CRYSTALLOGRAPHY ONLINE: WORKSHOP ON THE USE AND APPLICATIONS OF THE BILBAO CRYSTALLOGRAPHIC SERVER

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CRYSTALLOGRAPHY ONLINE: BILBAO CRYSTALLOGRAPHIC SERVER

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS I

GENERAL INTRODUCTION

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Representations of Groups

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

$\downarrow \Phi$

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

$D(g_j)$: n x n matrices

$\det D(g_j) \neq 0$

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

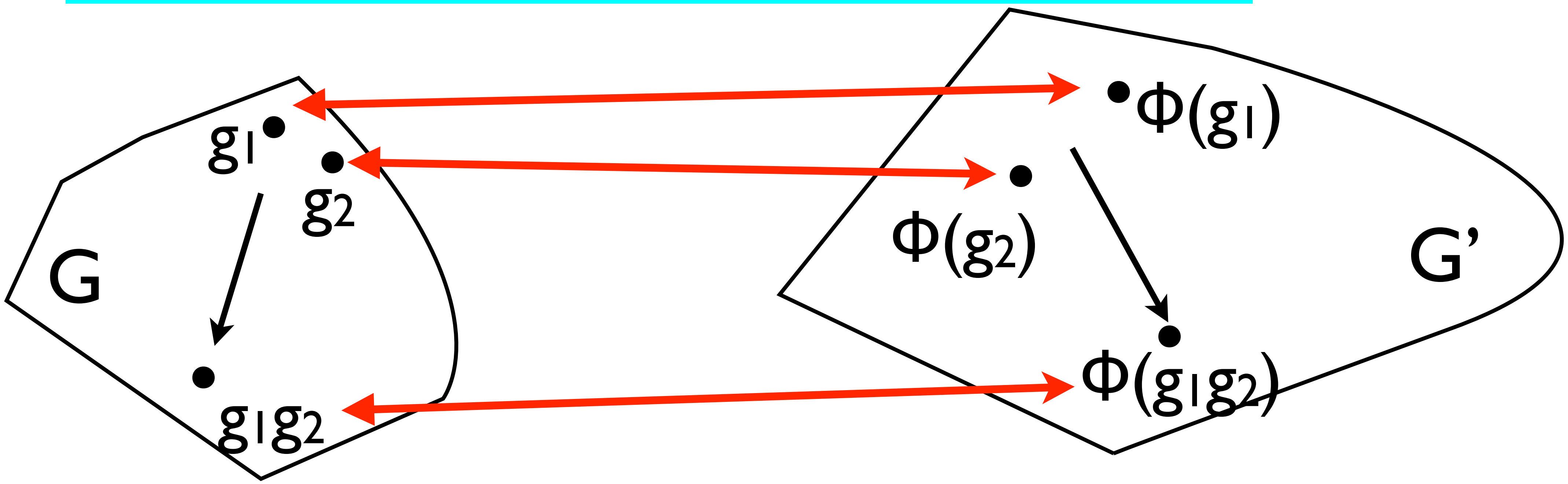
dimension of representation

kernel of representation

Examples: trivial (identity) representation

faithful representation

Homomorphism and Isomorphism



$$G=\{g\} \xrightarrow{\Phi(g)=g'} G'=\{g'\}$$

$$\Phi: G \rightarrow G'$$

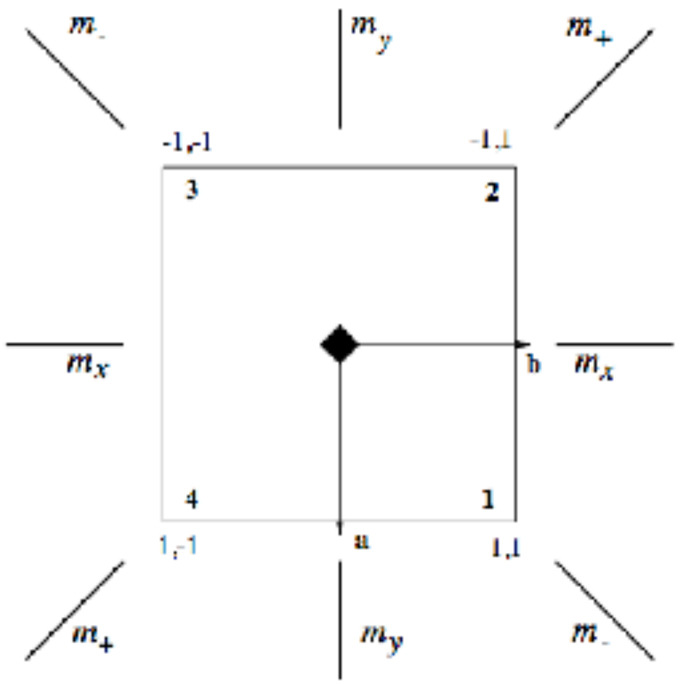
homomorphic condition $\quad \Phi(g_1)\Phi(g_2)=\Phi(g_1\ g_2)$

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

$4mm \rightarrow \{1,-1\}$

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

EXERCISE 3.1a



Two-dimensional faithful representation of 4mm

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

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \qquad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

?

Determine the rest of the matrices:

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

	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

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

Representation

G ⟷ isomorphic mapping ⟷ R_G

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

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

Carrier space of representation

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

P_G-invariant space

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

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

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

G ⟷ 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

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

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

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

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

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

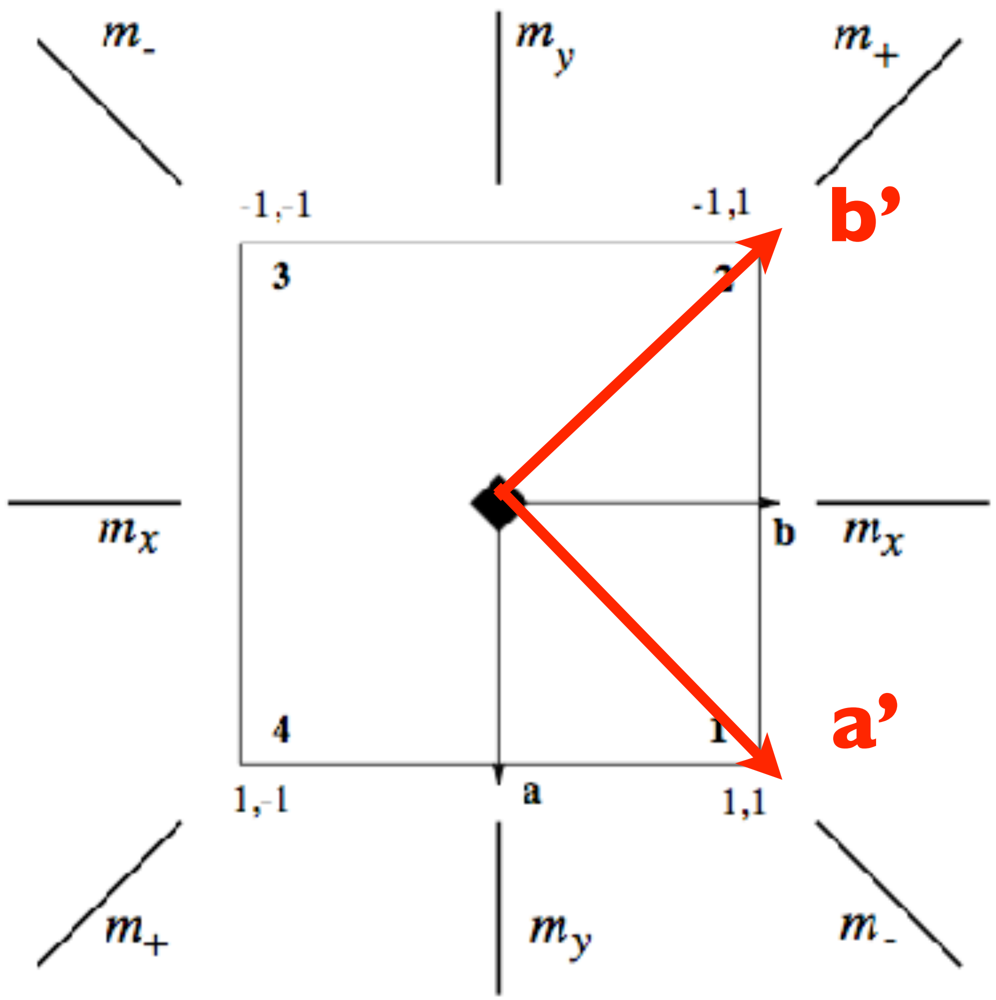
$$= (\mathbf{e}'_1,\mathbf{e}'_2,\mathbf{e}'_3)P^{-1}D(g)P$$

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

EXERCISE 3.1b

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

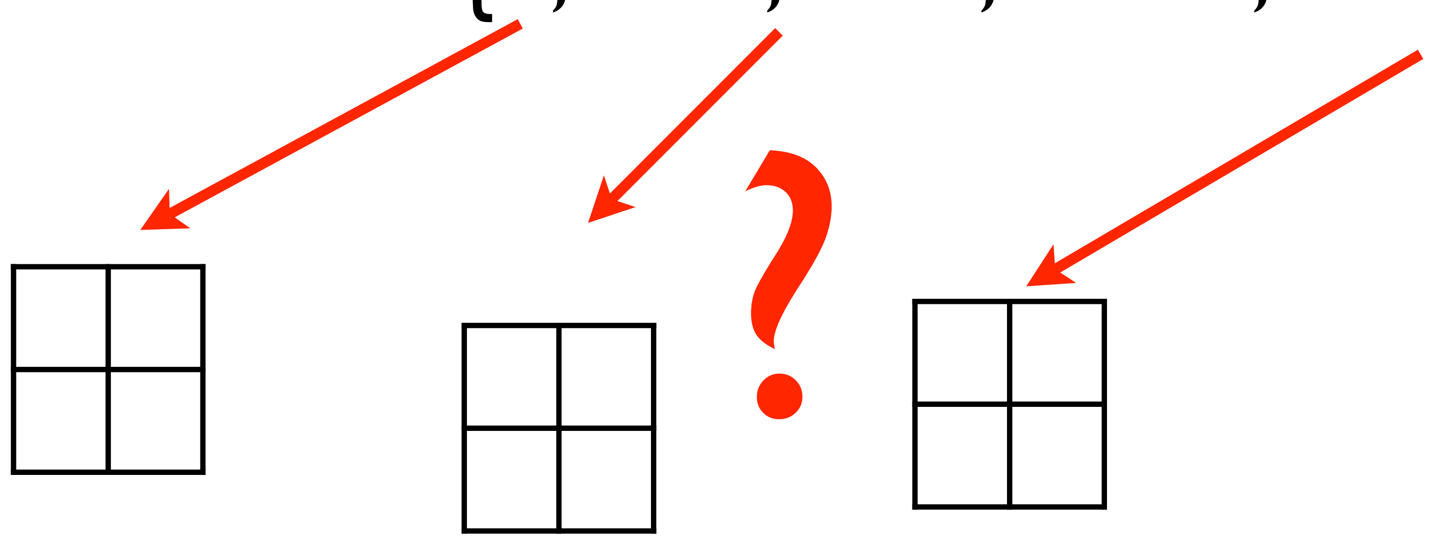


$$D(4)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix} \qquad D(m_x)=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}$$

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

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

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



Hint:

{**a'**,**b'**} = {**a**,**b**}P

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

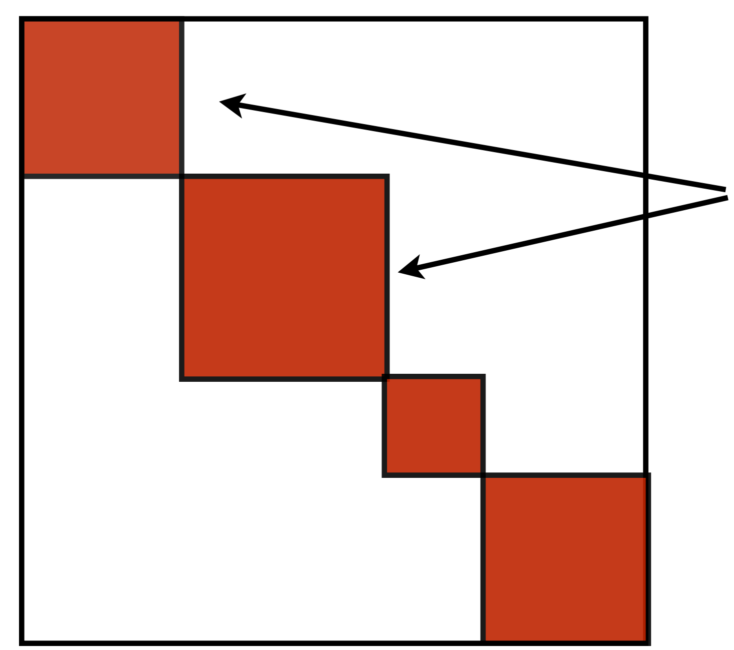
Reducible and Irreducible Representations of Groups

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



$D_i(G)$

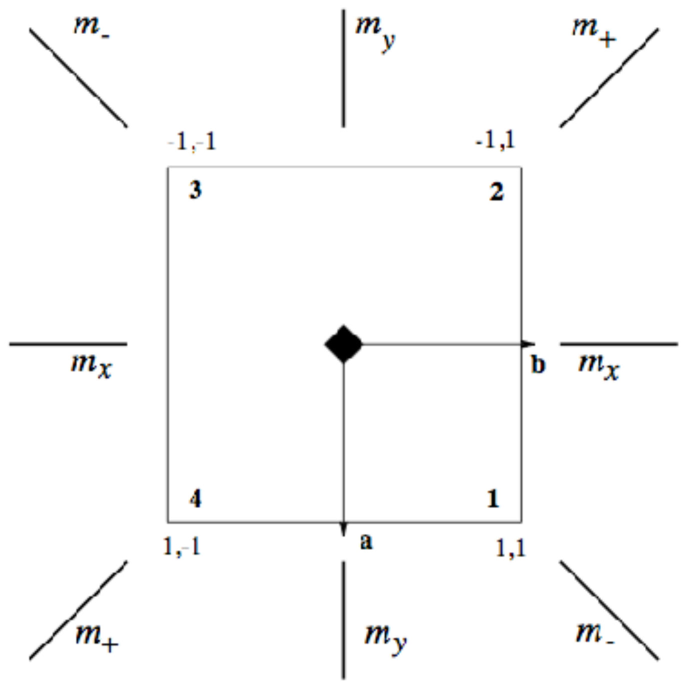
reps of G

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

$$\bigoplus m_i D_i(G)$$

EXAMPLE

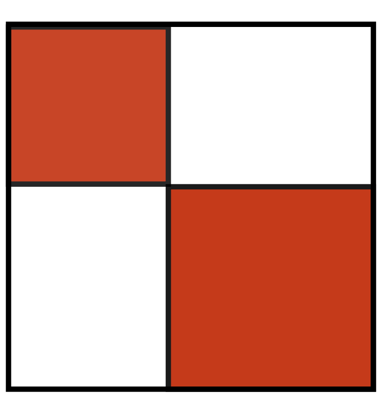
Reducible rep of 4mm



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

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

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



$D_1(4)=1$

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

$D_1(m_-)=-1$

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

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

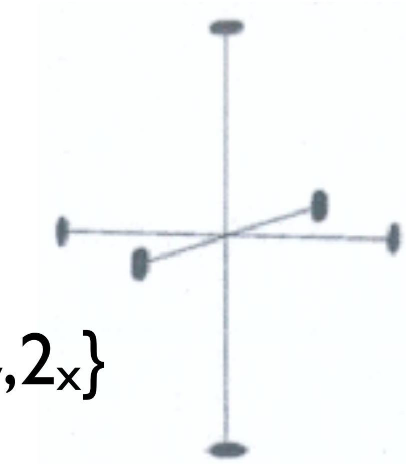
$\dim D_1(G)=d$

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

EXAMPLE: Irreps of 222

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

$\{e, 2_z, 2_y, 2_x\}$



2. Irreps of 222

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

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

$D(2_i) = \mp 1$

$D_2(222)$	#	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

irreps labels:

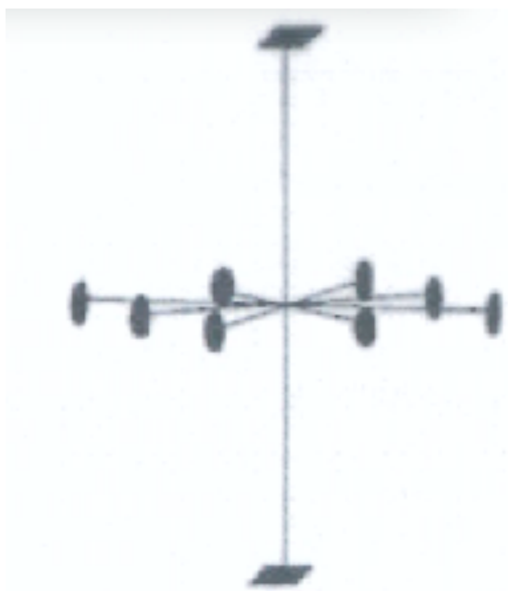
Mulliken labels: A, B, E, F or T

Bethe labels: Γ_i

EXERCISES 3.2

Problems

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



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

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

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

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

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

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 $\mathbf{X} = \mathbf{X}(G)$

rows: irrep labels (Mulliken, Bethe)

columns: conjugacy classes

Character Tables

Character Table of G:

r x **r** matrix **X**=**X**(G)

$\mathbf{X}_{ij} = \mu_{D_i}(g_j)$

$D_2(222)$	#	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

orthogonality

rows

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

columns

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

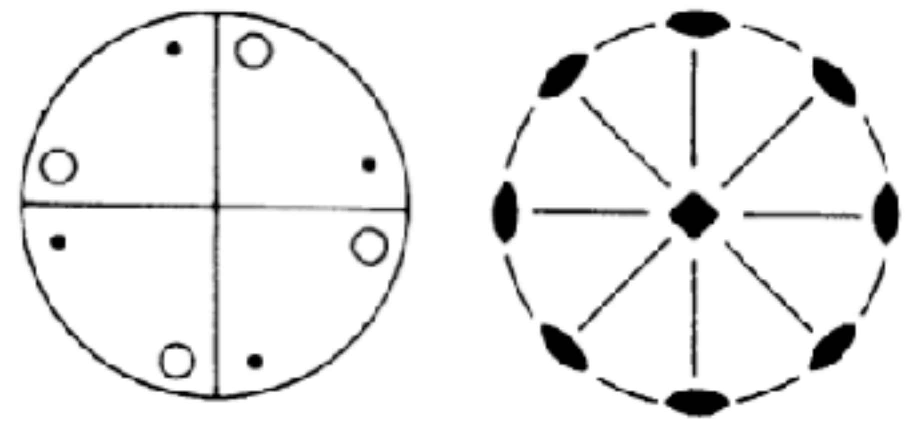
Additional data: order of the elements

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

length of the conjugacy classes

Mulliken

Bethe

rows

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

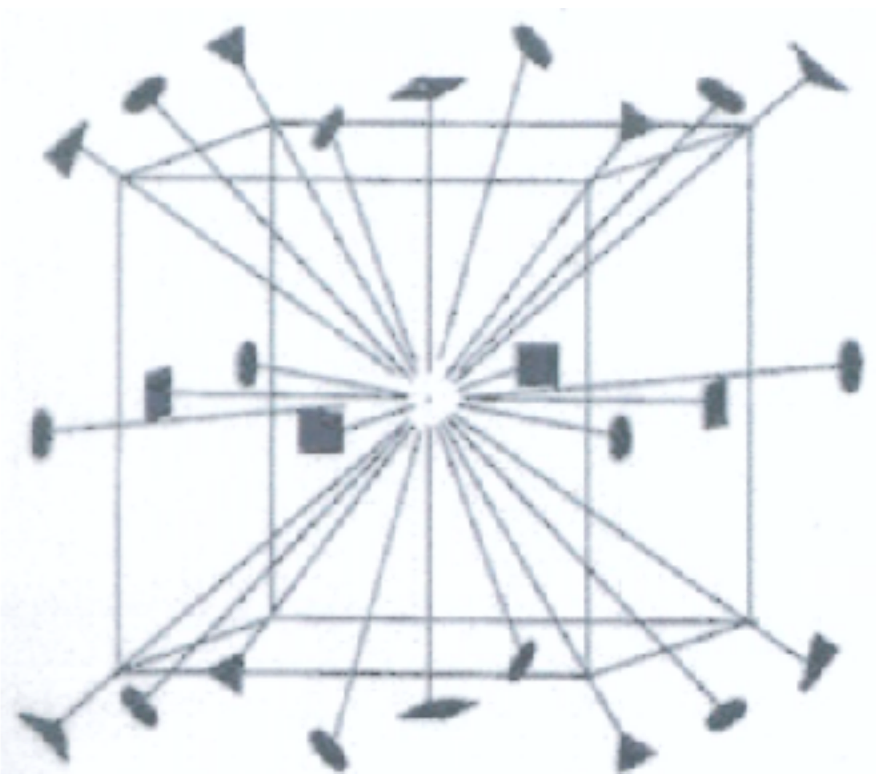
columns

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

Exercise 3.3

Characters of Representations

Character table of 432



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

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

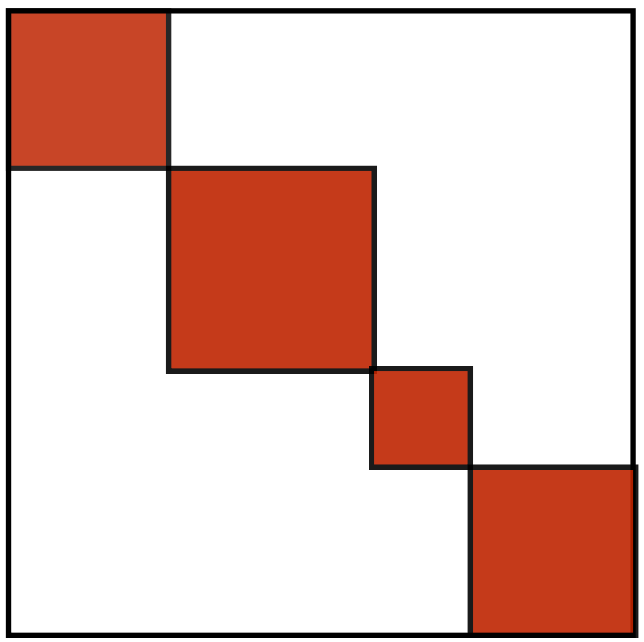
columns $$\frac{1}{|G|}\sum_p \eta_p^*(C_j)\,\eta_p(C_k)\,|C_j| = \delta_{jk}$$

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 3.4

Irreps of 222

Consider the group 222 and its irreps.

$D_2(222)$	#	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

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 + magic formula

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

DIRECT PRODUCT OF REPRESENTATIONS

Direct-product (Kronecker) product of matrices

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

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

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

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

tr$(A \otimes B) = $ tr$(A) \cdot$ tr(B)

EXERCISE 3.5

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

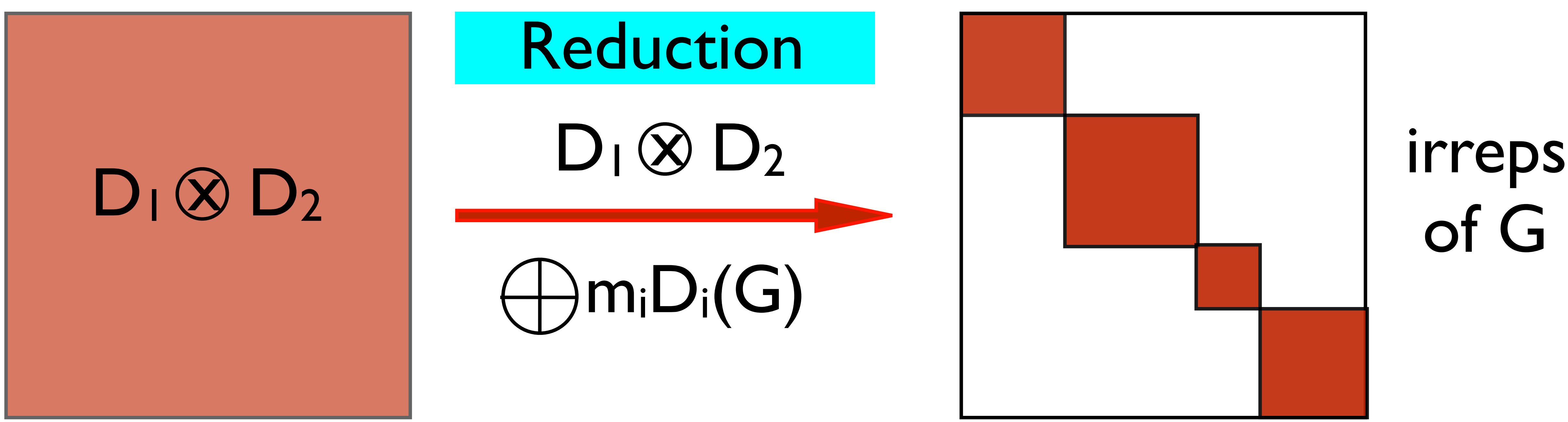
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

Direct-product representation

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



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

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

$$B_1 \otimes B_2 \sim A_2$$

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

Direct-product groups

Let G_1 and G_2 are two groups. The set of all pairs $\{(g_1,g_2), g_1 \in G_1, g_2 \in G_2\}$ forms a group $G_1 \otimes G_2$ with respect to the product: $(g_1,g_2)(g'_1,g'_2) = (g_1 g'_1, g_2 g'_2)$.

The group $G = G_1 \otimes G_2$ is called a **direct-product** group

Point group mm2 = $\{1, 2_{001}, m_{100}, m_{010}\}$

$G_1 = \{1, 2_{001}\}$ $G_2 = \{1, m_{100}\}$

$G_1 \otimes G_2 = \{1.1,\ 2_{001}.1,\ 1.m_{100},\ 2_{001} m_{100} = m_{010}\}$

Centro-symmetrical groups

G_1: rotational groups $G_2 = \{1, \bar{1}\}$ group of inversion

$G_1 \otimes \{1, \bar{1}\} = G_1 + \bar{1}.G_1$

$\{1, 2_{001}, m_{100}, m_{010}\} \otimes \{1, \bar{1}\} =$

$\{1.1,\ 2_{001}.1,\ m_{100}.1, m_{010}.1,\ 1.\bar{1},\ 2_{001}.\bar{1},\ m_{100}.\bar{1}, m_y.\bar{1}\}$

$\{1, 2_{001}, m_{100}, m_{010}, \bar{1}, m_{001}, 2_{100}, 2_{010}\} = 2/m2/m2/m$ or mmm

Direct-product groups and their representations

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

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

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

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

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

EXAMPLE

Irreps of 222=2⊗2'

Irreps of 2

	e	2
A	1	1
B	1	-1

	e	2'
A	1	1
B	1	-1

Irreps of 2'

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 3.6

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 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

Representations of finite Abelian groups

Finite Abelian groups { cyclic groups; direct product of cyclic groups

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

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

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

SUBDUCED REPRESENTATIONS

SUBDUCED REPRESENTATION

group G

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

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

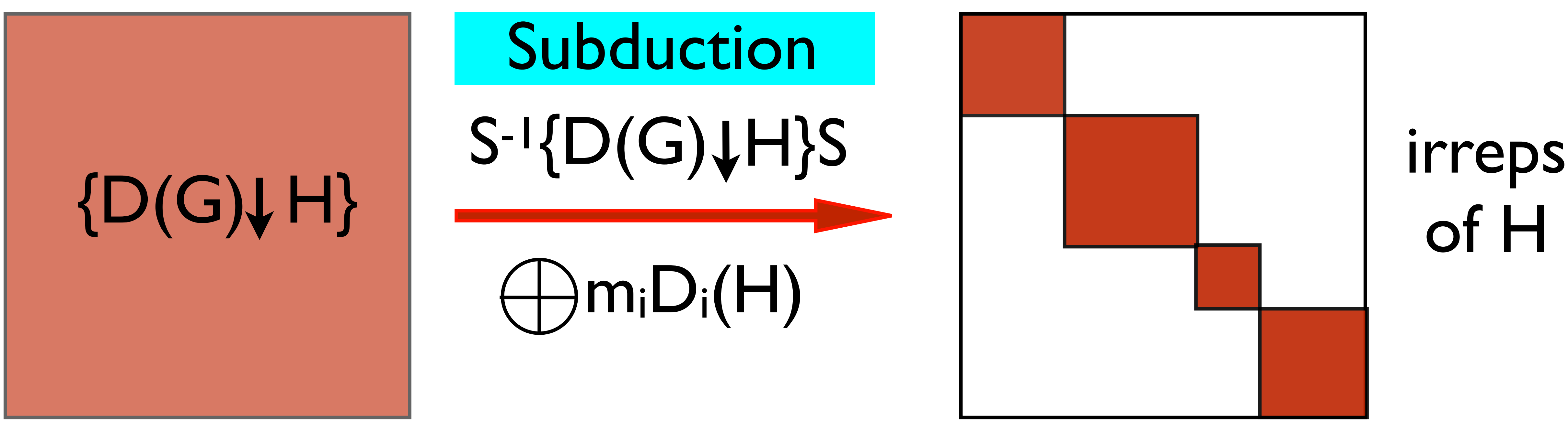
subgroup $H<G$

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 $H<G$



EXERCISES

Problem 3.7

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 3.7

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