Basic representation theory

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A group $\mathcal{G} = (G, \circ)$ consists of a set G and an operation $\circ$ s.t.

(1) $\forall\, a, b \in G \,, \quad a \circ b \in G$

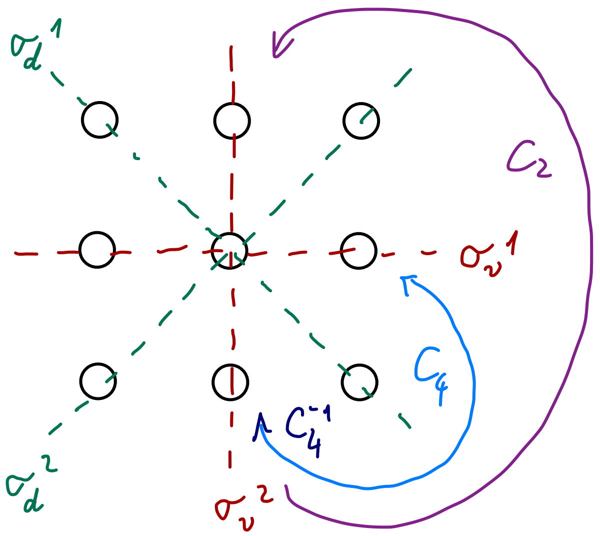
(2) $(a \circ b) \circ c = a \circ (b \circ c) \quad \forall\, a, b, c \in G$

(3) $\exists\, e \in G \,, \quad a \circ e = e \circ a = a \quad \forall\, a \in G$

(4) $\forall\, a \in G \;\exists\, a^{-1} \in G \,, \quad a \circ a^{-1} = a^{-1} \circ a = e$.

Example: Set of transformations which map a given lattice into itself by leaving one point fixed.

In the case of the 2D square lattice:



$C_{4v} = \{\; E,$ identity

$C_2,$ rotations by π (self-inverse)

$C_4,$ rotations by $\pi/2$

$C_4^{-1},$ inverse of C_4^{-1}

$\sigma_v^1,$ reflection about the horizontal axis (self-inverse)

$\sigma_v^2,$ % vertical %

$\sigma_d^1,$ % the first diagonal

σ_d^2 % second %

$\}$

Conjugate elements and classes in a group

(1) Two elements a, b of the group $\mathcal{G} = (G, \circ)$ are <u>conjugate</u> $a \sim b$, if and only if there is another element $x \in G$ such that $b = x \circ a \circ x^{-1}$.

(2) A <u>class</u> is the entirety of conjugate elements.

Example:

Classes of C_{4v}: $\{E\}$, $\{C_2\}$, $\{C_4, C_4^{-1}\} \equiv 2C_4$,
$\{\sigma_v^1, \sigma_v^2\} \equiv 2\sigma_v$, $\{\sigma_d^1, \sigma_d^2\} \equiv 2\sigma_d$

Side note: # of classes = # irreducible representations

Representation of a group

A group $\mathcal{R} = (R, \cdot)$ is a representation of another group $\mathcal{G} = (G, \circ)$, if there is a one-to-one mapping $M: G \mapsto R$ such that $M(a \circ b) = M(a) \cdot M(b)$ $\forall a, b \in G$.

Of interest here: R: set of n-dimensional square matrices
"$\cdot$": usual matrix multiplication

(1) If a representation Γ consists of $(n \times n)$-matrices, it is called <u>n-dimensional</u>.

(2) Two n-dimensional representations Γ_1, Γ_2 of a group $\mathcal{G}$ are <u>equivalent</u>, if $\exists$ a regular $(n \times n)$-matrix $\mathcal{U}$ s.t. $N(a) = \mathcal{U} \cdot M(a) \cdot \mathcal{U}^{-1}$ $\forall a \in G$ with $N(a) \in \Gamma_1$ and $M(a) \in \Gamma_2$.

(3) A representation Γ is called <u>reducible</u> if it is equivalent to a representation, where all matrices have a common block structure:

$$M(a) = \begin{pmatrix} M_1(a) & 0 \\ 0 & M_2(a) \end{pmatrix}$$

Otherwise, it is called <u>irreducible</u>.

How to determine all irreducible representations of a group? Use

Characters

The character of a group element g in a representation Γ_i is determined by the trace $\chi_i(g) = \mathrm{tr}(D_i(g))$ of its representing matrix $D_i(g)$.

(1) The dimension n_i of a representation Γ_i is given by the character of the idenbity map e: $n_i = \chi_i(e)$.

(2) The number of classes n_c in a given group equals the number of inequivalent irreducible representations.

(3) The characters χ_i of a representation Γ_i are equivalent for all elements in the same class, we can hence arrange all characters in a $(n_c \times n_c)$ character table:

g	$\mathcal{C}_1$	$\cdots$	$\mathcal{C}_{n_c}$	$\leftarrow$ classes
Γ_1	$\chi_1(\mathcal{C}_1)$	$\cdots$	$\chi_1(\mathcal{C}_{n_c})$	
$\vdots$	$\vdots$		$\vdots$	
Γ_{n_c}	$\chi_{n_c}(\mathcal{C}_1)$	$\cdots$	$\chi_{n_c}(\mathcal{C}_{n_c})$	
$\uparrow$ irreps				

(4) To compute character tables, one can use these two identities:

$$\sum_{i=1}^{n_c} \chi_i(\mathcal{C}_q)\, \chi_i^*(\mathcal{C}_{q'}) = \delta_{q,q'}\, N/h_q \qquad (1)$$

$$\sum_{q=1}^{n_c} h_q\, \chi_i(\mathcal{C}_q)\, \chi_{i'}^*(\mathcal{C}_q) = \delta_{i,i'}\, N, \qquad (2)$$

where N is the total number of elements of the group and h_q is the number of elements in the class $\mathcal{C}_q$.

Example: Character table of C_{4v}

We have five classes and hence the same number of irreps:

	C_{4v}	E	C_2	$2C_4$	$2\sigma_v$	$2\sigma_d$
1D	A_1	1	1	1	1	1
	A_2	1	1	1	-1	-1
	B_1	1	1	-1	1	-1
	B_2	1	1	-1	-1	1
2D	E_1	2	-2	0	0	0

- Use (1) for the class $\{E\}$ and use $\chi_i(e) = n_i$ ($\leftarrow$ dimension of irrep Γ_i):

$$n_1^2 + n_2^2 + n_3^2 + n_4^2 + n_5^2 = \frac{\overset{\swarrow \text{ \# of elements of } C_{4v}}{8}}{1} = 8$$

$\Rightarrow$ w.l.o.g. $n_1 = n_2 = n_3 = n_4 = 1$ and $n_5 = 2$.

- Each group has a trivial representation with $D(g) = 1 \quad \forall g \in G$

$\Rightarrow \quad \chi_{\text{trivial}}(g) = \operatorname{tr}(D(g)) \overset{1D}{=} 1 \Rightarrow$ trivial row (w.l.o.g. the first)

- Use (1) and (2) to determine the other entries (lengthy task).

Side note: One can determine whether a given representation is irreducible or not by computing its characters. If they coincide with a row in the character table, it is.

Basis functions of irreducible representations

We want basis functions (best computed in real space) $f_i(r_1 - r_2)$ which transform as an irreducible representation of the point group (in this case C_{4v})

For this we use that the operator

$$P(\Gamma_i) = \sum_{g \in \mathcal{G}} \chi_i^*(g)\, g$$

projects out the contribution of a trial wave-function, which transforms as the irrep Γ_i.

To classify the basis functions according to their extent in real-space, we use the trial wave-functions

$$\phi^{start}(\vec{x}) \in \{ \delta_{\vec{x}, \vec{e}_x} , \delta_{\vec{x}, \vec{e}_x + \vec{e}_y} , \delta_{\vec{x}, 2\vec{e}_x} , \dots \}$$

For the irrep E_1, we need a second, linear-independent trial wave-function, as this irrep is two-dimensional. We use

$$\phi_2^{start}(\vec{x}) \in \{ \delta_{\vec{x}, \vec{e}_y} , \delta_{\vec{x}, -\vec{e}_x + \vec{e}_y} , \delta_{\vec{x}, 2\vec{e}_y} , \dots \} .$$

Some comments

- The phrase "a function f transforms as (or according to) the irreducible representation Γ_i of the group $\mathcal{G}$" means

$$g\, f = D_i(g)\, f \qquad \forall\, g \in \mathcal{G}$$

where $D_i(g)$ is the representing matrix of the group element g in the irreducible representation Γ_i.
This means in particular that functions with this property can be used to build a basis for the representation Γ_i.

- An alternative to the notation Γ_i to label irreducible representations of point groups are the "Mullikan symbols" alredy used in the character table for C_{4v} above. They work as follows (only relevant parts for C_{4v} here):

  - One-dimensional representations are labelled either A or B.
    Two- " E.

  - One-dimensional representations which are symmetric with respect to rotation about $2\pi/n$ (i.e. $\chi(C_n) = 1$) are labelled A;
    those which are anti-symmetric (i.e. $\chi(C_n) = -1$) are labelled B.

  - there are more conventions...

Explicit calculations

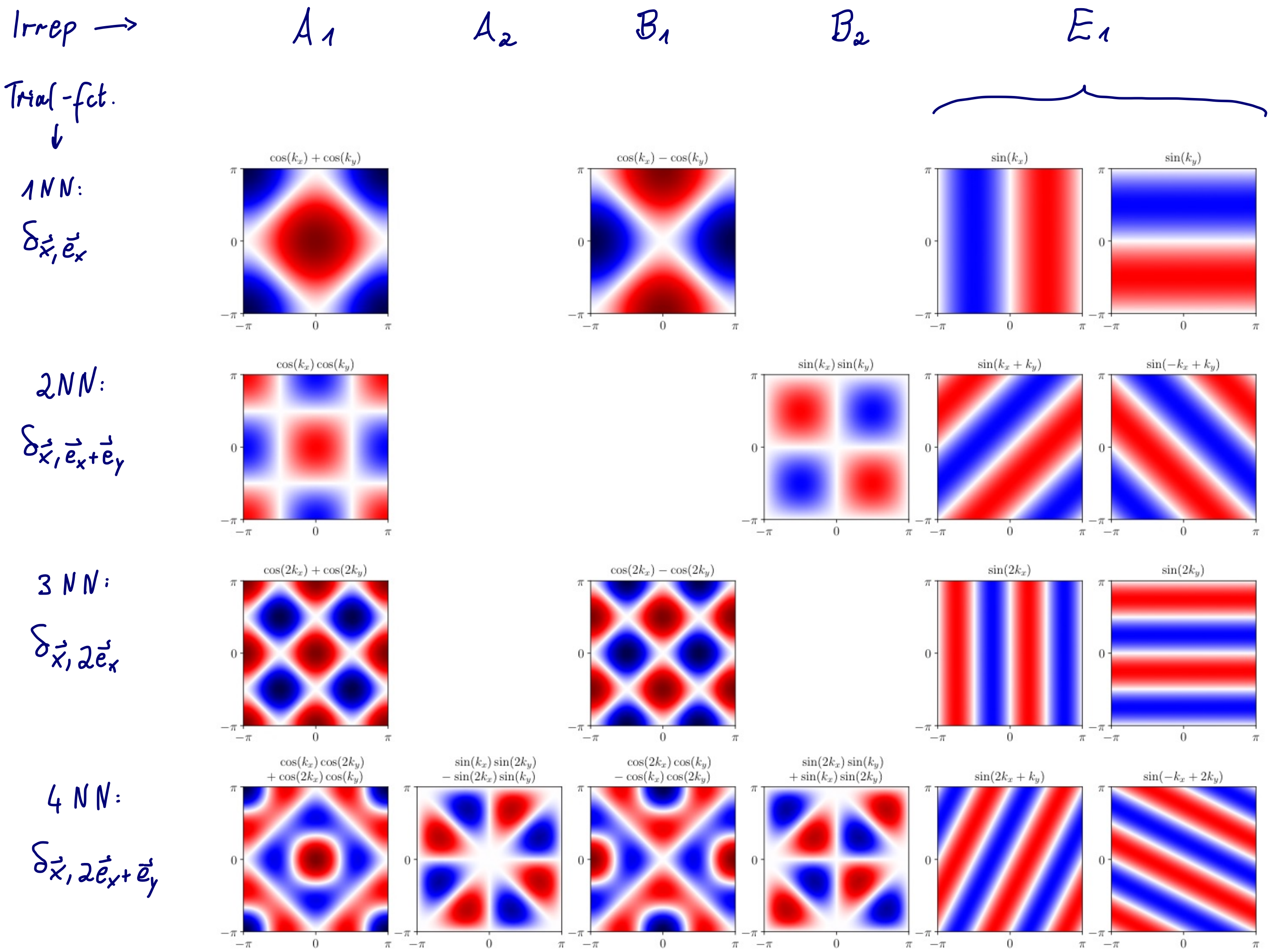
1. NN $\quad \phi^{start} = \delta_{\vec{x},\vec{e}_x}$

$$
\begin{aligned}
\mathcal{P}(A_1)\,\phi^{start}(\vec{x}) = \quad & \chi^*_{A_1}(E)\ \delta_{\vec{x},\vec{e}_x} && \text{identity} \\
+ & \chi^*_{A_1}(C_2)\ \delta_{\vec{x},-\vec{e}_x} && \text{rotation by } \pi \\
+ & \chi^*_{A_1}(C_4)\ \delta_{\vec{x},\vec{e}_y} && \text{rotation by } \pi/2 \\
+ & \chi^*_{A_1}(C_4^{-1})\ \delta_{\vec{x},-\vec{e}_y} && \text{rotation by } -\pi/2 \\
+ & \chi^*_{A_1}(\sigma_v^1)\ \delta_{\vec{x},\vec{e}_x} && \text{reflection about the horizontal axis} \\
+ & \chi^*_{A_1}(\sigma_v^2)\ \delta_{\vec{x},-\vec{e}_x} && \text{\%} \quad \text{vertical} \quad \text{\%} \\
+ & \chi^*_{A_1}(\sigma_d^1)\ \delta_{\vec{x},-\vec{e}_y} && \text{\% the first diagonal} \\
+ & \chi^*_{A_1}(\sigma_d^2)\ \delta_{\vec{x},\vec{e}_y} && \text{\%} \quad \text{second} \quad \text{\%}
\end{aligned}
$$

all characters are one for A_1 $\quad = 2\left(\delta_{\vec{x},\vec{e}_x} + \delta_{\vec{x},-\vec{e}_x} + \delta_{\vec{x},\vec{e}_y} + \delta_{\vec{x},-\vec{e}_y}\right)$

This expression now needs to be transformed to momentum space (and normalized) to yield the form-factor $\cos(K_x) + \cos(K_y)$.

Continuing this procedure for the other representations and for other trial-functions generates the complete set of form-factors, see next page.



(not all normalized)