Introduction to Group Theory Note 2 Theory of Representation

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1 Group Representation

In physical application, the group representation plays a very important role in deducing the consequence of the symmetries of the system. Roughly speaking, representation of a group is just some way to realize the same group operation other than the original definition of the group. Of particular interest to most physical application is the realization of group operation by the matrices whose multiplication operation can be naturally associated with group multiplication.

1.1 Definition of Representation

Given a group $G = \{A_i, i = 1 \cdots n\}$. If for each $A_i \in G$, there is an $n \times n$ matrix $D(A_i)$ such that

$$D(A_i)D(A_i) = D(A_iA_i) \tag{1}$$

then D's forms a n-dimensional representation of the group G. In other words, the correspondence $A_i \to D(A_i)$ is a homomorphism. The condition in Eq(1) simply means that the matrices $D(A_i)$ satisfy the same multiplication law as the group elments. If this homomorphism turns out to be an isomorphism (1-1) then the representation iscalled <u>faithful</u>. Note that a matrice M_{ij} can be viewed as linear operators M acting on some vector space V with respect to some choice of basis e_i ,

$$Me_i = \sum_i e_j M_{ji}$$

One way to generate such matrices for the symmetry of certain geometric objects is to use the group induced transformations, discussed before. Recall that each group element A_a will induce a transformation of the coordinate vector \vec{r} ,

$$\vec{r} \rightarrow A_a \vec{r}$$

Then we can take any function of \vec{r} , say $\varphi(\vec{r})$ and for any group element A_a define a new transformation P_{A_a} by

$$P_{A_a}\varphi\left(\vec{r}\right) = \varphi\left(A_a^{-1}\vec{r}\right)$$

Among the transformed functions obtained this way, $P_{A_1}\varphi\left(\vec{r}\right)$, $P_{A_2}\varphi\left(\vec{r}\right)$, $\cdots P_{An}\varphi\left(\vec{r}\right)$, we select the linearly independent set $\varphi_1\left(\vec{r}\right)$, $\varphi_2\left(\vec{r}\right)\cdots\varphi_\ell\left(\vec{r}\right)$. Then it is clear that $P_A\varphi_a$ can be expressed as linear combination of φ_i ,

$$P_{A_i}\varphi_a = \sum_{b=1}^{\ell} \varphi_b D_{ba} \left(A_i \right)$$

and $D_{ba}(A_i)$ forms a representation of G. This can be seen as follows.

$$P_{A_{i}A_{j}}\varphi_{a}=P_{A_{i}}P_{A_{j}}\varphi_{a}=P_{A_{i}}\sum_{b}\phi_{b}D_{ba}\left(A_{j}\right)=\sum_{b,c.}\phi_{c}D_{cb}\left(A_{i}\right)D_{ba}\left(A_{j}\right)$$

On the other hand,

$$P_{A_i A_j} \varphi_a = \sum_{c} \varphi_c D \left(A_i A_j \right)_{ca}$$

This gives

$$D\left(A_{i}A_{j}\right)_{ca} = D_{cb}\left(A_{i}\right)D_{ba}\left(A_{j}\right)$$

which means that $D(A_i)'s$ form representation of the group.

Example: Group D_3 , symmetry of the triangle.

As we have discussed in the previous chapter, choosing a coordinate system on the plane, we can represent the group elements by the following matrices,

$$A = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \qquad B = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \qquad E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$
$$K = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad L = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \qquad M = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

Choose $f(\vec{r}) = f(x,y) = x^2 - y^2$, we get

$$P_A f(\vec{r}) = f(A^{-1}\vec{r}) = \frac{1}{4} (x + \sqrt{3}y)^2 - \frac{1}{4} (\sqrt{3}x - y)^2 = -\frac{1}{2} (x^2 - y^2) + \sqrt{3}xy.$$

We now have a new function g(x,y) = -2xy. We can operate on g(r) to get,

$$P_{A}g\left(\vec{r}\right) = g\left(A^{-1}\vec{r}\right) = 2\left(-\frac{1}{2}\right)\left(x + \sqrt{3}y\right)\frac{1}{2}\left(\sqrt{3x} - y\right) = -\frac{1}{2}\left[\left(\sqrt{3}\right)\left(x^{2} - y^{2}\right) - 2xy\right] = -\frac{\sqrt{3}}{2}\left(x^{2} - y^{2}\right) - \frac{1}{2}\left(2xy\right)$$

Thus we have

$$P_A(f,g) = (f,g) \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

The matrix generated this way is the same as A as given above. Similarly

$$P_{B}f(\vec{r}) = f\left(B^{-1}\vec{r}\right) = \frac{1}{4}\left(x - \sqrt{3}y\right)^{2} - \frac{1}{4}\left(\sqrt{3}x + y\right)^{2} = -\frac{1}{2}\left(x^{2} - y^{2}\right) + \sqrt{3}\left(-xy\right)$$

$$P_{B}g(\vec{r}) = g\left(B^{-1}\vec{r}\right) = -2\left(\frac{1}{2}\right)\left(x - \sqrt{3}y\right)\left(-\frac{1}{2}\right)\left(\sqrt{3}x + y\right) = -\sqrt[4]{\frac{1}{2}}\left[\sqrt[4]{3}\left(x^{2} - y^{2}\right) - 2xy\right] = -\frac{\sqrt{3}}{2}\left(x^{2} - y^{2}\right) - \frac{1}{2}\left(-2xy\right)$$

$$P_{B}\left(f,g\right) = \left(f,g\right) \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

same as B as given before.

Remarks

1. If $D^{(1)}(A)$ and $D^{(2)}(A)$ are both representation of the group, then it is clear that

$$D^{(3)}(A) = \begin{pmatrix} D^{(1)}(A) & 0\\ 0 & D^{(2)}(A) \end{pmatrix}$$
 (block diagonal form)

also forms a representation. We will denote it as a direct sum \oplus ,

$$D^{(3)}(A) = D^{(1)}(A) \oplus D^{(2)}(A)$$
 direct sum

2. If $D^{(1)}(A)$ and $D^{(2)}(A)$ are 2 representations of G with same dimension and there exists a square matrix U such that

$$D^{(1)}(A_i) = UD^{(2)}(A_i)U^{-1}$$
 for all $A_i \in G$.

then $D^{(1)}$ and $D^{(2)}$ are said to be equivalent representations. Recall that if we change the basis used to represent the linear operators, the corresponding matrices undergo similar transformation. Since they represent the same operators, we consider them the "same" representation but with respect to different choice of basis.

1.2 Reducible and Irreducible Representations

A representation D of a group G is called **irreducible** if it is defined on a vector space V(D) which has no non-trivial invariant subspace. Otherwise, it is reducible. In essence this definition simply means that for a reducible representation, the linear opertors corresponding to the group elements will leave some smaller vector space invariant. In other words, all the group actions can be realized in some subspace.

We need to convert these statment into more practical criterion. Suppose the representation D is reducible on the vector space V. Then there exists a subspace S which is invariant under D. For any vector $v \in V$, we can decomposit as,

$$v = s + s_{\perp}$$

where $s \in S$ and s_{\perp} belongs to the complement S_{\perp} of S. If we write the vector v in the block form,

$$v = \begin{pmatrix} s \\ s_{\perp} \end{pmatrix}$$

then the representation matrix can be written as

$$Av = D(A) v = \begin{pmatrix} D_1(A) & D_2(A) \\ D_3(A) & D_4(A) \end{pmatrix} \begin{pmatrix} s \\ s_{\perp} \end{pmatrix}$$

For the space S to be invariant under group operators means that

$$D_3(A_i) = 0, \quad \forall A_i \in G$$

i.e. the matrices $D(A_i)$ are all of the upper triangular form,

$$D(A_i) = \begin{pmatrix} D_1(A_i) & D_2(A_i) \\ 0 & D_4(A_i) \end{pmatrix}, \quad \forall A_i \in G$$
 (2)

A representation is **completely reducible** if all the matrices in the representations $D(A_i)$ can be simultaneously brought into block diagonal form by the same similarity transformation U,

$$UD(A_i)U^{-1} = \begin{pmatrix} D_1(A_i) & 0\\ 0 & D_2(A_i) \end{pmatrix}, \quad \text{for all } A_i \in G$$

i.e. $D_2(A_i) = 0$ in the upper triangular matrices given in Eq (2). In other words, the space complement to S is also invariant under the group operation. This will be the case if the representation matrices are unitary as stated in the theorem;

Theorem: Any **unitary** reducible representation is completely reducible.

Proof: For simplicity we assume that the vector space V is equipped with a scalar product (u, v). It is easy to see in this case we can choose the complement space $S \perp$ to be perpendicular to S, i.e.

$$(u, v) = 0,$$
 if $u \in S, v \in S_{\perp}$

Recall that the scalar product is invariant under the unitary transformation,

$$0 = (u, v) = (D(A_i) u, D(A_i) v)$$

Thus if $D(A_i)u \in S$, then $D(A_i)v \in S_{\perp}$ which implies that S_{\perp} is also invariant under the group operation. In physical applications, we deal mostly with unitary representations and they are completely reducible.

1.3 Unitary Representation

Since unitary operators preserve the scalar product of a vector space, representation by unitary matrices will simplify the analysis of group theory. In the realm of finite groups, it turns out that we can always transform the representation into unitary one. This is the content of the following theorem.

Fundamental Theorem

Every irrep of a finite group is equivalent to a unitary irrep (rep by unitary matrices)

<u>Proof</u>:

Let $D(A_r)$ be a representation of the group $G = \{E, A_2 \cdots A_n\}$

Consider the sum

$$H = \sum_{r=1}^{n} D(A_r) D^{\dagger}(A_r)$$
 then $H^{\dagger} = H$

Since H is positive semidefinite, we can define squre root h by

$$h^2 = H$$
, $h^{\dagger} = h$

Define new set of matrices by

$$\bar{D}(A_r) = h^{-1}D(A_r)h$$
 $r = 1, 2, \dots, n$

Since this is a similarity transformation, $\bar{D}(A_r)$ also forms a rep which is equivalent to $D(A_r)$. We will now demonstrate that $\bar{D}(A_r)$ is unitary,

$$\bar{D}(A_r)\bar{D}^{\dagger}(A_r) = \left[h^{-1}D(A_r)h\right] \left[hD^{\dagger}(A_r)h^{-1}\right] = h^{-1}D(A_r)\sum_{s=1}^{n} \left[D(A_s)D^{\dagger}(A_s)\right]D^{\dagger}(A_r)h^{-1}$$

$$= h^{-1}\left[\sum_{s=1}^{n}D(A_rA_s)D^{\dagger}(A_rA_s)\right]h^{-1} = h^{-1}\sum_{s'=1}^{n}D(A_{s'})D^{\dagger}(A_{s'})h = h^{-1}h^2h = 1$$

where we have used the rearrangement theorem.

2 Schur's Lemma

One of the most important theorems in the study of the irreducible reprentation is the following lemma.

Schur's Lemma

(i) Any matrix which commutes with all matrices of irrep is a multiple of identity matrix.

Proof: Assume $\exists M$ such that

$$MD(A_r) = D(A_r) M \quad \forall A_r \in G$$

then by taking the hermitian conjugate, we get

$$D^{\dagger}(A_r) M^{\dagger} = M^{\dagger} D^{\dagger}(A_r)$$

As shown above, we can take $D(A_r)$ to be unitary, so we can write

$$M^{\dagger} = D(A_r) M^{\dagger} D^{\dagger}(A_r)$$
 or $M^{\dagger} D(A_r) = D(A_r) M^{\dagger}$

This means that M^{\dagger} also commutes with all D's and so are the combination $M + M^{\dagger}$ and $i \left(M - M^{\dagger} \right)$, which are hermitian. Thus, we only have to consider the case where M is hermitian. Start by diagonalizing M by unitary matrix U,

$$M = UdU^{\dagger}$$
 d : diagonal

Define $\bar{D}(A_r) = U^{\dagger}D(A_r)U$, then we have

$$d\bar{D}(A_r) = \bar{D}(A_r) d$$

or in terms of matrix elements,

$$\sum_{\beta} d_{\alpha\beta} \bar{D}_{\beta r} (A_s) = \sum_{\beta} \bar{D}_{\alpha\beta} (A_s) d_{\beta\gamma}$$

Since the matrix d is diagonal, we get

$$(d_{\alpha\alpha} - d_{\gamma\gamma}) \, \bar{D}_{\alpha\gamma} \, (A_s) = 0 \Longrightarrow \quad \text{if } d_{\alpha\alpha} \neq d_{\gamma\gamma}, \text{ then } \bar{D}_{\alpha\gamma} \, (A_s) = 0$$

This means if diagonal elements d_{ii} are all different, then the off-diagonal elements of \bar{D} are all zero. In this case, \bar{D} s are all diagonal and hence all reducible. The only possible non-zero off-diagonal elements of \bar{D} can arise when some of $d'_{\alpha\alpha}s$ are equal. For example, if $d_{11}=d_{22}$, then \bar{D}_{12} can be non-zero. Thus \bar{D} will be in the block diagonal form, i.e.

$$\text{if } d = \begin{bmatrix} d_1 & & & & & & \\ & d_1 & & & & & \\ & & \ddots & & & & \\ & & & d_1 & & & \\ & & & d_2 & & \\ & & & & d_2 & \\ & & & & & \ddots \end{bmatrix} \text{ then } \bar{D} = \begin{bmatrix} D_1 & 0 & & \\ 0 & D_2 & & \\ & & & \ddots \end{bmatrix}$$

This is true for every matrix in the representation. Thus all the matrices in the representation are in the block diagonal form. But D is irreducible which means that not all matrices can be brought into block diagonal form. Thus all d_i 's have to be equal

$$d=cI.$$
 or $M=UdU^{\dagger}=dUU^{\dagger}=d=cI$

(ii) If the only matrix that commutes with all the matrices of a representation is a multiple of identity, then the representation is irrep.

Proof: Suppose D is reducible, then we can transform them into

$$D\left(A_i\right)=\left[\begin{array}{cc}D^{(1)}\left(A_i\right)&\\D^{(2)}\left(A_i\right)\end{array}\right]\qquad\text{for all }A_i\in G$$
 construct $M=\begin{bmatrix}I&0\\0&2I\end{bmatrix}$ then clearly

$$D(A_i) M = MD(A_i)$$
 for all i

But M is not a multiple of identity (contradiction). Therefore D must be irreducible.

- 1. Any irrep of Abelian group is 1-dimensional. This is because for any element A, D(A) commutes with all $D(A_i)$. Then Schur's lemma $\Longrightarrow D(A) = cI \quad \forall A \in G$. But D is irrep, so D has to be 1×1 matrix.
 - 2. In any irrep, the identity element E is always represented by identity matrix. This follows Schur's lemma.
- 3. From $D(A)D(A^{-1}) = D(E) = I$, we see that $D(A^{-1}) = [D(A)]^{-1}$ and for unitary representation $D(A^{-1}) = D^{+}(A)$.
- (iii) If $D^{(1)}$ and $D^{(2)}$ are irreps of dimension l_1 , and dimension l_2 and

$$MD^{(1)}(A_i) = D^{(2)}(A_i) M$$
 .for all $A_i \in G$ (3)

then (a) if $l_1 \neq l_2$ M = 0

(b) if $l_1 = l_2$, then either M = 0 or $\det M \neq 0$ and reps are equivalent.

<u>Proof</u>: Without loss of generality we can take $l_1 \leq l_2$. Note that since Eq(3) is true for all elements we can replace A_i by A_i^{-1} ,

$$MD^{(1)}\left(A_{i}^{-1}\right) = D^{(2)}\left(A_{i}^{-1}\right)M$$

which can be written as

$$MD^{(1)}\left(A_{i}\right)^{\dagger}=D^{(2)}\left(A_{i}\right)^{\dagger}M$$

Hermitian conjugate of Eq(3) gives

$$D^{(1)^{\dagger}}M^{\dagger} = M^{\dagger}D^{(2)\dagger}, \quad MM^{\dagger}D^{(2)}(A_i)^{\dagger} = MD^{(1)}(A_i)^{\dagger}M^{\dagger} = D^{(2)}(A_i)^{\dagger}MM^{\dagger}$$

or

$$(MM^{\dagger}) D^{(2)} (A_i) = D^{(2)} (A_i) (MM^{\dagger}) \qquad \forall (A_i) \in G$$

Then from Schur's lemma (i) we get $MM^{\dagger}=cI$, where I is a l_2 -dimensional identity matrix.

First consider the case $l_1 = l_2$, where we get $|\det M|^2 = c^{\ell_1}$. Then either $\det M \neq 0$, which implies M is non-singular and from Eq(3)

$$D^{(1)}(A_i) = M^{-1}D^{(2)}(A_i) M \quad \forall (A_i) \in G$$

This means $D^{(1)}(A_i)$ and $D^{(2)}(A_i)$ are equivalent. Otherwise if the determinant is zero,

$$\det M = 0 \quad \Longrightarrow c = 0 \quad \text{or} \ M M^\dagger = 0 \quad \Longrightarrow \quad \sum_{\gamma} M_{\alpha\gamma} M_{\beta\gamma}^{\ *} = 0 \quad \forall \alpha.\beta.$$

In particular, for $\alpha = \beta$ $\sum_{\gamma} |M_{\alpha\gamma}|^2 = 0$ $M_{\alpha\gamma} = 0$ for all $\alpha.\gamma \Longrightarrow M = 0$.

Next, if $l_1 < l_2$, then M is a retangular $l_2 \times l_1$, matrix

$$M = \underbrace{\left(\begin{array}{c} \cdot \\ \cdot \end{array} \right)}_{l_1} l_2$$

we can define a square matrix by adding colums of zeros

$$N = \underbrace{[M,0]}^{l_2} l_2 \qquad l_2 \times l_2 \text{ square matrix}$$

then

$$N^\dagger = \left(egin{array}{c} M^\dagger \ 0 \end{array}
ight) \quad {
m and} \quad NN^\dagger = (M,0) \left(egin{array}{c} M^\dagger \ 0 \end{array}
ight) = MM^\dagger = cI$$

where I is the $l_2 \times l_2$ identity matrix. But from construction we see that $\det N = 0$, Hence $c = 0, \Longrightarrow NN^{\dagger} = 0$ or M = 0 identically.

3 Great Orthogonality Theorem

The most useful theorem for the representation of the finite group is the following one.

Theorem(Great orthogonality theorem): Suppose G is a group with n elements, $\{A_i, i = 1, 2, \dots, n\}$, and $D^{(\alpha)}(A_i)$, $\alpha = 1, 2 \dots$ are all the inequivalent irreps of G with dimension l_{α} .

Then

$$\sum_{\alpha=1}^{n} D_{ij}^{(\gamma)} \left(A_{\alpha} \right) D_{k\ell}^{(\beta)*} \left(A_{\alpha} \right) = \frac{n}{l_{\gamma}} \delta_{\gamma\beta} \delta_{ik} \delta_{j\ell}$$

Proof: Define

$$M = \sum_{a} D^{(\alpha)} (A_a) X D^{(\beta)} (A_a^{-1})$$

where X is an arbitrary $l_{\alpha} \times l_{\beta}$ matrix. Then multiplying M by representation matrices, we get

$$D^{(\alpha)}(A_b) M = D^{(\alpha)}(A_b) \sum_{a} D^{(\alpha)}(A_a) X D^{(\beta)}(A_a^{-1}) \left[D^{(\beta)}(A_b^{-1}) D^{(\beta)}(A_b) \right]$$
$$= \sum_{a} D^{(\alpha)}(A_b A_a) X D^{(\beta)}((A_b A_a)^{-1}) D^{(\beta)}(A_b) = M D^{(\beta)}(A_b)$$

(i) If $\alpha \neq \beta$, then M=0 from Schur's lemma, we get

$$M = \sum_{a} D_{ir}^{(\alpha)} (A_a) X_{rs} D_{sk}^{(\beta)} (A_a^{-1}) = \sum_{a} D_{ir}^{(\alpha)} (A_a) X_{rs} D_{ks}^{(\beta)*} (A_a) = 0$$

Choose $X_{rs} = \delta_{rj}\delta_{sl}$ (i.e. X is zero except the jl element). Then we have

$$\sum D_{ij}^{(\alpha)}(A_{\alpha}) D_{k\ell}^{(\beta)*}(A_{\alpha}) = 0$$

This shows that for different irreducible representations, the matrix elements, after summing over group elements, are orthogonal to each other.

(ii) $\alpha = \beta$ then we can write $M = \sum_{a} D^{(\alpha)}(A_a) X D^{(\alpha)}(A_a^{-1})$. This implies

$$D^{(\alpha)}(A_a) M = M D^{(\alpha)}(A_b) \implies M = c R$$

which gives,

$$\sum_{a} T_r \left[D^{(\alpha)} \left(A_a \right) X D^{(\alpha)} \left(A_a^{-1} \right) \right] = c l_2 \quad \text{or } n T_r X = c l_2, \quad \text{or } c = \frac{\left(T_r X \right) n}{l_\alpha}$$

Take $X_{rs} = \delta_{rj}\delta_{s\ell}$ then $T_rX = \delta_{j\ell}$ and

$$\sum_{\alpha} D^{(\alpha)} (A_a)_{ij} D^{(\alpha)} (A_a)_{k\ell}^* = \frac{n}{l_{\alpha}} \delta_{ik} \delta_{j\ell}$$

This gives the orthogonality for different matrix elements within a given irreducible representation.

Geometric Interpretation

Imagine a complex n-dimensional vector space in which axes (or components) are labeled by group elements $E, A_2.A_3...A_n$ (Group element space). Consider the vector in this space with componets made out of the matrix element of irreducible representation matrix $D^{(\alpha)}(A_a)_{ij}$. Each vector in this n-dimensionl space is labeled by 3 indices, $i, \mu.\nu$

$$\vec{D}_{\mu\nu}^{(i)} = \left(D_{\mu\nu}^{(i)}(E), D_{\mu\nu}^{(i)}(A_2), \cdots D_{\mu\nu}^{(i)}(A_n)\right)$$
(4)

Great orthogonality theorem says that all these vectors are \bot to each other. As a result

$$\sum_{i} l_i^2 \le n$$

because there can be no more than n mutually \perp vectors in n-dimensiona vector space.

As an example, we take the 2-dimensional representation we have work out before,

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad A = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \qquad B = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$
$$K = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad L = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \qquad M = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

Label the axises by the groupl elements in the order (E, A, B, K, L, M). Then we can construct four 6-dimensional ectors from these 2×2 matrices,

$$\begin{array}{llll} D_{11}^{(2)} &= (1 & , -\frac{1}{2} & , -\frac{1}{2} & , -1 & , \frac{1}{2} & , \frac{1}{2}) \\ D_{12}^{(2)} &= (0 & , \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} & , 0 & , -\frac{\sqrt{3}}{2} & , \frac{\sqrt{3}}{2}) \\ D_{21}^{(2)} &= (0 & , -\frac{\sqrt{3}}{2} & , \frac{\sqrt{3}}{2} & , 0 & -\frac{\sqrt{3}}{2} & , \frac{\sqrt{3}}{2}) \\ D_{21}^{(2)} &= (1 & , -\frac{1}{2} & , -\frac{1}{2} & , 1 & , -\frac{1}{2} & , -\frac{1}{2}) \end{array}$$

It is straightforward to check that these 4 vectors are perpendicular to each other.

Note that the other two vectors which are orthogonal to these vectors are of the form,

$$D_E = (1 , 1 , 1 , 1 , 1 , 1 , 1)$$

$$D_A = (1 , 1 , 1 , 1 , -1 , -1 , -1)$$

coming from the identity representation and other 1-dimensional representation.

4 Character of Representation

The matrices in irrep are not unique, because we can generate another equivalent irrep by similarity transformation. However, the trace of a matrix is invariant under such transformation,

$$Tr\left(SAS^{-1}\right) = TrA$$

We can use the trace, or <u>character</u>, to characterize the irrep.

$$\chi^{(\alpha)}(A_i) \equiv T_r \left[D^{(\alpha)}(A_i) \right] = \sum_a D_{aa}^{(\alpha)}(A_i)$$

Useful Properties

1. If $D^{(\alpha)}$ and $D^{(\beta)}$ are equivalent, then

$$\chi^{(\alpha)}(A_i) = \chi^{(\beta)}(A_i) \qquad \forall A_i \in G$$

2. If A and B are in the same class,

$$\chi^{(\alpha)}(A) = \chi^{(\alpha)}(B)$$

Proof: If A and B are in same class $\implies \exists x \in G \text{ such that } xAx^{-1} = B \implies D^{(\alpha)}(x) D^{(\alpha)}(A) D^{(\alpha)}(x^{-1}) = D^{(\alpha)}(B)$

Using

$$D^{(\alpha)}(x^{-1}) = D^{(\alpha)}(x)^{-1}$$

we get

$$T_r\left[D^{(\alpha)}\left(x\right)D^{(\alpha)}\left(A\right)D^{(\alpha)}\left(x\right)^{-1}\right] = T_r\left[D^{(\alpha)}\left(B\right)\right] \quad \text{or } \chi^{(\alpha)}\left(A\right) = \chi^{(\alpha)}\left(B\right)$$

Hence $\chi^{(\alpha)}$ is a function of class, not of each element.

3. Denote $\chi_i = \chi(\mathcal{C}_i)$, the character of ith class. Let n_c be the number of classes in G, and n_i the number of group elements in \mathcal{C}_i .

From great orthogonality theorem

$$\sum_{r} D_{ij}^{(\alpha)}(A_r) D_{k\ell}^{(\beta)*}(A_r) = \frac{n}{l_{\alpha}} \delta_{\alpha\beta} \delta_{ik} \delta_{jl}$$

we get

$$\sum_{r} \chi^{(\alpha)} (A_r) \chi^{(\beta)*} (A_r) = \frac{n}{l_{\alpha}} \cdot \delta_{\alpha\beta} l_{\alpha} = n \delta_{\alpha\beta}$$

or
$$\sum_{i} n_{i} \chi_{i}^{(\alpha)} \chi_{i}^{(\beta)*} = n \delta_{\alpha\beta}$$

This is the great orthogonality theorem for the characters.

Define $U_{\alpha i} = \sqrt{\frac{n_i}{n}} \chi^{(\alpha)} (\mathcal{C}_i)$, then great orthogonality theorem implies,

$$\sum_{i=1}^{n_c} U_{\alpha i} U_{\beta i}^* = \delta_{\alpha \beta}$$

Thus, if we consider $U_{\alpha i}$ as components in n_c dimensional vector space, $\vec{U}_{\alpha} = (U_{\alpha 1}U_{\alpha 2}\cdots U_{\alpha n_c})$, then \vec{U}_{α} $\alpha = 1, 2, 3 \cdots n_r$ $(n_r : \# \text{ of indep irreps})$ form an othornormal set of vectors, i.e.

$$U_{eta}U_{lpha}=\sum_{i=1}^{n_c}\!U_{lpha i}U_{eta i}^{\,*}=\delta_{lphaeta}$$

This implies that

$$n_r \le n_c$$

i. e. number of irreps is smaller than the number of classes. This greatly restricts the number of possible irreps.

4.1 Decomposition of Reducible Representation

For a reducible representation, we can write

$$D = D^{(1)} \oplus D^{(2)}$$
 i.e. $D(A_i) = \begin{pmatrix} D^{(1)}(A_i) \\ D^{(2)}(A_i) \end{pmatrix}$ $\forall A_i \in G$

Then we have for the trace

$$\chi\left(A_{i}\right)=\chi^{\left(1\right)}\left(A_{i}\right)+\chi^{\left(2\right)}\left(A_{i}\right)$$

Denote by $D^{(\alpha)}$, $\alpha = 1, 2 \cdots n_r$, all the inequivalent unitary irrep. Then any rep D can be decomposed as

$$D = \sum_{\alpha} c_{\alpha} D^{(\alpha)}$$
 c_{α} : some integer, $(\# \text{ of time } D^{(\alpha)} \text{ appears})$

In terms of traces, we get

$$\chi\left(\mathcal{C}_{i}\right) = \sum_{\alpha} c_{\alpha} \chi^{(\alpha)}\left(\mathcal{C}_{i}\right)$$

where we indicate that the trace is a function of class C_i . The coefficient can be calculated as follows (by using orthogonity theorem). Multiply by $n_i \chi_i^{(\beta)*}$ and sum over i

$$\sum_{i} \chi_{i} \chi_{i}^{(\beta)*} n_{i} = \sum_{i} \sum_{\alpha} c_{\alpha} \chi_{i}^{(\alpha)} \chi_{i}^{(\beta)*} n_{i} = \sum_{\alpha} c_{\alpha} \cdot n \delta_{\alpha\beta} = n c_{\beta}$$

or

$$c_{\beta} = \frac{1}{n} \sum_{i} \chi_{i} \chi_{i}^{(\beta)*} \mathbf{n}_{i}$$

From this we also get,

$$\sum_{i} n_{i} \chi_{i} \chi_{i}^{*} = \sum_{i} n_{i} \sum_{\alpha, \beta} c_{\alpha} \chi_{i}^{(\alpha)} c_{\beta} \chi_{i}^{(\beta)*} = n \sum_{\alpha} |c_{\alpha}|^{2}$$

This leads to the following theorem:

<u>Theorem</u>: If the rep D with character χ_i satisfies the relation,

$$\sum_{i} n_i \chi_i \chi_i^* = n$$

then the representation D is irreducible.

4.2 Regular Representation

Given a group $G = \{A_1 = E, A_2...A_n\}$. We can construct the <u>regular rep</u> as follows: Take any $A \in G$. If

$$AA_2 = A_3 = 0A_1 + 0A_2 + 1 \cdot A_3 + 0A_4 + \cdots$$

i.e. we write the product "formally" as linear combination of group elements,

$$AA_s = \sum_{r=1}^{n} C_{rs} A_r = \sum_{r=1}^{n} A_r D_{rs} (A),$$
 i.e. $C_{rs} = D_{rs} (A)$ is either 0 or 1. (5)

i.e.
$$D_{rs}(A) = 1$$
 if $AA_s = A_r$ or $A = A_rA_s^{-1}$
= 0 otherwise

Note strictly speaking, the sum over group elements is undefined. But here only one group element shows up in the right-hand side in Eq(5), we do not need to define the sum of group elements. Then D(A)'s form a rep of G: regular representation with dimensional n. This can be seen as follows:

$$\sum_{r} A_{r} D_{rs} (AB) = ABA_{s} = A \sum_{t} A_{t} D_{ts} (B) = \sum_{t \cdot r} D_{ts} (B) A_{r} D_{rt} (A)$$

or

$$D_{rs}(AB) = D_{rt}(A) D_{ts}(B)$$

From the definition of the regular representation

$$D_{rs}(A) = 1$$
 iff $AA_s = A_r$

we see that the diagonal elements are of the form,

$$D_{rr}(A) = 1$$
 iff $AA_r = A_r$ or $A = E$

Therefore every character is zero except for identity class,

$$\chi^{(reg)}(\mathcal{C}_i) = 0 \qquad i \neq 1$$

$$\chi^{(reg)}(\mathcal{C}_i) = n \qquad i = 1$$
 (6)

From this we can work out how $D^{(reg)}$ reduces to irreps. Write

$$D^{(reg)} = \sum_{\alpha} c_{\alpha} D^{(\alpha)}$$

then

$$c_{\alpha} = \frac{1}{n} \sum_{i} \chi_{i}^{(reg)} \chi_{i}^{(\alpha)*} n_{i} = \frac{1}{n} \chi_{1}^{(reg)} \chi_{1}^{(\alpha)*} = \frac{1}{n} \cdot nl_{\alpha} = l_{\alpha}$$

This means that D_{reg} contains the irreps as many times as its dimension,

$$\chi_i^{(reg)} = \sum_{\alpha}^{n_r} l_{\alpha} \chi_i^{(\alpha)}$$
 or $\chi_i^{(reg)} = \sum_{\alpha=1}^{n_r} \chi_i^{(\alpha)*} \chi_i^{(\alpha)} = n \delta_{i1}$

For the identity class $\chi_1^{reg}=n, \quad \chi_1^{(\alpha)}=l_{\alpha},$ then we get

$$\left[\sum_{\alpha} l_{\alpha}^2 = n \right]$$
(7)

This severely constraints the possible dimensionalities of irreps because both n and l_{α} have to be integers. For D_3 , with n=6, the only possible solution for $\sum_{\alpha} l_{\alpha}^2 = 6$ is $l_1 = 1$. $l_2 = 1$. $l_3 = 2$, and their permutations.

The relation in Eq(7) implies that the vector space formed by vectors defined in Eq(4) has dimension n, the number of elements in the group. Since those vectors in Eq(4) are orthogonal to each other, hence linearly independent, and there are n such vectors, they must satisfy the completeness relation,

$$\sum_{\alpha,\mu,\nu} \frac{l_{\alpha}}{n} D_{\mu\nu}^{(\alpha)} (A_k)^* D_{\mu\nu}^{(\alpha)} (A_l) = \delta_{kl} \qquad \text{completeness relation}$$
 (8)

The factor $\frac{l_{\alpha}}{n}$ comes from the normalization of the vectors in Eq(4).

We now want to show that

$$n_c = n_r$$

i.e. # of classes = # of irreps.

Define $D_i^{(\alpha)}$ by adding up all matrices corresponding to elements in the same class C_i ,

$$D_{i}^{(\alpha)} = \sum_{A \in \mathcal{C}_{i}} D^{(\alpha)}(A)$$

Then,

$$D^{(\alpha)}(A_j) D_i^{(\alpha)} D^{(\alpha)}(A_j^{-1}) = \sum_A D^{(\alpha)}(A_j) D^{(\alpha)}(A) D^{(\alpha)}(A_j^{-1})$$
$$= \sum_A D^{(\alpha)}(A_j A A_j^{-1}) = D_i^{(\alpha)}$$

Using

$$D^{(\alpha)}\left(A_j^{-1}\right) = D^{(\alpha)}\left(A_j\right)^{-1}$$

we get

$$D^{(\alpha)}(A_i) D_i^{(\alpha)} = D_i^{(\alpha)} D^{(\alpha)}(A_i)$$

i.e. $D_i^{(\alpha)}$ commutes with all matrice in the irrep. From Schur's lemma, we get

$$D_i^{(\alpha)} = \lambda_i^{(\alpha)} 1$$
 where $\lambda_i^{(\alpha)}$ is some number

Taking the trace, we get

$$n_i \chi_i^{(\alpha)} = \lambda_i^{(\alpha)} l_i \quad \text{or} \quad \lambda_i^{(\alpha)} = \frac{n_i \chi_i^{(\alpha)}}{l_i} = \frac{n_i \chi_i^{(\alpha)}}{\chi_i^{(\alpha)}}$$
 (9)

where $\chi_1^{(\alpha)}$ is the character of identity class. In the completeness relation in Eq(8), we can sum A_k over group elements in class C_r and A_l over class C_s to get

$$\sum_{\alpha,\mu,\nu} \frac{l_i}{n} \left[D_r^{(\alpha)*} \right]_{\mu\nu} \left[D_s^{(\alpha)} \right]_{\mu\nu} = n_r \delta_{rs}$$

Using value of $\lambda_i^{(\alpha)}$ in Eq(9) we have

$$\sum_{\alpha=1}^{n_r} \chi_r^{(\alpha)} \chi_s^{(\alpha)*} = \frac{n}{n_r} \delta_{rs}$$
 completeness

This the completeness relation for the characters. If we now consider $\chi_i^{(\alpha)}$ as a vector in n_r dim space $\overrightarrow{\chi}_i = \left(\chi_i^{(1)}, \chi_i^{(2)}, \dots, \chi_i^{(n_r)}\right)$ we get

$$n_c \le n_r$$

Combine this with the result $n_r \leq n_c$, we have derived before, we get

$$n_r = n_c$$

4.3 Character Table

For a finite group, the essential information about the irreducible representations can be summarized in a table which lists the characters of each irreducible representation in terms of the classes. This table has many useful applications. To construct such table we can use the following useful information:

- 1. # of columns = # of rows = # of classes
- $2. \quad \sum_{\alpha} l_{\alpha}^2 = n$
- 3. $\sum_{i} n_{i} \chi_{i}^{(\alpha)} \chi_{i}^{(\beta)*} = n \delta_{\alpha\beta}$ and $\sum_{\alpha} \chi_{i}^{(\alpha)} \chi_{j}^{(\alpha)*} = \frac{n}{n_{i}} \delta_{ij}$
- 4. If $l_{\alpha} = 1$, χ_i is itself a rep.
- 5. $\chi^{(\alpha)}(A^{-1}) = T_r(D^{(\alpha)}(A^{-1})) = T_r(D^{(\alpha)^+}(A^{-1})) = \chi^{(\alpha)*}(A)$

If A and A^{-1} are in the same class then $\chi(A)$ is real.

- 6. $D^{(\alpha)}$ is a rep $\implies D^{(\alpha)*}$ is also a rep so if $\chi^{(\alpha)}$'s are complex numbers, another row will be their complex conjugate
- 7. If $l_{\alpha} > 1, \chi_{i}^{(\alpha)} = 0$ for at least one class. This follows from the relation

$$\sum_{i} n_i |\chi_i|^2 = n \text{ and } \sum_{i} n_i = n$$

8. For physical symmetry group, x.y and z form a basis of a rep.

Example: D_3 character table

In this table, the typical basis functions up to quadratic in coordinate system are listed.

Remark: the basis functions listed in the usual character table are not necessarily normalized. In particular, the quadratic functions have to be handled carefully. The danger is that if we use the basis functions given in the character table, we might not generate unitary matrices.

Using the transformation properties of the coordinate, we can also infer the transformation properties of any vectors.

For example, the usual coordinates have the transformation property,

$$\vec{r} = (x, y, z) \sim A_2 \oplus E$$
 in D_3

This means that electric field of \vec{E} or magnetic field \vec{B} will have same transformation property,

$$\vec{B} \sim \vec{E} \sim A_2 \oplus E$$

because they all transform the same way under the rotation.

5 Product Representation (Kronecker product)

Let x_i be the basis for $D^{(\alpha)}$, i.e. $x_i' = \sum_{j=1}^{\ell_{\alpha}} x_j D_{ji}^{(\alpha)}(A)$

$$y_{\ell}$$
 be the basis for $D^{(\beta)}$, i.e. $y_{k}' = \sum_{\ell=1}^{\ell_{\beta}} y_{\ell} D_{\ell k}^{(\beta)}(A)$

then the products $x_j y_l$ transform as

$$x_i'y_k' = \sum_{j \cdot \ell} D_{ij}^{(\alpha)}(A) D_{k\ell}^{(\beta)}(A) x_j y_\ell \equiv \sum_{j \cdot \ell} D_{j\ell;ik}^{(\alpha \times \beta)}(A) x_j y_\ell$$

where

$$D_{j\ell;ik}^{(\alpha\times\beta)}(A) = D_{ij}^{(\alpha)}(A) D_{\ell k}^{(\beta)}(A)$$

Note that in these matrices, row and column are labelled by 2 indices, instead of one. It is easy to show that $D^{(\alpha \times \beta)}$ forms a rep of the group.

$$\begin{split} \left[D^{(\alpha\times\beta)}\left(A\right)D^{(\alpha\times\beta)}\left(B\right)\right]_{ij;k\ell} &= \sum_{s.t} D^{(\alpha\times\beta)}\left(A\right)_{ij,st} D^{(\alpha\times\beta)}\left(B\right)_{st;k\ell} \\ &= \sum_{s.t} \quad D^{(\alpha)}_{is}\left(A\right) \ D^{(\beta)}_{j\ell}\left(A\right) \ D^{(\alpha)}_{sk}\left(B\right) \ D^{(\beta)}_{t\ell}\left(B\right) = D^{(\alpha)}_{ik}\left(AB\right) D^{(\beta)}_{j\ell}\left(AB\right) = D^{(\alpha\times\beta)}\left(AB\right)_{ik;k\ell} \end{split}$$

or

$$D^{(\alpha \times \beta)}(A) D^{(\alpha \times \beta)}(B) = D^{(\alpha \times \beta)}(AB)$$

The basis functions for $D^{(\alpha \times \beta)}$ are $x_i y_j$

The character of this new rep can be calculated by making the row and colum indices the same and sum over,

$$\chi^{(\alpha \times \beta)}(A) = \sum_{j \cdot \ell} D_{j\ell;j\ell}^{(\alpha \times \beta)}(A) = \sum_{j \cdot \ell} D_{jj}^{(\alpha)}(A) D_{\ell\ell}^{(\beta)}(A) = \chi^{(\alpha)}(A) \chi^{(\beta)}(A)$$

$$\chi^{(\alpha \times \beta)}(A) = \chi^{(\alpha)}(A) \chi^{(\beta)}(A)$$

If $\alpha = \beta$, we can further decompose the product rep by symmetrization or antisymmetrization;

$$D_{ik,j\ell}^{\{\alpha \times \alpha\}}(A) = \frac{1}{2} \left[D_{ij}^{(\alpha)}(A) D_{k\ell}^{(\alpha)}(A) + D_{i\ell}^{(\alpha)}(A) D_{kj}^{(\alpha)}(A) \right] \quad \text{basis } \frac{1}{\sqrt{2}} \left(x_i y_k + x_k y_i \right)$$

$$D_{ik,j\ell}^{\left[\alpha\times\alpha\right]}\left(A\right) = \frac{1}{2}\left[D_{ij}^{\left(\alpha\right)}\left(A\right)D_{k\ell}^{\left(\alpha\right)}\left(A\right) - D_{i\ell}^{\left(\alpha\right)}\left(A\right)D_{kj}^{\left(\alpha\right)}\left(A\right)\right] \qquad \text{basis } \frac{1}{\sqrt{2}}\left(x_{i}y_{k} - x_{k}y_{i}\right)$$

These matrices also form rep of G and the characters are given by

$$\chi^{\{\alpha \times \alpha\}}\left(A\right) = \frac{1}{2} \left[\left(\chi^{(\alpha)}\left(A\right)\right)^2 + \chi^{(\alpha)}\left(A^2\right) \right], \qquad \chi^{[\alpha \times \alpha]}\left(A\right) = \frac{1}{2} \left[\left(\chi^{(\alpha)}\left(A\right)\right)^2 - \chi^{(\alpha)}\left(A^2\right) \right]$$

Example D_3

6 Direct Product Group

Given 2 groups $G_1 = \{E, A_2 \cdots A_n\}$, $G_2 = \{E, B_2 \cdots B_m\}$, we can define the product group as $G_1 \otimes G_2 = \{A_i B_j; i = 1 \cdots n, j = 1 \cdots m\}$ with multiplication law

$$(A_k B_\ell) \times (A_{k'} B_{\ell'}) = (A_k A_{k'}) (B_\ell B_{\ell'})$$

It turns out that irrep of $G_1 \otimes G_2$ are just direct product of irreps of G, and G_2 . Let $D^{(\alpha)}(A_i)$ be an irrep of G_1 and $D^{(\beta)}(B_i)$ an irrep of G_2 then the matrices defined by

$$D^{(\alpha \times \beta)} (A_i B_j)_{ab;cd} \equiv D^{(\alpha)} (A_i)_{ac} D^{(\beta)} (B_j)_{bd}$$

will have the property

$$\begin{split} \left[D^{(\alpha \times \beta)} \left(A_{i} B_{j} \right) D^{(\alpha \times \beta)} \left(A_{k} B_{\ell} \right) \right]_{ab;cd} &= \sum_{e \cdot f} \left[D^{(\alpha \times \beta)} \left(A_{i} B_{j} \right) \right]_{ab;ef} \left[D^{(\alpha \times \beta)} \left(A_{k} B_{\ell} \right) \right]_{ef;cd} \\ &= \sum_{e \cdot f} \left[D^{(\alpha)} \left(A_{i} \right)_{ac} D^{(\alpha)} \left(A_{k} \right)_{ec} \right] \left[D^{(\beta)} \left(B_{j} \right)_{bf} D^{(\beta)} \left(B_{e} \right)_{fd} \right] \\ &= D^{(\alpha)} \left(A_{i} A_{k} \right)_{ac} D^{(\beta)} \left(B_{j} B_{\ell} \right)_{bd} = D^{(\alpha \times \beta)} \left(A_{i} A_{k} B_{j} B_{\ell} \right)_{ab;cd} \end{split}$$

This means that the matrice $D^{(\alpha \times \beta)}(A_i B_j)$ form a representation of the product group $G_1 \otimes G_2$. The characters can be calculated,

$$\chi^{(\alpha \times \beta)}\left(A_{i}B_{j}\right) = \sum_{ab} D^{(\alpha \times \beta)}\left(A_{i}B_{j}\right)_{ab;ab} = \sum_{ab} D^{(\alpha)}\left(A_{i}\right)_{aa} D^{(\beta)}\left(B_{j}\right)_{bb} = \chi^{(\alpha)}\left(A_{i}\right)\chi^{(\beta)}\left(B_{j}\right)_{ab;ab}$$

Then

$$\sum_{i \cdot j} \left| \chi^{(\alpha \times \beta)} \left(A_i B_j \right) \right|^2 = \left(\sum_i \left| \chi^{(\alpha)} \left(A_i \right) \right|^2 \right) \left(\sum_j \left| \chi^{(\beta)} \left(B_j \right) \right|^2 \right) = nm \quad \Longrightarrow \quad D^{(\alpha \times \beta)} \text{ is irrep.}$$

Example, $G_1 = D_3 = \{E, 2C_3, 3C_2'\}$, $G_2 = \{E, \sigma_h\} = \varphi$ where σ_h : reflection on the plane of triangle. Direct product group is then $D_{3h} \equiv D_3 \otimes \varphi = E, A, B = \{E, 2C_3, 3C_2', \sigma_h, 2C_3\sigma_h, 3C_2'\sigma_h\}$

Character Table

Character Table

	$\mid E \mid$	$2C_3$	$2C_2'$	σ_h		$2C_2'\sigma_h$
					1	1
Γ_2^+	1	1	-1	1	1	-1
Γ_3^+			0			0
Γ_1^+			1		-1	-1
Γ_2^+	1	1	-1		-1	1
Γ_3^{-1}	2	-1	0	-2	1	0