3. Characters of a representation

Def: CHARACTER The character of the matrix representation $\chi^j(R)$ for a symmetry operation R is the trace of the matrix representation $\Gamma^j(\hat{R})$

$$\chi^j(R) = Tr\{\Gamma^j(\hat{R})\} = \sum_{\mu=1}^{l_j} \Gamma^j_{\mu\mu}(\hat{R})$$

Notice: - the character does NOT distinguish among equivalent representation

- the character is associated to a CLASS of symmetry operations $\mathcal{C}_R$.

proof: Given 2 matrices A and B $Tr\{AB\} = Tr\{BA\}$. It follows that

$Tr\{U^{-1}AU\} = Tr\{UU^{-1}A\} = Tr\{A\}$.

- Γ_1 is equivalent to Γ_2 if $\Gamma_1(\hat{R}) = U^{-1}\Gamma_2(\hat{R})U \ \forall R \in \mathcal{G}$

$\Rightarrow \quad \chi^1(\hat{R}) = \chi^2(\hat{R})$

- $S \in \mathcal{C}_R$ if $\exists T \in \mathcal{G}: \ S = T^{-1}RT \Rightarrow \Gamma(\hat{S}) = \Gamma(\hat{T})^{-1}\Gamma(\hat{R})\Gamma(\hat{T})$

$\Rightarrow \quad \chi^\Gamma(\hat{S}) = \chi^\Gamma(\hat{R})$

The character capture a more general property of the representations with respect to the single matrix element

By applying the WOT we can establish several connections between the concepts of character, class and irreducible representation:

3.1 Basic theorems on characters

Theorem The sum over the group elements of the modulus square of the characters of an irreducible representation equals the order of the group.

proof:

$$\sum_{R\in\mathcal{G}} \sqrt{\frac{l_j}{h}}\,\Gamma^{j}_{\mu\nu}(\hat{R})\sqrt{\frac{l_{j'}}{h}}\,\Gamma^{j'\,*}_{\mu'\nu'}(\hat{R}) = \delta_{jj'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

we set $j=j'$ $\mu=\nu$ $\mu'=\nu'$ and $\sum_{\mu\mu'}$

$$\frac{l_j}{h}\sum_{R\,\mu\mu'} \Gamma^{j}_{\mu\mu}(\hat{R})\,\Gamma^{j\,*}_{\mu'\mu'}(\hat{R}) = \sum_{\mu\mu'}(\delta_{\mu\mu'})^2$$

$$\frac{\cancel{l_j}}{h}\sum_{R}\left|\chi^j(\hat{R})\right|^2 = \cancel{l_j} \quad\Rightarrow\quad \sum_{k=1}^{N_k} c_k\left|\chi^j(\mathcal{C}_k)\right|^2 = h\,.$$

where we have introduced the number of classes N_k, the order of the class c_k and the class $\mathcal{C}_k$.

Notice: The result of the theorem above can be used to check the reducible nature of a representation.

Theorem First orthogonality theorem for characters

Let's consider 2 irreducible representations Γ^j and $\Gamma^{j'}$ associated to the group $\mathcal{G}$. The following orthogonality relation among their characters holds:

$$\sum_{k=1}^{N_c}\sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k)\sqrt{\frac{c_k}{h}}\,\chi^{j}(\mathcal{C}_k)^* = \delta_{jj'}$$

proof: We start again from WOT

$$\sum_{R\in\mathcal{G}}\sqrt{\frac{l_j}{h}}\,\Gamma^{j}_{\mu\nu}(\hat{R})\sqrt{\frac{l_{j'}}{h}}\,\Gamma^{j'\,*}_{\mu'\nu'}(\hat{R}) = \delta_{jj'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

$\mu=\nu$ $\mu'=\nu'$

$$\frac{\cancel{l_j}}{h}\sum_{R\in\mathcal{G}}\chi^j(\hat{R})\,\chi^{j'}(\hat{R})^* = \delta_{jj'}\cancel{l_j}$$

$$\sum_{k=1}^{N_k}\frac{c_k}{h}\,\chi^j(\mathcal{C}_k)\,\chi^{j'}(\mathcal{C}_k)^* = \delta_{jj'}$$

The first orthogonality theorem for classes allows to make a fundamental statement about the number of irreducible representations

Theorem : The number of non-equivalent irreducible repr. associated to a finite order group equals the number of classes contained into the group.

proof The first orthogonality theorem for characters is conveniently rewritten as:

$$(v^{j'}, v^{j}) = \delta_{jj'}$$

having introduced the vectors v^j in $\mathbb{C}^{N_k}$ with elements:

$$v^j_k = \sqrt{\frac{c_k}{h}}\, \chi^j(\mathcal{C}_k)$$

It follows immediately, for the number of non-equivalent irrepr. N_{ir}

$$N_{ir} \leqslant N_k$$

since orthogonal vectors are linearly independent and $\mathbb{C}^{N_k}$ is a vector space of dimension N_k.

Let's now assume $N_{ir} < N_k$ => it is possible to construct a vector v^{red} such that $(v^{red}, v^j) = 0 \quad \forall j : \Gamma^j$ is irreducible.

But, by definition

$$\Gamma^{red}(\hat{R}) = \bigoplus_{j=1}^{N_{ir}} \alpha_i \Gamma^j \Rightarrow \chi^{red}(\mathcal{C}_k) = \sum_{j=1}^{N_{ir}} \alpha_j \chi^j(\mathcal{C}_k)$$

$$v^{red} = \sum_j \alpha_j v^j$$ in contraddiction with $(v^{red}, v^j) = 0$

$\forall j = 1 \dots N_{ir}$

=> $N_{ir} = N_k$

■

Theorem <u>Second orthogonality theorem for characters</u>

Let's take a finite order group $\mathcal{G}$ with its N_K classes and its N_{ir} irreducible representations. It holds that:

$$\sum_{j=1}^{N_{ir}} \sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k)\,\sqrt{\frac{c_{k'}}{h}}\,\chi^j(\mathcal{C}_{k'})^* = \delta_{kk'}$$

<u>proof</u>:

Using the notation introduced in the previous theorem, out of the $N_{ir}=N_K$ orthogonal vectors v^j we can construct the square matrix Q whose element Q_{ik} reads:

$$Q_{ik} = \sqrt{\frac{c_k}{h}}\,\chi^i(\mathcal{C}_k)$$

$$\Rightarrow (Q^+)_{kj} = Q_{jk}^* = \sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k)^*$$

The first orthogonality theorem for characters reads, in this notation

$$QQ^+ = \mathbb{1} \qquad (QQ^+)_{ij} = \sum_{k=1}^{N_K} Q_{ik}\,Q_{jk}^* = \delta_{ij}$$

The relation above implies that $|\det Q| = 1 \Rightarrow Q^{-1} = Q^+ . \Rightarrow Q^+Q = \mathbb{1}$

In components

$$(Q^+Q)_{k'k} = \sum_{j=1}^{N_{ir}} (Q^+)_{k'j}\,Q_{jk} = \sum_{j=1}^{N_{ir}} Q_{jk'}^*\,Q_{jk} = \delta_{k'k}$$

or, in other terms:

$$\sum_{j=1}^{N_{ir}} \sqrt{\frac{c_{k'}}{h}}\,\chi^j(\mathcal{C}_{k'})^*\,\sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k) = \delta_{k'k}$$

■

An interesting consequence of the previous theorem is given in the following corollary.

Corollary: The sum of the squares of the dimensions of the irreducible representations equals the order of the group.

$$\sum_{j=1}^{N_{ir}} \ell_j^2 = h$$

proof:

from the second orthogonality theorem for characters:

$$\sum_{j=1}^{N_{ir}} \sqrt{\frac{C_k}{h}}\, \chi^j(\mathcal{C}_k) \sqrt{\frac{C_{k'}}{h}}\, \chi^j(\mathcal{C}_{k'})^* = \delta_{kk'} \quad (*)$$

Let's assume $k=k'$ to be the class of the identity $\mathcal{C}_E = E \Rightarrow C_k = 1$

Since $\Gamma^j(E) = \mathbb{1}_{\ell_j} \Rightarrow \chi^j(E) = \ell_j$. By combining these observations with $(*)$ we obtain the thesis of the corollary. ■

There is a bunch of useful observation which we can deduce from the previous theorems.

+ Criteria of irreducibility
  - Orthogonality relation for characters
  - $\sum_R |\chi^j(R)|^2 = h$

+ Maximal dimension of irrep. $\sum_j \ell_j^2 = h \Rightarrow \ell_j < \sqrt{h}$
+ All irrep of Abelian groups have dimension 1. $N_k = N_{ir} = h \quad \sum_j \ell_j^2 = h$.
+ Two irreducible repr. are equivalent iff they share the same characters.

proof: $\{\chi^i(\mathcal{C}_k)\} = \{\chi^j(\mathcal{C}_k)\} \Rightarrow v_k^i = \sqrt{\frac{C_k}{h}}\, \chi^i(\mathcal{C}_k) = \sqrt{\frac{C_k}{h}}\, \chi^j(\mathcal{C}_k) = v_k^j$

but if $\Gamma^j \not\approx \Gamma^i \Rightarrow (v^i, v^j) = 0$ which contradicts $v^j = v^i$

Viceversa relies on the cyclic property of the trace. ■

<u>Theorem</u> Let's consider a reducible representation $\Gamma(\hat{R})$ $R \in \mathcal{G}$. By definition of reducibility we can write:

$$\Gamma(\hat{R}) = \bigoplus_{j=1}^{N_{ir}} \alpha_j \Gamma^j(\hat{R}) \qquad (*)$$

where $\alpha_i \in \mathbb{N}^+$ indicates how many times is Γ^j contained in Γ.

The coefficients α_j are unique and can be calculated as:

$$\alpha_j = \sum_{k=1}^{N_K} \frac{c_k}{h} \chi^j(\mathcal{C}_k)^* \chi^\Gamma(\mathcal{C}_k) \qquad (**)$$

where $\{\chi^\Gamma(\mathcal{C}_k)\}$ is called the character set of the representation Γ and (**) is called <u>REDUCTION FORMULA</u>.

<u>proof</u>

From (*) we immediately deduce $\chi^\Gamma(\mathcal{C}_k) = \sum_{j'=1}^{N_{ir}} \alpha_{j'} \chi^{j'}(\mathcal{C}_k)$. We can use the second orthogonality theorem for characters:

$$\sum_{j'=1}^{N_{ir}} \alpha_{j'} \chi^{j'}(\mathcal{C}_k) \chi^j(\mathcal{C}_k)^* \frac{c_k}{h} = \sum_{j'=1}^{N_{ir}} \alpha_{j'} \delta_{jj'} = \alpha_j$$

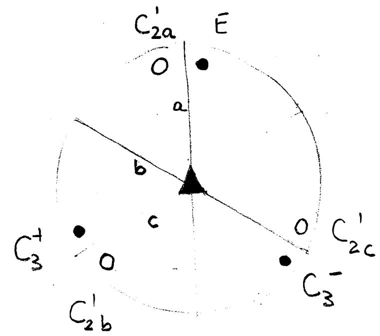
The uniqueness stems from the fact Γ^i is an orthonormal basis in $\mathbb{C}^{N_c}$

3.2 Character tables

A character table is, in its essence, a square table with N columns for the classes and N rows for the irreducible representations containing the characters for all possible combinations (class, irrep) associated to a given group. Example for D_3

N_k ↓ classes ←

		E	$2C_3$	$3C_2'$
irreducible representation	Γ_1	1	1	1
	Γ_2	1	1	-1
	Γ_3	2	-1	0



For analyzing the classes it is usefull to construct the table associating $(g_1, g_2) \to g_2^{-1} g_1 g_2$

conj	E	C_3^+	C_3^-	C_{2a}'	C_{2b}'	C_{2c}'
E	E	E	E	E	E	E
C_3^+	C_3^+	C_3^+	C_3^+	C_3^-	C_3^-	C_3^-
C_3^-	C_3^-	C_3^-	C_3^-	C_3^+	C_3^+	C_3^+
C_{2a}'	C_{2a}'	C_{2b}'	C_{2c}'	C_{2a}'	C_{2c}'	C_{2b}'
C_{2b}'	C_{2b}'	C_{2c}'	C_{2a}'	C_{2c}'	C_{2b}'	C_{2a}'
C_{2c}'	C_{2c}'	C_{2a}'	C_{2b}'	C_{2b}'	C_{2a}'	C_{2c}'

This table can be constructed from the projection diagram or remembering (we will return to it) that conjugation transforms the symmetry element correspondingly. i.e. $B^{-1}AB$ is the symmetry operation associated to $B(A)$.

The character tables for all common groups are listed in books and articles. They can be though derived without explicit calculation of the matrix representatives. Let's make two examples:

$\boxed{D_3}$ The dihedral group D_3

- Order of the group $h = 6$
- Number of classes $N_K = 3$ $E \quad 2C_3 \quad 3C_2'$

Every group admits the trivial irreducible representation of dimension 1

$$6 = \sum_{j=1}^{N_{IR}} l_j^2 = 1 + l_2^2 + l_3^2$$

If $l_j < 3$ since $3^2 = 9 > 6$ order of the group. We can write

$n_i = \#$ IR of dimension i

$$\begin{cases} n_1 + n_2 = 3 \\ n_1 + 4n_2 = 6 \end{cases}$$

$\Rightarrow \quad n_2 = 1$ and $n_1 = 2$.

We can already fill up the first column and row of the character table of D_3

D_3	E	$2C_3$	$3C_2'$
Γ_1	1	1	1
Γ_1'	1	1	-1
Γ_2	2		

Bethe notation.

We can proceed further remembering that

$$1 = \chi^{\Gamma_1'}(E) = \chi^{\Gamma_1'}(C_2'^2) = \left(\chi^{\Gamma_1'}(C_2')\right)^2 \Rightarrow \chi^{\Gamma_1'}(C_2') = \pm 1$$

$$\chi^{\Gamma_1'}(C_3^2) = \chi^{\Gamma_1'}(C_3^-) = \chi^{\Gamma_1'}(C_2' C_3^+ C_2') =$$

$$= \chi^{\Gamma_1'}(C_2')^2 \chi^{\Gamma_1'}(C_3^+) = \chi^{\Gamma_1'}(C_3^+) = 1$$

The first orthogonality theorem for characters further implies.

$$1 + 2 + 3 \cdot 1 \cdot \chi^{\Gamma_2'}(C_2') = 0 \Rightarrow \chi^{\Gamma_2'}(C_2') = -1.$$

D_3	E	$2C_3$	$3C_2'$
Γ_1	1	1	1
Γ_1'	1	1	-1
Γ_2	2	-1	0

The last two entries can be completed using the second orthogonality theorem for characters.

$\boxed{C_n}$

- The group is Abelian $\Rightarrow$ each element is a class $\Rightarrow N_k = N_{IR} = h = n$
- Using the relation $\sum_{i=1}^{n} l_i^2 = n$ with $l_i > 0 \Rightarrow l_i = 1 \ \forall i$
- $C_n^n = E$. Having to do with 1D representations $\left(\chi^j(C_n)\right)^n = 1$

  $\Rightarrow \chi^{\Gamma_j}(C_n) = e^{i\frac{2\pi}{n}j}$ $j = 1, \dots, n$ These n different solutions of the equation are the n different matrix representatives of the element C_n.
- $\chi^j(C_n^m) = e^{i\frac{2\pi}{n}mj}$ which is associated to the unitary matrix

$$Q_{jm} = \frac{1}{\sqrt{n}} e^{i\frac{2\pi}{n}mj}$$ fulfilling all orthogonality relations.

$j = n$ is the trivial representation. $m = n$ is the identity class.

Irreducible representations are classified with different nomenclatures
The Mulliken notation is the one mostly used in atomic and molecular physics.

IR	conditions
A	$l=1$ $\chi(C_n)=1$ ($\chi(S_n)=1$ in case $C_n \notin \mathcal{G}$)
B	$l=1$ $\chi(C_n)=-1$ ($\chi(S_n)=-1$ in case $C_n \notin \mathcal{G}$)
A_1 or B_1	$l=1$ $\chi(C_2')=1$ ($\chi(\sigma_v)=1$ in case $C_2' \notin \mathcal{G}$)
A_2 or B_2	$l=1$ $\chi(C_2')=-1$ ($\chi(\sigma_v)=-1$ in case $C_2' \notin \mathcal{G}$)
E	$l=2$ E comes from German Entartet
T	$l=3$
A' or B' or E' or T'	$l=1,2,3$ $\chi(\sigma_h)>0$
A'' or B'' or E'' or T''	$l=1,2,3$ $\chi(\sigma_h)<0$
A_g or B_g or E_g or T_g	$l=1,2,3$ $\chi(i)>0$
A_u or B_u or E_u or T_u	$l=1,2,3$ $\chi(i)<0$

Examples D_3

	E	$2C_3$	$3C_2'$
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

D_{3h}

	E	$2C_3$	$3C_2'$	σ_h	$2S_3$	$3\sigma_v$
A_1'	1	1	1	1	1	1
A_2'	1	1	-1	1	1	-1
E'	2	-1	0	2	-1	0
A_1''	1	1	1	-1	-1	-1
A_2''	1	1	-1	-1	-1	1
E''	2	-1	0	-2	1	0

The example of the character table $D_{3h} = D_3 \otimes C_\sigma$ brings forward the natural questions about the characters of:

i) The direct product of 2 subgroups

ii) The direct product of 2 irreducible representations.

Theorem If $\mathcal{G} = \mathcal{G}_a \otimes \mathcal{G}_b$ is the direct product of 2 finite order subgroups and Γ^a and Γ^b are irrep of $\mathcal{G}_a$ and $\mathcal{G}_b$ => the representation

$$\Gamma(AB) = \Gamma^a(A) \otimes \Gamma^b(B) \qquad (*).$$

is an irreducible representation for $\mathcal{G}$. Moreover, every irrep. of $\mathcal{G}$ is equivalent to a representation written in the form (*)

proof: In order to prove that Γ is irreducible we can use the criterion $\sum_{R\in\mathcal{G}} |\chi^\Gamma(R)|^2 = h$ the order of $\mathcal{G}$.

The order of $\mathcal{G}$. $h = h_a h_b$ if $h_{a/b}$ is the order of $\mathcal{G}_{a/b}$. In fact $A_1B_1 \neq A_2B_2$ if $A_1 \neq A_2$ or $B_1 \neq B_2$. Otherwise $E = A_2^{-1}A_1B_1B_2^{-1}$.

$$\chi^\Gamma(AB) = \sum_{\mu\nu} \left(\Gamma^a(A) \otimes \Gamma^b(B)\right)_{\mu\nu,\mu\nu} = \sum_{\mu\nu} \Gamma^a_{\mu\mu}(A)\, \Gamma^b_{\nu\nu}(B) = \chi^a(A)\chi^b(B)$$

$$\sum_{R\in\mathcal{G}} |\chi^\Gamma(R)|^2 = \sum_{A\in\mathcal{G}^a\, B\in\mathcal{G}^b} |\chi^a(A)\chi^b(B)|^2 = \sum_{A\in\mathcal{G}^a} |\chi^a(A)|^2 \sum_{B\in\mathcal{G}^b} |\chi^b(B)|^2 = h_a h_b$$

Viceversa we can show that $\Gamma^a(A) \otimes \Gamma^b(B)$ varying a and b exhaust all possible irreducible representations since they are orthogonal and:

$$\sum_{ab} |\chi^\Gamma(E)|^2 = \sum_a |\chi^a(E)|^2 \sum_b |\chi^b(E)|^2 = \sum_a l_a^2 \sum_b l_b^2 = h_a h_b.$$

The direct product of 2 irreducible representations of the same group $\mathcal{C}$ is defined as:

$$\Gamma^{j\otimes j'}(R) = \Gamma^{j}(R) \otimes \Gamma^{j'}(R)$$

From which we obtain, following the same line of thoughts as for $\Gamma^{a} \otimes \Gamma^{b}$

$$\chi^{j\otimes j'}(R) = \chi^{j}(R)\,\chi^{j'}(R)$$

which is, in general, the set of characters of an irreducible representation

Example: $D_3^{E\otimes E}$: $\chi^{E\otimes E} = \{4 \quad 1 \quad 0\}$, using the reduction formula we obtain.

$$\alpha_{A_1} = \frac{1}{6}\left(4\cdot 1\cdot 1 + 1\cdot 1\cdot 2 + 0\cdot 1\cdot 3\right) = 1$$

$$\alpha_{A_2} = \frac{1}{6}\left(4\cdot 1\cdot 1 + 1\cdot 1\cdot 2 + 0\cdot(-1)\cdot 3\right) = 1$$

$$\alpha_{E} = \frac{1}{6}\left(4\cdot 2\cdot 1 + 1\cdot(-1)\cdot 2 + 0\cdot 0\cdot 3\right) = 1$$

$$E\otimes E = A_1 \oplus A_2 \oplus E$$