REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS I.

GENERAL INTRODUCTION

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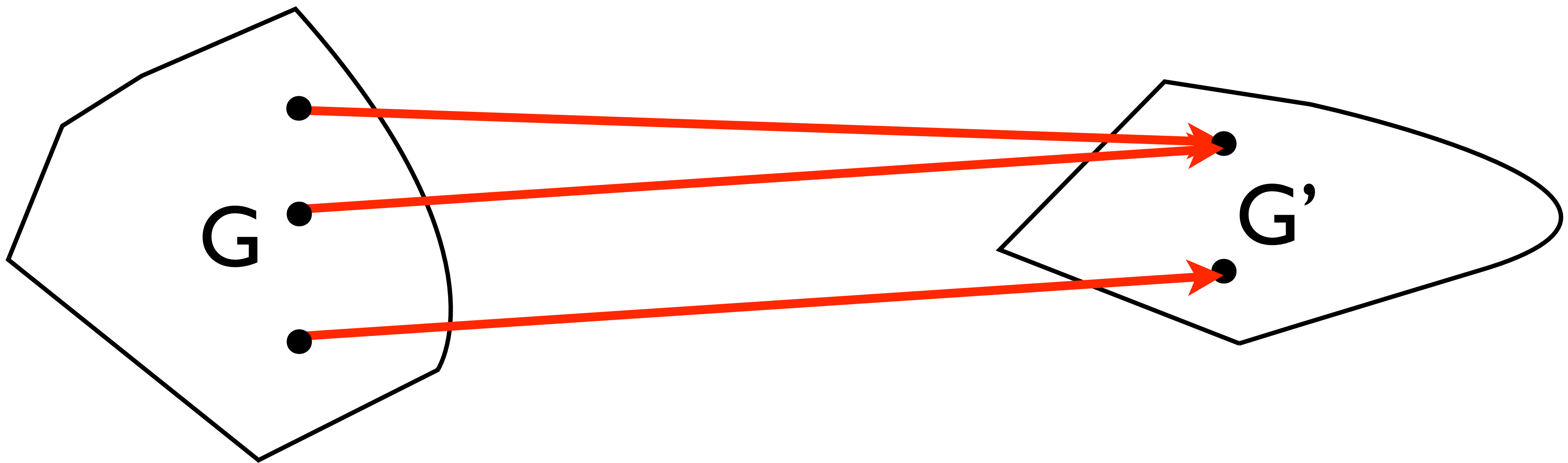
Homomorphism and Isomorphism



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

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

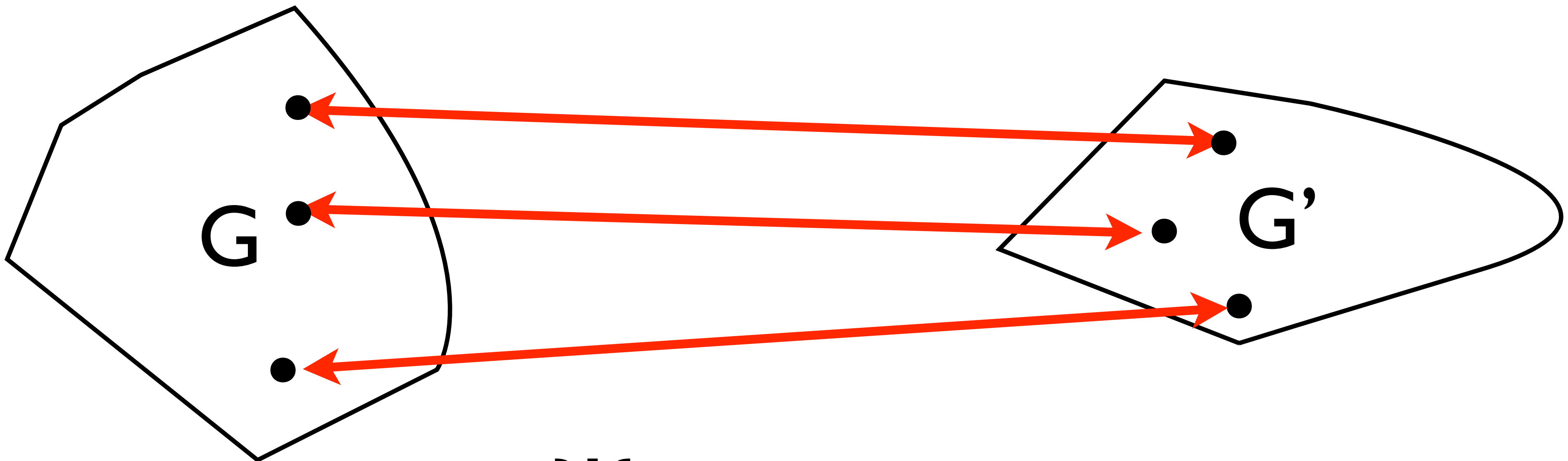
$$\Phi: G \longrightarrow G'$$

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

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

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

Isomorphism



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

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

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

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

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

$\downarrow$ $\quad$?

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

Representations of Groups

group G

$\downarrow \Phi$

D(G): rep of G

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

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

$D(g_j)$: nxn matrices

$\det D(g_j) \neq 0$

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

Example: trivial (identity) representation

faithful representation

EXERCISES

Two-dimensional faithful representation of 4mm

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

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

Determine the rest of the matrices

Representations of Groups

equivalent representations

reps of G: $D_1(G)=\{D_1(g_i),\ g_i \in G\}$ $\quad D_2(G)=\{D_2(g_i),\ g_i \in G\}$

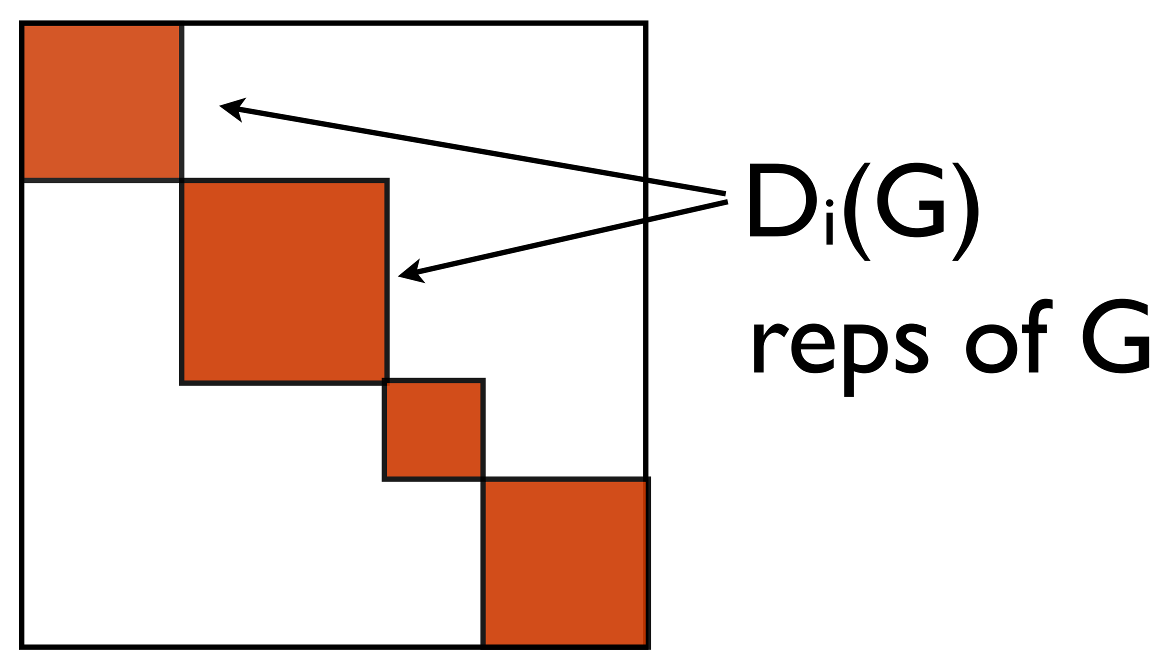
$\dim D_1(G) = \dim D_2(G)$

$D_1(G) \sim D_2(G)$ if $\exists\ S:\ D_1(G) = S^{-1} D_2(G) S$

reducible and irreducible

D(G) reducible

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



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

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

Schur lemma II

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

if $\exists$ B: $D_1(G)B = B\, D_1(G)$

then $B=cI$

irreps of abelian groups

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

$\dim D_1(G)=d$

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

Representations of Groups

example irreps of 222

abelian group

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

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

$D(2_i)=\mp 1$

Point Group Tables of $D_2(222)$

Character Table

$D_2(222)$	#	1	2_z	2_y	2_x	functions
A	Γ_1	1	1	1	1	x^2,y^2,z^2
B_1	Γ_3	1	1	-1	-1	z,xy,J_z
B_2	Γ_2	1	-1	1	-1	y,xz,J_y
B_3	Γ_4	1	-1	-1	1	x,yz,J_x

Characters of Representations
Basic results

character properties

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

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

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

orthogonality

rows

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

columns

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

Characters of Representations

example: 422

Point Group Tables of D_4(422)

Character Table

D_4(422)	#	1	2	4	2_h	$2_{h'}$	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	x^2+y^2, z^2
A_2	Γ_3	1	1	1	-1	-1	z, J_z
B_1	Γ_2	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	$(x,y),(xz,yz),(J_x,J_y)$

rows

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

columns

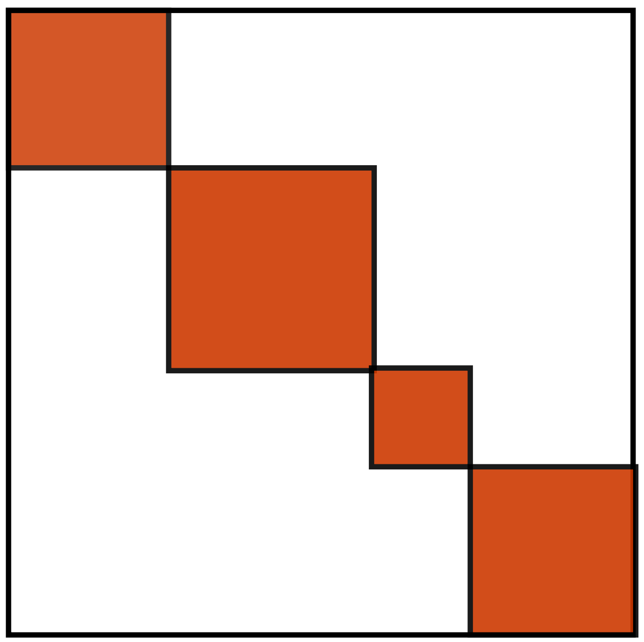
$$\frac{1}{|G|}\sum_p \eta_p^*(C_j)\,\eta_p(C_k)\,|C_j| = \delta_{jk}$$

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

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

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 $-w^2$	$(x,y),(xz,yz),(J_x,J_y)$

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

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

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

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

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

Point Group Tables of $D_4(422)$

Character Table

$D_4(422)$	#	1	2	4	2_h	$2_{h'}$	functions
Mult.	-	1	1	2	2	2	.
A_1	Γ_1	1	1	1	1	1	x^2+y^2,z^2
A_2	Γ_3	1	1	1	-1	-1	z,J_z
B_1	Γ_2	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 $C_i(-1)$

Character Table

$C_i(-1)$	#	1	-1	functions
A_g	Γ_1^+	1	1	$x^2,y^2,z^2,xy,xz,yz,J_x,J_y,J_z$
A_u	Γ_1^-	1	-1	x,y,z

Point Group Tables of $D_{4h}(4/mmm)$

Character Table

$D_{4h}(4/mmm)$	#	1	2	4	2_h	$2_{h'}$	-1	m_z	-4	m_v	m_d	functions
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	x^2+y^2,z^2
A_{2g}	Γ_2^+	1	1	1	-1	-1	1	1	1	-1	-1	J_z
B_{1g}	Γ_3^+	1	1	-1	1	-1	1	1	-1	1	-1	x^2-y^2
B_{2g}	Γ_4^+	1	1	-1	-1	1	1	1	-1	-1	1	xy
E_g	Γ_5^+	2	-2	0	0	0	2	-2	0	0	0	$(xz,yz),(J_x,J_y)$
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	z
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	(x,y)

Direct product of representations

$D_1(G)$: irrep of G

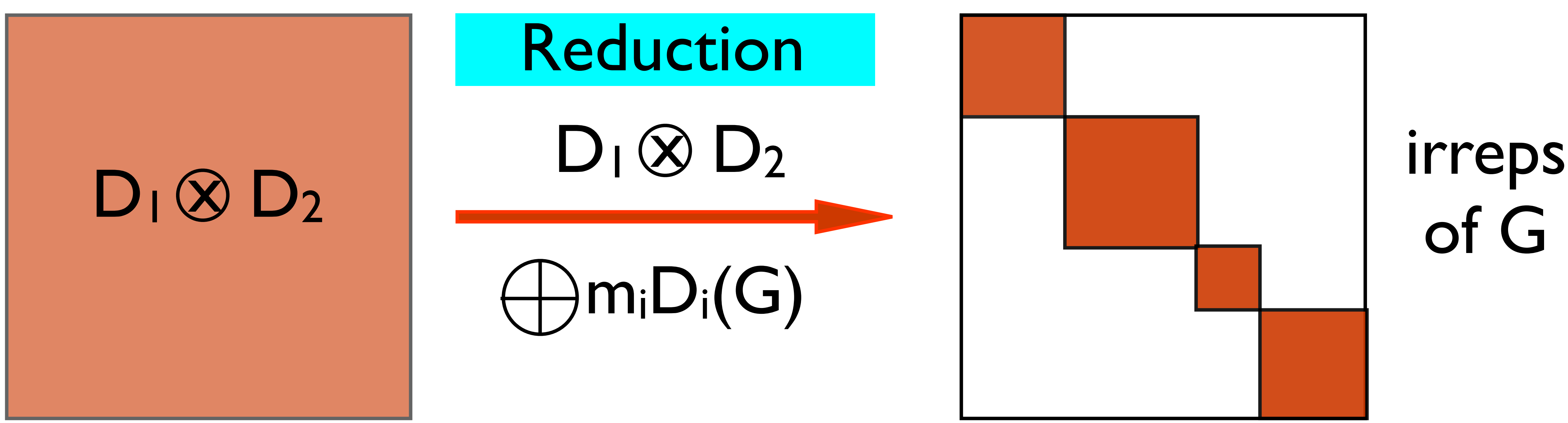
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

Direct-product representation

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



Direct-product (Kronecker) product of matrices

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

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

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

$$\eta(A \otimes B)(g_i) = \eta_A(g_i)\,\eta_B(g_i)$$

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

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	.	.	.	.	$A_1+A_2+B_1+B_2$

EXERCISES

Problem 1

Direct-product representation

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

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

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

Decompose the direct product representation ExE into irreps of 4mm

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

SUBDUCED REPRESENTATION

group G

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

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

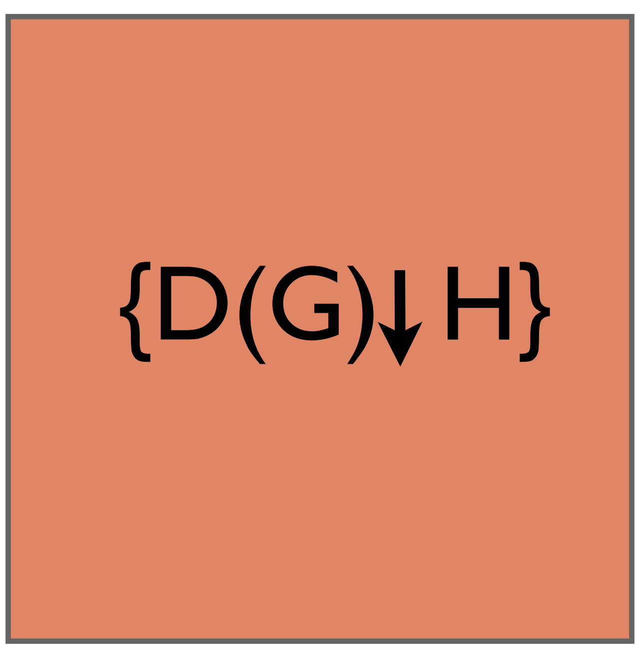
subgroup H<G

D(G): irrep of G

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

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

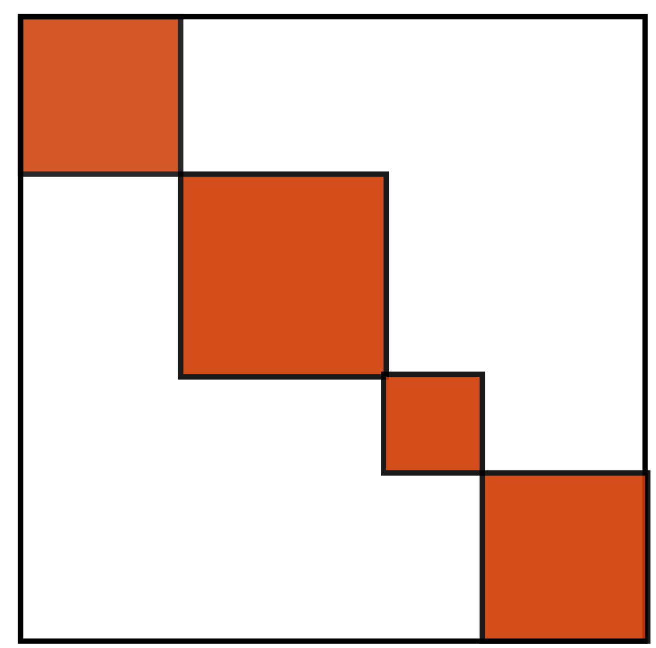
$\{D(G)\downarrow H\}$: subduced rep of H<G



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 $\mathbf{D}^r(\mathcal{G}) \downarrow \mathcal{H}$

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

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

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

2. Subduction matrix

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

EXERCISES

Problem 1

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 1

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

Conjugate representations

conjugate representation

$G \triangleright H$: $D^S(H)=\{D^S(g^{-1}h_i g),\ h_i \in H,\ g \in G, g \notin H\}$

$H = \{e, h_2, h_3, \ldots, h_i, \ldots, h_n\}$

$\{D(e), D(h_2), \ldots, D(h_n)\}$

conjugated irrep

$\{D(g^{-1}eg), D(g^{-1}h_2 g), \ldots, D(g^{-1}h_n g)\}$

$D^S(H) = \{D(e), D(h'_2), \ldots, D(h'_n)\}$

Conjugate representations

properties

CONJUGATE REPRESENTATION

$$(\mathbf{D}^s(\mathcal{H}))_g = \{\mathbf{D}^s(g^{-1}\,h\,g),\ \ h \in \mathcal{H}\},$$
$$\text{where} g \in \mathcal{G},\ \ g \notin \mathcal{H}$$

1. $dim(\mathbf{D}^s(\mathcal{H})) = dim((\mathbf{D}^s(\mathcal{H}))_g)$;
2. $(\mathbf{D}^s(\mathcal{H}))_g$ is an irrep if $\mathbf{D}^s(\mathcal{H})$ is.
3. Equivalent or nonequivalent conjugate rep

$$(\mathbf{D}^s(\mathcal{H}))_g \begin{cases} \sim \mathbf{D}^s(\mathcal{H}) \\ \not\sim \mathbf{D}^s(\mathcal{H}) \end{cases}$$

Conjugate representations and orbits

Group–normal subgroup pair $\mathcal{G} \triangleright \mathcal{H}$

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

ORBIT OF CONJUGATE REPS

$O\,(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}),\, (\mathbf{D}^s(\mathcal{H}))_{g_2}, \ldots,\, (\mathbf{D}^s(\mathcal{H}))_{g_r}\}$,

where $g \in \mathcal{G}$

EXERCISES

Problem 2.

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	1	-1	-1j	1j	$(x,y),(xz,yz),(J_x,J_y)$
	Γ_3	1	-1	1j	-1j	

(i) Consider the irreps of the group 4 and distribute them into orbits with respect to the group 422

Point Group Tables of $D_2(222)$

Character Table

$D_2(222)$	#	1	2_z	2_y	2_x	functions
A	Γ_1	1	1	1	1	x^2, y^2, z^2
B_1	Γ_3	1	1	-1	-1	z, xy, J_z
B_2	Γ_2	1	-1	1	-1	y, xz, J_y
B_3	Γ_4	1	-1	-1	1	x, yz, J_x

(ii) Consider the irreps of the group 222 and distribute them into orbits with respect to the group 422

SOLUTION

Problem 2(i).

Distribution of the irreps of *4* into orbits of conjugate irreps relative to *422*

- Coset decomposition of *422* relative to *4*
  $422 = 4 \cup 2_x\, 4$
- Conjugation of 4 under 2_x
  $2_x^{-1}\, 4_z\, 2_x = 4_z^{-1}; \qquad 2_x^{-1}\, 2_z\, 2_x = 2_z$
- irreps of *4* and their conjugates by 2_x

SOLUTION

Problem 2(i).

4	1	4_z	2_z	4_z^{-1}
Γ_1	1	1	1	1
Γ_2	1	-1	1	-1
Γ_3	1	i	-1	$-i$
Γ_4	1	$-i$	-1	i

4	1	4_z	2_z	4_z^{-1}
$(\Gamma_1)_{2_x}$	1	1	1	1
$(\Gamma_2)_{2_x}$	1	-1	1	-1
$(\Gamma_3)_{2_x}$	1	$-i$	-1	i
$(\Gamma_4)_{2_x}$	1	i	-1	$-i$

- Orbits of irreps of *4* relative to *422*
  - Γ_1 and Γ_2 - selfconjugate;
  - $\{\Gamma_3, \Gamma_4\}$ - orbit of conjugate irreps.

SOLUTION

Problem 2(ii).

Distribution of the irreps of *222* into orbits of conjugate irreps relative to *422*.

- coset decomposition
  $422 = 222 \cup 4_z\, 222$
- conjugation of *222* under 4_z
  $4_z^{-1}\, 2_x\, 4_z = 2_y$; $4_z^{-1}\, 2_y\, 4_z = 2_x$;
  $4_z^{-1}\, 2_z\, 4_z = 2_z$.
- irreps of *222* and their conjugates by 4_z

SOLUTION

Problem 2(ii).

222	1	2_x	2_y	2_z
Γ_1	1	1	1	1
Γ_2	1	1	−1	−1
Γ_3	1	−1	1	−1
Γ_4	1	−1	−1	1

222	1	2_x	2_y	2_z
$(\Gamma_1)_{4_z}$	1	1	1	1
$(\Gamma_2)_{4_z}$	1	−1	1	−1
$(\Gamma_3)_{4_z}$	1	1	−1	−1
$(\Gamma_4)_{4_z}$	1	−1	−1	1

.

- orbits of irreps of *222* under *422*

  $\{\Gamma_1\}$, $\{\Gamma_2, \Gamma_3\}$, $\{\Gamma_4\}$

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

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

EXERCISES

Problem 3.

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

$4mm$	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:
$m_y = m_{xz}$

Hint to Problem 3.

Step 1. Decompostion 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}

SOLUTION

Problem 3.

Example: Determine representations of 4mm induced from the irreps of m

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

$$4mm = \{1, m_{xz}\} \cup m_{yz}\{1, m_{xz}\} \cup 4_z\{1, m_{xz}\} \cup m_{x-x}\{1, m_{xz}\}$$

coset representatives $\{1, m_{yz}, 4_z, m_{x-x}\}$

SOLUTION

Problem 3.

Step 2. Construction of the induction matrix

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

$4mm$	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

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}
	4_z	4_z^{-1}	4_z^{-1}	4_z	1	M_{33}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	$m_{x\bar{x}}$	$m_{x\bar{x}}$	1	M_{44}

SOLUTION

Problem 3.

The induction matrix for the induction of reps of 4mm from irreps of {1,m_{xz}}

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}
	4_z	4_z^{-1}	4_z^{-1}	4_z	1	M_{33}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	$m_{x\bar{x}}$	$m_{x\bar{x}}$	1	M_{44}
m_{xz}	1	1	m_{xz}	1	m_{xz}	M_{11}
	m_{yz}	m_{yz}	2_z	m_{yz}	m_{xz}	M_{22}
	4_z	4_z^{-1}	$m_{x\bar{x}}$	$m_{x\bar{x}}$	1	M_{34}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	4_z^{-1}	4_z	1	M_{43}
m_{yz}	1	1	m_{yz}	m_{yz}	1	M_{12}
	m_{yz}	m_{yz}	1	1	1	M_{21}
	4_z	4_z^{-1}	m_{xx}	4_z	m_{xz}	M_{33}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	4_z	$m_{x\bar{x}}$	m_{xz}	M_{44}
4_z	1	1	4_z	$m_{x\bar{x}}$	m_{xz}	M_{14}
	m_{yz}	m_{yz}	m_{xx}	4_z	m_{xz}	M_{23}
	4_z	4_z^{-1}	1	1	1	M_{31}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	m_{yz}	m_{yz}	1	M_{42}
$m_{x\bar{x}}$	1	1	$m_{x\bar{x}}$	$m_{x\bar{x}}$	1	M_{14}
	m_{yz}	m_{yz}	4_z^{-1}	4_z	1	M_{23}
	4_z	4_z^{-1}	m_{yz}	m_{yz}	1	M_{32}
	$m_{x\bar{x}}$	$m_{x\bar{x}}$	1	1	1	M_{41}

SOLUTION

Problem 3.

Matrices of the induced representation for some of the elements of 4mm

$$\mathbf{D}_i^{Ind}(1) = \begin{pmatrix} D^{(i)}(1) & 0 & 0 & 0 \\ 0 & D^{(i)}(1) & 0 & 0 \\ 0 & 0 & D^{(i)}(1) & 0 \\ 0 & 0 & 0 & D^{(i)}(1) \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(m_{xz}) = \begin{pmatrix} D^{(i)}(m_{xz}) & 0 & 0 & 0 \\ 0 & D^{(i)}(m_{xz}) & 0 & 0 \\ 0 & 0 & 0 & D^{(i)}(1) \\ 0 & 0 & D^{(i)}(1) & 0 \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(m_{yz}) = \begin{pmatrix} 0 & D^{(i)}(1) & 0 & 0 \\ D^{(i)}(1) & 0 & 0 & 0 \\ 0 & 0 & D^{(i)}(m_{xz}) & 0 \\ 0 & 0 & 0 & D^{(i)}(m_{xz}) \end{pmatrix};$$

$$\mathbf{D}_i^{Ind}(4_z) = \begin{pmatrix} 0 & 0 & 0 & D^{(i)}(m_{xz}) \\ 0 & 0 & D^{(i)}(m_{xz}) & 0 \\ D^{(i)}(1) & 0 & 0 & 0 \\ 0 & D^{(i)}(1) & 0 & 0 \end{pmatrix};$$

LITTLE GROUP AND LITTLE-GROUP REPRESENTATIONS

LITTLE GROUP $\mathcal{G}^s$:

Group-normal subgroup pair $\mathcal{G} \triangleright \mathcal{H}$; Irrep $\mathbf{D}^s(\mathcal{H})$

$\mathcal{G}^s \equiv \mathcal{G}^s(\mathbf{D}^s(\mathcal{H})) = \{g \in \mathcal{G} : (\mathbf{D}^s(\mathcal{H}))_g \sim \mathbf{D}^s(\mathcal{H})\}$

$\mathcal{G} > \mathcal{G}^s \triangleright \mathcal{H}.$

ALLOWED IRREP OF THE LITTLE GROUP:

$\mathbf{D}^j(\mathcal{G}^s(\mathbf{D}^s(\mathcal{H}))) \downarrow \mathcal{H} \ni \mathbf{D}^s(\mathcal{H})$

INDUCTION THEOREM

1. Let $\mathbf{D}^j(\mathcal{H})$ be an irrep from the orbit $O(\mathbf{D}^j(\mathcal{H}))$ with the little group $\mathcal{G}^j(\mathbf{D}^j(\mathcal{H}))$ relative to $\mathcal{G}$. Then each allowed irrep $\mathbf{D}^m(\mathcal{G}^j(\mathbf{D}^j(\mathcal{H})))$ of $\mathcal{G}^j(\mathbf{D}^j(\mathcal{H}))$ induces an irrep $\mathbf{D}^{Ind}(\mathcal{G})$, whose subduction to $\mathcal{H}$ yields the orbit $O(\mathbf{D}^j(\mathcal{H}))$.

2. All irreps of $\mathcal{G}$ are obtained exactly once if the procedure described in 1 is applied on one irrep $\mathbf{D}^j(\mathcal{H})$ from each orbit $O(\mathbf{D}^j(\mathcal{H}))$ of irreps of $\mathcal{H}$ relative to $\mathcal{G}$.

ADDITIONAL

Point Group Tables of $D_4(422)$

Character Table

$D_4(422)$	#	1	2	4	2_h	$2_{h'}$	functions
Mult.	-	1	1	2	2	2	·
A_1	Γ_1	1	1	1	1	1	x^2+y^2,z^2
A_2	Γ_3	1	1	1	-1	-1	z,J_z
B_1	Γ_2	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	$(x,y),(xz,yz),(J_x,J_y)$

Multiplication Table

$D_4(422)$	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	·	·	·	·	$A_1+A_2+B_1+B_2$

The k-vector Types of Group 99 [*P4mm*]

(Table for arithmetic crystal class 4mmP)

(P4mm-C_{4v}^1 (99) to P4_2bc-C_{4v}^8 (106))

Reciprocal-space group (P4mm)*, No. 99

Brillouin zone

k-vector label		Wyckoff position			Parameters
CDML		ITA			ITA
GM	0,0,0	1	a	4mm	0,0,z: z=0
Z	0,0,1/2	1	a	4mm	0,0,z: z=1/2
LD	0,0,u	1	a	4mm	0,0,z: 0<z<1/2
LE	0,0,-u	1	a	4mm	0,0,-z: 0<z<1/2
LE + SM + LD + Z					
[Z$_1$Z]		1	a	4mm	o,o,z: -1/2<z<=1/2
M	1/2,1/2,0	1	b	4mm	1/2,1/2,z:z=0
A	1/2,1/2,1/2	1	b	4mm	1/2,1/2,z:z=1/2
V	1/2,1/2,u	1	b	4mm	1/2,1/2,z: 0<z<1/2
VA	1/2,1/2,-u	1	b	4mm	1/2,1/2,-z: 0<z<1/2
VA + M + V + A					
[A$_1$A]		1	b	4mm	0,1/2,z: -1/2<z<=1/2
X	0,1/2,0	2	c	2mm.	0,1/2,z:z=0
R	0,1/2,1/2	2	c	2mm.	0,1/2,z: z=1/2
W	0,1/2,u	2	c	2mm.	0,1/2,z: 0<z<1/2
WA	0,1/2,-u	2	c	2mm.	0,1/2,-z: 0<z<1/2
WA + X + W + R					
[R$_2$R]		2	c	2mm.	0,1/2,z: -1/2<z<=1/2

SM	u,u,0	4	d	..m	x,x,z: 0=z<x<1/2
S	u,u,1/2	4	d	..m	x,x,z: 0<x<z=1/2
C	u,u,v	4	d	..m	x,x,z: 0<x,z<1/2
CA	u,u,-v	4	d	..m	x,x,-z: 0<x,z<1/2
CA + SM + C + S					
[ZZ$_1$A$_1$A]		4	d	..m	x,x,z: 0<x<1/2, -1/2<z<=1/2
DT	0,u,0	4	e	.m.	0,y,z: 0=z<y<1/2
U	0,u,1/2	4	e	.m.	0,y,z: 0<y<z=1/2
B	0,u,v	4	e	.m.	0,y,z: 0<y,z<1/2
BA	0,u,-v	4	e	.m.	0,y,-z: 0<y,z<1/2
BA + DT + B + U					
[ZZ$_1$R$_2$R]		4	e	.m.	x,x,z: 0<x<1/2, -1/2<z<=1/2
Y	u,1/2,0	4	f	.m.	x,1/2,z: 0=z<x<1/2
T	u,1/2,1/2	4	f	.m.	x,1/2,z: 0<x<z=1/2
F	u,1/2,v	4	f	.m.	x,1/2,z: 0<x,z<1/2
FA	u,1/2,-v	4	f	.m.	x,1/2,-z: 0<x,z<1/2
FA + Y + F + T					
[AA$_1$R$_2$R]		4	f	.m.	x,1/2,z: 0<x<1/2, -1/2<z<=1/2
GP	u,v,w	8	g	1	x,y,z: -1/2<x<y<1/2, -1/2<z<=1/2.