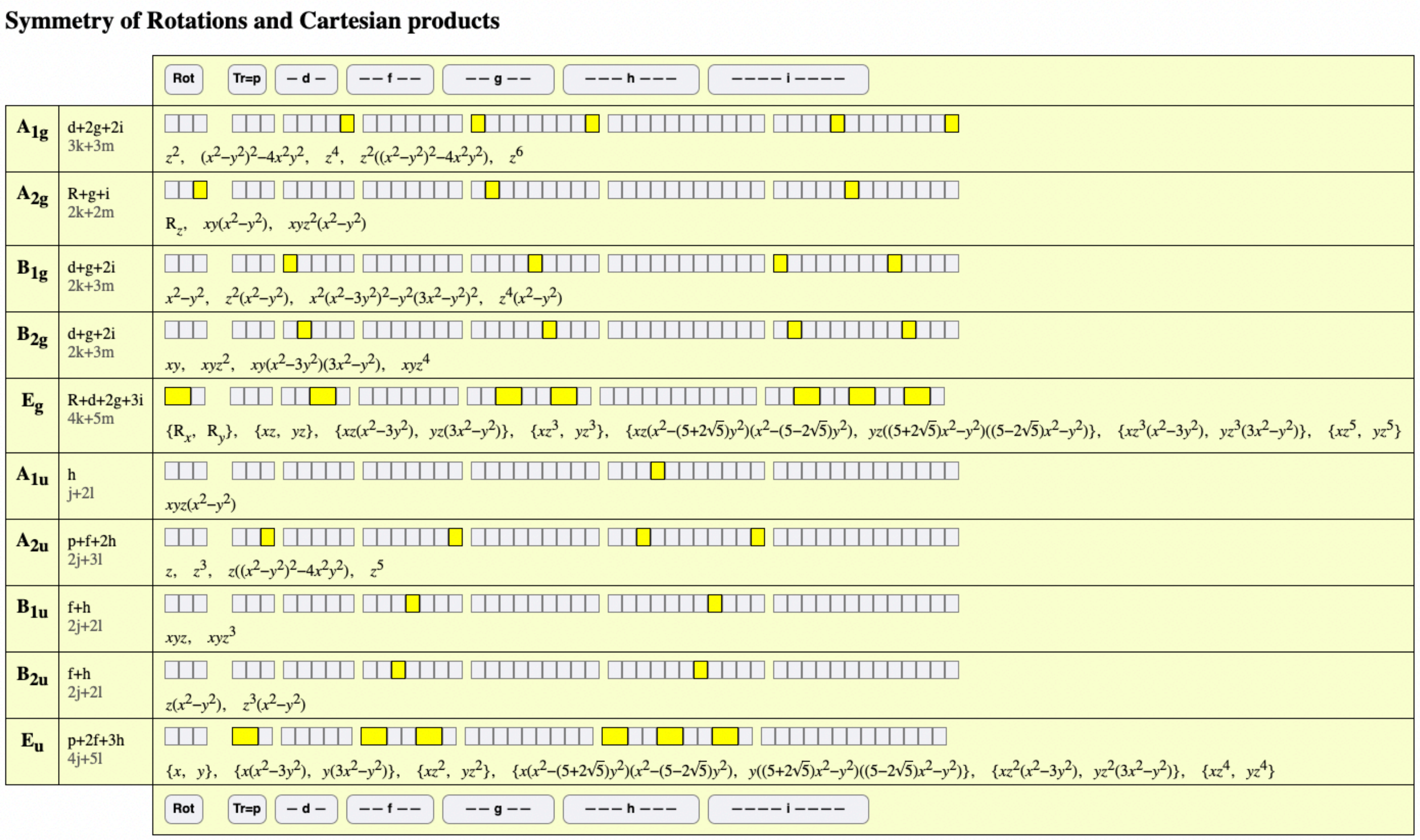
D_{4h} = D_4 + inversion





D_{4h} h=16	E	2 C_4	C_2	2 C_2'	2 C_2''	i	2 S_4	σ_h	2 σ_v	2 σ_d
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	1	−1	−1	1	1	1	−1	−1
B_{1g}	1	−1	1	1	−1	1	−1	1	1	−1
B_{2g}	1	−1	1	−1	1	1	−1	1	−1	1
E_g	2	0	−2	0	0	2	0	−2	0	0
A_{1u}	1	1	1	1	1	−1	−1	−1	−1	−1
A_{2u}	1	1	1	−1	−1	−1	−1	−1	1	1
B_{1u}	1	−1	1	1	−1	−1	1	−1	−1	1
B_{2u}	1	−1	1	−1	1	−1	1	−1	1	−1
E_u	2	0	−2	0	0	−2	0	2	0	0

Only gives us information about the k-dependent part of the gap function.



Symmetry of Rotations and Cartesian products

Rot | Tr=p | – d – | – – f – – | – – g – – | – – – h – – – | – – – – i – – – –

A_{1g}	d+2g+2i 3k+3m	z^2, $(x^2-y^2)^2-4x^2y^2$, z^4, $z^2((x^2-y^2)^2-4x^2y^2)$, z^6
A_{2g}	R+g+i 2k+2m	R_z, $xy(x^2-y^2)$, $xyz^2(x^2-y^2)$
B_{1g}	d+g+2i 2k+3m	x^2-y^2, $z^2(x^2-y^2)$, $x^2(x^2-3y^2)^2-y^2(3x^2-y^2)^2$, $z^4(x^2-y^2)$
B_{2g}	d+g+2i 2k+3m	xy, xyz^2, $xy(x^2-3y^2)(3x^2-y^2)$, xyz^4
E_g	R+d+2g+3i 4k+5m	$\{R_x, R_y\}$, $\{xz, yz\}$, $\{xz(x^2-3y^2), yz(3x^2-y^2)\}$, $\{xz^3, yz^3\}$, $\{xz(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), yz((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{xz^3(x^2-3y^2), yz^3(3x^2-y^2)\}$, $\{xz^5, yz^5\}$
A_{1u}	h j+2l	$xyz(x^2-y^2)$
A_{2u}	p+f+2h 2j+3l	z, z^3, $z((x^2-y^2)^2-4x^2y^2)$, z^5
B_{1u}	f+h 2j+2l	xyz, xyz^3
B_{2u}	f+h 2j+2l	$z(x^2-y^2)$, $z^3(x^2-y^2)$
E_u	p+2f+3h 4j+5l	$\{x, y\}$, $\{x(x^2-3y^2), y(3x^2-y^2)\}$, $\{xz^2, yz^2\}$, $\{x(x^2-(5+2\sqrt{5})y^2)(x^2-(5-2\sqrt{5})y^2), y((5+2\sqrt{5})x^2-y^2)((5-2\sqrt{5})x^2-y^2)\}$, $\{xz^2(x^2-3y^2), yz^2(3x^2-y^2)\}$, $\{xz^4, yz^4\}$

Rot | Tr=p | – d – | – – f – – | – – g – – | – – – h – – – | – – – – i – – – –

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Phenomenological theory of unconventional superconductivity

Manfred Sigrist and Kazuo Ueda

Rev. Mod. Phys. **63**, 239 – Published 1 April 1991

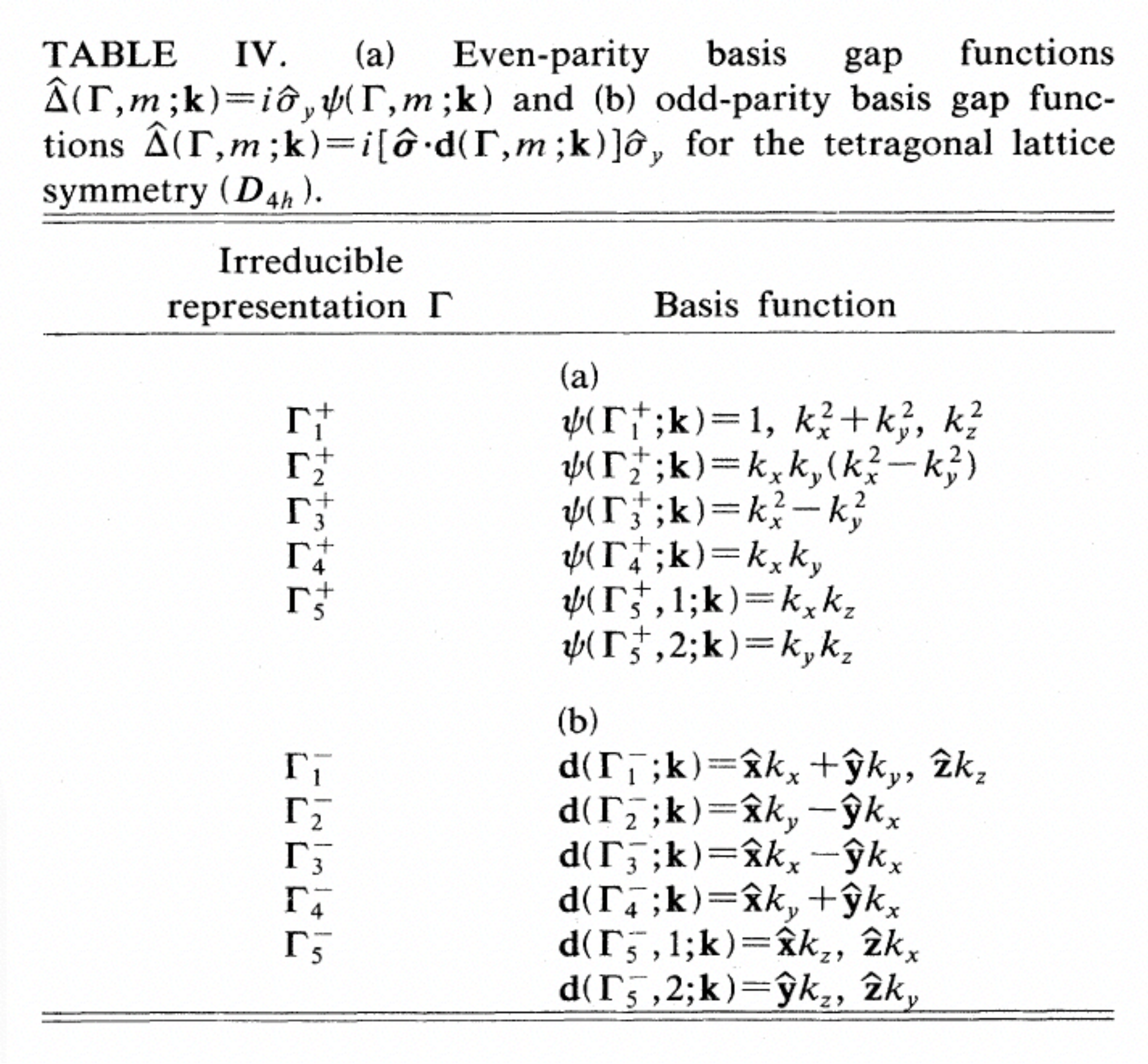

TABLE IV. (a) Even-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i\hat{\sigma}_y\psi(\Gamma,m;\mathbf{k})$ and (b) odd-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i[\hat{\boldsymbol{\sigma}}\cdot\mathbf{d}(\Gamma,m;\mathbf{k})]\hat{\sigma}_y$ for the tetragonal lattice symmetry (D_{4h}).

Irreducible representation Γ	Basis function
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-k_y^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_x^2-k_y^2$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_xk_y$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$
	$\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$

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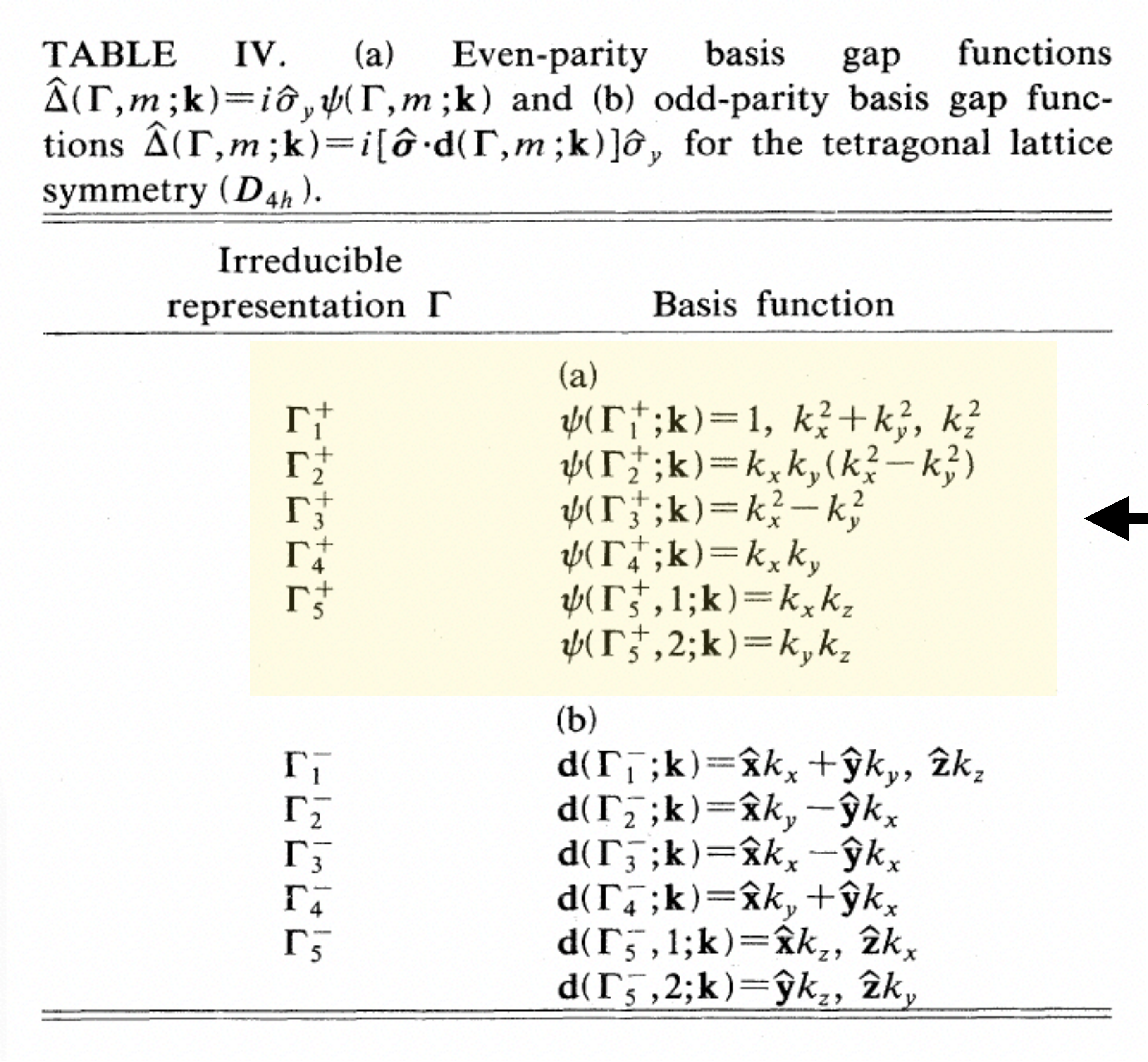

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Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
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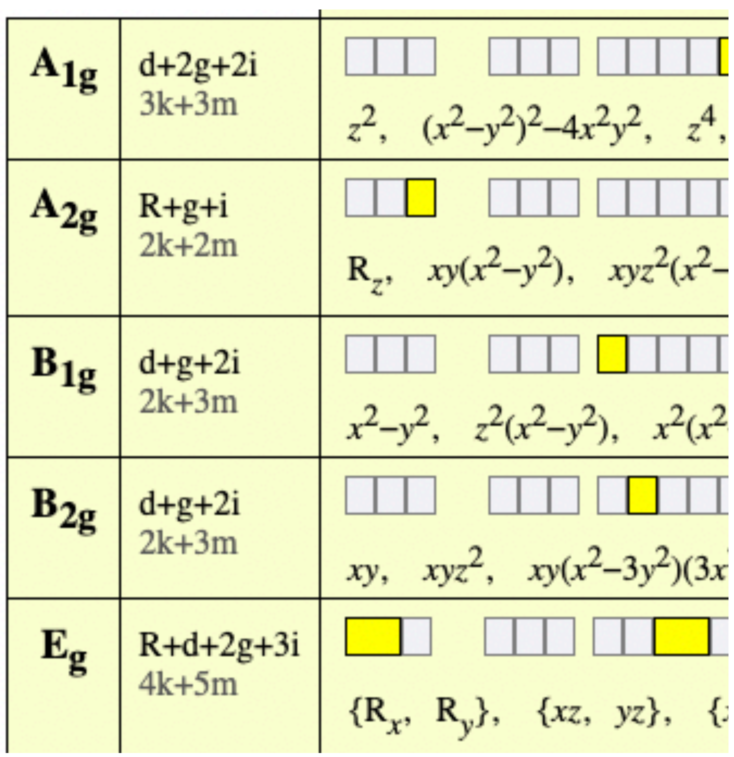
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$



A_{1g}	d+2g+2i 3k+3m	☐☐☐ ☐☐☐ ☐☐☐☐🟨 z^2, $(x^2-y^2)^2-4x^2y^2$, z^4,
A_{2g}	R+g+i 2k+2m	☐☐🟨 ☐☐☐ ☐☐☐☐☐ R_z, $xy(x^2-y^2)$, $xyz^2(x^2-$
B_{1g}	d+g+2i 2k+3m	☐☐☐ ☐☐☐ 🟨☐☐☐☐ x^2-y^2, $z^2(x^2-y^2)$, $x^2(x^2$
B_{2g}	d+g+2i 2k+3m	☐☐☐ ☐☐☐ ☐🟨☐☐☐ xy, xyz^2, $xy(x^2-3y^2)(3x$
E_g	R+d+2g+3i 4k+5m	🟨☐ ☐☐☐ ☐☐🟨☐ $\{R_x,\ R_y\}$, $\{xz,\ yz\}$, $\{$

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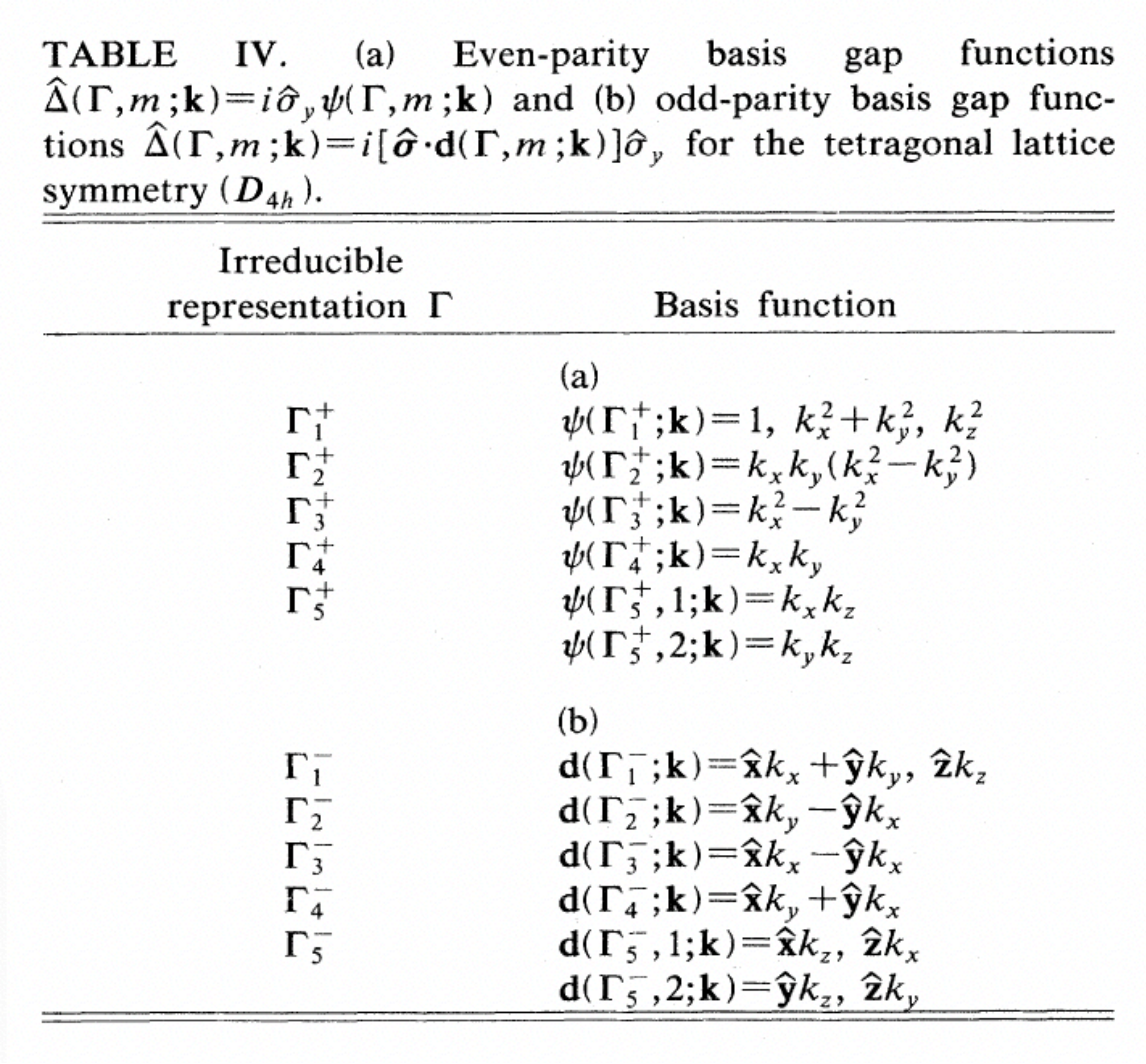

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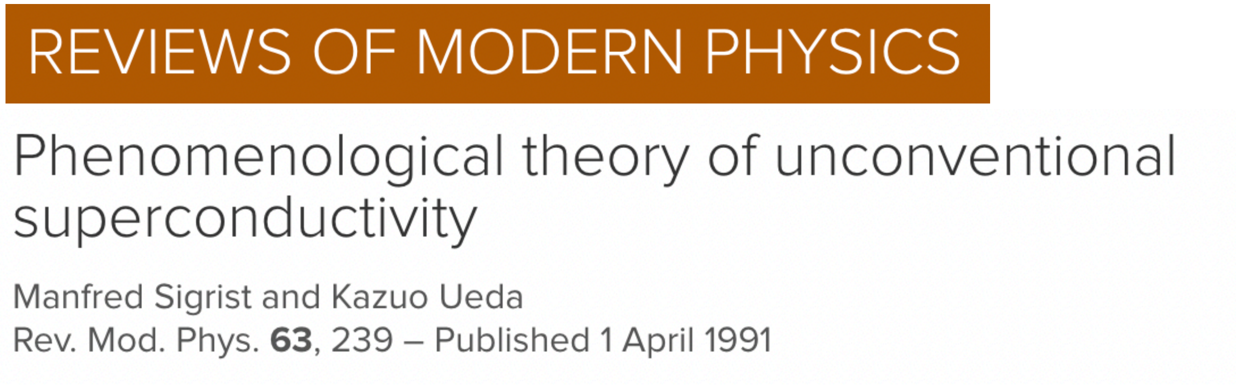
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_xk_y$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$
	$\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$



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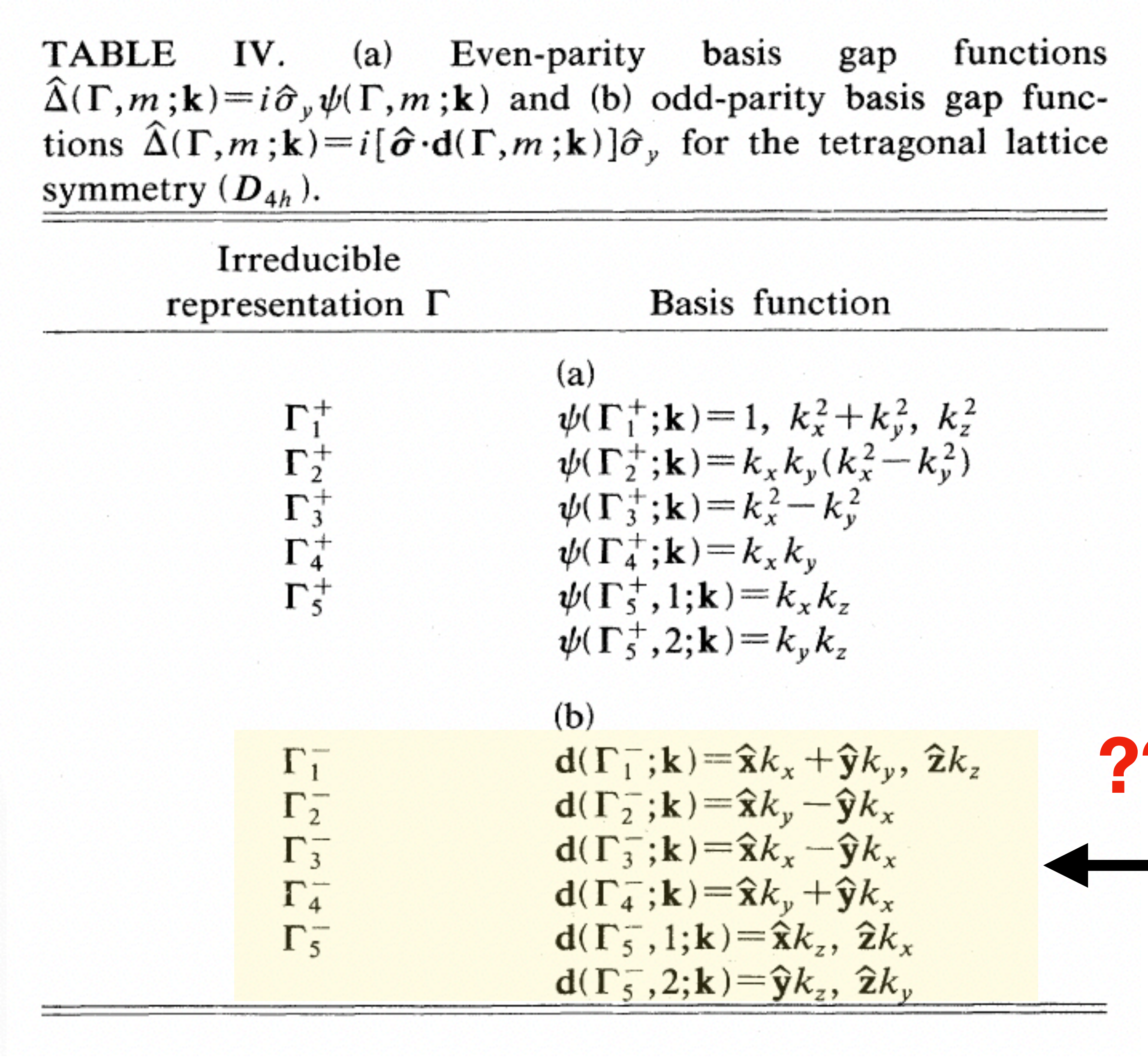
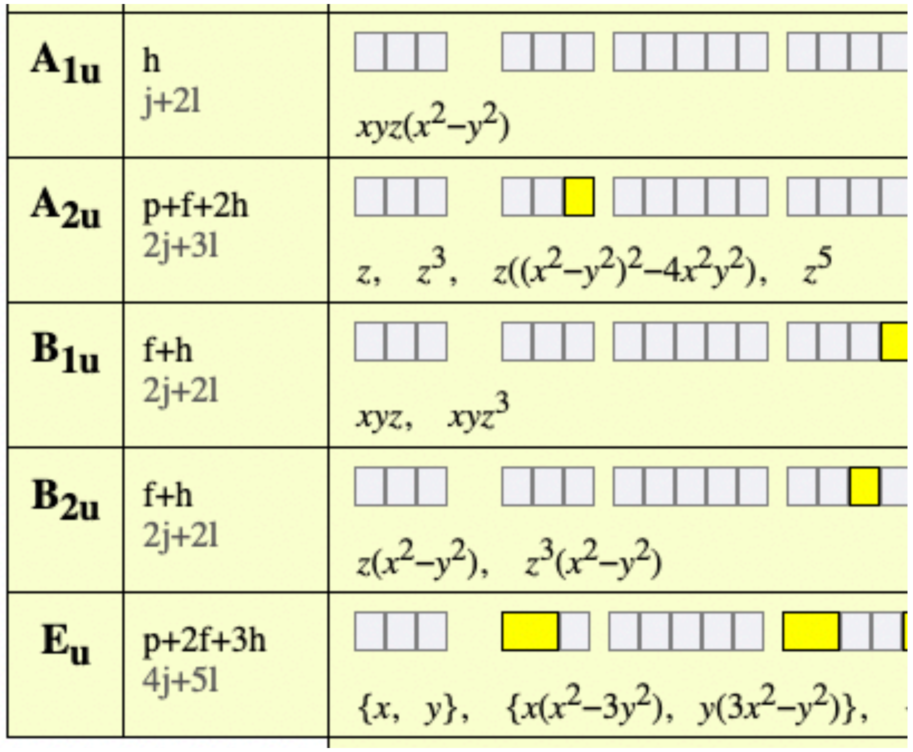


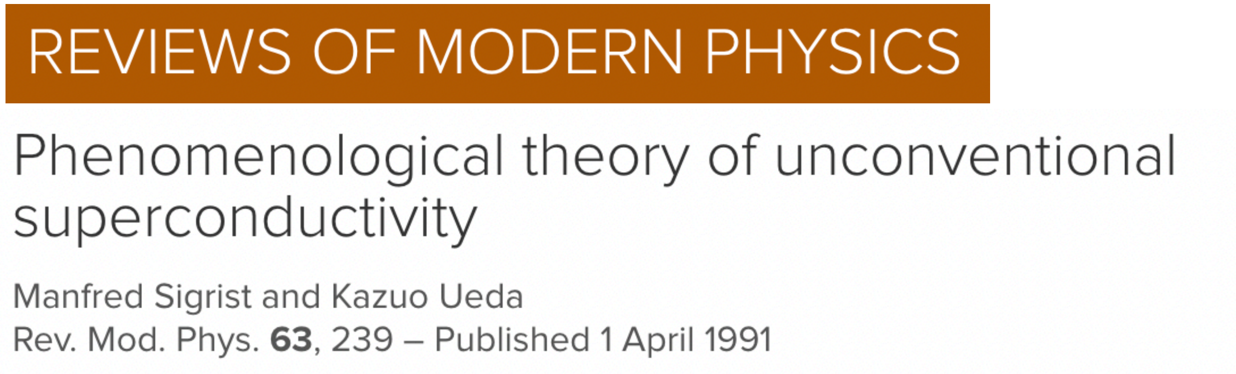
TABLE IV. (a) Even-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i\hat{\sigma}_y\psi(\Gamma,m;\mathbf{k})$ and (b) odd-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i[\hat{\boldsymbol{\sigma}}\cdot\mathbf{d}(\Gamma,m;\mathbf{k})]\hat{\sigma}_y$ for the tetragonal lattice symmetry (D_{4h}).

Irreducible representation Γ	Basis function
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-k_y^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_x^2-k_y^2$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_xk_y$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$
	$\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$

???



A_{1u}	h j+2l	$xyz(x^2-y^2)$
A_{2u}	p+f+2h 2j+3l	$z,\ z^3,\ z((x^2-y^2)^2-4x^2y^2),\ z^5$
B_{1u}	f+h 2j+2l	$xyz,\ xyz^3$
B_{2u}	f+h 2j+2l	$z(x^2-y^2),\ z^3(x^2-y^2)$
E_u	p+2f+3h 4j+5l	$\{x,\ y\},\ \{x(x^2-3y^2),\ y(3x^2-y^2)\},$



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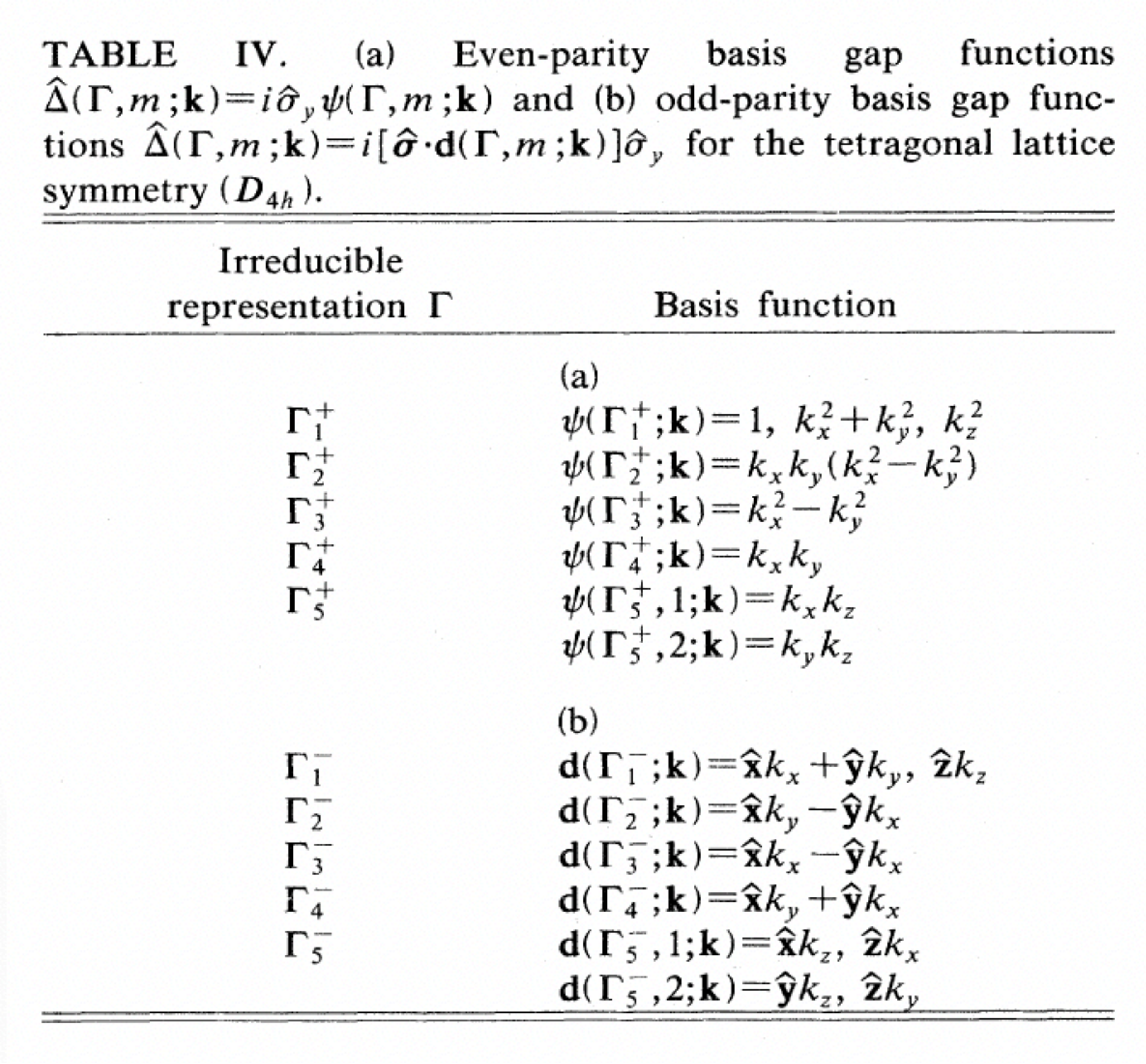


TABLE IV. (a) Even-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i\hat{\sigma}_y\psi(\Gamma,m;\mathbf{k})$ and (b) odd-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i[\hat{\boldsymbol{\sigma}}\cdot\mathbf{d}(\Gamma,m;\mathbf{k})]\hat{\sigma}_y$ for the tetragonal lattice symmetry (D_{4h}).

Irreducible representation Γ	Basis function
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-k_y^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_x^2-k_y^2$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_xk_y$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$
	$\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$
	$\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$

In the presence of SOC:

Symmetry operations also act on the spin DOF and influence the classification of SC order parameters.

Spin singlet (associated with σ_0) always transforms trivially;

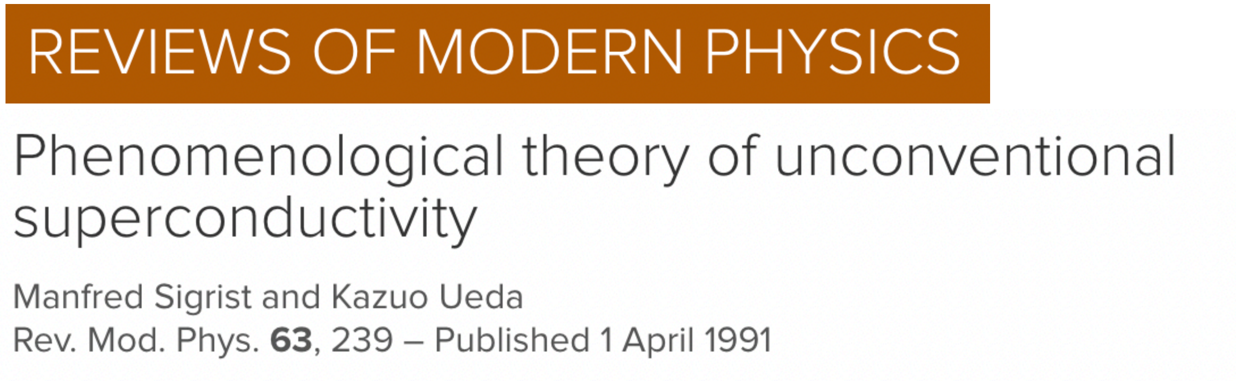
The irreps associated with each spin configuration in the triplet sector can be deduced from the explicit form of the generators:

$$C_{4z} = e^{i\pi\sigma_3/4} = \frac{\sigma_0 - i\sigma_3}{\sqrt{2}}$$

$$C_{2x} = e^{i\pi\sigma_1/2} = i\sigma_1$$

$$P = \sigma_0$$

Homework!



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Complete classification of SC order parameters from the perspective of point groups!

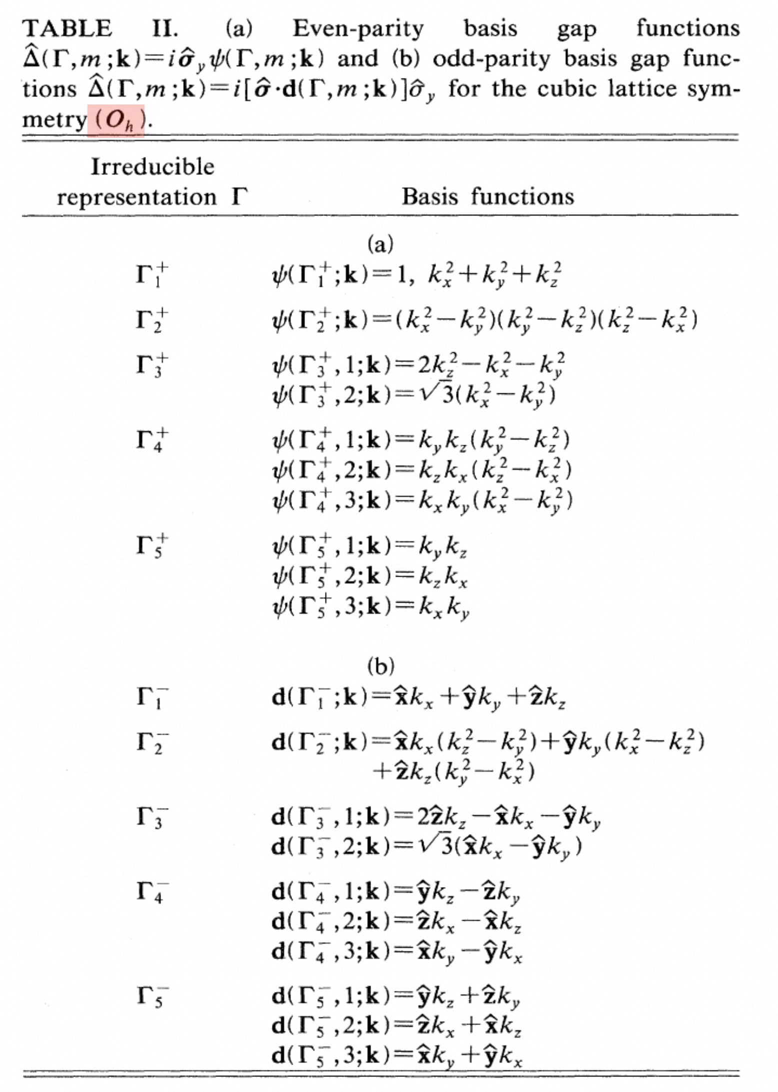


TABLE II. (a) Even-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i\hat{\sigma}_y\psi(\Gamma,m;\mathbf{k})$ and (b) odd-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i[\hat{\boldsymbol{\sigma}}\cdot\mathbf{d}(\Gamma,m;\mathbf{k})]\hat{\sigma}_y$ for the cubic lattice symmetry (O_h).

Irreducible representation Γ	Basis functions
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2+k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=(k_x^2-k_y^2)(k_y^2-k_z^2)(k_z^2-k_x^2)$
Γ_3^+	$\psi(\Gamma_3^+,1;\mathbf{k})=2k_z^2-k_x^2-k_y^2$ $\psi(\Gamma_3^+,2;\mathbf{k})=\sqrt{3}(k_x^2-k_y^2)$
Γ_4^+	$\psi(\Gamma_4^+,1;\mathbf{k})=k_yk_z(k_y^2-k_z^2)$ $\psi(\Gamma_4^+,2;\mathbf{k})=k_zk_x(k_z^2-k_x^2)$ $\psi(\Gamma_4^+,3;\mathbf{k})=k_xk_y(k_x^2-k_y^2)$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_yk_z$ $\psi(\Gamma_5^+,2;\mathbf{k})=k_zk_x$ $\psi(\Gamma_5^+,3;\mathbf{k})=k_xk_y$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y+\hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_x(k_z^2-k_y^2)+\hat{\mathbf{y}}k_y(k_x^2-k_z^2)$ $+\hat{\mathbf{z}}k_z(k_y^2-k_x^2)$
Γ_3^-	$\mathbf{d}(\Gamma_3^-,1;\mathbf{k})=2\hat{\mathbf{z}}k_z-\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y$ $\mathbf{d}(\Gamma_3^-,2;\mathbf{k})=\sqrt{3}(\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y)$
Γ_4^-	$\mathbf{d}(\Gamma_4^-,1;\mathbf{k})=\hat{\mathbf{y}}k_z-\hat{\mathbf{z}}k_y$ $\mathbf{d}(\Gamma_4^-,2;\mathbf{k})=\hat{\mathbf{z}}k_x-\hat{\mathbf{x}}k_z$ $\mathbf{d}(\Gamma_4^-,3;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{y}}k_z+\hat{\mathbf{z}}k_y$ $\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{z}}k_x+\hat{\mathbf{x}}k_z$ $\mathbf{d}(\Gamma_5^-,3;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$

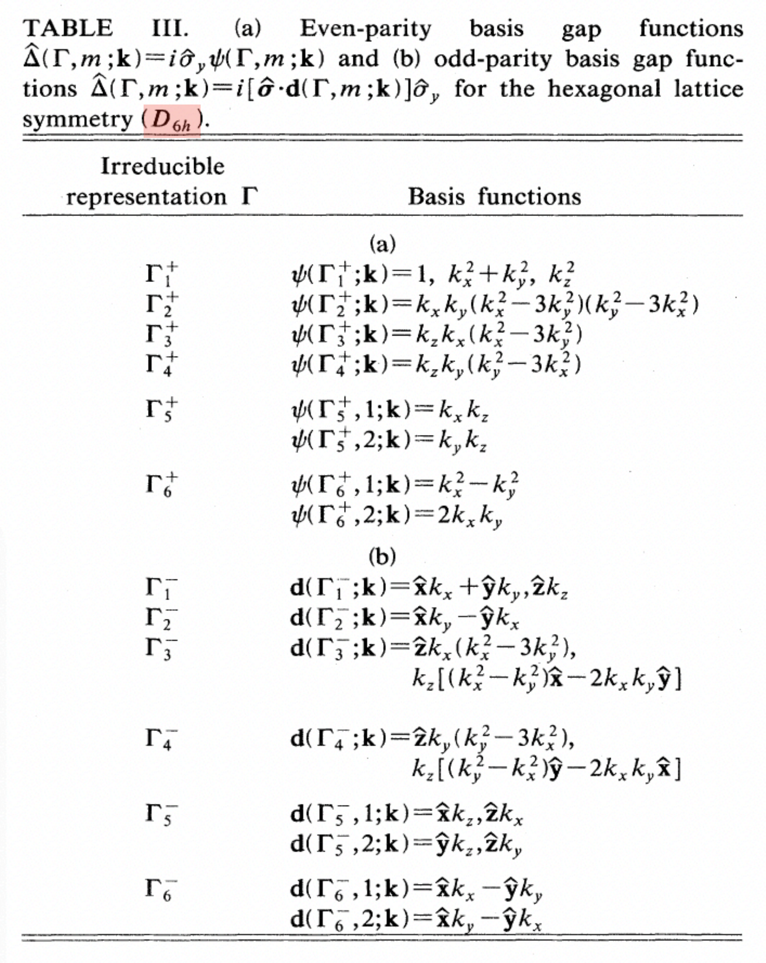
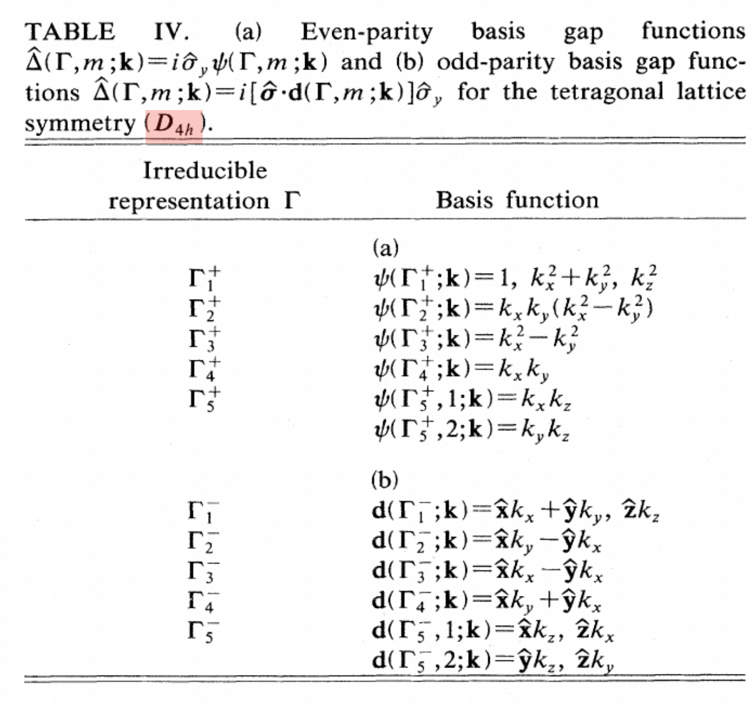


TABLE III. (a) Even-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i\hat{\sigma}_y\psi(\Gamma,m;\mathbf{k})$ and (b) odd-parity basis gap functions $\hat{\Delta}(\Gamma,m;\mathbf{k})=i[\hat{\boldsymbol{\sigma}}\cdot\mathbf{d}(\Gamma,m;\mathbf{k})]\hat{\sigma}_y$ for the hexagonal lattice symmetry (D_{6h}).

Irreducible representation Γ	Basis functions
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-3k_y^2)(k_y^2-3k_x^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_zk_x(k_x^2-3k_y^2)$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_zk_y(k_y^2-3k_x^2)$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$ $\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
Γ_6^+	$\psi(\Gamma_6^+,1;\mathbf{k})=k_x^2-k_y^2$ $\psi(\Gamma_6^+,2;\mathbf{k})=2k_xk_y$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{z}}k_x(k_x^2-3k_y^2),$ $k_z[(k_x^2-k_y^2)\hat{\mathbf{x}}-2k_xk_y\hat{\mathbf{y}}]$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{z}}k_y(k_y^2-3k_x^2),$ $k_z[(k_y^2-k_x^2)\hat{\mathbf{y}}-2k_xk_y\hat{\mathbf{x}}]$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\hat{\mathbf{z}}k_x$ $\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\hat{\mathbf{z}}k_y$
Γ_6^-	$\mathbf{d}(\Gamma_6^-,1;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y$ $\mathbf{d}(\Gamma_6^-,2;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$



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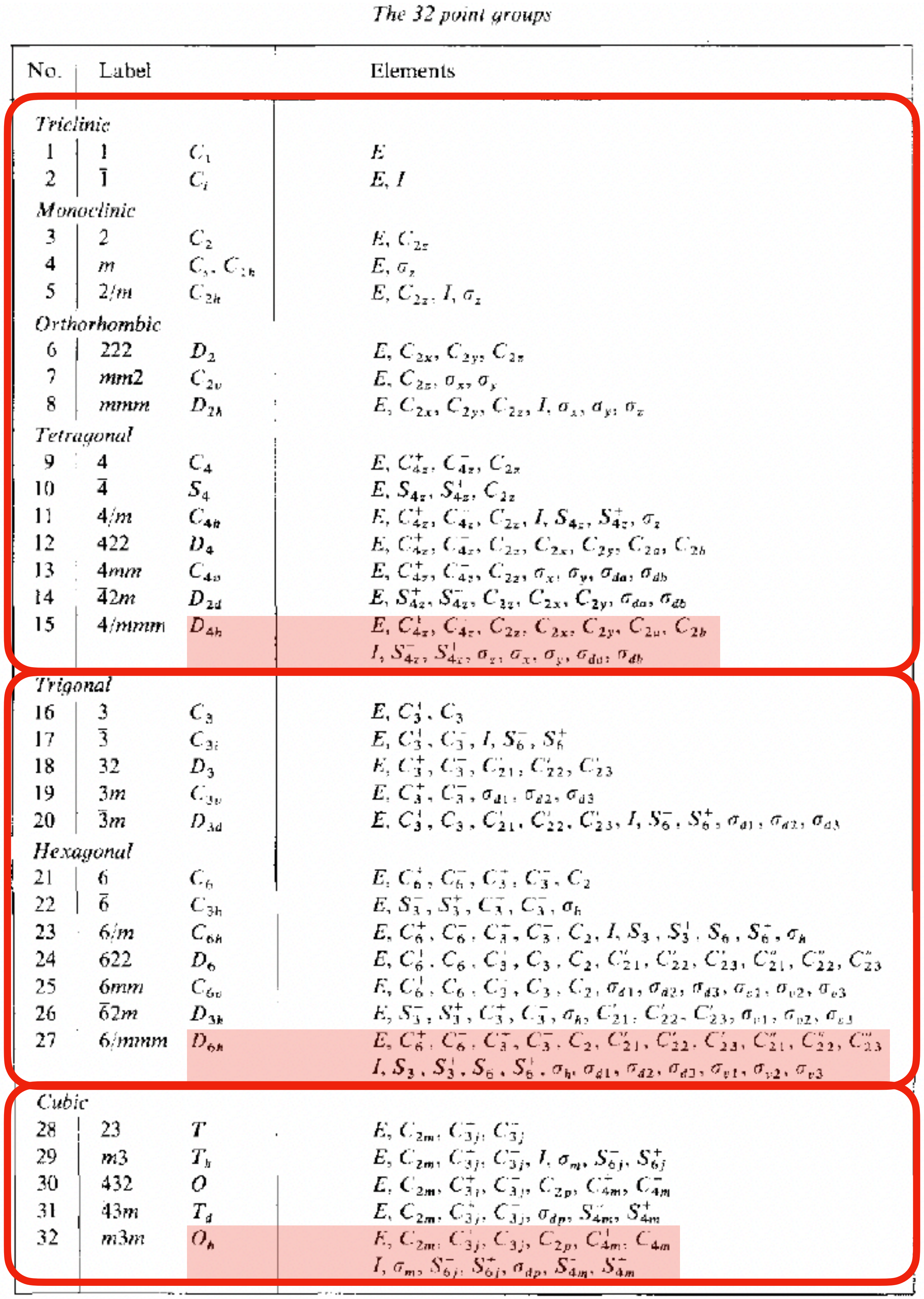
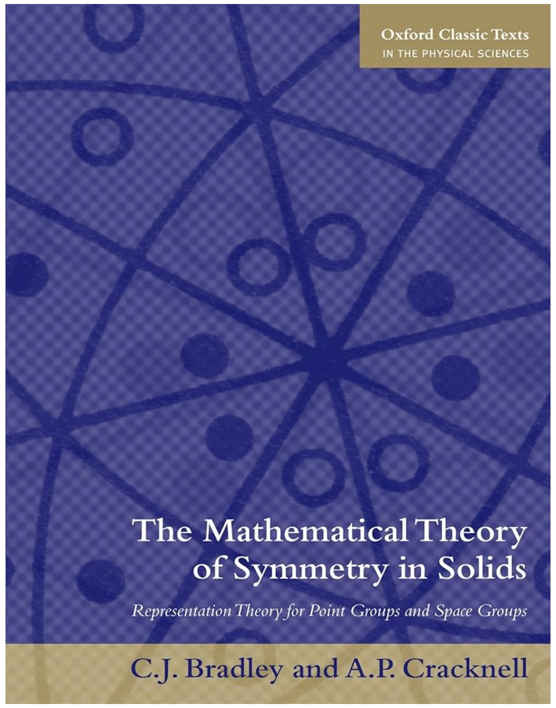
Irreducible representation Γ	Basis function
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-k_y^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_x^2-k_y^2$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_xk_y$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$ $\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\ \hat{\mathbf{z}}k_z$
Γ_2^-	$\mathbf{d}(\Gamma_2^-;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_x$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{x}}k_y+\hat{\mathbf{y}}k_x$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\ \hat{\mathbf{z}}k_x$ $\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\ \hat{\mathbf{z}}k_y$

Can deduce irreps for all other point groups by “symmetry descent”



The 32 point groups

No.	Label		Elements
Triclinic			
1	1	C_1	E
2	$\bar{1}$	C_i	E, I
Monoclinic			
3	2	C_2	E, C_{2z}
4	m	C_s, C_{1h}	E, σ_z
5	$2/m$	C_{2h}	E, C_{2z}, I, σ_z
Orthorhombic			
6	222	D_2	$E, C_{2x}, C_{2y}, C_{2z}$
7	$mm2$	C_{2v}	$E, C_{2z}, \sigma_x, \sigma_y$
8	mmm	D_{2h}	$E, C_{2x}, C_{2y}, C_{2z}, I, \sigma_x, \sigma_y, \sigma_z$
Tetragonal			
9	4	C_4	$E, C_{4z}^+, C_{4z}^-, C_{2z}$
10	$\bar{4}$	S_4	$E, S_{4z}^-, S_{4z}^+, C_{2z}$
11	$4/m$	C_{4h}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, I, S_{4z}^-, S_{4z}^+, \sigma_z$
12	422	D_4	$E, C_{4z}^+, C_{4z}^-, C_{2z}, C_{2x}, C_{2y}, C_{2a}, C_{2b}$
13	$4mm$	C_{4v}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db}$
14	$\bar{4}2m$	D_{2d}	$E, S_{4z}^+, S_{4z}^-, C_{2z}, C_{2x}, C_{2y}, \sigma_{da}, \sigma_{db}$
15	$4/mmm$	D_{4h}	$E, C_{4z}^+, C_{4z}^-, C_{2z}, C_{2x}, C_{2y}, C_{2a}, C_{2b}$ $I, S_{4z}^-, S_{4z}^+, \sigma_z, \sigma_x, \sigma_y, \sigma_{da}, \sigma_{db}$
Trigonal			
16	3	C_3	E, C_3^+, C_3^-
17	$\bar{3}$	C_{3i}	$E, C_3^+, C_3^-, I, S_6^-, S_6^+$
18	32	D_3	$E, C_3^+, C_3^-, C'_{21}, C'_{22}, C'_{23}$
19	$3m$	C_{3v}	$E, C_3^+, C_3^-, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}$
20	$\bar{3}m$	D_{3d}	$E, C_3^+, C_3^-, C'_{21}, C'_{22}, C'_{23}, I, S_6^-, S_6^+, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}$
Hexagonal			
21	6	C_6	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2$
22	$\bar{6}$	C_{3h}	$E, S_3^-, S_3^+, C_3^+, C_3^-, \sigma_h$
23	$6/m$	C_{6h}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, I, S_3^-, S_3^+, S_6^-, S_6^+, \sigma_h$
24	622	D_6	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, C'_{21}, C'_{22}, C'_{23}, C''_{21}, C''_{22}, C''_{23}$
25	$6mm$	C_{6v}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
26	$\bar{6}2m$	D_{3h}	$E, S_3^-, S_3^+, C_3^+, C_3^-, \sigma_h, C'_{21}, C'_{22}, C'_{23}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
27	$6/mmm$	D_{6h}	$E, C_6^+, C_6^-, C_3^+, C_3^-, C_2, C'_{21}, C'_{22}, C'_{23}, C''_{21}, C''_{22}, C''_{23}$ $I, S_3^-, S_3^+, S_6^-, S_6^+, \sigma_h, \sigma_{d1}, \sigma_{d2}, \sigma_{d3}, \sigma_{v1}, \sigma_{v2}, \sigma_{v3}$
Cubic			
28	23	T	$E, C_{2m}, C_{3j}^+, C_{3j}^-$
29	$m3$	T_h	$E, C_{2m}, C_{3j}^+, C_{3j}^-, I, \sigma_m, S_{6j}^-, S_{6j}^+$
30	432	O	$E, C_{2m}, C_{3j}^+, C_{3j}^-, C_{2p}, C_{4m}^+, C_{4m}^-$
31	$\bar{4}3m$	T_d	$E, C_{2m}, C_{3j}^+, C_{3j}^-, \sigma_{dp}, S_{4m}^-, S_{4m}^+$
32	$m3m$	O_h	$E, C_{2m}, C_{3j}^+, C_{3j}^-, C_{2p}, C_{4m}^+, C_{4m}^-$ $I, \sigma_m, S_{6j}^-, S_{6j}^+, \sigma_{dp}, S_{4m}^-, S_{4m}^+$



Oxford Classic Texts IN THE PHYSICAL SCIENCES

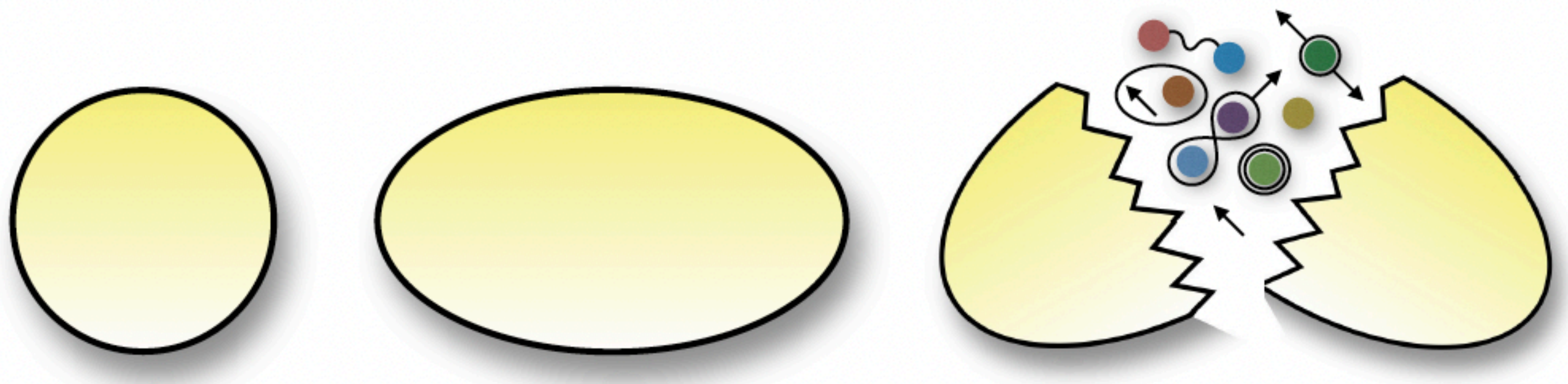
The Mathematical Theory of Symmetry in Solids

Representation Theory for Point Groups and Space Groups

C.J. Bradley and A.P. Cracknell

Have we covered everything?
Is the Sigrist-Ueda classification “complete”?

“Yes and No!”



Have we covered everything?
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[Generalizations]

I) Multiple internal DOF

II) Nonsymmorphic systems [Space group]

Have we covered everything?
Is the Sigrist-Ueda classification “complete”?

[Generalizations]

I) Multiple internal DOF

II) Nonsymmorphic systems [Space group]

How to describe the superconducting states in complex materials with multiple internal DOFs?

Considering multiple internal DOF (orbitals/sublattice)

Annica’s Lecture:

The mean-field BdG Hamiltonian

$$\hat{H}_{BdG}(\mathbf{k}) = \begin{pmatrix} \hat{H}_0(\mathbf{k}) & \hat{\Delta}(\mathbf{k}) \\ \hat{\Delta}^\dagger(\mathbf{k}) & -\hat{H}_0^*(-\mathbf{k}) \end{pmatrix}$$

$$\hat{\Delta}(\mathbf{k}) = \sum_{ab} d_{ab}(\mathbf{k}) \hat{\tau}_a \otimes \hat{\sigma}_b (i\hat{\sigma}_2)$$

Orbital/SL **Spin**

Considering multiple internal DOF (orbitals/sublattice)

Annica's Lecture:

The mean-field BdG Hamiltonian

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$$\hat{\Delta}(\mathbf{k}) = \sum_{ab} d_{ab}(\mathbf{k}) \hat{\tau}_a \otimes \hat{\sigma}_b (i\hat{\sigma}_2)$$

Orbital/SL

Spin

In principle parametrised in terms of (3+1)x(3+1) = 16 functions d_{ab}(k)

If $a = 0{,}3$: Intra-orbital/SL

If $a = 1{,}2$: Inter-orbital/SL

If $b = 0$: Spin Singlet

If $b = 1{,}2{,}3$: Spin Triplet

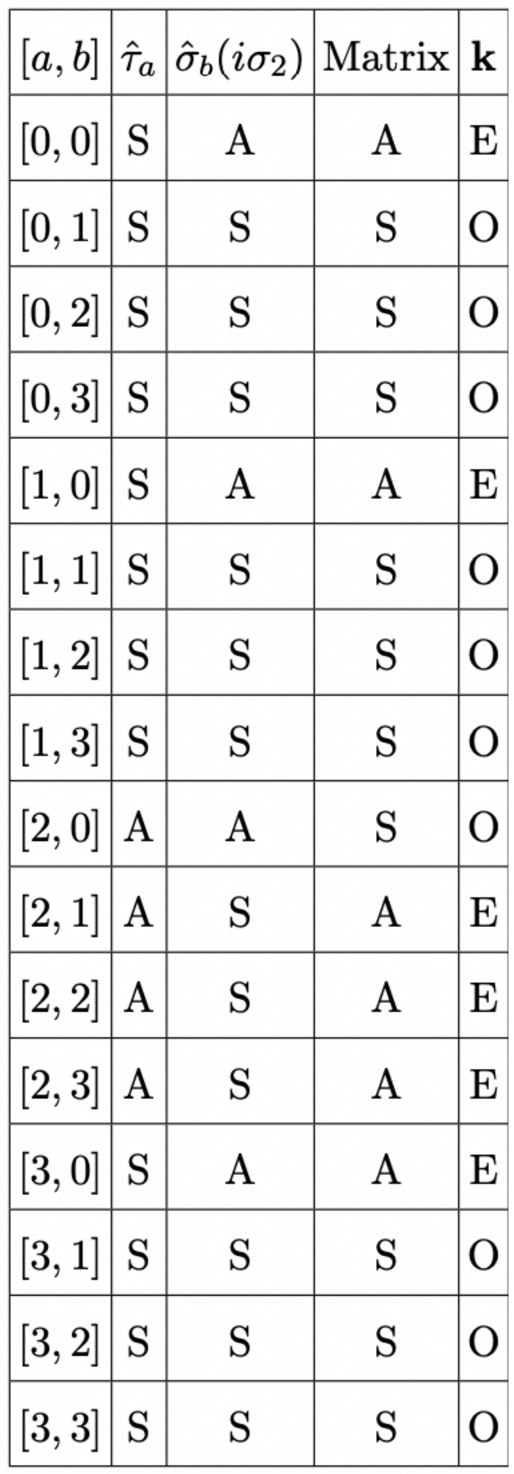
$$\sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_2 = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

The basic symmetries of the order parameter

$$\hat{\Delta}(\mathbf{k}) = \sum_{ab} d_{ab}(\mathbf{k})\hat{\tau}_a \otimes \hat{\sigma}_b(i\hat{\sigma}_2)$$



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$
$[0,0]$	S	A	A	E
$[0,1]$	S	S	S	O
$[0,2]$	S	S	S	O
$[0,3]$	S	S	S	O
$[1,0]$	S	A	A	E
$[1,1]$	S	S	S	O
$[1,2]$	S	S	S	O
$[1,3]$	S	S	S	O
$[2,0]$	A	A	S	O
$[2,1]$	A	S	A	E
$[2,2]$	A	S	A	E
$[2,3]$	A	S	A	E
$[3,0]$	S	A	A	E
$[3,1]$	S	S	S	O
$[3,2]$	S	S	S	O
$[3,3]$	S	S	S	O

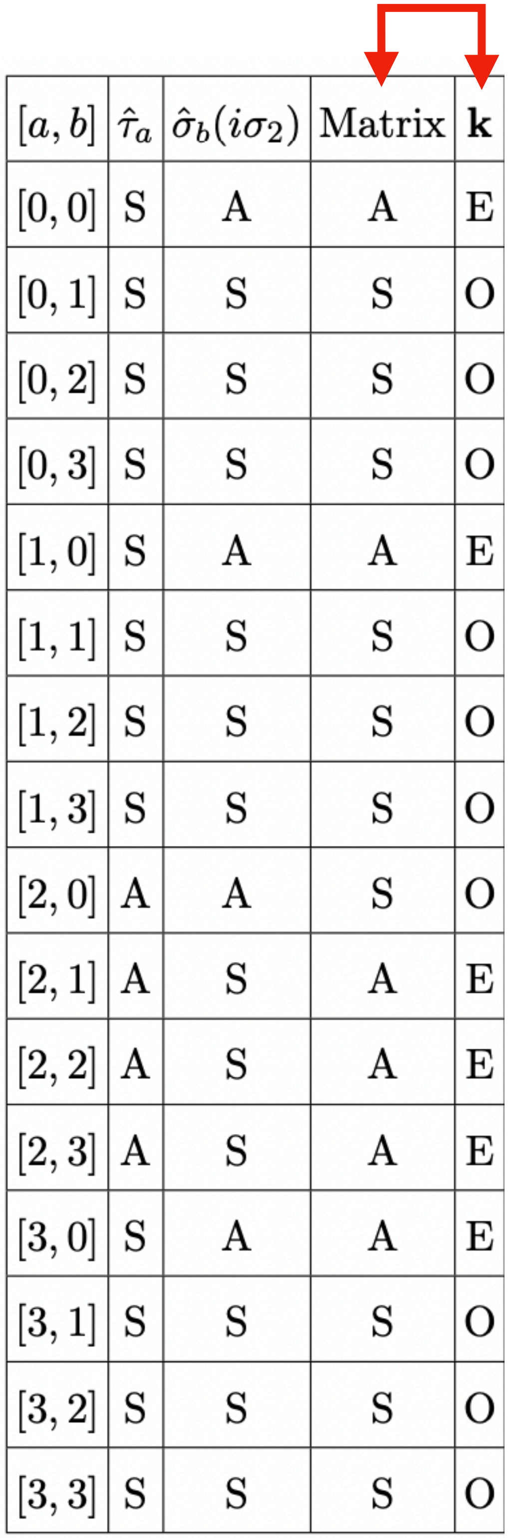
The basic symmetries of the order parameter

Annica's Lecture:

$$\hat{\Delta}(\mathbf{k}) = -\hat{\Delta}^T(-\mathbf{k})$$

If the matrix is anti-symmetric: k-even
If the matrix is symmetric: k-odd

$$\hat{\Delta}(\mathbf{k}) = \sum_{ab} d_{ab}(\mathbf{k})\hat{\tau}_a \otimes \hat{\sigma}_b(i\hat{\sigma}_2)$$



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$
$[0,0]$	S	A	A	E
$[0,1]$	S	S	S	O
$[0,2]$	S	S	S	O
$[0,3]$	S	S	S	O
$[1,0]$	S	A	A	E
$[1,1]$	S	S	S	O
$[1,2]$	S	S	S	O
$[1,3]$	S	S	S	O
$[2,0]$	A	A	S	O
$[2,1]$	A	S	A	E
$[2,2]$	A	S	A	E
$[2,3]$	A	S	A	E
$[3,0]$	S	A	A	E
$[3,1]$	S	S	S	O
$[3,2]$	S	S	S	O
$[3,3]$	S	S	S	O

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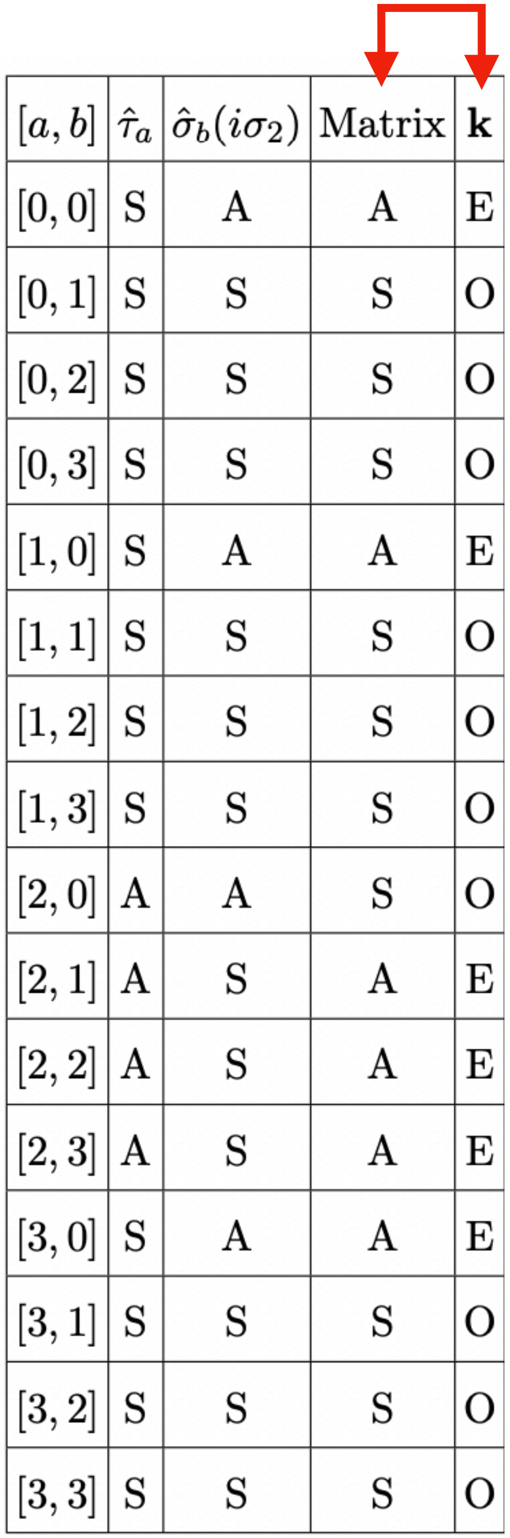
Sublattice: $P = \hat{\tau}_1 \otimes \hat{\sigma}_0$



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$
$[0,0]$	S	A	A	E
$[0,1]$	S	S	S	O
$[0,2]$	S	S	S	O
$[0,3]$	S	S	S	O
$[1,0]$	S	A	A	E
$[1,1]$	S	S	S	O
$[1,2]$	S	S	S	O
$[1,3]$	S	S	S	O
$[2,0]$	A	A	S	O
$[2,1]$	A	S	A	E
$[2,2]$	A	S	A	E
$[2,3]$	A	S	A	E
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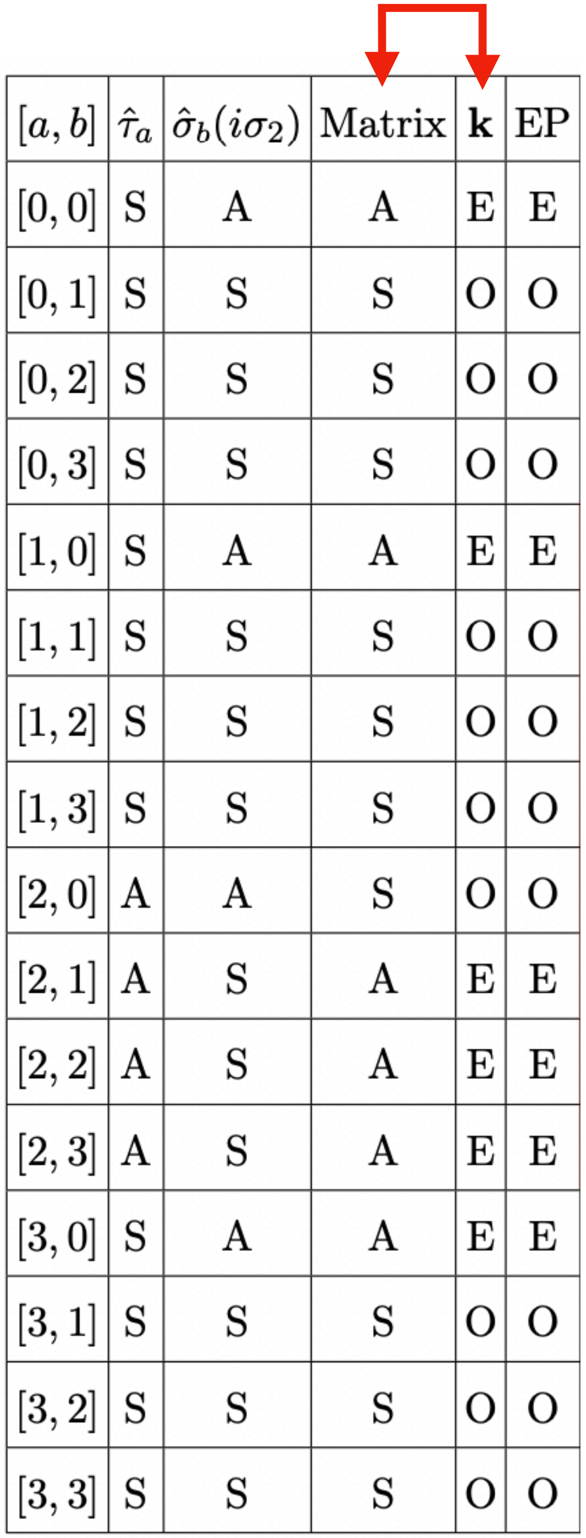

$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$	EP
$[0,0]$	S	A	A	E	E
$[0,1]$	S	S	S	O	O
$[0,2]$	S	S	S	O	O
$[0,3]$	S	S	S	O	O
$[1,0]$	S	A	A	E	E
$[1,1]$	S	S	S	O	O
$[1,2]$	S	S	S	O	O
$[1,3]$	S	S	S	O	O
$[2,0]$	A	A	S	O	O
$[2,1]$	A	S	A	E	E
$[2,2]$	A	S	A	E	E
$[2,3]$	A	S	A	E	E
$[3,0]$	S	A	A	E	E
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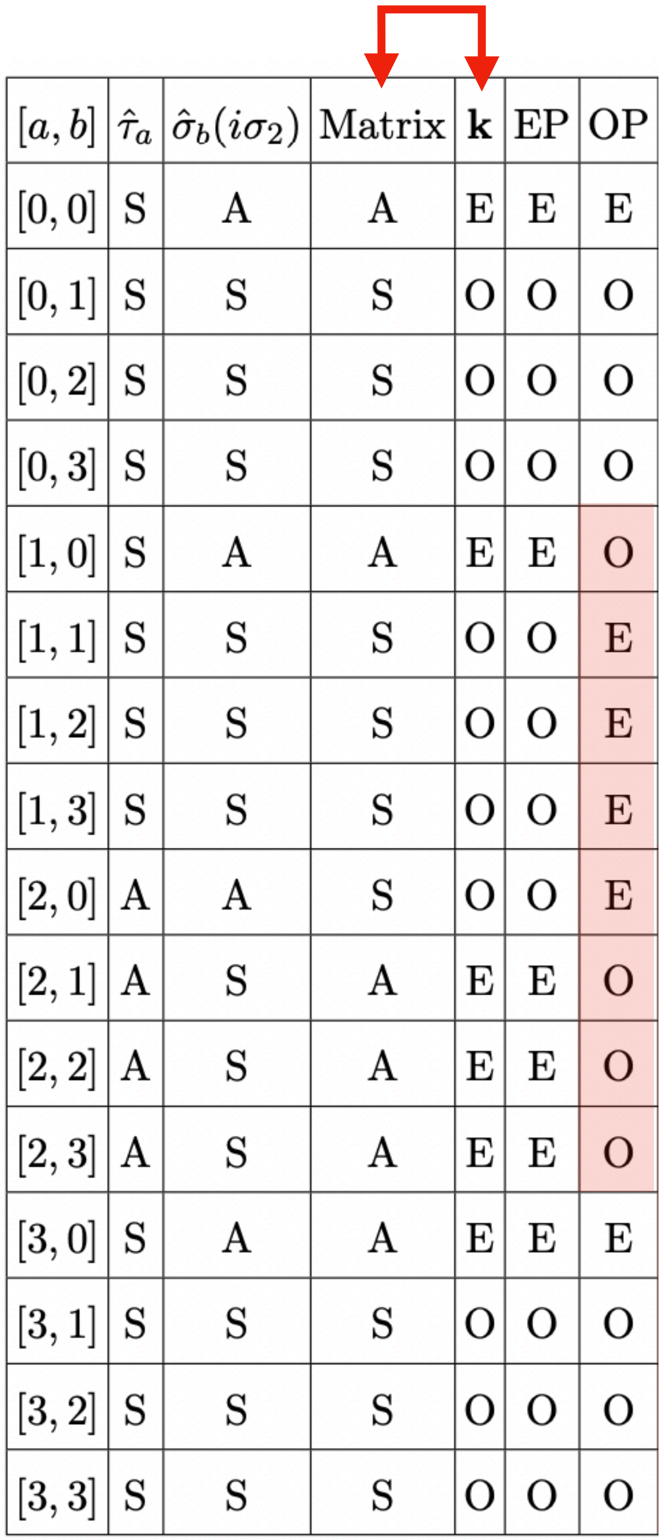

$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$	EP	OP
$[0,0]$	S	A	A	E	E	E
$[0,1]$	S	S	S	O	O	O
$[0,2]$	S	S	S	O	O	O
$[0,3]$	S	S	S	O	O	O
$[1,0]$	S	A	A	E	E	O
$[1,1]$	S	S	S	O	O	E
$[1,2]$	S	S	S	O	O	E
$[1,3]$	S	S	S	O	O	E
$[2,0]$	A	A	S	O	O	E
$[2,1]$	A	S	A	E	E	O
$[2,2]$	A	S	A	E	E	O
$[2,3]$	A	S	A	E	E	O
$[3,0]$	S	A	A	E	E	E
$[3,1]$	S	S	S	O	O	O
$[3,2]$	S	S	S	O	O	O
$[3,3]$	S	S	S	O	O	O

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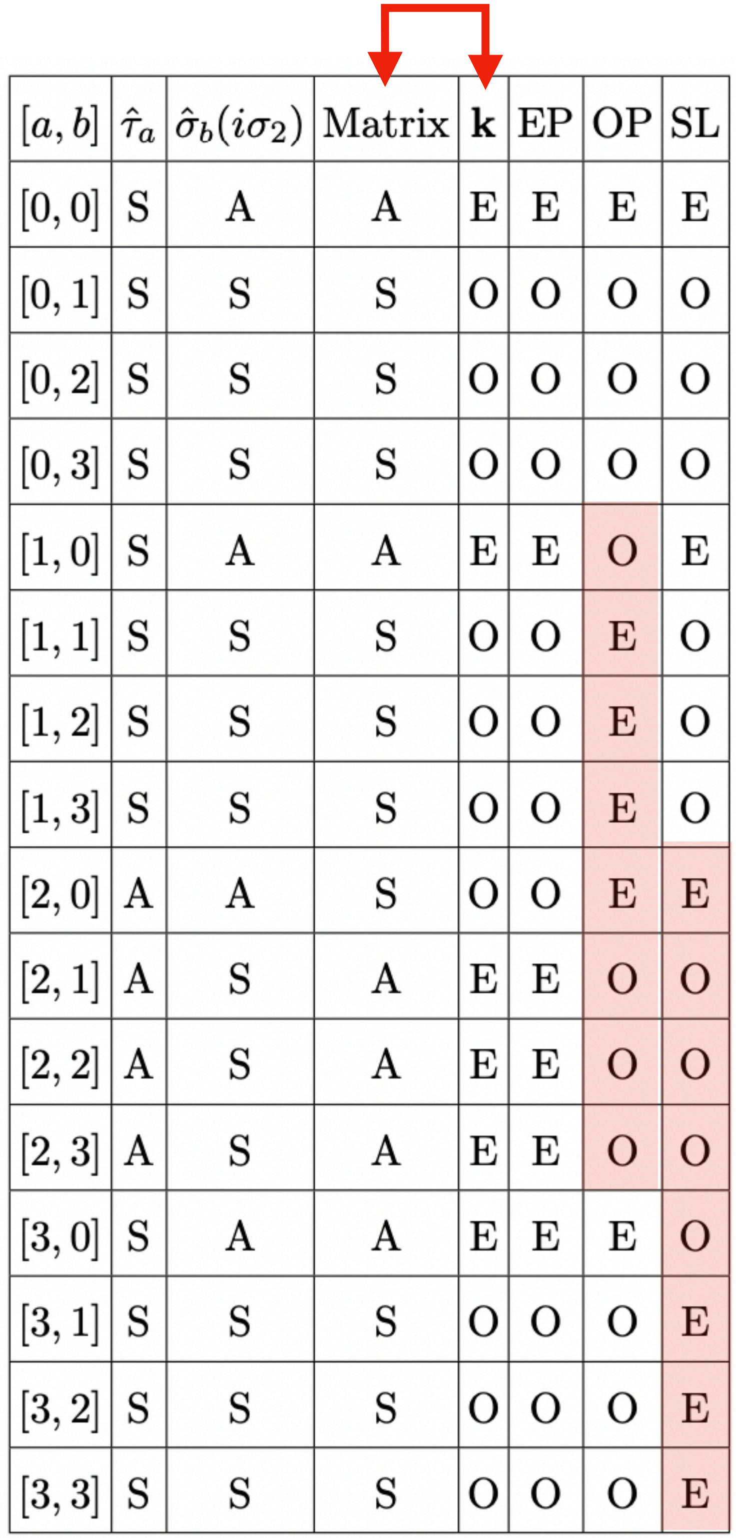
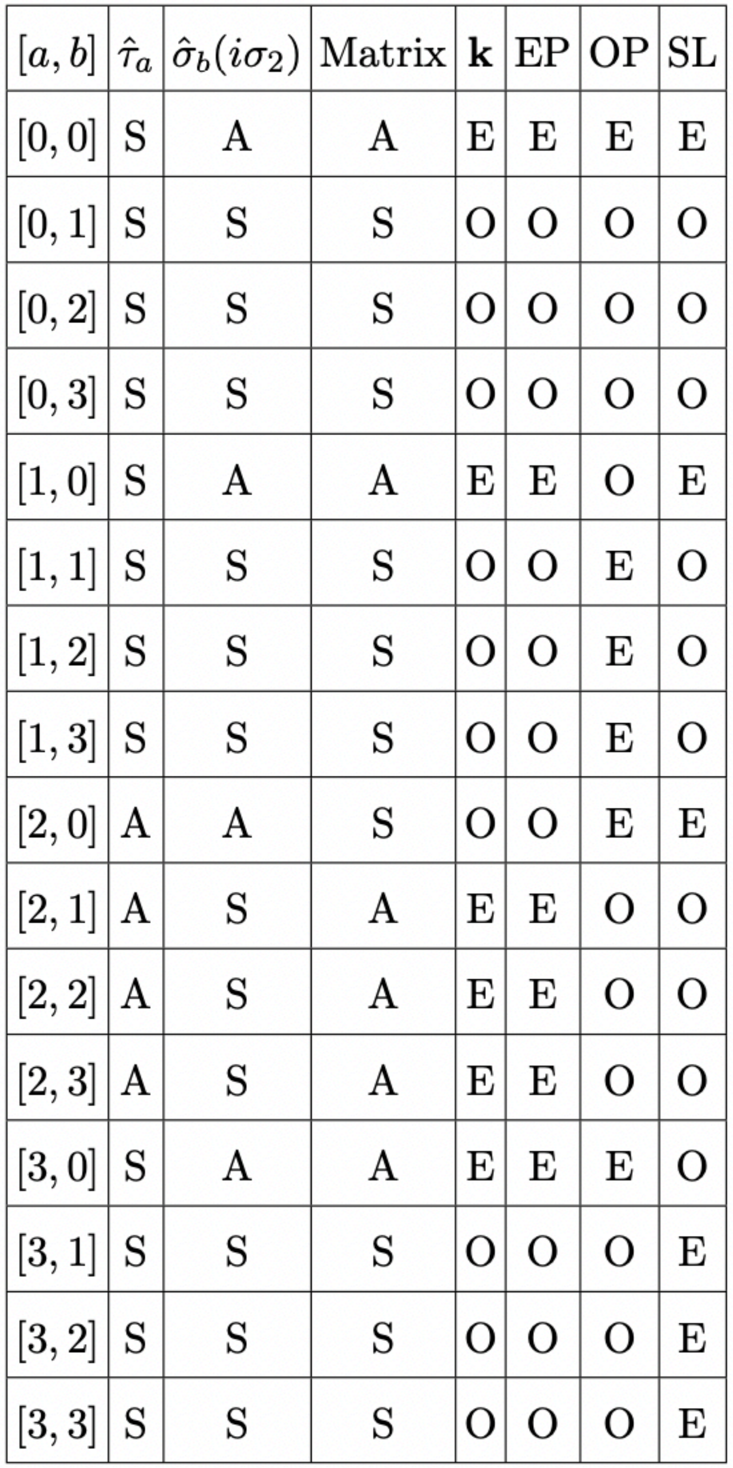


$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	**k**	EP	OP	SL
$[0,0]$	S	A	A	E	E	E	E
$[0,1]$	S	S	S	O	O	O	O
$[0,2]$	S	S	S	O	O	O	O
$[0,3]$	S	S	S	O	O	O	O
$[1,0]$	S	A	A	E	E	O	E
$[1,1]$	S	S	S	O	O	E	O
$[1,2]$	S	S	S	O	O	E	O
$[1,3]$	S	S	S	O	O	E	O
$[2,0]$	A	A	S	O	O	E	E
$[2,1]$	A	S	A	E	E	O	O
$[2,2]$	A	S	A	E	E	O	O
$[2,3]$	A	S	A	E	E	O	O
$[3,0]$	S	A	A	E	E	E	O
$[3,1]$	S	S	S	O	O	O	E
$[3,2]$	S	S	S	O	O	O	E
$[3,3]$	S	S	S	O	O	O	E

Considering multiple internal DOF (orbitals)

$$\hat{\Delta}(\mathbf{k}) = \sum_{ab} d_{ab}(\mathbf{k}) \hat{\tau}_a \otimes \hat{\sigma}_b (i\hat{\sigma}_2)$$



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$	EP	OP	SL
$[0,0]$	S	A	A	E	E	E	E
$[0,1]$	S	S	S	O	O	O	O
$[0,2]$	S	S	S	O	O	O	O
$[0,3]$	S	S	S	O	O	O	O
$[1,0]$	S	A	A	E	E	O	E
$[1,1]$	S	S	S	O	O	E	O
$[1,2]$	S	S	S	O	O	E	O
$[1,3]$	S	S	S	O	O	E	O
$[2,0]$	A	A	S	O	O	E	E
$[2,1]$	A	S	A	E	E	O	O
$[2,2]$	A	S	A	E	E	O	O
$[2,3]$	A	S	A	E	E	O	O
$[3,0]$	S	A	A	E	E	E	O
$[3,1]$	S	S	S	O	O	O	E
$[3,2]$	S	S	S	O	O	O	E
$[3,3]$	S	S	S	O	O	O	E

Singlet/triplet are not directly associated with even/odd k or with even/odd parity!

Considering multiple internal DOF (orbitals)

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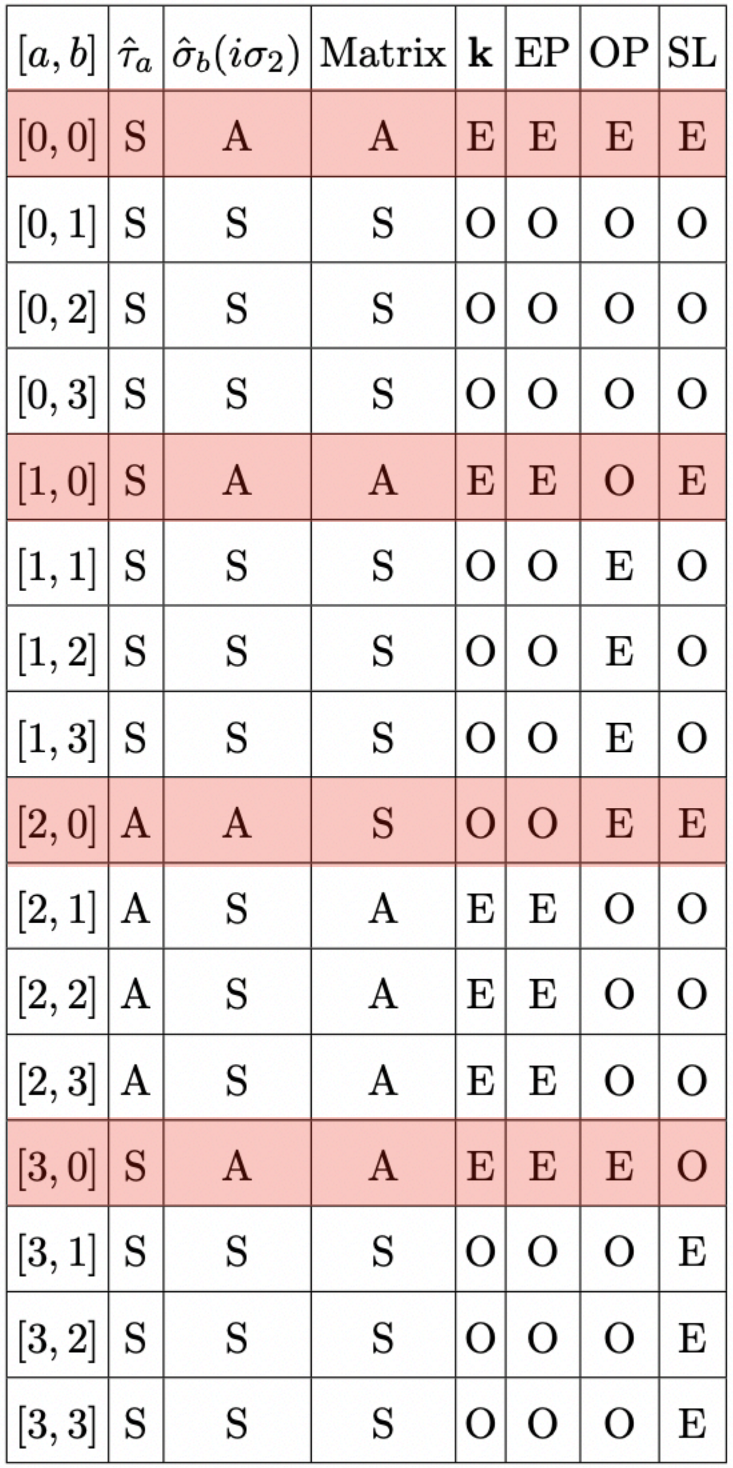
Spin Singlet [b=0]



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$	EP	OP	SL
$[0,0]$	S	A	A	E	E	E	E
$[0,1]$	S	S	S	O	O	O	O
$[0,2]$	S	S	S	O	O	O	O
$[0,3]$	S	S	S	O	O	O	O
$[1,0]$	S	A	A	E	E	O	E
$[1,1]$	S	S	S	O	O	E	O
$[1,2]$	S	S	S	O	O	E	O
$[1,3]$	S	S	S	O	O	E	O
$[2,0]$	A	A	S	O	O	E	E
$[2,1]$	A	S	A	E	E	O	O
$[2,2]$	A	S	A	E	E	O	O
$[2,3]$	A	S	A	E	E	O	O
$[3,0]$	S	A	A	E	E	E	O
$[3,1]$	S	S	S	O	O	O	E
$[3,2]$	S	S	S	O	O	O	E
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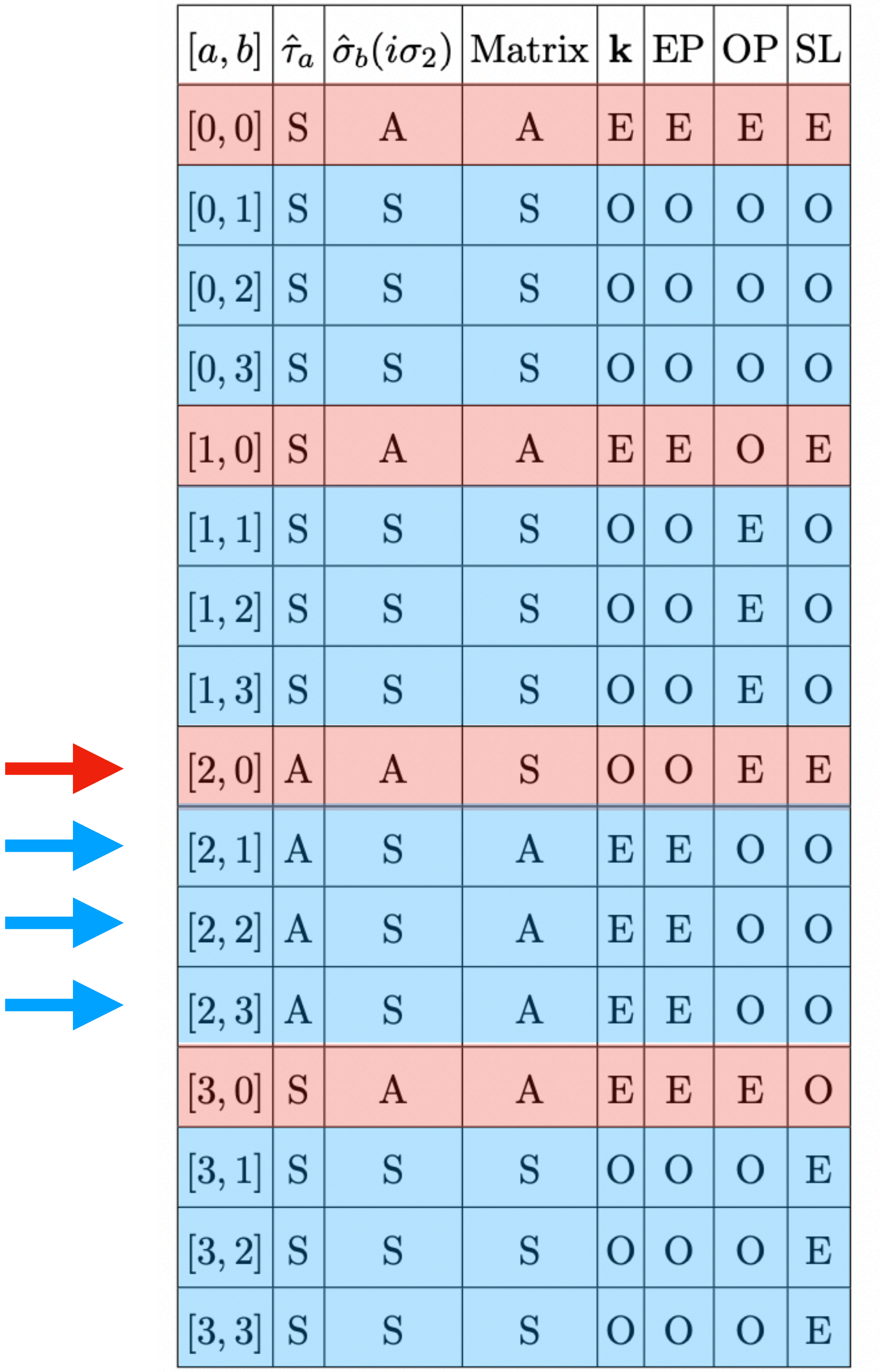
Spin Singlet [b=0]

Spin Triplet [b=1,2,3]



$[a,b]$	$\hat{\tau}_a$	$\hat{\sigma}_b(i\sigma_2)$	Matrix	$\mathbf{k}$	EP	OP	SL
$[0,0]$	S	A	A	E	E	E	E
$[0,1]$	S	S	S	O	O	O	O
$[0,2]$	S	S	S	O	O	O	O
$[0,3]$	S	S	S	O	O	O	O
$[1,0]$	S	A	A	E	E	O	E
$[1,1]$	S	S	S	O	O	E	O
$[1,2]$	S	S	S	O	O	E	O
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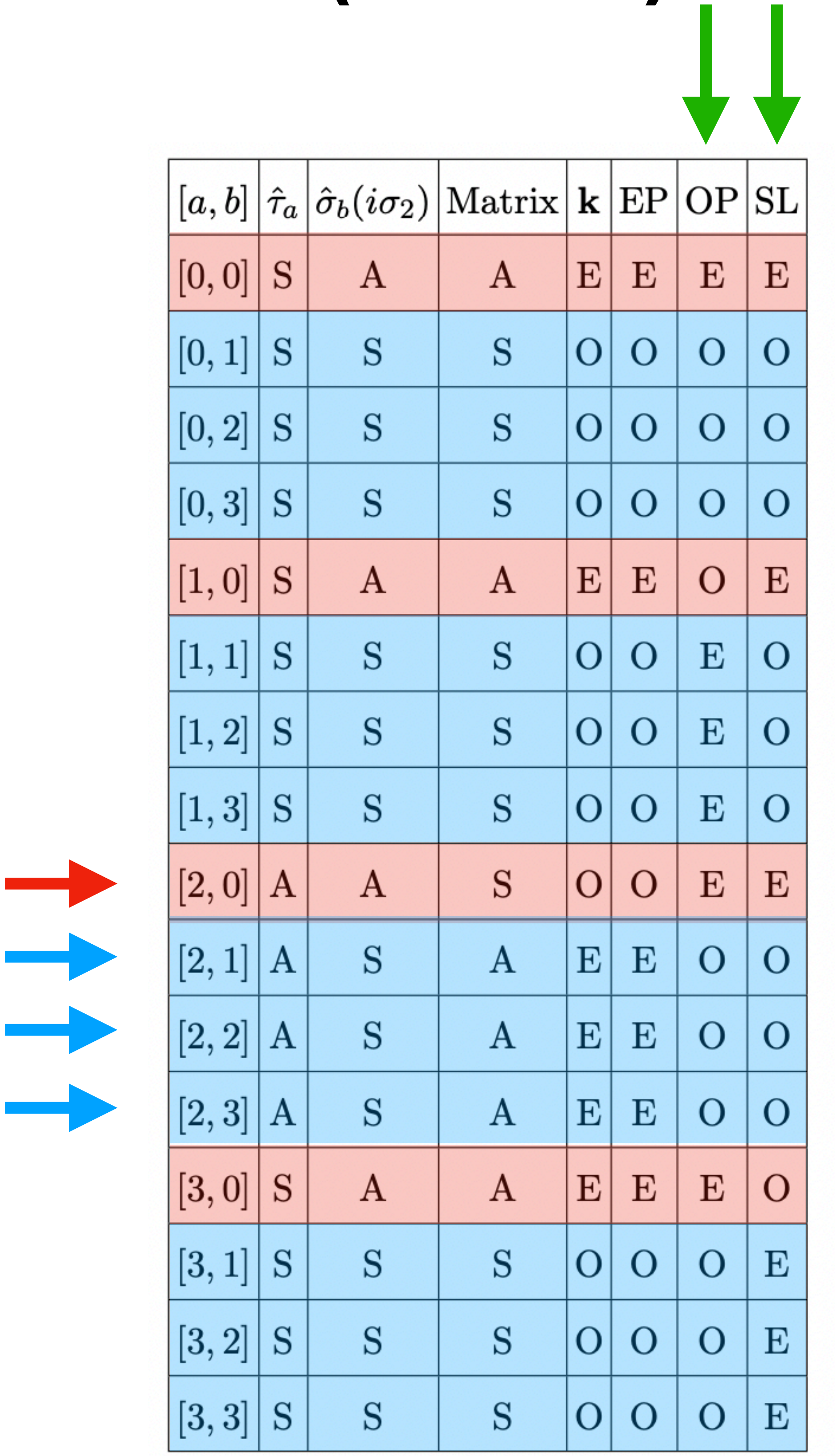
Spin Triplet [b=1,2,3]

k-dependence does not uniquely define the parity of the SC order parameter!

Singlet/triplet are not directly associated with even/odd k or with even/odd parity!



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$[0,0]$	S	A	A	E	E	E	E
$[0,1]$	S	S	S	O	O	O	O
$[0,2]$	S	S	S	O	O	O	O
$[0,3]$	S	S	S	O	O	O	O
$[1,0]$	S	A	A	E	E	O	E
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$[2,2]$	A	S	A	E	E	O	O
$[2,3]$	A	S	A	E	E	O	O
$[3,0]$	S	A	A	E	E	E	O
$[3,1]$	S	S	S	O	O	O	E
$[3,2]$	S	S	S	O	O	O	E
$[3,3]$	S	S	S	O	O	O	E

Some examples of nontrivial phenomenology

Superconductivity in Complex Quantum Materials

$$\hat{\Delta}(\mathbf{k}) = -\hat{\Delta}^T(-\mathbf{k}) \xrightarrow[\text{Only spin}]{} \hat{\Delta}(\mathbf{k}) = d_a(\mathbf{k})\hat{\sigma}_a(i\hat{\sigma}_2)$$

$$\xrightarrow[\text{Orbital/Layer/Sublattice+Spin}]{} \hat{\Delta}(\mathbf{k}) = d_{ab}(\mathbf{k})\hat{\tau}_a \otimes \hat{\sigma}_b(i\hat{\sigma}_2)$$

Can transform non-trivially under inversion!

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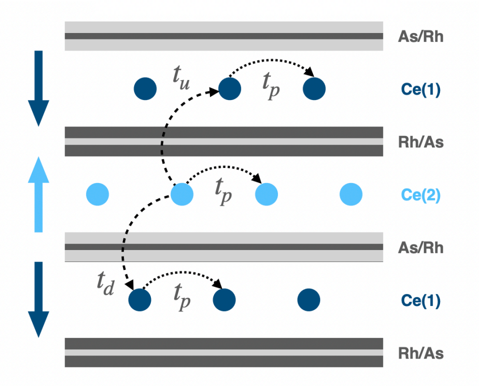
The case of $CeRh_2As_2$

Sublattice structure

$$P = \hat{\tau}_1$$



$$\hat{\Delta}(\mathbf{k}) = d_{33}(\mathbf{k})\hat{\tau}_3 \otimes \hat{\sigma}_3(i\hat{\sigma}_2)$$

Even-parity, k-odd,
intra-layer, **spin-triplet**

Two superconducting phases!

D. Möckli and A. Ramires, Phys. Rev. Research **3**, 023204 (2021)

Superconductivity in Complex Quantum Materials

$$\hat{\Delta}(\mathbf{k}) = -\hat{\Delta}^T(-\mathbf{k}) \xrightarrow[\text{Only spin}]{\hspace{3cm}} \hat{\Delta}(\mathbf{k}) = d_a(\mathbf{k})\hat{\sigma}_a(i\hat{\sigma}_2)$$

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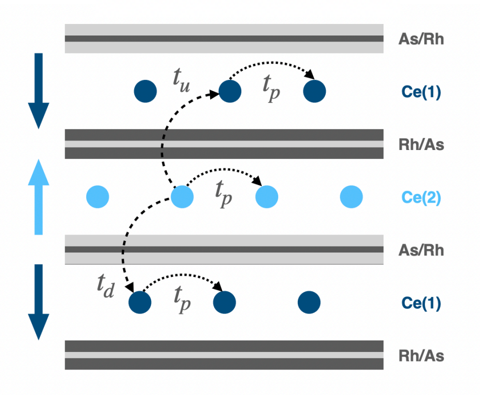

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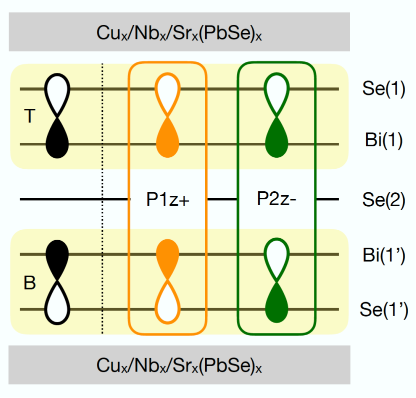
The case of d-Bi_2Se_3

Even- and odd-P orbitals

$$P = \hat{\tau}_3$$



$$\hat{\Delta}(\mathbf{k}) = d_0\hat{\tau}_1 \otimes \hat{\sigma}_0(i\hat{\sigma}_2)$$

Odd-parity, s-wave,
inter-orbital, **spin-singlet**

Generalized Anderson's Theorem

L. Andersen*, A. Ramires* et al., Sci. Adv. **6**, eaay6502 (2020)

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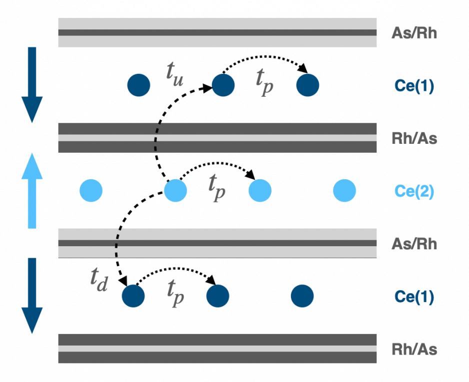
The case of CeRh$_2$As$_2$

Sublattice structure

$$P = \hat{\tau}_1$$



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Even-parity, k-odd,
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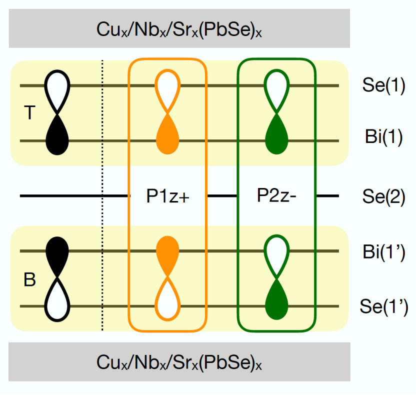

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Odd-parity, s-wave,
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Generalized Anderson's Theorem

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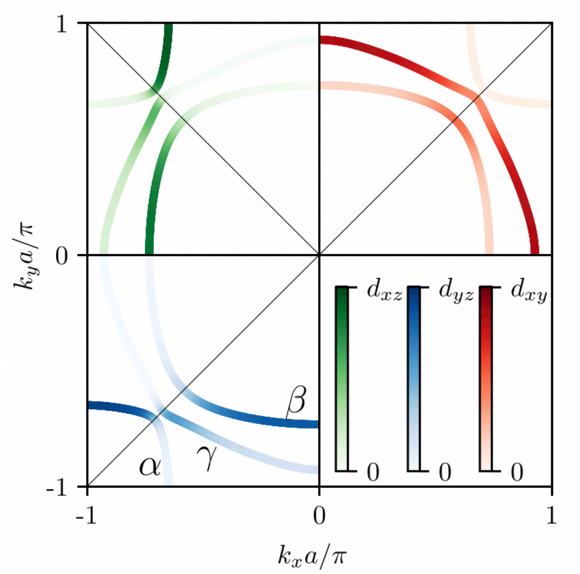
The case of Sr$_2$RuO$_4$

3 orbitals



$$[6,3] + i[5,3]$$

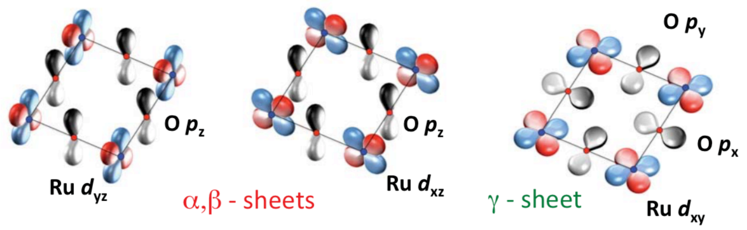
Chiral d-wave superconductivity
[Orbital antisymmetric spin-triplet]

Chiral d-wave in 2D FS!

S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

Three orbitals with same parity: Sr_2RuO_4

3 t_{2g} orbitals/3 bands system



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S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

H. G. Suh, A. Ramires et al., Phys. Rev. Res. **2**, 032023(R) (2020)

Three orbitals with same parity: Sr_2RuO_4

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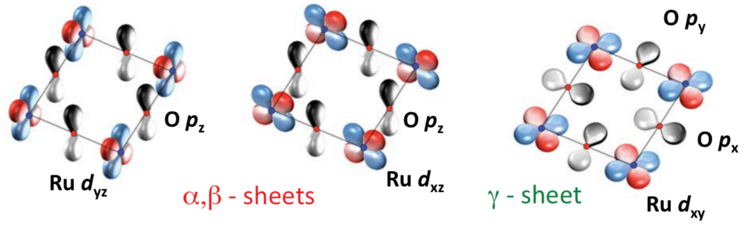

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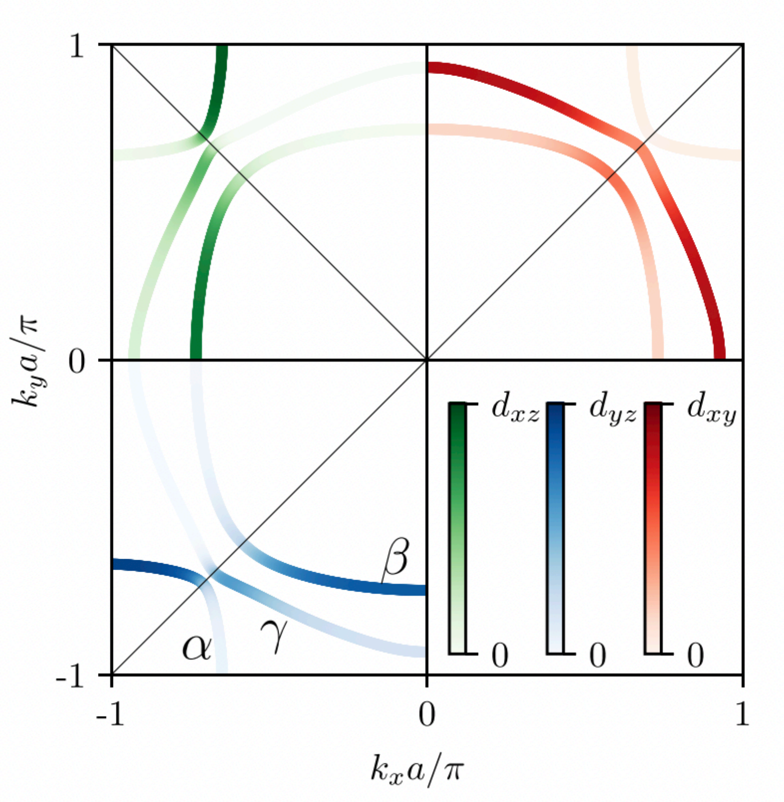
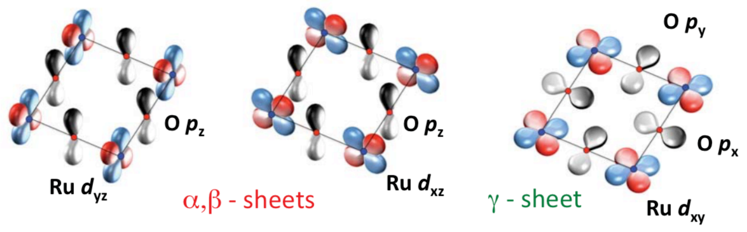


S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

H. G. Suh, A. Ramires et al., Phys. Rev. Res. **2**, 032023(R) (2020)

Three orbitals with same parity: Sr_2RuO_4

3 t_{2g} orbitals/3 bands system



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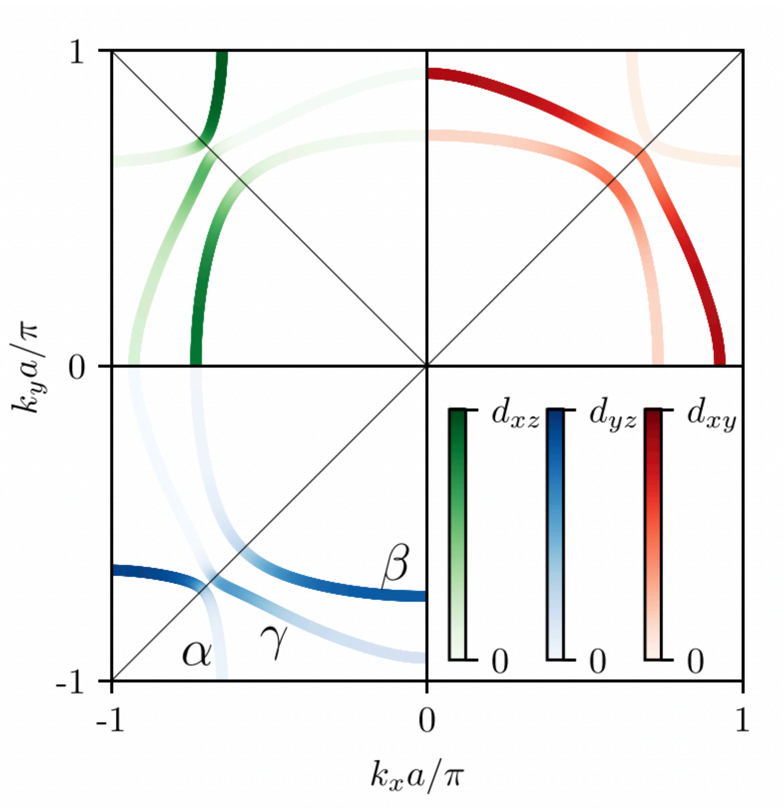
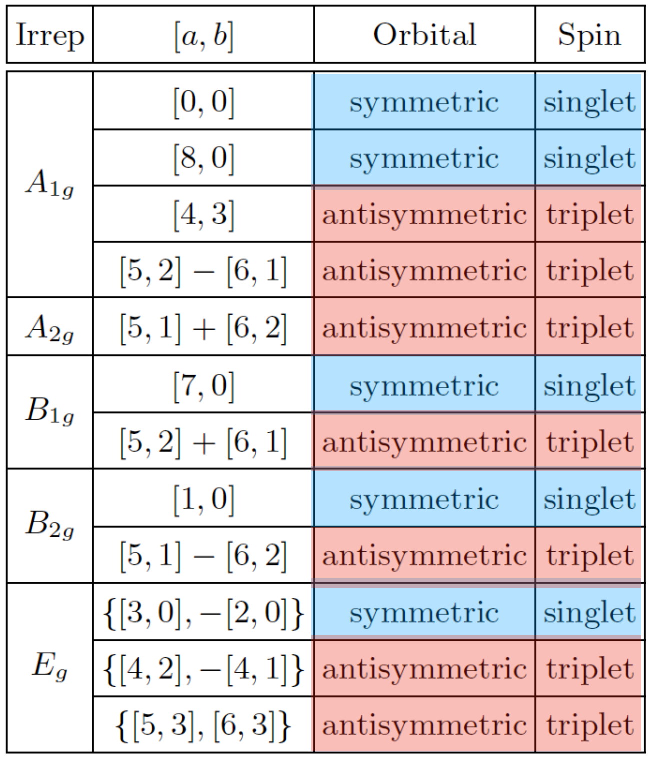


SC states [Even-parity sector]



Irrep	$[a,b]$	Orbital	Spin
A_{1g}	$[0,0]$	symmetric	singlet
	$[8,0]$	symmetric	singlet
	$[4,3]$	antisymmetric	triplet
	$[5,2]-[6,1]$	antisymmetric	triplet
A_{2g}	$[5,1]+[6,2]$	antisymmetric	triplet
B_{1g}	$[7,0]$	symmetric	singlet
	$[5,2]+[6,1]$	antisymmetric	triplet
B_{2g}	$[1,0]$	symmetric	singlet
	$[5,1]-[6,2]$	antisymmetric	triplet
E_g	$\{[3,0],-[2,0]\}$	symmetric	singlet
	$\{[4,2],-[4,1]\}$	antisymmetric	triplet
	$\{[5,3],[6,3]\}$	antisymmetric	triplet

Microscopic basis: E-parity/S-Triplet
Band basis: pseudospin-S

S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

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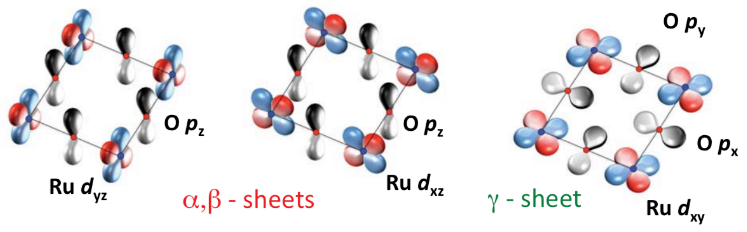

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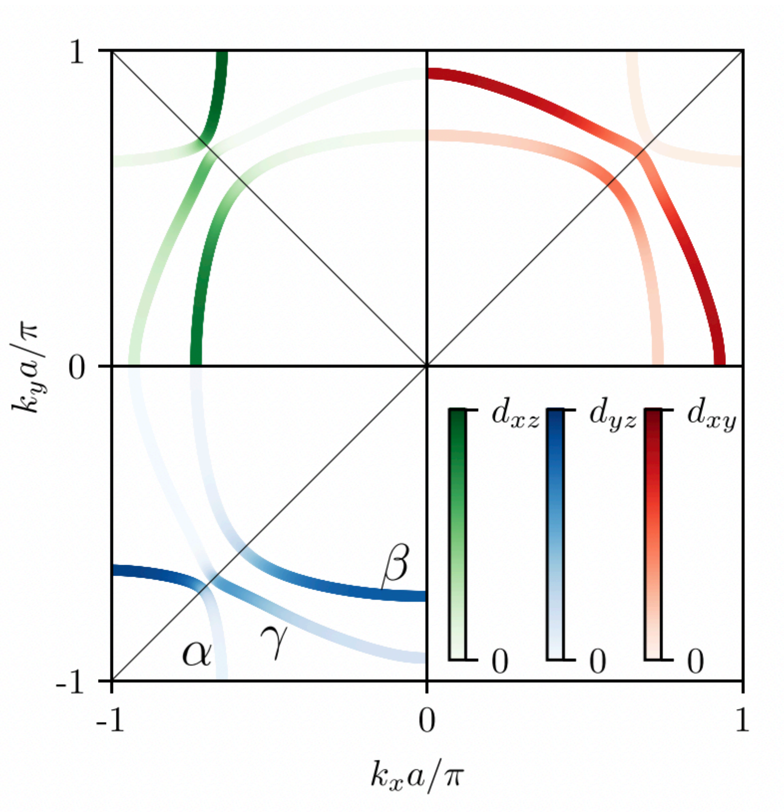

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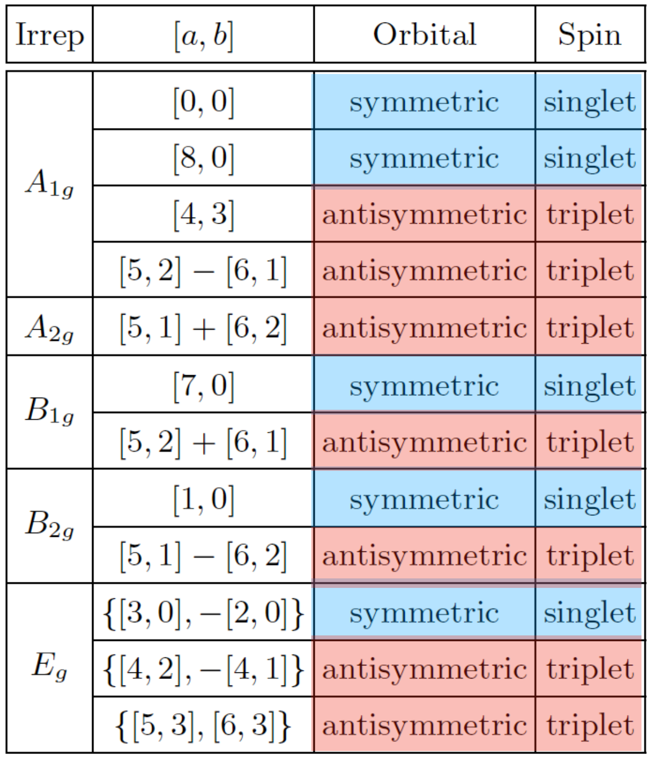

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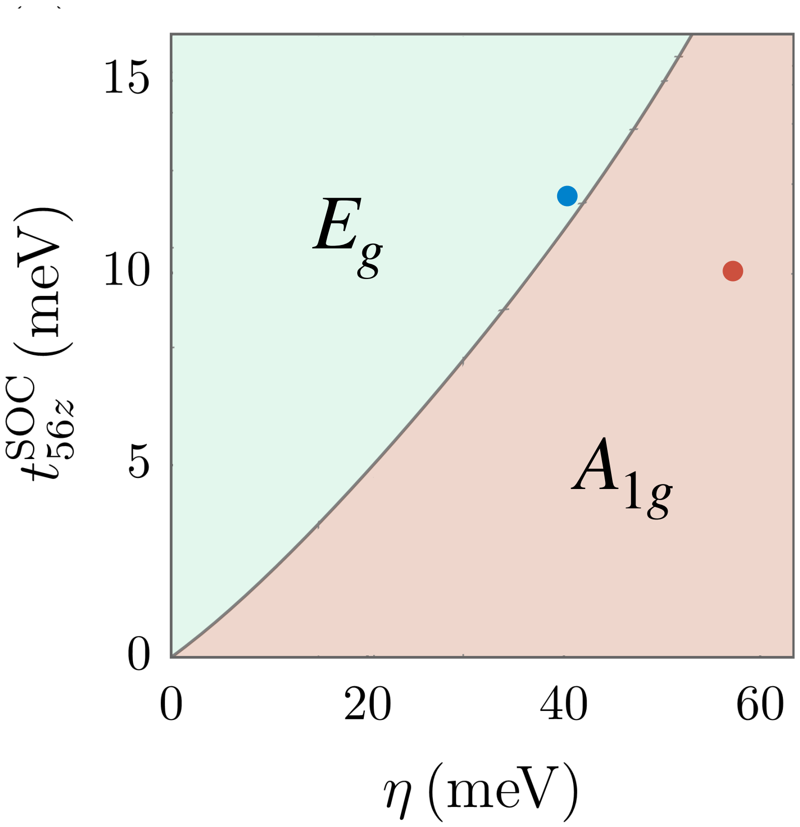
Phase diagram
[atomic x k-dependent SOC]



Hund’s interaction
[inter-orbital]

S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

H. G. Suh, A. Ramires et al., Phys. Rev. Res. **2**, 032023(R) (2020)

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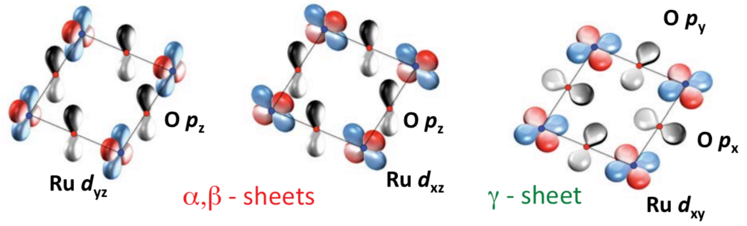

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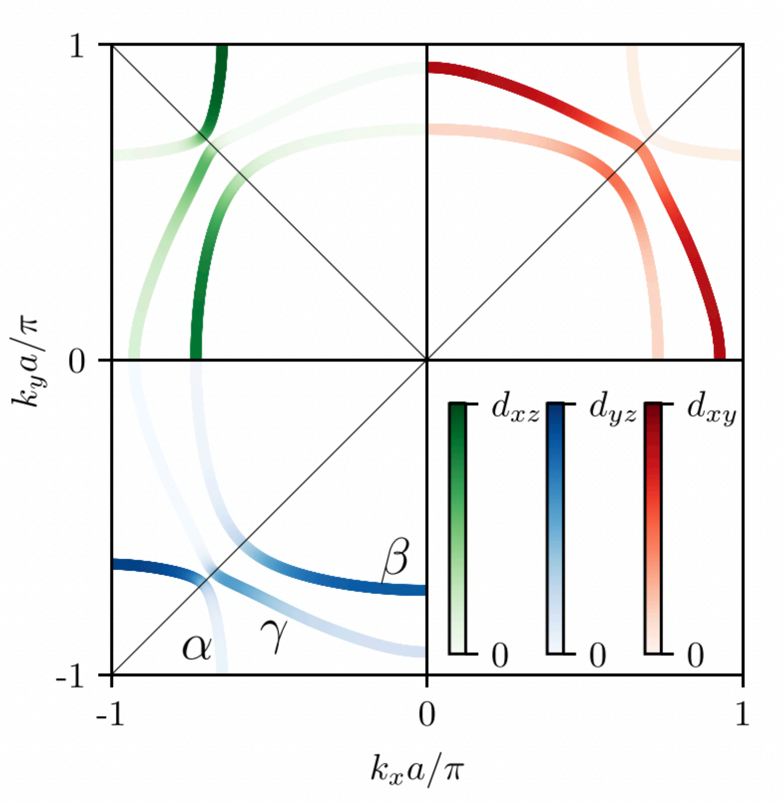

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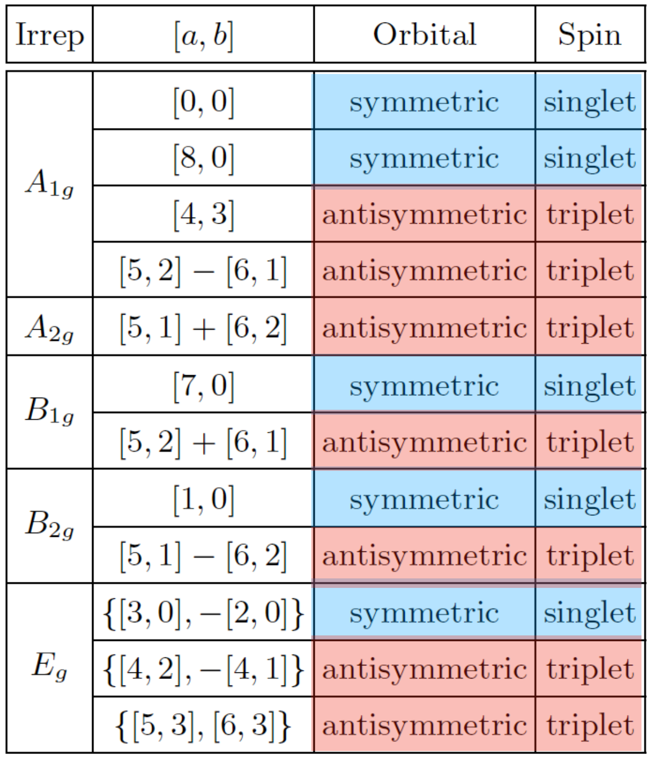

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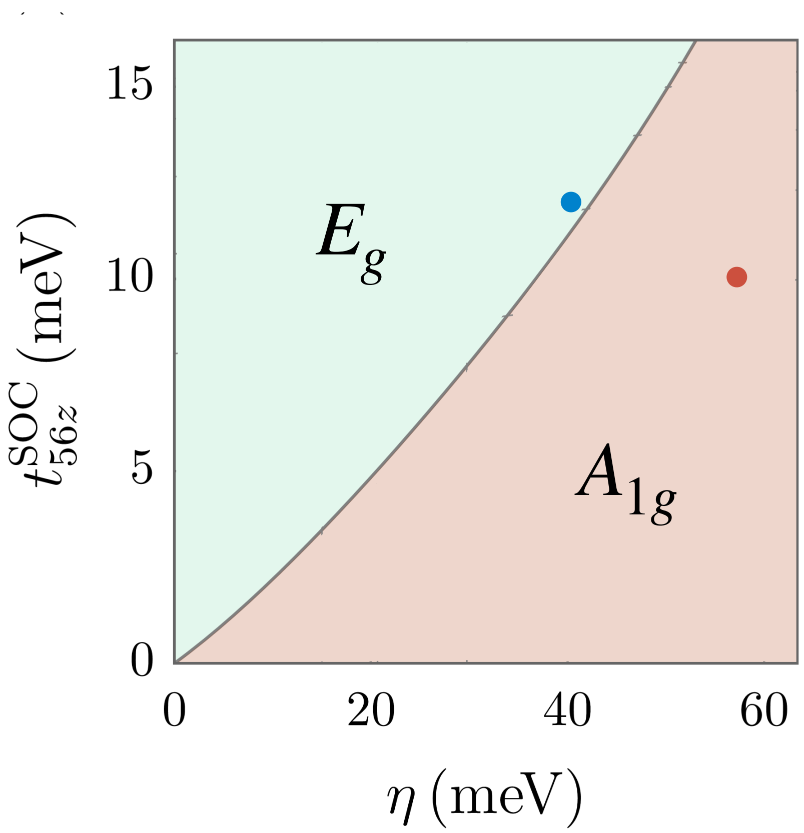

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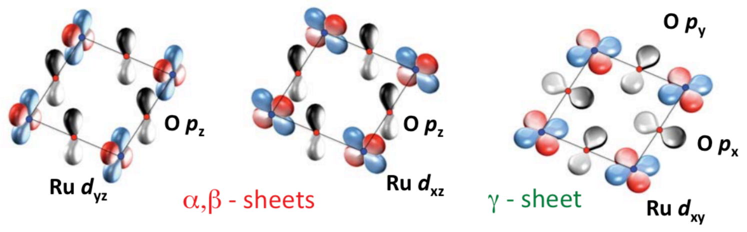

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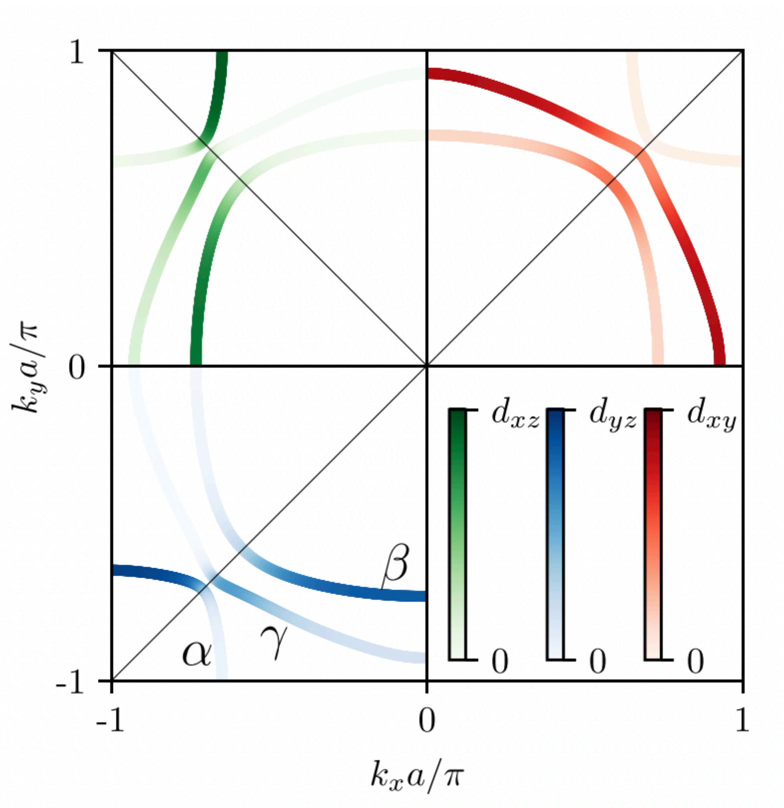

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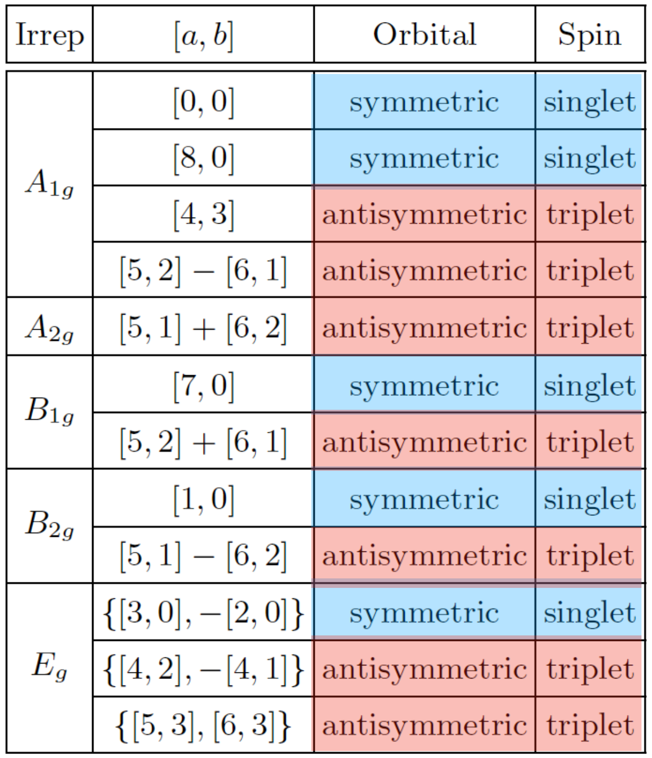

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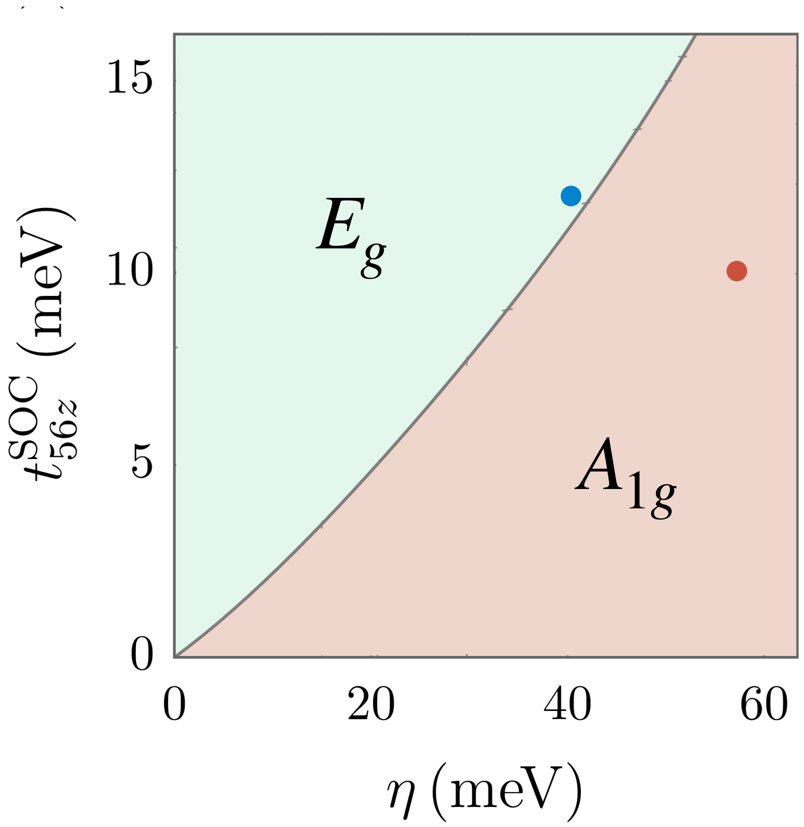


Hund's interaction
[inter-orbital]

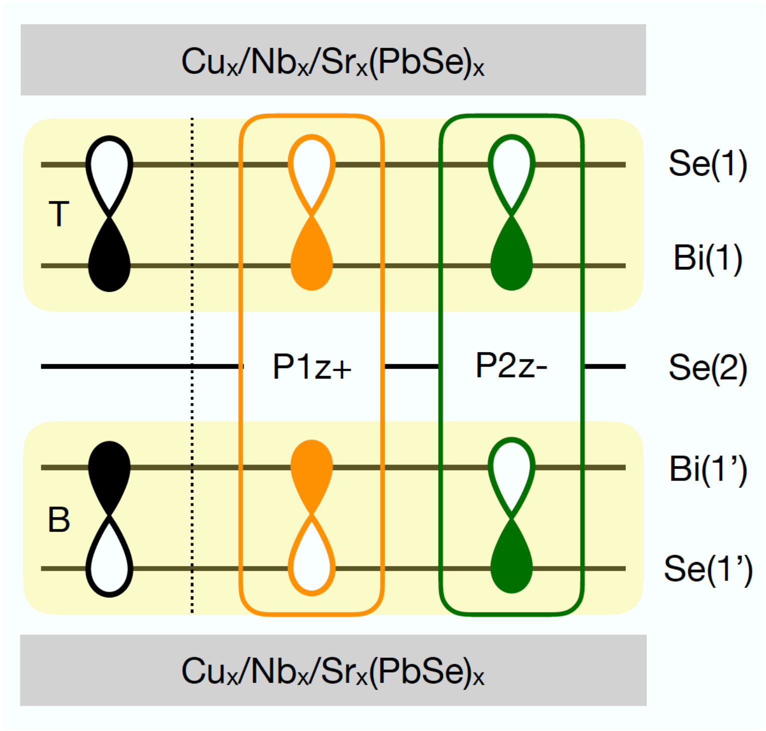
- **Uncovered mechanism for chiral d-wave!**
- **Engineering the normal state to enhance T_c!**

S. Beck, A. Ramires et al., Phys. Rev. Research **4**, 023060 (2022)

H. G. Suh, A. Ramires et al., Phys. Rev. Res. **2**, 032023(R) (2020)

Two-orbitals with opposite parity: d-Bi_2Se_3

Pz-like orbitals in a quintuple layer



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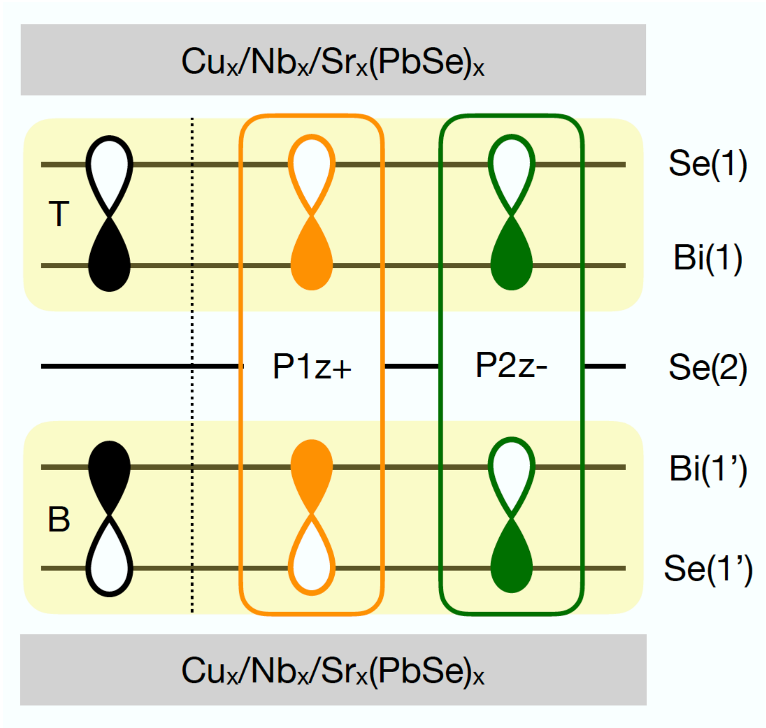

K-independent sector

Irrep	Spin	Orbital	Parity	Matrix Form
A_{1g}	Singlet	Trivial	Even	$\hat{\tau}_0 \otimes \hat{\sigma}_0(i\hat{\sigma}_2)$
				$\hat{\tau}_3 \otimes \hat{\sigma}_0(i\hat{\sigma}_2)$
A_{1u}	Triplet	Singlet	Odd	$\hat{\tau}_2 \otimes \hat{\sigma}_3(i\hat{\sigma}_2)$
A_{2u}	Singlet	Triplet	Odd	$\hat{\tau}_1 \otimes \hat{\sigma}_0(i\hat{\sigma}_2)$
E_u	Triplet	Singlet	Odd	$i\hat{\tau}_2 \otimes \hat{\sigma}_1(i\hat{\sigma}_2)$
				$\hat{\tau}_2 \otimes \hat{\sigma}_2(i\hat{\sigma}_2)$

Odd parity ⇒ Nodes!

[Sensitive to disorder]

Two-orbitals with opposite parity: d-Bi$_2$Se$_3$

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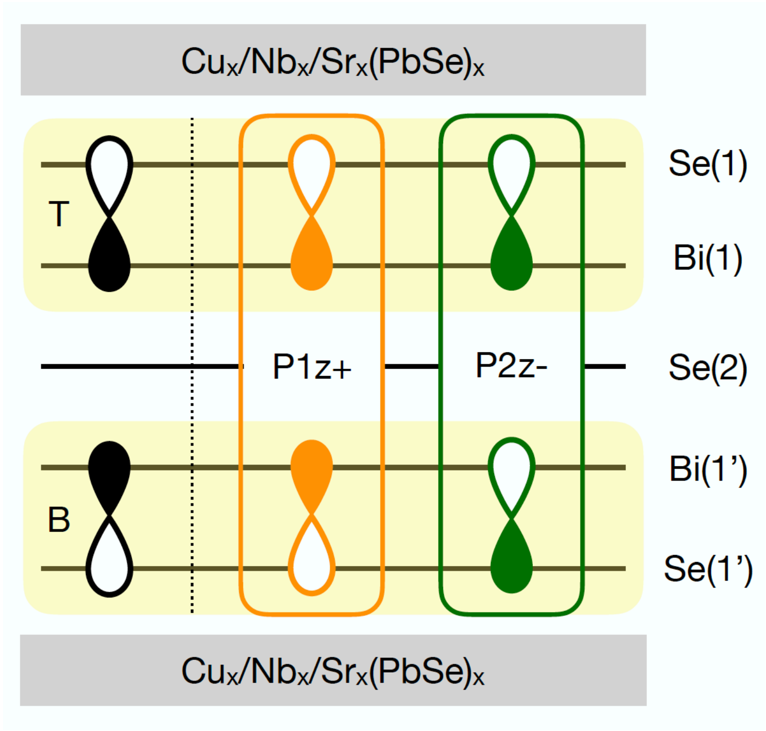

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Odd parity ⇒ Nodes!
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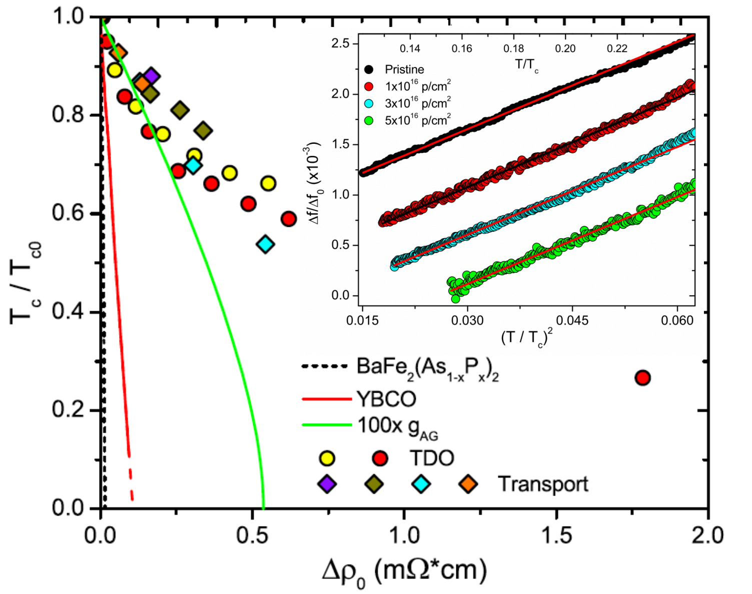
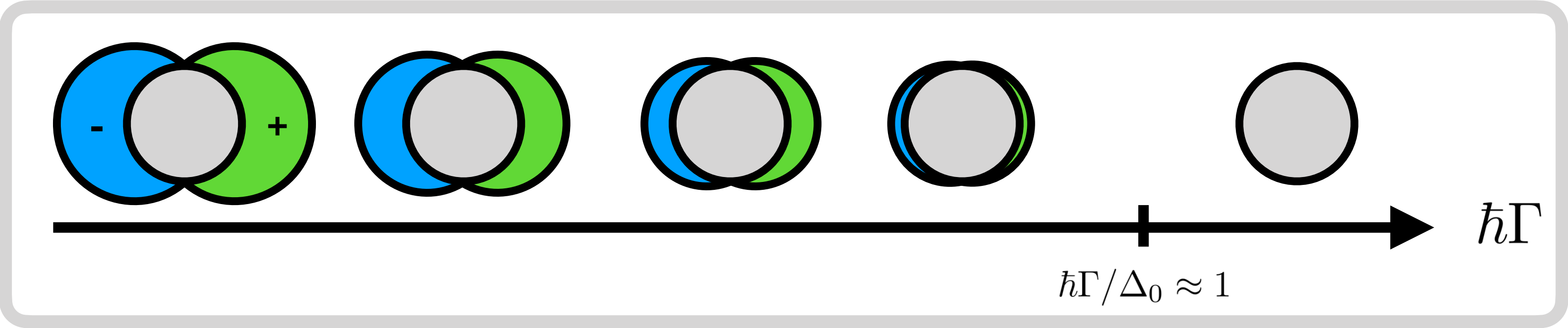
Experiment/Theory



M. P. Smylie et al., PRB **96**, 115145 (2017)



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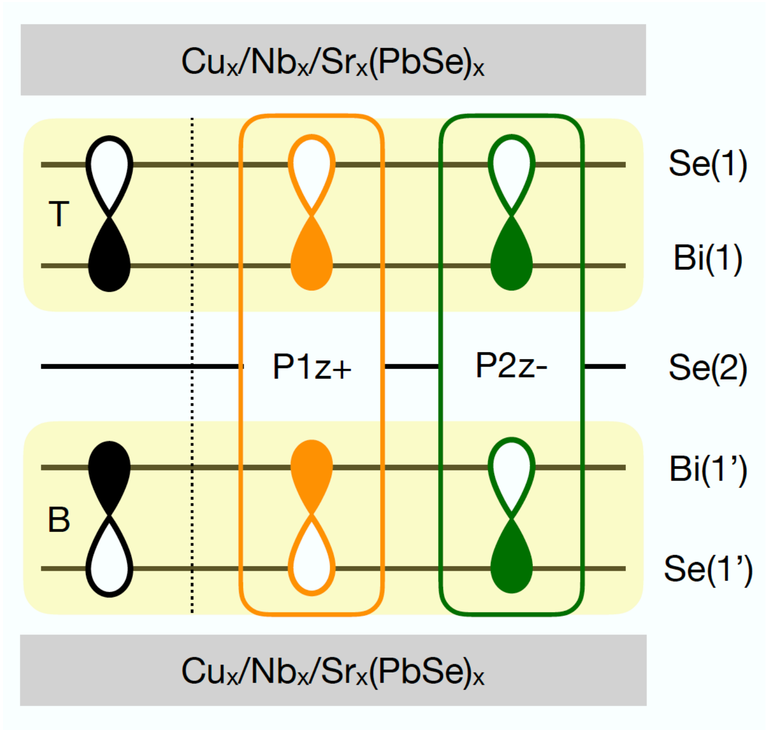

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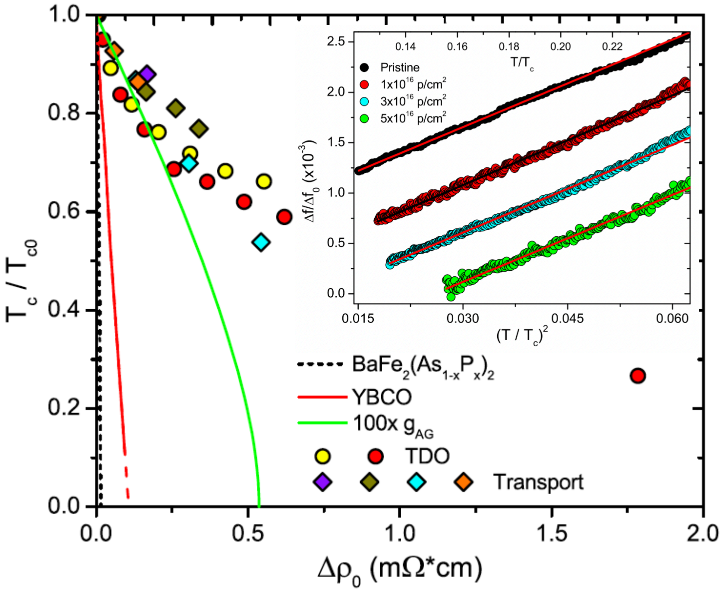
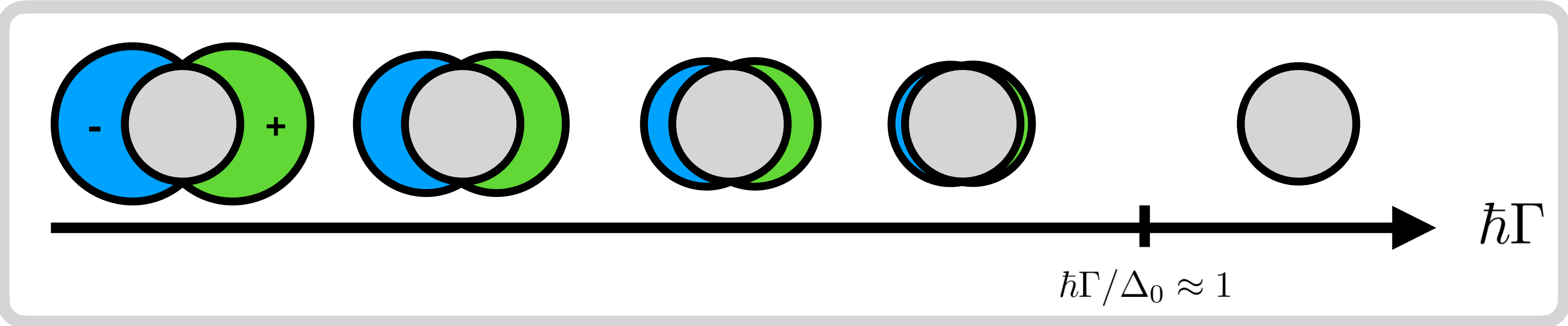
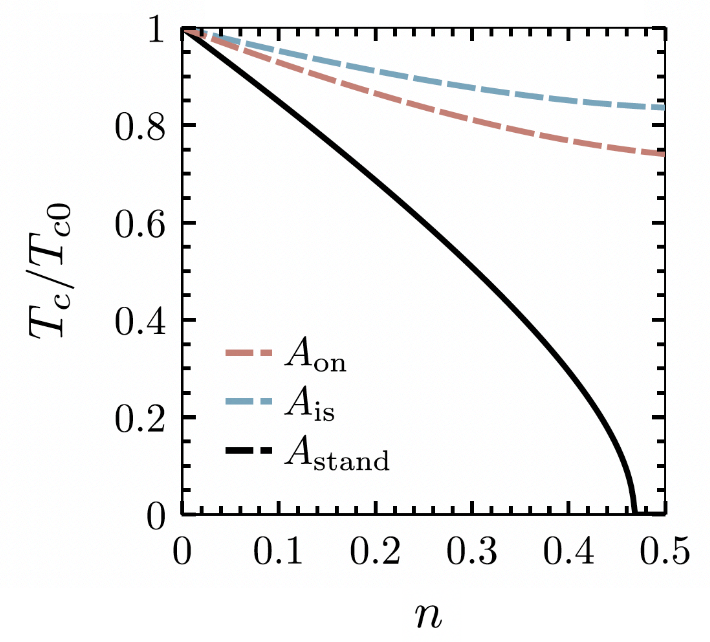


M. P. Smylie et al., PRB **96**, 115145 (2017)



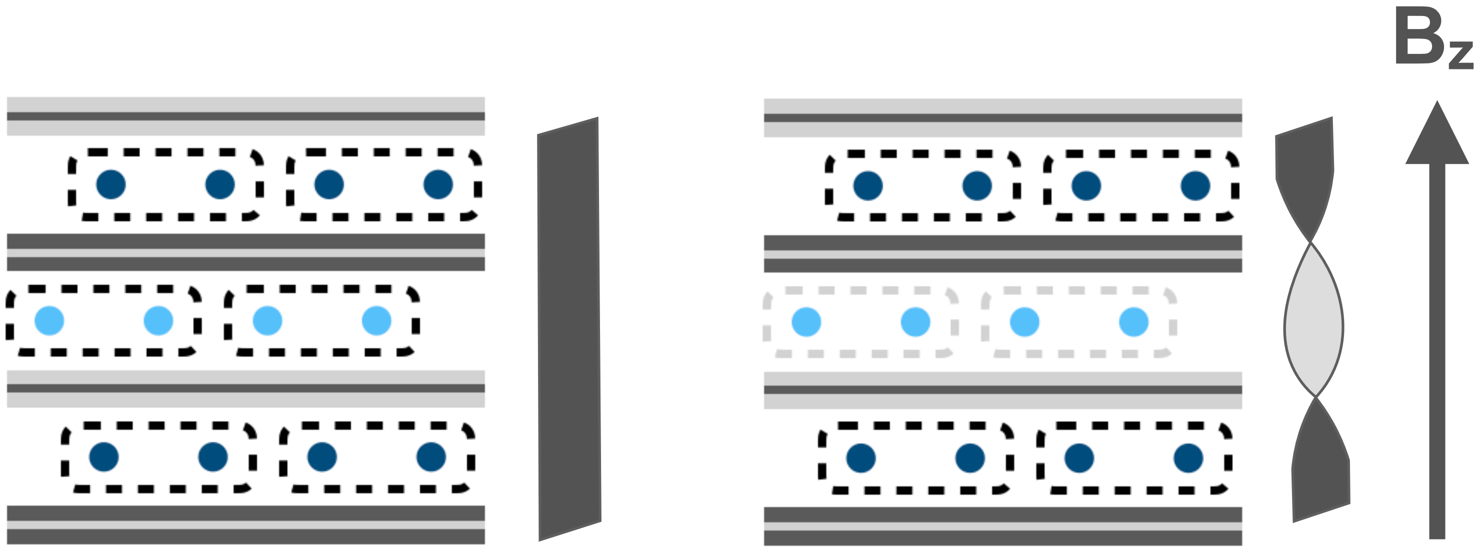


"Generalised Anderson's Theorem"

L. Andersen*, A. Ramires* et al., Sci. Adv. **6**, eaay6502 (2020)
B. Zinkl and A. Ramires, Phys. Rev. B **106**, 014515 (2022)

Two sublattices/layers: $CeRh_2As_2$

Cartoon picture:



“Trivial”
Even-parity SC

B_z-robust
Odd-parity SC

M. Sigrist et al., J. Phys. Soc. Jpn. **83**, 061014 (2014)
T. Yoshida et al., Phys. Rev. B **86**, 134514 (2012)
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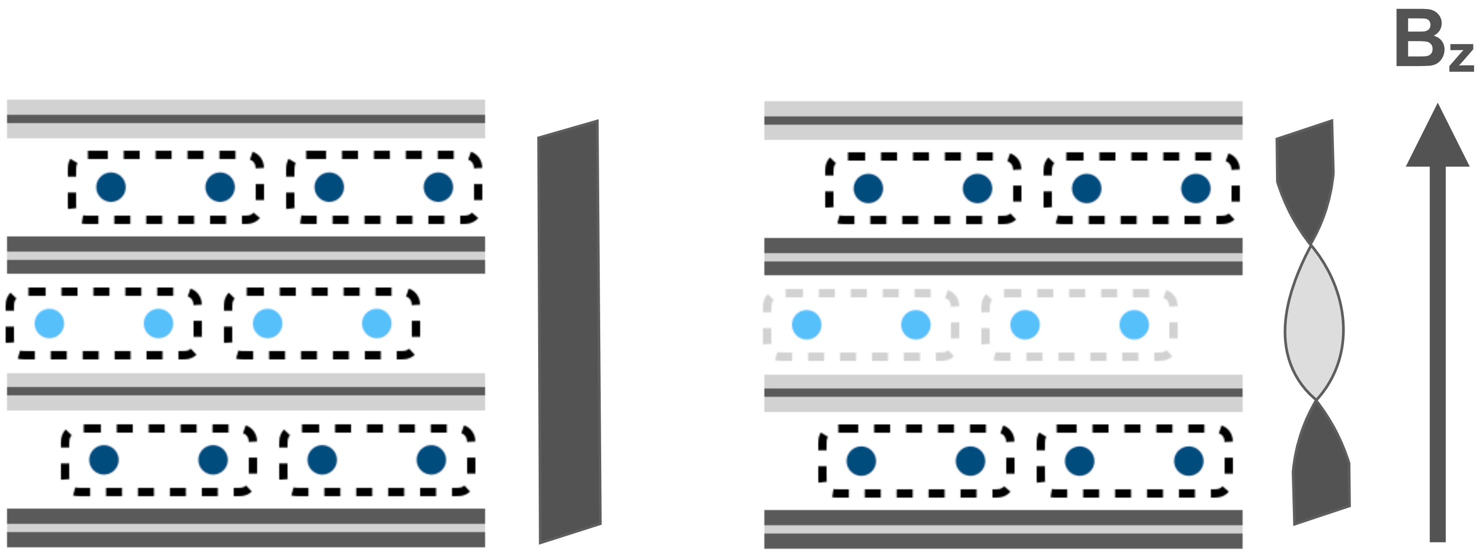

“Trivial”
Even-parity SC

B_z-robust
Odd-parity SC

Trivial pairing + Twist = Odd parity SC

⇕

w.r.t. an extra internal DOF
[SL/layers/orbitals/…]

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Elena’s Lecture

Two sublattices/layers: $CeRh_2As_2$

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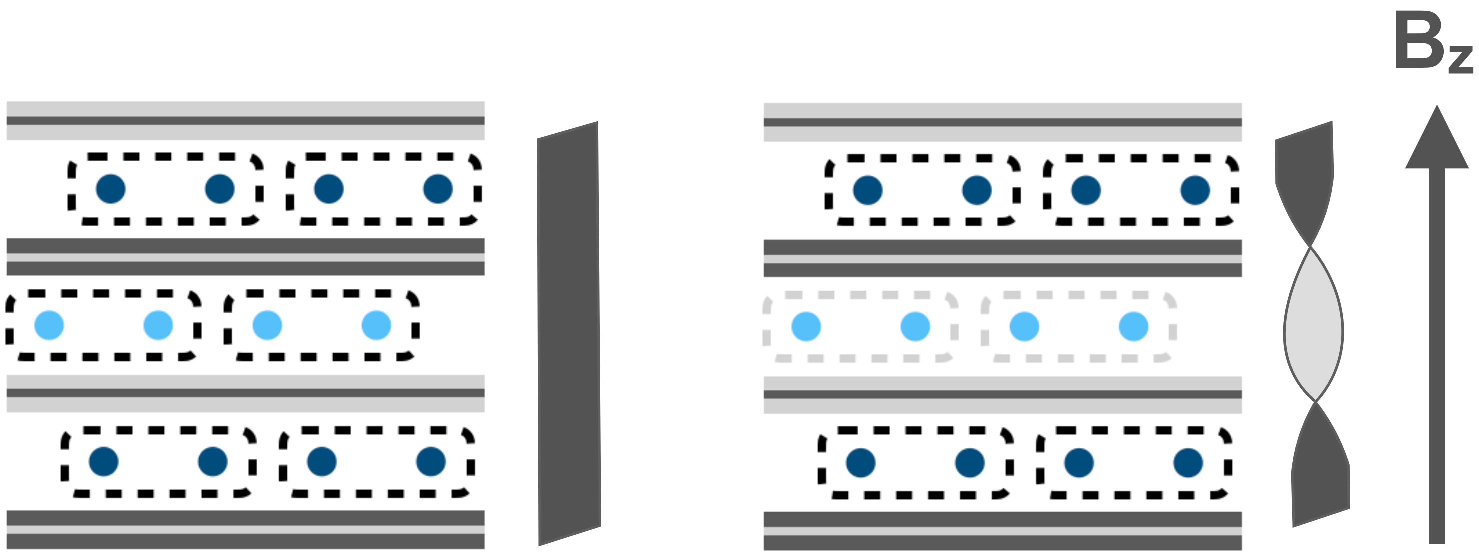

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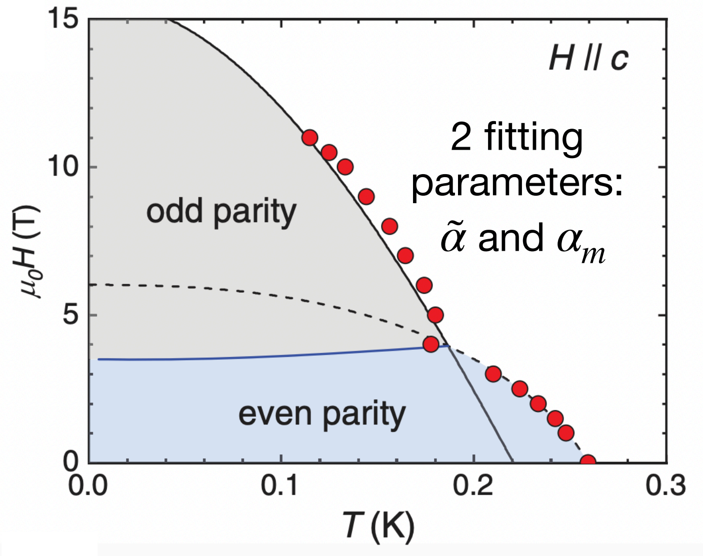
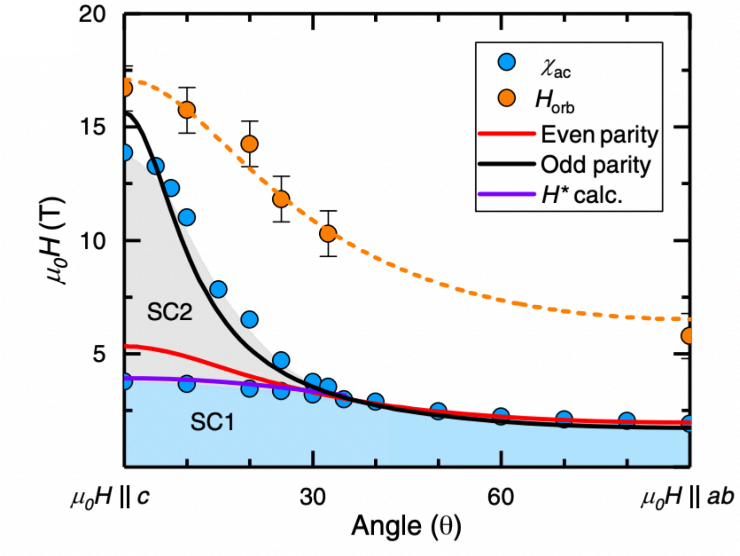
D. Möckli and A. Ramires, Phys. Rev. B **104**, 134517 (2021)

Successfully fits the HxT phase diagram



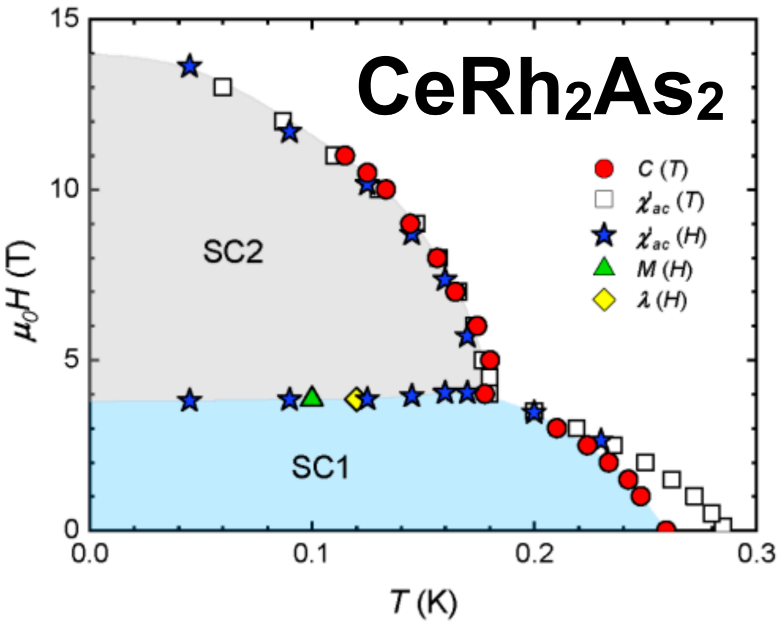
Khim et al., Science **373**, 1012 (2021)

Successfully addresses the magnetic field anisotropy



Landaeta et al., PRX **12**, 031001 (2022)

Some common themes…



S. Khim et al., Science **373**, 1012 (2021)
S. Adenwalla et a., Phys. Rev. Lett. **65**, 2298 (1990)
D. Aoki et al., J. Phys. Soc. Jpn. **89**, 053705 (2020)
S. Ran et al., Nature Physics 15, 1250 (2019)

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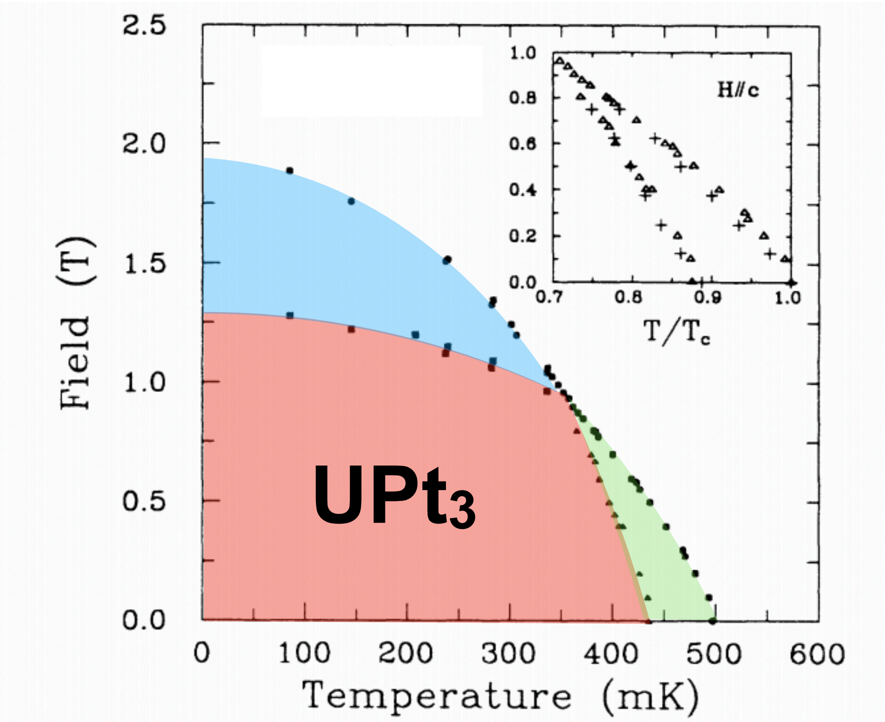

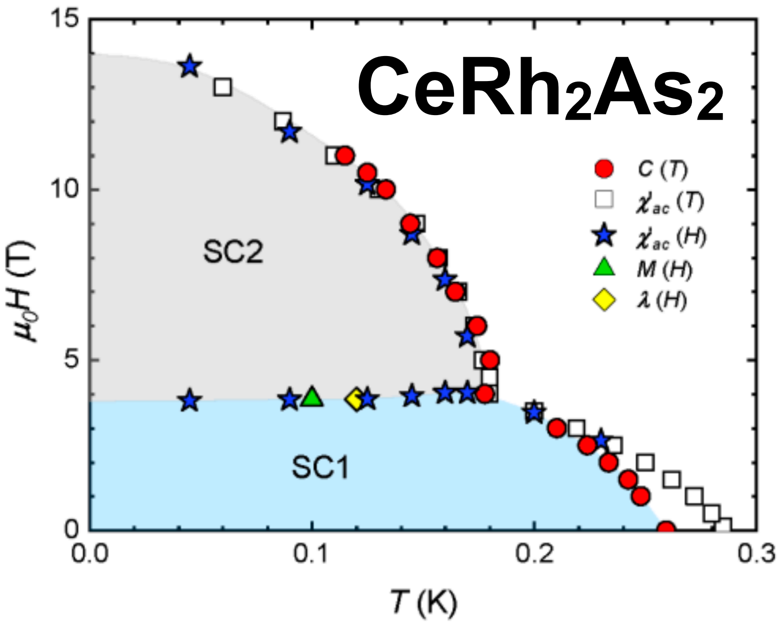

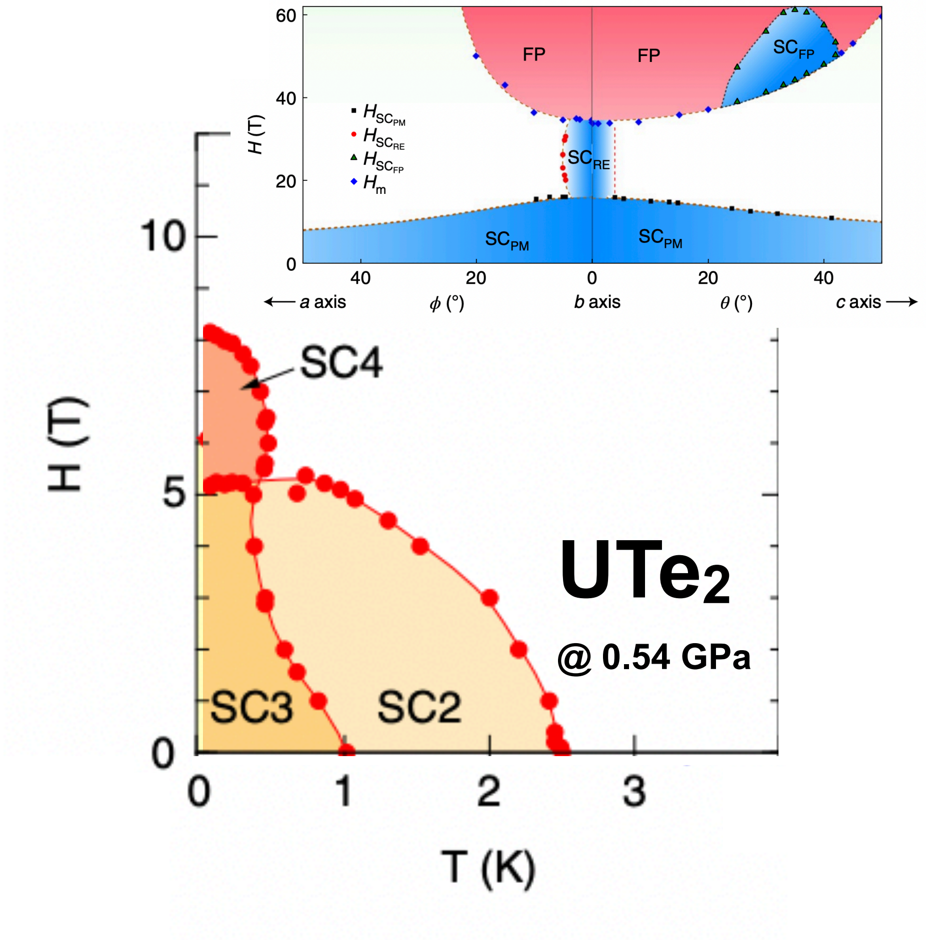

- **Phase diagrams with multiple SC phases are rare!**
- **Only observed in other two HF materials!**
- **Indication of unconventional SC state!**

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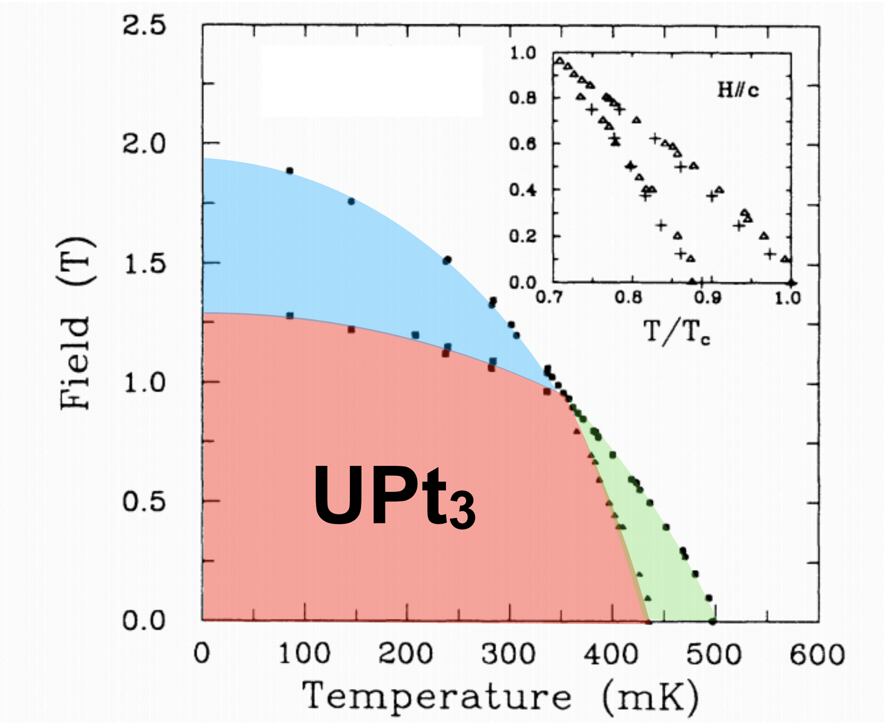

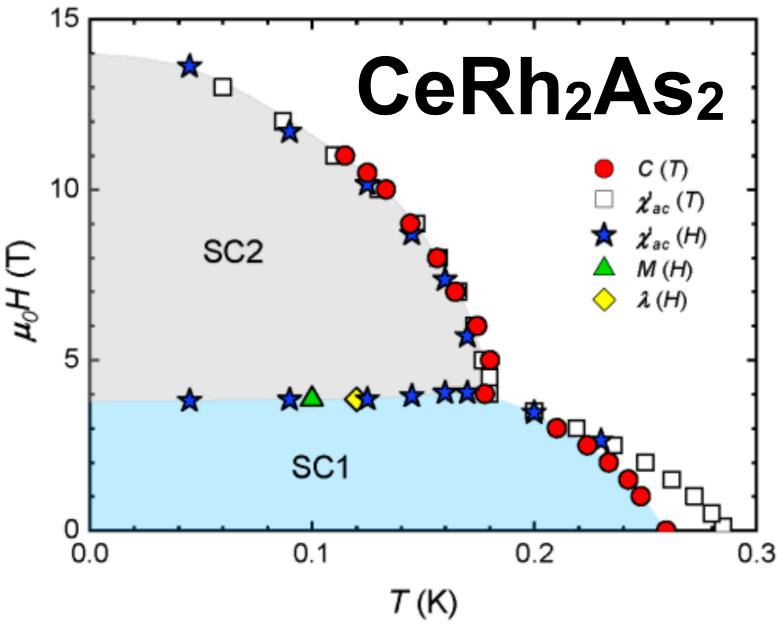

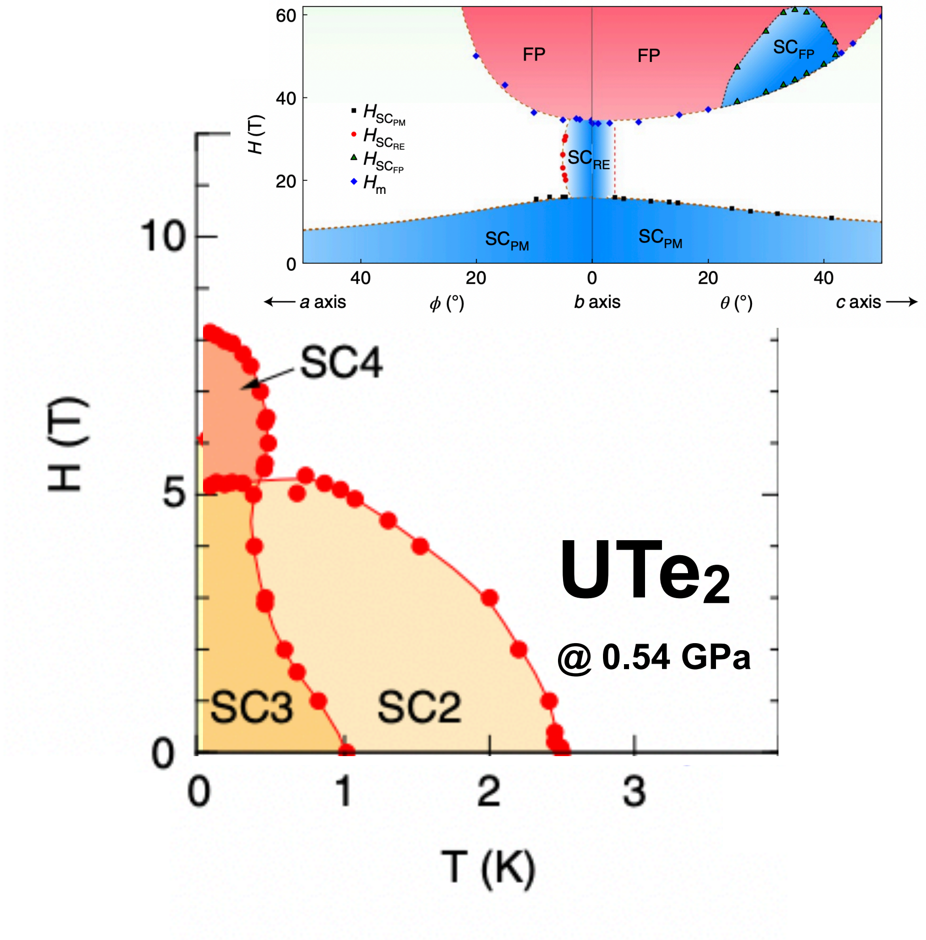

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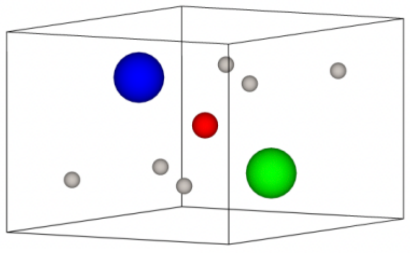
- **Common theme: sublattice DOF?!**

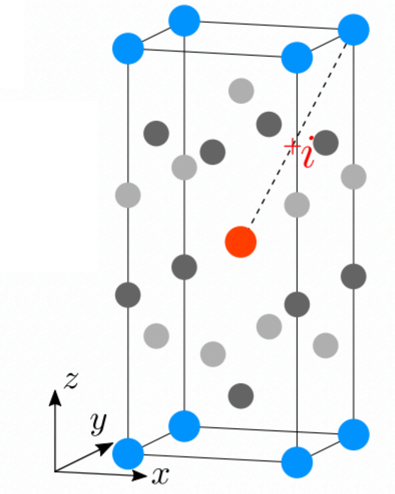
T. Hazra et al., Phys. Rev. Lett. **130**, 136002 (2023)

$P6_3/mmc$



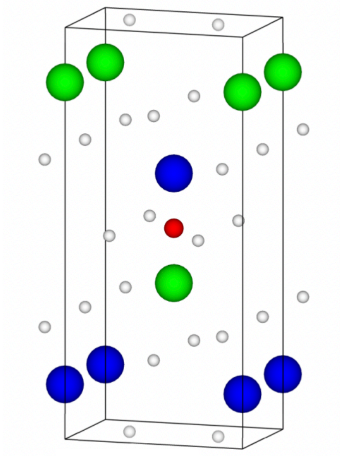
Nonsymmorphic

P4/nmm



Nonsymmorphic

I/mmm



Body-centered

S. Khim et al., Science **373**, 1012 (2021)
S. Adenwalla et a., Phys. Rev. Lett. **65**, 2298 (1990)
D. Aoki et al., J. Phys. Soc. Jpn. **89**, 053705 (2020)
S. Ran et al., Nature Physics 15, 1250 (2019)

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Rev. Mod. Phys **63**, 239 (1991)

Symmetry aspects of Chiral Superconductors
Aline Ramires
Contemporary Physics **63**(2), 71 (2022)

Nonunitary Superconductivity in Complex Quantum Materials
Aline Ramires
J. Phys.: Condens. Matter **34** 304001(2022)

Still mystery after all these years -- Unconventional SC of Sr_2RuO_4
Yoshiteru Maeno, Shingo Yonezawa, Aline Ramires
arXiv:2402.12117 [Invited review to appear in JPSJ]

Have we covered everything?
Is the Sigrist-Ueda classification “complete”?

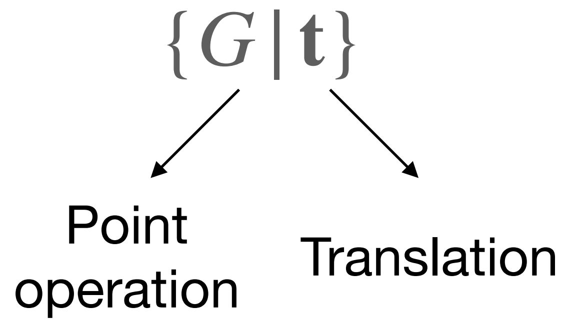
[Generalizations]

I) Multiple internal DOF

II) Nonsymmorphic systems [Space group]

Crystallographic Space Groups in 3D

A general space-group operation can be written as [Seitz notation]:



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Point operation

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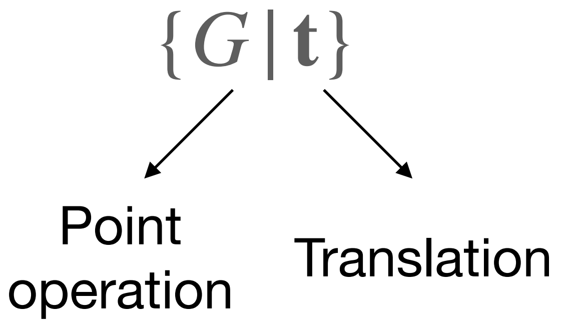

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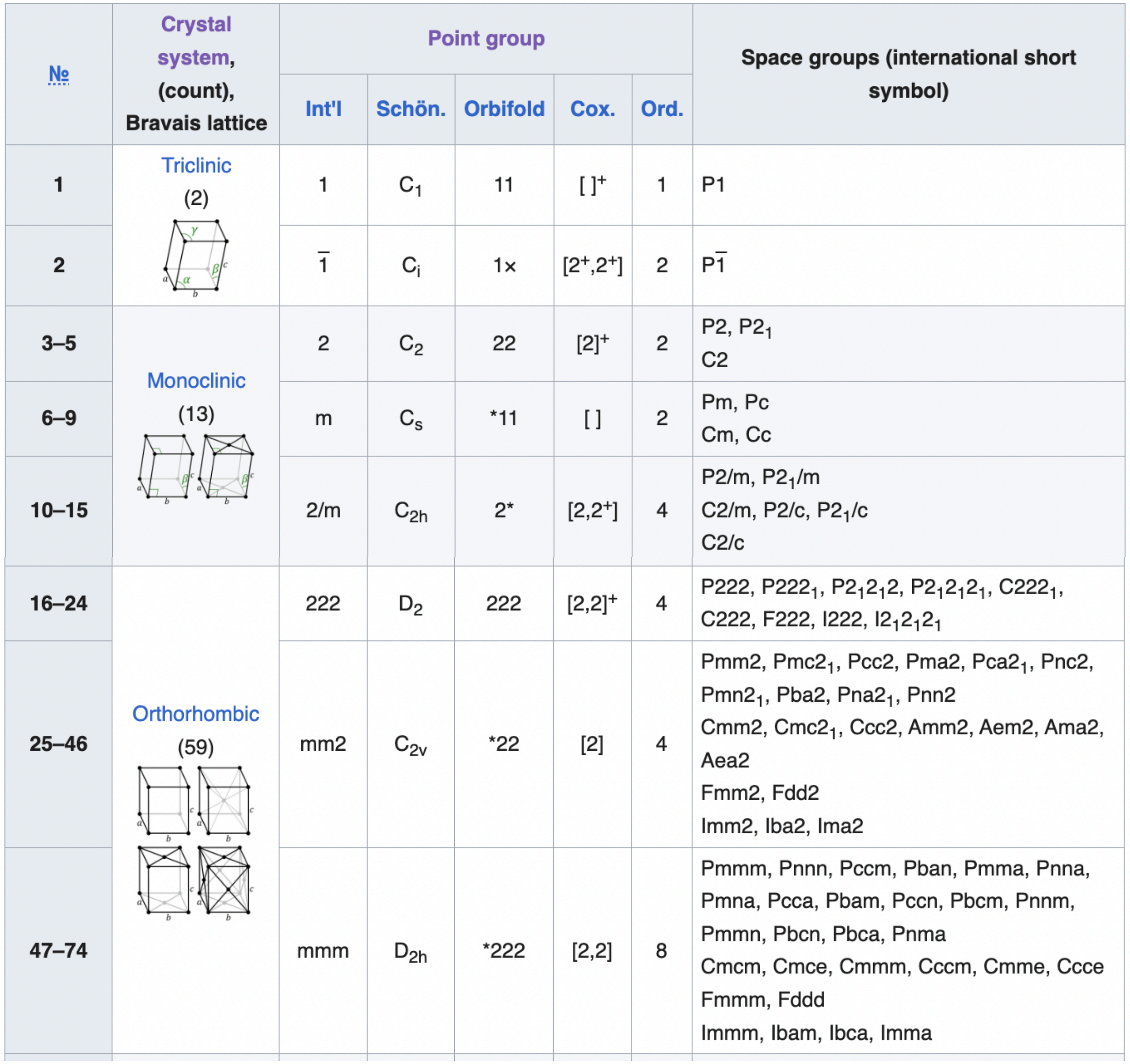
[There are 230 space groups in 3D]



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		Int'l	Schön.	Orbifold	Cox.	Ord.	
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3–5	Monoclinic (13)	2	C_2	22	[2]$^+$	2	P2, $P2_1$ C2
6–9		m	C_s	*11	[ ]	2	Pm, Pc Cm, Cc
10–15		2/m	C_{2h}	2*	[2,2^+]	4	P2/m, $P2_1$/m C2/m, P2/c, $P2_1$/c C2/c
16–24	Orthorhombic (59)	222	D_2	222	[2,2]$^+$	4	P222, $P222_1$, $P2_12_12$, $P2_12_12_1$, $C222_1$, C222, F222, I222, $I2_12_12_1$
25–46		mm2	C_{2v}	*22	[2]	4	Pmm2, $Pmc2_1$, Pcc2, Pma2, $Pca2_1$, Pnc2, $Pmn2_1$, Pba2, $Pna2_1$, Pnn2 Cmm2, $Cmc2_1$, Ccc2, Amm2, Aem2, Ama2, Aea2 Fmm2, Fdd2 Imm2, Iba2, Ima2
47–74		mmm	D_{2h}	*222	[2,2]	8	Pmmm, Pnnn, Pccm, Pban, Pmma, Pnna, Pmna, Pcca, Pbam, Pccn, Pbcm, Pnnm, Pmmn, Pbcn, Pbca, Pnma Cmcm, Cmce, Cmmm, Cccm, Cmme, Ccce Fmmm, Fddd Immm, Ibam, Ibca, Imma

Continues with tetragonal, trigonal, hexagonal and cubic…

https://en.wikipedia.org/wiki/Space_group

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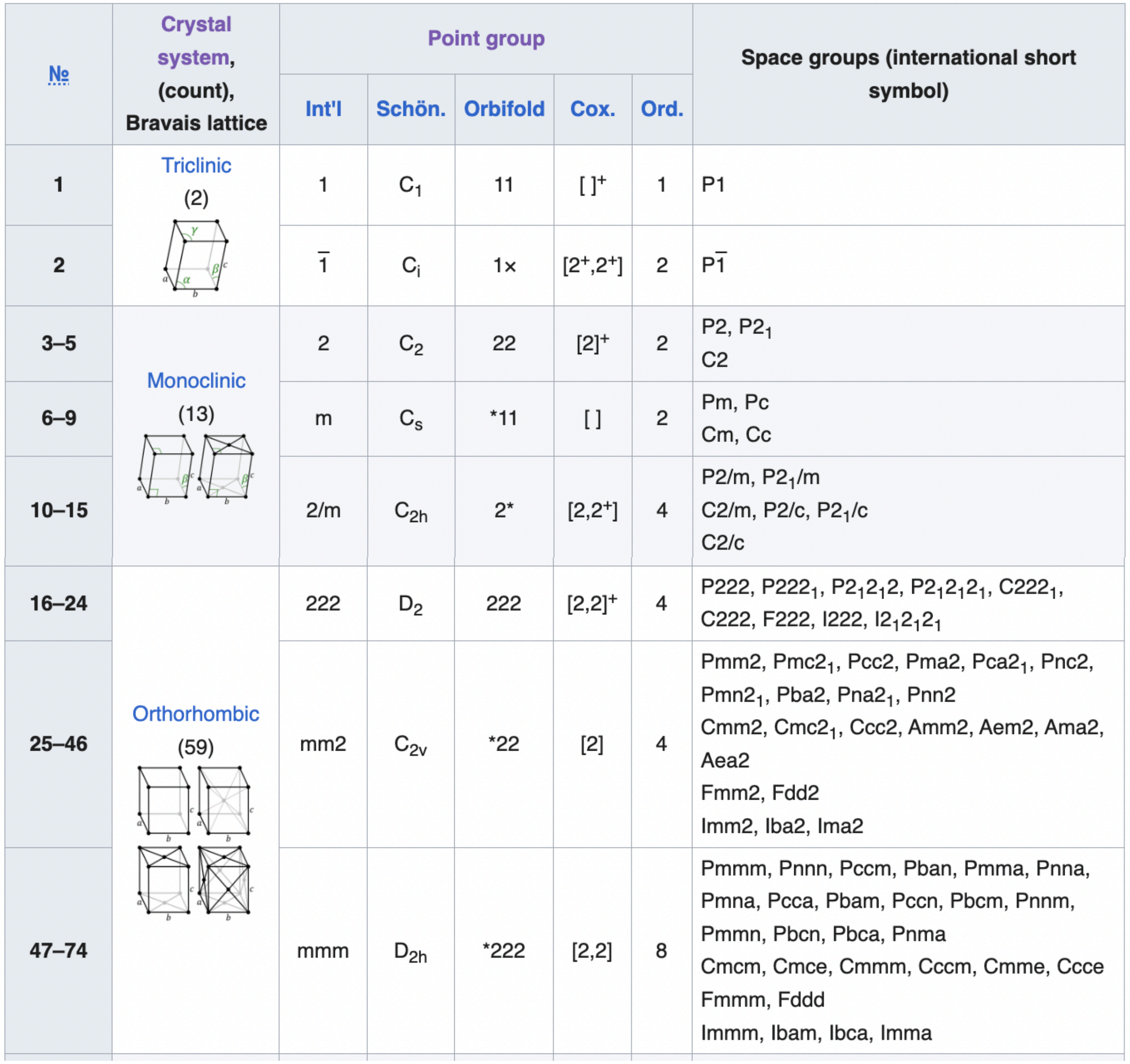

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Note: Order of the SG is infinite (translations!)

Compound space group operations (I)

Glide Plane: $\{M \,|\, \mathbf{t}_{||}\}$

Definition: A glide plane consists of a reflection followed by a (non-primitive) translation parallel to the plane of reflection.

1D Example

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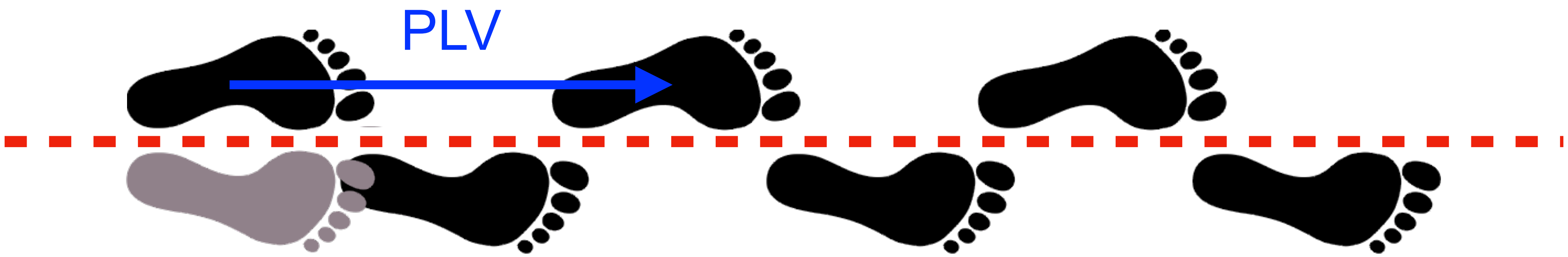

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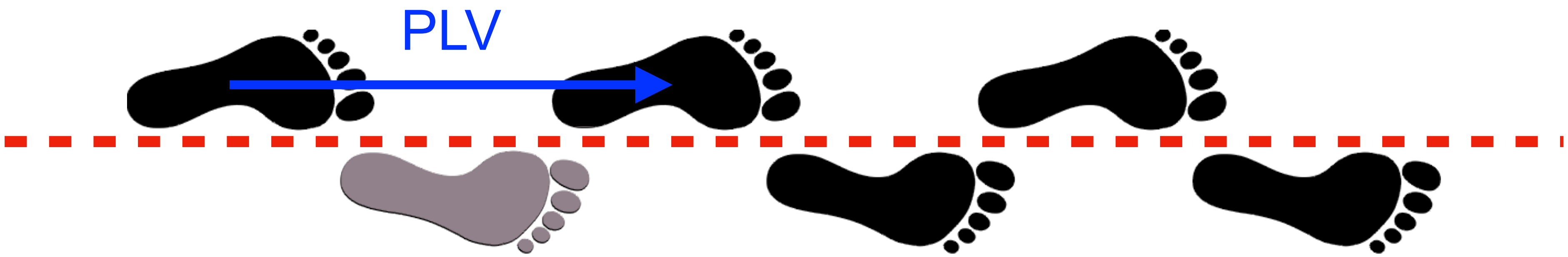

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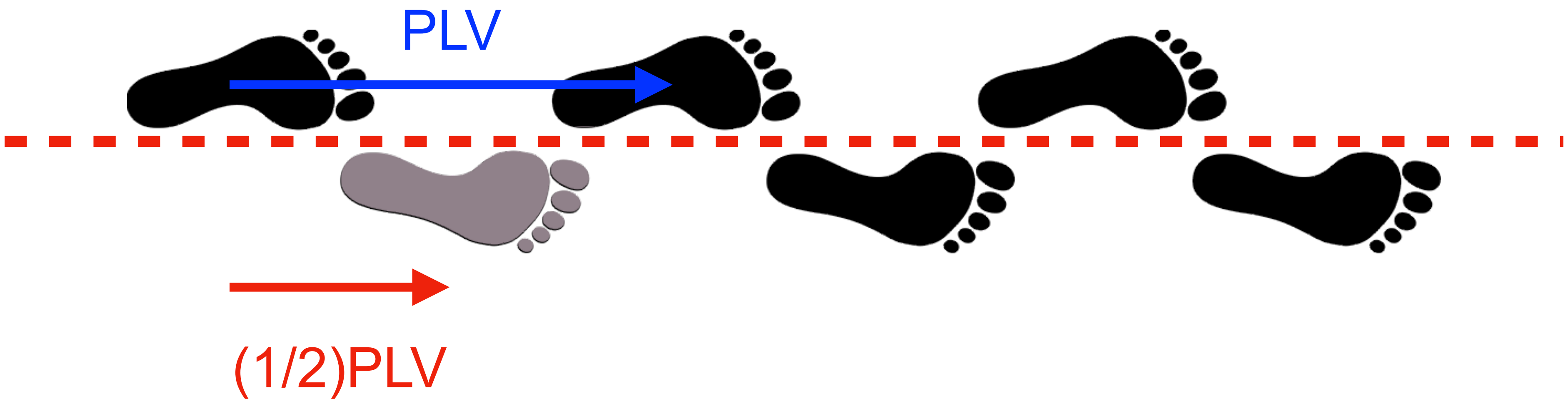

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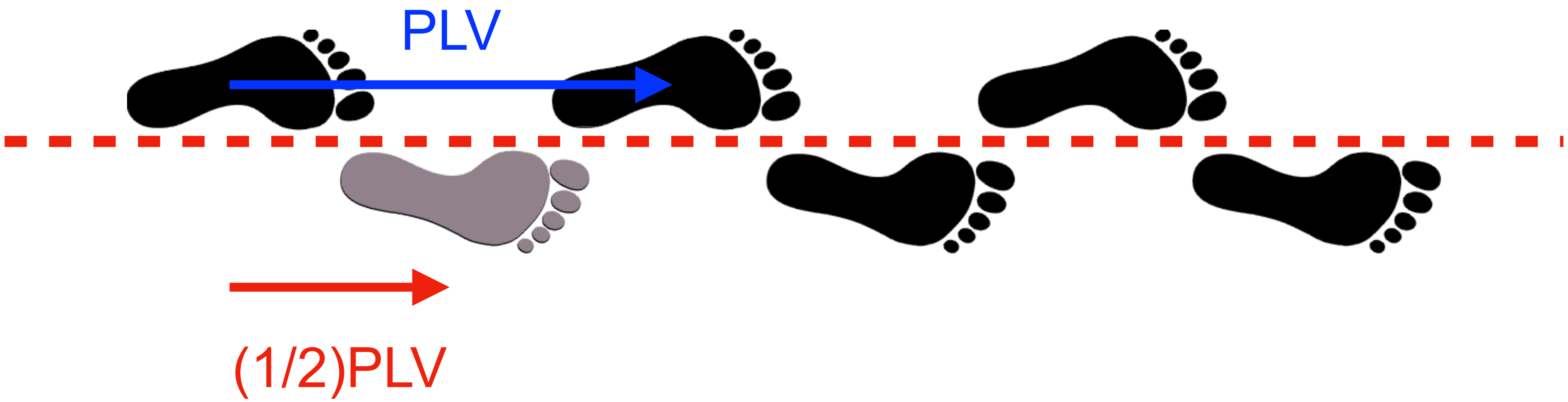
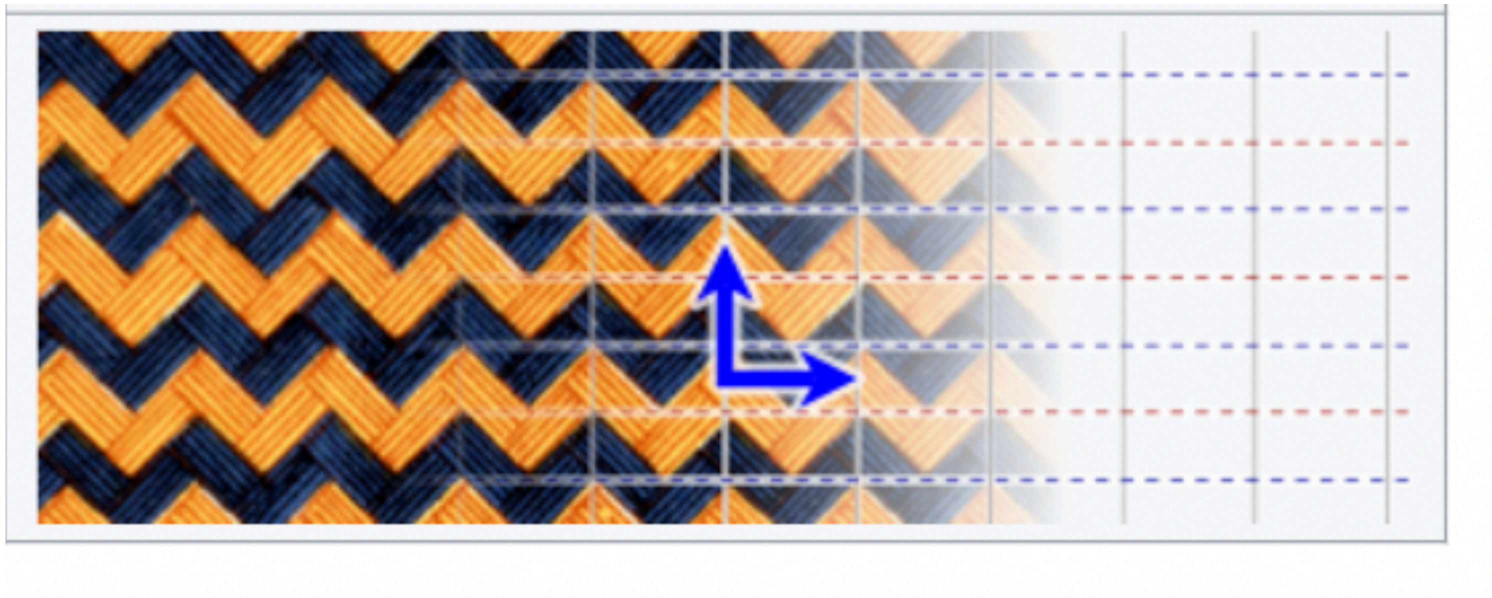


2D Example



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Compound space group operations (II)
Screw axis: $\{R\,|\,\mathbf{t}_{||}\}$

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J. Li et al., Phil. Mag. **93**, 3216 (2013)

A. Sazbo and A. Ramires arXiv.2309.05664 (2023)

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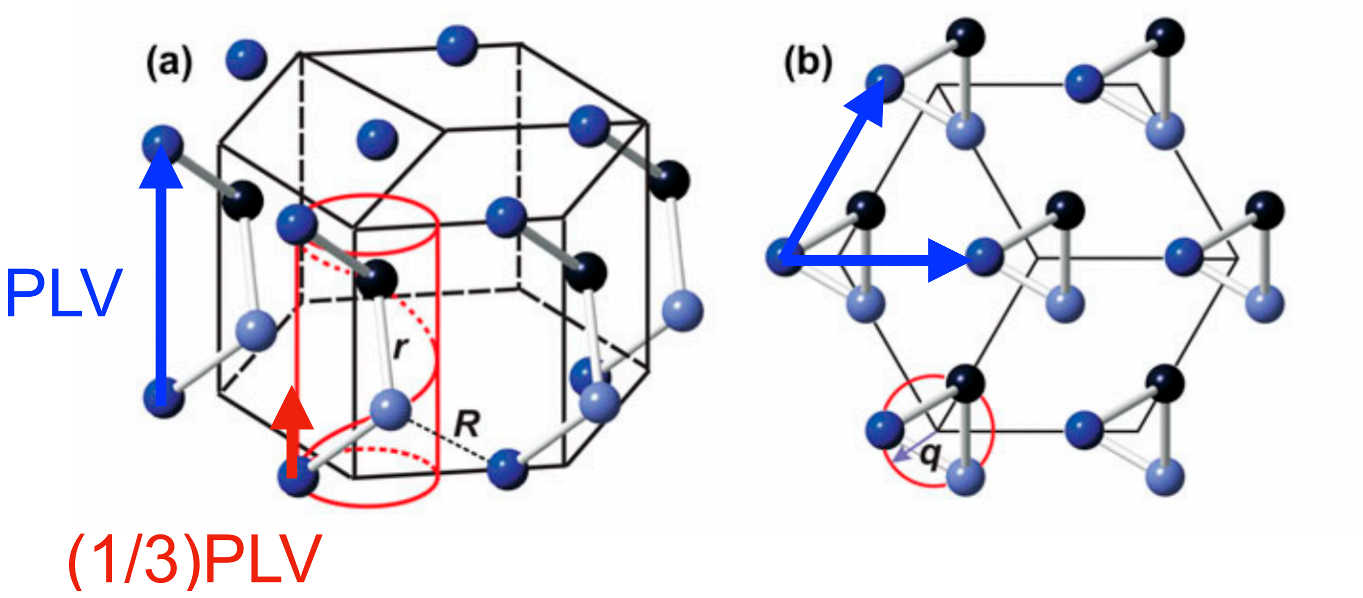

[P$3_1$21]

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Elena's Lecture

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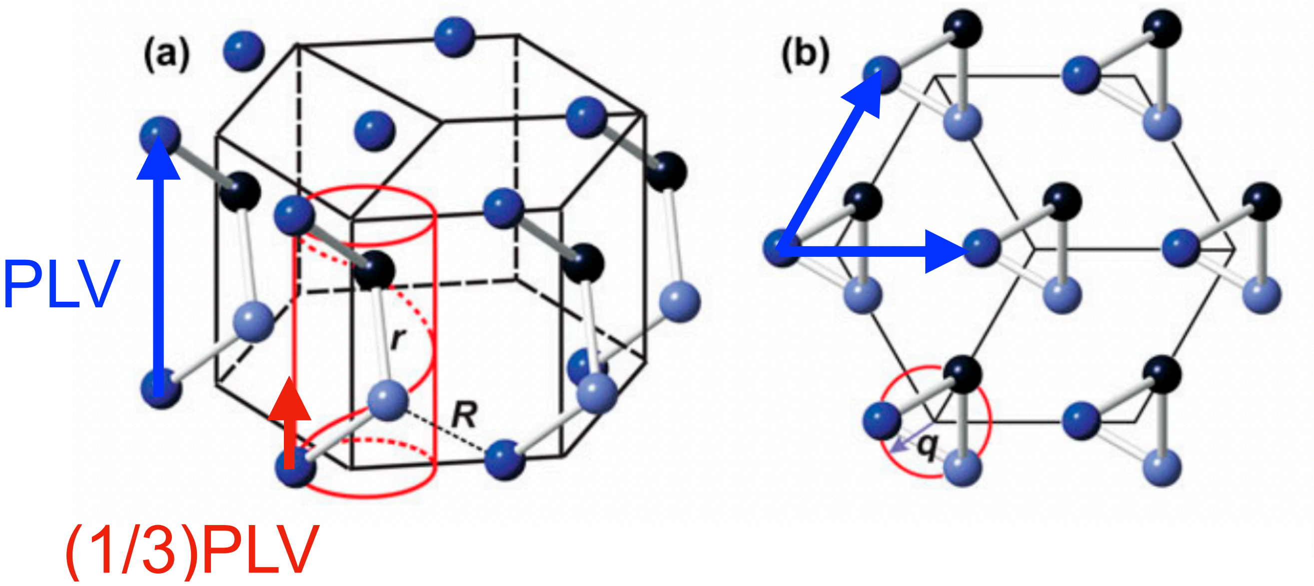

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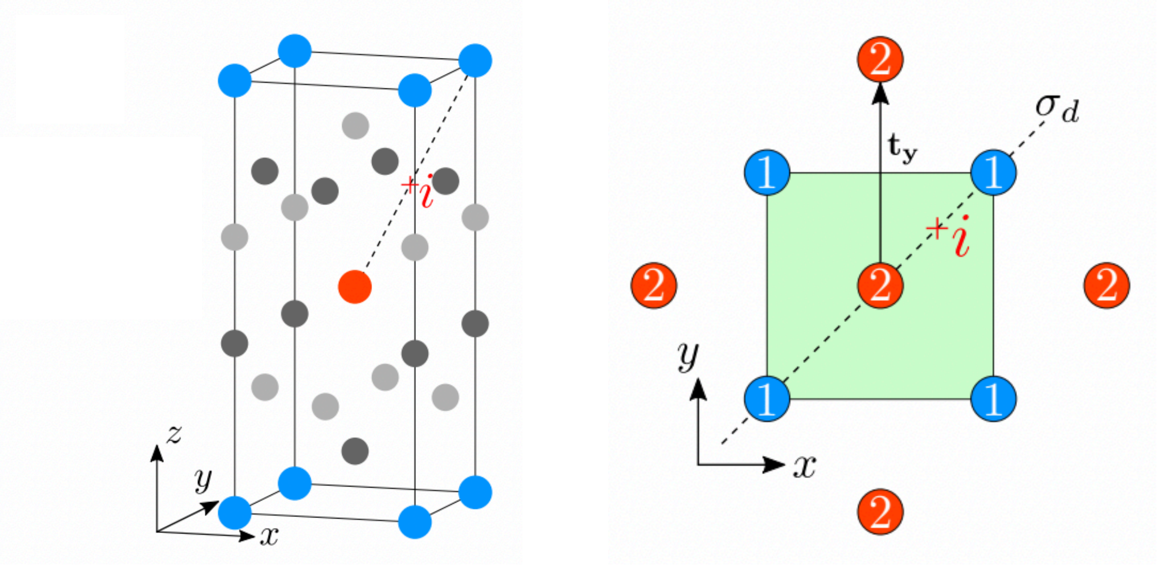

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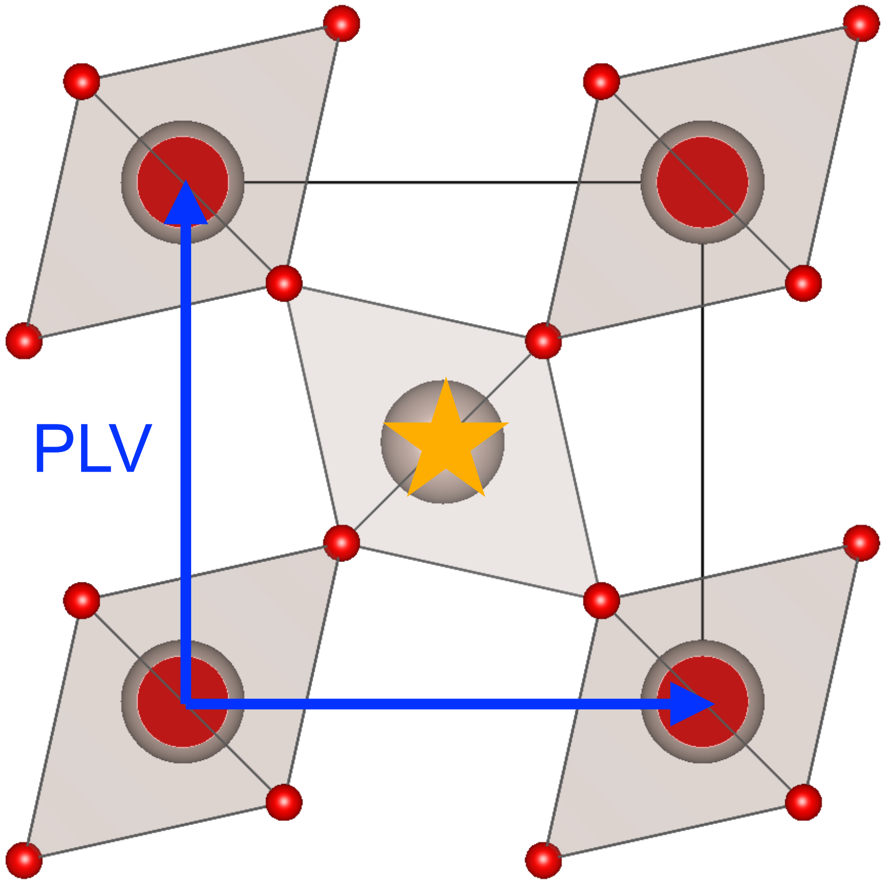

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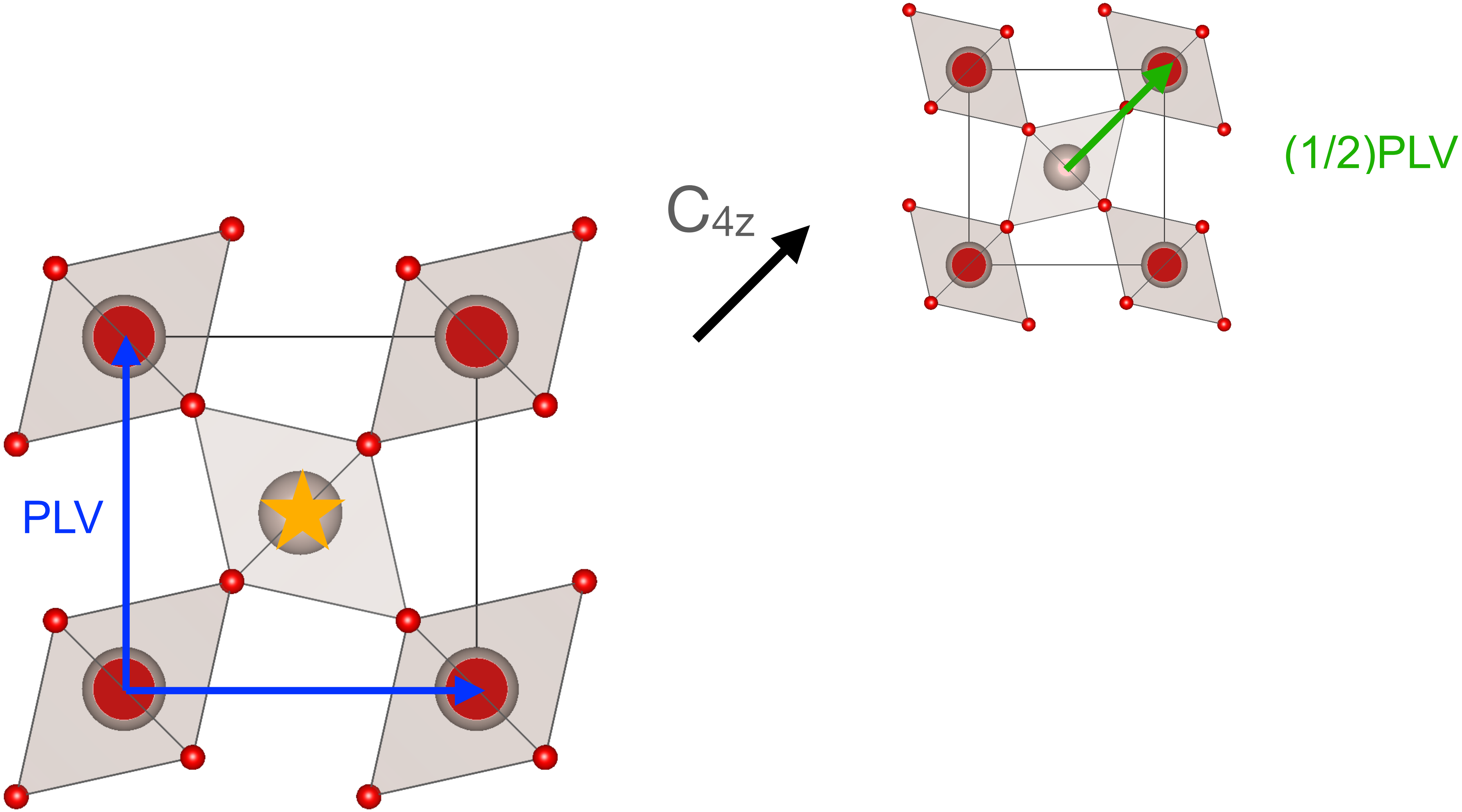

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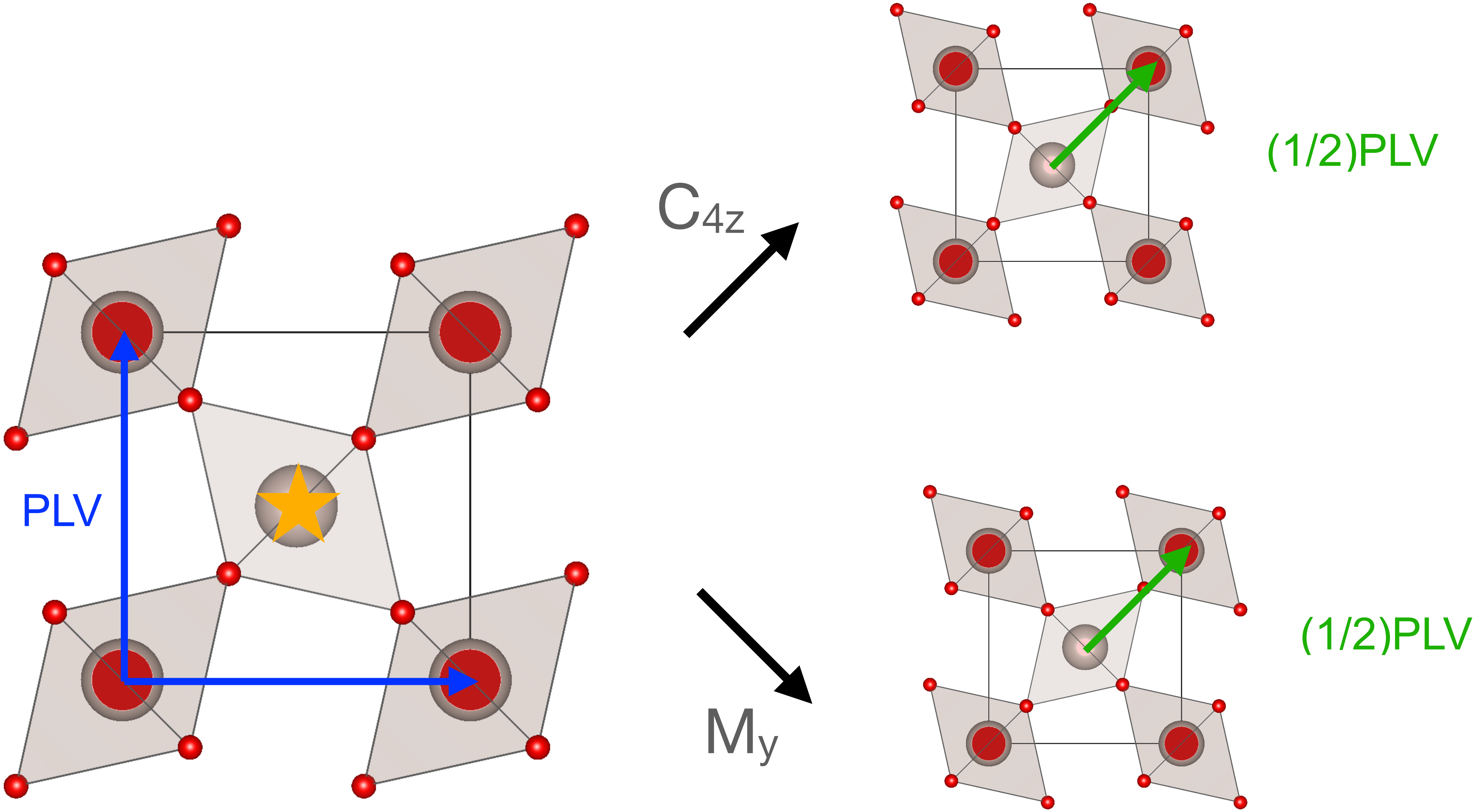

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Nonsymmorphic Space groups

Consider a space group G with operations $\{G\,|\,\mathbf{t}\}$ which leave a given lattice invariant. We can rewrite each operation as:

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If, by ANY choice of origin we find that AT LEAST ONE of the elements of G have

$$\tilde{\mathbf{t}} \neq 0$$

the space group is called NONSYMMORPHIC

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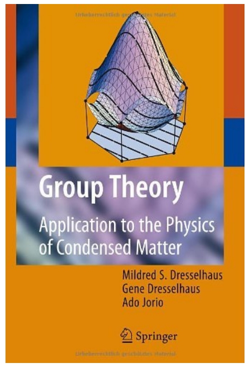
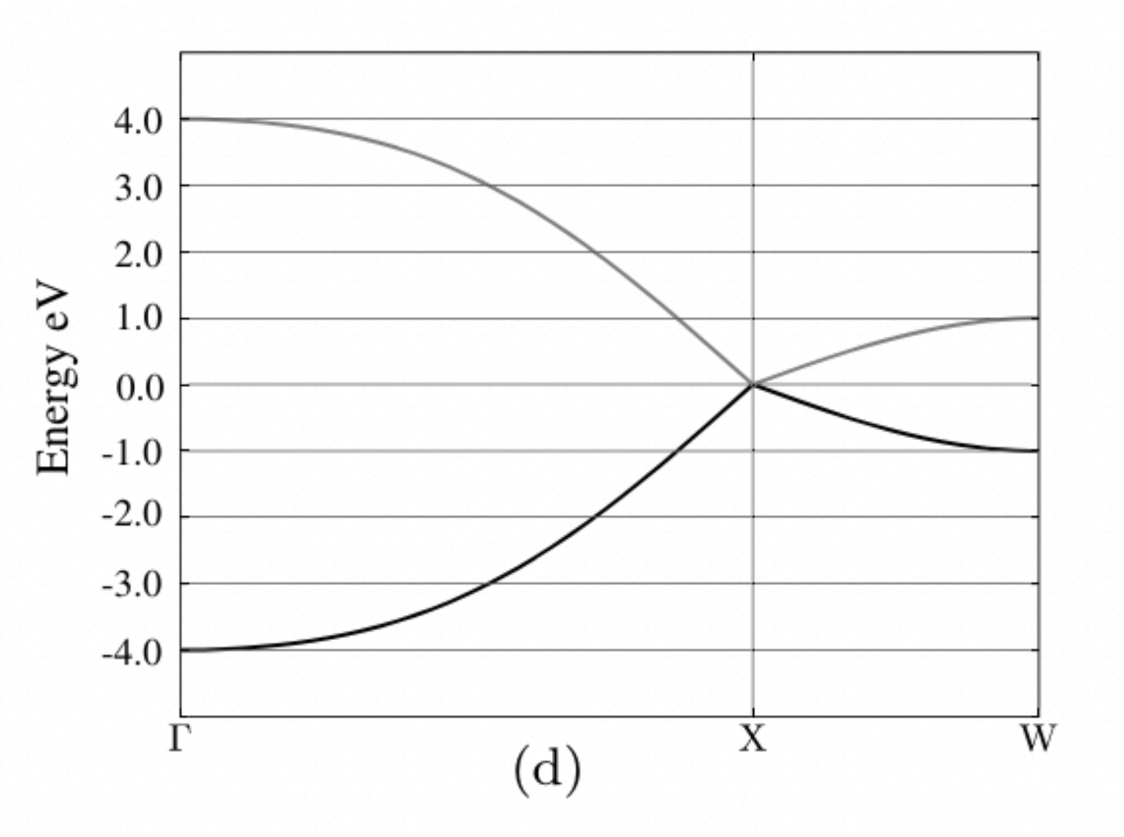
Nonsymmorphic groups: More complicated…but there are tables!



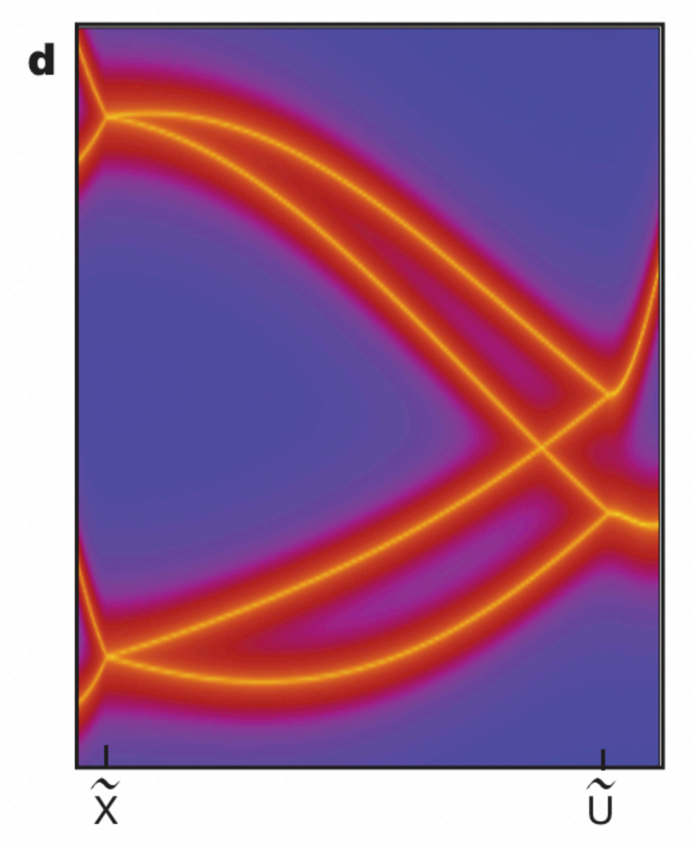
Nonsymmorphic symmetry
Manifestation #1: Symmetry-protected band crossings

s-states in a diamond lattice
[Fd-3m]



S. M. Young et al., PRL **108**, 140405 (2012)

Hourglass fermions in KHgSb
[$P6_3$/mmc]

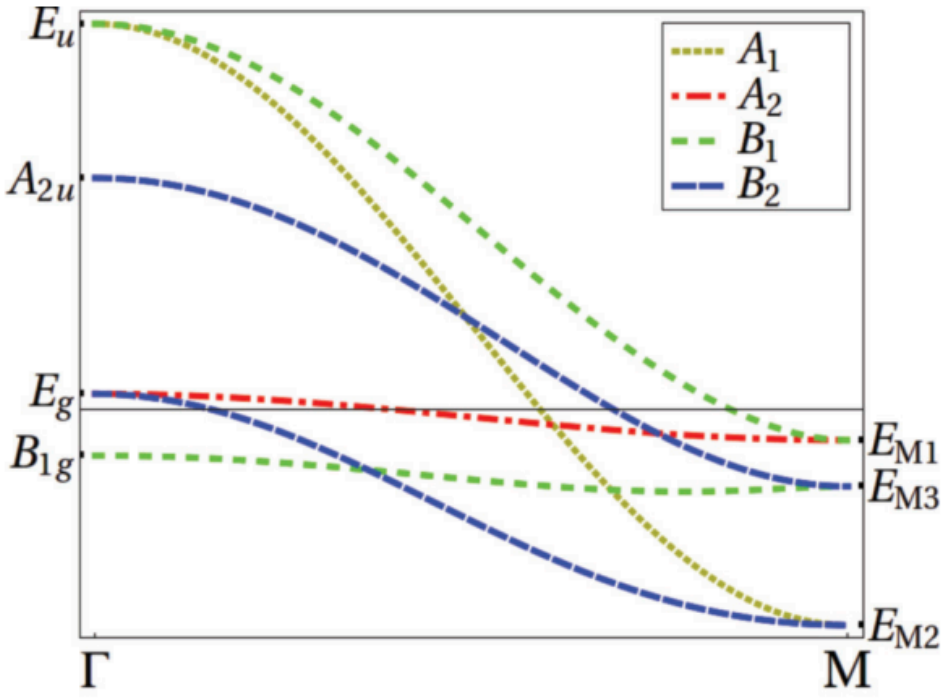


S. Wang et al., Nature **532**, 189 (2016)

Nonsymmorphic symmetry Manifestation #2: New OP connectivities in modulated systems

Band perspective

Fe-based SC [P4/nmm]



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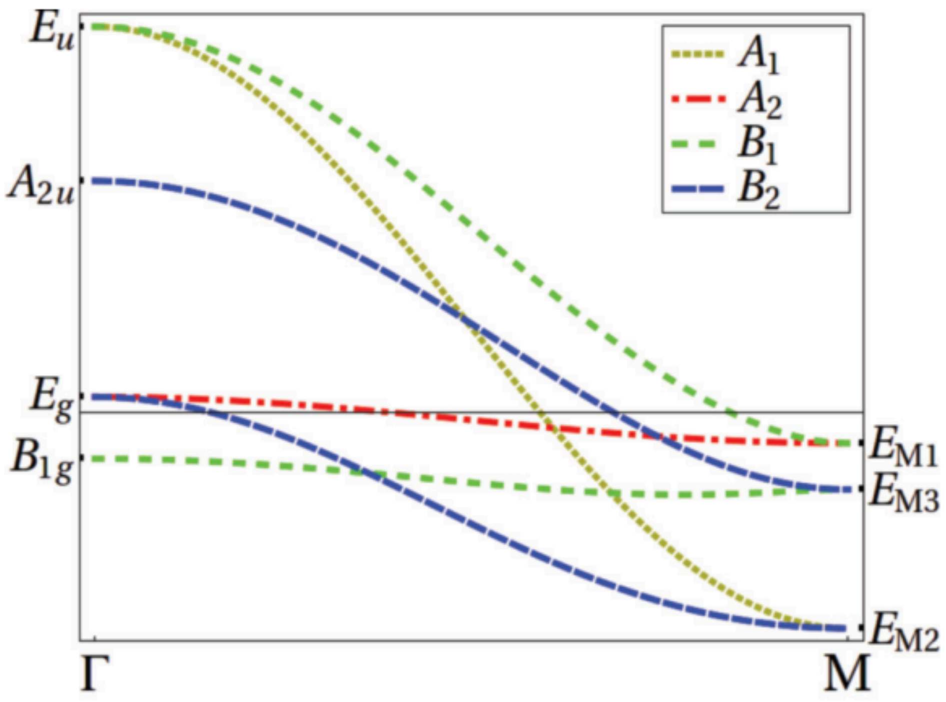

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If a multi-component order parameter:

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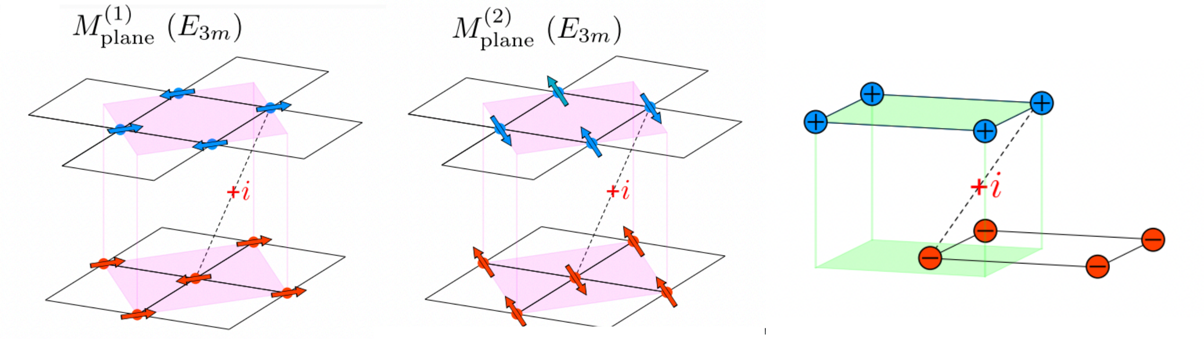

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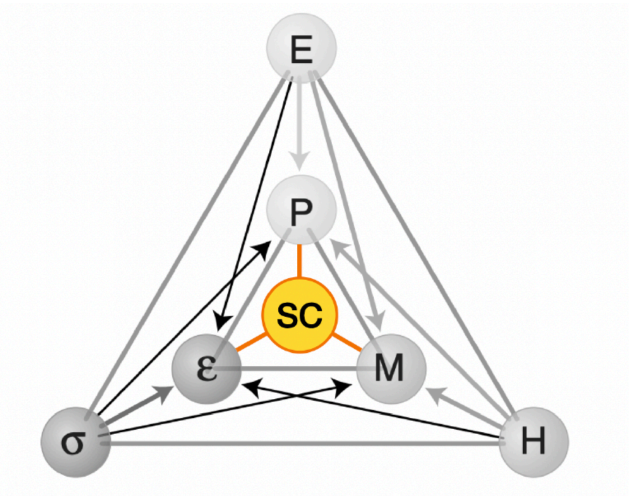

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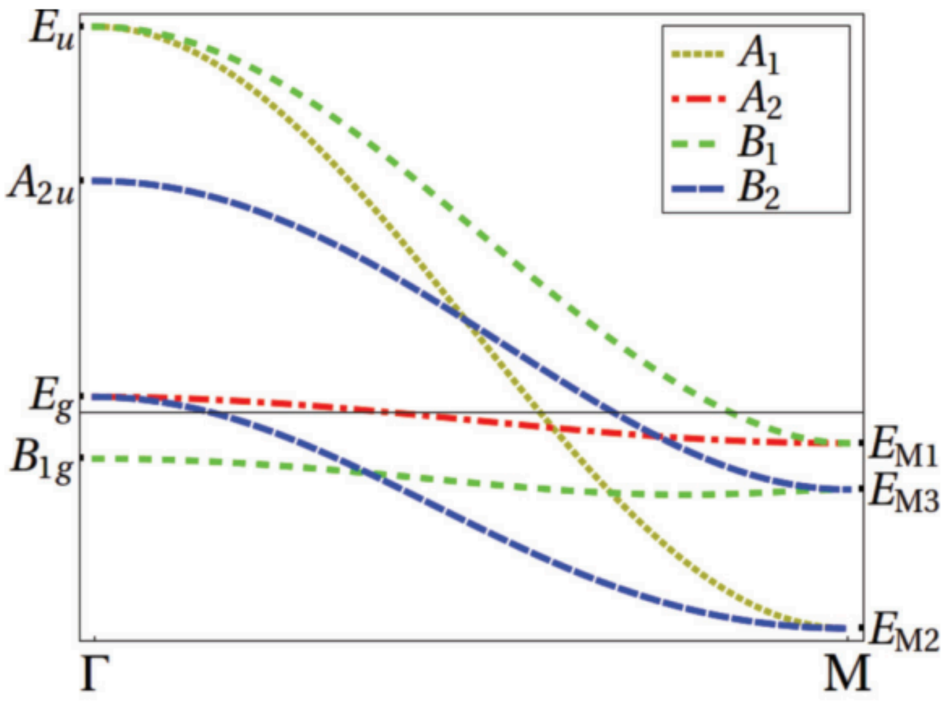

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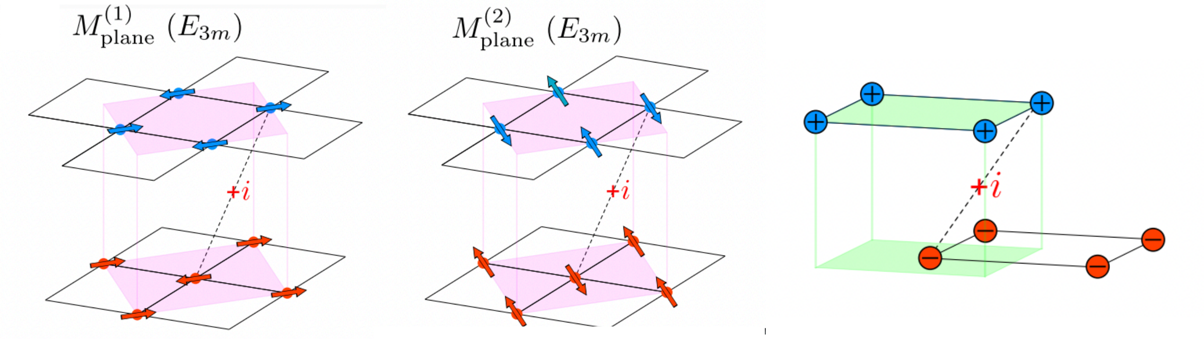

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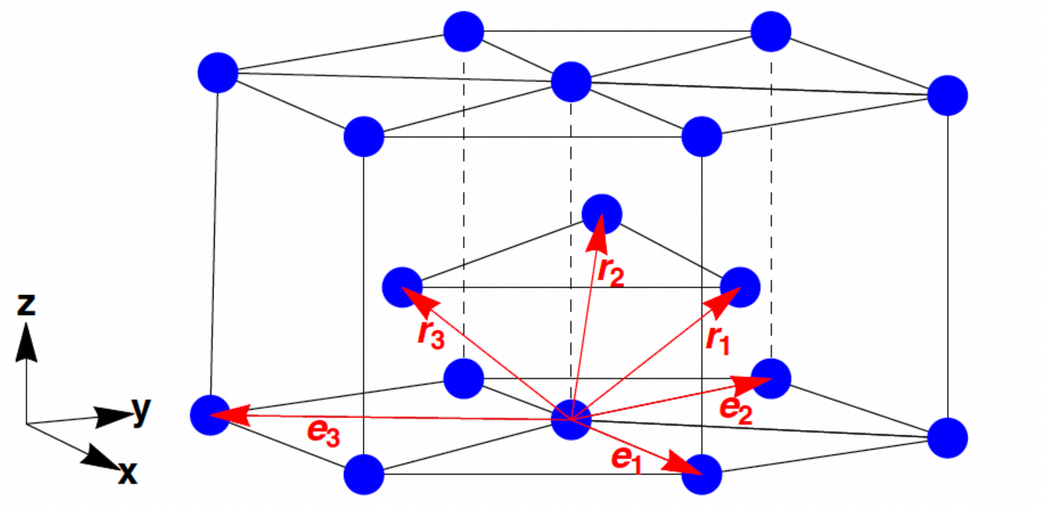
UPt_3 [$P6_3/mmc$]



M. R. Norman, PRB **52**, 15093 (1995)

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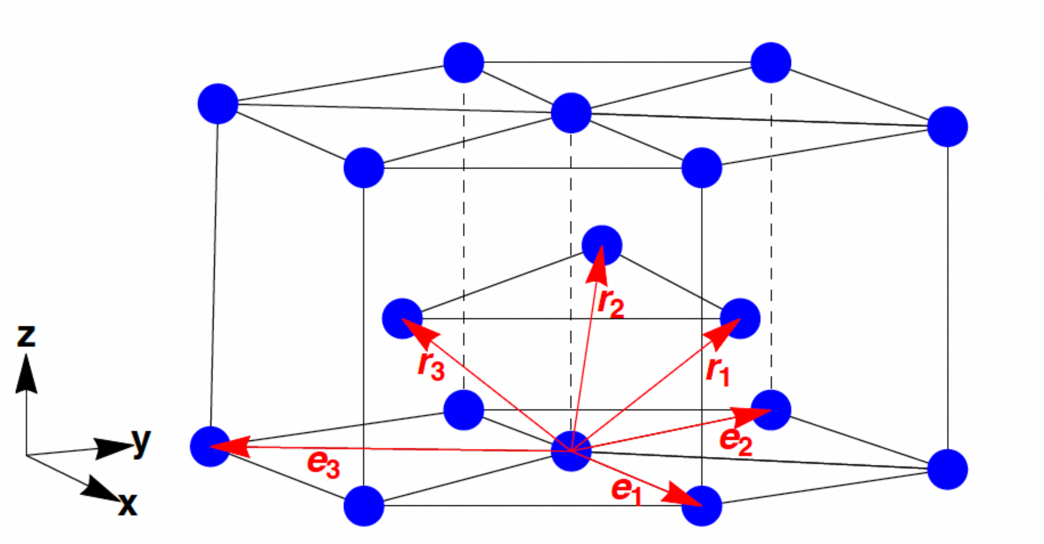
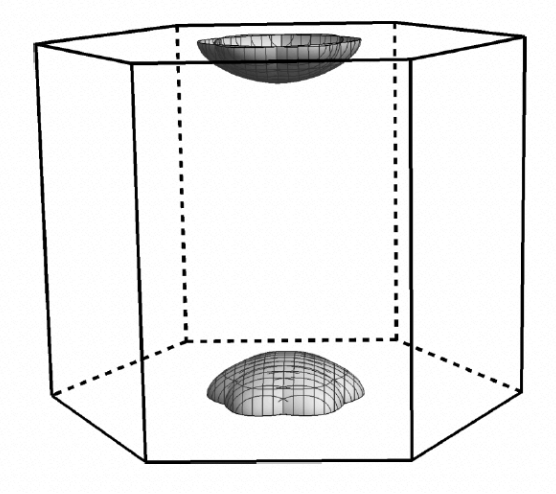
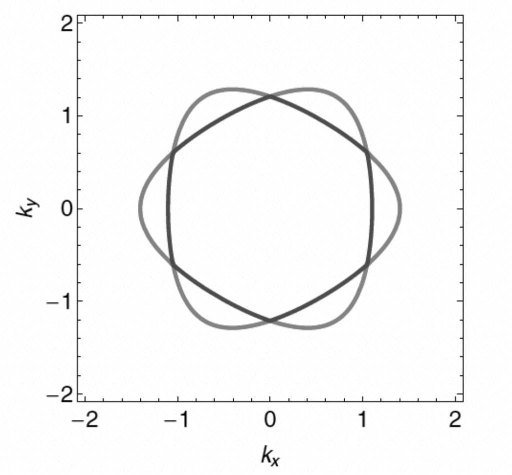


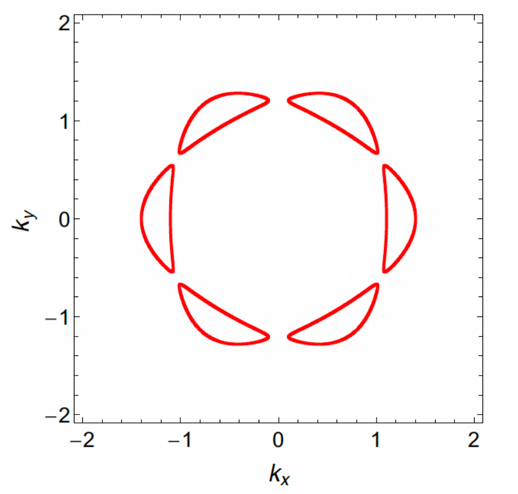
M. R. Norman, PRB **52**, 15093 (1995)

FS in 3D BZ



FS in $k_z = \pi$ plane





In the SC state:
Line nodes!

Z. Wang et al., PRB **96**, 174511 (2017)

S. Kobayashi et al., PRB **94**, 134512 (2016)
T. Micklitz et al., PRL **118**, 207001 (2017)
T. Micklitz et al., PRB **95**, 024508 (2017)
S. Sumita Ph.D. Thesis (2019)
...

Summary/Conclusion

Brief introduction to group theory concepts:

Group ⇒ Conjugacy Classes ⇒ Group Representation
⇒ Character ⇒ Irreducible Representations

Crystallographic Point Groups:

⇒ SC order parameter classification
⇒ Conventional/unconventional
⇒ Nematic/Chiral

Beyond the Sigrist-Ueda Classification:

⇒ Multiple internal DOFs (orbitals/layers/sublattices)
⇒ Nonsymmorphic symmetries

"Loopholes" to what we have thought were very well-established concepts and theorems in the field…are there more of them?

Homework!