8
Group Theoretical Methods

The methods of group theory are of valuable service for the analysis of the mathematical structure of tensors, in particular for the investigation and the determination of the number and type of independent tensor components. We mention especially the general importance of the application of group theoretical methods for the description of electronic states and their transitions, for the analysis of the vibrational states of molecular and crystalline systems as well as for the classification of phase transitions based on symmetry properties. In this book, however, we shall only discuss a few basic aspects.

In the following we will recapitulate some important definitions and theorems to provide a helpful introduction for those unfamiliar with group theory. In particular, this chapter should be read in conjunction with introductory books on group theory and the rules practiced by working through concrete examples.

8.1
Basics of Group Theory

A set of elements $g_1, g_2, \ldots, g_3$ forms a *group* G, when the following conditions are fulfilled:

1. Between any two elements g_i and g_j of the group an operation is defined which also leads to an element belonging to the group, hence $g_i g_j = g_k$. The commutative law for "multiplication" need not be fulfilled.

2. The operation is associative, i.e., for arbitrary g_i, g_j, g_k then it is always true that $g_i(g_j g_k) = (g_i g_j) g_k$.

3. There is an identity element e of the group, also called the neutral element, such that $e g_i = g_i e = g_i$ for all elements g_i of the group.

4. Each element g_i possesses an inverse element g_i^{-1} also belonging to the group such that $g_i g_i^{-1} = e$.

The number of elements of a group is called the order h of the group. We denote a *subgroup* as a subset of the group satisfying all the conditions of a group.

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Table 8.1 Some symmetry operations for transformations of cartesian frames in matrix notation.

n-fold rotation (n) parallel to $\boldsymbol{e}_3$; angle $\varphi = 2\pi/n$:

$$A_{n\|e_3} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

n-fold rotation–inversion ($\bar{n}$) parallel to $\boldsymbol{e}_3$:

$$A_{\bar{n}\|e_3} = \begin{pmatrix} -\cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & \bar{1} \end{pmatrix};$$

threefold rotation parallel to the space diagonal of the cartesian frame:

$$A_{3\|[111]} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix};$$

twofold rotation parallel to the axis dissecting $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$:

$$A_{2\|[110]} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix};$$

reflection at a mirror plane perpendicular to the axis dissecting $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$:

$$A_{\bar{2}\|[110]} = \begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

All other symmetry operations with different orientations with respect to the crystallographic reference frame can be deduced from those indicated by a similarity transformation $\boldsymbol{A} = \boldsymbol{U}^{-1}\boldsymbol{A}'\boldsymbol{U}$. The transformation matrix $\boldsymbol{U}$ creates from the crystallographic reference frame $\{\boldsymbol{e}_i\}$ the new reference frame $\{\boldsymbol{e}'\}$ according to $\boldsymbol{e}' = \boldsymbol{U}\boldsymbol{e}$, in which the respective symmetry operator assumes the form $\boldsymbol{A}'$ of one of the matrices given above.

Those elements of a group, which through their operation build a complete group are called generating elements. If the elements are concrete things such as geometric figures, permutations of numbers or letters, functions of the position vector or matrices then we speak of concrete *representations* of the group. In the broader sense, we will be mainly dealing with groups whose elements consist of quadratic matrices (number of rows = number of columns). Among these, in particular, are all transformation matrices describing symmetry operations. Table 8.1 lists these matrices for distinct directions.

The properties of a group are taken from the associated *group table*. This contains all products $g_i g_j$. In the case of point symmetry groups the simplest way to generate the table is by means of a stereographic projection in which all the symmetry operations occurring are written. We select a point P inside the respective elementary triangle and first let the symmetry element g_j act on P to generate $g_jP = P'$. Then we let g_i act on P' and obtain $g_ig_jP = g_iP' = P''$. From the stereographic projection we can see how P'' is to be directly generated with a single operation g_k of the group according to $P'' = g_kP$. Hence, we find the product $g_ig_j = g_k$, which we then write in the ith row and jth column of the group table.

Two elements g_i and g_j are *conjugated* when there exists one element x in G such that $g_i = x^{-1}g_jx$. All elements conjugated to an element g_i form a *class*. If g_i and g_j as well as g_j and g_k are conjugated, then g_i and g_k are also conjugated. Since two classes of a group do not possess a common element, one can decompose each finite group in a finite number of classes $K_1, K_2 \ldots$. The number of elements n_i of a class K_i is a divisor of the order of G, hence, $h = n_ih'$, h' whole. As an example we select PSG 3m. The generating symmetry elements are the threefold axis and a symmetry plane containing the threefold axis. The group consists of six elements $g_1 = e$, $g_2 = R_3$, $g_3 = R_3^2$, $g_4 = m_1 = R_{\bar{2}\|a_1}$, $g_5 = m_2 = R_{\bar{2}\|a_2}$ and $g_6 = m_3 = R_{\bar{2}\|a_1'}$ with $\boldsymbol{a}_1' = -\boldsymbol{a}_1 - \boldsymbol{a}_2$. In order to carry out the decomposition into classes, we multiply each element g_i with all elements x according to $x^{-1}g_ix$. This procedure can be carried out comfortably by means of the given group table. Groups with the same group table are called *isomorphic groups* (example, m3 and 23).

Group table of PSG 3m

$g_1 = e$	$g_2 = R_3$	$g_3 = R_3^2$	$g_4 = m_1$	$g_5 = m_2$	$g_6 = m_3$
g_2	g_3	g_1	g_6	g_4	g_5
g_3	g_1	g_2	g_5	g_6	g_4
g_4	g_5	g_6	g_1	g_2	g_3
g_5	g_6	g_4	g_3	g_1	g_2
g_6	g_4	g_5	g_2	g_3	g_1

The following classes result K_1: $g_1 = e$, K_2: g_2, g_3; K_3: g_4, g_5, g_6. The class K_1 with the identity element exists in each group. The three elements of class K_3 belong to the three symmetry equivalent symmetry planes of PSG 3m. In case the group is represented by matrices $g_k = (a_{ij})_k$ then each class can be characterized by an invariant quantity, namely the *trace* $S = \sum_i a_{ii}$ of one of the matrices of the class since all elements of a class possess the same trace; hence, $S(g_i) = S(g_j)$ for the case $g_i = x^{-1}g_jx$. The proof for

$$S(\boldsymbol{A}^{-1}\boldsymbol{B}\boldsymbol{A}) = S(\boldsymbol{B}) = S(\boldsymbol{A}\boldsymbol{B}\boldsymbol{A}^{-1})$$

results from the relation

$$S(\boldsymbol{A}\boldsymbol{B}\boldsymbol{C}) = S(\boldsymbol{B}\boldsymbol{C}\boldsymbol{A}) = S(\boldsymbol{C}\boldsymbol{A}\boldsymbol{B}) = A_{ij}B_{jk}C_{ki}$$

for the case $\boldsymbol{C} = \boldsymbol{A}^{-1}$. The quadratic matrices $\boldsymbol{A}$, $\boldsymbol{B}$ and $\boldsymbol{C}$ are of the same order.

The trace assigned to a class, which we will denote by χ in what is to follow, is called the *character* of the class. The invariance of the character consists in the fact that a transformation matrix retains its trace even after a change of the reference system. From a reference system $\{\boldsymbol{e}'_i\}$ let new basic vectors $\boldsymbol{a}'_i$ arise according to $\boldsymbol{a}'_i = a'_{ij}\boldsymbol{e}'_j$, or in the matrix notation $\boldsymbol{a}' = \boldsymbol{A}'\boldsymbol{e}'$. The basic vectors $\boldsymbol{e}'_i$ and $\boldsymbol{a}'_i$ with the transformation matrix $\boldsymbol{U}$ shall result from the unprimed basic vectors according to

$$\boldsymbol{e}'_i = u_{ij}\boldsymbol{e}_j \quad \text{or} \quad \boldsymbol{a}'_i = u_{ij}\boldsymbol{a}_j \quad (\boldsymbol{e}' = \boldsymbol{U}\boldsymbol{e}, \boldsymbol{a}' = \boldsymbol{U}\boldsymbol{a}).$$

Hence, $\boldsymbol{a} = \boldsymbol{U}^{-1}\boldsymbol{A}'\boldsymbol{U}\boldsymbol{e}$ when we solve the relation $\boldsymbol{a}' = \boldsymbol{U}\boldsymbol{a}$ with the help of the inverse matrix in $\boldsymbol{a} = \boldsymbol{U}^{-1}\boldsymbol{a}'$ and substitute $\boldsymbol{a}'$ by $\boldsymbol{A}'\boldsymbol{e}'$ and $\boldsymbol{e}'$ by $\boldsymbol{U}\boldsymbol{e}$. We denote the matrix $\boldsymbol{A} = \boldsymbol{U}^{-1}\boldsymbol{A}'\boldsymbol{U}$ as a to $\boldsymbol{A}'$ equivalent matrix or symmetry operation. The same relation applies to the coordinates when $\boldsymbol{U}$ represents a unitary matrix, i.e., when $\boldsymbol{U} = (\bar{\boldsymbol{U}}^T)^{-1}$. T means transposed matrix and $\bar{}$ means conjugate complex for the case that the components of the matrix are complex. Consequently, the elements of a class represent the set of symmetry equivalent operations of a certain type within the group. The elements of an arbitrary finite group can always be represented in the form of matrices. This is seen from the *regular representation*, directly constructed from the group table. This is done by rearranging the columns of the group table such that the identity element is present in each principal diagonal. The matrix of the ith element of the regular representation is obtained by writing the number 1 for the element g_i and 0 for all remaining positions in the rearranged group table. The order of these matrices is equal to the order of the group.

The element $g_i g_j^{-1}$ is in the ith row and jth column of the rearranged group table and the element $g_j g_i^{-1} = (g_i g_j^{-1})^{-1}$ is in the jth row and ith column. This means that the transposed matrices are equivalent to the inverse matrices, hence, unitary. That the regular representation actually obeys the group table is recognized as follows. To each three elements g_i, g_j, g_k there always exists two elements g_m and g_n with the property

$$g_i g_k = g_m, \quad g_j g_n = g_k, \quad \text{hence} \quad g_i = g_m g_k^{-1} \quad \text{and} \quad g_j = g_k g_n^{-1}.$$

The associated matrices of the regular representation have the components $(\boldsymbol{A}_i)_{mk} = 1$ and $(\boldsymbol{A}_j)_{kn} = 1$. All the components with other values for mk or nk than those resulting from the above conditions vanish.

We now inquire as to the elements $g_l = g_i g_j$ with the matrix $\boldsymbol{A}_l$. Because $g_l = g_i g_j = g_m g_k^{-1} g_k g_n^{-1}$, we have $(\boldsymbol{A}_l)_{mn} = 1$. If the regular representation were to obey the group table, then we would have $\boldsymbol{A}_l = \boldsymbol{A}_i\boldsymbol{A}_j$. In point of fact the components

$$(\boldsymbol{A}_i\boldsymbol{A}_j)_{mn} = \sum_k (\boldsymbol{A}_i)_{mk}(\boldsymbol{A}_j)_{kn} = 1$$

agree with $(\boldsymbol{A}_l)_{mn}$ for each pair mn with the above value of k. All other mn yield the component 0 in both the cases. This proves our assertion.

The matrices g_i can be simultaneously transformed into the so-called block matrices with the aid of the unitary transformation $\boldsymbol{U}^{-1}g_i\boldsymbol{U}$ (by applying a suitable unitary matrix). Representations whose matrices cannot be reduced into still smaller block matrices are called *irreducible representations*. These are of fundamental importance in group theory applications. In all further unitary transformations, the individual blocks (see the irreducible representation for the PSG 3m in Table 8.2 arising from the regular representation) are transformed among one another without involving other block matrices and their coefficients. This means that the corresponding block matrices among themselves are also irreducible representations of the given group fulfilling the conditions of the group table. These irreducible representations in the form of block matrices possess a number of important properties which we cite without proof:

1. The number of different nonequivalent irreducible representations of a finite group is equal to the number S of the class.

2. The number of equivalent matrices of an irreducible representation contained in the regular representation is equal to the order of the given matrices. If one divides the identity element of the regular representation, i.e., the unit matric of order h, into unit matrices of the block matrices of the irreducible representation, one sees that the sum of the squares of the matrices of all nonequivalent irreducible representations is equal to the order of the group; hence, $\sum_{s=1}^{S} l_s^2 = h$, where l_s is the order of the block matrix of the sth irreducible representation.

3. If $\chi_k(g_i)$ is the trace of the matrix of the ith element in the kth irreducible representation then the following orthogonality relations are valid:

$$\sum_{s=1}^{S} n_s \chi_k^{\text{irr}}(s)\bar{\chi}_{k'}^{\text{irr}}(s) = \sum_{i=1}^{h} \chi_k^{\text{irr}}(i)\bar{\chi}_{k'}^{\text{irr}}(i) = h\delta_{kk'}.$$

   As an abbreviation, we write $\chi(i)$ instead of $\chi(g_i)$. One sums over the classes in the first summation and over all elements of the group in the second summation. n_s is the number of elements in the sth class. A similar relation for the products of the characters of the different classes is given by

$$\sum_{k=1}^{S} \chi_k^{\text{irr}}(s)\bar{\chi}_k^{\text{irr}}(s') = \delta_{ss'}h/n_s.$$

Table 8.2 Representations of PSG 3m.

Rearranged group table:

g_1	g_3	g_2	g_4	g_5	g_6
g_2	g_1	g_3	g_6	g_4	g_5
g_3	g_2	g_1	g_5	g_6	g_4
g_4	g_6	g_5	g_1	g_2	g_3
g_5	g_4	g_6	g_3	g_1	g_2
g_6	g_5	g_4	g_2	g_3	g_1

Regular representation:

$$g_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}, \quad g_3 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix},$$

$$g_4 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad g_5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad g_6 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

Table 8.2 *(continued)*

Equivalent representation constructed from irreducible block-diagonal matrices:

$$g_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad g_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/2 & \sqrt{3}/2 & 0 & 0 \\ 0 & 0 & -\sqrt{3}/2 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/2 & \sqrt{3}/2 \\ 0 & 0 & 0 & 0 & -\sqrt{3}/2 & -1/2 \end{pmatrix},$$

$$g_3 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/2 & -\sqrt{3}/2 & 0 & 0 \\ 0 & 0 & \sqrt{3}/2 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1/2 & -\sqrt{3}/2 \\ 0 & 0 & 0 & 0 & \sqrt{3}/2 & -1/2 \end{pmatrix}, \quad g_4 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$g_5 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & -\sqrt{3}/2 & 0 & 0 \\ 0 & 0 & -\sqrt{3}/2 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & -\sqrt{3}/2 \\ 0 & 0 & 0 & 0 & -\sqrt{3}/2 & -1/2 \end{pmatrix}, \quad g_6 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & \sqrt{3}/2 & 0 & 0 \\ 0 & 0 & \sqrt{3}/2 & -1/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/2 & \sqrt{3}/2 \\ 0 & 0 & 0 & 0 & \sqrt{3}/2 & -1/2 \end{pmatrix},$$

The character of an element of an arbitrary representation $\Gamma(g_i)$ can be resolved according to

$$\chi(g_i) = \sum_{k=1}^{S} m_k \chi_k^{\text{irr}}(i).$$

Hence, m_k specifies how often the kth irreducible representation is contained in the representation $\Gamma(g_i)$. From the orthogonality relation it follows that

$$m_k = \frac{1}{h} \sum_{s=1}^{S} n_s \chi(s) \bar{\chi}_k^{\text{irr}}(s) = \frac{1}{h} \sum_{i=1}^{h} \chi_k(g_i) \bar{\chi}_k^{\text{irr}}(g_i),$$

whereby in the first summation one again sums over the classes and in the second over the elements of the group. For each arbitrary representation Γ it is true that

$$\Gamma = \sum_{k=1}^{S} m_k \Gamma_k^{\text{irr}},$$

where Γ_k^{irr} is the kth irreducible representation.

For many problems it is sufficient to consider the character table of a group instead of the group table. Each column contains the characters of a certain class for the different irreducible representations and the rows contain the characters of the elements of the different classes for a fixed irreducible representation.

In point symmetry groups, the order h of the group, i.e., the number of symmetry operations, is always equal to the number of surface elements of a general form; hence, one can specify h from the known morphological rules.

8.2 Construction of Irreducible Representations

The irreducible representations of the crystallographic point symmetry groups can always be derived without difficulty with the help of the above relations, in particular, with the orthogonality relations. Thus we can forgo a description of a general procedure for the construction of irreducible representations here.

In some cases it is useful to apply an additional rule concerning the *direct matrix product* (*inner Kronecker product*), which also plays an important role in other relationships. The direct matrix product of two matrices $\boldsymbol{A} = (a_{ij})$ and $\boldsymbol{B} = (b_{kl})$, denoted by $\boldsymbol{A} \times \boldsymbol{B}$, is a matrix with the elements

$$(\boldsymbol{A} \times \boldsymbol{B})_{ij,kl} = a_{ik} b_{jl}.$$

The direct product of two representations

$$\Gamma_a(g) \times \Gamma_b(g) = \Gamma_c(g)$$

consists of matrices formed by the direct product of the matrices belonging to each element g of both representations. The direct product is also a representation of the group when the matrices Γ_a and Γ_b are permutable for all elements g. This results because

$$\begin{aligned}(\Gamma_c(f)\Gamma_c(g))_{ij,kl} &= (\Gamma_a(f) \times \Gamma_b(f))_{ij,mn}(\Gamma_a(g) \times \Gamma_b(g))_{mn,kl} \\ &= (\Gamma_a(f)_{im}\Gamma_b(f)_{jn})(\Gamma_a(g)_{mk}\Gamma_b(g)_{nl}) \\ &= (\Gamma_a(f)\Gamma_a(g))_{ik}(\Gamma_b(f)\Gamma_b(g))_{jl} \\ &= (\Gamma_a(fg) \times \Gamma_b(fg))_{ij,kl} \\ &= (\Gamma_c(fg))_{ij,kl}.\end{aligned}$$

Since an arbitrary representation can be resolved according to $\Gamma_s(g) = \sum_{k=1}^{S} m_k \Gamma_k^{\text{irr}}$, and for m_k the relation

$$m_k = \frac{1}{h}\sum_{s=1}^{S} n_s \chi(s)\bar{\chi}_k^{\text{irr}}(s)$$

holds as well as the relation

$$\chi(\Gamma_a(g) \times \Gamma_b(g)) = \chi(\Gamma_a(g))\chi(\Gamma_b(g)),$$

proved directly from the Kronecker relation, one has

$$\Gamma_a(g) \times \Gamma_b(g) = \frac{1}{h}\sum_{k=1}^{S}\sum_{g}\chi_a(g)\chi_b(g)\bar{\chi}_k^{\text{irr}}(g)\Gamma_k.$$

If $\Gamma_a(g)$ and $\Gamma_b(g)$ are two irreducible representations, then one can obtain other irreducible representations via the direct product as long as $\Gamma_a(g)$ and $\Gamma_b(g)$ are different from the identity representation.

The construction of the irreducible representation is now made as follows:

1. The group is decomposed into classes by calculating the product $x^{-1}gx$, whereby with given g for x all elements of the group are written down. As already mentioned, this operation can be comfortably carried out using the group table.

2. From the relation $\sum_{s=1}^{S} l_s^2 = h$, one obtains in almost all important applications an unambiguous statement concerning the dimensions of the individual representations. From 1. the number of irreducible representations is known ($S =$ number of classes!).

3. $\Gamma_1 = (1;1;1;\ldots;1)$ is always an irreducible representation (total symmetrical representation, trivial representation). We use the following scheme

for the construction of nontrivial representations for $l = 1, 2$ and 3 (angle of rotation $\varphi = 2\pi/n$):

	$g = 1$	$\bar{1}$	$\mathrm{m} = \bar{2} \parallel \boldsymbol{e}_1$	$\mathrm{n} \parallel \boldsymbol{e}_3$	$\bar{\mathrm{n}} \parallel \boldsymbol{e}_3$
$l = 1$	(1)	$(\bar{1})$	$(\bar{1})$	(1)	$(\bar{1})$
$l = 2$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}$	$\begin{pmatrix} -\cos\varphi & -\sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix}$
$l = 3$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -\cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$

From the similarity transformation $\boldsymbol{U}\boldsymbol{A}\boldsymbol{U}^{-1}$ one obtains the corresponding matrices $\boldsymbol{A}'$ for the different orientations of the symmetry operators. For example, one has for $g_5 = \boldsymbol{R}_{\bar{2}\parallel \boldsymbol{a}_2}$ in the PSG 3m, in two-dimensional representation:

$$
\begin{aligned}
g_5 = \boldsymbol{U} g_4 \boldsymbol{U}^{-1} &= \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \\
&= \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}
\end{aligned}
$$

with $\varphi = 120°$ (rotation of the symmetry plane about the threefold axis).

In any case, one must check whether the orthogonality conditions are adhered to. For cyclic groups, in which all group elements are powers of the generating elements, hence, with all rotation axes and rotation–inversion axes, each element forms a class on its own, i.e., only one-dimensional representations exist. In these cases we can immediately specify the complete irreducible representations. For an n-fold rotation axis, one always has $g^n = 1$, hence, $g = e^{2\pi i k/n}$ (unit roots of nth degree) for the one-dimensional representations. The irreducible representations are then the n powers $\Gamma_k = (e^{2\pi i k m/n})$ with $m = 0, 1, 2, \ldots, n-1$. Thus, for example, for a sixfold rotation axis $\Gamma_2 = (1; e^{2\pi i 2/6}; e^{2\pi i 4/6}; e^{2\pi i 6/6}; e^{2\pi i 8/6}; e^{2\pi i 10/6})$. We recognize the validity of the orthogonality relation when we form the "scalar product" of two such representations

$$
\begin{aligned}
\Gamma_k \cdot \bar{\Gamma}_{k'} &= \sum_{m=0}^{n-1} e^{2\pi i k m/n} e^{-2\pi i k' m/n} = \sum_{m=0}^{n-1} e^{2\pi i (k-k') m/n} \\
&= \frac{e^{2\pi i (k-k')} - 1}{e^{2\pi i (k-k')/n} - 1} = \left\{ \begin{matrix} 0 & \text{for} & k \neq k' \\ 1 & \text{for} & k = k' \end{matrix} \right\} .
\end{aligned}
$$

For rotation inversions with even orders of symmetry one obtains the same irreducible representations (the PSGs n and $\bar{n}$ are isomorphic). In the case of odd orders of symmetry, one makes use of the fact that the group $\bar{n} = n \times \bar{1}$. This results in $2n$ irreducible representations when one writes the identity element

(1) and the element $(\bar{1})$ for the group $\bar{1}$. The irreducible representations then follow directly from the product of the representations of n and $\bar{1}$, because the one-dimensional representations are identical with the corresponding character values.

We will illustrate the procedure using the PSGs 3m, 23, and m3 as examples. As already shown, 3m has six elements divided into three classes[1]:

$$K_1 : g_1 = e;$$
$$K_2 : g_2 = 3^1, g_3 = 3^2;$$
$$K_3 : g_4 = m_1, g_5 = m_2, g_6 = m_3.$$

The dimensions of the irreducible representations result from $\sum_{s=1}^{3} l_s^2 = 6 = 1 + 1 + 4$; thus there exists two one-dimensional representations and one two-dimensional irreducible representation. The table below gives the values $\chi(\Gamma_2) = (1, 1, \bar{1})$ for the character values of Γ_2 and $\chi(\Gamma_3) = (2, \bar{1}, 0)$ for the two-dimensional representation. Consequently, the complete character table for the PSG 3m looks like

	e	$(3^1, 3^2)$	(m_1, m_2, m_3)
$\chi(\Gamma_1)$	1	1	1
$\chi(\Gamma_2)$	1	1	$\bar{1}$
$\chi(\Gamma_3)$	2	$\bar{1}$	0

The associated irreducible representations can be calculated with the help of the above table when one generates the elements g_5 and g_6 from g_4, as demonstrated above:

	$g_1 = e$	$g_2 = 3^1$	$g_3 = 3^2$	$g_4 = m_1$	$g_5 = m_2$	$g_6 = m_3$
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	$\bar{1}$	$\bar{1}$	$\bar{1}$
Γ_3	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}$	$\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$

At this point we note that all groups $n2$ or nm with arbitrary n-fold axis possess easily manageable character tables and irreducible representations. If n is even we have the classes K_1: e; K_2: n^1, n^{n-1}; K_3: n^2, n^{n-2}; $\ldots$ $K_{n/2+1}$: $n^{n/2}$; $K_{n/2+2}$: $2'$ ($n/2$ times) or m$'$ ($n/2$ times); $K_{n/2+3}$: $2''$ ($n/2$ times) or m$''$ ($n/2$ times). $2'$ and m$'$ are the generating elements of the group $n2$ and nm, respectively; $2''$ and m$''$ are further symmetry elements bisecting the angles between the axes $2'$ and the symmetry planes m$'$, respectively. Thus a total of $n/2 + 3$ classes exist. From $\sum_{s=1}^{S} l_s^2 = h = 2n$ follows the unique decomposition $2n = 4 + 4(n-2)/2$, i.e., there exists four one-dimensional irreducible representations and $(n-2)/2$ two-dimensional representations.

1) In the following we use the symbol n^q as an abbreviation for $\boldsymbol{R}_n^q$.

If n is odd, then the groups $n2$ and nm, respectively, possess the following classes: K_1: e, K_2: n^1, n^{n-1}; K_3: n^2, n^{n-2}; ...; $K_{(n+1)/2}$: $n^{(n-1)/2}, n^{(n+1)/2}$; $K_{(n+1)/2+1}$: 2 (n-times) and m (n-times) respectively. Thus there exists $(n+1)/2+1 = (n+3)/2$ classes. With $\sum_{s=1}^{S} l_s^2 = h = 2n$, one obtains uniquely $2n = 2 + 4(n-1)/2$ and hence, two one-dimensional irreducible representations and $(n-1)/2$ two-dimensional irreducible representations. The construction of the character table for these groups and the complete determination of the associated irreducible representations for arbitrary n is unproblematic.

We now come to the PSG 23, possessing two threefold axes running in the direction of the space diagonals of a cube, as the generating symmetry operations. The elements of the group, aside from the identity element, are the three twofold axes along the edges of the cube, the four threefold axes 3^1 along the space diagonals and the four threefold axes with an angle of rotation of 240°, which we denote as 3^2. The group contains a total of 12 elements. From the relation $\sum_{s=1}^{S} l_s^2 = 12$, we recognize the following:

If a three-dimensional representation exists, then there must also exist three one-dimensional representations. In the case of a two-dimensional representation we would have eight additional one-dimensional representations and in the case of two two-dimensional representations, a further four one-dimensional representations. From the equivalent symmetry operations mentioned above it clearly emerges that only four classes exist. Thus only the first alternative comes into question: three one-dimensional representations and one three-dimensional representation.

The characters of the nontrivial one-dimensional representations of the classes $K_3 = 3^1$ (4-times) and $K_4 = 3^2$ (4-times) are found by setting the values $e^{2\pi i m/3} = 1$.

We then obtain

$$\chi(\Gamma_2) = (1, 1, e^{2\pi i/3}, e^{2\pi i 2/3})$$

and

$$\chi(\Gamma_3) = (1, 1, e^{2\pi i 2/3}, e^{2\pi i 4/3}).$$

The character values of the three-dimensional representation are obtained by using the values from our table and we find

$$(\Gamma_4) = (3, -1, 0, 0).$$

Checking the orthogonality relation confirms the correctness.

The associated irreducible representations are found directly from the matrix representation of the symmetry elements of the group when one performs the respective transformations. For Γ_4 the result is

	e	$2' \parallel [100]$	$2'' \parallel [010]$	$2''' \parallel [001]$
Γ_4	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$
	$3^{1'} \parallel [111]$	$3^{1''} \parallel [\bar{1}\bar{1}1]$	$3^{1'''} \parallel [1\bar{1}\bar{1}]$	$3^{1''''} \parallel [\bar{1}1\bar{1}]$
	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{pmatrix}$
	$3^{2'} \parallel [111]$	$3^{2''} \parallel [\bar{1}\bar{1}1]$	$3^{2'''} \parallel [1\bar{1}\bar{1}]$	$3^{2''''} \parallel [\bar{1}1\bar{1}]$
	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{pmatrix}$

The irreducible representations and the respective character vectors for the PSG m3 are obtained from the Kronecker product according to $\mathrm{m3} = 23 \times \bar{1}$. The 24 elements are distributed over eight classes, of which the first four are identical with those of the PSG 23, and the second four result simply from the first four by multiplication with the element $g_{13} = \bar{1}$. Formally, we can represent a group G, formed from a group G' by a Kronecker product with the group $\bar{1} = (g_1 = 1, g_2 = -1)$ as $G = G' \times \bar{1} = G'g_1 + G'g_2$. The character table then has the form

	$K(G')$	$K(G'g_2)$
$\chi(\Gamma(G'))$	$\chi(G')$	$\chi(G')$
$\chi(\Gamma(G'g_2))$	$\chi(G')$	$-\chi(G')$

$K(G')$ means the classes of G' and $K(G'g_2)$ means the classes of $G'g_2$. Correspondingly, $\Gamma(G')$ and $\Gamma(G'g_2)$ are the irreducible representations of G' and $G'g_2$, respectively.

Exercises 37 to 40 provide further practice.

As we have seen from the concrete examples, each individual irreducible representation includes certain partial aspects of the group law. The irreducible representations are therefore associated with the concept of symmetry types referred to the respective group. For example, the identity representation Γ_1 contains absolutely no specific group properties. It is therefore called as totally symmetric. The decomposition of an arbitrary representation into irreducible representations sheds light on the analysis of different symmetry types.

8.3 Tensor Representations

If one carries out an arbitrary symmetry operation, one finds that certain tensor components transform among themselves, independent of the position and the order of symmetry of the rotation axis or the rotation–inversion axis. This is illustrated by taking a general second-rank tensor as an example. We already know the scalar invariant

$$I = t_{ij}\delta_{ij} = t_{11} + t_{22} + t_{33} = t'_{11} + t'_{22} + t'_{33}.$$

A vector invariant is the vector

$$\begin{aligned} \boldsymbol{t} &= t_{ij}e_{ijk}\boldsymbol{e}_k \\ &= (t_{23} - t_{32})\boldsymbol{e}_1 + (t_{31} - t_{13})\boldsymbol{e}_2 + (t_{12} - t_{21})\boldsymbol{e}_3 \\ &= \boldsymbol{t}', \end{aligned}$$

where e_{ijk} are the components of the Levi-Cività tensor. The components of $\boldsymbol{t}$ transform like the coordinates, i.e., only the components of $\boldsymbol{t}$ appear in $\boldsymbol{t}'$.

If we consider a general mth-rank tensor in three-dimensional space, not subject to secondary conditions, we then have 3^m independent components, which we can conceive as the coordinates of a 3^m-dimensional space. The second-rank tensor is then represented as a vector of the form $\boldsymbol{T} = t_i\boldsymbol{e}_i$, where, for example $t_{11} = t_1$, $t_{22} = t_2$, $t_{33} = t_3$, $t_{23} = t_4$, $t_{31} = t_5$, $t_{12} = t_6$, $t_{32} = t_7$, $t_{13} = t_8$ and $t_{21} = t_9$. We now go over to a new reference system with the basic vectors $\boldsymbol{e}_i^0$, which are orthogonal, hence, $\boldsymbol{e}_i^0 \cdot \boldsymbol{e}_j^0 = \delta_{ij}$, and so selected that the invariants I and $\boldsymbol{t}$ fix the first four of these basic vectors, namely

$$\begin{aligned} \boldsymbol{e}_1^0 &= (\boldsymbol{e}_1 + \boldsymbol{e}_2 + \boldsymbol{e}_3)/\sqrt{3} \\ \boldsymbol{e}_2^0 &= (\boldsymbol{e}_4 - \boldsymbol{e}_7)/\sqrt{2} \\ \boldsymbol{e}_3^0 &= (\boldsymbol{e}_5 - \boldsymbol{e}_8)/\sqrt{2} \\ \boldsymbol{e}_4^0 &= (\boldsymbol{e}_6 - \boldsymbol{e}_9)/\sqrt{2}. \end{aligned}$$

For the remaining five new basic vectors $\boldsymbol{e}_i^0 = a_{ij}\boldsymbol{e}_j$, the orthogonality to the first four demands $\boldsymbol{e}_i^0 \cdot \boldsymbol{e}_k^0 = 0$ for $i \neq k$, hence, $a_{i1} + a_{i2} + a_{i3} = 0$ as well as

$$a_{i4} - a_{i7} = a_{i5} - a_{i8} = a_{i6} - a_{i9} = 0.$$

These relationships are fulfilled, for example, by the following mutually orthogonal vectors:

$$\boldsymbol{e}_5^0 = (\boldsymbol{e}_1 + \boldsymbol{e}_2 - 2\boldsymbol{e}_3)/\sqrt{6}$$
$$\boldsymbol{e}_6^0 = (\boldsymbol{e}_1 - \boldsymbol{e}_2)/\sqrt{2}$$
$$\boldsymbol{e}_7^0 = (\boldsymbol{e}_4 + \boldsymbol{e}_7)/\sqrt{2}$$
$$\boldsymbol{e}_8^0 = (\boldsymbol{e}_5 + \boldsymbol{e}_8)/\sqrt{2}$$
$$\boldsymbol{e}_9^0 = (\boldsymbol{e}_6 + \boldsymbol{e}_9)/\sqrt{2}.$$

In the abbreviated notation we have $\boldsymbol{e}_i^0 = D_{ij}\boldsymbol{e}_j$ and correspondingly $t_i^0 = D_{ij}t_j$. In this representation I, the vector $\boldsymbol{t}$ as well as each vector composed of the basic vectors $\boldsymbol{e}_5^0$ to $\boldsymbol{e}_9^0$ remain within the space spanned by $\boldsymbol{e}_1^0$, $\boldsymbol{e}_2^0$, $\boldsymbol{e}_3^0$, $\boldsymbol{e}_4^0$ or $\boldsymbol{e}_5^0$, $\boldsymbol{e}_6^0$, $\boldsymbol{e}_7^0$, $\boldsymbol{e}_8^0$, $\boldsymbol{e}_9^0$ during the transformation (rotation or rotation inversion). This means that the space spanned by the new basic vectors is resolved into three subspaces of dimensions 1, 3, and 5. We call these subspaces the invariant linear subspaces of the corresponding 3^m-dimensional space formed by an mth-rank tensor of that three-dimensional space. The search for these subspaces is carried out in a manner analogous to the above example, even for tensors of higher rank, whereby a knowledge of the tensor invariants is of valuable help. Conversely, resolving a tensor into its invariant linear subspaces allows an overview of the tensor invariants, which in many cases are amenable to a direct geometric interpretation.

A transformation of the basic system, which we introduced with the definition of the tensor concept, that is

$$t'_{ij} = u_{ii^*}u_{jj^*}t_{i^*j^*},$$

takes the form $t'_i = R_{ij}t_j$ or abbreviated $\boldsymbol{t}' = \boldsymbol{R}\boldsymbol{t}$ in the respective linear vector space. The matrix $\boldsymbol{R}$ is derived from the three-dimensional transformation matrix $\boldsymbol{U}$, which carries over the Cartesian basic vectors $\boldsymbol{e}_i$ to the new basic vectors $\boldsymbol{e}'_i$ according to $\boldsymbol{e}'_i = u_{ii^*}\boldsymbol{e}_{i^*}$. From the definition given above for the inner Kronecker product, we recognize straight away that the matrix $\boldsymbol{R}$ is to be understood as the Kronecker product of $\boldsymbol{U}$ with itself. Accordingly, with a mth-rank tensor, we have to use the m-fold Kronecker product of the matrix $\boldsymbol{U}$ for the transformation $\boldsymbol{R}$.

We now have the possibility of calculating the number of independent tensor components for the case that the tensor belongs to a certain symmetry group. The tensor, even in the linear vector space representation, is carried over by the respective symmetry operations into itself. The number of independent components must be equal to the dimension of the linear vector space which the tensor takes up because of symmetry operations or other conditions. For example, the three-dimensional subspace spanned by $\boldsymbol{e}_2^0$, $\boldsymbol{e}_3^0$,

$\boldsymbol{e}_4^0$ remains empty for the case of a symmetric second-rank tensor, i.e., a symmetric second-rank tensor only possesses the one-dimensional and the five-dimensional invariant linear subspace.

The symmetry operations of the given symmetry group carry the tensor over into itself, i.e., the individual tensor components experience an identical transformation, which in the representation of the matrices $\boldsymbol{R}$ must be conserved as identity representations. Consequently, the number of independent tensor components is equal to the number of identity representations conserved in the representation by the matrices $\boldsymbol{R}$. This number, according to the rules discussed above, is

$$m_1 = \frac{1}{h}\sum_{s=1}^{S} n_s \chi(s)\chi_1(s) \quad \text{and with } \chi_1(s) = 1:$$

$$m_1 = \frac{1}{h}\sum_{s=1}^{S} n_s \chi(s) \quad (n_s \text{ number of elements in the } s\text{-th class}).$$

As an example, consider the third-rank tensor t_{ijk} (without permutability of the indices) in the PSG 3m. The character of the $\boldsymbol{R}$-representation is obtained as the third power of the character value of the three-dimensional representation Γ_3' of the PSG 3m. It is $\Gamma_3' = \Gamma_1 + \Gamma_3$ (Γ_3 is two-dimensional!), hence,

$$\chi(\Gamma_3') = \chi(\Gamma_1) + \chi(\Gamma_3) = (3, 0, 1).$$

Thus

$$\chi(\Gamma_3' \times \Gamma_3' \times \Gamma_3') = (27, 0, 1) \quad \text{and} \quad m_1 = \frac{1}{6}(27 + 3) = 5.$$

This result is obtained far more laboriously as with the method of symmetry reduction discussed in Section 4.4. However, the other way of determining the independent tensor components with the methods of the linear vector space representation of the tensor in linear vector space and the explicit calculation of the invariant subspaces is not essentially different from those discussed in Section 3.8. Nevertheless, there does not exist a simpler method as that just discussed to calculate the number of independent tensor components, particularly with tensors of higher rank. In this regard, let us consider a further example of a ninth-rank tensor (without permutability of the indices) in the PSG 3m. The character values of the representation of the $\boldsymbol{R}$-matrices are the ninth powers of the character of the representation Γ_3'. Hence, $\chi(\boldsymbol{R}) = (3^9, 0, 1^9)$ and thus

$$m_1 = \frac{1}{6}(19683 + 3) = 3281.$$

We now have to investigate the effects of secondary conditions, such as the permutability of indices, which can arise, for example, from physical reasons in almost all tensors describing physical properties (most second-rank tensors, piezoelectric tensor, elasticity tensor etc.).

In many cases one can obtain the transformation matrix $\boldsymbol{R}$ of the tensors through the Kronecker products $\boldsymbol{R} = \boldsymbol{A} \times \boldsymbol{B}$. The associated character values can be calculated with the help of the product rule $\chi(\boldsymbol{A} \times \boldsymbol{B}) = \chi(\boldsymbol{A})\chi(\boldsymbol{B})$, where $\boldsymbol{A}$ and $\boldsymbol{B}$ may themselves be Kronecker products.

The situation in the case of the permutability of indices is less clear. A general derivation of the valid relations is found, for example, in Ljubarski (1962). For our purposes, it suffices to discuss practical applications for some important cases. Firstly, we consider the permutability of indices of second-rank tensors ($t_{ij} = t_{ji}$, second-rank symmetric tensors). To calculate the character of $\boldsymbol{R}$ we need only sum the factors in the principal diagonal of the transformation table:

$$
\begin{aligned}
t_{11} &= u_{11}u_{11}t_{11} + \cdots \\
t_{22} &= \cdots + u_{22}u_{22}t_{22} + \cdots \\
t_{33} &= \cdots + u_{33}u_{33}t_{33} + \cdots \\
t_{12} &= t_{21} = \cdots + (u_{11}u_{22} + u_{12}u_{21})t_{12} + \cdots \\
t_{23} &= t_{32} = \cdots + (u_{22}u_{33} + u_{23}u_{32})t_{23} + \cdots \\
t_{31} &= t_{13} = \cdots + (u_{33}u_{11} + u_{31}u_{13})t_{31} + \cdots
\end{aligned}
$$

hence,

$$
\begin{aligned}
\chi(\boldsymbol{R}) = \chi_{(3\times3)_s}(\boldsymbol{R}) &= \sum_{i=1} u_{ii}^2 + \frac{1}{2}\sum_{i\neq j}(u_{ii}u_{jj} + u_{ij}u_{ji}) \\
&= \frac{1}{2}\sum_{i,j} u_{ij}u_{ji} + \frac{1}{2}\left(\sum_i u_{ii}\right)^2 .
\end{aligned}
$$

As one can immediately verify with

$$
\boldsymbol{U} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix},
$$

the first sum is just the half trace of $\boldsymbol{U}^2$. The second sum is half the square of the trace of $\boldsymbol{U}$. Hence,

$$
\chi_{(3\times3)_s}(\boldsymbol{R}) = \frac{1}{2}\chi_3(\boldsymbol{U}^2) + \frac{1}{2}\chi_3^2(\boldsymbol{U}),
$$

where the symbols $(3 \times 3)_s$ denote the symmetric second-rank tensor, 3×3 denote the general second-rank tensor and corresponding higher tensors. For example, $(3 \times 3)_s \times (3 \times 3)$ means a fourth rank tensor in which two index positions are permutable.

Since in this connection we must always use the three-dimensional representation for $\boldsymbol{U}$, it is convenient to note the characters for the simple products: $\chi(\boldsymbol{U}) = \pm(1 + 2\cos\varphi)$ with $\varphi = 2\pi/n$. $+$ specifies rotation operations, $-$ specifies rotation-inversion. Furthermore, $\chi_3(\boldsymbol{U}^2) = (1 + 2\cos 2\varphi)$ and thus

$$\chi_{(3\times3)_s}(\boldsymbol{R}) = 2\cos\varphi + 4\cos^2\varphi \quad \text{for } n \text{ and } \bar{n}.$$

Again, we take the PSG 3m as an example. In this PSG, a symmetric second-rank tensor has

$$m_1 = \frac{1}{6}(6 + 2\cdot 0 + 3\cdot(-2+4)) = 2 \quad \text{independent components.}$$

For $\boldsymbol{U}$ we have written the three-dimension representation Γ_3' already given above.

As the next example, we consider the piezoelectric tensor and other third-rank tensors in which two index positions are permutable, hence, $t_{ijk} = t_{ikj}$. We use the product formula to calculate the character values

$$\begin{aligned}\chi_{3\times(3\times3)_s} &= \chi_3(\boldsymbol{U})\chi_{(3\times3)_s}(\boldsymbol{U})\\ &= \pm(1+2\cos\varphi)(2\cos\varphi + 4\cos^2\varphi)\\ &= \pm2(\cos\varphi + 4\cos^2\varphi + 4\cos^3\varphi),\end{aligned}$$

where we write $+$ for n and $-$ for $\bar{n}$.

In the PSG 3m, we then have $\chi(\boldsymbol{R}) = (18, 0, 2)$ and thus

$$m_1 = \frac{1}{6}(18 + 6) = 4 \quad \text{independent components}$$

in agreement with the result in Section 4.4.1.

To calculate $\chi(\boldsymbol{R})$ in the case of three and more mutually permutable index positions we proceed as in the case of second-rank tensors and construct the respective transformation formulae. The result is then, for example,

$$\chi_{(3\times3\times3)_s} = \pm2\cos\varphi(-1 + 2\cos\varphi + 4\cos^2\varphi)$$

with $+$ for n and $-$ for $\bar{n}$ as well as

$$\chi_{(3\times3\times3\times3)_s} = 1 - 2\cos\varphi - 8\cos^2\varphi + 8\cos^3\varphi + 16\cos^4\varphi$$

for n and $\bar{n}$.

Table 8.3 presents a compilation of the more important formulae for the calculation of the characters of tensor representations (polar tensors).

Table 8.3 Characters of tensor representations.

Tensor	Character $\chi(\boldsymbol{R})$ ($+$ for n, $-$ for $\bar{n}$)
t_i	$\chi_3 = \pm(1+2\cos\varphi)$
t_{ij}	$\chi_{(3\times 3)} = (1+2\cos\varphi)^2$
$t_{ij\ldots s}$ (mth rank)	$\chi_{(3\times 3\times \ldots 3)} = (\pm 1)^m(1+2\cos\varphi)^m$
$t_{ij} = t_{ji}$ (totally symmetric)	$\chi_{(3\times 3)_s} = \frac{1}{2}\chi_3(\boldsymbol{U}^2) + \frac{1}{2}\chi_3^2(\boldsymbol{U}) = 2\cos\varphi(1+2\cos\varphi)$
$t_{ijk} = t_{ikj}$ (interchangeable within one pair)	$\chi_{3\times(3\times 3)_s} = \chi_3\chi_{(3\times 3)_s} = \pm 2\cos\varphi(1+2\cos\varphi)^2$
t_{ijk} (totally symmetric)	$\chi_{(3\times 3\times 3)_s} = \frac{1}{3}\chi_3(\boldsymbol{U}^3) + \frac{1}{2}\chi_3(\boldsymbol{U}^2)\chi_3(\boldsymbol{U}) + \frac{1}{6}\chi_3^3(\boldsymbol{U}) = \pm 2\cos\varphi(-1+2\cos\varphi+4\cos^2\varphi)$
$t_{ijkl} = t_{ijlk}$	$\chi_{(3\times 3)\times(3\times 3)_s} = \chi_{3\times 3}\chi_{(3\times 3)_s} = 2\cos\varphi(1+2\cos\varphi)^3$
$t_{ijkl} = t_{klij}$ (pairwise interchangeable)	$\chi_{((3\times 3)\times(3\times 3))_s} = \frac{1}{2}\chi_{(3\times 3)}(\boldsymbol{U}^2)+\frac{1}{2}\chi_{(3\times 3)}^2(\boldsymbol{U}) = 1+4\cos\varphi(1+2\cos\varphi+4\cos^2\varphi+4\cos^3\varphi)$
$t_{ijkl} = t_{jikl} = t_{ijlk} = t_{jilk}$ (interchangeable within pairs)	$\chi_{(3\times 3)_s\times(3\times 3)_s} = \chi_{(3\times 3)_s}^2 = 4\cos^2\varphi(1+2\cos\varphi)^2$
$t_{ijkl} = t_{iklj} = t_{ilkj} = \ldots$ (interchangeable within a triple)	$\chi_{(3)\times(3\times 3\times 3)_s} = \chi_3\chi_{(3\times 3\times 3)_s} = 2\cos\varphi(1+2\cos\varphi)(-1+2\cos\varphi+4\cos^2\varphi)$
$t_{ijkl} = t_{ijlk} = t_{lkij} = \ldots$ (pairwise and within pairs interchangeable)	$\chi_{((3\times 3)_s\times(3\times 3)_s)_s} = \frac{1}{2}\chi_{(3\times 3)_s}(\boldsymbol{U}^2) + \frac{1}{2}\chi_{(3\times 3)_s}^2(\boldsymbol{U})$ $= 1+4\cos^2\varphi(-1+2\cos\varphi+4\cos^2\varphi)$
t_{ijkl} (totally symmetric)	$\chi_{(3\times 3\times 3\times 3)_s} = 1+2\cos\varphi(-1-4\cos\varphi+4\cos^2\varphi+8\cos^3\varphi)$
t_{ijklm} (totally symmetric)	$\chi_{(3\times 3\times 3\times 3\times 3)_s} = \pm 1 \pm 4\cos\varphi(1-2\cos\varphi-6\cos^2\varphi+4\cos^3\varphi+8\cos^4\varphi)$
$t_{ijklmn} = t_{ijklnm} = t_{ijlknm} = \ldots$ (interchangeable within pairs)	$\chi_{(3\times 3)_s\times(3\times 3)_s\times(3\times 3)_s} = \chi_{(3\times 3)_s}^3(\boldsymbol{U}) = 8\cos^3\varphi(1+2\cos\varphi)^3$
$t_{ijklmn} = t_{klijmn} = t_{klijnm} = \ldots$ (pairwise and within pairs interchangeable)	$\chi_{((3\times 3)_s\times(3\times 3)_s\times(3\times 3)_s)_s} = \frac{1}{3}\chi_{(3\times 3)_2}(\boldsymbol{U}^3) + \frac{1}{2}\chi_{(3\times 3)_s}(\boldsymbol{U}^2)\chi_{(3\times 3)_s}(\boldsymbol{U}) + \frac{1}{6}\chi_{(3\times 3)_s}^3(\boldsymbol{U})$ $= 8\cos^2\varphi(2-\cos\varphi-6\cos^2\varphi+4\cos^3\varphi+8\cos^4\varphi$

With axial tensors (pseudo tensors), $\chi(\boldsymbol{R})$ must be furnished with an additional factor (-1) when applying a symmetry operation $\bar{n}$.

All further cases are calculated in an analogous fashion. The formulae for the totally symmetric sixth and higher rank tensors can be easily derived by the reader by summing the coefficients in the principal diagonals of the system of the transformation formulae (see also Exercise 7)

$$t'_{ij\ldots s} = t_{ij\ldots s} = u_{ii}u_{jj}\ldots u_{ss}t_{ij\ldots s},$$

where

$$\boldsymbol{U} = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

as previously.

8.4
Decomposition of the Linear Vector Space into Invariant Subspaces

We now return to the decomposition of a tensor into invariant linear subspaces. Since, in a unitary transformation, the components spanning a certain invariant subspace again join to an invariant subspace of the same dimension, the transformation matrices can be split into irreducible blocks. In doing so, the basic vectors are selected corresponding to the invariant subspaces, as we explained on hand of the example of the second-rank tensor (see section 8.3). Accordingly, the characters (traces) of the transformation matrices are equal to the sum of the characters of the transformations in the individual subspaces. If one knows the character values for a tensor representation $\chi(\boldsymbol{R})$, then one can extract the nature of the subspace formed by the given tensor. It is $\chi(\boldsymbol{R}) = \sum_j m_j\chi_j(\boldsymbol{R})$. $\chi_j(\boldsymbol{R})$ is the character of the transformation matrix for the j-dimensional subspace for a certain symmetry operation $\boldsymbol{U}$. Accordingly, the tensor representation is then $\Gamma(\boldsymbol{R}) = \sum_j m_j\Gamma_j(\boldsymbol{R})$.

The following matrices furnish a $(2l+1)$-dimensional representation of the group of n-fold rotation axis:

$$\Gamma_{q;2l+1}(\boldsymbol{R}) = \begin{pmatrix} e^{ilq\varphi} & 0 & & \vdots & \\ 0 & e^{i(l-1)q\varphi} & & \cdots 0 \cdots & \\ & \vdots & \ddots & \vdots & \\ \cdots & 0 & \cdots & e^{-i(l-1)q\varphi} & 0 \\ & \vdots & & 0 & e^{-ilq\varphi} \end{pmatrix},$$

where $\varphi = 2\pi/n$. Allowing q to run through the values $0, 1, \ldots, n-1$, results in n matrices, which fulfil the group properties of the existent rotation group.

This representation has the character

$$\chi_{2l+1}(\boldsymbol{R}^q) = \sum_{m=-l}^{m=+l} e^{imq\varphi} = 1 + 2\sum_{m=+1}^{m=+l} \cos mq\varphi = \frac{\sin(2l+1)q\varphi/2}{\sin q\varphi/2}.$$

The simplest way of deriving this relation is with the help of a proof by induction or through the summation formula for a geometric series

$$\begin{aligned}\sum_{m=-l}^{m=+l} e^{imq\varphi} = \frac{e^{i(l+1)q\varphi} - e^{-ilq\varphi}}{e^{iq\varphi}-1} &= \frac{(e^{i(l+1)q\varphi} - e^{-ilq\varphi})(e^{-iq\varphi}+1)}{(e^{iq\varphi}-1)(e^{-iq\varphi}+1)} \\ &= \frac{\sin(l+1)q\varphi + \sin lq\varphi}{\sin q\varphi} = \frac{\sin(2l+1)q\varphi/2}{\sin q\varphi/2}\end{aligned}$$

(with $\sin\alpha + \sin\beta = 2\sin(\alpha+\beta)/2 \cdot \cos(\alpha-\beta)/2$). In practice, it is convenient to expand the cos terms in powers of $\cos\varphi$. Then one obtains the following values for $q = 1$:

$$\begin{aligned}
\chi_1(\boldsymbol{R}) &= 1 \\
\chi_3(\boldsymbol{R}) &= 1 + 2\cos\varphi \\
\chi_5(\boldsymbol{R}) &= -1 + 2\cos\varphi + 4\cos^2\varphi \\
\chi_7(\boldsymbol{R}) &= -1 - 4\cos\varphi + 4\cos^2\varphi + 8\cos^3\varphi \\
\chi_9(\boldsymbol{R}) &= 1 - 4\cos\varphi - 12\cos^2\varphi + 8\cos^3\varphi + 16\cos^4\varphi \\
\chi_{11}(\boldsymbol{R}) &= 1 + 6\cos\varphi - 12\cos^2\varphi - 32\cos^3\varphi + 16\cos^4\varphi + 32\cos^5\varphi \\
\chi_{13}(\boldsymbol{R}) &= -1 + 6\cos\varphi + 24\cos^2\varphi - 32\cos^3\varphi - 80\cos^4\varphi \\
&\qquad + 32\cos^5\varphi + 64\cos^6\varphi \\
\chi_{15}(\boldsymbol{R}) &= -1 - 8\cos\varphi + 24\cos^2\varphi + 80\cos^3\varphi - 80\cos^4\varphi - 192\cos^5\varphi \\
&\qquad + 64\cos^6\varphi + 128\cos^7\varphi
\end{aligned}$$

and so on.

As an example, we consider the tensor $t_{ijk} = t_{ikj}$ (for example, the piezoelectric tensor) and the tensor $t_{ijkl} = t_{klij} = t_{jikl} = \ldots$ (for example, the elasticity tensor). Because

$$\chi_{3\times(3\times3)_s} = 2\cos\varphi + 8\cos^2\varphi + 8\cos^3\varphi$$

(see Table 8.3) one obtains the unique decomposition

$$\chi_{3\times(3\times3)_s}(\boldsymbol{R}) = 2\chi_3(\boldsymbol{R}) + \chi_5(\boldsymbol{R}) + \chi_7(\boldsymbol{R}).$$

One begins by assigning the respective highest power to the corresponding $\chi_{2l+1}(\boldsymbol{R})$. The result is that there does not exist a scalar invariant (one-dimensional subspace), rather, two three-dimensional and a five- and seven-dimensional invariant subspace. In the other example we have

$$\chi_{((3\times3)_s\times(3\times3)_s)_s}(\boldsymbol{R}) = 2\chi_1(\boldsymbol{R}) + 2\chi_5(\boldsymbol{R}) + \chi_9(\boldsymbol{R}).$$

Here we have two scalar (one-dimensional) invariants as well as two five-dimensional subspaces and one nine-dimensional subspace. For the elasticity tensor this means, for example, that except for the dynamic elasticity $\bar{E} = \sum_{i,j} c_{ijij} = c_{ijkl}\delta_{ik}\delta_{jl}$ and the trace $\sum_{m=1}^{3} g_{mm}$ of the second-rank tensor describing the deviation from the Cauchy relations, where $g_{mm} = 1/2 e_{mik} e_{njl} c_{ijkl}$, that no further scalar invariants exist that cannot be formed from these two. The same applies accordingly to both second-rank tensor invariants, the dynamic elasticity, and the deviations from the Cauchy relations (see Sections 4.5.1 and 4.5.5).

8.5 Symmetry Matched Functions

For the description of the directional dependence of properties and even of functions of the position coordinates or a wave function of a quantum mechanical system, one can employ upon a system of functions which in themselves obey a certain point symmetry. Of particular interest are homogeneous polynomials in the coordinates x_1, x_2, x_3 of the Cartesian reference system. These polynomials can also be represented as functions of the angles ξ and η with the aid of polar coordinates. ξ is the angle between the position vector $\boldsymbol{x} = x_i \boldsymbol{e}_i$ and the vector $\boldsymbol{e}_3$ and η is the angle between the projection of the position vector on the plane spanned by $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ and the vector $\boldsymbol{e}_1$. Accordingly,

$$x_1 = |\boldsymbol{x}| \cos\eta \sin\xi, \quad x_2 = |\boldsymbol{x}| \sin\eta \sin\xi$$

and

$$x_3 = |\boldsymbol{x}| \cos\xi \quad \text{with} \quad |\boldsymbol{x}| = \sqrt{x_1^2 + x_2^2 + x_3^2}.$$

If a symmetry operation n or $\bar{n}$ exists, then each polynomial of the lth degree $\Theta = A_{ijk\ldots s} x_i x_j \ldots x_s$ is carried over in an identical form by the respective transformation, i.e., one has $A'_{ijk\ldots s} = A_{ijk\ldots s}$. Hence, these polynomials transform as the quadric of degree l.

The scheme of independent coefficients for each polynomial of the lth degree and the relationships of the coefficients among one another corresponds to the conditions for the components of a totally symmetric lth-rank tensor in the respective PSG. For example, a third-degree polynomial has the following form in the PSG 3m

$$\Theta_3 = A_{113} x_1^2 x_3 - 3A_{222} x_1^2 x_2 + A_{222} x_2^3 + A_{113} x_2^2 x_3 + A_{333} x_3^3$$

in accordance with the result of symmetry reduction in the PSG 3m under the condition of total symmetry (see Section 4.4).

We now consider functions dependent only on the direction of the position vector and not on its magnitude and those containing the radial dependence in a separate factor respectively. We then have

$$\Theta = \Theta(r)\Theta(\xi,\eta) \quad \text{with} \quad r = |\boldsymbol{x}|.$$

Analogous to the expansion of a periodic function in a Fourier series, the angular dependent function $\Theta(\xi,\eta)$ can be expanded in a series with respect to the terms of a suitable system of functions $\{F_l\}$ according to

$$\Theta(\xi,\eta) = \sum_{l=0}^{q} A_l F_l.$$

If we demand that F_l is a polynomial of the lth degree in x_i/r and further, that the function $\Theta(\xi,\eta)$ is optimally approximated by the functions $S_q = \sum_{l=0}^{q} A_l F_l$ in each stage q according to the least squares method, i.e., that

$$\Delta q = \int_{\text{sphere}} [\Theta(\xi,\eta) - S_q(\xi,\eta)]^2 d\Omega$$

becomes a minimum for each q, then we come to the system of spherical harmonic functions, well known from potential theory. These functions are solutions of the Laplace differential equation

$$\frac{\partial^2 Y}{\partial x_1^2} + \frac{\partial^2 Y}{\partial x_2^2} + \frac{\partial^2 Y}{x_3^2} = 0.$$

Since this quantity is a scalar invariant of the differential operator $\{\partial^2/\partial x_i \partial x_j\}$, the solutions always have the same form independent of the respective reference system. The spherical harmonic functions are expressed as follows:

$$Y_l^m = N_l^m P_l^m(\zeta) e^{im\eta}.$$

The index m is an integer number and can only take on the values $|m| \leq l$. They obey the orthogonality- and normalization condition

$$\int_{\text{sphere}} Y_l^m \bar{Y}_{l'}^{m'} d\Omega = \int_{\eta=0}^{2\pi} \int_{\xi=0}^{\pi} Y_l^m \bar{Y}_{l'}^{m'} \sin\xi d\xi d\eta = \delta_{ll'} \delta_{mm'}$$

with

$$d\Omega = \sin\xi d\xi d\eta.$$

For P_l^m there exist a simple recursion formula

$$P_l^m = \frac{(1-\zeta^2)^{m/2} d^{l+m} (\zeta^2 - 1)^l}{2^l l! d\zeta^{l+m}},$$

with

$$\zeta = \cos\xi \quad \text{and} \quad (1-\zeta^2) = \sin^2\xi.$$

The normalization factor N_l^m has the form

$$N_l^m = \left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right)^{1/2}.$$

Hence, we can expand any arbitrary function $\Theta(\xi,\eta)$, which is numerically or analytically known, in a series with respect to the functions Y_l^m, according to

$$\Theta(\xi,\eta) = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=+l} A_{lm}Y_l^m.$$

We obtain the coefficients A_{lm} directly from the orthogonality relation by inserting the series

$$A_{lm} = \int_{\text{sphere}} \Theta(\xi,\eta)\bar{Y}_l^m d\Omega.$$

Some low indexed Y_l^m are presented in Table 8.4.

We now come to discuss two further important properties of the functions Y_l^m. Let us carry out a transformation of the Cartesian reference system according to $\boldsymbol{e}_i' = u_{ij}\boldsymbol{e}_j$, we then have $Y_l^{m'} = R_{mn}Y_l^n$. This means that $Y_l^{m'}$, a polynomial of the lth degree, can be constructed from a linear combination of Y_l^n. This results from the fact that $Y_l^{m'}$ must also be a polynomial of the lth degree, as well as from the expansion formula. A rotation about $\boldsymbol{e}_3$ with the angle $2\pi/n$ (n-fold rotation axis) carries Y_l^m over in $Y_l^m e^{2\pi im/n}$, as is directly seen from the definition of Y_l^m. In a rotation-inversion $\bar{n} \parallel \boldsymbol{e}_3$, one must distinguish between the cases "l even" and "l odd." These are

$$Y_l^{m'} = Y_l^m e^{2\pi im/n} \quad \text{for } l \text{ even and}$$
$$Y_l^{m'} = Y_l^m e^{2\pi im/n}(-1) \quad \text{for } l \text{ odd.}$$

Thus the spherical harmonics are subject to the following conditions under the existence of symmetry properties (aside from the condition $|m| \leq l$):

n: $e^{2\pi im/n} = 1$ hence, $m = nq$, q integer,
$\bar{n}$: $e^{2\pi im/n} = -1$ for l odd, hence, $m = n(2q+1)/2$, q integer
$\bar{n}$: $e^{2\pi im/n} = 1$ for l even, hence, $m = nq$, q integer, as in the case of n.

From these we read the following rules, which we have come to know in part already in Section 3 with regards to tensor transformations:

1. All homogeneous polynomials of odd order and thus all odd-rank polar tensors vanish for the case that the respective symmetry groups contain a rotation-inversion $\bar{n}$ with odd n ($\bar{1}$, $\bar{3}$, $\bar{5}$, and so on).

Table 8.4 Spherical harmonics Y_l^m for $l = 0$ to 3 ($r = \sqrt{x_1^2 + x_2^2 + x_3^2}$; $x_1 = r\sin\xi\cos\eta$; $x_2 = r\sin\xi\sin\eta$; $x_3 = r\cos\xi$).

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^{-1} = -\sqrt{\frac{3}{8\pi}}\frac{(x_1 - ix_2)}{r}; \qquad Y_1^0 = \sqrt{\frac{3}{4\pi}}\frac{x_3}{r}; \qquad Y_1^1 = \sqrt{\frac{3}{8\pi}}\frac{(x_1 + ix_2)}{r}$$

$$Y_2^{-2} = \sqrt{\frac{15}{32\pi}}\frac{(x_1 - ix_2)^2}{r^2}; \qquad Y_2^{-1} = \sqrt{\frac{15}{8\pi}}\frac{x_3(x_1 - ix_2)}{r^2}; \qquad Y_2^0 = \sqrt{\frac{5}{16\pi}}\frac{(3x_3^2 - r^2)}{r^2};$$

$$Y_2^1 = \sqrt{\frac{15}{8\pi}}\frac{x_3(x_1 + ix_2)}{r^2}; \qquad Y_2^2 = \sqrt{\frac{15}{32\pi}}\frac{(x_1 + ix_2)^2}{r^2}$$

$$Y_3^{-3} = -\sqrt{\frac{35}{64\pi}}\frac{(x_1 - ix_2)^3}{r^3}; \qquad Y_3^{-2} = \sqrt{\frac{105}{32\pi}}\frac{x_3(x_1 - ix_2)^2}{r^3};$$

$$Y_3^{-1} = -\sqrt{\frac{21}{64\pi}}\frac{(5x_3^2 - r^2)(x_1 - ix_2)}{r^3}; \qquad Y_3^0 = \sqrt{\frac{7}{16\pi}}\frac{x_3(5x_3^2 - 3r^2)}{r^3};$$

$$Y_3^1 = \sqrt{\frac{21}{64\pi}}\frac{(5x_3^2 - r^2)(x_1 + ix_2)}{r^3}; \qquad Y_3^2 = \sqrt{\frac{105}{32\pi}}\frac{x_3(x_1 + ix_2)^2}{r^3}; \qquad Y_3^3 = \sqrt{\frac{35}{64\pi}}\frac{(x_1 + ix_2)^3}{r^3}.$$

Real functions can be constructed from simple linear combinations of the complex Y_l^m, e.g.

$$Y_2^2 + Y_2^{-2} = \sqrt{\frac{15}{8\pi}}\frac{(x_1^2 - x_2^2)}{r^2}; \qquad i(Y_2^2 - Y_2^{-2}) = -2\sqrt{\frac{15}{8\pi}}\frac{x_1x_2}{r^2};$$

$$i(Y_2^1 + Y_2^{-1}) = -2\sqrt{\frac{15}{8\pi}}\frac{x_3x_2}{r^2}; \qquad (Y_2^1 - Y_2^{-1}) = 2\sqrt{\frac{15}{8\pi}}\frac{x_3x_1}{r^2}.$$

In general, for each l a total of $(2l + 1)$ real orthogonal and normalized functions can be constructed according to

$$\frac{1}{\sqrt{2}}(Y_l^m \pm Y_l^{-m})i^{(m-1/2\pm 1/2)} \quad \text{mit} \quad 0 < m \leq l \quad \text{und} \quad Y_l^0.$$

This statement can easily be proven from the relation $Y_l^{-m} = (-1)^m\overline{Y_l^m}$ that derives directly from the definition of the Y_l^m.

2. All homogeneous polynomials of even order and thus all even-rank polar tensors have the same form when a rotation axis n or a rotation-inversion $\bar{n}$ of the same order of symmetry exists. This means that polynomials and tensors of even order and rank respectively are "centrosymmetric"!

Furthermore, due of the limitations of m, we can take in at a glance which spherical harmonics, at all, can be found with the existence of an n-fold axis or a rotation-inversion $\bar{n}$. Thus, we can now derive all symmetry matched spherical harmonics for the PSG of type n, $\bar{n}$ and n/m. For the PSG $n2$, $n\mathrm{m}$ and the cubic PSG, the respective conditions for a second distinct direction must also be fulfilled. In this manner, the homogeneous polynomials, allowed for each l (degree of the polynomial), are now accessible for each arbitrary point symmetry group.

From the transformation behavior of Y_l^m we obtain a $(2l+1)$-dimensional representation, which in the case of a rotation axis n assumes the form of the representation $\Gamma_{m;2l+1}(\boldsymbol{R})$ discussed in the previous section. The individual Y_l^m for a respective fixed l represent, to a certain extent, the coordinates of a $(2l+1)$-dimensional vector. Thus, we also recognize the character of the given transformation matrices and are then in the position to apply the known rules of group theory to analyze symmetry matched functions.

As an example, consider the PSG 3m and m3, for which we want to calculate the $(2l+1)$-dimensional representation. We use the formula for the number m_j of the jth irreducible representation Γ_j of the group contained in an arbitrary representation Γ

$$m_j = \frac{1}{h}\sum_{s=1}^{S} n_s \chi(s)\bar{\chi}_j(s)^{\mathrm{irr}}.$$

It is

$$\chi(\boldsymbol{R}) = \pm\frac{\sin(2l+1)\varphi/2}{\sin\varphi/2},$$

where $\varphi = 2\pi/n$; $+$ for n and $\bar{n}$ when l is even and $-$ for $\bar{n}$ when l is odd. The procedure runs as follows:

1. Calculate the characters of the classes for each l with the help of the above formula,

2. Calculate the values m_j and hence, the decomposition

   $$\Gamma_{(2l+1)} = \sum_{j=1}^{S} m_j\Gamma_j.$$

   The index "$2l+1$" was placed in brackets to distinguish irreducible representations.

Tables 8.5 and 8.6 present the results for the PSGs m3 and 3m.

Table 8.5 Decomposition of the $(2l+1)$-dimensional representations in irreducible representations of the PSG m3 = 23×$\bar{1}$. Classes: $K_1 = e$; $K_2 = 2$ (3×); $K_3 = 3^1$ (4×); $K_4 = 3^2$ (4×); $K_5 = K_1' = \bar{1}$; $K_6 = K_2' = m$ (3×); $K_7 = K_3' : \bar{3}^1$ (4×); $K_8 = K_4' = \bar{3}^2$ (4×).

Characters of irreducible representations

	e	2 (3×)	3^1 (4×)	3^2 (4×)	$\bar{1}$	m (3×)	$\overline{3^1}$ (4×)	$\overline{3^2}$ (4×)
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	$e^{2\pi i/3}$	$e^{2\pi i2/3}$	1	1	$e^{2\pi i/3}$	$e^{2\pi i2/3}$
Γ_3	1	1	$e^{2\pi i2/3}$	$e^{2\pi i4/3}$	1	1	$e^{2\pi i2/3}$	$e^{2\pi i4/3}$
Γ_4	3	$\bar{1}$	0	0	3	$\bar{1}$	0	0
$\Gamma_5 = \Gamma_1'$	1	1	1	1	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$
$\Gamma_6 = \Gamma_2'$	1	1	$e^{2\pi i/3}$	$e^{2\pi i2/3}$	$\bar{1}$	$\bar{1}$	$-e^{2\pi i/3}$	$-e^{2\pi i2/3}$
$\Gamma_7 = \Gamma_3'$	1	1	$e^{2\pi i2/3}$	$e^{2\pi i4/3}$	$\bar{1}$	$\bar{1}$	$-e^{2\pi i2/3}$	$-e^{2\pi i4/3}$
$\Gamma_8 = \Gamma_4'$	3	$\bar{1}$	0	0	$\bar{3}$	1	0	0

Characters $\chi_{(2l+1)}$ of the $(2l+1)$-dimensional representations

	e	2 (3×)	3^1 (4×)	3^2 (4×)	$\bar{1}$	m (3×)	$\overline{3^1}$ (4×)	$\overline{3^2}$ (4×)	$\Gamma_{(2l+1)}$
$\Gamma_{(1)}$	1	1	1	1	1	1	1	1	Γ_1
$\Gamma_{(3)}$	3	$\bar{1}$	0	0	$\bar{3}$	1	0	0	Γ_4'
$\Gamma_{(5)}$	5	1	$\bar{1}$	$\bar{1}$	$\bar{5}$	$\bar{1}$	1	1	$\Gamma_2' + \Gamma_3' + \Gamma_4'$
$\Gamma_{(7)}$	7	$\bar{1}$	1	1	$\bar{7}$	1	$\bar{1}$	$\bar{1}$	$\Gamma_1' + 2\Gamma_4'$
$\Gamma_{(9)}$	9	1	0	0	$\bar{9}$	$\bar{1}$	0	0	$\Gamma_1' + \Gamma_2' + \Gamma_3' + 2\Gamma_4'$
$\Gamma_{(11)}$	11	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\overline{11}$	1	1	1	$\Gamma_2' + \Gamma_3' + 3\Gamma_4'$

Table 8.6 Decomposition of the $(2l+1)$-dimensional representations in irreducible representations of the PSG 3m. Classes: $K_1 = e$; $K_2 = 3^1, 3^2$; $K_3 =$ m (3×).

Characters of irreducible representations

	e	$3^1, 3^2$	m (3×)
Γ_1	1	1	1
Γ_2	1	1	$\bar{1}$
Γ_3	2	$\bar{1}$	0

Characters $\chi_{(2l+1)}$ of the $(2l+1)$-dimensional representations

	e	$3^1, 3^2$	m (3×)	$\Gamma_{(2l+1)}$
$\Gamma_{(1)}$	1	1	1	Γ_1
$\Gamma_{(3)}$	3	0	1	$\Gamma_1 + \Gamma_3$
$\Gamma_{(5)}$	5	$\bar{1}$	$\bar{1}$	$\Gamma_2 + 2\Gamma_3$
$\Gamma_{(7)}$	7	1	1	$2\Gamma_1 + \Gamma_2 + 2\Gamma_3$
$\Gamma_{(9)}$	9	0	$\bar{1}$	$\Gamma_1 + 2\Gamma_2 + 3\Gamma_3$
$\Gamma_{(11)}$	11	$\bar{1}$	1	$2\Gamma_1 + \Gamma_2 + 4\Gamma_3$
$\Gamma_{(13)}$	13	1	$\bar{1}$	$2\Gamma_1 + 3\Gamma_2 + 4\Gamma_3$
$\Gamma_{(15)}$	15	0	1	$3\Gamma_1 + 2\Gamma_2 + 5\Gamma_3$
$\Gamma_{(25)}$	25	1	$\bar{1}$	$4\Gamma_1 + 5\Gamma_2 + 8\Gamma_3$