Lecture Course
GROUP THEORY AND TOPOLOGY

Donostia - San Sebastian

23-26 August 2018

ikerbasque
Basque Foundation for Science

UPV EHU

EUSKO JAURLARITZA
GOBIERNO VASCO

REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

FURTHER DEVELOPMENTS

Bradley & Cracknell. The Mathematical Theory of Symmetry in Solids (1972)

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

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

EXERCISE 3.1

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:

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

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, $\det X\neq 0$.

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

$\dim D_1(G)=d$

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

Characters of Representations
Basic results

character properties

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

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

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

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

orthogonality

rows

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

columns

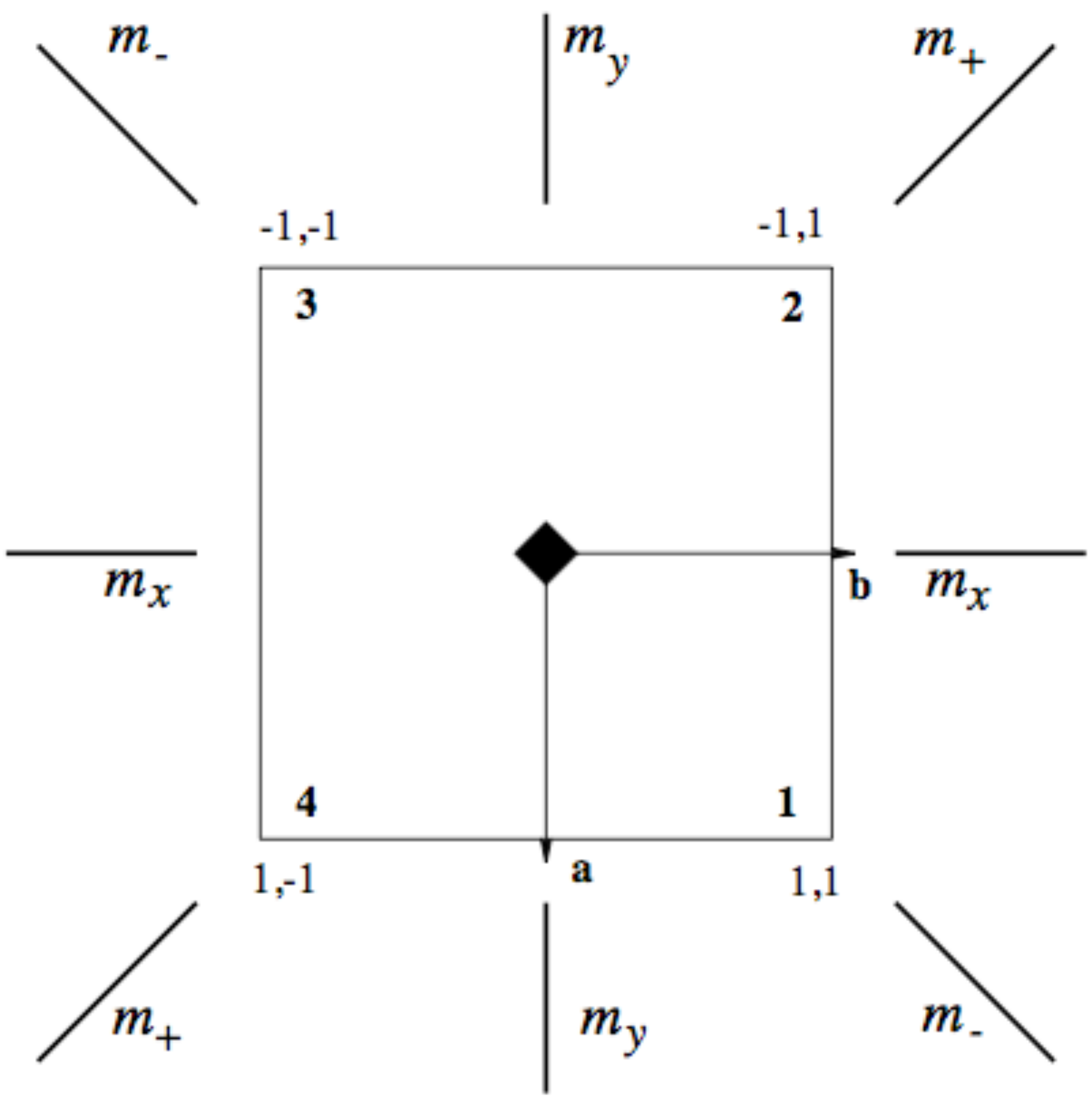
$$\frac{1}{|G|} \sum_{p} \eta_p^*(C_j)\, \eta_p(C_k)\, |C_j| = \delta_{jk}$$

$D_2(222)$	#	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 3.2

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 $4mm$

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

$$\begin{array}{ccccc} G_1 & & G_2 & \longrightarrow & G_1 \otimes G_2 \\ \downarrow & & \downarrow & & \downarrow \\ D_1 & & D_2 & & D_1 \otimes D_2 \end{array}$$

Kronecker product

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

Direct-product (Kronecker) product of matrices

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

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

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

dim (A ⊗ B) = dim(A) . dim(B)

tr(A ⊗ B)= tr(A). tr(B)

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

EXERCISE 3.3

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

A $\{a, a^2, \dots, a^s\}$

B $\{b, b^2, \dots, b^r\}$

A × B $\{(a^m, b^n)\}$ $m=1,\dots,s;$ $n=1,\dots,r$

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

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

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

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

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

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

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

Direct product of representations

$D_1(G)$: irrep of G

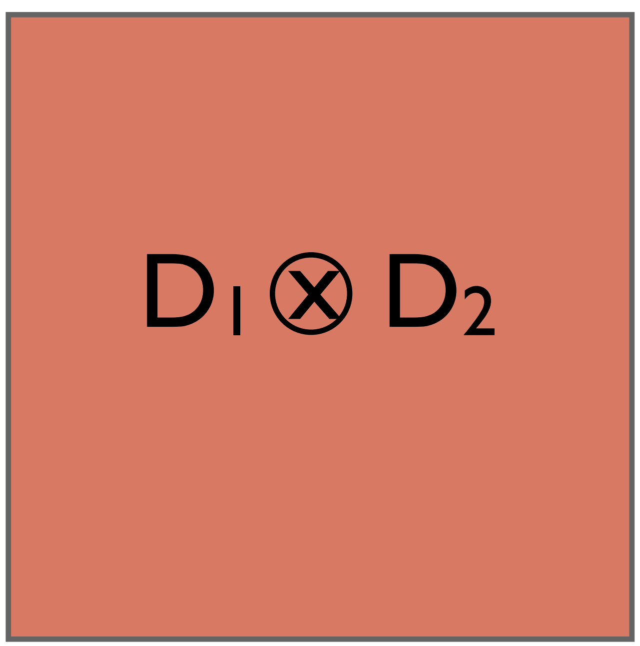
$\{D_1(e), D_1(g_2), \ldots, D_1(g_n)\}$

$D_2(G)$: irrep of G

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

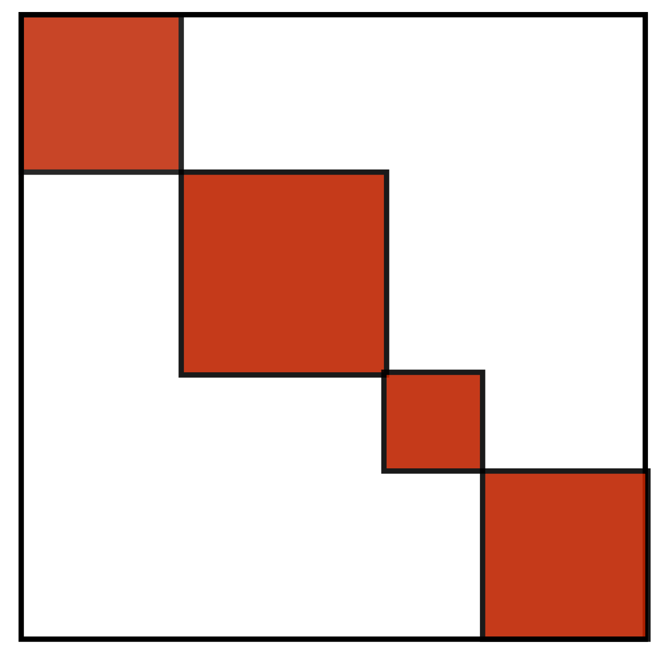
Direct-product representation

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



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

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

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

EXERCISES

Problem 3.5

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 direct-product representation $\mathbf{E} \otimes \mathbf{E}$ reducible or irreducible?

2. If reducible, find its decomposition into irreps of *4mm.*

3. If the functions ($\mathbf{f}_x$, $\mathbf{f}_y$) form the basis of **E**, can you guess if it would be possible to construct invariants from the functions of the product carrier space $\{\mathbf{f_x^2}, \mathbf{f}_1\mathbf{f_2}, \mathbf{f_2}\mathbf{f}_1, \mathbf{f_y^2}\}$?

4. If possible, how many invariants can be constructed, and what are the corresponding linear combinations of $\mathbf{f_i f_j}$?

EXERCISES

Problem 3.5

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

Click here to get more detailed information on the symmetry operations

Character Table of the group C_{4v}(4mm) *

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

Irreducibility criterion + magic formula

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

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

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

Clebsch-Gordan coefficients

$$S^{-1}(D_1 \otimes D_2)S = \bigoplus m_i D_i(G)$$

the matrices of the so-called Clebsch-Gordan coefficients

determine the linear combinations of products of basis functions that transform according to irreps

Problem 3.5

SOLUTION

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

$$B_1 \otimes B_2 \sim A_2$$

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

INVARIANTS? HOW MANY?

Problem 3.5

SOLUTION

Clebsch-Gordan coefficients

$$S^{-1}(D_1 \otimes D_2)S = \bigoplus m_i D_i(G)$$

$$(D_1 \otimes D_2)S = S \bigoplus m_i D_i(G)$$

Calculation of invariants

$$(D_1 \otimes D_2)S^1 = S^1 \bigoplus m_i D_i(G)$$

S^1: the column(s) of S corresponding to the identity irrep

$$(E \otimes E)(g) \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} \boxed{1} \longrightarrow S^1 = \begin{pmatrix} a \\ 0 \\ 0 \\ a \end{pmatrix}$$

sufficiently to solve for the generators $\mathbf{g} = 4^+, m_x$:

invariant $\sim$ $\mathbf{f_x^2 + f_y^2}$

REPRESENTATIONS OF DOUBLE GROUPS

Double Groups Representations

Bete (1929)
Opechowski (1940)

Definition (Opechowski, 1940):

The double group $^d\mathbf{G}$ of a group $\mathbf{G}$ of order $|\mathbf{G}|$ (which is a subgroup of the 3-dim rotational group $\mathbf{O}(3)$), is an abstract group of order $2|\mathbf{G}|$ having the same group-multiplication table as the $2|\mathbf{G}|$ matrices of $\mathbf{SU}(2)$ which correspond to the elements of $\mathbf{G}$.

$$^d\mathbf{G} = \mathbf{G} + \bar{E}\mathbf{G} = \{R\} + \{\bar{R}\}$$

$\underline{\mathbf{G}} = \{R\} < O(3)$

$\bar{E}$ rotation of 2π $\quad \bar{E}R = \bar{R}$

number and dimensions of irreps

number of irreps = number of conjugacy classes

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

great orthogonality theorem $\quad \sum D_1(g)^*_{jk} D_2(g)_{st} = \frac{|G|}{d}\,\delta_{12}\delta_{js}\delta_{kt}$

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

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

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

orthogonality

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

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

Double Groups Representations

Theorem 1 (Opechowski, 1940):

Each representation of a group **G** is also a representation of the double group ^{d}**G** where $\eta(\overline{E}g)=+\eta(g)$; it is called a single-valued representation of **G.**

Theorem 2 (Opechowski, 1940):

The rest of the representations of the double group ^{d}**G** are called double-valued representation of **G** and are such that $\eta(\overline{E}g)=-\eta(g)$.

notation of double-valued irreps:

Bethe: Γ_k, Γ_{k+1},…
Mulliken-Herzberg: $\overline{E}_k$, $\overline{F}_k$, $\overline{G}_k$…
[2], [4], [6]

Example Irreps of the group $^{d}222$

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

$^{d}222$	D_2	1	$2_z,\overline{2}_z$	$2_y,\overline{2}_y$	$2_x,\overline{2}_x$	$\overline{E}$
A	Γ_1	1	1	1	1	1
B_1	Γ_2	1	1	-1	-1	1
B_2	Γ_3	1	-1	1	-1	1
B_3	Γ_4	1	-1	-1	1	1
$\overline{E}$	Γ_5	2	0	0	0	-2

Note on terminology

We can either talk about single-valued and double-valued representations of a point or space group G or alternatively one can simply talk about the representations of the double point (or space) group ^dG.

In the second case they are ordinary single-valued irreducible representations of ^dG for which are valid all basic properties and results.

Bradley & Cracknell, 1972

EXERCISE 3.4

Determine the character table of the double group $^{d}422$ starting from the character table of the group 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

Hints:

Distribute the elements of $^{d}422$ into conjugacy classes

Determine the number and dimensions of the irreps of $^{d}422$?

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

Classes of conjugate elements

Double Groups

OPECHOWSKI RULES

To each class of G → one or two classes of ${}^{d}G$

self-conjugated operations

$$\{E\},\ \{\bar{E}\},\ \{\bar{1}\},\{\bar{1}\bar{E}\}$$

$$\{C_n\},\ \{\bar{C}_n\} \text{ iff, } n \neq 2$$

$$\{C_2(n),\ \bar{C}_2(n)\} \text{ iff } \exists\ C_2(n') \text{ or } m(n') \text{ with } n \perp n'$$

$$\{m(n),\ \bar{m}(n)\} \text{ iff } \exists\ C_2(n') \text{ or } m(n') \text{ with } n \perp n'$$

$$\{\bar{C}_n^k,\ \bar{C}_n^{k-1}\} \text{ iff } \{C_n^k,\ C_n^{k-1})\},\ n > 2$$

Symbols of 'double-group' symmetry operations

$$\boxed{\begin{aligned}\bar{E} &= {}^{d}1\\ \bar{R} &= {}^{d}1R = {}^{d}R\end{aligned}}$$

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

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

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

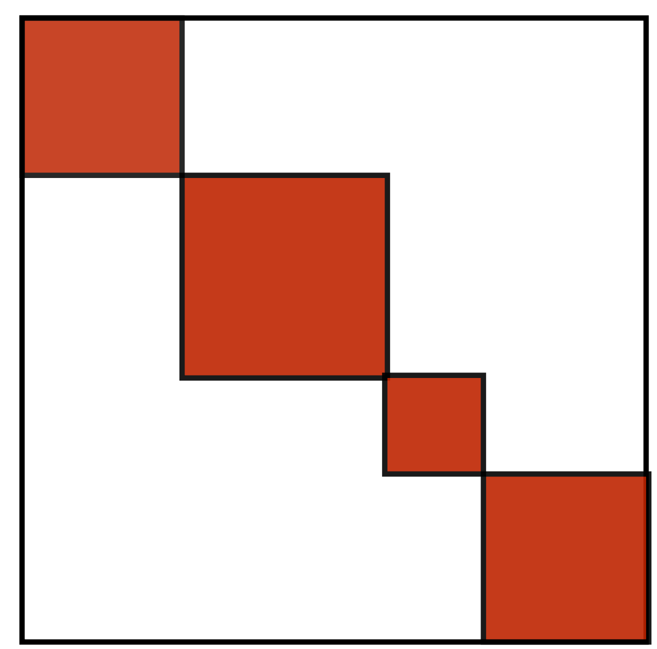
$\{D(G)\downarrow H\}$: subduced rep of H<G

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

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

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

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

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 3.5

Let $\mathbf{E}$ 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 $\mathbf{S}$, 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 3.5

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

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

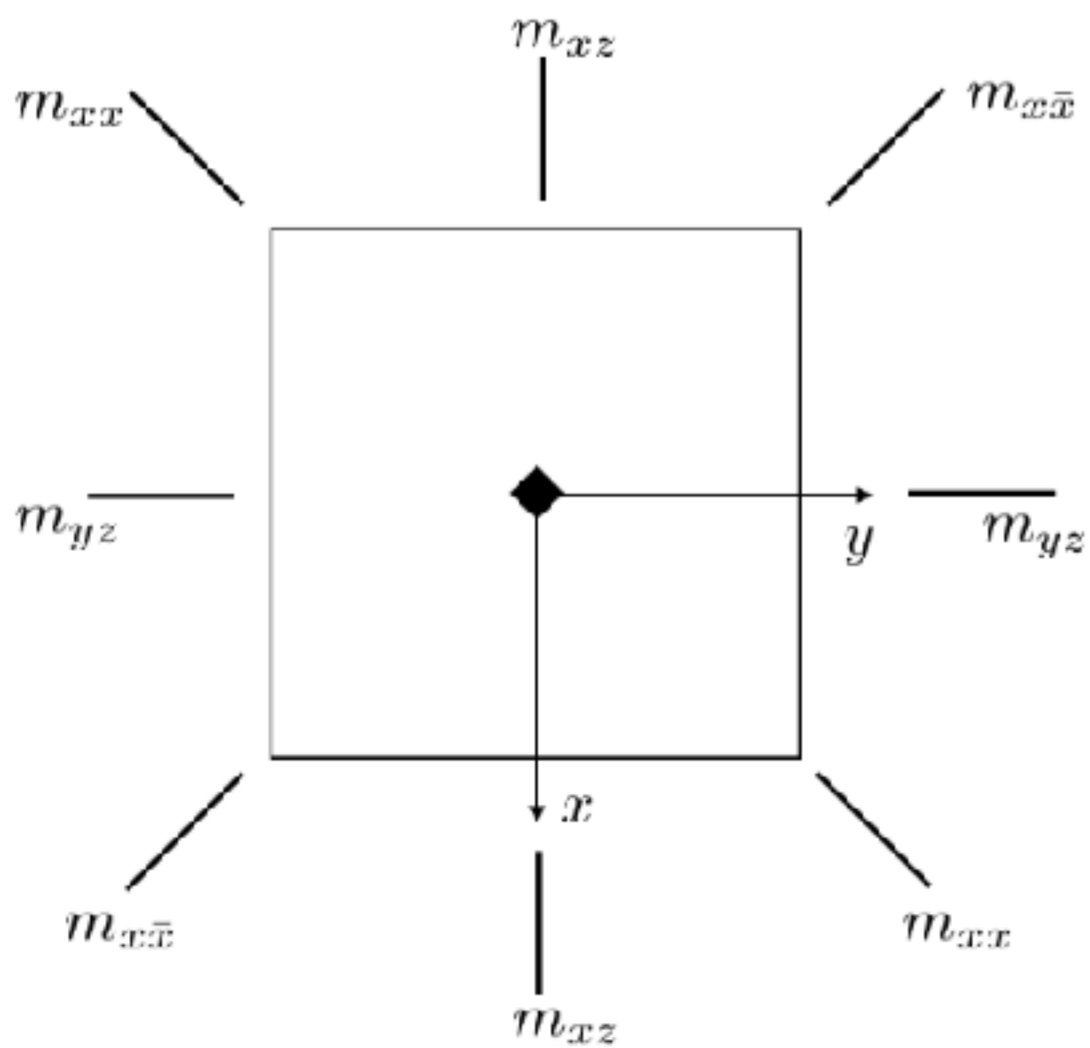
EXERCISES

Problem 3.6

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

Problem 3.7

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



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:

$m_{01} = m_{xz}$ $m_{10} = m_{yz}$

$m_{1\text{-}1} = m_{xx}$ $m_{11} = m_{x\text{-}x}$

Hint to Problem 3.7

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}

REPRESENTATIONS OF A GROUP IN TERMS OF THE IRREPS OF AN INVARIANT SUBGROUP

Conjugate representations

conjugate representation $G \triangleright H$:

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

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

conjugate irrep

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

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

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

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 $g \in \mathcal{G}$

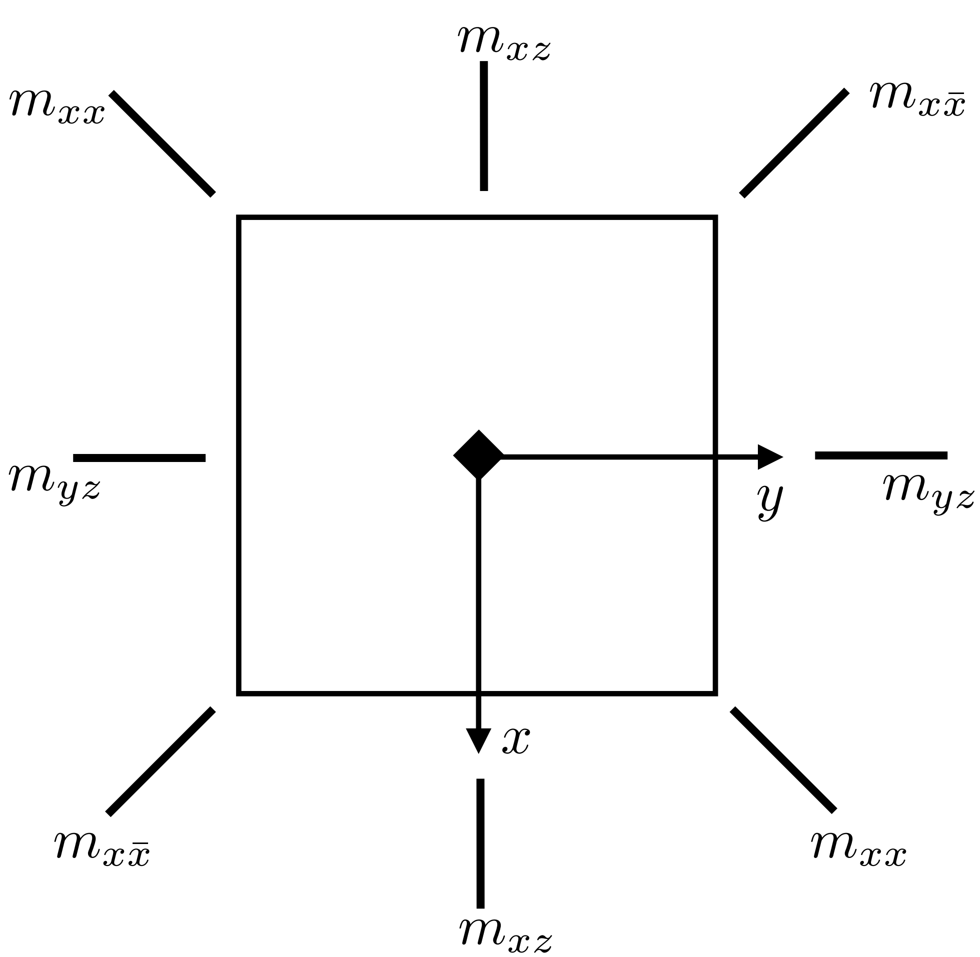
EXERCISES

Problem 3.8

Consider the irreps of the group 4 and distribute them into orbits with respect to the group 4mm

Irreps of 4

4	1	4_z	2_z	4_z^{-1}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	i	-1	$-i$
$\mathbf{D}^{(4)}$	1	$-i$	-1	i



Multiplication table of **4mm**

$4mm$	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_{xx}
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_{xx}	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_{xx}	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

EXERCISES

Problem 3.9

Consider the irreps of the group 222 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

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:

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

NOTE: terminology

allowed irrep or ***allowable*** irrep or ***small*** irrep

EXERCISES

Problem 3.8 (cont)

Consider the group-subgroup pair

$$4mm \triangleright 4$$

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

Determine the little groups and the corresponding allowed irreps for all irreps of the group 4

EXERCISES

Problem 3.9 (cont)

Consider the group-subgroup pair

$$422 \vartriangleright 222$$

Point Group Tables of $D_4(422)$

Character Table of the group $D_4(422)$ *

$D_4(422)$	#	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_2	1	1	1	-1	-1	z,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 $D_2(222)$

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

Determine the little groups and the corresponding allowed irreps for all irreps of the group 222.

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 $\mathcal{G}$.

Procedure for the construction of Irreducible Representations

Method: Construct the irreps of the space group G starting from the irreps of one of its normal subgroups $H \lhd G$

1. Construct all irreps of H
2. Distribute the irreps of H into orbits under G and select a representative
3. Determine the little group for each representative
4. Find the small (allowed) irreps of the little group
5. Construct the irreps of G by induction from the the small (allowed) irreps of the little group

Special cases: Subgroups of index 2

$G \trianglerighteq H$: $|G|/|H|=2$ $G=H \cup qH$, $q\notin H$, $q\in G$

I. Orbits of $D^s(H)$ with respect to G

(i) $O(D^s(H))=\{D^s(H), D^s(H)_q \neq D^s(H)\}$

(ii) $O(D^s(H))=\{D^s(H)\}$

II. Little group and allowed irreps

(i) $O(D^s(H))=\{D^s(H), D^s(H)_q\}$

$L=H$, $D^s(H)$: allowed

(ii) $O(D^s(H))=\{D^s(H)\}$

$L=G$, $D(G)\downarrow H \ni D^s(H)$: allowed

III. Induction procedure: G=H ∪ qH

(i) $O(D^s(H))=\{D^s(H), D^s(H)_q\}$

Induction matrix

g	g_i	$g_i^{-1} g$	g_j	$g_i^{-1} g\, g_j$	$M_{ij} \neq 0$
h	e	h	e	$e\, h\, e = h$	M_{11}
	q	$q^{-1} h$	q	$q^{-1} h\, q = (h)_q$	M_{22}
q	e	q	q	q^2	M_{12}
	q	$q^{-1} q = e$	e	e	M_{21}

Matrices of the induced irrep

$$\mathbf{D}^{Ind}(h) = \begin{pmatrix} \boldsymbol{D}^{(s)}(h) & \boldsymbol{O} \\ \boldsymbol{O} & (\boldsymbol{D}^{(s)}(h))_q \end{pmatrix} \qquad h \in H$$

$$\mathbf{D}^{Ind}(q) = \begin{pmatrix} \boldsymbol{O} & \boldsymbol{D}^{(s)}(q^2) \\ \boldsymbol{I} & \boldsymbol{O} \end{pmatrix} \qquad q \notin H,\ q \in G$$

III. Induction procedure: $G=H \cup qH$

$$
\begin{tikzcd}[row sep=small]
 & D^{Ind}_{+}(G) \\
D^{s}(H) \arrow[ur] \arrow[dr] & \\
 & D^{Ind}_{-}(G)
\end{tikzcd}
$$

$\dim D^{Ind}_{+}(G) = \dim D^{s}(H)$

$\dim D^{Ind}_{-}(G) = \dim D^{s}(H)$

$D^{Ind}_{+}(G)$	$D^{Ind}_{-}(G)$
$D^{Ind}_{+}(h)=D^{s}(h)$	$D^{Ind}_{-}(h)=D^{s}(h)$
$D^{Ind}_{+}(q)=U$	$D^{Ind}_{-}(q)=-U$

$$U^{-1}D^{s}(h)U=D^{s}(h)_{q}$$

$$U^{2}=D^{Ind}_{\pm}(q^{2})=D^{s}(h'),\ q^{2}=h'\in H$$

Induction procedure for normal subgroups of index 2 and 3

Start from the irreps $\mathbf{D}^s$ of a normal subgroup $\mathcal{H} \lhd \mathcal{G}$, where $|\mathcal{G}/\mathcal{H}| = 2$ or 3.

1. Characterize the group-subgroup chain $\mathcal{G} \rhd \mathcal{H}$ by

   (a) choice of appropriate generators for $\mathcal{H}$ and $\mathcal{G}$

   (b) decompose $\mathcal{G}$ into cosets relative to $\mathcal{H}$ with coset representative q: $q \in \mathcal{G}$ but $q \notin \mathcal{H}$

      i. $\mathcal{G} = \mathcal{H} \cup q\,\mathcal{H}$ for index 2

      ii. $\mathcal{G} = \mathcal{H} \cup q\,\mathcal{H} \cup q^2\,\mathcal{H}$ for index 3.

2. Determine the orbits of irreps of $\mathcal{H}$ relative to $\mathcal{G}$

- index 2:
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}) = (\mathbf{D}^s(\mathcal{H}))_q\}$ (self-conjugate)
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}), (\mathbf{D}^s(\mathcal{H}))_q\}$
- index 3:
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}) = (\mathbf{D}^s(\mathcal{H}))_q = (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$ (self-conjugate)
  - $O(\mathbf{D}^s(\mathcal{H})) = \{\mathbf{D}^s(\mathcal{H}), (\mathbf{D}^s(\mathcal{H}))_q, (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$

3. Construction of irreps of G

- index 2
  - $\{\mathbf{D}^s(\mathcal{H})\}$: selfconjugate irrep

$$\mathbf{D}^1(h) = \mathbf{D}^2(h) = \mathbf{D}^s(h), h \in \mathcal{H}$$

$$\mathbf{D}^1(q) = -\mathbf{D}^2(q) = \mathbf{U}$$

$\mathbf{U}$ is determined by the conditions

$$\mathbf{D}^s(q^{-1}\,h\,q) = \mathbf{U}^{-1}\,\mathbf{D}^s(h)\,\mathbf{U},\ \ h \in \mathcal{H};$$

$$\mathbf{U}^2 = \mathbf{D}^s(q^2)$$

-orbits of length 2

– $\{\mathbf{D}^s(\mathcal{H}),\ (\mathbf{D}^s(\mathcal{H}))q\}$

$$\mathbf{D}(h) = \begin{pmatrix} \mathbf{D}^s(h) & \mathbf{O} \\ \mathbf{O} & (\mathbf{D}^s(h))_q \end{pmatrix}$$

$$\mathbf{D}(q) = \begin{pmatrix} \mathbf{O} & \mathbf{D}^s(q^2) \\ \mathbf{I} & \mathbf{O} \end{pmatrix}$$

3. Construction of irreps of G

- index 3
  - $\{\mathbf{D}^s(\mathcal{H})\}$: selfconjugate irrep

$$\mathbf{D}^m(h) = \mathbf{D}^s(h),\ m = 1,\ 2,\ 3$$

$$\mathbf{D}^m(q) = \omega^m \mathbf{U}$$

$\mathbf{U}$ is determined by the conditions

$$\mathbf{D}^s(q^{-1}\,h\,q) = \mathbf{U}^{-1}\,\mathbf{D}^s(h)\,\mathbf{U},\ h \in \mathcal{H};$$

$$\omega^3 \mathbf{U}^3 = \mathbf{D}^s(q^3)$$

-orbits of length 3

– $\{\mathbf{D}^s(\mathcal{H}),\ (\mathbf{D}^s(\mathcal{H}))_q,\ (\mathbf{D}^s(\mathcal{H}))_{q^2}\}$

$$\mathbf{D}(h) = \begin{pmatrix} \mathbf{D}^s(h) & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & (\mathbf{D}^s(h))_q & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & (\mathbf{D}^s(h))_{q^2} \end{pmatrix}$$

$$\mathbf{D}(q) = \begin{pmatrix} \mathbf{O} & \mathbf{O} & \mathbf{D}^s(q^3) \\ \mathbf{I} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{I} & \mathbf{O} \end{pmatrix} .$$

POINT-GROUP IRREPS BY INDUCTION PROCEDURE

Generation of point groups

Crystallographic groups are **solvable** groups

Composition series: $1 \triangleleft Z_2 \triangleleft Z_3 \triangleleft \ldots \triangleleft G$

index 2 or 3

Set of generators of a group is a set of group elements such that each element of the group can be obtained as an ordered product of the generators

$$W = (g_h)^{k_h} * (g_{h-1})^{k_{h-1}} * \ldots * (g_2)^{k_2} * g_1$$

g_1 - identity

$g_2, g_3, \ldots$ - generate the rest of elements

Example

Generation of the group of the square

Composition series: $\boldsymbol{1} \overset{2_z}{\underset{[2]}{\triangleleft}} \boldsymbol{2} \overset{4_z}{\underset{[2]}{\triangleleft}} \boldsymbol{4} \overset{m_x}{\underset{[2]}{\triangleleft}} \boldsymbol{4mm}$

Step 1:

$\boldsymbol{1} = \{1\}$

Step 2:

$\boldsymbol{2} = \{1\} + 2_z \{1\}$

Step 3:

$\boldsymbol{4} = \{1,2\} + 4_z \{1,2\}$

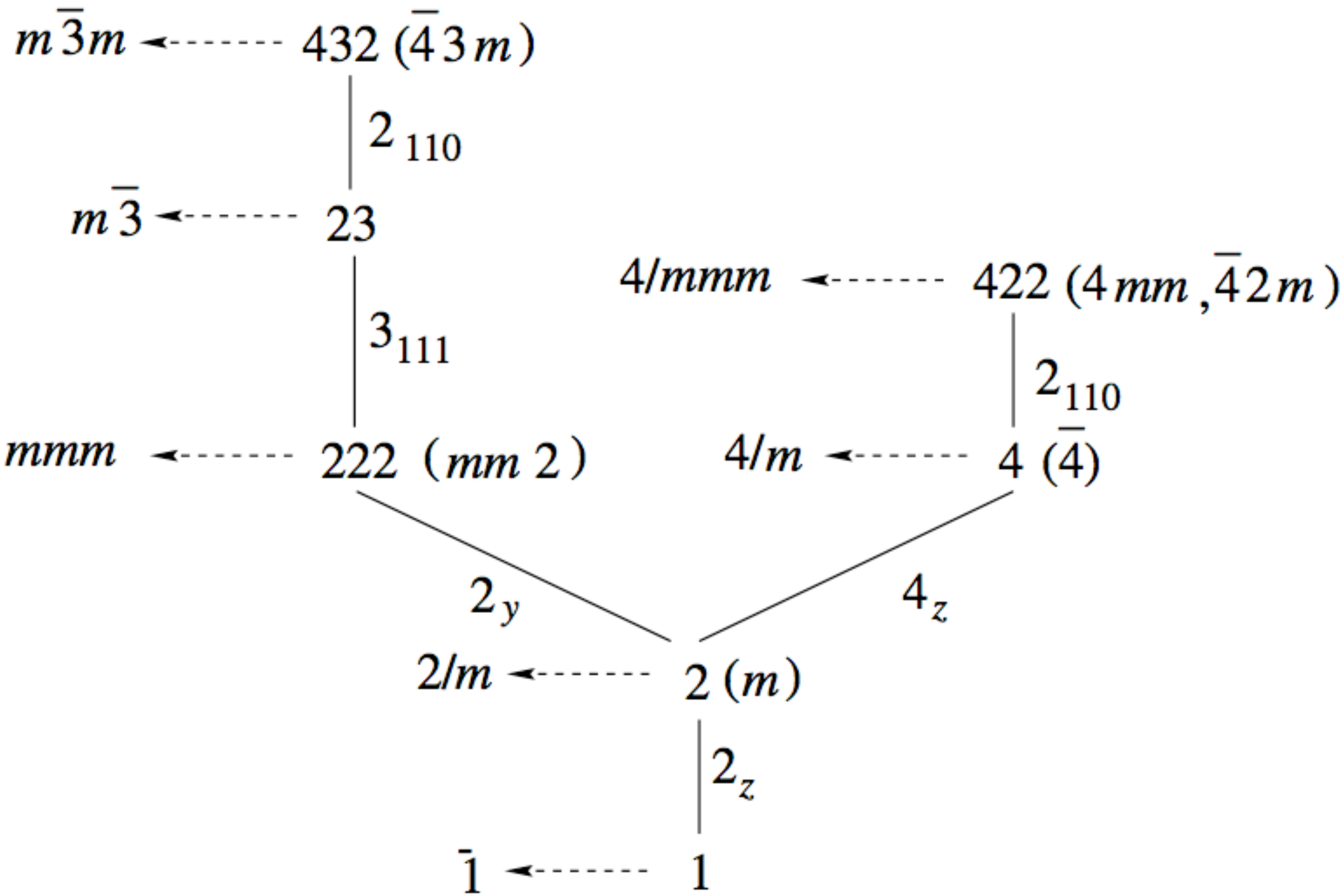
Step 4:

$\boldsymbol{4mm} = \boldsymbol{4} + m_x \boldsymbol{4}$

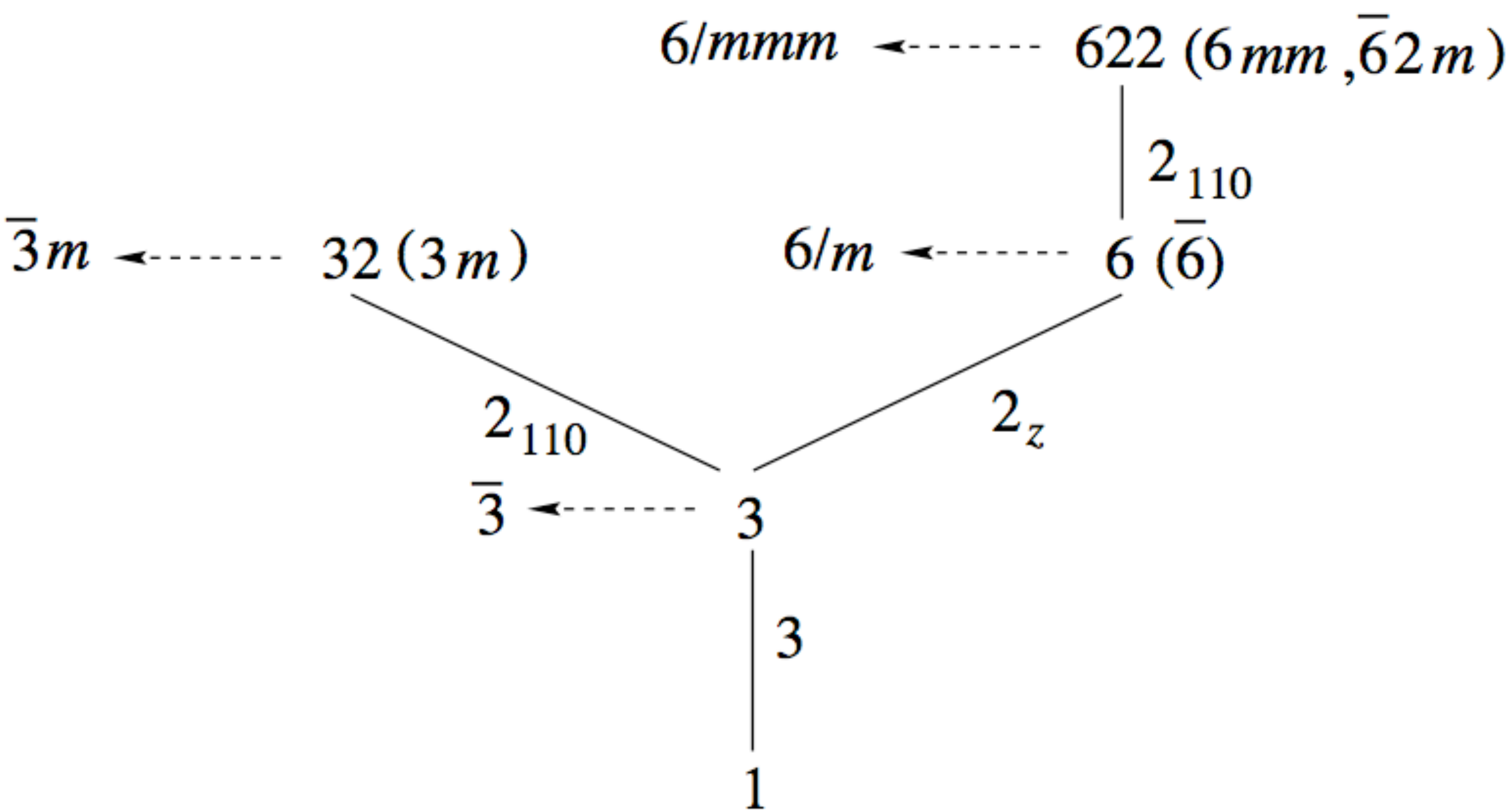
	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
1	1	2	4	4^{-1}	m_x	m_+	m_y	m_-
2	2	1	4^{-1}	4	m_y	m_-	m_x	m_+
4	4	4^{-1}	2	1	m_+	m_y	m_-	m_x
4^{-1}	4^{-1}	4	1	2	m_-	m_x	m_+	m_y.
m_x	m_x	m_y	m_-	m_+	1	4^{-1}	2	4
m_+	m_+	m_-	m_x	m_y	4	1	4^{-1}	2
m_y	m_y	m_x	m_+	m_-	2	4	1	4^{-1}
m_-	m_-	m_+	m_y	m_x	4^{-1}	2	4	1

Multiplication table of $4mm$

Generation of sub-cubic point groups



Generation of sub-hexagonal point groups



Problem 3.10

Generate the symmetry operations of the group *4/mmm* following its composition series.

Generate the symmetry operations of the group $\bar{3}m$ following its composition series.

Example: Determination of the irreps of the group $C_4(4)$

composition series for C_4: $C_4 \rhd C_2 \rhd C_1$

Irreps of C_2

Decomposition of $\mathcal{C}_2$ relative to $\mathcal{C}_1$:

$\mathcal{C}_2 = \mathcal{C}_1 \cup a\mathcal{C}_1$

-coset representative q is the element a.

Determination of the matrix $\mathbf{U}$:

1. $\mathbf{U}^{-1}\mathbf{A}(e)\mathbf{U} = \mathbf{1}$: self-conjugacy;

2. $\mathbf{U}^2 = \mathbf{A}(e) = 1$; $\mathbf{U} = \pm 1$.

The irreps of the group $\mathcal{C}_2$ are

$\mathcal{C}_2$	e	a
$\mathbf{D}_1$	1	1
$\mathbf{D}_2$	1	-1

Irreps of C_4: $C_4 = C_2 \cup aC_2$, $a = 4$

Multiplication table of C_4

C_4	e	a^2	a	a^3
e	e	a^2	a	a^3
a^2	a^2	e	a^3	a
a	a	a^3	a^2	e
a^3	a^3	a	e	a^2

C_4 is Abelian: $q^{-1}a^2q=a^2$

	e	a^2
A	1	1
B	1	-1

Irreps of C_2 (relative to C_4): selfconjugate

{**A**}, {**B**}

Construction of irreps of C_4

1. Irreps of the group $\mathcal{C}_4$, induced from the irrep **A**

   Matrix **U** for $\mathcal{O}(\mathbf{A})$:

   (a) $\mathbf{U}^{-1}\,\mathbf{A}(h)\,\mathbf{U} = \mathbf{A}(h)$, $h \in \mathcal{C}_2$: self-conjugacy

   (b) $\mathbf{U}^2 = \mathbf{D}(q^2) = \mathrm{a}^2 = +1$; $\mathbf{U} = \pm 1$.

   From the irrep **A** of $\mathcal{C}_2$ the irreps **A** and **B** of $\mathcal{C}_4$ have been induced.

$\mathcal{C}_4$	e	a^2	a	a^3
A	1	1	1	1
B	1	1	-1	-1

Construction of irreps of C_4

2. Irreps of $\mathcal{C}_4$, induced **B** of $\mathcal{C}_2$

Matrix **U** for $O(\mathbf{A})$:

(a) $\mathbf{U}^{-1}\,\mathbf{B}(h)\,\mathbf{U} = \mathbf{B}(h)$, $h \in \mathcal{C}_2$: self-conjugacy

(b) $\mathbf{U}^2 = \mathbf{B}(q^2) = \mathbf{B}(a^2) = -1$; $\mathbf{U} = \pm i$.

From the irrep **B** of $\mathcal{C}_2$ the irreps ${}^1\mathbf{E}$ and ${}^2\mathbf{E}$ of $\mathcal{C}_4$ are induced.

$\mathcal{C}_4$	e	a^2	a	a^3
${}^1\mathbf{E}$	1	-1	$-i$	i
${}^2\mathbf{E}$	1	-1	i	$-i$

EXERCISES

Problem 3.11

By the `induction procedure', derive the irreps of 4mm from those of group 4

Irreps of 4

4	1	4_z	2_z	4_z^{-1}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	i	-1	$-i$
$\mathbf{D}^{(4)}$	1	$-i$	-1	i

Multiplication table of **4mm**

$4mm$	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

EXERCISES

Problem 3.12

By the `induction procedure', derive: ;

(a) the irreps of the group $\bar{1} \otimes G$ from those of the group G;

(b) applying the results from (a) write down the irreps of 4/mmm starting from the irreps of 422

REALITY OF REPRESENTATIONS

Representations of Groups
Basic results

classification of irreps

type I or real irrep: if $D(G)$ is real

type II or pseudoreal: if $D(G) \sim D(G)^*$ but $D(G)$ is not real

type III or complex: if $D(G) \nsim D(G)^*$

irrep reality criterion

$$\frac{1}{|G|} \sum_g \eta_I(g^2) = \begin{cases} +1 & \text{type I or real} \\ -1 & \text{type II or pseudoreal} \\ 0 & \text{type III or complex} \end{cases}$$

Reality of representations induced from little groups

Consider the irrep $D^i(H)$ of the subgroup $H \lhd G$ with a little group G^i. The irrep $D^{Ind}(G)$ induced from a small irrep $D^m(G^i)$ of the little group G^i is of the first, second or third kind according to:

$$\frac{q_i}{h} \sum_{\alpha} \chi^i_m(r^2_\alpha) = 1, -1, 0$$

where the sum over α is restricted so that $D^i(H)_\alpha = D^i(H)^{-1}$

χ^i_m - the character of the small irrep $D^m(G^i)$

$h = |G|/|H|$ - the index of H in G

q_i - the order of the orbit of $D^i(H)$ in G

Example: 2dim irrep of 4mm

Step 1. Coset decomposition of *4mm* relative to *4*

$$4mm = 4 \cup m_{xz}\, 4$$

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

Step 2. Orbits of irreps

Conjugation of the elements of 4 under m_{xz}

$$m_{xz}^{-1}\, 4_z\, m_{xz} = 4_z^{-1}; \qquad m_{xz}^{-1}\, 2_z\, m_{xz} = 2_z$$

$$(\mathbf{D}^{(i)})_{m_{xz}}(4_z) = \mathbf{D}^{(i)}(4_z^{-1})$$

$$(\mathbf{D}^{(i)})_{m_{xz}}(2_z) = \mathbf{D}^{(i)}(2_z)$$

Irreps of *4*

4	1	4_z	2_z	4_z^{-1}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	i	-1	$-i$
$\mathbf{D}^{(4)}$	1	$-i$	-1	i

$\{\mathbf{D}^{(3)}, \mathbf{D}^{(4)}\}$ --- orbit of conjugate irreps

Example: 2dim irrep of 4mm

		E	4	2	4^{-1}
	D^3	1	-i	-1	i
	$(D^3)^{-1}$	1	i	-1	-i
r_α=E	$(D^3)_\alpha$	1	-i	-1	i
$r_\alpha=m_{xz}$	$(D^3)_\alpha$	1	i	-1	-i

$$\frac{q_i}{h}\chi^{D^3}(m_{xz}^2) = \frac{2}{2}\chi^{D^3}(E) = +1$$

the 2dim irrep of 4mm induced by D^3 of 4 is real