3. Character of a representation

CHARACTER

Def: The character of the matrix representation $\chi^{\Gamma_j}(R)$ for a symmetry operation R in a representation $\Gamma_j(R)$ is the trace of the matrix of the representation.

$$\chi^{j}(R) = \text{trace}\ \Gamma_j(R) = \sum_{\mu=1}^{l_j} \Gamma^{j}_{\mu\mu}(R)$$

Notice that the trace of a matrix is invariant under similarity transformation => the character does not distinguish between equivalent representations. Also, within one representation, all elements of a class will have the same character. (exercise) This property was defined by van Vleck as "the great beauty of characters".

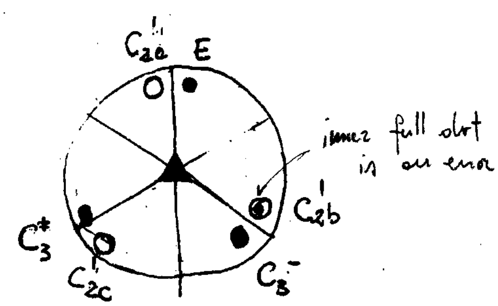
Now we are ready to combine the concept of irreducible representations and the one of character in the celebrated

CHARACTER TABLE for D_3

number of elements in the class

	E	$3C_2'$	$2C_3$ ← classes
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

irreducible representations



$$C_{2a}' = C_3^+ C_{2b}' C_3^- = C_3^- C_{2c}' C_3^+ \qquad \text{remembering } C_3^+ = (C_3^-)^{-1}$$

$$C_3^+ = C_{2b}'^{-1} C_3^- C_{2b}' = (C_{2a}')^{-1} C_3^- C_{2a}' = (C_{2c}')^{-1} C_3^- C_{2c}'$$

A few fundamental properties of the characters:

i) The sum of the squares of the characters is equal to the order of the group

proof:

$$\sum_R \sqrt{\frac{\ell_j}{h}}\, \Gamma^{j}_{\mu\nu}(R) \sqrt{\frac{\ell_{j'}}{h}}\, \Gamma^{j'}_{\mu'\nu'}{}^{*}(R) = \delta_{jj'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

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

$$\frac{\cancel{\ell_j}}{h} \sum_{R,\mu\nu} \Gamma^{j}_{\mu\mu}(R)\, \Gamma^{j}_{\mu'\mu'}(R) = \sum_{\mu\mu'} \delta_{\mu\mu'} = \cancel{\ell_j}$$

$$\sum_R \left|\chi^j(R)\right|^2 = h \qquad \blacksquare$$

ii) First orthogonality theorem for characters:

$$\frac{1}{h} \sum_{k=1}^{N_c} c_k\, \chi^j(C_k)\, \chi^{j'}(C_k) = \delta_{jj'}$$

proof

$$\sum_R \sqrt{\frac{\ell_j}{h}}\, \Gamma^{j}_{\mu\nu}(R) \sqrt{\frac{\ell_{j'}}{h}}\, \Gamma^{j'}_{\mu'\nu'}{}^{*}(R) = \delta_{jj'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'}$$

$\mu = \nu$ $\mu' = \nu'$ $\sum_{\mu\mu'}$

$$\frac{1}{h} \sum_R \chi^j(R)\, \chi^{j'*}(R) = \delta_{jj'}$$

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

but the characters are all the same for elements of the same class.

$\blacksquare$

this equation describes the orthogonality of the rows of the character table (if the normalization $\sqrt{c_k}$ is introduced)

iii) The number of irreducible representations is equal to the number of classes.

NOT
$$\sum_{k=1}^{N_k} c_k \, \chi^i(\mathcal{C}_k) \, \chi^j(\mathcal{C}_k)^* = h\,\delta_{ij}$$

$$\sum_{k=1}^{N_k} \underbrace{\left[\sqrt{\frac{c_k}{h}}\,\chi^i(\mathcal{C}_k)\right]^*}_{(v_i)_k} \underbrace{\left[\sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k)\right]}_{(v_j)_k} = \delta_{ij}$$

$i = 1, \dots, N_{ir}$ $\quad N_{ir}$ is the number of irred. repr.

$k = 1, \dots N_k$ $\quad N_k$ is the number of classes.

$\vec{v}_i \perp \vec{v}_j \quad \forall\, i,j$ But since $\vec{v}_i$ is in a vector space of dimension at most N_k one cannot find more than N_k vectors all orthogonal to each others. $\Rightarrow N_{ir} \leq N_k$. On the other hand if $N_{ir} < N_k$ it means that in principle it is possible to construct a reducible representation that is NOT a linear combination of irreducible ones since the characters of a linear combination of representations are the same combination of the irreducible characters. This is absurd

■

It can be proven that if a square complex matrix is composed of a set of orthonormal vectors $\Rightarrow$ the matrix is unitary. The character table with normalized coefficients is thus <u>unitary</u>. Easy: $Q^+Q = \mathbb{1}$ by construction

if $Q = \left(v^{(1)} \middle| v^{(2)} \middle| v^{(3)} \middle| \dots \middle| v^{(N)}\right)$ and $\sum_{k=1}^{N_k} v_k^{(i)*} v_k^{(j)} = \delta_{ij}$

$N = N_k$ $\quad Q$ is square and $v^{(i)}$ are linearly independent $\Rightarrow \det Q \neq 0$

$\Rightarrow \exists\, Q^{-1} \quad \Rightarrow \quad Q^+Q = \mathbb{1} \Rightarrow Q^+ = Q^{-1} \quad \Rightarrow \quad QQ^+ = \mathbb{1}.$

proof of iii): The number of irreducible representations is equal to the number of classes

$$\text{WOT} \Rightarrow \sum_{k=1}^{N_k} c_k \chi^i(\mathcal{C}_k) \chi^j(\mathcal{C}_k)^* = h\,\delta_{ij}$$

conveniently rewritten as

$$\sum_{k=1}^{N_k} \underbrace{\left[\sqrt{\frac{c_k}{h}}\,\chi^i(\mathcal{C}_k)\right]}_{v_k^{(i)}} \underbrace{\left[\sqrt{\frac{c_k}{h}}\,\chi^j(\mathcal{C}_k)\right]^*}_{v_k^{(j)}} = \delta_{ij}$$

$$\sum_{k=1}^{N_k} v_k^{(i)}\, v_k^{(j)*} = \delta_{ij}$$

$v^{(i)}$ and $v^{(j)}$ are orthogonal vectors in $\mathbb{C}^{N_k}$

1) $\Rightarrow$ $N_{i2} \leq N_k$ since there are at maximum N_k mutually orthogonal vectors in $\mathbb{C}^{N_k}$.

2) Let us assume $N_{i2} < N_k$ $\Rightarrow$ I can construct a vector $v^{(i')}$ orthogonal to all others. This vector must contain the caracters of ~~a~~ reducible representation. (due to the Hyp $N_{i2} < N_k$)

$$\Gamma^{red} = \bigoplus_{i=1}^{N_{i2}} \alpha_i \Gamma_i^{in} \Rightarrow \chi(\Gamma^{red}) = \sum_{i=1}^{N_{in}} \alpha_i \chi(\Gamma_i^{in})$$

$$\Rightarrow v_k^{(i')} = \sum_i \alpha_i \chi^i(\mathcal{C}_k^*).$$

iv) Second orthogonality theorem for characters

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

this relation describes the orthogonality of the columns of the character table.

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

$k \in$ Classes
$i \in$ irrepresentations

$$(QQ^+)_{ij} = \sum_k Q_{ik}(Q^+)_{kj} = \sum_k \sqrt{\frac{c_k}{h}}\,\chi^i(\mathcal{C}_k)\,\chi^j(\mathcal{C}_k)^*\sqrt{\frac{c_k}{h}}$$

$$\frac{1}{h}\sum_k c_k\,\chi^i(\mathcal{C}_k)\,\chi^j(\mathcal{C}_k)^* \overset{(ii)}{=} \delta_{ij}$$

In matrix form $QQ^+ = \mathbb{1}_{N_2}$ $\qquad N_2$ = Number of irreducible representations = Nclasses

Q is unitary $\Rightarrow$ also $Q^+Q = \mathbb{1}$

$$(Q^+Q)_{k\ell} = \sum_i (Q^+)_{ki}\,Q_{i\ell} = \delta_{k\ell}$$

$$= \sum_i \sqrt{\frac{c_k}{h}}\,\chi^i(\mathcal{C}_k)^*\,\sqrt{\frac{c_\ell}{h}}\,\chi^i(\mathcal{C}_\ell) = \delta_{k\ell}$$

And, by taking the complex conjugation.

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

$\Rightarrow k=\ell \quad \sum_i c_k|\chi^i(\mathcal{C}_k)|^2 = h \qquad$ and, if $\mathcal{C}_k = E \quad c_k = 1 \quad \chi^i(E) = \ell_i$

$$\sum_i \ell_i^2 = h .$$

There are a number of important consequences of the orthogonality relations that we have just proven.

* Characters tell us if a representation is irreducible or not. Reducible representations do not respect the orthogonality relations we just proved.

* Characters tells us whether or not we have found ALL the irreducible representations.

  D_3 for example has order 6 => it cannot have an irreducible representation of dimension 3.

* A necessary and sufficient condition that 2 irreducible representations are equivalent is that the characters are the same

$$\chi^i = \chi^j \quad \Rightarrow \quad v^i_k \equiv \frac{\sqrt{c_k}}{\sqrt{g}}\chi^i(\mathcal{C}_k) = v^j_k \equiv \frac{\sqrt{c_k}}{\sqrt{g}}\chi^j(\mathcal{C}_k)$$

but 2 non equivalent irreducible representations would generate $\vec{v}^i \perp \vec{v}^j$. The other way is trivial.

* The reduction of any reducible representation into its irreducible constituents is unique.

* The number of irreducible representations for Abelian groups (e.g. C_n) is the number of elements of the group.

$$\sum_j \ell_j^2 = h \quad \Rightarrow \quad \ell_j = 1 \quad \forall j$$

The irreducible representations have all dimension 1.

SETTING UP CHARACTER TABLES

The character tables for all common groups are listed in books and articles. Nevertheless, as an application of the theorems that we have just proven we will now construct the character tables of 2 small groups: D_3 and C_3.

Before starting let us set up a certain number of rules derived from the orthogonality theorems:

$\boxed{A}$ # irr. repr. = # classes

$\boxed{B}$ $\sum_i l_i^2 = h$ $\quad$ l_i is the dimensionality of Γ_i; h is the order of the group.

$\boxed{C}$ There is always a row of ones in the character table for the "identity" representation. For point groups think to the isomorphism to the transformation of (wave)functions and then take the 1-dimensional Hilbert space generated by a spherically symmetrical function.

$\boxed{D}$ The first column of the character table is l_i since it is the trace of $\mathbb{1}_{l_i}$.

$\boxed{E}$ $\forall i : \Gamma_i \neq$ identity $\quad \sum_k c_k \chi^i(\mathcal{C}_k) = 0$

$\boxed{F}$ Normalization or Orthogonalization $\Big\}$ of rows $\quad \sum_k \chi^i(\mathcal{C}_k)\,\chi^{j*}(\mathcal{C}_k)\,c_k = h\,\delta_{ij}$

$\boxed{G}$ Normalization or Orthogonalization $\Big\}$ of columns $\quad \sum_i \chi^i(\mathcal{C}_k)\,\chi^i(\mathcal{C}_l) = \frac{h}{c_k}\,\delta_{kl}$

$\boxed{H}$ $\forall k : \mathcal{C}_k \neq E \quad \sum_i l_i\,\chi^i(\mathcal{C}_k) = 0$

$\boxed{D_3}$ $E \quad 2C_3 \quad 3C_2'$ ← These are the 3 classes. 6 elements in total

- ⟹ 3 irreducible representations
- $6 = 1^2 + ?^2 + ?^2$ solution $1^2 + 1^2 + 2^2$.

Both notation of IR. Only specifies the dimensionality

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

- Orthogonalization rows: $1 \cdot 1 + 2 \cdot ? + 3 \cdot ? = 0$

Remember that $|?| = 1$ since we are speaking of simmetry operations for a 1 dimensional representation.

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

- Orthogonalization columns: $1 \cdot 2 \times 1 + 1 \cdot 2 \times 1 + 2 \cdot 2 \times ? = 0$

$? = -1$

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

$1 \cdot 3 \times 1 + 1 \cdot 3 \times -1 + 2 \cdot 3 \times ? = 0$

$? = 0$

$\boxed{C_3}$ $\quad E \quad C_3^+ \quad C_3^- \longleftarrow$ these are the 3 classes

$\Rightarrow$ 3 irreducible representations all 1 dimensional.

$3 = 1^2 + ?^2 + ?^2$ solution $1^2 + 1^2 + 1^2$

	E	C_3^+	C_3^-
Γ_1	1	1	1
Γ_1'	1	a	b
Γ_1''	1	c	d

$$\left.\begin{aligned} 1 + a + b &= 0 \\ 1 + c + d &= 0 \end{aligned}\right\} \text{row orth}$$

$$\left.\begin{aligned} 1 + a + c &= 0 \\ 1 + b + d &= 0 \end{aligned}\right\} \text{column orth}$$

$$\underbrace{\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}}_{\det = 0.} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ -1 \\ -1 \end{pmatrix}$$

We can use another information coming from the multiplication table.

$$(C_3^+)^2 = C_3^- \quad \text{and} \quad (C_3^+)^3 = E$$

$$a^2 = b \qquad a^3 = 1 \Rightarrow a = \exp\left[i\frac{2\pi}{3}\right]$$

$$b = \exp\left[i\frac{4\pi}{3}\right]$$

	E	C_3^+	C_3^-
Γ_1	1	1	1
Γ_1'	1	ω	ω^2
Γ_1''	1	c	d

$$\omega + c = -1 \Rightarrow c = \omega^2$$

$$\omega^2 + d = -1 \Rightarrow d = \omega$$

Since $\sum_{i=1}^{N} \omega^i = 0$ if $\omega^N = 1$.

	E	C_3^+	C_3^-
Γ_1	1	1	1
Γ_1'	1	ω	ω^2
Γ_1''	1	ω^2	ω

Mulliken Notation for irreducible representations

ℓ	Notation IR	$\chi(C_n)$ or $\chi(S_n)$ if C_n is not there	$\chi(C_2')$ or $\chi(\sigma_v)$	$\chi(\sigma_h)$	$\chi(i)$
1	A	+1			
	B	-1			
1, [redacted]	subscript 1		+1		
	subscript 2		-1		
2	E (entartet)				
3	T				
1, 2 or 3	superscript $'$			+	
	superscript $''$			−	
	subscript g				+
	subscript u				−

example D_3

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

How can we reduce a reducible representation? The basic idea is to use the orthogonality theorems for the characters.

Let's take a generic representation Γ. We know that by definition of irreducible representation

$$\Gamma = \bigoplus_{i=1}^{N_{ir}} c_i \Gamma^i$$

Correspondingly $\chi^{\Gamma}(R) = \sum_{i=1}^{N_{ir}} \alpha_i \chi^{\Gamma^i}(R)$ (*) $\forall R$ in the group.

~~(N.B. c_i has nothing to do with the order of the classes)~~

The relation (*) in page 28 can also be written for classes

$$(**) \qquad \chi^{\Gamma}(\mathcal{C}_k) = \sum_{i=1}^{N_{ir}} \alpha_i \chi^{\Gamma^i}(\mathcal{C}_k) \qquad \forall\, k=1,\dots,N_{\text{classes}}$$

But now we can use the I orthogonality theorem for characters

$$\sum_{k=1}^{N} \sqrt{\frac{c_k}{h}}\, \chi^{\Gamma^i}(\mathcal{C}_k) \sqrt{\frac{c_k}{h}}\, \chi^{\Gamma^j}(\mathcal{C}_k)^* = \delta_{ij} \qquad N = N_{ir} = N_{\text{classes}}$$

We take then $(**)$, multiply by $c_k/h\, \chi^{\Gamma^j}(\mathcal{C}_k)^*$ and sum over k

$$\sum_{k=1}^{N} \frac{c_k}{h} \chi^{\Gamma^j}(\mathcal{C}_k)^* \chi^{\Gamma}(\mathcal{C}_k) = \sum_{i,k=1}^{N} \frac{\alpha_i c_k}{h} \chi^{\Gamma^j}(\mathcal{C}_k)^* \chi^{\Gamma^i}(\mathcal{C}_k)$$

$$= \sum_{i=1}^{N} \alpha_i \delta_{ij} = \alpha_j$$

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

This is called REDUCTION FORMULA. It gives the coefficients of the expansion of a reducible representation in terms of its irreducible components.

the sizes of the blocks is l_j.

$\Gamma(R) =$