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Overview

Representations of space groups

- subduced and induced representations
- induction from normal subgroups
- special case of index 2 and 3
- representations of the translation subgroup
- Brillouin zone
- little group representations
- full-group representations of space groups

Subduced representations

Definition

A representation **D** of $\mathcal{G}$ can be regarded as a representation of a subgroup $\mathcal{H}$ of $\mathcal{G}$ by considering only the elements of $\mathcal{H}$. This restriction of **D** to $\mathcal{H}$ is called the subduced representation or subduction of $\mathcal{H}$ from $\mathcal{G}$.

The subduced representation is denoted by $\mathbf{D}(\mathcal{G}) \downarrow \mathcal{H}$, or simply by $\mathbf{D} \downarrow \mathcal{H}$ (if there is no doubt about $\mathcal{G}$).

Some properties of the subduction

- The degree of the subduction $\mathbf{D} \downarrow \mathcal{H}$ is equal to the degree of **D**.
- If **D** is reducible, then also the subduction $\mathbf{D} \downarrow \mathcal{H}$ is reducible.
- If **D** is 1-dimensional, then also the subduction $\mathbf{D} \downarrow \mathcal{H}$ is 1-dimensional and thus irreducible.

Decomposition into irreducibles

- In general, the subduction $\mathbf{D} \downarrow \mathcal{H}$ of an irrep $\mathbf{D}$ may be irreducible or not, the decomposition into irreps of $\mathcal{H}$ can be computed from the character $\chi \downarrow \mathcal{H}$ of $\mathbf{D} \downarrow \mathcal{H}$ by the magic formula.
- If $\chi^{(1)}, \ldots, \chi^{(s)}$ are the characters of the irreps $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(s)}$ of $\mathcal{H}$, then

$$\mathbf{D} \downarrow \mathcal{H} = m_1 \mathbf{D}^{(1)} \oplus \ldots \oplus m_s \mathbf{D}^{(s)} = \bigoplus_{i=1}^{s} m_i \mathbf{D}^{(i)} \quad \text{with}$$

$$m_i = (\chi \downarrow \mathcal{H}, \chi^{(i)})_{\mathcal{H}} = \frac{1}{|\mathcal{H}|} \sum_{h \in \mathcal{H}} \chi \downarrow \mathcal{H}(h)\, \chi^{(i)}(h)^*.$$

- Unless the multiplicities are large, they can often be read off easily from the character table of $\mathcal{H}$.

Example

Let **D** be the 2-dimensional irrep of $\mathcal{G} = 4mm$ given by

$$\mathbf{D}(4^+) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}(m_{10}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

Then the subduction of **D** to $\mathcal{H} = 4 = \langle 4^+ \rangle$ is given by

$$\mathbf{D} \downarrow \mathcal{H}(4^+) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

and this is equivalent to the direct sum $\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}$ for the 1-dimensional irreps

$$\mathbf{D}^{(1)}(4^+) = \big(i\big) \quad \text{and} \quad \mathbf{D}^{(2)}(4^+) = \big(-i\big)$$

of $\mathcal{H}$.

Exercise

Let **D** be the 2-dimensional irrep of $\mathcal{G} = 4mm$ given by

$$\mathbf{D}(4^+) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}(m_{10}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

and take $\mathcal{H} = \{1, 2, m_{10}, m_{01}\} = 2mm$ that has the character table

	1	2	m_{10}	m_{01}
$\chi^{(1)}$	1	1	1	1
$\chi^{(2)}$	1	-1	-1	1
$\chi^{(3)}$	1	1	-1	-1
$\chi^{(4)}$	1	-1	1	-1

Give the matrices $\mathbf{D} \downarrow \mathcal{H}(h)$ of the subduction $\mathbf{D} \downarrow \mathcal{H}$ of **D** to $\mathcal{H}$ and decompose $\mathbf{D} \downarrow \mathcal{H}$ into irreps of $2mm$.

Answer

The matrices are $\mathbf{D} \downarrow \mathcal{H}(1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\mathbf{D} \downarrow \mathcal{H}(2) = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$, $\mathbf{D} \downarrow \mathcal{H}(m_{10}) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$, $\mathbf{D} \downarrow \mathcal{H}(m_{01}) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, and since they are in diagonal form one can immediately see that $\mathbf{D} \downarrow \mathcal{H} = \mathbf{D}^{(2)} \oplus \mathbf{D}^{(4)}$.

Induced representations

Reversal of subduction

- Goal: construct a representation of a supergroup $\mathcal{G} \geq \mathcal{H}$ from a representation of $\mathcal{H}$.
- Idea: combine the known action of $\mathcal{H}$ on a vector space $\mathbb{V}$ with the permutation action of $\mathcal{G}$ on the cosets of $\mathcal{G}$ relative to $\mathcal{H}$.
- Let $\mathcal{G} = \mathcal{H} \cup g_2\mathcal{H} \cup \ldots \cup g_m\mathcal{H}$ be the coset decomposition of $\mathcal{G}$ relative to $\mathcal{H}$, with coset representatives $e, g_2, \ldots, g_m$.
- $\mathcal{G}$ permutes the cosets $g_i\mathcal{H}$ (by left multiplication), since $g(g_i\mathcal{H}) = (gg_i)\mathcal{H} = g_j\mathcal{H}$ for some j.
- For $gg_i\mathcal{H} = g_j\mathcal{H}$ we have $g_j^{-1}gg_i = h \in \mathcal{H}$, thus we know the matrix for $\mathbf{D}(g_j^{-1}gg_i)$.
- Define

$$\dot{\mathbf{D}}(x) = \begin{cases} \mathbf{D}(x) & \text{if } x \in \mathcal{H} \\ 0 & \text{if } x \notin \mathcal{H} \end{cases}$$

Definition

The representation $\mathbf{D} \uparrow \mathcal{G} = \mathbf{D}(\mathcal{H}) \uparrow \mathcal{G}$ given by

$$\mathbf{D} \uparrow \mathcal{G}(g) = \begin{pmatrix} \dot{\mathbf{D}}(g_1^{-1} g g_1) & \dot{\mathbf{D}}(g_1^{-1} g g_2) & \cdots & \dot{\mathbf{D}}(g_1^{-1} g g_m) \\ \dot{\mathbf{D}}(g_2^{-1} g g_1) & \dot{\mathbf{D}}(g_2^{-1} g g_2) & \cdots & \dot{\mathbf{D}}(g_2^{-1} g g_m) \\ \vdots & & \ddots & \vdots \\ \dot{\mathbf{D}}(g_m^{-1} g g_1) & \dot{\mathbf{D}}(g_m^{-1} g g_2) & \cdots & \dot{\mathbf{D}}(g_m^{-1} g g_m) \end{pmatrix}$$

is called the induced representation or induction from $\mathcal{H}$ to $\mathcal{G}$.

Some comfort

Every row and column of $\mathbf{D} \uparrow \mathcal{G}(g)$ contains precisely one block which is not zero, all other blocks are zero, a typical matrix of an induced representation will look like

$$\mathbf{D} \uparrow \mathcal{G}(g) = \left(\begin{array}{c|c|c} \mathbf{0} & \mathbf{D}(g_1^{-1} g g_2) & \mathbf{0} \\ \hline \mathbf{D}(g_2^{-1} g g_1) & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} & \mathbf{D}(g_3^{-1} g g_3) \end{array}\right)$$

Interpretation of the induction

- Let $\mathbf{v}_1, \dots, \mathbf{v}_n$ be a basis for the vector space $\mathbb{V}$ on which $\mathcal{H}$ acts by **D**.
- Make a new vector space $\mathbb{V} \uparrow \mathcal{G}$ of dimension mn with basis

$$\begin{aligned} g_1 \otimes \mathbf{v}_1, \dots, g_1 \otimes \mathbf{v}_n, &\quad g_2 \otimes \mathbf{v}_1, \dots, g_2 \otimes \mathbf{v}_n, \\ \dots, &\quad g_m \otimes \mathbf{v}_1, \dots, g_m \otimes \mathbf{v}_n \end{aligned}$$

- An element $g \in \mathcal{G}$ for which $gg_i\mathcal{H} = g_j\mathcal{H}$ and $g_j^{-1}gg_i = h$ maps the basis vector $g_i \otimes \mathbf{v}_k$ as follows:

$$g(g_i \otimes \mathbf{v}_k) = g_j \otimes \mathbf{D}(g_j^{-1}gg_i)\mathbf{v}_k = g_j \otimes \mathbf{D}(h)\mathbf{v}_k = \sum_{l=1}^{n} \mathbf{D}(h)_{lk}(g_j \otimes \mathbf{v}_l)$$

- Note that all basis vectors in the i-th block $g_i \otimes \mathbf{v}_1, \dots, g_i \otimes \mathbf{v}_n$ are mapped to linear combinations of basis vectors in the j-th block $g_j \otimes \mathbf{v}_1, \dots, g_j \otimes \mathbf{v}_n$.

Description by a permutation matrix

- Define an $m \times m$-matrix $\mathbf{M}(g)$ by

$$\mathbf{M}(g)_{ji} = \begin{cases} 1 & \text{if } g_j^{-1} g g_i \in \mathcal{H}, \\ 0 & \text{otherwise} \end{cases}$$

  then $\mathbf{M}$ permutes the basis vectors $\mathbf{e}_1, \ldots, \mathbf{e}_m$ in the same way as g permutes the cosets $g_1\mathcal{H}, \ldots, g_m\mathcal{H}$, i.e. $\mathbf{M}(g)$ describes the permutation action of $\mathcal{G}$ on the cosets of $\mathcal{G}$ relative to $\mathcal{H}$.
- With a slight abuse of notation, the induced representation can then be described as a Kronecker product

$$\mathbf{D} \uparrow \mathcal{G}(g) = \mathbf{M}(g) \otimes \mathbf{D}(\underline{h})$$

  where $\underline{h}$ is different in every column of the block matrix: in the i-th column, $\underline{h}$ is the element $\underline{h} = g_j^{-1} g g_i$ which lies in $\mathcal{H}$.

Example: Induction from $2mm$ to $4mm$

- Take $\mathcal{G} = \langle 4^+, m_{10} \rangle = 4mm$ and $\mathcal{H} = \langle 2, m_{10} \rangle = 2mm$, coset representatives: $g_1 = 1$, $g_2 = 4^+$
- It is sufficient to determine the induction on the generators 4^+ and m_{10}.
- $1^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{m_{10}}_{g_1^{-1} g g_1} \in \mathcal{H}, \quad (4^+)^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{4^+}_{g_2} = \underbrace{m_{01}}_{g_2^{-1} g g_2} \in \mathcal{H}$

  $\Rightarrow \mathbf{M}(m_{10}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\mathbf{D} \uparrow \mathcal{G}(m_{10}) = \begin{pmatrix} \mathbf{D}(m_{10}) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(m_{01}) \end{pmatrix}$
- $(4^+)^{-1} \cdot \underbrace{4^+}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{1}_{g_2^{-1} g g_1} \in \mathcal{H}, \quad 1^{-1} \cdot \underbrace{4^+}_{g} \cdot \underbrace{4^+}_{g_2} = \underbrace{2}_{g_1^{-1} g g_2} \in \mathcal{H}$

  $\Rightarrow \mathbf{M}(4^+) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\mathbf{D} \uparrow \mathcal{G}(4^+) = \begin{pmatrix} \mathbf{0} & \mathbf{D}(2) \\ \mathbf{D}(1) & \mathbf{0} \end{pmatrix}$

Example: Induction from $2mm$ to $4mm$ (ctd.)

Filling in the different irreps of $2mm$ gives the following results:

$2mm$	1	2	m_{10}	m_{01}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	-1	-1	1
$\mathbf{D}^{(3)}$	1	1	-1	-1
$\mathbf{D}^{(4)}$	1	-1	1	-1

$4mm$	1	2	4^+	m_{10}	m_{11}
$\chi^{(1)}$	1	1	1	1	1
$\chi^{(2)}$	1	1	1	-1	-1
$\chi^{(3)}$	1	1	-1	-1	1
$\chi^{(4)}$	1	1	-1	1	-1
$\chi^{(5)}$	2	-2	0	0	0

irrep of $\mathcal{H}$	$\mathbf{D} \uparrow \mathcal{G}(m_{10})$	$\mathbf{D} \uparrow \mathcal{G}(4^+)$	decomposition
$\mathbf{D}^{(1)}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(1)} + \chi^{(4)}$
$\mathbf{D}^{(2)}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(5)}$
$\mathbf{D}^{(3)}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(2)} + \chi^{(3)}$
$\mathbf{D}^{(4)}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(5)}$

Example: Induction from m to $3m$

- $\mathcal{G} = \langle 3^+, m_{10} \rangle$, $\mathcal{H} = \langle m_{10} \rangle$, coset representatives: 1, 3^+, 3^-
- $1^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{m_{10}}_{g_1^{-1} g g_1} \in \mathcal{H}, \quad (3^-)^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{3^+}_{g_2} = \underbrace{m_{10}}_{g_3^{-1} g g_2} \in \mathcal{H}$

  $(3^+)^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{3^-}_{g_3} = \underbrace{m_{10}}_{g_2^{-1} g g_3} \in \mathcal{H} \Rightarrow \mathbf{M}(m_{10}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$ and

  $$\mathbf{D} \uparrow \mathcal{G}(m_{10}) = \begin{pmatrix} \mathbf{D}(m_{10}) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}(m_{10}) \\ \mathbf{0} & \mathbf{D}(m_{10}) & \mathbf{0} \end{pmatrix}$$

- $(3^+)^{-1} \cdot \underbrace{3^+}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{1}_{g_2^{-1} g g_1} \in \mathcal{H}, \; (3^-)^{-1} \cdot \underbrace{3^+}_{g} \cdot \underbrace{3^+}_{g_2} = \underbrace{1}_{g_3^{-1} g g_2} \in \mathcal{H}$

  $1^{-1} \cdot \underbrace{3^+}_{g} \cdot \underbrace{3^-}_{g_2} = \underbrace{1}_{g_1^{-1} g g_3} \in \mathcal{H} \Rightarrow \mathbf{M}(3^+) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$ and

  $$\mathbf{D} \uparrow \mathcal{G}(3^+) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{D}(1) \\ \mathbf{D}(1) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(1) & \mathbf{0} \end{pmatrix}$$

Example: Induction from m to $3m$ (ctd.)

m	1	m_{10}
$\mathbf{D}^{(1)}$	1	1
$\mathbf{D}^{(2)}$	1	-1

$3m$	1	3^+	m_{10}
$\chi^{(1)}$	1	1	1
$\chi^{(2)}$	1	1	-1
$\chi^{(3)}$	2	-1	0

irrep of $\mathcal{H}$	$\mathbf{D}\uparrow\mathcal{G}(m_{10})$	$\mathbf{D}\uparrow\mathcal{G}(3^+)$	decomposition
$\mathbf{D}^{(1)}$	$\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\chi^{(1)}+\chi^{(3)}$
$\mathbf{D}^{(2)}$	$\begin{pmatrix}-1&0&0\\0&0&-1\\0&-1&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\chi^{(2)}+\chi^{(3)}$

Exercise: Induction from 4 to $4mm$

- Take $\mathcal{G} = \langle 4^+, m_{10} \rangle = 4mm$ and $\mathcal{H} = \langle 4^+ \rangle = 4$ and choose the coset representatives $g_1 = 1$, $g_2 = m_{10}$.
- Determine for the irreps **D** of $\mathcal{H}$ the induction **D** $\uparrow \mathcal{G}$ and decompose them into irreps of $4mm$.

  It is sufficient to determine **D** $\uparrow \mathcal{G}$ on the generators 4^+ and m_{10}.
- The character tables of 4 and $4mm$ are as follows:

4	1	4^+	2	4^-
$\mathbf{D}^{(0)}$	1	1	1	1
$\mathbf{D}^{(1)}$	1	i	-1	$-i$
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	$-i$	-1	i

$4mm$	1	2	4^+	m_{10}	m_{11}
$\chi^{(1)}$	1	1	1	1	1
$\chi^{(2)}$	1	1	1	-1	-1
$\chi^{(3)}$	1	1	-1	-1	1
$\chi^{(4)}$	1	1	-1	1	-1
$\chi^{(5)}$	2	-2	0	0	0

Answer

- $1^{-1} \cdot \underbrace{4^+}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{4^+}_{g_1^{-1} g g_1} \in \mathcal{H}, \quad m_{10}^{-1} \cdot \underbrace{4^+}_{g} \cdot \underbrace{m_{10}}_{g_2} = \underbrace{4^-}_{g_2^{-1} g g_2} \in \mathcal{H}$

  $\Rightarrow \mathbf{M}(4^+) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $\mathbf{D} \uparrow \mathcal{G}(4^+) = \begin{pmatrix} \mathbf{D}(4^+) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(4^-) \end{pmatrix}$

- $m_{10}^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{1}_{g_1} = \underbrace{1}_{g_2^{-1} g g_1} \in \mathcal{H}, \quad 1^{-1} \cdot \underbrace{m_{10}}_{g} \cdot \underbrace{m_{10}}_{g_2} = \underbrace{1}_{g_1^{-1} g g_2} \in \mathcal{H}$

  $\Rightarrow \mathbf{M}(m_{10}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\mathbf{D} \uparrow \mathcal{G}(m_{10}) = \begin{pmatrix} \mathbf{0} & \mathbf{D}(1) \\ \mathbf{D}(1) & \mathbf{0} \end{pmatrix}$

irrep of $\mathcal{H}$	$\mathbf{D} \uparrow \mathcal{G}(4^+)$	$\mathbf{D} \uparrow \mathcal{G}(m_{10})$	decomposition
$\mathbf{D}^{(0)}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(1)} + \chi^{(2)}$
$\mathbf{D}^{(1)}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(5)}$
$\mathbf{D}^{(2)}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(3)} + \chi^{(4)}$
$\mathbf{D}^{(3)}$	$\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\chi^{(5)}$

Induced character

- If χ is the character of **D**, the character $\chi \uparrow \mathcal{G}$ of **D** $\uparrow \mathcal{G}$, called the induced character, is equal to

$$\chi \uparrow \mathcal{G}(g) = \sum_{i=1}^{m} \dot{\chi}(g_i^{-1} g g_i) \quad \text{where} \quad \dot{\chi}(x) = \begin{cases} \chi(x) & \text{if } x \in \mathcal{H}, \\ 0 & \text{otherwise.} \end{cases}$$

- The induced character $\chi \uparrow \mathcal{G}$ can also be written as

$$\chi \uparrow \mathcal{G}(g) = \frac{1}{|H|} \sum_{x \in \mathcal{G}} \dot{\chi}(x^{-1} g x)$$

Decomposition into irreducibles

- In general, the induction $\mathbf{D} \uparrow \mathcal{G}$ of an irrep $\mathbf{D}$ of $\mathcal{H}$ may be irreducible or not, the decomposition into irreps of $\mathcal{G}$ can be computed from the character $\chi \uparrow \mathcal{G}$ of $\mathbf{D} \uparrow \mathcal{G}$ by the magic formula.
- If $\chi^{(1)}, \ldots, \chi^{(r)}$ are the characters of the irreps $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ of $\mathcal{G}$, then

$$\mathbf{D} \uparrow \mathcal{G} = m_1 \mathbf{D}^{(1)} \oplus \ldots \oplus m_r \mathbf{D}^{(r)} = \bigoplus_{i=1}^{r} m_i \mathbf{D}^{(i)} \quad \text{with}$$

$$m_i = (\chi \uparrow \mathcal{G}, \chi^{(i)})_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi \uparrow \mathcal{G}(g)\, \chi^{(i)}(g)^*.$$

- As for the subduction, the multiplicities can often be read off easily from the character table of $\mathcal{G}$.

Induction from normal subgroups

Soluble groups

- In an abelian group, all subgroups are normal subgroups.
- For induction from a normal subgroup $\mathcal{H} \trianglelefteq \mathcal{G}$ one has much more control over the properties of the induced representations.
- This is in particular the case if the index $[\mathcal{G} : \mathcal{H}]$ of $\mathcal{H}$ in $\mathcal{G}$ is a prime number p.
- A finite group $\mathcal{G}$ is called a soluble group if it has a chain of subgroups

$$\{1\} = \mathcal{G}_0 \leq \mathcal{G}_1 \leq \ldots \leq \mathcal{G}_{s-1} \leq \mathcal{G}_s = \mathcal{G}$$

  such that for each i:
  - $\mathcal{G}_i \trianglelefteq \mathcal{G}_{i+1}$ is a normal subgroup of its successor $\mathcal{G}_{i+1}$;
  - the index $|\mathcal{G}_{i+1}|/|\mathcal{G}_i|$ is a prime number p.

Point groups are soluble groups

All point groups in 2D and 3D are soluble groups and the only primes that occur as index are 2 and 3.

Induction from a normal subgroup of index 2

- $\mathcal{H} \trianglelefteq \mathcal{G}$ with $[\mathcal{G} : \mathcal{H}] = 2$, coset decomposition $\mathcal{G} = \mathcal{H} \cup g\mathcal{H}$, i.e. coset representatives $1, g$
- $h \in \mathcal{H}$: $1^{-1} \cdot h \cdot 1 = h \in \mathcal{H}, \quad g^{-1} \cdot h \cdot g = g^{-1}hg \in \mathcal{H}$

$$\Rightarrow \mathbf{M}(h) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbf{D} \uparrow \mathcal{G}(h) = \begin{pmatrix} \mathbf{D}(h) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(g^{-1}hg) \end{pmatrix}$$

- g: $g^{-1} \cdot g \cdot 1 = 1 \in \mathcal{H}, \quad 1^{-1} \cdot g \cdot g = g^2 \in \mathcal{H}$

$$\Rightarrow \mathbf{M}(g) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D} \uparrow \mathcal{G}(g) = \begin{pmatrix} \mathbf{0} & \mathbf{D}(g^2) \\ \mathbf{D}(1) & \mathbf{0} \end{pmatrix}$$

Induction from a normal subgroup of index 3

- $\mathcal{H} \trianglelefteq \mathcal{G}$ with $[\mathcal{G} : \mathcal{H}] = 3$, coset decomposition $\mathcal{G} = \mathcal{H} \cup g\mathcal{H} \cup g^2\mathcal{H}$, i.e. coset representatives $1, g, g^2$
- $h \in \mathcal{H}$: $1^{-1} \cdot h \cdot 1 = h \in \mathcal{H}$, $\quad g^{-1} \cdot h \cdot g = g^{-1}hg \in \mathcal{H}$
  $g^{-2} \cdot h \cdot g^2 = g^{-2}hg^2 \in \mathcal{H}$

$$\Rightarrow \mathbf{M}(h) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; \mathbf{D} \uparrow \mathcal{G}(h) = \begin{pmatrix} \mathbf{D}(h) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(g^{-1}hg) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}(g^{-2}hg^2) \end{pmatrix}$$

- g: $g^{-1} \cdot g \cdot 1 = 1 \in \mathcal{H}$, $\quad (g^2)^{-1} \cdot g \cdot g = 1 \in \mathcal{H}$
  $1^{-1} \cdot g \cdot g^2 = g^3 \in \mathcal{H}$

$$\Rightarrow \mathbf{M}(g) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{D} \uparrow \mathcal{G}(g) = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{D}(g^3) \\ \mathbf{D}(1) & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}(1) & \mathbf{0} \end{pmatrix}$$

Conjugate representations

- If $\mathcal{H} \trianglelefteq \mathcal{G}$ and $\mathbf{D}$ is an irrep of $\mathcal{H}$ with character χ, then

$$\mathbf{D}^g \text{ with } \mathbf{D}^g(h) = \mathbf{D}(g^{-1}hg)$$

  is also an irrep of $\mathcal{H}$, which is called the conjugate representation of $\mathbf{D}$ by g.
- The character χ^g of $\mathbf{D}^g$ is given by $\chi^g(h) = \chi(g^{-1}hg)$.
- $[\mathcal{G} : \mathcal{H}] = 2$ with coset representatives $1, g$

$$\Rightarrow (\mathbf{D} \uparrow \mathcal{G}) \downarrow \mathcal{H} = \mathbf{D} \oplus \mathbf{D}^g$$

- $[\mathcal{G} : \mathcal{H}] = 3$ with coset representatives $1, g, g^2$

$$\Rightarrow (\mathbf{D} \uparrow \mathcal{G}) \downarrow \mathcal{H} = \mathbf{D} \oplus \mathbf{D}^g \oplus \mathbf{D}^{g^2}$$

Little group

- Mapping **D** to $\mathbf{D}^g$ and χ to χ^g is an action of $\mathcal{G}$ on the equivalence classes of irreps of $\mathcal{H}$ and on the corresponding characters.
- The stabilizer $\mathcal{G}^{(s)} = \mathcal{G}^{(s)}(\mathbf{D}^{(s)})$ of an irrep $\mathbf{D}^{(s)}$ of $\mathcal{H}$ under this action is called the little group of $\mathbf{D}^{(s)}$ relative to $\mathcal{G}$:

$$\begin{aligned}\mathcal{G}^{(s)} &= \{g \in \mathcal{G} \mid (\mathbf{D}^{(s)})^g \text{ is equivalent to } \mathbf{D}^{(s)}\} \\ &= \{g \in \mathcal{G} \mid (\chi^{(s)})^g = \chi^{(s)}\}\end{aligned}$$

- $\mathcal{H} \leq \mathcal{G}^{(s)}$, since $\chi(x^{-1}hx) = \chi(h)$ for $x \in \mathcal{H}$ (recall that χ is constant on the conjugacy classes of $\mathcal{H}$).
  Conjugation by $g \in \mathcal{G}$, however, may take a conjugacy class of $\mathcal{H}$ to a different one.
- The number of inequivalent irreps in the orbit of $\mathbf{D}^{(s)}$ is the index $[\mathcal{G} : \mathcal{G}^{(s)}]$ of the little group in $\mathcal{G}$.

Example: $4 \trianglelefteq 4mm$

- $\mathcal{G} = 4mm = \langle 4^+, m_{10} \rangle$, $\mathcal{H} = \langle 4^+ \rangle$
- $\mathcal{H}$ has character table

	1	4^+	2	4^-
$\mathbf{D}^{(0)}$	1	1	1	1
$\mathbf{D}^{(1)}$	1	i	-1	$-i$
$\mathbf{D}^{(2)}$	1	-1	1	-1
$\mathbf{D}^{(3)}$	1	$-i$	-1	i

- $m_{10}^{-1} \cdot 4^+ \cdot m_{10} = 4^-$, thus conjugation by m_{10} interchanges $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(3)}$ (it interchanges the conjugacy classes of 4^+ and 4^-)
- $\mathbf{D}^{(0)}$ and $\mathbf{D}^{(2)}$ are fixed under conjugation by all elements of $\mathcal{G}$
- $\mathcal{G}^{(0)} = \mathcal{G}^{(2)} = \mathcal{G}$, $\mathcal{G}^{(1)} = \mathcal{G}^{(3)} = \mathcal{H}$
- orbits of conjugate irreps: $\{\mathbf{D}^{(0)}\}$, $\{\mathbf{D}^{(2)}\}$, $\{\mathbf{D}^{(1)}, \mathbf{D}^{(3)}\}$

Example: $222 \trianglelefteq 4/mmm$

- $\mathcal{G} = 4/mmm = \langle 4^+_{001}, 2_{100}, \bar{1}\rangle$, $\mathcal{H} = \langle 2_{100}, 2_{010}\rangle$, $[\mathcal{G} : \mathcal{H}] = 4$
- $\mathcal{H}$ has character table

	1	2_{100}	2_{010}	2_{001}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	1	-1	-1
$\mathbf{D}^{(3)}$	1	-1	1	-1
$\mathbf{D}^{(4)}$	1	-1	-1	1

- $\bar{1}$ commutes with all elements of $\mathcal{H}$ and is contained in every little group
- $(4^+_{001})^{-1} \cdot 2_{100} \cdot 4^+_{001} = 2_{010}$, thus conjugation by 4^+_{001} interchanges $\mathbf{D}^{(2)}$ and $\mathbf{D}^{(3)}$
- $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(4)}$ are fixed under conjugation by all elements of $\mathcal{G}$
- $\mathcal{G}^{(1)} = \mathcal{G}^{(4)} = \mathcal{G}$, $\mathcal{G}^{(2)} = \mathcal{G}^{(3)} = \langle \mathcal{H}, \bar{1}\rangle = mmm$
- orbits of conjugate irreps: $\{\mathbf{D}^{(1)}\}$, $\{\mathbf{D}^{(4)}\}$, $\{\mathbf{D}^{(2)}, \mathbf{D}^{(3)}\}$

Exercise: $222 \trianglelefteq 23$

- $\mathcal{G} = 23 = \langle 3^+_{111}, 2_{100} \rangle$, $\mathcal{H} = \langle 2_{100}, 2_{010} \rangle$, $[\mathcal{G} : \mathcal{H}] = 3$
- $\mathcal{H}$ has character table

	1	2_{100}	2_{010}	2_{001}
$\mathbf{D}^{(1)}$	1	1	1	1
$\mathbf{D}^{(2)}$	1	1	-1	-1
$\mathbf{D}^{(3)}$	1	-1	1	-1
$\mathbf{D}^{(4)}$	1	-1	-1	1

Find the little groups of the irreps of $\mathcal{H}$ and the orbits of conjugate irreps under the action of $\mathcal{G}$.

Answer

- Since there is no group between $\mathcal{G}$ and $\mathcal{H}$, the little groups are either $\mathcal{G}$ (character fixed under 3^+_{111}) or $\mathcal{H}$ (character not fixed under 3^+_{111}).
- 3^+_{111} conjugates 2_{100} to 2_{010} and 2_{010} to 2_{001}, thus $\{\mathbf{D}^{(2)}, \mathbf{D}^{(3)}, \mathbf{D}^{(4)}\}$ form one orbit of conjugate irreps and all have little group $\mathcal{H}$.
- The trivial irrep forms an orbit on its own with little group $\mathcal{G}$.

Allowed representations

- An irrep $\mathbf{\Delta}$ of the little group $\mathcal{G}^{(s)}$ is called allowed or a small irrep with respect to the irrep $\mathbf{D}^{(s)}$ of $\mathcal{H}$ if its subduction $\Delta \downarrow \mathcal{H}$ contains $\mathbf{D}^{(s)}$ with multiplicity > 0.

Clifford's theorem

Let $\mathbf{D}^{(s)}$ be an irrep of $\mathcal{H}$ with little group $\mathcal{G}^{(s)}$.

- The induction $\mathbf{\Delta} \uparrow \mathcal{G}$ of each allowed irrep $\mathbf{\Delta}$ of $\mathcal{G}^{(s)}$ is an irrep of $\mathcal{G}$ and these irreps are inequivalent for different allowed irreps.
- Every irrep $\mathbf{D}$ of $\mathcal{G}$ that has $\mathbf{D}^{(s)}$ in its subduction $\mathbf{D} \downarrow \mathcal{H}$ is obtained in this way.
- The subduction $(\mathbf{\Delta} \uparrow \mathcal{G}) \downarrow \mathcal{H}$ of $\mathbf{\Delta} \uparrow \mathcal{G}$ to $\mathcal{H}$ contains each irrep in the orbit of $\mathbf{D}^{(s)}$ under $\mathcal{G}$ with the same multiplicity and no irreps which do not lie in the orbit of $\mathbf{D}^{(s)}$.

Example

- $\mathcal{G} = 4/mmm = \langle 4^+_{001}, 2_{100}, \bar{1}\rangle$, $\mathcal{H} = \langle 2_{100}, 2_{010}\rangle$,
  $\mathcal{G}^{(2)} = \mathcal{H} \times \langle \bar{1}\rangle = mmm$
- $\mathcal{G}^{(2)}$ has character table

	1	2_{100}	2_{010}	2_{001}	$\bar{1}$	m_{100}	m_{010}	m_{001}
$\mathbf{D}^{(11)}$	1	1	1	1	1	1	1	1
$\mathbf{D}^{(12)}$	1	1	-1	-1	1	1	-1	-1
$\mathbf{D}^{(13)}$	1	-1	1	-1	1	-1	1	-1
$\mathbf{D}^{(14)}$	1	-1	-1	1	1	-1	-1	1
$\mathbf{D}^{(21)}$	1	1	1	1	-1	-1	-1	-1
$\mathbf{D}^{(22)}$	1	1	-1	-1	-1	-1	1	1
$\mathbf{D}^{(23)}$	1	-1	1	-1	-1	1	-1	1
$\mathbf{D}^{(24)}$	1	-1	-1	1	-1	1	1	-1

- allowed irreps are $\mathbf{D}^{(12)}$ and $\mathbf{D}^{(22)}$
- subduction of $\mathbf{D}^{(12)} \uparrow \mathcal{G}$ to $\mathcal{G}^{(2)}$ is $\mathbf{D}^{(12)} \oplus \mathbf{D}^{(13)}$,
- subduction of $\mathbf{D}^{(22)} \uparrow \mathcal{G}$ to $\mathcal{G}^{(2)}$ is $\mathbf{D}^{(22)} \oplus \mathbf{D}^{(23)}$
- subductions of $\mathbf{D}^{(12)} \uparrow \mathcal{G}$ and $\mathbf{D}^{(22)} \uparrow \mathcal{G}$ to $\mathcal{H}$ are both $\mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)}$

Special case $[\mathcal{G} : \mathcal{H}] = p$

- If the index of $\mathcal{H}$ in $\mathcal{G}$ is a prime p, the little group is either $\mathcal{H}$ or $\mathcal{G}$, since there are no groups between $\mathcal{H}$ and $\mathcal{G}$.
- $\mathcal{G}^{(s)} = \mathcal{G}$: $\mathbf{D}^{(s)}$ forms an orbit on its own, in this case it is called a self-conjugate irrep:
  - $\mathbf{D}^{(s)}$ can be extended in p different ways to an irrep of $\mathcal{G}$
  - each of these inequivalent irreps of $\mathcal{G}$ subduces to $\mathbf{D}^{(s)}$
- $\mathcal{G}^{(s)} = \mathcal{H}$: the orbit of $\mathbf{D}^{(s)}$ consists of p irreps:
  - the induction $\mathbf{D}^{(s)} \uparrow \mathcal{G}$ is irreducible
  - the subduction of $\mathbf{D}^{(s)} \uparrow \mathcal{G}$ to $\mathcal{H}$ is the sum of the p irreps in the orbit of $\mathbf{D}^{(s)}$
- We have already seen how to deal with the induction case, let's take a brief look at the extension case.

Extending a representation

- $\mathcal{H} \trianglelefteq \mathcal{G}$ with $[\mathcal{G} : \mathcal{H}] = p$ prime, coset representatives $1, g, \ldots, g^{p-1}$
- If $\mathcal{G}^{(s)} = \mathcal{G}$, $\mathbf{D}^{(s)}$ can be extended to an irrep $\mathbf{\Delta}$ of $\mathcal{G}$.
- The only matrix missing is $\mathbf{U} = \mathbf{\Delta}(g)$.
- $\mathcal{H} \trianglelefteq \mathcal{G} \Rightarrow g^{-1}hg \in \mathcal{H}$ for all $h \in \mathcal{H}$, the coset $g\mathcal{H}$ has order p, therefore $g^p \in \mathcal{H}$
- The matrix $\mathbf{U}$ has to fulfill the conditions
  - $\mathbf{U}^{-1}\mathbf{D}^{(s)}(h)\mathbf{U} = \mathbf{D}^{(s)}(g^{-1}hg)$ for generators h of $\mathcal{H}$;
  - $\mathbf{U}^p = \mathbf{D}^{(s)}(g^p)$.
- From one solution $\mathbf{U}$, the p different extensions of $\mathbf{D}^{(s)}$ to $\mathcal{G}$ are obtained as $\mathbf{\Delta}^{(k)}(g) = e^{2\pi i \frac{k}{p}}\mathbf{U}$.
- In particular, for $p = 2$ the two extensions are given by

$$\mathbf{\Delta}^{+}(g) = \mathbf{U} \text{ and } \mathbf{\Delta}^{-}(g) = -\mathbf{U},$$

  for $p = 3$ the three extensions are given by

$$\mathbf{\Delta}^{(0)}(g) = \mathbf{U},\ \mathbf{\Delta}^{(1)}(g) = e^{\frac{2\pi i}{3}}\mathbf{U} \text{ and } \mathbf{\Delta}^{(2)}(g) = e^{-\frac{2\pi i}{3}}\mathbf{U}.$$

Example: $2 \trianglelefteq 4$

- The irrep $\mathbf{D}^{(2)}$ of $\mathcal{H} = \{1, 2\}$ with $\mathbf{D}^{(2)}(2) = \begin{pmatrix} -1 \end{pmatrix}$ is self-conjugate with respect to $\mathcal{G} = \langle 4^+ \rangle$ and thus has little group $\mathcal{G}^{(2)} = \mathcal{G}$.
- The coset decomposition is $\mathcal{G} = \mathcal{H} \cup 4^+\mathcal{H}$.
- The conjugation relations are automatically fulfilled, since $\mathcal{G}$ is abelian, but we require $\mathbf{\Delta}(g)^2 = \mathbf{D}^{(2)}(2) = \begin{pmatrix} -1 \end{pmatrix}$, thus the two extensions are $\mathbf{\Delta}^+(g) = \begin{pmatrix} i \end{pmatrix}$ and $\mathbf{\Delta}^-(g) = \begin{pmatrix} -i \end{pmatrix}$.

Example: $222 \trianglelefteq 23$

- The trivial representation is always a self-conjugate irrep.
- For $\mathcal{G} = 23$ the rotation group of the tetrahedron and $\mathcal{H} = 222$ is a normal subgroup of index 3, the coset decomposition is $\mathcal{G} = \mathcal{H} \cup 3^+_{111}\mathcal{H} \cup 3^-_{111}\mathcal{H}$.
- Since $(3^+_{111})^3 = 1$, the three extensions of the trivial irrep are

$$\mathbf{\Delta}^{(0)}(3^+_{111}) = \begin{pmatrix} 1 \end{pmatrix}, \ \mathbf{\Delta}^{(1)}(3^+_{111}) = \begin{pmatrix} e^{\frac{2\pi i}{3}} \end{pmatrix}, \ \mathbf{\Delta}^{(2)}(3^+_{111}) = \begin{pmatrix} e^{-\frac{2\pi i}{3}} \end{pmatrix}.$$

Exercise

- The irrep $\mathbf{D}^{(2)}$ of $\mathcal{H} = \langle 4^+ \rangle = 4$ with $\mathbf{D}^{(2)}(4^+) = \big(-1\big)$ is self-conjugate with respect to $\mathcal{G} = \langle 4^+, m_{10} \rangle = 4mm$ and thus has little group $\mathcal{G}^{(2)} = \mathcal{G}$.
- The coset decomposition is $\mathcal{G} = \mathcal{H} \cup m_{10}\mathcal{H}$.
- Determine the extensions $\mathbf{\Delta}^+$ and $\mathbf{\Delta}^-$ of $\mathbf{D}^{(2)}$ to $\mathcal{G}$.

Answer

The conjugation relations are automatically fulfilled, since $\mathbf{D}^{(2)}$ is 1-dimensional and $m_{10}^{-1} \cdot 4^+ \cdot m_{10} = 4^-$ and $\mathbf{D}^{(2)}(4^+) = \mathbf{D}^{(2)}(4^-)$.

We require $\mathbf{\Delta}(m_{10})^2 = \mathbf{D}^{(2)}(1) = \big(1\big)$, thus the two extensions are $\mathbf{\Delta}^+(m_{10}) = \big(1\big)$ and $\mathbf{\Delta}^-(m_{10}) = \big(-1\big)$.

Irreps of space groups

General idea

- Start with an irrep of the translation subgroup $\mathcal{T}$, this has to be 1-dimensional because $\mathcal{T}$ is abelian.
- Compute the little group and the allowed representations.
- Induce the allowed representations of the little group to $\mathcal{G}$.

Irreps of the translation subgroup

Born-von Karman boundary condition

- Let $\mathbf{\Gamma}$ be an irrep of the translation subgroup $\mathcal{T}$ and thus 1-dimensional.
- Fix a basis $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of the translation lattice $\mathbf{L}$.
- Assume that $\mathbf{\Gamma}((\mathbf{I}, \mathbf{a}_j))$ has (large) finite order N_j for $j = 1, 2, 3$, then $\mathbf{\Gamma}((\mathbf{I}, \mathbf{t}))$ has finite order for all $\mathbf{t} \in \mathbf{L}$.
  This is called the Born-von Karman boundary condition.
- Then there are integers q_1, q_2, q_3 with $0 \leq q_j < N_j$ such that

$$\mathbf{\Gamma}((\mathbf{I}, \mathbf{a}_j)) = \left(e^{-2\pi i \frac{q_j}{N_j}} \right)$$

  and for an arbitrary $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ one has

$$\mathbf{\Gamma}((\mathbf{I}, \mathbf{t})) = \left(e^{-2\pi i (\frac{q_1}{N_1} n_1 + \frac{q_2}{N_2} n_2 + \frac{q_3}{N_3} n_3)} \right)$$

Description by a $\mathbf{k}$-vector

- Define the reciprocal basis $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$ by the conditions

$$\mathbf{a}_i \cdot \mathbf{a}_j^* = 2\pi\delta_{ij} = \begin{cases} 2\pi & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

  and let $\mathbf{L}^* = \{h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^* \mid h_j \in \mathbb{Z}\}$ be the reciprocal lattice.
  Mind the scaling factor 2π!

- Take $k_j = \dfrac{q_j}{N_j}$ and define the $\mathbf{k}$-vector $\mathbf{k} = k_1\mathbf{a}_1^* + k_2\mathbf{a}_2^* + k_3\mathbf{a}_3^*$, also called a wave vector.

  Then the irrep $\boldsymbol{\Gamma}$ is labelled as $\boldsymbol{\Gamma}^{\mathbf{k}}$ and takes the more convenient form

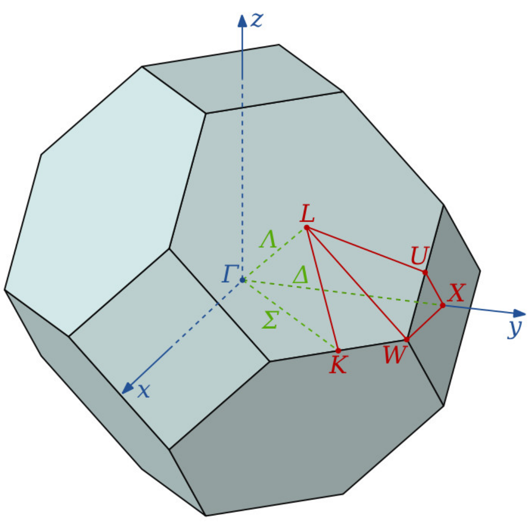
$$\boldsymbol{\Gamma}^{\mathbf{k}}((\mathbf{I}, \mathbf{t})) = \left(e^{-i\mathbf{k}\cdot\mathbf{t}}\right) = \left(e^{-2\pi i\left(\frac{q_1}{N_1}n_1 + \frac{q_2}{N_2}n_2 + \frac{q_3}{N_3}n_3\right)}\right)$$

  since
  $(n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3) \cdot (k_1\mathbf{a}_1^* + k_2\mathbf{a}_2^* + k_3\mathbf{a}_3^*) = 2\pi(n_1k_1 + n_2k_2 + n_3k_3)$.

Fundamental regions

- Two irreps $\Gamma^{\mathbf{k}}$ and $\Gamma^{\mathbf{k}'}$ are equal if the difference $\mathbf{k} - \mathbf{k}'$ of their $\mathbf{k}$-vectors lies in $\mathbf{L}^*$, since for $\mathbf{K} \in \mathbf{L}^*$ one has $\mathbf{K} \cdot \mathbf{t} = 2\pi N$ for some integer N and thus $e^{-i\mathbf{K}\cdot\mathbf{t}} = 1$.
- It is sufficient to consider $\mathbf{k}$-vectors from a fundamental region with respect to translations by $\mathbf{L}^*$, i.e. from a region which contains precisely one vector from each coset $\mathbf{k} + \mathbf{L}^*$.
- There are two standard choices for such a fundamental region **F**:
    - First Brillouin zone or Wigner-Seitz cell:
      F $= \{\mathbf{k} \mid |\mathbf{k}| \le |\mathbf{K} - \mathbf{k}| \text{ for all } \mathbf{K} \in \mathbf{L}^*\}$. These are the points which are closer to the origin $\mathbf{o}$ than to any other point of the reciprocal lattice $\mathbf{L}^*$.
      This is the fundamental region which is usually used in the context of representations of space groups.
    - Crystallographic unit cell: **F** $= \{k_1\mathbf{a}_1^* + k_2\mathbf{a}_2^* + k_3\mathbf{a}_3^* \mid 0 \le k_i < 1\}$.

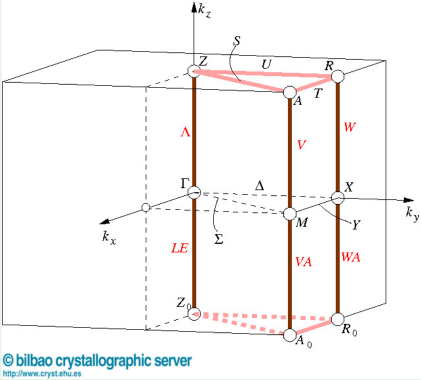
Brillouin zone of an fcc-lattice



Running example: irreps of $P4mm$

To illustrate the procedure, we construct the irreps of $\mathcal{G} = P4mm$ for two selected $\mathbf{k}$-vectors from the Brillouin zone:

- $\mathbf{k}$-vector Γ $(0,0,0)$: $\mathbf{\Gamma^k}((\mathbf{I},\mathbf{t})) = \big(1\big)$
- $\mathbf{k}$-vector X $(0,\frac{1}{2},0)$: $\mathbf{\Gamma^k}((\mathbf{I},\mathbf{t})) = \big(e^{-\pi i n_2}\big) = \big((-1)^{n_2}\big)$ for $\mathbf{t} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$



Brillouin zone of the reciprocal primitive tetragonal lattice

Conjugation action on the $\mathbf{\Gamma^k}$

- Since $(\mathbf{W},\mathbf{w})^{-1}(\mathbf{I},\mathbf{t})(\mathbf{W},\mathbf{w}) = (\mathbf{I},\mathbf{W}^{-1}\mathbf{t})$, the conjugate irrep $(\mathbf{\Gamma^k})^{(\mathbf{W},\mathbf{w})}$ is given by

$$(\mathbf{\Gamma^k})^{(\mathbf{W},\mathbf{w})}((\mathbf{I},\mathbf{t})) = \mathbf{\Gamma^k}((\mathbf{I},\mathbf{W}^{-1}\mathbf{t}))$$
$$= \left(e^{-i\mathbf{k}\cdot\mathbf{W}^{-1}\mathbf{t}}\right) = \left(e^{-i\mathbf{k}\mathbf{W}^{-1}\cdot\mathbf{t}}\right) = \mathbf{\Gamma}^{\mathbf{k}\mathbf{W}^{-1}}((\mathbf{I},\mathbf{t}))$$

  and thus $\mathbf{\Gamma^k}$ is mapped to $\mathbf{\Gamma}^{\mathbf{k}\mathbf{W}^{-1}}$.
- The irreps $\mathbf{\Gamma^k}$ and $\mathbf{\Gamma}^{\mathbf{k}\mathbf{W}^{-1}}$ are equivalent if $\mathbf{k}\mathbf{W}^{-1} - \mathbf{k} \in \mathbf{L}^*$ or, equivalently, $\mathbf{k} - \mathbf{k}\mathbf{W} \in \mathbf{L}^*$.
- The little group $\mathcal{G}^{\mathbf{k}}$ stabilizing $\mathbf{\Gamma^k}$ is therefore given by

$$\mathcal{G}^{\mathbf{k}} = \{(\mathbf{W},\mathbf{w}) \in \mathcal{G} \mid \mathbf{k} - \mathbf{k}\mathbf{W} \in \mathbf{L}^*\}.$$

- $\mathcal{G}^{\mathbf{k}}$ is the t-subgroup of $\mathcal{G}$ consisting of the cosets of $\mathcal{G}$ relative to $\mathcal{T}$ with linear parts fulfilling $\mathbf{k} - \mathbf{k}\mathbf{W} \in \mathbf{L}^*$.

The star of a $\mathbf{k}$-vector

- If $\boldsymbol{\Gamma}^{\mathbf{k}_1}, \ldots, \boldsymbol{\Gamma}^{\mathbf{k}_s}$ is the orbit of $\boldsymbol{\Gamma}^{\mathbf{k}}$ under the action of $\mathcal{G}$ where the $\mathbf{k}$-vectors $\mathbf{k}_i$ lie in the Brillouin zone, then $\star(\mathbf{k}) = \{\mathbf{k}_1, \ldots, \mathbf{k}_s\}$ is called the star of $\mathbf{k}$ and the $\mathbf{k}_i$ are the arms of the star.
- The number of arms of the star is the index $[\mathcal{G} : \mathcal{G}^{\mathbf{k}}]$ and if $(\mathbf{W}_1, \mathbf{w}_1), \ldots, (\mathbf{W}_s, \mathbf{w}_s)$ are coset representatives of $\mathcal{G}$ relative to the little group $\mathcal{G}^{\mathbf{k}}$, then $\mathbf{k}_i$ is the unique vector in $\mathbf{k}\mathbf{W}_i + \mathbf{L}^*$ that lies in the Brillouin zone.

Running example: irreps of $P4mm$

- $\mathbf{k}$-vector Γ $(0,0,0)$: $\star(\mathbf{k}) = \{(0,0,0)\}$,
  little group $\mathcal{G}^{\mathbf{k}} = \mathcal{G}$
- $\mathbf{k}$-vector X $(0, \frac{1}{2}, 0)$: $\star(\mathbf{k}) = \{(0, \frac{1}{2}, 0), (\frac{1}{2}, 0, 0)\}$,
  little group $\mathcal{G}^{\mathbf{k}} = Pmm2 = \langle (2_{001}, \mathbf{o}), (m_{100}, \mathbf{o}), (1, \mathbf{a}_i) \rangle$,
  coset representatives of $\mathcal{G}$ relative to $\mathcal{G}^{\mathbf{k}}$: $(1, \mathbf{o})$, $(4^+_{001}, \mathbf{o})$

Allowed irreps of the little group

The trivial case

- If the number of arms in the star $\star(\mathbf{k})$ equals the order of the point group of $\mathcal{G}$, $\mathbf{k}$ is a vector in general position and $\mathcal{G}^{\mathbf{k}} = \mathcal{T}$.
- In this case, $\mathbf{\Gamma}^{\mathbf{k}}$ is the only allowed irrep of $\mathcal{G}^{\mathbf{k}}$ and the induction $\mathbf{\Gamma}^{\mathbf{k}} \uparrow \mathcal{G}$ is the only irrep of $\mathcal{G}$ having $\mathbf{\Gamma}^{\mathbf{k}}$ in its subduction to $\mathcal{H}$.
- The subduction of $\mathbf{\Gamma}^{\mathbf{k}} \uparrow \mathcal{G}$ to $\mathcal{H}$ is the sum $\bigoplus_{\mathbf{k}_i \in \star(\mathbf{k})} \mathbf{\Gamma}^{\mathbf{k}_i}$.

The easy case

- Let $\overline{\mathcal{G}}^{\mathbf{k}}$ be the point group of the little group $\mathcal{G}^{\mathbf{k}}$, this is called the little co-group of $\mathbf{k}$.
- If either $\mathcal{G}^{\mathbf{k}}$ is a symmorphic space group or $\mathbf{k}$ is a vector in the interior of the Brillouin zone, the allowed irreps of $\mathcal{G}^{\mathbf{k}}$ are of the form

$$\mathbf{D}^{\mathbf{k},i}((\mathbf{W},\mathbf{w})) = e^{-i\mathbf{k}\cdot\mathbf{w}}\,\overline{\mathbf{D}}^{\mathbf{k},i}(\mathbf{W})$$

where $\overline{\mathbf{D}}^{\mathbf{k},i}$ runs over the irreps of the little co-group $\overline{\mathcal{G}}^{\mathbf{k}}$.

The harder case

- If $\mathcal{G}^{\mathbf{k}}$ is a non-symmorphic space group and $\mathbf{k}$ is a vector on the surface of the Brillouin zone, we choose a symmorphic subgroup $\mathcal{H}_0$ of $\mathcal{G}^{\mathbf{k}}$.
- Construct the allowed irreps of $\mathcal{H}_0$ as in the easy case.
- Find a proper supergroup $\mathcal{H}_1$ of $\mathcal{H}_0$ such that $\mathcal{H}_0 \trianglelefteq \mathcal{H}_1$, $\mathcal{H}_1 \leq \mathcal{G}^{\mathbf{k}}$ and $[\mathcal{H}_1 : \mathcal{H}_0] = 2$ or 3.
- Obtain the allowed irreps of $\mathcal{H}_1$ from those of $\mathcal{H}_0$ by applying the special case of Clifford's theorem for $p = 2, 3$:
  - self-conjugate irreps are extended from $\mathcal{H}_0$ to $\mathcal{H}_1$;
  - irreps which are not self-conjugate are induced to $\mathcal{H}_1$.
- Construct in the same way allowed irreps along an ascending chain of subgroups $\mathcal{H}_2, \mathcal{H}_3, \ldots$ until the little group $\mathcal{G}^{\mathbf{k}}$ is reached.

Running example: irreps of $P4mm$

- For both cases we are in the easy case.
- $\mathbf{k}$-vector $\Gamma\ (0,0,0)$: little co-group $\overline{\mathcal{G}}^{\mathbf{k}} = 4mm$, allowed irreps coincide with the irreps of the point group $4mm$

	$(4^{+}_{001}, \mathbf{o})$	$(m_{100}, \mathbf{o})$	$(1, \mathbf{t})$
$\mathbf{D}^{\mathbf{k},1}$	(1)	(1)	(1)
$\mathbf{D}^{\mathbf{k},2}$	(1)	(-1)	(1)
$\mathbf{D}^{\mathbf{k},3}$	(-1)	(-1)	(1)
$\mathbf{D}^{\mathbf{k},4}$	(-1)	(1)	(1)
$\mathbf{D}^{\mathbf{k},5}$	$\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Running example: irreps of $P4mm$ (ctd.)

- $\mathbf{k}$-vector X $(0, \frac{1}{2}, 0)$: little co-group $\overline{\mathcal{G}}^{\mathbf{k}} = mm2$, allowed irreps from irreps of little co-group and $e^{-i\mathbf{k}\cdot\mathbf{t}} = (-1)^{n_2}$ for $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$

	$(2_{001}, \mathbf{o})$	$(m_{100}, \mathbf{o})$	$(1, \mathbf{t})$
$\mathbf{D}^{\mathbf{k},1}$	(1)	(1)	$((-1)^{n_2})$
$\mathbf{D}^{\mathbf{k},2}$	(1)	(-1)	$((-1)^{n_2})$
$\mathbf{D}^{\mathbf{k},3}$	(-1)	(-1)	$((-1)^{n_2})$
$\mathbf{D}^{\mathbf{k},4}$	(-1)	(1)	$((-1)^{n_2})$

The finishing touch

Finally, induce all allowed irreps $\mathbf{D}^{\mathbf{k},i}$ of the little group $\mathcal{G}^{\mathbf{k}}$ to irreps $\mathbf{D}^{\mathbf{k},i} \uparrow \mathcal{G}$ of $\mathcal{G}$.

Running example: irreps of $P4mm$

- $\mathbf{k}$-vector Γ $(0,0,0)$: already finished
- $\mathbf{k}$-vector X $(0,\frac{1}{2},0)$: apply induction procedure for index 2

	$(4^+_{001},\mathbf{o})$	$(m_{100},\mathbf{o})$	$(1,\mathbf{t})$
$\mathbf{D}^{\mathbf{k},1} \uparrow \mathcal{G}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{\mathbf{k},2} \uparrow \mathcal{G}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{\mathbf{k},3} \uparrow \mathcal{G}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$
$\mathbf{D}^{\mathbf{k},4} \uparrow \mathcal{G}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} (-1)^{n_2} & 0 \\ 0 & (-1)^{n_1} \end{pmatrix}$

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News:

- **New Article in Nature**
  07/2017: Bradlyn *et al.* "Topological quantum chemistry" *Nature* (2017). **547**, 298-305.
- **New program: BANDREP**
  04/2017: Band representations and Elementary Band representations of Double Space Groups.
- **New section: Double point and space groups**
  - **New program: DGENPOS**
    04/2017: General positions of Double Space Groups
  - **New program: REPRESENTATIONS DPG**
    04/2017: Irreducible representations of the Double Point Groups
  - **New program: REPRESENTATIONS DSG**
    04/2017: Irreducible representations of the Double Space Groups
  - **New program: DSITESYM**
    04/2017: Site-symmetry induced representations of Double Space Groups
  - **New program: DCOMPREL**
    04/2017: Compatibility relations between the irreducible representations of Double Space Groups

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Space-group symmetry

Magnetic Symmetry and Applications

Group-Subgroup Relations of Space Groups

Representations and Applications

REPRES	Space Groups Representations
Representations PG	Irreducible representations of the crystallographic Point Groups
Representations SG	Irreducible representations of the Space Groups
Get_irreps	Irreps and order parameters in a space group-subgroup phase transition
Get_mirreps	Irreps and order parameters in a paramagnetic space group- magnetic subgroup phase transition
DIRPRO	Direct Products of Space Group Irreducible Representations
CORREL	Correlations relations between the irreducible representations of a group-subgroup pair
POINT	Point Group Tables
SITESYM	Site-symmetry induced representations of Space Groups
COMPATIBILITY RELATIONS	Compatibility relations between the irreducible representations of a space group
MECHANICAL REP. ⚠	Decomposition of the mechanical representation into irreps
MAGNETIC REP. ⚠	Decomposition of the magnetic representation into irreps
BANDREP ⚠	Band representations and Elementary Band representations of Double Space Groups

Solid State Theory Applications

Structure Utilities

Quick access to some tables

- Space Groups
- Plane Groups
- Layer Groups
- Rod Groups
- Frieze Groups
- 2D Point Groups
- 3D Point Groups
- Magnetic Space Groups