Now taking (k, s) element

$$\sum_{A\in G}\sum_{p,q} \Gamma^{(i)}_{kp}(A)\, X_{pq}\, \Gamma^{(i)}_{qs}(A^{-1}) = a\,\delta_{ks}$$

If $X_{pq} = \delta_{pm}\delta_{qn}$

$$\sum_{A\in G} \Gamma^{(i)}_{km}(A)\,\Gamma^{(i)}_{ns}(A^{-1}) = a\delta_{ks}$$

To find a, we trace the matrix N, we get

$$\text{trace } N = a l_i = \sum_{k=1}^{l_i}\sum_{A\in G}\sum_{p,q} \Gamma^{(i)}_{kp}(A)\, X_{pq}\, \Gamma^{(i)}_{qk}(A^{-1})$$

$$= \sum_{pq} X_{pq} \sum_{A\in G}\sum_{k} \Gamma^{(i)}_{qk}(A^{-1})\,\Gamma^{(i)}_{kp}(A)$$

$$= \sum_{pq} X_{pq} \sum_{A\in G} \Gamma^{(i)}(E)$$

$$= g \sum_{pq} X_{pq}\,\delta_{pq} = g \text{ trace } X$$

$$a = g(\text{trace } X)/l_i$$

But trace $X = 0$, unless $m = n$, ~~then~~ in which case trace $X = 1$

trace $X = \delta_{mn}$.

$$\sum_{A\in G} \Gamma^{(i)}_{km}(A)\,\Gamma^{(i)}_{ns}(A^{-1}) = (g/l_i)\,\delta_{ks}\,\delta_{mn},$$

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Now we combine the two results in single equation

$$\sum_{A \in G} \Gamma^{(i)}_{km}(A)\,\Gamma^{(j)}_{ns}(A^{-1}) = (g/l_i)\,\delta_{ij}\,\delta_{ks}\,\delta_{mn}$$

or

$$\sum_{A \in G} \Gamma^{(i)}_{km}(A)\,\Gamma^{(j)*}_{sn}(A) = (g/l_i)\,\delta_{ij}\,\delta_{ks}\,\delta_{mn}$$

This is known as the great orthogonality theorem for I.R. of a group.

Characters of a Representation:-

The traces of all the matrices of a representation would uniquely characterised a representation irrespective of the choice of the basis vectors

Let Γ be a representation of a group G. then character of representation can be written as

$$\chi(A) = \sum \Gamma_{kk}(A) \quad -(1)$$

If representation is one dimensional, then character is the same as the representation The character of conjugate elements in a representation are same because the traces of matrix is invariant under similarity transformation. If A and B are conjugate elements such that $A = C^{-1}BC$, or

$$\Gamma(A) = \Gamma(C^{-1})\,\Gamma(B)\,\Gamma(C)$$

taking the traces of both sides.

$$\mathrm{trace}(\Gamma(A)) = \mathrm{trace}(\Gamma(B))$$

$$\chi(A) = \chi(B)$$

where we have used the cyclic property of traces, that is, for any matrices P, Q and R we have

$$\mathrm{trace}\,(PQR) = \mathrm{trace}(QRP) = \mathrm{trace}\,(RPQ)$$

All the elements in a class thus have the same character in a representation. The character is therefore a function of the classes just as a representation is a function of the group elements

Reduction of a reducible representation: —

we can find the number of times an IR $\Gamma^{(i)}$ occurs in the reduction of Γ. For this we take the traces of both side of eqn

$$\Gamma = \sum_i a_i\,\Gamma^{(i)}. \qquad (1)$$

If $\chi(A)$ ... etc denote the characters of the elements in the representation Γ, then we have

$$\chi(A) = \sum_i a_i\,\chi^{(i)}(A) \qquad (1) \quad \forall \; A \in G$$

Multiplying both sides by $\chi^{(j)*}(A)$ and summing over the elements of G, we get

$$\sum_{A \in G} \chi^{(j)*}(A)\, \chi(A) = \sum_i a_i \sum_{A \in G} \chi^{(j)*}(A)\, \chi^{(i)}(A)$$

$$= a_j g.$$

$$a_j = \frac{1}{g} \sum_{A \in G} \chi^{(j)*}(A)\, \chi(A)$$

This gives a method for obtaining the coefficients in eq. (1). The characters of the irreducible representations are called primitive or simple characters, while the characters of the reducible representation are called compound characters. A compound character can be expressed as a linear combination of the simple character of a group.

A criterion for irreducibility :—

Let Γ be representation with character χ. The character can be written as linear combination of simple character of G with coefficient a_i. Let us multiply eq. $\chi(A) = \sum_i a_i \chi^{(i)}(A)$ by

its complex conjugate equation, and sum over all element of group G and divided by g.

we get

$$\frac{1}{g}\sum_{A\in G}\chi^*(A)\chi(A)=\frac{1}{g}\sum_{ij}a_i^*a_j\sum_{A\in G}\chi^{(i)*}(A)\,\chi^{(j)}(A)$$

$$=\sum_i |a_i|^2$$

If $|a_i|^2$ be unity then a_i be zero except one. the Γ must be identical with IR $\chi^k(A)$. we have simple criterion for the irreducibility of representation. The necessary and sufficient condition will be irreducible and satisfy the condition

$$\sum_{A\in G}\chi^*(A)\chi(A)=g$$

$$\sum_{k} n_k\chi_k^*\chi_k=g$$

where χ_k is the character of the k^{th} class of the group.

The character table of C_{4V}. – Since C_{4V} has five classes it must have five IR. say $\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}, \Gamma^{(4)}$ and $\Gamma^{(5)}$ whose dimensions may be denoted as l_1, l_2, l_3, l_4 and l_5, then

$$l_1^2+l_2^2+l_3^2+l_4^2+l_5^2=8.$$

The possible solution is

$l_1=l_2=l_3=l_4=1$ and

$l_5=2.$

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The character table can be constructed by making use of orthogonality relations as follows

$$\sum \sqrt{\left[\frac{n_k}{g}\right]} \chi_k^{(i)} \sqrt{\left[\frac{n_k}{g}\right]} \chi_k^{(j)*} = \delta_{ij}$$

and $$C_i C_j = \sum_k a_{ijk} C_k$$

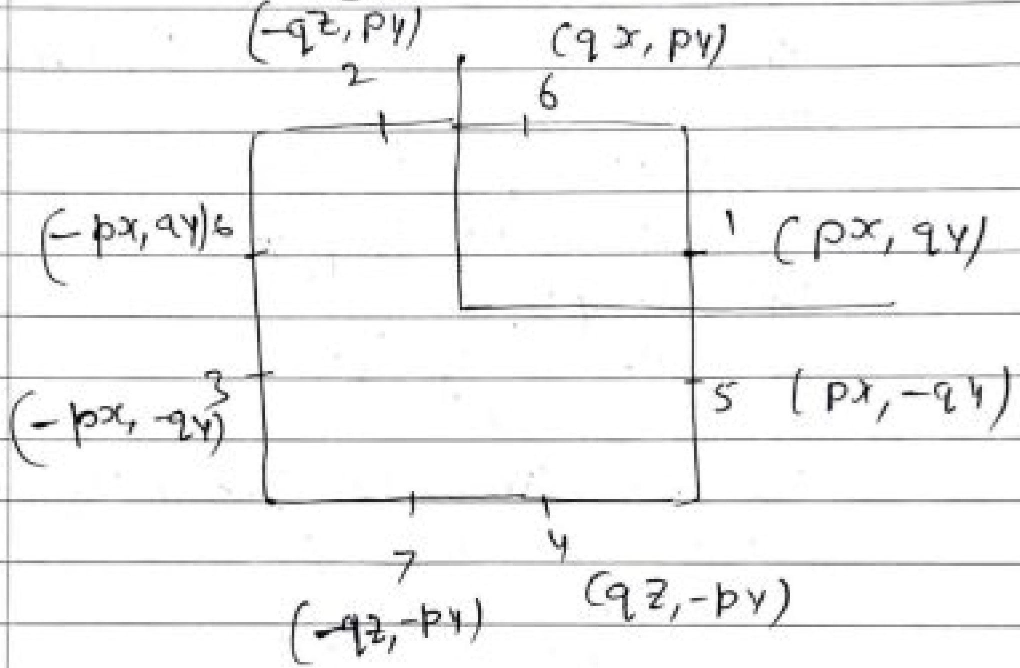
characters \ classes	C_1 (E)	C_2 (C_4, C_4^3)	C_3 (C_4^2)	C_4 (m_x, m_y)	C_5 (σ_u, σ_v)
$\chi^{(1)}$	1	1	1	1	1
$\chi^{(2)}$	1	−1	1	−1	1
$\chi^{(3)}$	1	−1	1	1	−1
$\chi^{(4)}$	1	1	1	−1	−1
$\chi^{(5)}$	2	0	−2	0	0

Symmeterized Basis functions for irreducible representations:-

We shall now study the method for obtaining suitable linear combinations of the basis functions and demostrati of the basis functions and demostrate the use of the method

The matrix representing an element A for basis functions $\{\phi_1 \dots \phi_n\}$ is written as

$$A\phi_i = \sum_{j=1}^{n} \phi_j \Gamma_{ji}(A) \quad (1)$$



The eight function ϕ_i of the positions for C_{4v} can be written as

$$(\phi_1', \phi_2' \dots \phi_8') = C_4(\phi_1, \phi_2, \phi_3 \dots \phi_8)$$
$$= (\phi_1, \phi_2 \dots \phi_8)\, \Gamma^{req}(C_4)$$

Where matrix representing C_4 in the regular representation is shown as above.

In order to reduce Γ, we take unitary representation matrix U

$$U^{-1}\Gamma(A)U = \Gamma_{red.}(A) \quad (2)$$

where $\Gamma_{red}(A)$ have the reduced or block diagonalized form Now eq.(1) in the matrix notation can be written as

$$A\Phi = \Phi\Gamma(A)$$

then U is required transformation, then

$$A\Phi U = \Phi U U^{-1}\Gamma(A)U$$

$$A(\Phi U) = (\Phi U)\Gamma_{red.}(A)$$

Let $\psi = \Phi U_n$

$$\psi_i = \sum_{J=1}^{n}\phi_J U_{Ji} \qquad (3)$$

The proper linear combination ψ_i can be written as

$$\chi^{\alpha}_{pm} = \sum_{i=1}^{n}\phi_i U^{i}_{\alpha pm} \qquad (4)$$

where ψ^{α}_{pm} is the m^{th} basis function for IR, $\Gamma^{(\alpha)}$ occuring for the pth time in the reduction of Γ

$$\Gamma = \sum_{\alpha=1}^{n}a_\alpha\Gamma^{(\alpha)} \qquad (5)$$

for $1 \leq \alpha \leq c$, $1 \leq p \leq a_\alpha$ and $1 \leq m \leq l_\alpha$

As eq (4), same as eq (3), the matrix $[U^{i}_{\alpha pm}]$ is just another label for the matrix $[U_{Ji}]$ as a set of values of (α, pm) denote

* a column of U and value i denotes row of U. Similarly ψ^{α}_{pm} is just another ψ_i. Since the dimension of the matrix on both sides of eq (5), must be the same, then

$$n = \sum_{\alpha=1}^{c} a_{\alpha} l_{\alpha} \qquad (5')$$

Now as the result of the othera operation of an element $A \in G$, on ψ^{α}_{pm} is to give linear combination of l_{α} function which generate IR $\Gamma^{(\alpha)}$ and which define an l_{α}-dimensional invariant subspace of the full space L_n. Thus

$$A\psi^{\alpha}_{pm} = \sum_{k=1}^{l_{\alpha}} \psi^{\alpha}_{pk} \Gamma^{(\alpha)}_{km}(A) \qquad (6)$$

ψ^{α}_{pm} is called transform according to the m^{th} column of IR $\Gamma^{(\alpha)}$. If ϕ_i be orthonogrnonal. Then U must be unitary matrix, and we have

$$\sum_{i=1}^{n} U^{i+}_{\alpha km} U^{i}_{\beta qk} = \delta_{\alpha\beta} \delta_{pq} \delta_{mn}$$

$$\sum_{\alpha pm} U^{i+}_{\alpha km} U^{J}_{\alpha pm} = \delta_{iJ} \qquad (7)$$

operating on both sides of eq(4) we get

$$A\psi^{\alpha}_{pm} = \sum_{i=1}^{n} A\phi_i U^{i}_{\alpha pm}$$

or $$\sum_{k=1}^{l_\alpha} \psi^{\alpha}_{pk} \Gamma^{(\alpha)}_{km}(A) = \sum_{i=1}^{n}\sum_{j=1}^{n} \phi_j \Gamma_{ji}(A) U^{i}_{\alpha pm}$$

Using eq (4) again we get

$$\sum_{k=1}^{l_\alpha}\sum_{s=1}^{n} \phi_s U^{s}_{\alpha pk} \Gamma^{\alpha}_{km}(A) = \sum_{i=j=1}^{n} \phi_j \Gamma_{ji}(A) U^{i}_{\alpha pm}$$

Since ϕ_i is independent, the coefficient on both sides must be equal. This gives

$$\sum_{k=1}^{l_\alpha} U^{s}_{\alpha pk} \Gamma^{(\alpha)}_{km}(A) = \sum_{i=1}^{n} \Gamma_{si}(A) U^{i}_{\alpha pM} \quad (8)$$

$\forall A \in G$, $1 \leq s \leq n$, $1 \leq m \leq l_\alpha$; Now we shall discuss the projection operator technique in next part

Let us apply eq (8) to the spacial case of regular representation. Changing indicis s and i we get

$$\sum_{k=1}^{l_\alpha} U^{B}_{\alpha pk} \Gamma^{(\alpha)}_{km}(A) = \sum_{C\in G} \Gamma^{reg}_{BC}(A) U^{C}_{\alpha pm} = U^{BA}_{\alpha pm}$$

$\forall\ 1 \leq m \leq l_\alpha$ Further for identity element we have $\sum_{k=1}^{l_k} U^{E}_{\alpha p E} \Gamma^{(\alpha)}_{km}(A) = U^{A}_{\alpha p m}$ (9)

This is used to find the matrix for the regular representation.

we shall apply the result to reduce C_{4V} and to determine the symmetrized basis functions for IR

$$\Gamma^{reg} = \Gamma^{(1)} \oplus \Gamma^{(2)} \oplus \Gamma^{(3)} \oplus \Gamma^{(4)} + 2\Gamma^{(5)}$$

For regular relation we take $U^{E}_{\alpha p m} = a$ which can be find by normalization ± 1.

Thus for obtaing two set of basis functions for $\Gamma^{(5)}$, we take

$$U^{E}_{5p1} = a, \quad U^{E}_{5p2} = b$$

we get

A	: E	C_4	C_4^2	C_4^3	m_x	m_y	σ_u	σ_v
U^{A}_{5p1}	: a	$-b$	$-a$	b	a	$-a$	$-b$	b
U^{A}_{5p2}	: b	a	$-b$	$-a$	$-b$	b	$-a$	a

If we choose $p=1$, $p=2$, as $a=a_1$, $b=b_1$ and $a=a_2$, $b=b_2$ respectively then orthogonality

$$a_1 a_2 + b_1 b_2 = 0$$

The matrix U for reduction of Γ^{reg} of C_{4V} (for $a_1=b_1=1$, $a_2=-b_2=1$).

$$\left[U^{A}_{\alpha p m}\right] = \begin{array}{c|cccccccc}
\alpha & 1 & 2 & 3 & 4 & 5 & 5 & 5 & 5 \\
p & 1 & 1 & 1 & 1 & 1 & 1 & 2 & 2 \\
m & 1 & 1 & 1 & 1 & 1 & 2 & 1 & 2 \\
\hline
E & + & + & + & + & + & + & + & - \\
C_4 & + & - & - & + & - & + & + & + \\
C_4^2 & + & + & + & + & - & - & - & + \\
C_4^3 & + & - & - & + & + & - & - & - \\
m_x & + & - & + & + & + & - & + & + \\
m_y & + & - & + & - & - & + & - & - \\
\sigma_u & + & + & - & - & - & - & + & - \\
\sigma_v & + & + & - & - & + & + & - & +
\end{array}$$

where a factor $8^{-1/2}$ is associated with each positive or negative sign.

* Representations of a direct product Group:—

Let $H = \{E = H_1, \ldots H_h\}$ and $G = \{E = G_1 \ldots G_g\}$ such that H_i commute with all G_i. Let this direct product of group of order $k = gh$

$$K = \{E = K_1, \ldots\ldots K_{hg}\}$$

$$K_{ij} = H_i G_j \quad (1)$$

Let $H_i H_m = H_p$ and $G_j G_n = G_q$, then

$$K_{ij} K_{mn} = (H_i G_j)(H_m G_n)$$
$$= (H_i H_m)(G_j G_n)$$
$$= H_p G_p$$
$$= K_{pq}$$