University of Science and Technology, Beijung
Optical Material and Device Lab

2022 SPRING FESTIVAL BEIJING CRYSTALLOGRAPHY SCHOOL

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REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

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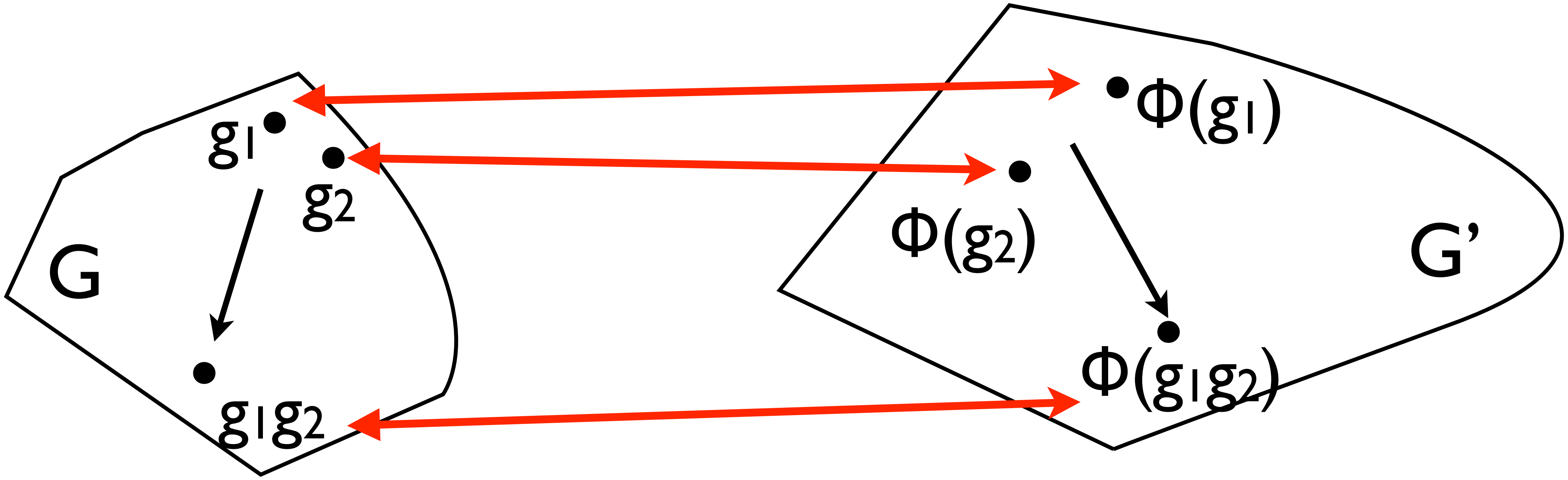
GENERAL INTRODUCTION

Homomorphism and Isomorphism



$$\Phi(g)=g'$$

$$G=\{g\} \longleftrightarrow G'=\{g'\}$$

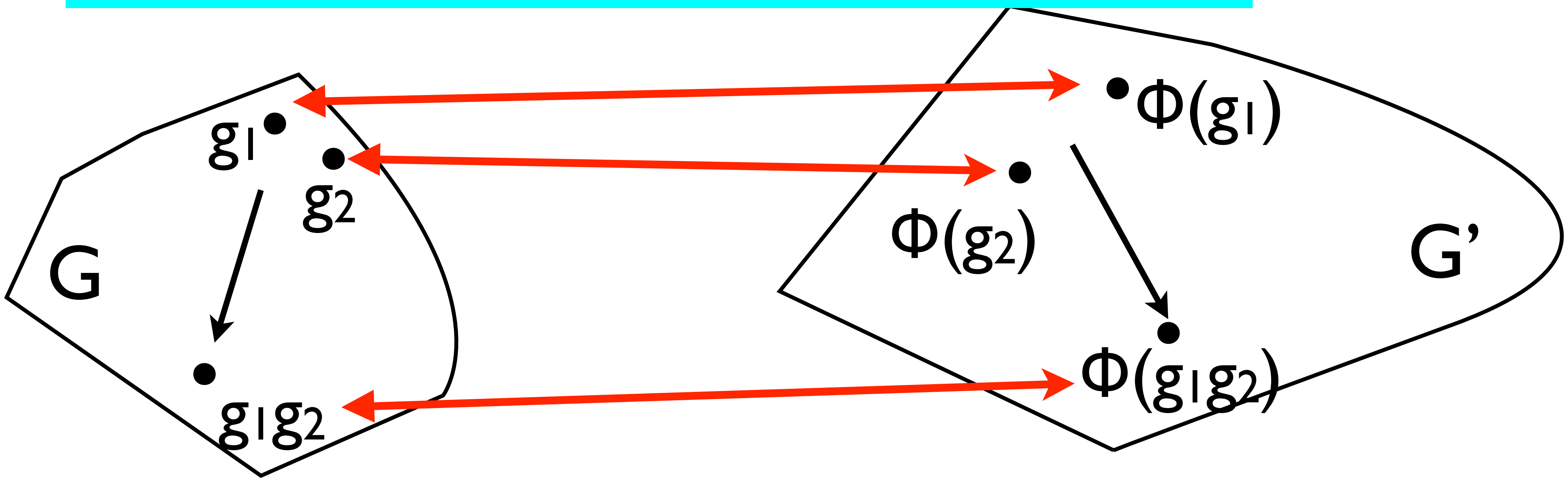
$$\Phi^{-1}(g')=g$$

$$\Phi: G \longrightarrow G' \qquad \Phi^{-1}: G' \longrightarrow G$$

homomorphic condition $\Phi(g_1)\Phi(g_2)= \Phi(g_1 g_2)$

Isomorphic groups -groups with the same multiplication table

Homomorphism and Isomorphism



$$\Phi(g) = g'$$

$$G = \{g\} \longrightarrow G' = \{g'\}$$

$$\Phi: G \longrightarrow G'$$

homomorphic condition $\Phi(g_1)\Phi(g_2) = \Phi(g_1\, g_2)$

Example

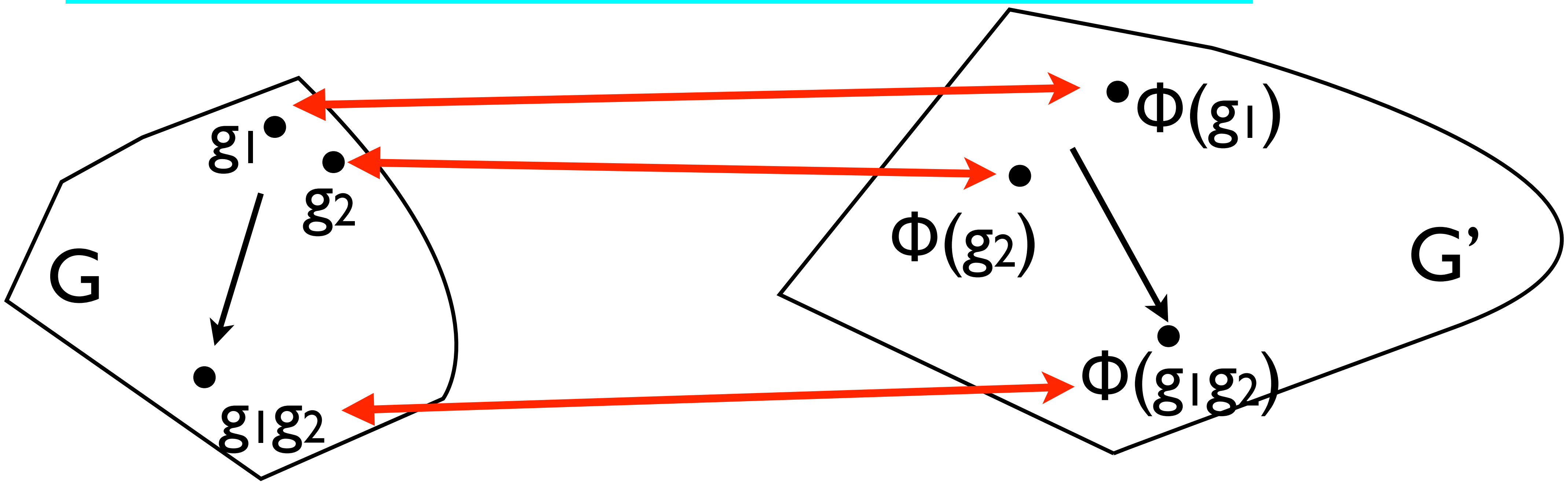
isomorphic groups

4mm $\{1, 4, 2, 4^{-1}, m_x, m_y, m_+, m_-\}$

↕ ↕ ?

422 $\{1, 4, 2, 4^{-1}, 2_x, 2_y, 2_+, 2_-\}$

Homomorphism and Isomorphism



$\Phi(g)=g'$

$G=\{g\} \longrightarrow G'=\{g'\}$

$\Phi: G \longrightarrow G'$

homomorphic condition $\Phi(g_1)\Phi(g_2)= \Phi(g_1\, g_2)$

Example

4mm $\{1, 4, 2, 4^{-1}, m_x, m_y, m_+, m_-\}$

$\downarrow$ $\{1,-1\}$ $\{1,-1\}$?

Representations of Groups

group G $\{e, g_2, g_3, \ldots, g_i, \ldots, g_n\}$

Φ

D(G): rep of G $\{D(e), D(g_2), D(g_3), \ldots, D(g_i), \ldots, D(g_n)\}$

$D(g_j)$: n x n matrices

$\det D(g_j) \neq 0$

$D(g_i)D(g_j) = D(g_i g_j)$

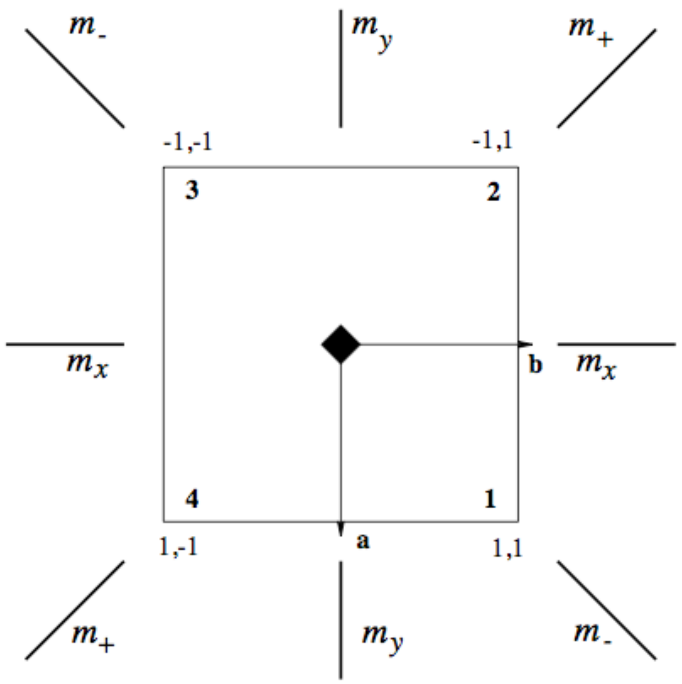
dimension of representation

kernel of representation

Examples: trivial (identity) representation

faithful representation

EXERCISE 1a



Two-dimensional faithful representation of 4mm

$\{1, \quad 4, \quad 2, \quad 4^{-1}, \quad m_x, \quad m_y, \quad m_+, \quad m_-\}$

$1 \rightarrow \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad 4 \rightarrow \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad m_x \rightarrow \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \qquad m_y \rightarrow ?$

Determine the rest of the matrices:

$$D(g_i)D(g_j)=D(g_ig_j)$$

Group G $= \{e, g_2, g_3, \ldots, g_k\}$

Representation

Vector space $\mathbf{V}^{(n)}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$

Group of operators P_G: $\{R_e, R_{g2}, \ldots, R_{gk}\}$

$$R_g(\mathbf{v}+\mathbf{w}) = R_g\mathbf{v} + R_g\mathbf{w}$$

$$R_g \alpha \mathbf{v} = \alpha R_g \mathbf{v}$$

Representation of G:

$$\{e, g_2, g_3, \ldots, g_k\}$$

$$\downarrow$$

$$\{R_e, R_{g2}, \ldots, R_{gk}\}$$

$$R_{g1g2} = R_{g1} R_{g2}$$

$$G \xrightarrow{\text{isomorphic mapping}} R_G$$

Vector space $\mathbf{V}^{(n)}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$

Representation

G —isomorphic mapping→ R_G

$\{e, g_2, g_3, \ldots, g_k\}$ $\{R_e, R_{g2}, \ldots, R_{gk}\}$

Carrier space of representation

$R_G\, \mathbf{V}^{(n)} = \mathbf{V}^{(n)}$

P_G-invariant space

$R_g \mathbf{v}_i = \sum \mathbf{v}_j D(g)_{ji}$ $j=1,\ldots,n$

Basis vectors $i=1,\ldots,n$

$R_g\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}=\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}D(g)$

Matrix representation

$D_G=\{D(e), D(g_2), \ldots, D(g_k)\}$

R_G —homomorphic mapping→ D_G

Equivalent Representations of Groups

Given two reps of G:

$D(G)=\{D(g_i), g_i \in G\}$

$D'(G)=\{D'(g_i), g_i \in G\}$

dim D(G)= dim D'(G)

equivalent representations

$D(G) \sim D'(G)$

if $\exists$ S: $D(g) = S^{-1} D'(g) S$ $\forall g \in G$

S: invertible matrix

Equivalent Representations

two sets of bases for $\mathbf{V}^{(3)}$

$$(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3) \text{ and } (\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3) = (\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)P$$

two reps of G

$$R_g(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)=(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)D(g), \quad g\in G$$

$$R_g(\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3) = (\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3)D'(g), \quad g\in G$$

D(G) and D'(G) are equivalent, as:

$$R_g(\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3) = R_g[(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)P]$$

$$=(\mathbf{e}_1,\mathbf{e}_2,\mathbf{e}_3)D(g)P$$

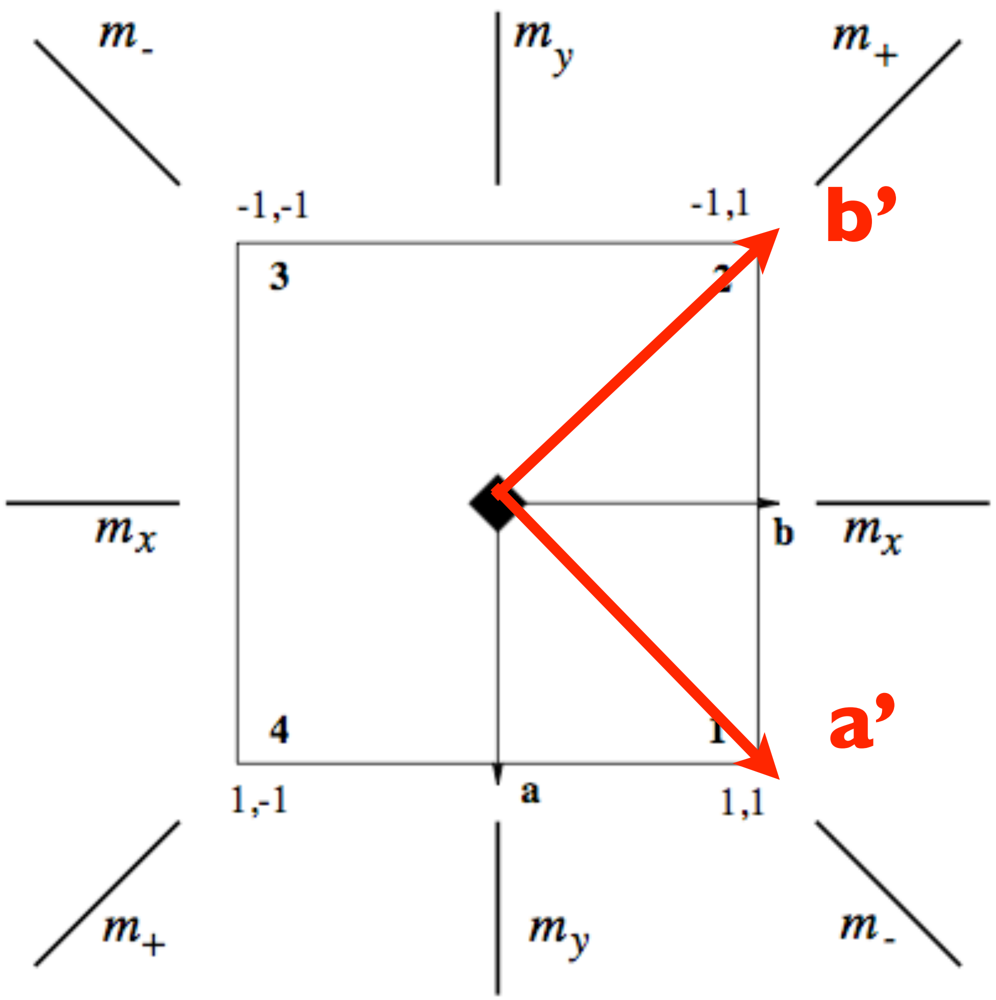
$$= (\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3)P^{-1}D(g)P$$

$$D'(g)= P^{-1}D(g)P, \quad g\in G$$

EXERCISE 1b

2-dim faithful representation of 4mm

In problem 1a we consider a representation of 4mm with respect to the basis {**a**,**b**} of the type



D(4)=

0	-1
1	0

$D(m_x)$=

-1	0
0	1

Determine the matrices of the representation of 4mm with respect to the new bases (**a'**,**b'**)

R_g{**a'**, **b'**}={**a'**, **b'**}D'(g)

{1, 4, 2, 4^{-1}, m_x, m_y, m_+, m_-}

?

Hint: $D'(g)= P^{-1}D(g)P$, $g\in G$

EXERCISE 3

The cyclic group C_4 of order 4 is generated by the element g. Two of the following three representations of C_4 are equivalent:

$$D_1(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \qquad D_2(g) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad D_3(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

Determine which of the two are equivalent and find the corresponding similarity matrix. Can you give an argument why the third representation is not equivalent?

Hint: The determination of X such that $D'(g)=X^{-1}D(g)X$ is equivalent to determine X such that $XD'(g)=D(g)X$, with the additional condition, $\det X \neq 0$.

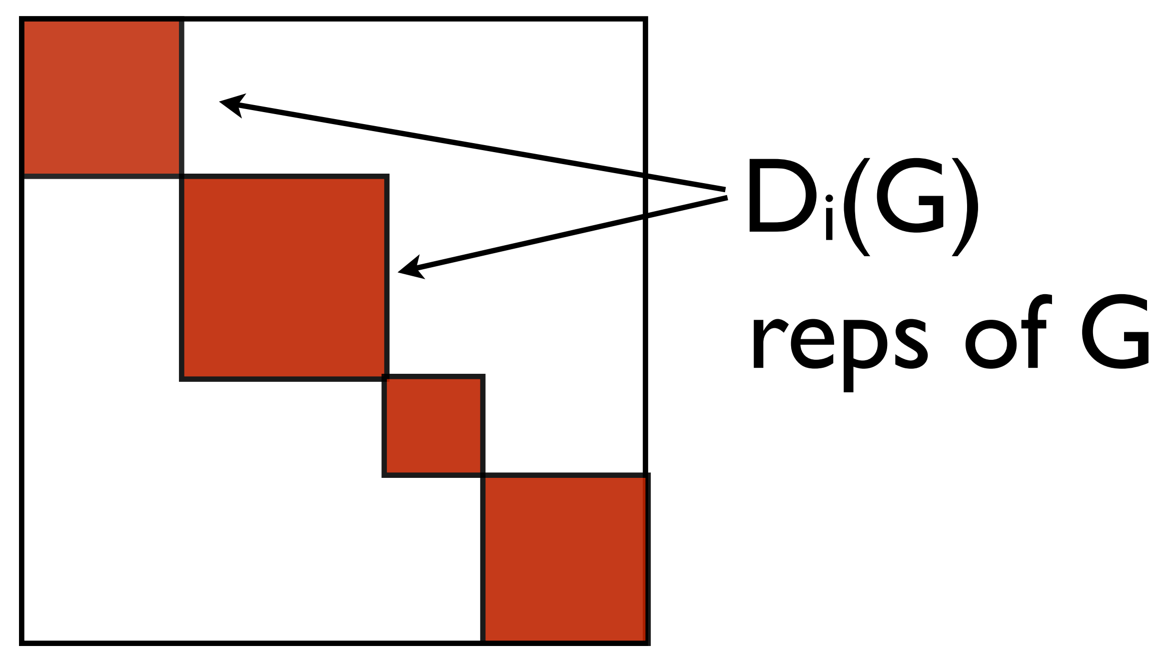
Reducible and Irreducible Representations of Groups

reps of G: $D(G)=\{D(g_i), g_i \in G\}$

$D(G) \sim D'(G)$ $D(G) = S^{-1} D'(G) S$

reducible and irreducible

D(G) reducible if $D(G) \sim D'(G) =$

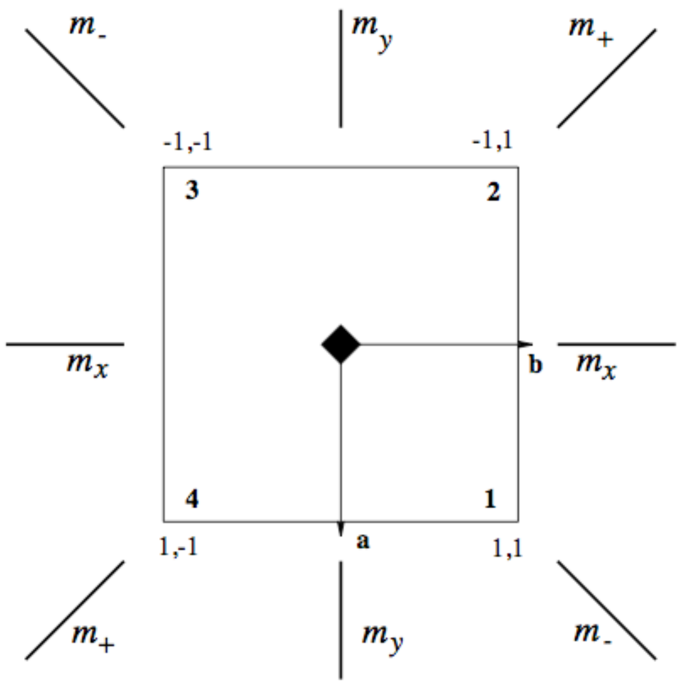


$$D(G) \sim m_1 D_1(G) \oplus m_2 D_2(G) \oplus \ldots \oplus m_k D_k(G)$$

$$\bigoplus m_i D_i(G)$$

EXAMPLE

Reducible rep of 4mm

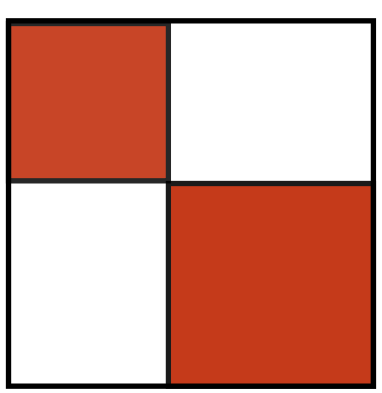


$\{1, \quad 4, \quad 2, \quad 4^{-1}, \quad m_x, \quad m_y, \quad m_+, \quad m_-\}$

$$D(4) \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad D(m_-)$$

$$D(G) \sim D_1(G) \oplus D_2(G)$$



$D_1(4)=1$

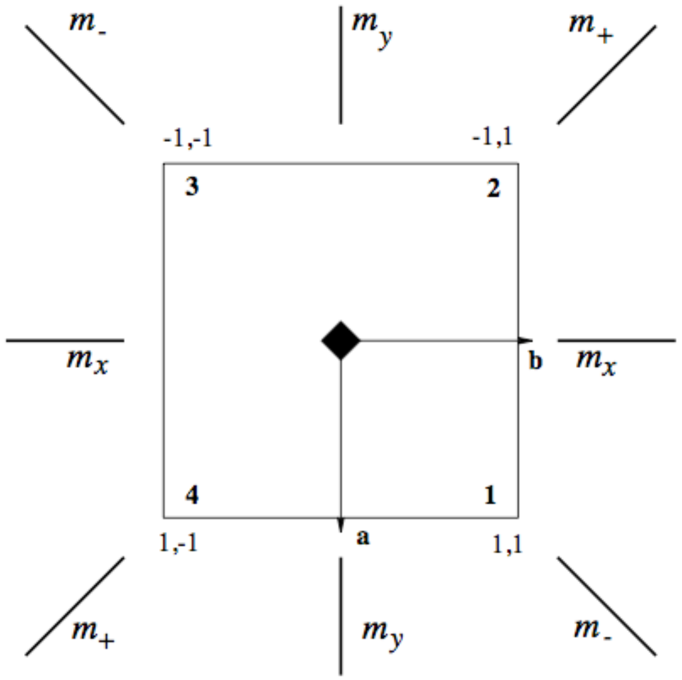
$$D_2(4)= \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$D_1(m_-)=-1$

$$D_2(m_-)= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

EXAMPLE

Group 4mm=$\langle 4, m_- \rangle$



Reducible or Irreducible representation?

$$D(4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad D(m_-) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Are there **common** eigenspaces/eigenvectors of D(4) and $D(m_-)$?

Eigenvectors of $D(m_-)$: $(1,1)^T$ and $(1,-1)^T$

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

EXERCISE 5

Irreps of 222

Consider the following matrices of a representation of 222 (D_2):

$$D(e)=D(2_z)=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D(2_x)=D(2_y)=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

(i) Show that it is a reducible representation

(ii) Determine the transformation matrix that transform the matrices of the reducible representation into direct sum of irreps.

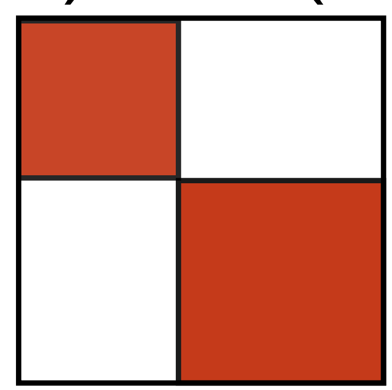
Reducible representations and invariant subspaces

rep D(G) of G: $D(G)=\{D(g_i),\ g_i \in G,\ \dim D(G)=n\}$

carrier space: $\mathbf{V}^{(n)}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$

$R_G\, \mathbf{V}^{(n)} = \mathbf{V}^{(n)}$ $\quad R_g \mathbf{v}_i = \sum \mathbf{v}_j D(g)_{ji}$

reducible rep: $D(G) \sim D_1(G) \oplus D_2(G)$



$\dim D_1(G)=n_1$

$\dim D_2(G)=n_2$

invariant subspaces:

$R_G\, \mathbf{V}^{(n1)} = \mathbf{V}^{(n1)}$ $\quad R_g \mathbf{v}_i = \sum \mathbf{v}_j D_1(g)_{ji}$

$R_G\, \mathbf{V}^{(n2)} = \mathbf{V}^{(n2)}$ $\quad R_g \mathbf{w}_i = \sum \mathbf{w}_j D_2(g)_{ji}$

$$\mathbf{V}^{(n)} = \mathbf{V}^{(n1)} \oplus \mathbf{V}^{(n2)}$$

EXAMPLE

Group $C_2=\{e,g\}$

Representation	Carrier space
$D(C_2)=\left\{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right\}$	$\mathbf{F}^{(2)}\{\mathbf{e}_1,\mathbf{e}_2\}$
↓ **reducible**	↓ **invariant subspaces**
$D'(C_2)=X^{-1}\,D(C_2)\,X$	$\mathbf{V}^{(1)}$ $\{\mathbf{e}_1+\mathbf{e}_2\}$
$D'(C_2)=\left\{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\}$	$\mathbf{W}^{(1)}$ $\{\mathbf{e}_1-\mathbf{e}_2\}$

$$X=\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$$

Representations of Groups
Basic results

Schur lemma I

irreps of G: $D_1(G)=\{D_1(g_i),\ g_i\in G\}$

$D_2(G)=\{D_2(g_i),\ g_i\in G\}$

if $\exists$ A: $D_1(G)A = A\ D_2(G)$

then $\begin{cases} A=0 \\ \dim D_1(G)=\dim D_2(G), \quad \det A\neq 0 \\ D_1(G) \sim D_2(G) \end{cases}$

Representations of Groups
Basic results

Schur lemma II

irrep of G: $D_I(G)=\{D_I(g_i), g_i \in G\}$

if $\exists$ B: $D_I(G)B = B\, D_I(G)$

then $B=cI$

irreps of Abelian groups

one-dimensional

WHY?

Representations of Groups
Basic results

number and dimensions of irreps

number of irreps = number of conjugacy classes

order of G = $\sum [\dim D_i(G)]^2$

great orthogonality theorem

irreps of G: $D_1(G), D_2(G),$

$\dim D_1(G) = d$

$$\sum_g D_1(g)^*_{jk} D_2(g)_{st} = \frac{|G|}{d} \delta_{12}\delta_{js}\delta_{kt}$$

EXAMPLE: Irreps of 222

1. Number and dimensions of the irreps of 222
   -abelian group

2. Irreps of 222

$(2_i)^2=(2_i\ 2_j)^2=1$

$[D(2_i)]^2=D[(2_i\ 2_j)]^2=D(1)=1$

$D(2_i)=\mp 1$

irreps labels:

Mulliken labels: A, B, E, F or T

Bethe labels: Γ_i

$D_2(222)$	#	1	2_z	2_y	2_x
A	Γ_1	1	1	1	1
B_1	Γ_3	1	1	-1	-1
B_2	Γ_2	1	-1	1	-1
B_3	Γ_4	1	-1	-1	1

EXERCISES 8a

Problems

1. Determine the number and dimensions of the irreps of 4mm. What about the irreps of 422? And of 4/mmm?

2. Determine the number and dimensions of the irreps of 3m. What about the irreps of 32? And of $\bar{3}$m?

CHARACTERS OF REPRESENTATIONS

Characters of Representations
Basic results

character properties

$$\eta(g) = \mathrm{trace}[D(g)] = \sum D(g)_{ii}$$

$$D_1(G) \sim D_2(G) \longleftrightarrow \eta_1(g) = \eta_2(g),\ g \in G$$

$$g_1 \sim g_2 \longleftrightarrow \eta_1(g) = \eta_2(g),\ g \in G$$

orthogonality

rows

$$\frac{1}{|G|} \sum_g \eta_1^*(g)\, \eta_2(g) = \delta_{12}$$

columns

$$\frac{1}{|G|} \sum_p \eta_p^*(C_j)\, \eta_p(C_k)\, |C_j| = \delta_{jk}$$

Character Tables

Finite group G: $\mathbf{r}$ conjugacy classes $\{e\}, \{g_2,\ldots, g_k\},\ldots,\{g_r, \ldots\}$

$\mathbf{r}$ irreducible representations $D_i(G)$

$$\mu_{D_i}(G)=\{\mu_{D_i}(e), \mu_{D_i}(g_2), \ldots, \mu_{D_i}(g_r)\}$$

Character Table of G: $\mathbf{r} \times \mathbf{r}$ matrix $\mathbf{X}=\mathbf{X}(G)$

$$\mathbf{X}_{\mathbf{ij}}= \mu_{D_\mathbf{i}}(g_\mathbf{j})$$

rows: irrep labels (Mulliken, Bethe)

columns: conjugacy classes

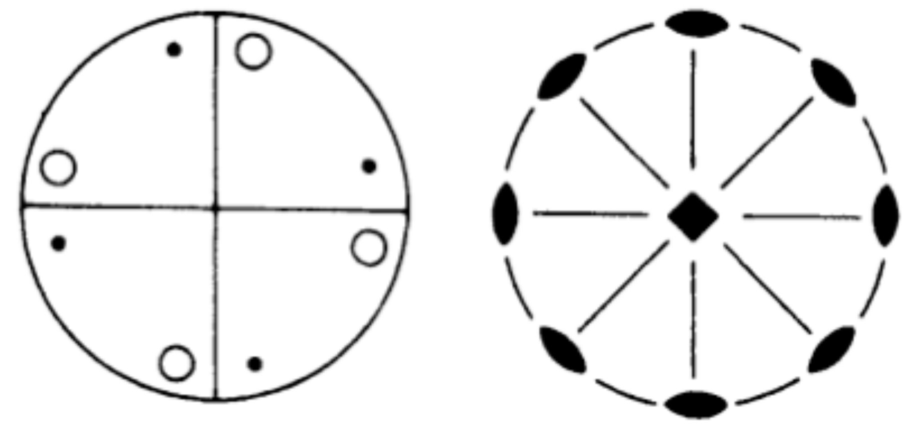
Additional data: order of the elements

length of conjugacy classes

basis functions

EXAMPLE

Characters of Representations



Character table of 422

422: $\{e\},\{4_z,4_z\}, \{2_z\},\{2_y,2_x\},\{2_+,2_-\}$

$D_4(422)$	#	1	2	4	2_h	$2_{h'}$
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_3	1	1	1	-1	-1
B_1	Γ_2	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	-2	0	0	0

Mult. row: length of the conjugacy classes

First column: Mulliken; second column: Bethe

rows

$$\frac{1}{|G|}\sum_{g} \eta_1^*(g)\, \eta_2(g) = \delta_{12}$$

columns

$$\frac{1}{|G|}\sum_{p} \eta_p^*(C_j)\,\eta_p(C_k)\,|C_j| = \delta_{jk}$$

EXAMPLE

Characters of Representations

Character table of 432

rows

$$\frac{1}{|G|}\sum_{g} \eta_1^*(g)\,\eta_2(g) = \delta_{12}$$

columns

$$\frac{1}{|G|}\sum_{p} \eta_p^*(C_j)\,\eta_p(C_k)\,|C_j| = \delta_{jk}$$

class length	1	3	6	8	6
element order	1	2	2	3	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	?	?	?	?
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

EXAMPLE

SOLUTION

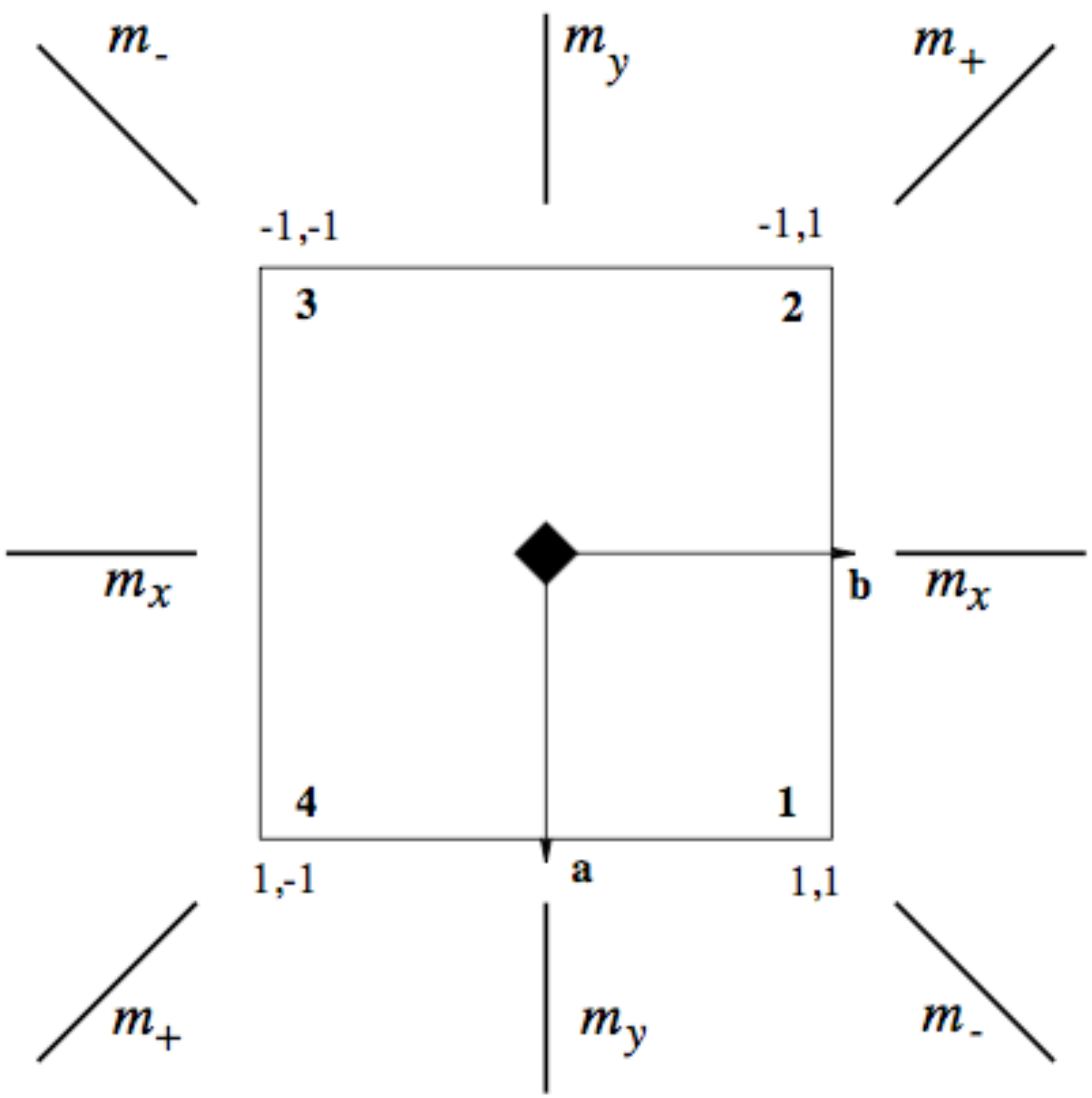
Example: Character table of 432

$\lvert C_j \rvert$	1	3	6	8	6
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

EXERCISES 8b

Character table of 4mm

Determine the characters of the irreps of 4mm and order them in a character table



	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
1	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
2	2	1	4^{-1}	4	m_y	m_-	m_x	m_+
4	4	4^{-1}	2	1	m_+	m_y	m_-	m_x
4^{-1}	4^{-1}	4	1	2	m_-	m_x	m_+	m_y
m_x	m_x	m_y	m_-	m_+	1	4^{-1}	2	4
m_+	m_+	m_-	m_x	m_y	4	1	4^{-1}	2
m_y	m_y	m_x	m_+	m_-	2	4	1	4^{-1}
m_-	m_-	m_+	m_y	m_x	4^{-1}	2	4	1

Multiplication table of $4mm$

Problem 8b

SOLUTION

-number and dimensions of the irreps of 4mm

5 irreps with dimensions: 1,1,1,1,2

-characters of one-dimensional irreps of 4mm

$m_y=m_+=\pm 1$ $m_y m_+=4=\pm 1$ $(4)^2=2=1$

-characters of 2-dim irrep

orthogonality by columns

$$\frac{1}{|G|}\sum_p \eta_p^*(C_j)\eta_p(C_k)\,|C_j| = \delta_{jk}$$

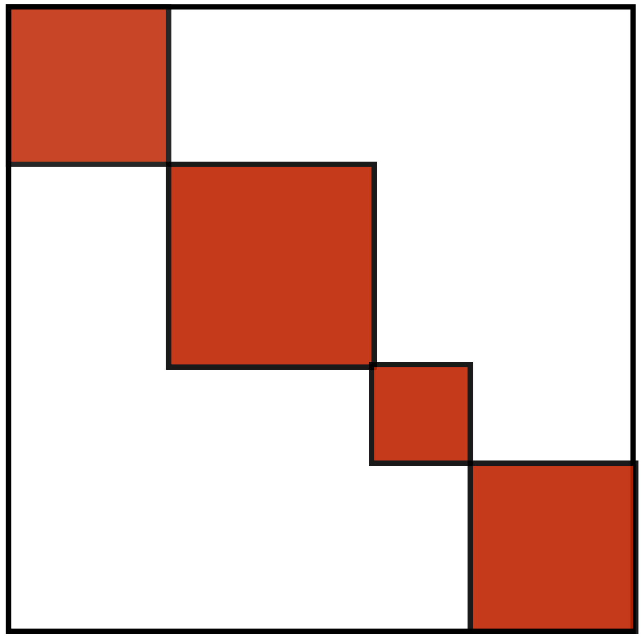
C_{4v}(4mm)	#	1	2	4	m_x	m_d
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_2	1	1	1	-1	-1
B_1	Γ_3	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	?	?	?	?

Characters of Representations

reducible rep

$$D(G) \sim m_1 D_1(G) \oplus m_2 D_2(G) \oplus \ldots \oplus m_k D_k(G)$$

$$\bigoplus m_i D_i(G)$$



magic formula

$$m_i = \frac{1}{|G|} \sum_g \eta(g) \eta_i(g)^*$$

irreducibility criteria

$$\frac{1}{|G|} \sum_g |\eta(g)|^2 = 1$$

EXERCISE 9

Irreps of 222

$D_2(222)$	#	1	2_z	2_y	2_x
A	Γ_1	1	1	1	1
B_1	Γ_3	1	1	-1	-1
B_2	Γ_2	1	-1	1	-1
B_3	Γ_4	1	-1	-1	1

Consider the group 222 and its irreps.

Show that the following matrices form a representation of 222 (D_2) that is reducible:

$$D(e)=D(2_z)=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad D(2_x)=D(2_y)=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Decompose the reducible representation into irreps of 222

Hint: Irreducibility criterion

$$\frac{1}{|G|}\sum_{g}|\eta(g)|^2 = 1$$

EXERCISE 10

'magic' formula

1. Consider the character table of the irreps of the group 422. The characters of reducible representations D1, D2 and D3 of 422 are given at the bottom of the table.

2. Determine the decomposition of the reps D1, D2 and D3 into irreps of 422.

Hint: 'magic formula

$$m_i = \frac{1}{|G|} \sum_g \eta(g)\eta_i(g)^*$$

$D_4(422)$	#	1	2	4	2_h	$2_{h'}$
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_3	1	1	1	-1	-1
B_1	Γ_2	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	-2	0	0	0
D1		6	2	0	0	0
D2		10	6	-2	-2	0
D3		11	7	-3	-3	-3

DIRECT PRODUCT OF REPRESENTATIONS

Direct-product (Kronecker) product of matrices

$$(A \otimes B)_{ik,jl} = A_{ij} B_{kl}$$

$$\boldsymbol{A} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad \boldsymbol{B} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

$$\boldsymbol{A} \otimes \boldsymbol{B} = \begin{pmatrix} 0\,\boldsymbol{B} & (-1)\,\boldsymbol{B} \\ 1\,\boldsymbol{B} & 0\,\boldsymbol{B} \end{pmatrix} = \left(\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \end{array}\right).$$

Properties of the Kronecker product

$$(A \otimes B)_{ik,jl} = A_{ij} B_{kl}$$

$$\dim(A \otimes B) = \dim(A) \,.\, \dim(B)$$

$$\mathrm{tr}(A \otimes B) = \mathrm{tr}(A) \,.\, \mathrm{tr}(B)$$

$$(A \otimes B)(C \otimes D) = (AC \otimes BD)$$

$\dim A = \dim C = n$

$\dim B = \dim D = m$

EXERCISE 11

Kronecker product

Calculate the Kronecker products $A \otimes B$ and $B \otimes A$ of the following two matrices

A=

-1	-2
1	2

B=

1	1	2
1	-1	1
0	2	-1

What is the trace of the matrix $A \otimes B$?
And of $B \otimes A$?

Direct product of representations

$D_1(G)$: irrep of G

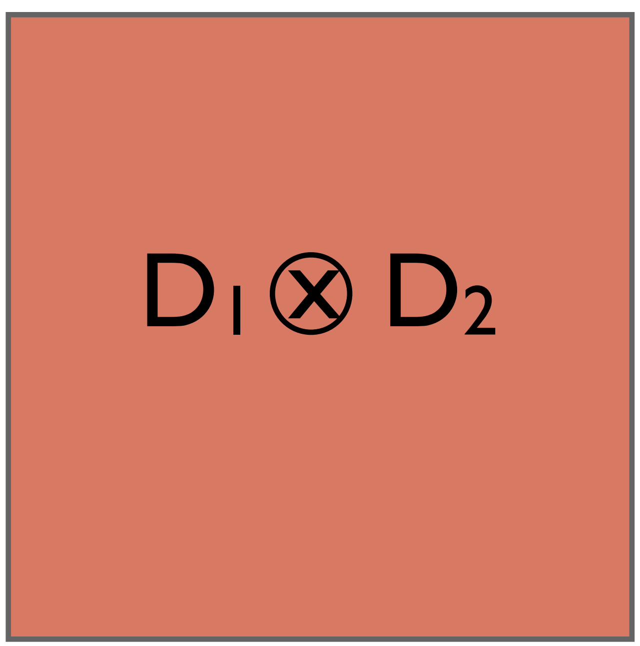
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

$\{D_2(e), D_2(g_2), \ldots, D_2(g_n)\}$

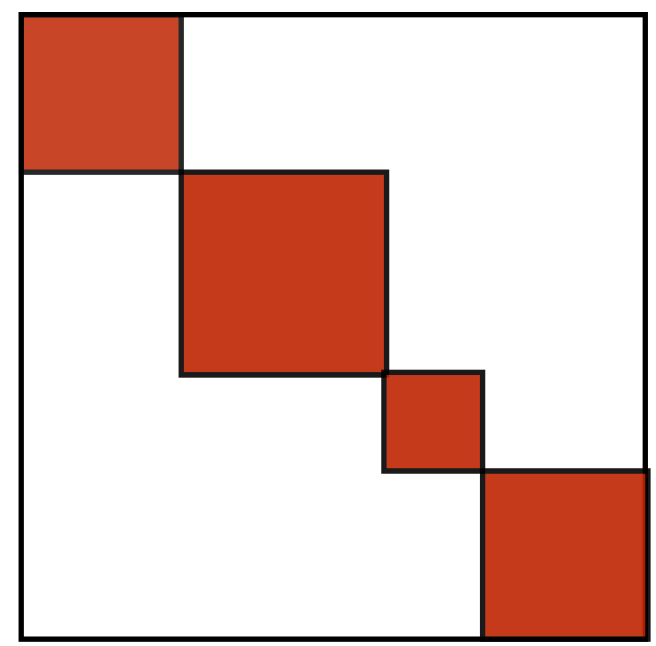
Direct-product representation

$$D_1 \otimes D_2 = \{D_1(e) \otimes D_2(e), \ldots, D_1(g_i) \otimes D_2(g_i), \ldots\}$$



Reduction

$$D_1 \otimes D_2 \longrightarrow \bigoplus m_i D_i(G)$$



irreps of G

$$m_i = \frac{1}{|G|} \sum_g \eta_1(g)\, \eta_2(g)\, \eta_i(g)^*$$

Direct product of representations

$D_1(G)$: irrep of G

$\mathbf{V}^{(h)}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_h\}$

$D_2(G)$: irrep of G

$\mathbf{W}^{(k)}$ $\{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_k\}$

Direct-product representation

$$D_1 \otimes D_2 = \{D_1(e) \otimes D_2(e), \ldots, D_1(g_i) \otimes D_2(g_i), \ldots\}$$

Carrier space

$$\mathbf{V}^{(h)} \otimes \mathbf{W}^{(k)} \; \{\mathbf{v}_1\mathbf{w}_1, \mathbf{v}_2\,\mathbf{w}_1, \ldots, \mathbf{v}_i\mathbf{w}_j, \ldots, \mathbf{v}_h\mathbf{w}_k\}$$

$$R_g\mathbf{v}_i\mathbf{w}_j = \sum \mathbf{v}_l\mathbf{w}_m (D_1 \otimes D_2)(g)_{lm}$$

EXAMPLE

Irreps of 4mm and their multiplication table

$$D_1 \otimes D_2 \sim \bigoplus m_i D_i(G) \qquad \eta(D_1 \otimes D_2)(g_i) = \eta_1(g_i)\,\eta_2(g_i)$$

$$m_i = \frac{1}{|G|} \sum_g \eta_1(g)\,\eta_2(g)\,\eta_i(g)^*$$

C_{4v}(4mm)	#	1	2	4	m_x	m_d
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_2	1	1	1	-1	-1
B_1	Γ_3	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	-2	0	0	0
$E \otimes E$		4	4	0	0	0

Multiplication Table

C_{4v}(4mm)	A_1	A_2	B_1	B_2	E
A_1	A_1	A_2	B_1	B_2	E
A_2	.	A_1	B_2	B_1	E
B_1	.	.	A_1	A_2	E
B_2	.	.	.	A_1	E
E	.	.	.	.	A_1+A_2+B_1+B_2

$$B_1 \otimes B_2 \sim A_2$$

$$E \otimes E \sim A_1 \oplus A_2 \oplus B_1 \oplus B_2$$

EXERCISE 12

Direct-product representation

Determine the multiplication table for the irreps of the group 3m

$$m_i = \frac{1}{|G|} \sum_g \eta_1(g)\, \eta_2(g)\, \eta_i(g)^*$$

C_{3v}(3m)	#	1	3	m
Mult.	-	1	2	3
A_1	Γ_1	1	1	1
A_2	Γ_2	1	1	-1
E	Γ_3	2	-1	0

EXERCISE 12

SOLUTION

Character table of 3m

C_{3v}(3m)	#	1	3	m
Mult.	-	1	2	3
A_1	Γ_1	1	1	1
A_2	Γ_2	1	1	-1
E	Γ_3	2	-1	0

Irrep multiplication table of 3m

Multiplication Table

C_{3v}(3m)	A_1	A_2	E
A_1	A_1	A_2	E
A_2	.	A_1	E
E	.	.	A_1+A_2+E

REPRESENTATIONS OF FINITE ABELIAN GROUPS

Representations of cyclic groups

$$G = \langle g \rangle = \{g, g^2, ...g^k, ...\}$$
$$g^n = e$$

$$\Gamma^p(g^k) = exp(2\pi i k)\frac{p-1}{n}$$
$$p = 1, ..., n$$

Point Group Tables of $C_4(4)$

Character Table

$C_4(4)$	#	1	2	4^+	4^-	functions
A	Γ_1	1	1	1	1	z, x^2+y^2, z^2, J_z
B	Γ_2	1	1	-1	-1	x^2-y^2, xy
E	Γ_4 Γ_3	1 1	-1 -1	-1j 1j	1j -1j	$(x,y),(xz,yz),(J_x,J_y)$

Point Group Tables of $C_6(6)$

Character Table

$C_6(6)$	#	E	6^+	3^+	2	3^-	6^-	functions
A	Γ_1	1	1	1	1	1	1	z, x^2+y^2, z^2, J_z
B	Γ_4	1	-1	1	-1	1	-1	.
E_2	Γ_3 Γ_2	1 1	w w^2	w^2 w	1 1	w w^2	w^2 w	(x^2-y^2, xy)
E_1	Γ_5 Γ_6	1 1	$-w^2$ -w	w w^2	-1 -1	w^2 w	-w $-w^2$	$(x,y),(xz,yz),(J_x,J_y)$

Examples: 1, 2, 3, 4, 6, T_1

Direct-product groups and their representations of

Direct-product groups

$$G_1 \otimes G_2 = \{(g_1,g_2),\ g_1 \in G_1,\ g_2 \in G_2\}$$

$$(g_1,g_2)\ (g'_1,g'_2) = (g_1 g'_1,\ g_2 g'_2)$$

$G_1 \otimes \{1,\bar{1}\}$ group of inversion

Irreps of direct-product groups

$$G_1 \quad G_2 \longrightarrow G_1 \otimes G_2$$

$$\downarrow \qquad \downarrow \qquad\qquad \downarrow$$

$$D_1 \quad D_2 \qquad\qquad D_1 \otimes D_2$$

$$\{D_1(e) \otimes D_2(e)\ ,\ldots,\ D_1(g_i) \otimes D_2(g_i)\ ,\ldots\}$$

EXAMPLE

Irreps of 222=2⊗2’

Irreps of 2

	e	2
A	1	1
B	1	-1

Irreps of 222

		e	2	2’	2.2’
AxA	A	1	1	1	1
AxB	B_2	1	-1	1	-1
BxA	B_1	1	1	-1	-1
BxB	B_3	1	-1	-1	1

+1 +1

+1 -1

EXERCISE 14

Irreps of 4/mmm=422 x $\bar{1}$

Determine the character table of the group 4/mmm=422⊗$\bar{1}$ from the character tables of groups 422 and $\bar{1}$

D_4(422)	#	1	2	4	2_h	$2_{h'}$
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_3	1	1	1	-1	-1
B_1	Γ_2	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	-2	0	0	0

C_i(-1)	#	1	-1
A_g	Γ_1^+	1	1
A_u	Γ_1^-	1	-1

EXERCISE 14

SOLUTION

D_4(422)	#	1	2	4	2_h	$2_{h'}$
Mult.	-	1	1	2	2	2
A_1	Γ_1	1	1	1	1	1
A_2	Γ_3	1	1	1	-1	-1
B_1	Γ_2	1	1	-1	1	-1
B_2	Γ_4	1	1	-1	-1	1
E	Γ_5	2	-2	0	0	0

C_i(-1)	#	1	-1
A_g	Γ_1^+	1	1
A_u	Γ_1^-	1	-1

Irreps of $4/mmm = 422 \otimes \bar{1}$

D_{4h}(4/mmm)	#	1	2	4	2_h	$2_{h'}$	-1	m_z	-4	m_v	m_d
Mult.	-	1	1	2	2	2	1	1	2	2	2
A_{1g}	Γ_1^+	1	1	1	1	1	1	1	1	1	1
A_{2g}	Γ_2^+	1	1	1	-1	-1	1	1	1	-1	-1
B_{1g}	Γ_3^+	1	1	-1	1	-1	1	1	-1	1	-1
B_{2g}	Γ_4^+	1	1	-1	-1	1	1	1	-1	-1	1
E_g	Γ_5^+	2	-2	0	0	0	2	-2	0	0	0
A_{1u}	Γ_1^-	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	Γ_2^-	1	1	1	-1	-1	-1	-1	-1	1	1
B_{1u}	Γ_3^-	1	1	-1	1	-1	-1	-1	1	-1	1
B_{2u}	Γ_4^-	1	1	-1	-1	1	-1	-1	1	1	-1
E_u	Γ_5^-	2	-2	0	0	0	-2	2	0	0	0

+ + + −

Representations of finite Abelian groups

Finite Abelian groups $\begin{cases} \text{cyclic groups} \\ \text{direct product of cyclic groups} \end{cases}$

A

$\{a, a^2, \ldots, a^s\}$

$D^p(a^m)$, $p=0,1,\ldots,s-1$

$$exp(-i2\pi m)\frac{p}{s}$$

B

$\{b, b^2, \ldots, b^r\}$

$D^q(b^n)$, $q=0,1,\ldots,r-1$

$$exp(-i2\pi n)\frac{q}{r}$$

A x B

$\{(a^m, b^n)\}$ $m=1,\ldots,s;$ $n=1,\ldots,r$

$D^p(a^m) \otimes D^q(b^n)$

$$D^{p,q}(a^m, b^n) = exp(-i2\pi m)\frac{p}{s}\ exp(-i2\pi n)\frac{q}{r}$$

$p=0,1,\ldots,s-1 \quad q=0,1,\ldots,r-1$

EXERCISE 15

Determine the character table of the group $4/m \cong 4 \otimes 2$ from the character tables of the cyclic groups 4 and 2.

Determine the character table of the group $6 \cong 3 \otimes 2$ from the character tables of the cyclic groups 3 and 2.

SUBDUCED REPRESENTATIONS

SUBDUCED REPRESENTATION

group G

$\{e, g_2, g_3, \ldots, g_i, \ldots, g_n\}$

$\{e, h_2, h_3, \ldots, h_m\}$

subgroup H<G

D(G): irrep of G

$\{D(e), D(g_2), D(g_3), \ldots, D(g_i), \ldots, D(g_n)\}$

$\{D(e), D(h_2), D(h_3), \ldots, D(h_m)\}$

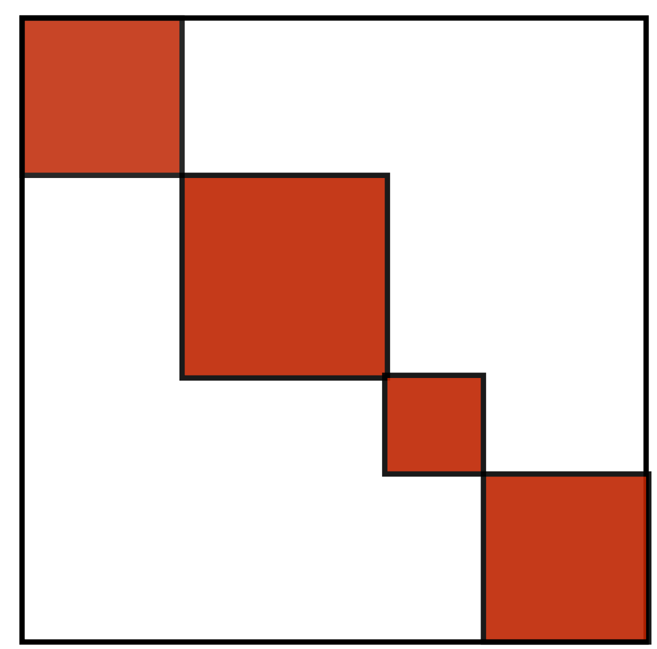
$\{D(G)\downarrow H\}$: subduced rep of H<G

$\{D(G)\downarrow H\}$

Subduction

$S^{-1}\{D(G)\downarrow H\}S$

$\bigoplus m_i D_i(H)$



irreps of H

SUBDUCED REPRESENTATION

$\{\mathbf{D}^r(g_i)\} = \mathbf{D}^r(\mathcal{G}) \downarrow \mathcal{H}$: reducible in general

1. Decomposition of $\mathbf{D}^r(\mathcal{G}) \downarrow \mathcal{H}$

   $\mathbf{D}^r(\mathcal{G}) \downarrow \mathcal{H} \sim \oplus m_i \, \mathbf{D}^i(h),\ h \in \mathcal{H}.$

$$\chi(\mathbf{D}^r(\mathcal{G} \downarrow \mathcal{H})) = \sum_i m_i \, \chi(\mathbf{D}^i(\mathcal{H}))$$

$$m_i = \frac{1}{|\mathcal{H}|} \sum_h \chi^r(h) \chi^i(h)^*$$

2. Subduction matrix

$$\mathbf{S}^{-1} \, (\mathbf{D}^r \downarrow \mathcal{H})(h) \, \mathbf{S} = \oplus m_i \, \mathbf{D}^i(h), h \in \mathcal{H}.$$

EXERCISES

Problem 20

Let **E** be the 2-dimensional irrep of *4mm*:

$$\mathbf{4} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}; \mathbf{m}_x = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

1. Is the subduced representation $\mathbf{E} \downarrow \mathbf{4}$ reducible or irreducible ?
2. If reducible, decompose it into irreps of *4*.
3. Determine the corresponding subduction matrix **S**, defined by $\mathbf{S}^{-1}(\mathbf{E} \downarrow \mathbf{4})(h)\,\mathbf{S} = \oplus m_i \mathbf{D}^i(h),\ h \in 4.$

EXERCISES

Problem 20

Point Group Tables of C_{4v}(4mm)

Character Table

C_{4v}(4mm)	#	1	2	4	m_x	m_d	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	1	-1	-1	J_z
B_1	Γ_3	1	1	-1	1	-1	x^2-y^2
B_2	Γ_4	1	1	-1	-1	1	xy
E	Γ_5	2	-2	0	0	0	$(x,y),(xz,yz),(J_x,J_y)$

Point Group Tables of C_4(4)

Character Table

C_4(4)	#	1	2	4^+	4^-	functions
A	Γ_1	1	1	1	1	z,x^2+y^2,z^2,J_z
B	Γ_2	1	1	-1	-1	x^2-y^2,xy
E	Γ_4 Γ_3	1 1	-1 -1	-1j 1j	1j -1j	$(x,y),(xz,yz),(J_x,J_y)$

BILBAO CRYSTALLOGRAPHIC SERVER

Space Groups Retrieval Tools	
GENPOS	Generators and General Positions of Space Groups
WYCKPOS	Wyckoff Positions of Space Groups
HKLCOND	Reflection conditions of Space Groups
MAXSUB	Maximal Subgroups of Space Groups
SERIES	Series of Maximal Isomorphic Subgroups of Space Groups
WYCKSETS	Equivalent Sets of Wyckoff Positions
NORMALIZER	Normalizers of Space Groups
KVEC	The k-vector types and Brillouin zones of Space Groups
SYMMETRY OPERATIONS	Geometric interpretation of matrix column representations of symmetry operations
IDENTIFY GROUP	Identification of a Space Group from a set of generators in an arbitrary setting

Representation Theory Applications	
REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
Get_mirreps	Irreps and order parameters in a paramagnetic space group-magnetic subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group

Databases of Representations

Representations of space and point groups

wave-vector data

Brillouin zones
representation domains
parameter ranges

POINT

character tables
multiplication tables
symmetrized products

Retrieval tools

Database on Representations of Point Groups

group-subgroup relations

Point Subgroups

Subgroup	Order	Index
6mm	12	1
6	6	2
3m	6	2
3	3	4
mm2	4	3
2	2	6
m	2	6
1	1	12

The Rotation Group D(L)

L	2L+1	A_1	A_2	B_1	B_2	E_2	E_1
0	1	1	.	.	.	.	.
1	3	1	.	.	.	.	1
2	5	1	.	.	.	1	1
3	7	1	.	1	1	1	1
4	9	1	.	1	1	2	1
5	11	1	.	1	1	2	2
6	13	2	1	1	1	2	2
7	15	2	1	1	1	2	3
8	17	2	1	1	1	3	3
9	19	2	1	2	2	3	3
10	21	2	1	2	2	4	3

Point Group Tables of C_{6v}(6mm)

Character Table

C_{6v}(6mm)	#	1	2	3	6	m_d	m_v	functions
Mult.	-	1	1	2	2	3	3	.
A_1	Γ_1	1	1	1	1	1	1	z,x^2+y^2,z^2
A_2	Γ_2	1	1	1	1	-1	-1	J_z
B_1	Γ_3	1	-1	1	-1	1	-1	.
B_2	Γ_4	1	-1	1	-1	-1	1	.
E_2	Γ_6	2	2	-1	-1	0	0	(x^2-y^2,xy)
E_1	Γ_5	2	-2	-1	1	0	0	$(x,y),(xz,yz),(J_x,J_y)$

[List of irreducible representations in matrix form]

character tables
matrix representations
basis functions

Direct (Kronecker) products of representations

Point-group Database

Multiplication Table

C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
A_1	A_1	A_2	B_1	B_2	E_2	E_1
A_2	·	A_1	B_2	B_1	E_2	E_1
B_1	·	·	A_1	A_2	E_1	E_2
B_2	·	·	·	A_1	E_1	E_2
E_2	·	·	·	·	$A_1+A_2+E_2$	$B_1+B_2+E_1$
E_1	·	·	·	·	·	$A_1+A_2+E_2$

Symmetrized Products of Irreps

C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
$[A_1 \times A_1]$	1	·	·	·	·	·
$[A_2 \times A_2]$	1	·	·	·	·	·
$[B_1 \times B_1]$	1	·	·	·	·	·
$[B_2 \times B_2]$	1	·	·	·	·	·
$[E_2 \times E_2]$	1	·	·	·	1	·
$[E_1 \times E_1]$	1	·	·	·	1	·

Irreps Decompositions

C_{6v}(6mm)	A_1	A_2	B_1	B_2	E_2	E_1
V	1	·	·	·	·	1
$[V^2]$	2	·	·	·	1	1
$[V^3]$	2	·	1	1	1	2
$[V^4]$	3	·	1	1	3	2
A	·	1	·	·	·	1
$[A^2]$	2	·	·	·	1	1
$[A^3]$	·	2	1	1	1	2
$[A^4]$	3	·	1	1	3	2
$[V^2]\text{x}V$	3	1	1	1	2	4
$[[V^2]^2]$	5	·	1	1	4	3
$\{V^2\}$	·	1	·	·	·	1
$\{A^2\}$	·	1	·	·	·	1
$\{[V^2]^2\}$	1	2	1	1	2	3