Lecture 3. Introduction to Representation Theory of Finite Groups[1]

1 Group representations

1.1 Basic definitions

Let us put into correspondence to each element G of the group $\mathbf{G}$ a square regular matrix $D(G)$ such that

1. if $G_1 \cdot G_2 = G_3$ then $D(G_1) \cdot D(G_2) = D(G_3)$
2. $(D(G_1) \cdot D(G_2)) \cdot D(G_3) = D(G_1) \cdot (D(G_2) \cdot D(G_3))$
3. $D(E)$ is an identity matrix
4. $[D(G)]^{-1} = D(G^{-1})$.

Then the set of the matrices $D(G)$ is called a *representation* of the group $\mathbf{G}$.
The dimension of the matrices $D(G)$ is called the *dimension* of the representation.

If the matrices corresponding to the different elements of the group are different then the group of matrices and the original group are isomorphic and such a representation is called a *faithful* (or *true*) representation.

If each matrix D represents more than one element of the group then the representation is called *unfaithful*.

Every group has a trivial one-dimensional *identity* representation obtained by representing each element by $+1$.

Let us consider two different representations of the group $\mathbf{G}$ of the same dimension: $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$. If there exists a regular matrix U such that

$$D^{(\alpha)}(G) = U^{-1} D^{(\beta)}(G) U \tag{1}$$

then the representations $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$ are *equivalent*.

The transformation of the type (1) is called a *similarity* transformation.

[1]Most of the results given below can be generalized to infinite discrete or continuous group under certain conditions [1, 2, 3].

1.2 Reducible and irreducible representations

Let us consider two representations $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$ of the dimensions l_α and l_β, respectively. We can construct a larger representation by adding these two:

$$D(G) = D^{(\alpha)}(G) \oplus D^{(\beta)}(G) = \left(\begin{array}{cc} D^{(\alpha)}(G) & 0 \\ 0 & D^{(\beta)}(G) \end{array} \right) \tag{2}$$

Such a form of the matrix is called a *block-diagonal* form, and $\oplus$ denotes the direct sum of the matrices. The dimension of the representation $D(G)$ is $l = l_\alpha + l_\beta$. The representation $D(G)$ is called a *reducible* representation because it consists of two smaller representations.

In general, if the representation which is not of a block-diagonal form (2) can be transformed to such a form by a similarity transformation then the representation is called a *reducible* representation.

For example, if a representation $D(G)$ can be transformed to a form

$$D(G) = \left(\begin{array}{cccc} D^{(1)}(G) & 0 & 0 & 0 \\ 0 & D^{(1)}(G) & 0 & 0 \\ 0 & 0 & D^{(2)}(G) & 0 \\ 0 & 0 & 0 & D^{(3)}(G) \end{array} \right) \tag{3}$$

then this representation is reducible and we can write schematically

$$D(G) = 2D^{(1)}(G) \oplus D^{(2)}(G) \oplus D^{(3)}(G) \; . \tag{4}$$

If the representation which is not of the block-diagonal form cannot be transformed to such a form by any similarity transformation then the representation is called an *irreducible* representation.

Remark

Any 1-dimensional representation is an irreducible representation.

1.3 Basis of the representation

Consider l linear independent functions $f_1(r)$, $f_2(r)$, ..., $f_l(r)$. Let $\mathbf{G}$ be a group of symmetry transformations of the space:

$$r' = Gr \; ,$$

where G is an element of $\mathbf{G}$. If under these transformations, the functions $f_1(r)$, $f_2(r)$, ..., $f_l(r)$ transform as

$$f_i'(r) = \sum_{j=1}^{l} D_{ji}(G) f_j(r) \tag{5}$$

where $D_{ji}(G)$ are the matrix elements of a representation $D(G)$ of the group $\mathbf{G}$, then it is said that these functions form a *basis* of the representation $D(G)$.

If the functions $f_1(r)$, $f_2(r)$, ..., $f_l(r)$ are orthogonal and normalized then the matrix elements $D_{ji}(G)$ are given by the integrals

$$D_{ji}(G) = \int f_j^*(r) D(G) f_i(r) dr \tag{6}$$

We say that the functions $f_1(r)$, $f_2(r)$, ..., $f_l(r)$ transform according to the representation $D(G)$ of the group $\mathbf{G}$.

Remark

We can construct a representation in any linear vector space (of sufficient dimension) and use a basis of this space as a basis of the representation with the appropriate definition of the scalar product. For example, in three dimensions the basis can be three unit vectors $\vec{e}_x$, $\vec{e}_y$ and $\vec{e}_z$ directed along the axes x, y and z and a scalar product be the usual scalar product of two vectors.

In quantum mechanics the properties of the system of N particles in a given state are described by a wave function $\psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ which is a function of the particle coordinates $\vec{r}_i$. The wave functions satisfy certain boundary conditions determined by the problem. All these functions form a linear vector space. The scalar product is defined as

$$(\psi', \psi) = \int \psi'^* \psi dV \tag{7}$$

where integration goes over coordinates of all particles and $dV = d\vec{r}_1 d\vec{r}_2 \ldots d\vec{r}_N$. If the Hamiltonian H is Hermitian, then its eigenfunctions ψ_i satisfying the Schrödinger equation

$$H\psi_i = E_i \psi_i \tag{8}$$

will be orthogonal

$$(\psi_i, \psi_j) = \int \psi_i^* \psi_j dV = \delta_{ij} \tag{9}$$

and therefore they form a basis in the linear space, which can serve as a *basis of the representation of a symmetry group of the Hamiltonian.*

1.4 Construction of group representations

1. Choose a basis of the representation (a set of linear independent vectors)
2. Look how the basis vectors transform under symmetry transformations of the group
3. Write down the matrices of the representation

Example 1

Construct the representation of the group $\mathbf{C}_4$ *in the basis of three orthogonal unit vectors* $\vec{e}_x$, $\vec{e}_y$ *and* $\vec{e}_z$ *and check if it is a reducible representation or an irreducible one.*

Group $\mathbf{C}_4$ contains 4 elements: E, C_4, C_2 and C_4^3.

Let us choose the symmetry axis C_4 perpendicular to the (x, y) plane and coincide with the vector $\vec{e}_z$. Now consider how the vectors $\vec{e}_x$, $\vec{e}_y$ and $\vec{e}_z$ transform under operations of the group $\mathbf{C}_4$:

$$\begin{array}{lll} E\vec{e}_x = \vec{e}_x\,, & E\vec{e}_y = \vec{e}_y\,, & E\vec{e}_z = \vec{e}_z \\ C_4\vec{e}_x = \vec{e}_y\,, & C_4\vec{e}_y = -\vec{e}_x\,, & C_4\vec{e}_z = \vec{e}_z \\ C_2\vec{e}_x = -\vec{e}_x\,, & C_2\vec{e}_y = -\vec{e}_y\,, & C_2\vec{e}_z = \vec{e}_z \\ C_4^3\vec{e}_x = -\vec{e}_y\,, & C_4^3\vec{e}_y = \vec{e}_x\,, & C_4^3\vec{e}_z = \vec{e}_z \end{array} \tag{10}$$

From (10) we can write down the matrices of these transformations:

$$
\begin{aligned}
D(E) &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \qquad D(C_4) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \\
D(C_2) &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad D(C_4^3) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} .
\end{aligned}
\tag{11}
$$

Matrices (11) realize a 3-dimensional representation of the group $\mathbf{C}_4$. It is seen from their explicit form that this representation is reducible. Under transformations of the group $\mathbf{C}_4$ the vector $\vec{e}_z$ remains unchanged. Thus it forms itself a basis of the identity representation of this group (let us denote it as $D^{(1)}$):

$$
D^{(1)}(E) = 1, \quad D^{(1)}(C_4) = 1, \quad D^{(1)}(C_2) = 1, \quad D^{(1)}(C_4^3) = 1 \,. \tag{12}
$$

The other component of (11) is a 2-dimensional representation of the group $\mathbf{C}_4$, which we denote as $D'(G)$:

$$
D'(E)= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \; D'(C_4)= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} , \; D'(C_2)= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} , \; D'(C_4^3)= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{13}
$$

This representation is also reducible. We can reduce it to two one-dimensional representations. In order to do this we should find a transformation U such that the representation $D''(G) = U^{-1}D'(G)U$ has a block-diagonal structure for each G. In Section 4 we will learn a special technique how to do this in a general case. At the moment, we will do it straightforwardly by a trial method for $\mathbf{C}_4$ group.

Let us choose U as

$$
U = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{\mathrm{i}}{\sqrt{2}} & -\frac{\mathrm{i}}{\sqrt{2}} \end{pmatrix} \tag{14}
$$

The operator U transform the basis vectors $\vec{e}_x$ and $\vec{e}_y$ to the vectors:

$$
\begin{aligned}
U\vec{e}_x &= \tfrac{1}{\sqrt{2}}(\vec{e}_x + \mathrm{i}\vec{e}_y) \equiv \vec{e}_{+1} \\
U\vec{e}_y &= \tfrac{1}{\sqrt{2}}(\vec{e}_x - \mathrm{i}\vec{e}_y) \equiv \vec{e}_{-1}
\end{aligned}
\tag{15}
$$

The matrices of the representation $D''(G)$ equivalent to $D'(G)$ look like

$$
D''(E)= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} , \; D''(C_4)= \begin{pmatrix} -\mathrm{i} & 0 \\ 0 & \mathrm{i} \end{pmatrix} , \; D''(C_2)= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} , \; D''(C_4^3)= \begin{pmatrix} \mathrm{i} & 0 \\ 0 & -\mathrm{i} \end{pmatrix} . \tag{16}
$$

It is seen that the representation $D''(G)$ consists of two 1-dimensional irreducible representations, which we call $D^{(2)}$ and $D^{(3)}$:

$$
\begin{aligned}
D^{(2)}(E) = 1, \quad D^{(2)}(C_4) = -\mathrm{i}, \quad D^{(2)}(C_2) = -1, \quad D^{(2)}(C_4^3) = \mathrm{i} \\
D^{(3)}(E) = 1, \quad D^{(3)}(C_4) = \mathrm{i}, \quad\;\; D^{(3)}(C_2) = -1, \quad D^{(3)}(C_4^3) = -\mathrm{i}
\end{aligned}
\tag{17}
$$

The vector $\vec{e}_{+1}$ is the basis vector of the representation $D^{(2)}$, while the vector $\vec{e}_{-1}$ is the basis vector of the representation $D^{(3)}$.

In summary, in this Example we have constructed a 3-dimensional representation of the group $\mathbf{C}_4$ and decomposed it to three 1-dimensional components (irreducible representations):

$$D(G) = D^{(1)}(G) \oplus D^{(2)}(G) \oplus D^{(3)}(G) \; . \tag{18}$$

Example 2

Construct the representation of the group $\mathbf{C}_{3v}$ in the basis of three orthogonal unit vectors $\vec{e}_x$, $\vec{e}_y$ and $\vec{e}_z$ and check if it is a reducible representation or an irreducible one.

Group $\mathbf{C}_{3v}$ contains 6 elements: E, two rotations C_3 and C_3^2, three reflections σ_1, σ_2, σ_3.

Let us choose the symmetry axis C_3 perpendicular to the (x, y) plane and coincide with the vector $\vec{e}_z$. Consider how the vectors $\vec{e}_x$, $\vec{e}_y$ and $\vec{e}_z$ transform under operations of the group $\mathbf{C}_{3v}$:

$$\begin{array}{lll}
E\vec{e}_x = \vec{e}_x, & E\vec{e}_y = \vec{e}_y, & E\vec{e}_z = \vec{e}_z \\
C_3\vec{e}_x = -\frac{1}{2}\vec{e}_x + \frac{\sqrt{3}}{2}\vec{e}_y, & C_3\vec{e}_y = -\frac{\sqrt{3}}{2}\vec{e}_x - \frac{1}{2}\vec{e}_y, & C_3\vec{e}_z = \vec{e}_z \\
C_3^2\vec{e}_x = -\frac{1}{2}\vec{e}_x - \frac{\sqrt{3}}{2}\vec{e}_y, & C_3^2\vec{e}_y = \frac{\sqrt{3}}{2}\vec{e}_x - \frac{1}{2}\vec{e}_y, & C_3^2\vec{e}_z = \vec{e}_z \\
\sigma_1\vec{e}_x = \frac{1}{2}\vec{e}_x + \frac{\sqrt{3}}{2}\vec{e}_y, & \sigma_1\vec{e}_y = \frac{\sqrt{3}}{2}\vec{e}_x - \frac{1}{2}\vec{e}_y, & \sigma_1\vec{e}_z = \vec{e}_z \\
\sigma_2\vec{e}_x = -\vec{e}_x, & \sigma_2\vec{e}_y = \vec{e}_y, & \sigma_2\vec{e}_z = \vec{e}_z \\
\sigma_3\vec{e}_x = \frac{1}{2}\vec{e}_x - \frac{\sqrt{3}}{2}\vec{e}_y, & \sigma_3\vec{e}_y = -\frac{\sqrt{3}}{2}\vec{e}_x - \frac{1}{2}\vec{e}_y, & \sigma_3\vec{e}_z = \vec{e}_z
\end{array} \tag{19}$$

From (19) we can write down the matrices of these transformations:

$$\begin{array}{l}
D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(C_3^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \\
D(\sigma_1) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(\sigma_2) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(\sigma_3) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{array} \tag{20}$$

Matrices (20) form a 3-dimensional representation of the group $\mathbf{C}_{3v}$. This representation is reducible. We can immediately see that it consists of a 2-dimensional and a 1-dimensional representations.

The vectors $\vec{e}_x$ and $\vec{e}_y$ form the basis of the 2-dimensional representation, which we denote as $D^{(3)}$:

$$\begin{array}{l}
D^{(3)}(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; D^{(3)}(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; D^{(3)}(C_3^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \\
D^{(3)}(\sigma_1) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; D^{(3)}(\sigma_2) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; D^{(3)}(\sigma_3) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.
\end{array} \tag{21}$$

The 1-dimensional representation is the identity representation, whose basis is the vector $\vec{e}_z$. We denote it as $D^{(1)}$:

$$D^{(1)}(E) = 1, \; D^{(1)}(C_3) = 1, \; D^{(1)}(C_3^2) = 1, \; D^{(1)}(\sigma_1) = 1, \; D^{(1)}(\sigma_2) = 1, \; D^{(1)}(\sigma_3) = 1 \; . \tag{22}$$

Thus we have found that

$$D(G) = D^{(1)}(G) \oplus D^{(3)}(G) \; . \tag{23}$$

Example 3

Construct the representation of the group $\mathbf{C}_{3v}$ in a 3-dimensional space of the functions of the type $f(\vec{r}) = c_1x^2 + c_2y^2 + c_3xy$.

We can choose as a basis three linear independent functions $f_1 = x^2$, $f_2 = y^2$, $f_3 = xy$ (this is not an orthogonal basis).

Let us see how these basis will change under transformations of the group $\mathbf{C}_{3v}$. For the identity element it is trivial:

$$Ef_1 = x^2 = f_1\,,\; Ef_2 = y^2 = f_2\,,\; Ef_3 = xy = f_3 \tag{24}$$

and the matrix looks like:

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{25}$$

Now, let us consider rotation C_3. Under this rotation, the coordinates x and y transform as

$$\begin{array}{l} C_3x = -\frac{1}{2}x + \frac{\sqrt{3}}{2}y \\ C_3y = -\frac{\sqrt{3}}{2}x - \frac{1}{2}y \end{array} \tag{26}$$

Inserting these expressions in the functions $f_1 = x^2$, $f_2 = y^2$, $f_3 = xy$, we get

$$\begin{array}{l} C_3f_1 = \frac{1}{4}x^2 + \frac{3}{4}y^2 - \frac{\sqrt{3}}{2}xy \\ C_3f_2 = \frac{3}{4}x^2 + \frac{1}{4}y^2 + \frac{\sqrt{3}}{2}xy \\ C_3f_3 = \frac{\sqrt{3}}{4}x^2 - \frac{\sqrt{3}}{4}y^2 - \frac{1}{2}xy \end{array} \tag{27}$$

and we obtain the matrix of the representation for C_3

$$D(C_3) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \tag{28}$$

In the same way, we can construct the other four matrices of the representation (see problems).

2 Some important properties of representations

1. Each representation is equivalent to a unitary representation, i.e. to a representation in which each group element is represented by a unitary matrix [2] .

2. The number of irreducible representations of a group equals to the number of group classes.

   Example

   Six elements of the group $\mathbf{C}_{3v}$ can be divided into three classes (see the exact definition of the class in the previous lecture):

[2] Remember that only finite groups are considered here

- E
- C_3, C_3^2
- σ_1, σ_2, σ_3

In the group of transformations, the classes unite physically equivalent transformations, e.g. identity, rotations, reflections.

Thus the group $\mathbf{C}_{3v}$ has three irreducible representations.

3. If l_α is the dimension of the irreducible representation $D^{(\alpha)}(G)$ then

$$\sum_\alpha l_\alpha^2 = n \ , \tag{29}$$

where n is the number of the group elements and the sum goes over all irreducible representations of the group.

Example

Let us apply this formula to the group $\mathbf{C}_{3v}$. The group has 6 elements divided into 3 classes and, therefore, it has 3 irreducible representations. From (29) we have:

$$l_1^2 + l_2^2 + l_3^2 = 6 \ . \tag{30}$$

It is easy to check that the only possible solution is $l_1 = 1$, $l_2 = 1$, $l_3 = 2$, i.e. the group $\mathbf{C}_{3v}$ has two 1-dimensional and one 2-dimensional irreducible representations.

4. *Orthogonality relation*: If $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$ are irreducible unitary representations, then

$$\sum_G D_{ij}^{(\alpha)*}(G) D_{km}^{(\beta)}(G) = \frac{n}{l_\alpha} \delta_{\alpha\beta} \delta_{ik} \delta_{jm} \tag{31}$$

where n is the number of the group elements, l_α is the dimension of the representation $D^{(\alpha)}(G)$ and the sum goes over all elements G of the group $\mathbf{G}$.

3 Characters

3.1 Basic definitions

The *character* $\chi(G)$ of the element G in the representation D is the trace of the matrix $D(G)$:

$$\chi(G) = \sum_i D_{ii}(G) \tag{32}$$

In order to apply the group in physics usually it is sufficient to know only the characters of the irreducible representations of the symmetry group of the Hamiltonian, without the explicit form of the matrices.

The characters of all irreducible representations of the point symmetry groups are usually given by tables, of the symmetric group $\mathbf{S}_n$ and of the continuous matrix groups are given by recurrent formulae and can be found in different books, e.g. [1, 2, 3].

Example

Find the characters of the 3-dimensional representation $D(G)$ of the group $\mathbf{C}_{3v}$ given by (20) and of its components $D^{(1)}(G)$ and $D^{(3)}(G)$ given by (22) and (21), respectively.

From the explicit form of the matrices of the representations $D(G)$, $D^{(1)}(G)$ and $D^{(3)}(G)$ we can easily calculate the characters, i.e. the traces of these matrices. The results are summarized in the table below:

	E	C_3	C_3^2	σ_1	σ_2	σ_3
$\chi^{(1)}$	1	1	1	1	1	1
$\chi^{(3)}$	2	-1	-1	0	0	0
χ	3	0	0	1	1	1

Remark

It is seen from table that the sum of the characters of the representation $D(G)$ equals to the sum of the characters of its components. In general, if

$$D(G) = D^{(1)}(G) \oplus D^{(2)}(G) \oplus D^{(3)}(G) \oplus \ldots, \tag{33}$$

then

$$\chi(G) = \chi^{(1)}(G) + \chi^{(2)}(G) + \chi^{(3)}(G) + \ldots \; . \tag{34}$$

3.2 Some important properties of group characters

1. Equivalent representations have the same set of characters.

2. In any representation the characters are the same for all elements from a given class (e.g., see the table of characters for the group $\mathbf{C}_{3v}$ above).

3. Since $D(E)$ is just an identity matrix, then the character $\chi(E)$ is always equal to the dimension of the representation.

4. If $\chi^{(\alpha)}(G)$ and $\chi^{(\beta)}(G)$ denote the characters of an element G in the irreducible unitary representations $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$, respectively, then

   $$\sum_G \chi^{(\alpha)*}(G)\chi^{(\beta)}(G) = n\delta_{\alpha\beta} \tag{35}$$

   where the sum goes over all group elements G and n is the total number of the group elements (the order of the group).

   Since the elements belonging to one class have the same characters, the formula (35) can be re-written as

   $$\sum_C n_C \chi^{(\alpha)*}(C)\chi^{(\beta)}(C) = n\delta_{\alpha\beta} \tag{36}$$

   where $\chi^{(\alpha)}(C)$ denotes the character of the elements from the class C, n_C is the number of the elements in a given class C and the sum goes over all classes of the group.

5. If the representation $D^{(\alpha)}(G)$ is irreducible, then from (35) we get

   $$\sum_G |\chi^{(\alpha)}(G)|^2 = n \; , \tag{37}$$

or, using the classes,

$$\sum_C n_C |\chi^{(\alpha)}(C)|^2 = n \ . \tag{38}$$

These formulae can be used as a check if a representation is irreducible or not.

Example 1

Check if the representation $D^{(3)}(G)$ of the group $\mathbf{C}_{3v}$ is irreducible.

From (37) we have:

$$2^2 + 1^2 + 1^2 + 0^2 + 0^2 + 0^2 = 6 \ . \tag{39}$$

Since the group contains exactly 6 elements, then the criterion (37) is satisfied and the representation $D^{(3)}(G)$ is irreducible.

Instead of (37), we can use (38) that brings us to the same result:

$$1 \cdot 2^2 + 2 \cdot 1^2 + 3 \cdot 0^2 = 6 \ . \tag{40}$$

Example 2

Find the third irreducible representation of the group $\mathbf{C}_{3v}$.

Below we constructed the table of the characters of two irreducible representations $D^{(1)}(G)$ and $D^{(3)}(G)$ of the group $\mathbf{C}_{3v}$. From the Example of Section 2 we know that there exists a third irreducible representation of this group, which we denote as $D^{(2)}(G)$, and it is 1-dimensional. Thus the character table for all irreducible representations of the group $\mathbf{C}_{3v}$ will look as follows:

	E	$C_3,\ C_3^2$	$\sigma_1,\ \sigma_2,\ \sigma_3$
$\chi^{(1)}$	1	1	1
$\chi^{(2)}$	1	a	b
$\chi^{(3)}$	2	-1	0

In this table we have already united elements into classes. We need to find two unknown characters, denoted by a and b in this table. To do this, let us use the formula (36):

$$\begin{aligned} &\sum_C n_C \chi^{(1)}(C) \chi^{(2)}(C) = 0 \ , \\ &\sum_C n_C \chi^{(3)}(C) \chi^{(2)}(C) = 0 \ . \end{aligned} \tag{41}$$

Inserting the required values from the table above into (41), we get two equations:

$$\begin{aligned} &1 \cdot 1 \cdot 1 + 2 \cdot 1 \cdot a + 3 \cdot 1 \cdot b = 0 \ , \\ &1 \cdot 2 \cdot 1 + 2 \cdot (-1) \cdot a + 3 \cdot 0 \cdot b = 0 \ , \end{aligned} \tag{42}$$

from which we find that $a = 1$ and $b = -1$. Thus, we get the final table of characters of all irreducible representations of the group $\mathbf{C}_{3v}$:

	E	$C_3,\ C_3^2$	$\sigma_1,\ \sigma_2,\ \sigma_3$
$\chi^{(1)}$	1	1	1
$\chi^{(2)}$	1	1	-1
$\chi^{(3)}$	2	-1	0

Example 3

Find the characters of all irreducible representations of the symmetric group $\mathbf{S}_3$.

Group $\mathbf{S}_3$ contains 6 elements:

$$\begin{aligned} E &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix} , \quad \pi_1 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} , \quad \pi_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} , \\ P_{12} &= \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} , \quad P_{23} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} , \quad P_{13} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} . \end{aligned} \tag{43}$$

These elements can be divided into three classes:

- E
- π_1, π_2
- P_{12}, P_{23}, P_{13}

Thus the group has three irreducible representations. From (29) we can find their dimensions:

$$l_1^2 + l_2^2 + l_3^2 = 6 , \tag{44}$$

and the only possible solution is $l_1 = 1$, $l_2 = 1$, $l_3 = 2$, i.e. the group $\mathbf{S}_3$ has two 1-dimensional and one 2-dimensional irreducible representations. Let us denote them as $D^{(1)}(G)$, $D^{(2)}(G)$ and $D^{(3)}(G)$. We already know the characters of the element E in this representations (they equal to the dimensions of the representations). Moreover, it is clear that one of the two 1-dimensional irreducible representations is an identity representation. Let us put all this information into a character table:

	E	π_1, π_2	P_{12}, P_{23}, P_{13}
$\chi^{(1)}$	1	1	1
$\chi^{(2)}$	1	a	b
$\chi^{(3)}$	2	c	d

In order to find four unknown characters, denoted by a, b, c and d, let us use the formulae (36) and (38):

$$\begin{aligned} &\sum_C n_C \chi^{(1)}(C) \chi^{(2)}(C) = 0 , \\ &\sum_C n_C \chi^{(1)}(C) \chi^{(3)}(C) = 0 , \\ &\sum_C n_C |\chi^{(2)}(C)|^2 = 6 , \\ &\sum_C n_C |\chi^{(3)}(C)|^2 = 6 . \end{aligned} \tag{45}$$

Inserting the known characters into (46), we get four equations:

$$\begin{aligned} &1 \cdot 1 \cdot 1 + 2 \cdot 1 \cdot a + 3 \cdot 1 \cdot b = 0 , \\ &1 \cdot 2 \cdot 1 + 2 \cdot 1 \cdot c + 3 \cdot 1 \cdot d = 0 , \\ &1 \cdot 1^2 + 2 \cdot a^2 + 3 \cdot b^2 = 6 , \\ &1 \cdot 1^2 + 2 \cdot c^2 + 3 \cdot d^2 = 6 , \end{aligned} \tag{46}$$

from which we find that $a = 1$, $b = -1$, $c = 2$, $d = 0$. Thus, we get the final table of characters of all irreducible representations of the group $\mathbf{S}_3$:

	E	π_1, π_2	P_{12}, P_{23}, P_{13}
$\chi^{(1)}$	1	1	1
$\chi^{(2)}$	1	1	-1
$\chi^{(3)}$	2	-1	0

Remarks

1. It is seen that the characters of the irreducible representations of the groups $\mathbf{C}_{3v}$ and $\mathbf{S}_3$ coincide. This is a natural result, since these two groups are isomorphic.

2. Usually the representations of the symmetric group $\mathbf{S}_n$ are labelled by the so-called Young tableau. The Young tableau is a scheme consisting of n small boxes (the number of boxes equals the number of particles). The boxes can be placed in one row, two rows, and so on. If we have n_1 particles in the first row, n_2 particles in the second row, ..., n_i particles in the *ith* row, then the scheme is denoted as $[n_1, n_2, \ldots, n_i]$ where $n_1 + n_2 + \ldots + n_i = n$. It is always required that $n_1 \geq n_2 \geq \ldots \geq n_i$.

   The same notations can be used to label the basis functions of the representation. The physical meaning of these schemes is that the particles which are in the same row are in a totally symmetric state (the sign of the wave function does not change under any permutation of any number of the particles from the row), while the particles which are in the same column are in a totally antisymmetric state (the sign of the basis function changes under permutation of any two particles from the column).

   The irreducible representations of $\mathbf{S}_3$ obtained in the Example 3, can be labelled by the following Young tableaux:

$$\begin{aligned} D^{(1)}(G) &= [3]\,, \\ D^{(2)}(G) &= [111]\,, \\ D^{(3)}(G) &= [21]\,. \end{aligned} \tag{47}$$

   It means that the representation [3] is realized on the functions which are symmetric with respect to interchange of any of three particles, the representation [111] is realized on the functions which are antisymmetric with respect to interchange of any of three particles, while the representation [21] is realized on the functions which is of mixed symmetry (symmetric with respect to interchange of some of three particles, but antisymmetric with respect to interchange of the other particles).

4 Decomposition of representation into irreducible components

Suppose that we know all irreducible representations $D^{(1)}(G)$, $D^{(2)}(G)$, ... of a given group. Then we can represent any arbitrary reducible representation in a form:

$$D(G) = m_1 D^{(1)}(G) \oplus m_2 D^{(2)}(G) \oplus \ldots\ , \tag{48}$$

where m_α denote how many times a representation $D^{(\alpha)}(G)$ contains in the representation $D(G)$.

How to find these m_α?

From (35) it follows that

$$m_\alpha = \frac{1}{n} \sum_G \chi^{(\alpha)\,*}(G)\chi(G) \ , \tag{49}$$

where $\chi^{(\alpha)}(G)$ is the character of the representation $D^{(\alpha)}(G)$ (it is complex conjugate in the formula (49)) and $\chi(G)$ is the character of the representation $D(G)$.

Example

Construct the representation of the symmetric group $\mathbf{S}_3$ *in the basis formed by the vectors* ($\vec{e}_1$,$\vec{e}_2$,$\vec{e}_3$) *supposing that each permutation of the group interchanges the vectors having the corresponding indices. Decompose this representation into irreducible components.*

To construct the representation, let us first look how the basis transforms under permutations. Since we have three basis vectors, the representation which we want to construct is 3-dimensional. for the identity element we have

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{50}$$

Now, let us consider P_{12}. Under this permutation, the vectors $\vec{e}_1$ and $\vec{e}_2$ interchange their places:

$$D(P_{12})(\vec{e}_1, \vec{e}_2, \vec{e}_3) = (\vec{e}_2, \vec{e}_1, \vec{e}_3) \tag{51}$$

and we get a matrix

$$D(P_{12}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{52}$$

In the same way, we can construct the other four matrices of the representation:

$$\begin{gathered} D(P_{23}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \ , \quad D(P_{13}) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \ , \\ D(\pi_1) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \ , \quad D(\pi_2) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \ . \end{gathered} \tag{53}$$

the characters of these representation are given in the table below:

	E	π_1, π_2	P_{12}, P_{23}, P_{13}
χ	3	0	1

Now, let us decompose this representation into irreducible components. The characters of all three irreducible representations were found in Example 3 of the section 3.2. Thus we have:

$$D(G) = m_1 D^{(1)}(G) \oplus m_2 D^{(2)}(G) \oplus m_3 D^{(3)}(G) \ . \tag{54}$$

In order to find how many times each of these representations are contained in $D(G)$ (the values m_α, let us use the formula (35):

$$\begin{aligned} m_1 &= \frac{1}{6}(3\cdot 1+1\cdot 0+1\cdot 0+1\cdot 1+1\cdot 1+1\cdot 1)=1\ ,\\ m_2 &= \frac{1}{6}(3\cdot 1+1\cdot 0+1\cdot 0-1\cdot 1-1\cdot 1-1\cdot 1)=0\ ,\\ m_3 &= \frac{1}{6}(3\cdot 2-1\cdot 0-1\cdot 0+0\cdot 1+0\cdot 1+0\cdot 1=1)\ , \end{aligned} \tag{55}$$

from where we get the final result:

$$D(G)=D^{(1)}(G)\oplus D^{(3)}(G)\ . \tag{56}$$

5 Direct product of representations

Suppose that two sets of the functions $f_1^{(\alpha)}(r)$, $f_2^{(\alpha)}(r)$, ..., $f_{l_\alpha}^{(\alpha)}(r)$ and $f_1^{(\beta)}(r)$, $f_2^{(\beta)}(r)$, ..., $f_{l_\beta}^{(\beta)}(r)$ form the bases of two representations of the group **G**: $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$ of the dimensions l_α and l_β, respectively. Then the $l_\alpha l_\beta$ products $f_i^{(\alpha)}(r)f_j^{(\beta)}(r)$ form a basis of some representation of the group **G**, which we denote as $D^{(\alpha\times\beta)}$ and whose matrix elements are

$$D_{ik,jm}^{(\alpha\times\beta)}(G)=D_{ij}^{(\alpha)}(G)D_{km}^{(\beta)}(G) \tag{57}$$

This representation is called a *direct product* of two representations $D^{(\alpha}(G)$ and $D^{(\beta)}(G)$ and its dimension $l=l_\alpha l_\beta$.

If $\chi^{(\alpha)}(G)$ and $\chi^{(\beta)}(G)$ denote the characters of an element G in the irreducible unitary representations $D^{(\alpha)}(G)$ and $D^{(\beta)}(G)$, respectively, then

$$\chi^{(\alpha\times\beta)}(G)=\chi^{(\alpha)}(G)\chi^{(\beta)}(G)\ . \tag{58}$$

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