CRYSTALLOGRAPHY ONLINE Workshop

on the use and applications of the structural and magnetic tools of the

BILBAO CRYSTALLOGRAPHIC SERVER

Leioa, 27 June -1 July 2022

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

GENERAL INTRODUCTION

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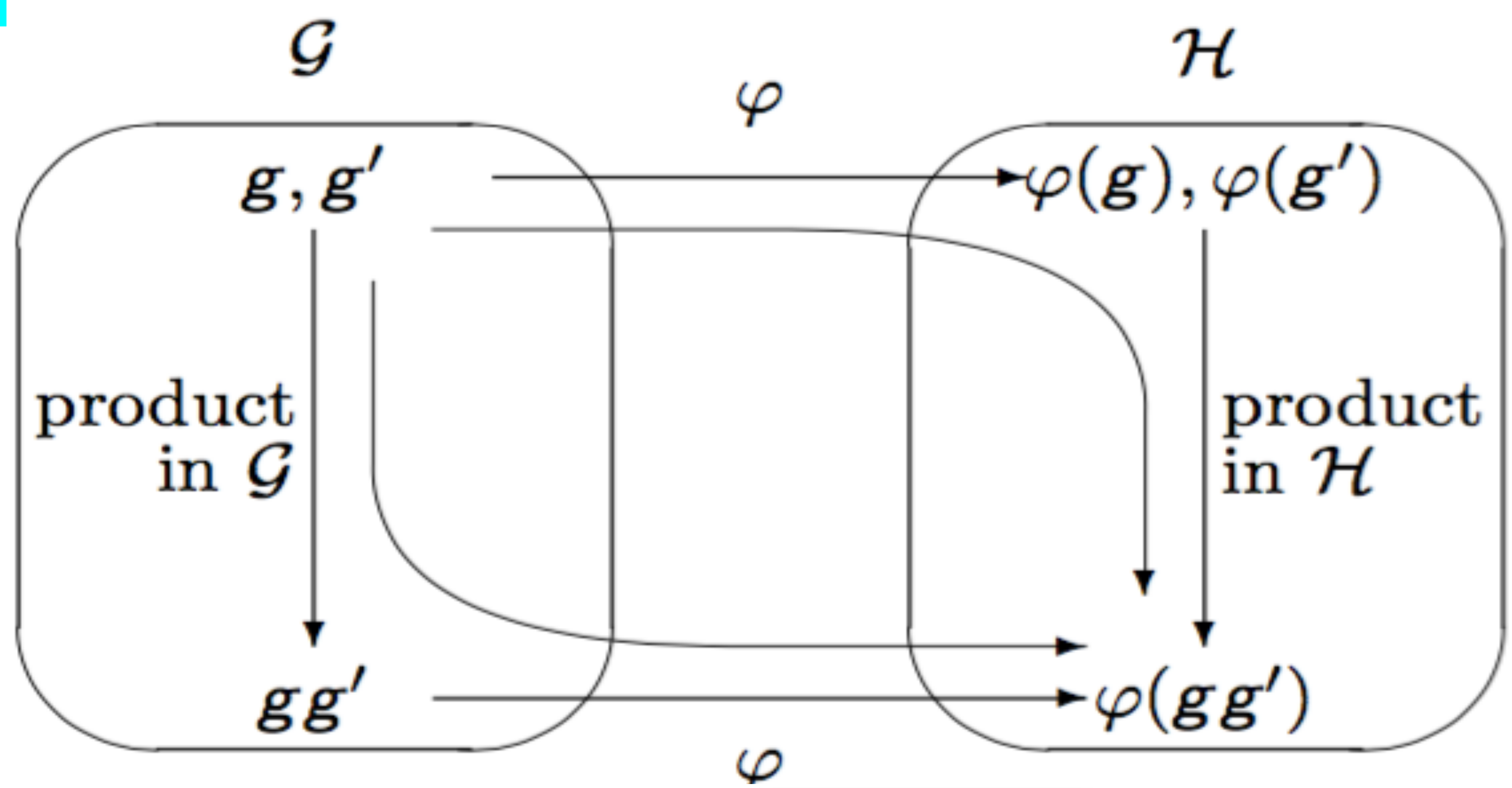
Homomorphism

mapping G={g} $\xrightarrow{\phi(g)=h}$ H={h}

homomorphic condition $\varphi(gg') = \varphi(g)\varphi(g')$ for all $g, g' \in \mathcal{G}$



The set $\{g \in \mathcal{G} \mid \varphi(g) = e\}$ is called the *kernel of* φ, denoted by $\ker(\varphi)$

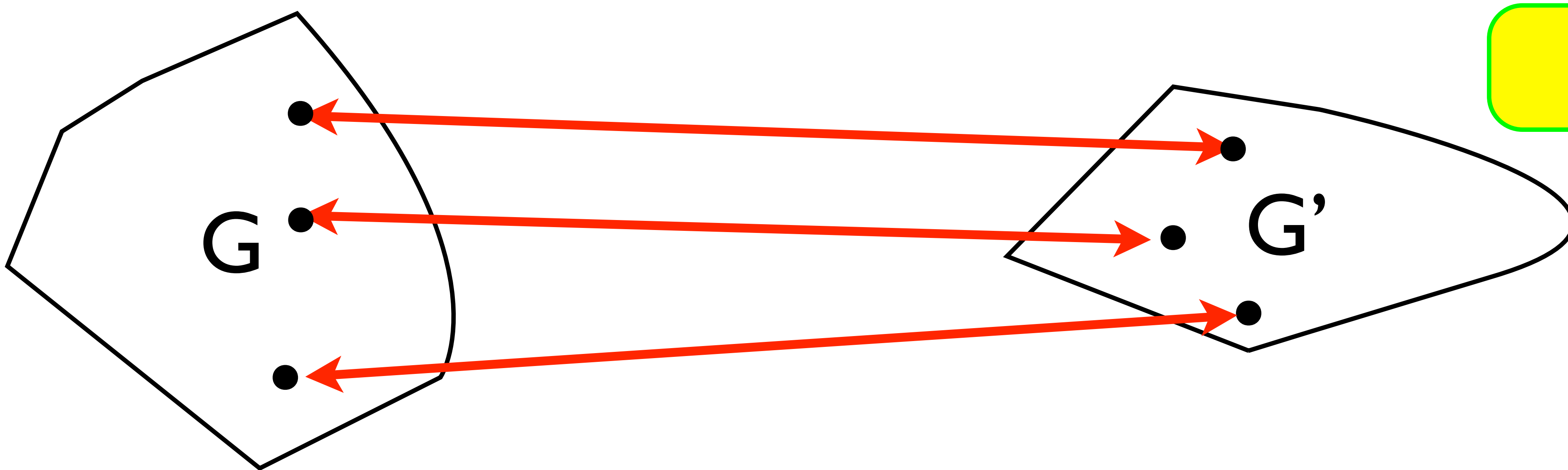
The set $\varphi(\mathcal{G}) = \{\varphi(g) \mid g \in \mathcal{G}\}$ is called the *image of* φ, denoted by $\mathrm{im}(\varphi)$

homomorphism for which $\ker(\varphi) = \{e\}$ is called *injective* or a *monomorphism*,
homomorphism for which $\mathrm{im}(\varphi) = \mathcal{H}$ is called *surjective* or an *epimorphism*.

isomorphism

homomorphism which is both injective and surjective is called *bijective*

Isomorphism



$$\Psi: G \longleftrightarrow G'$$

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

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

$$\Psi(g_1)\ \Psi(g_2) = \Psi(g_1\ g_2)$$

Isomorphic groups -groups with the same multiplication table

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

$\updownarrow$?

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

Representations of Groups

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

Φ

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

$D(g_j)$: n x n matrices

$\det D(g_j) \neq 0$

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

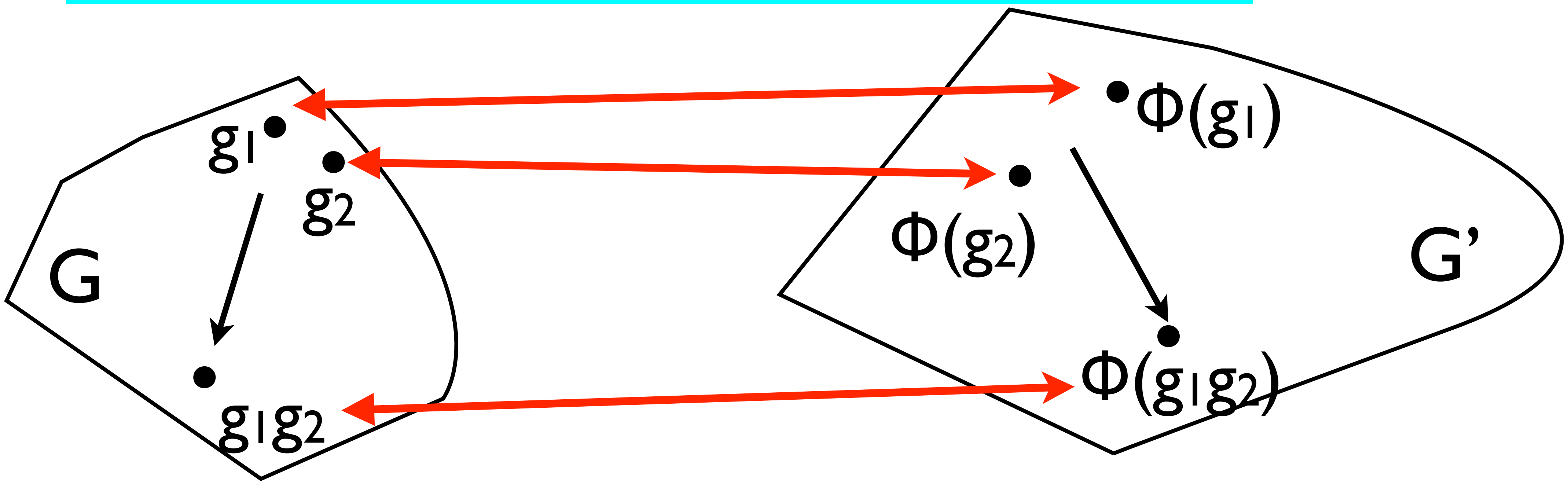
dimension of representation

kernel of representation

Examples: trivial (identity) representation

faithful representation

Homomorphism and Isomorphism



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

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

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

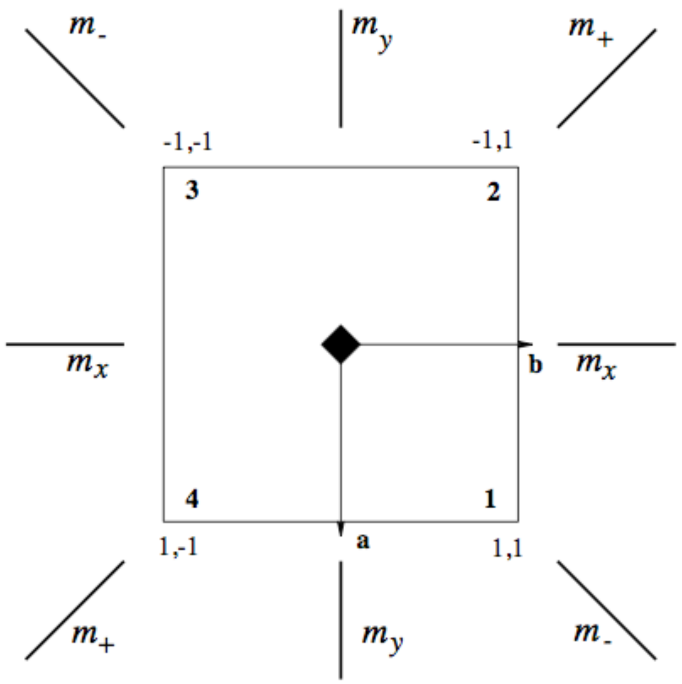
homomorphic condition $\Phi(g_1)\Phi(g_2)= \Phi(g_1\ g_2)$

Example

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

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

EXERCISE 2.6.1.1(a)



Two-dimensional faithful representation of 4mm

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

$D(1)$:

1	0
0	1

$D(4)$:

0	-1
1	0

$D(m_x)$:

-1	0
0	1

$D(m_y)$: ?

Determine the rest of the matrices:

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

Representation

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

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:

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

$$\downarrow$$

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

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

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

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

Representation

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

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

Carrier space of representation

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

P_G-invariant space

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

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

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

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

Matrix representation

$$R_G \xrightarrow{\text{homomorphic mapping}} D_G$$

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

S: invertible matrix

Equivalent Representations

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

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

two reps of G

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

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

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

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

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

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

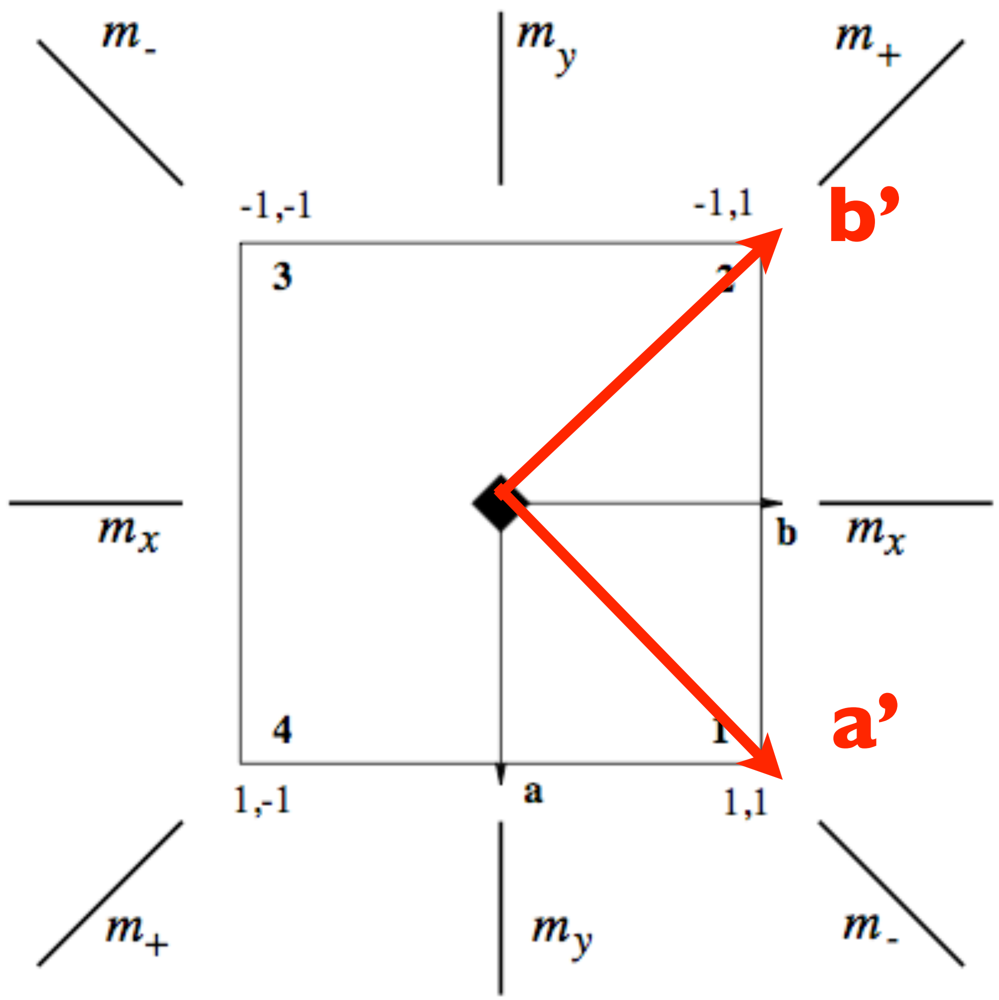
$$D'(g)= P^{-1}D(g)P,\ g\in G$$

EXERCISE 2.6.1.1(b)

2-dim faithful representation of 4mm

In problem 2.6.1.1(a) we consider a representation of 4mm with respect to the basis {**a**,**b**} of the type

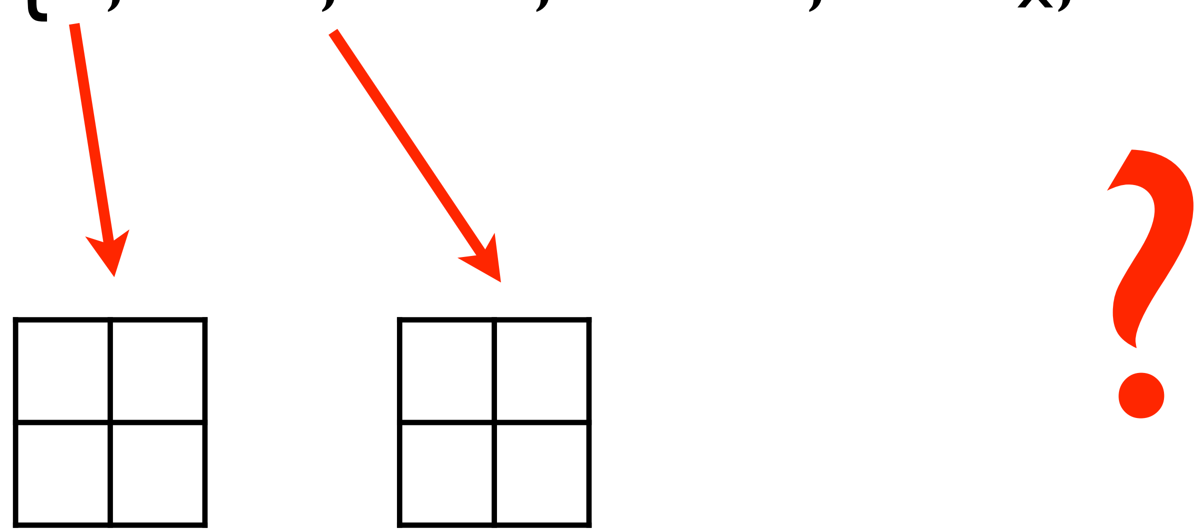
$$D(4)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \qquad D(m_x)=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$$



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

$$R_g\{\mathbf{a'}, \mathbf{b'}\}=\{\mathbf{a'}, \mathbf{b'}\}D'(g)$$

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



Problem 2.6.1.1 (c)

Show that the representations D and D'of the group 4mm determined in problems 2.6.1.1(a) and 2.6.1.1(b) are equivalent, *i.e* show that there exists a matrix S such that: $S^{-1}D(g)S=D'(g)$, $g\in 4mm$.

2.6.1.1a: $D(4)=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ $D(m_x)=\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

2.6.1.1b: $D'(4)=\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ $D'(m_x)=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

EXERCISE 2.6.1.2

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

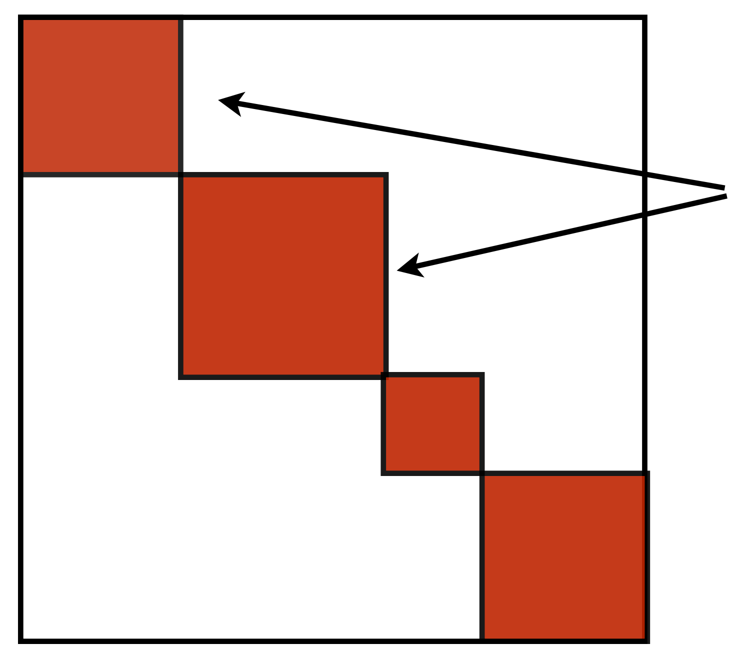
reps of G: $D(G)=\{D(g_i), g_i \in G\}$

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

reducible and irreducible

D(G) reducible

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



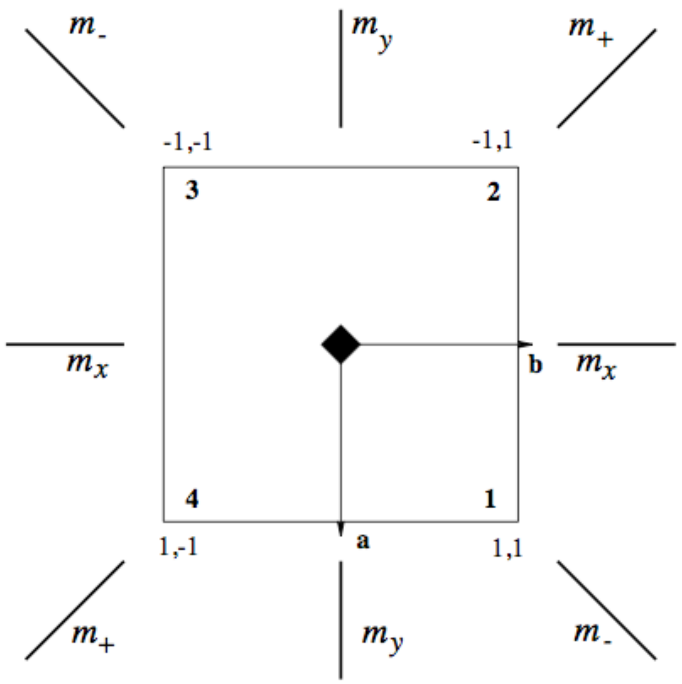
$D_i(G)$ reps of G

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

$$\bigoplus m_i D_i(G)$$

EXAMPLE

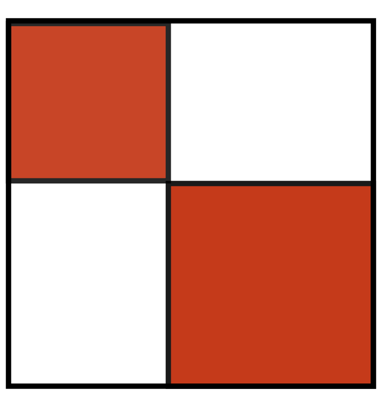
Reducible rep of 4mm



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

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

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



$D_1(4)=1$

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

$D_1(m_-)=-1$

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

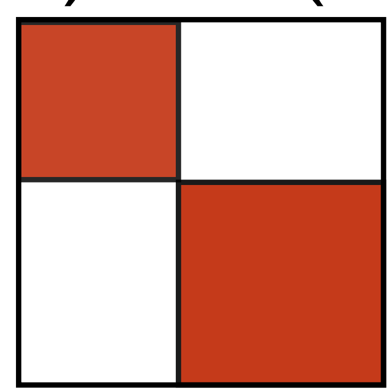
Reducible representations and invariant subspaces

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**

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

$$D'(C_2)=X^{-1}\,D(C_2)\,X$$

$$D'(C_2)=\left\{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\right\}$$

$\mathbf{V}^{(1)}$ $\{\mathbf{e}_1+\mathbf{e}_2\}$ $\mathbf{W}^{(1)}$ $\{\mathbf{e}_1-\mathbf{e}_2\}$

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 $B=cI$

Problem: 2.6.1.3 (ii)

Irreps of Abelian groups **are one-dimensional**

WHY?

Problem 2.6.1.3 | Exercises

(i) Determine the general form of the matrix B that commutes with the matrices of all elements of the 2-dim irrep E of *4mm*

$$E(g)B = B\, E(g),\ g \in 4mm \quad (*)$$

where $E(4) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ $E(m_{yz}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

Hint: To determine B it is sufficient to consider the commuting equations (*) for the generators of 4mm

(ii) Show that the irreps of Abelian groups are one-dimensional

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

$\dim D_1(G)=d$

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

Problem: 2.6.1.4

Exercise

1. Determine the number and dimensions of the irreps of 222.

Can you write down the irrep table of 222?

Problem: 2.6.1.4 (cont.)

Exercise

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

3. 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: **r** conjugacy classes $\{e\}, \{g_2, \ldots, g_k\}, \ldots, \{g_r, \ldots\}$

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

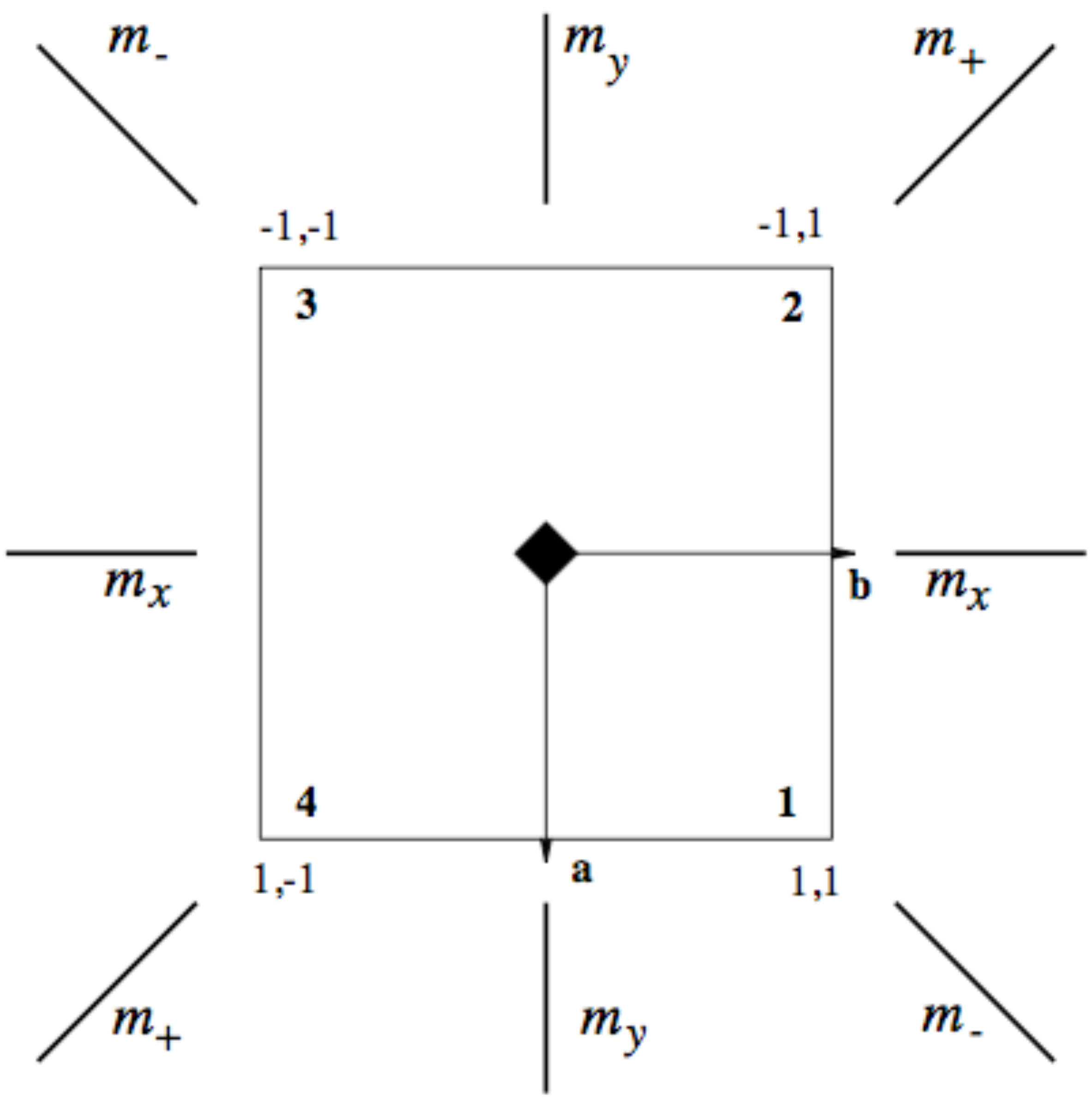
length of conjugacy classes

basis functions

Problem 2.6.1.5

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 2.6.1.5 (cont)

Characters of Representations

Character table of 432

rows

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

columns

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

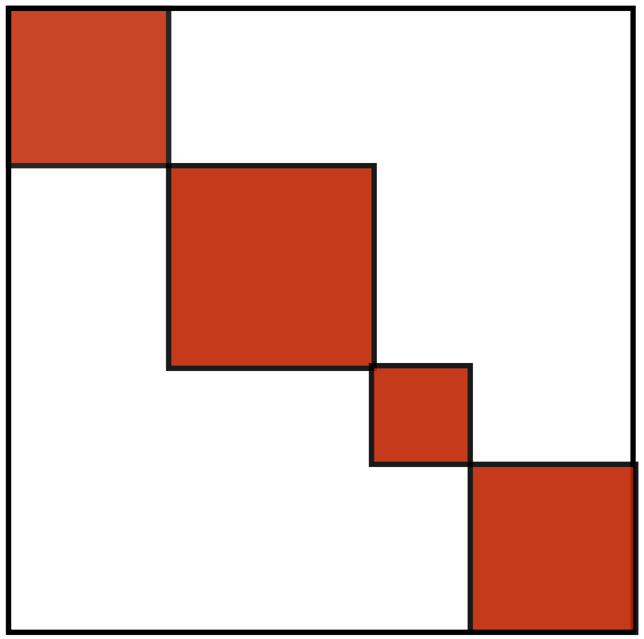
class length	1	3	6	8	6
element order	1	2	2	3	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	?	?	?	?
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

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

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

Problem 2.6.1.6

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:

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

1. Decompose the reducible representation into irreps of 222
2. Determine the matrix **S** that transforms the matrices of the reducible representation into direct sum of irreps.

Hint: $D(G)\mathbf{S}=\mathbf{S}[\bigoplus m_i D_i(G)]$

Problem 2.6.1.8

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.

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

$D_4(422)$	#	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

Hint: 'magic' formula

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

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

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

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

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

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

$$\dim A = \dim C = n$$

$$\dim B = \dim D = m$$

Problem 2.6.2.1

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

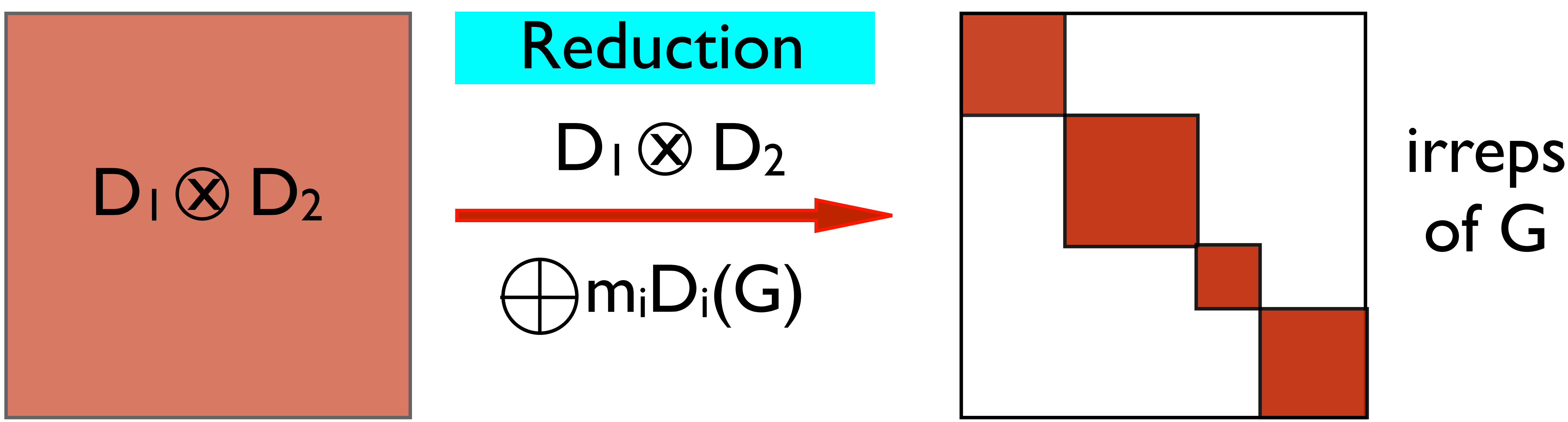
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

Direct-product representation

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



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

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

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

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

Problem 2.6.2.2

Determine the multiplication table of the irreps of 4mm

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

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

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

Problem 2.6.2.2

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

Symmetrized and anti-symmetrized squares

$\mathbf{V}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$: D(G)

$\mathbf{V} \otimes \mathbf{V}$ $\{\mathbf{v}_1\mathbf{v}_1, \mathbf{v}_2\mathbf{v}_1, \ldots, \mathbf{v}_i\mathbf{v}_j, \ldots, \mathbf{v}_n\mathbf{v}_n\}$

symmetrized square $[\mathbf{V}]^2$: $\mathbf{v}\,\mathbf{v'} = \mathbf{v'}\mathbf{v}$

basis $[\mathbf{V}]^2$: $\{\mathbf{v}_i\mathbf{v}_j+\mathbf{v}_j\mathbf{v}_i,\ 1 \leq i < j \leq n\}$

dim $[\mathbf{V}]^2 = 1/2n(n+1)$

anti-symmetrized square $\{\mathbf{V}\}^2$: $\mathbf{v}\,\mathbf{v'} = -\mathbf{v'}\mathbf{v}$

basis $\{\mathbf{V}\}^2$: $\{\mathbf{v}_i\mathbf{v}_j-\mathbf{v}_j\mathbf{v}_i,\ 1 \leq i < j \leq n\}$

dim $\{\mathbf{V}\}^2 = 1/2n(n-1)$

Symmetrized and anti-symmetrized squares

$\mathbf{V}$ $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$: D(G) rep of G:

character of D(G): $\mu(G)=\{\mu(e), \mu(g_2), \ldots, \mu(g_n)\}$

symmetrized square $[\mathbf{V}]^2$: $[D(G)]^2$

character of $[D(G)]^2$: $[\mu(g)]^2=1/2(\mu^2(g)+\mu(g^2))$

anti-symmetrized square $\{\mathbf{V}\}^2$: $\{D(G)\}^2$

character of $\{D(G)\}^2$: $\{\mu(g)\}^2=1/2(\mu^2(g)-\mu(g^2))$

Problem 2.6.2.3

Symmetrized and anti-symmetrized squares

Calculate the characters of the symmetrized and anti-symmetrized squares of the two-dimensional irreps of 4mm and 3m.

If $\{E\}^2$ and/or $[E]^2$ are reducible, decompose them into irreps.

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

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

REPRESENTATIONS OF FINITE ABELIAN GROUPS

Representations of cyclic groups

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

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

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

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

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

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

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

Problem 2.6.2.4 (1)

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

Problem 2.6.2.4 (2)

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

Representations of finite Abelian groups

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

A	B	A × B
$\{a, a^2, \ldots, a^s\}$	$\{b, b^2, \ldots, b^r\}$	$\{(a^m, b^n)\}$ $m=1,\ldots,s;$ $n=1,\ldots,r$
$D^p(a^m), p=0,1,\ldots,s-1$	$D^q(b^n), q=0,1,\ldots,r-1$	$D^p(a^m) \otimes D^q(b^n)$
$exp(-i2\pi m)\frac{p}{s}$	$exp(-i2\pi n)\frac{q}{r}$	

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

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

Problem 2.6.2.4 (cont)

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

4. 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

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

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

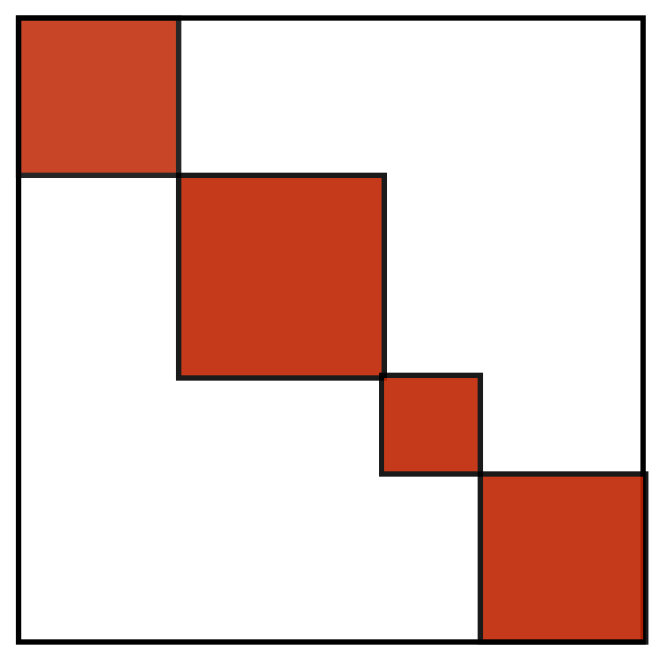
$\{D(G)\downarrow H\}$: subduced rep of $H<G$

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

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

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

Problem 2.6.2.5

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 2.6.2.5

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	$(x,y),(xz,yz),(J_x,J_y)$

INDUCED REPRESENTATIONS

INDUCED REPRESENTATION

Group-subgroup pair $\mathcal{G} > \mathcal{H}$; Irrep $\mathbf{D}^j(\mathcal{H})$

$\mathcal{G} = \mathcal{H} \cup g_2 \mathcal{H} \cup \ \ldots \ \cup g_r \mathcal{H}$

Induced rep of $\mathcal{G}$: The set of $(r\,d \times r\,d)$ matrices

$$\mathbf{D}^{Ind}(g)_{mt,ns} = \begin{cases} \mathbf{D}^j(g_m^{-1}\, g\, g_n)_{t,s} & \text{if } g_m^{-1}\, g\, g_n = h \\ 0 & \text{if } g_m^{-1}\, g\, g_n \notin \mathcal{H} \end{cases}$$

$$\mathbf{D}^{Ind}(g)_{mt,ns} = \mathbf{M}(g)_{m,n} \mathbf{D}^j(h)_{t,s}$$

INDUCED REPRESENTATION

Induction matrix M(g)
monomial matrix

	g_1	g_2		...	g_r
g_1	0	1	0	...	0
g_2	0	0	0	...	1
	1			...	
...	...	...			
g_r	0	0	1	...	0

Induced representation $D^{Ind}(g)$
super-monomial matrix

	g_1	g_2		...	g_r
g_1	0	$D^J(h)$	0		0
g_2	0	0	0	...	$D^J(h)$
	$D^J(h)$			...	
...	...	...			
g_r	0	0	$D^J(h)$	...	0

$$M(g)_{mn} = \begin{cases} 1 & \text{if } g_m^{-1} g g_n = h \\ 0 & \text{if } g_m^{-1} g g_n \notin H \end{cases}$$

EXAMPLE

Problem 2.6.2.9

Determine representations of 4mm induced from the irreps of $\{1, m_{010}\}$.

4mm	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\bar{x}}$
1	1	2_z	4_z	4_z^{-1}	m_{xz}	m_{yz}	m_{xx}	$m_{x\bar{x}}$
2_z	2_z	1	4_z^{-1}	4_z	m_{yz}	m_{xz}	$m_{x\bar{x}}$	m_{xx}
4_z	4_z	4_z^{-1}	2_z	1	m_{xx}	$m_{x\bar{x}}$	m_{yz}	m_{xz}
4_z^{-1}	4_z^{-1}	4_z	1	2_z	$m_{x\bar{x}}$	m_{xx}	m_{xz}	m_{yz}
m_{xz}	m_{xz}	m_{yz}	$m_{x\bar{x}}$	m_{xx}	1	2_z	4_z^{-1}	4_z
m_{yz}	m_{yz}	m_{xz}	m_{xx}	$m_{x\bar{x}}$	2_z	1	4_z	4_z^{-1}
m_{xx}	m_{xx}	$m_{x\bar{x}}$	m_{xz}	m_{yz}	4_z	4_z^{-1}	1	2_z
$m_{x\bar{x}}$	$m_{x\bar{x}}$	m_{xx}	m_{yz}	m_{xz}	4_z^{-1}	4_z	2_z	1

Notation:
$m_{010} = m_{xz}$

Hint to 2.6.2.9

Step 1. Decomposition of 4mm with respect to the subgroup $\{1, m_{xz}\}$

Step 2. Construction of the induction matrix

$$M(g)_{mn} = \begin{cases} 1 & \text{if } g_m^{-1} g g_n = h \\ 0 & \text{if } g_m^{-1} g g_n \notin H \end{cases}$$

g	g_m	g_m^{-1}	$g_m^{-1}\,g$	g_n	$h = g_m^{-1}\,g\,g_n$	$M_{mn} \neq 0$
1	1	1	1	1	1	M_{11}
	m_{yz}	m_{yz}	m_{yz}	m_{yz}	1	M_{22}

EXERCISES

Problem 2.6.2.7

Construct the general form of the matrices of a representation of G induced by the irreps of a subgroup $H<G$ of index 2.