Solution to Problems 3

1. *Construct the representation of the group* $\mathbf{D}_3$ *in a 3-dimensional space formed by the vectors* $\vec{e}_x$, $\vec{e}_y$ *and* $\vec{e}_z$. *What is the difference in comparison with the group* $\mathbf{C}_{3v}$?

Group $\mathbf{D}_3$ contains 6 elements: E, two rotations C_3 and C_3^2, three rotations C_2, C_2', C_2'' around C_2-axes passing one of the triangle vertices and its centre. In the basis ($\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$), the representation matrices are

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; D(C_3^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$D(C_2) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}, \; D(C_2') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}, \; D(C_2'') = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{1}$$

This representation of the group $\mathbf{D}_3$ is reducible. 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 $D^{(3)}$:

$$D^{(3)}(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; D^{(3)}(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; D^{(3)}(C_3^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},$$
$$D^{(3)}(C_2) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; D^{(3)}(C_2') = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; D^{(3)}(C_2'') = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{2}$$

The vector $\vec{e}_z$ is the basis vector of the 1-dimensional representation, which we call $D^{(2)}$:

$$D^{(2)}(E) = 1, \; D^{(2)}(C_3) = 1, \; D^{(2)}(C_3^2) = 1, \; D^{(2)}(C_2) = -1, \; D^{(2)}(C_2'') = -1, \; D^{(2)}(C_2'') = -1\,. \tag{3}$$

Thus we have found that

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

The group $\mathbf{D}_3$ is isomorphic to the group $\mathbf{C}_{3v}$. The characters of their irreducible representations are identical, but in the basis ($\vec{e}_x$, $\vec{e}_y$, $\vec{e}_z$), the constructed reducible representations consist of different irreducible components in two cases.

2. *Elements of the group* $\mathbf{C}_{4v}$ *can be divided into 5 classes. How many irreducible representations has this group? What are their dimensions? (See definitions of all point symmetry groups in the previous lecture).*

The 8 elements of the group $\mathbf{C}_{4v}$ can be divided into 5 classes. Therefore, the group has five irreducible representations: four 1-dimensional representations and one 2-dimensional representation.

3. *Elements of the group* **T** *can be divided into 4 classes. How many irreducible representations has this group? What are their dimensions?*

The 12 elements of the group **T** can be divided into 4 classes. Therefore, the group has four irreducible representations: three 1-dimensional representations and one 3-dimensional representation.

4. *Elements of the group* **O** *can be divided into 5 classes. How many irreducible representations has this group? What are their dimensions?*

The 24 elements of the group **O** can be divided into 5 classes. Therefore, the group has five irreducible representations: two 1-dimensional representations, one 2-dimensional representation and two 3-dimensional representations.

5. *How many irreducible representations has the group* $\mathbf{C}_4$*? Find their dimensions and characters, using the result of Example 1 of the section 1.4.*

The group $\mathbf{C}_4$ has four irreducible representations.

	E	C_4	C_4^2	C_4^3
$\chi^{(1)}$	1	1	1	1
$\chi^{(2)}$	1	-1	1	-1
$\chi^{(3)}$	1	i	-1	$-$i
$\chi^{(4)}$	1	$-$i	-1	i

6. *Construct the representation of the group* $\mathbf{C}_{3v}$ *in the 3-dimensional space formed by the functions* $f_1 = x^2$, $f_2 = y^2$, $f_3 = xy$ *(continue the procedure started in Example 3 of the section 1.4). Decompose this representation into irreducible components using and the known characters of the irreducible representations.*

$$D(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ D(C_3) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},\ D(C_3^2) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & -\frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},$$
$$D(\sigma_1) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{2} & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix},\ D(\sigma_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},\ D(\sigma_3) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & -\frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{1}{4} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{5}$$

$$D(G) = D^{(1)}(G) \oplus D^{(3)}(G)\ . \tag{6}$$

7. *Find the matrices of the direct product of two representations of the group* $\mathbf{C}_{3v}$*:* $D^{(2)}(G)$ *and* $D^{(3)}(G)$*.*

See the matrices $D(G)$ of the problem 1.

8. *Decompose the direct product of two representations* $D^{(3)}(G)$ *of the group* $\mathbf{C}_{3v}$ *into irreducible components.*

$$D^{(3)}(G) \otimes D^{(3)}(G) \equiv D^{(3\times 3)}(G) = D^{(1)}(G) \oplus D^{(2)}(G) \oplus D^{(3)}(G) \, . \qquad (7)$$