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1.2. Representations of crystallographic groups

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1.2.1. Introduction

Symmetry arguments play an important role in science. Often one can use them in a heuristic way, but the correct formulation is in terms of group theory. This remark is in fact superfluous for crystallographers, who are used to point groups and space groups as they occur in the description of structures. However, besides these structural problems there are many others where group theory may play a role. A central role in this context is played by representation theory, which treats the action of a group on physical quantities, and usually this is done in terms of linear transformations, although nonlinear representations may also occur.

To start with an example, consider a spin system, an arrangement of spins on sites with a certain symmetry, for example space-group symmetry. The elements of the space group map the sites onto other sites, but at the same time the spins are rotated or transformed otherwise in a well defined fashion. The spins can be seen as elements of a vector space (spin space) and the transformation in this space is an image of the space-group element. In a similar way, all symmetric tensors of rank 2 form a vector space, because one can add them and multiply them by a real factor. A linear change of coordinates changes the vectors, and the transformations in the space of tensors are the image of the coordinate transformations. Probably the most important use of such representations is in quantum mechanics, where transformations in coordinate space are mapped onto linear transformations in the quantum mechanical space of state vectors.

To see the relation between groups of transformations and the use of their representations in physics, consider a tensor which transforms under a certain point group. Let us take a symmetric rank 2 tensor T_{ij} in three dimensions. We take as example the point group 222. From Section 1.1.3.2 one knows how such a tensor transforms: it transforms into a tensor T'_{ij} according to

$$T'_{ij} = \sum_{k=1}^{3}\sum_{m=1}^{3} R_{ik}R_{jm}T_{km} \qquad (1.2.1.1)$$

for all orthogonal transformations R in the group 222. This action of the point group 222 is obviously a linear one:

$$\left(c_1T_{ij}^{(1)} + c_2T_{ij}^{(2)}\right)' = c_1T_{ij}^{(1)\prime} + c_2T_{ij}^{(2)\prime}.$$

The transformations on the tensors really form an image of the group, because if one writes $D(R)T$ for T', one has for two elements $R^{(1)}$ and $R^{(2)}$ the relation

$$\left(D(R^{(1)}R^{(2)})\right)T = D(R^{(1)})\left(D(R^{(2)})T\right)$$

or

$$D(R^{(1)}R^{(2)}) = D(R^{(1)})D(R^{(2)}). \qquad (1.2.1.2)$$

This property is said to define a (linear) representation. Because of the representation property, it is sufficient to know how the tensor transforms under the generators of a group. In our example, one could be interested in symmetric tensors that are invariant under the group 222. Then it is sufficient to consider the rotations over 180° along the x and y axes. If the point group is a symmetry group of the system, a tensor describing the relation between two physical quantities should remain the same. For invariant tensors one has

$$\begin{pmatrix} a_{11} & a_{12} & a_{13}\\ a_{12} & a_{22} & a_{23}\\ a_{13} & a_{23} & a_{33}\end{pmatrix} = \begin{pmatrix} 1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix} a_{11} & a_{12} & a_{13}\\ a_{12} & a_{22} & a_{23}\\ a_{13} & a_{23} & a_{33}\end{pmatrix}\begin{pmatrix} 1 & 0 & 0\\ 0 & -1 & 0\\ 0 & 0 & -1\end{pmatrix},$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13}\\ a_{12} & a_{22} & a_{23}\\ a_{13} & a_{23} & a_{33}\end{pmatrix} = \begin{pmatrix} -1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix} a_{11} & a_{12} & a_{13}\\ a_{12} & a_{22} & a_{23}\\ a_{13} & a_{23} & a_{33}\end{pmatrix}\begin{pmatrix} -1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & -1\end{pmatrix}$$

and the solution of these equations is

$$\begin{pmatrix} a_{11} & a_{12} & a_{13}\\ a_{12} & a_{22} & a_{23}\\ a_{13} & a_{23} & a_{33}\end{pmatrix} = \begin{pmatrix} a_{11} & 0 & 0\\ 0 & a_{22} & 0\\ 0 & 0 & a_{33}\end{pmatrix}.$$

The matrices of rank 2 form a nine-dimensional vector space. The rotation over 180° around the x axis can also be written as

$$R\begin{pmatrix} a_{11}\\ a_{12}\\ a_{13}\\ a_{21}\\ a_{22}\\ a_{23}\\ a_{31}\\ a_{32}\\ a_{33}\end{pmatrix} = \begin{pmatrix} 1&0&0&0&0&0&0&0&0\\ 0&-1&0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&0&0&0\\ 0&0&0&-1&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&-1&0&0\\ 0&0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&0&1\end{pmatrix}\begin{pmatrix} a_{11}\\ a_{12}\\ a_{13}\\ a_{21}\\ a_{22}\\ a_{23}\\ a_{31}\\ a_{32}\\ a_{33}\end{pmatrix}.$$

This nine-dimensional matrix together with the one corresponding to a rotation along the y axis generate a representation of the group 222 in the nine-dimensional space of three-dimensional rank 2 tensors. The invariant tensors form the subspace $(a_{11}, 0, 0, 0, a_{22}, 0, 0, 0, a_{33})$. In this simple case, group theory is barely needed. However, in more complex situations, the calculations may become quite cumbersome without group theory. Moreover, group theory may give a wealth of other information, such as selection rules and orthogonality relations, that can be obtained only with much effort without group theory, or in particular representation theory. Tables of tensor properties, and irreducible representations of point and space groups, have been in use for a long time. For point groups see, for example, Butler (1981) and Altmann & Herzig (1994); for space groups, see Miller & Love (1967), Kovalev (1987) and Stokes & Hatch (1988).

In the following, we shall discuss the representation theory of crystallographic groups. We shall adopt a slightly abstract language, which has the advantage of conciseness and generality, but we shall consider examples of the most important notions. Another point that could give rise to some problems is the fact that we shall consider in part the theory for crystallographic groups in arbitrary dimension. Of course, physics occurs in three-dimensional space, but often it is useful to see what is general and what is special for one, two or three dimensions. In Section 1.2.2, the point groups are discussed, together with their representations. In Section 1.2.3, the same is done for space groups. Tensors for point and space groups are then treated in terms of representation theory in Section 1.2.4. Besides transformations in space, transformations involving time reversal are important as well. They are discussed in Section 1.2.5. Information on crystallographic groups and their representations is presented in tabular form in Section 1.2.6. This section can be consulted independently.

1.2.2. Point groups

1.2.2.1. *Finite point groups in one, two and three dimensions*

The crystallographic point groups are treated in Volume A of *International Tables for Crystallography* (2005). Here we just give a brief summary of some important notions. To maintain generality, we consider the case of n-dimensional point groups.

Point groups in n dimensions are subgroups of the orthogonal group $O(n)$ in n dimensions. By definition they leave a point, the origin, invariant. They are of importance in physics because physical laws are invariant under such transformations. In this case $n = 1$, 2 or 3. For crystallography, the crystallographic point groups are the most relevant ones. A *crystallographic point group* is a subgroup of $O(n)$ that leaves an n-dimensional lattice invariant. A *lattice* is a collection of points

$$\mathbf{r} = \mathbf{r}_o + \sum_{i=1}^{n} n_i \mathbf{e}_i, \quad n_i \in \mathbb{Z}, \tag{1.2.2.1}$$

where the n vectors $\mathbf{e}_i$ form a basis of n-dimensional space. In other words, the points of the lattice can be obtained by the action of translations

$$\mathbf{t} = \sum_{i=1}^{n} n_i \mathbf{e}_i \tag{1.2.2.2}$$

on the lattice origin $\mathbf{r}_o$. These translations form a *lattice translation group* in n-dimensional space, *i.e.* a discrete subgroup of the group of all translations $T(n)$ in n dimensions, generated by n linearly independent translations.

Because a crystallographic point group leaves a lattice of points invariant, (*a*) it is a finite group of linear transformations and (*b*) on a basis of the lattice it is represented by integer matrices. On the other hand, as will be shown in Section 1.2.2.2, there is for every finite group of matrices an invariant scalar product, *i.e.* a positive definite metric tensor left invariant by the group. If one uses this metric tensor for the definition of the scalar product, the matrices represent orthogonal transformations. Moreover, when the matrices are integer, the group of matrices can be considered to be a crystallographic point group. In this sense, every finite group of integer matrices is a crystallographic point group. Consider as an example the group of matrices

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix},$$

which leaves invariant the metric tensor

$$g = \begin{pmatrix} \mathbf{a}_1 \cdot \mathbf{a}_1 & \mathbf{a}_1 \cdot \mathbf{a}_2 \\ \mathbf{a}_2 \cdot \mathbf{a}_1 & \mathbf{a}_2 \cdot \mathbf{a}_2 \end{pmatrix} = \begin{pmatrix} a & -a/2 \\ -a/2 & a \end{pmatrix}.$$

The lattice points $n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ go over into lattice points and the transformation leaves the scalar product of two such vectors the same if the scalar product of the two vectors $n_1\mathbf{a}_1 + n_2\mathbf{a}_2$ and $n'_1\mathbf{a}_1 + n'_2\mathbf{a}_2$ is defined as

$$n_1 n'_1 a - n_1 n'_2 a/2 - n_2 n'_1 a/2 + n_2 n'_2 a.$$

After a basis transformation,

$$\mathbf{e}_1 = \mathbf{a}_1/\sqrt{a}, \quad \mathbf{e}_2 = (\mathbf{a}_1 + 2\mathbf{a}_2)/\sqrt{3a},$$

the metric tensor is in standard form (see Section 1.1.2.2):

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}.$$

This means that with respect to the basis $\mathbf{e}_1$, $\mathbf{e}_2$, the three transformations become orthogonal matrices.

To be able to give a list of all crystallographic point groups in n dimensions it is necessary to state which point groups should be considered as different. Two point groups belong to the same *geometric crystal class* if they are conjugated subgroups of $O(n)$. This means that $K \subset O(n)$ and $K' \subset O(n)$ belong to the same class if there is an element $R \in O(n)$ such that $K' = RKR^{-1}$, which implies that there are two orthonormal bases in the vector space related by an orthogonal transformation R such that the matrices of K for one basis are the same as those for K' on the second basis.

In *one-dimensional space*, there are only two different point groups, the first consisting of the identity, the second of the numbers ± 1. These groups are isomorphic to C_1 and C_2, respectively, where C_m is the cyclic group of integers modulo m (also denoted by $\mathbb{Z}_m$). Both are crystallographic because their 1×1 'matrices' are the integers ± 1.

In *two-dimensional space*, the orthogonal group $O(2)$ is the union of the subgroup $SO(2)$, consisting of all orthogonal transformations with determinant $+1$, and the coset $O(2)\backslash SO(2)$, consisting of all orthogonal transformations with determinant -1. The group $SO(2)$ is Abelian, and therefore all its subgroups are Abelian. The finite ones are the rotation groups denoted by n ($n \in \mathbb{Z}^+$). Every element of $O(2)\backslash SO(2)$ is of order two, and corresponds to a mirror line. Therefore, all the other finite point groups are nmm (n even) or nm (n odd). The rotation groups are isomorphic with the cyclic groups C_n and the others with the dihedral groups D_n. Only the groups 1, 2, 3, 4, 6, m, $2mm$, $3m$, $4mm$ and $6mm$ leave a lattice invariant and are crystallographic.

The isomorphism class of a group can be given by its *generators* and *defining relations*. For example, the elements of the group $4mm$ can be written as products (with generally more than two factors) of the two matrices

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which satisfy the relations $A^4 = B^2 = ABAB = E$, and every group whose elements are products of two generating elements with the same and not more independent relations is isomorphic. One calls the relations the defining relations. The set of generators and defining relations is not unique. In an extreme case, one can consider all elements of the group as generators, and the product rules $ab = c$ as the defining relations.

For the two-dimensional groups, the generators and defining relations are

C_n: one generator A, with $A^n = E$;

D_n: two generators A and B, with $A^n = B^2 = (AB)^2 = E$, where E is the unit element.

The determination of all finite point groups in *three-dimensional space* is more involved. A derivation can, for example, be found in Janssen (1973). The group $O(3)$ is again the union of $SO(3)$ and $O(3)\backslash SO(3)$, and in fact the direct product of $SO(3)$ and the group generated by the inversion $I = -E$. One may distinguish between three different classes of finite point groups:

(*a*) point groups that belong fully to the rotation group $SO(3)$;

(*b*) point groups that contain the inversion $-E$ and are, consequently, the direct product of a point group of the first class and the group generated by $-E$;

(*c*) point groups that have elements in common with $O(3)\backslash SO(3)$ but do not contain $-E$; such groups are isomorphic to a group of the first class, as one can see if one multiplies all elements with determinant equal to -1 by $-E$.

The list of three-dimensional finite point groups is given in Table 1.2.6.1. All isomorphism classes of two-dimensional point groups occur in three dimensions as well. The isomorphism classes occurring here for the first time are:

$C_n \times C_2$: A, B, with $A^n = B^2 = ABA^{-1}B^{-1} = E$;

$D_n \times C_2$: A, B, C with $A^n = B^2 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

T: A, B, with $A^3 = B^2 = (AB)^3 = E$;

O: A, B, with $A^4 = B^3 = (AB)^2 = E$;

$T \times C_2$: A, B, C, with $A^3 = B^2 = (AB)^3 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

$O \times C_2$: A, B, C, with $A^4 = B^3 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$;

I: A, B, with $A^5 = B^3 = (AB)^2 = E$;

$I \times C_2$: A, B, C, with $A^5 = B^3 = (AB)^2 = C^2 = ACA^{-1}C^{-1} = BCB^{-1}C^{-1} = E$.

The crystallographic groups among them are given in Table 1.2.6.2.

1.2.2.2. *Representations of finite groups*

As stated in Section 1.2.1, elements of point groups act on physical properties (like tensorial properties) and on wave functions as linear operators. These linear operators therefore generally act in a different space than the three-dimensional configuration space. We denote this new space by V and consider a mapping D from the point group K to the group of nonsingular linear operators in V that satisfies

$$D(R)D(R') = D(RR') \quad \forall\ R, R' \in K. \qquad (1.2.2.3)$$

In other words D is a *homomorphism* from K to the group of nonsingular linear transformations $GL(V)$ on the vector space V. Such a homomorphism is called a *representation* of K in V. Here we only consider finite-dimensional representations.

With respect to a basis $\mathbf{e}_i$ $(i = 1, 2, \ldots n)$ the linear transformations are given by matrices $\Gamma(R)$. The mapping Γ from K to the group of nonsingular $n \times n$ matrices $GL(n, R)$ (for a real vector space V) or $GL(n, C)$ (if V is complex) is called an n-dimensional *matrix representation* of K.

If one chooses another basis for V connected to the former one by a nonsingular matrix S, the same group of operators $D(K)$ is represented by another matrix group $\Gamma'(K)$, which is related to $\Gamma(K)$ by S according to $\Gamma'(R) = S^{-1}\Gamma(R)S$ $(\forall\ R \in K)$. Two such matrix representations are called *equivalent*. On the other hand, two such equivalent matrix representations can be considered to describe two different groups of linear operators [$D(K)$ and $D'(K)$] on the same basis. Then there is a nonsingular linear operator T such that $D(R)T = TD'(R)$ $(\forall\ R \in K)$. In this case, the representations $D(K)$ and $D'(K)$ are also called equivalent.

It may happen that a representation $D(K)$ in V leaves a subspace W of V invariant. This means that for every vector $v \in W$ and every element $R \in K$ one has $D(R)v \in W$. Suppose that this subspace is of dimension $m < n$. Then one can choose m basis vectors for V inside the invariant subspace. With respect to this basis, the corresponding matrix representation has elements

$$\Gamma(R) = \begin{pmatrix} \Gamma_1(R) & \Gamma_3(R) \\ 0 & \Gamma_2(R) \end{pmatrix}, \qquad (1.2.2.4)$$

where the matrices $\Gamma_1(R)$ form an m-dimensional matrix representation of K. In this situation, the representations $D(K)$ and $\Gamma(K)$ are called *reducible*. If there is no proper invariant subspace the representation is *irreducible*. If the representation is a direct sum of subspaces, each carrying an irreducible representation, the representation is called *fully reducible* or *decomposable*. In the latter case, a basis in V can be chosen such that the matrices $\Gamma(R)$ are direct sums of matrices $\Gamma_i(R)$ such that the $\Gamma_i(R)$ form an irreducible matrix representation. If $\Gamma_3(R)$ in (1.2.2.4) is zero and Γ_1 and Γ_2 form irreducible matrix representations, Γ is fully reducible. For finite groups, each reducible representation is fully reducible. That means that if $\Gamma(K)$ is reducible, there is a matrix S such that

$$\Gamma(R) = S\big[\Gamma_1(R) \oplus \ldots \oplus \Gamma_n(R)\big]S^{-1} = S\begin{pmatrix} \Gamma_1(R) & 0 & \ldots & 0 \\ 0 & \Gamma_2(R) & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \Gamma_n(R) \end{pmatrix}S^{-1}. \qquad (1.2.2.5)$$

In this way one may proceed until all matrix representations $\Gamma_i(K)$ are *irreducible*, *i.e.* do not have invariant subspaces. Then each representation $\Gamma(K)$ can be written as a direct sum

$$\Gamma(R) = S\big[m_1\Gamma_1(R) \oplus \ldots \oplus m_s\Gamma_s(R)\big]S^{-1}, \qquad (1.2.2.6)$$

where the representations $\Gamma_1 \ldots \Gamma_s$ are all nonequivalent and the *multiplicities* m_i are the numbers of times each irreducible representation occurs. The nonequivalent irreducible representations Γ_i for which the multiplicity is not zero are the *irreducible components* of $\Gamma(K)$.

We first discuss two special representations. The simplest representation in one-dimensional space is obtained by assigning the number 1 to all elements of K. Obviously this is a representation, called the *identity* or *trivial representation*. Another is the *regular representation*. To obtain this, one numbers the elements of K from 1 to the order N of the group ($|K| = N$). For a given $R \in K$ there is a one-to-one mapping from K to itself defined by $R_i \to R_j \equiv RR_i$. Consider the $N \times N$ matrix $\Gamma(R)$, which has in the ith column zeros except on line j, where the entry is unity. The matrix $\Gamma(R)$ then has as only entries 0 or 1 and satisfies

$$RR_i = \Gamma(R)_{ji}R_j, \quad (i = 1, 2, \ldots, N). \qquad (1.2.2.7)$$

These matrices $\Gamma(R)$ form a representation, the *regular representation* of K of dimension N, as one sees from

$$(R_iR_j)R_k = R_i\sum_{l=1}^{N}\Gamma(R_j)_{lk}R_l = \sum_{l=1}^{N}\sum_{m=1}^{N}\Gamma(R_j)_{lk}\Gamma(R_i)_{ml}R_m = \sum_{m=1}^{N}\big[\Gamma(R_i)\Gamma(R_j)\big]_{mk}R_m = \sum_{m=1}^{N}\Gamma(R_iR_j)_{mk}R_m.$$

A representation in a real vector space that leaves a positive definite metric invariant can be considered on an orthonormal basis for that metric. Then the matrices satisfy

$$\Gamma(R)\Gamma(R)^T = E$$

[^{T} denotes transposition of the matrix: $\Gamma(R)^T_{ij} = \Gamma(R)_{ji}$] and the representation is *orthogonal*. If V is a complex vector space with positive definite metric invariant under the representation, the latter gives on an orthonormal basis matrices satisfying

$$\Gamma(R)\Gamma(R)^\dagger = E$$

[† denotes Hermitian conjugation: $\Gamma(R)^\dagger_{ij} = \Gamma(R)^*_{ji}$] and the representation is *unitary*. A real representation of a finite group is always equivalent with an orthogonal one, a complex representation of a finite group is always equivalent with a unitary one. As a proof of the latter statement, consider the standard Hermitian metric on V: $f(x, y) = \sum_i x_i^* y_i$. Then the positive definite form

$$F(x, y) = (1/N) \sum_{R \in K} f(D(R)x, D(R)y) \qquad (1.2.2.8)$$

is invariant under the representation. To show this, take an arbitrary element R'. Then

$$F(D(R')x, D(R')y) = (1/N) \sum_{R \in K} f(D(R'R)x, D(R'R)y) = F(x, y). \qquad (1.2.2.9)$$

With respect to an orthonormal basis for this metric $F(x, y)$, the matrices corresponding to $D(R)$ are unitary. The complex representation can be put into this unitary form by a basis transformation. For a real representation, the argument is fully analogous, and one obtains an orthogonal transformation.

From two representations, $D_1(K)$ in V_1 and $D_2(K)$ in V_2, one can construct the sum and product representations. The *sum representation* acts in the direct sum space $V_1 \oplus V_2$, which has elements $(\mathbf{a}, \mathbf{b})$ with $\mathbf{a} \in V_1$ and $\mathbf{b} \in V_2$. The representation $D_1 \oplus D_2$ is defined by

$$\big[(D_1 \oplus D_2)(R)\big](\mathbf{a}, \mathbf{b}) = (D_1(R)\mathbf{a}, D_2(R)\mathbf{b}). \qquad (1.2.2.10)$$

The matrices $\Gamma_1 \oplus \Gamma_2(R)$ are of dimension $n_1 + n_2$.

The *product representation* acts in the tensor space, which is the space spanned by the vectors $\mathbf{e}_i \otimes \mathbf{e}_j$ ($i = 1, 2, \ldots, \dim V_1$; $j = 1, 2 \ldots, \dim V_2$). The dimension of the tensor space is the product of the dimensions of both spaces. The action is given by

$$\big[(D_1 \otimes D_2)(R)\big]\mathbf{a} \otimes \mathbf{b} = D_1(R)\mathbf{a} \otimes D_2(R)\mathbf{b}. \qquad (1.2.2.11)$$

For bases $\mathbf{e}_i$ ($i = 1, 2, \ldots, d_1$) for V_1 and $\mathbf{e}'_j$ ($j = 1, 2, \ldots, d_2$) for V_2, a basis for the tensor product of spaces is given by

$$\mathbf{e}_i \otimes \mathbf{e}'_j, \quad i = 1, \ldots, d_1;\ j = 1, 2, \ldots, d_2, \qquad (1.2.2.12)$$

and with respect to this basis the representation of K is given by matrices

$$(\Gamma_1 \otimes \Gamma_2)(R)_{ik,jl} = \Gamma_1(R)_{ij}\Gamma_2(R)_{kl}. \qquad (1.2.2.13)$$

As an example of these operations, consider

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \oplus \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix};$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

If two representations $D_1(K)$ and $D_2(K)$ are equivalent, there is an operator S such that

$$SD_1(R) = D_2(R)S \quad \forall\, R \in K.$$

This relation may also hold between sets of operators that are not necessarily representations. Such an operator S is called an *intertwining operator*. With this concept we can formulate a theorem that strictly speaking does not deal with representations but with intertwining operators: *Schur's lemma*.

Proposition. Let M and N be two sets of nonsingular linear transformations in spaces V (dimension n) and W (dimension m), respectively. Suppose that both sets are irreducible (the only invariant subspaces are the full space and the origin). Let S be a linear transformation from V to W such that $SM = NS$. Then either S is the null operator or S is nonsingular and $SMS^{-1} = N$.

Proof: Consider the image of V under S: $\mathrm{Im}_S V \subseteq W$. That means that $S\mathbf{r} \in \mathrm{Im}_S V$ for all $\mathbf{r} \in V$. This implies that $NS\mathbf{r} = SM\mathbf{r} \in \mathrm{Im}_S V$. Therefore, $\mathrm{Im}_S V$ is an invariant subspace of W under N. Because N is irreducible, either $\mathrm{Im}_S V = 0$ or $\mathrm{Im}_S V = W$. In the first case, S is the null operator. In the second case, notice that the kernel of S, the subspace of V mapped on the null vector of W, is an invariant subspace of V under M: if $S\mathbf{r} = 0$ then $NS\mathbf{r} = 0$. Again, because of the irreducibility, either Ker_S is the whole of V, and then S is again the null operator, or $\mathrm{Ker}_S = 0$. In the latter case, S is a one-to-one mapping and therefore nonsingular. Therefore, either S is the null operator or it is an isomorphism between the vector spaces V and W, which are then both of dimension n. With respect to bases in the two spaces, the operator S corresponds to a nonsingular matrix and $M = S^{-1}NS$.

This is a very fundamental theorem. Consequences of the theorem are:

(1) If N and M are nonequivalent irreducible representations and $SM = NS$, then $S = 0$.

(2) If a matrix S is singular and links two irreducible representations of the same dimension, then $S = 0$.

(3) A matrix S that commutes with all matrices of an irreducible complex representation is a multiple of the identity. Suppose that an $n \times n$ matrix S commutes with all matrices of a complex irreducible representation. S can be singular and is then the null matrix, or it is nonsingular. In the latter case it has an eigenvalue $\lambda \neq 0$ and $S - \lambda E$ commutes with all the matrices. However, $S - \lambda E$ is singular and therefore the null matrix: $S = \lambda E$. This reasoning is only valid in a complex space, because, generally, the eigenvalues λ are complex.

1.2.2.3. *General tensors*

Suppose a group K acts linearly on a d-dimensional space V: for any $v \in V$ one has

$$Rv \in V \quad \forall\, R \in K, v \in V.$$

For a basis $\mathbf{a}_i$ in V this gives a matrix group $\Gamma(K)$ *via*

$$R\mathbf{a}_i = \sum_{j=1}^{d} \Gamma(R)_{ji}\mathbf{a}_j, \quad R \in K. \qquad (1.2.2.14)$$

The matrix group $\Gamma(K)$ is a matrix representation of the group K.

Consider now a linear function f on V. Because

$$f\left(\sum_{i=1}^{d} \xi_i \mathbf{a}_i\right) = \sum_{i=1}^{d} \xi_i f(\mathbf{a}_i),$$

the function is completely determined by its value on the basis vectors $\mathbf{a}_i$. A second point is that these linear functions form a vector space because for two functions f_1 and f_2 the function $\alpha_1 f_1 + \alpha_2 f_2$ is a well defined linear function. The vector space is called the *dual space* and is denoted by V^*. A basis for this space is given by functions $f_1, \ldots, f_d$ such that

$$f_i(\mathbf{a}_j) = \delta_{ij},$$

because any linear function f can be written as a linear combination of these vectors with as coefficients the value of f on the basis vectors $\mathbf{a}_i$:

$$f = \sum_{i=1}^{d} f(\mathbf{a}_i) f_i \Leftrightarrow f\Big(\sum_{k=1}^{d} \xi_k \mathbf{a}_k\Big) = \sum_{k=1}^{d} \xi_k \sum_{i=1}^{d} f(\mathbf{a}_i) f_i(\mathbf{a}_k) = \sum_{k=1}^{d} \xi_k f(\mathbf{a}_k).$$

Therefore, the space V^* also has d dimensions. If V has in addition a nonsingular scalar product, there is for each linear function f a vector $\mathbf{k}$ such that

$$f(\mathbf{r}) = \mathbf{k} \cdot \mathbf{r}, \quad (1.2.2.15)$$

and the vectors $\mathbf{k}_i$ corresponding to the basis functions f_i above satisfy

$$\mathbf{k}_i \cdot \mathbf{a}_j = f_i(\mathbf{a}_j) = \delta_{ij}. \quad (1.2.2.16)$$

The vectors $\mathbf{k}_i$ (with $i = 1, 2, \ldots, d$) form the *reciprocal basis* (see also Section 1.1.2.4).

The transformation properties of the vectors in dual (or reciprocal) space can be derived from those of the vectors in V if one puts

$$(Rf)(R\mathbf{r}) = f(\mathbf{r}). \quad (1.2.2.17)$$

Then

$$Rf_i = \sum_{i=1}^{d} \Gamma^*(R)_{ji} f_j \leftrightarrow \sum_{i=1}^{d} \Gamma^*(R)_{ji} \sum_{l=1}^{d} \Gamma(R)_{lk} f_j(\mathbf{a}_l) = f_i(\mathbf{a}_k) = \delta_{ik},$$

from which follows the relation

$$\Gamma^*(R)_{ij} = \Gamma^{-1}(R)_{ji}. \quad (1.2.2.18)$$

The matrices $\Gamma^*(R)$ form also a representation of K, the *contragredient representation*. In general, the latter is not equivalent with the former. The elements of the space V^* are *dual vectors*.

One can generalize the procedure that gave the dual space, and this leads to a more abstract definition of a tensor. Consider a bilinear function on V.

$$f(r, s): \quad f(\alpha r_1 + \beta r_2, \gamma s_1 + \delta s_2) = \alpha\gamma f(r_1, s_1) + \alpha\delta f(r_1, s_2) + \beta\gamma f(r_2, s_1) + \beta\delta f(r_2, s_2).$$

Again, such bilinear functions form a vector space of dimension d^2. Any function $f(\mathbf{r}, \mathbf{s})$ is fixed by its value on the d^2 pairs of basis vectors, and these values are the coefficients of the function on a basis

$$f_{ij}(\mathbf{a}_k, \mathbf{a}_l) = \delta_{ik}\delta_{jl}. \quad (1.2.2.19)$$

One has

$$f(\mathbf{r}, \mathbf{s}) = \sum_{ij} f(\mathbf{a}_i, \mathbf{a}_j) f_{ij}(\mathbf{r}, \mathbf{s}). \quad (1.2.2.20)$$

Analogously to the former case, one can determine the transformation properties of the elements of the *tensor space* $V^* \otimes V^*$:

$$Rf_{ij} = \sum_{k=1}^{d} \sum_{l=1}^{d} \Gamma^*(R)_{ki} \Gamma^*(R)_{lj} f_{kl}. \quad (1.2.2.21)$$

The space carries the product representation of the contragredient representation Γ^* with itself.

That this is really the same concept of tensor as usually used in physics can be seen from the example of the dielectric tensor ε_{ij}. For an electric field $\mathbf{E}$, the energy is given by $\sum_{ij} \varepsilon_{ij} E_i E_j$ and this is a bilinear function $f_\varepsilon(\mathbf{E}, \mathbf{E})$.

The most general situation occurs if one considers all multilinear functions of p vectors and q dual vectors. The function

$$f(\mathbf{r}_1, \ldots, \mathbf{r}_p, \mathbf{k}_1, \ldots, \mathbf{k}_q)$$

is linear in each of its arguments. Again, the function is determined by its value on the basis vectors $\mathbf{a}_i$ of V and $\mathbf{b}_j$ of V^*. The (p, q)-linear functions form a vector space with basis vectors $f_{i_1,\ldots,j_q}$ given by

$$f_{i_1,\ldots,i_p,j_1,\ldots,j_q}(\mathbf{a}_{k_1}, \ldots, \mathbf{b}_{l_q}) = \delta_{i_1k_1} \ldots \delta_{j_ql_q}.$$

The $d^{(p+q)}$-dimensional space carries a representation of the group K:

$$Rf_{i_1,\ldots,i_p,j_1,\ldots,j_q} = \sum_{k_1=1}^{d} \ldots \sum_{k_p=1}^{d} \sum_{l_1=1}^{d} \ldots \sum_{l_q=1}^{d} \Gamma(R)_{k_1i_1} \ldots \Gamma(R)_{k_pi_p} \Gamma^*(R)_{l_1j_1} \ldots f_{k_1\ldots l_q}. \quad (1.2.2.22)$$

Therefore, the space of (p, q) tensors carries a representation which is the tensor product of the pth tensor power of $\Gamma(K)$ and the qth tensor power of the contragredient representation $\Gamma^*(K)$.

If the $(0, 2)$ tensor $f(\mathbf{r}, \mathbf{s})$ is symmetric in its arguments, the space of such tensors carries the symmetrized tensor product of the representation $\Gamma(K)$ with itself. Similarly the (anti)symmetric $(2, 0)$ tensors form a space that carries the symmetrized, respectively antisymmetrized, tensor product of $\Gamma^*(K)$ with itself. This can be generalized to (p, q) tensors with all kinds of symmetry. One can have a $(0, 4)$ tensor that is symmetric in all its four arguments. Such tensors form a space that not only carries a representation of K, but one of the symmetric group S_4 (the permutation group on four letters) as well. We shall come back to such symmetric tensors in Section 1.2.2.7.

1.2.2.4. *Orthogonality relations*

Important consequences from symmetry for physical systems are related to orthogonality relations. The vanishing of matrix elements is one example. Consider two irreducible representations $\Gamma_1(K)$ and $\Gamma_2(K)$ of dimensions d_1 and d_2, respectively. Then take an arbitrary $d_1 \times d_2$ matrix M and construct with this a new matrix S:

$$S = \sum_{R \in K} \Gamma_1(R) M \Gamma_2^{-1}(R).$$

For this matrix one has

$$\begin{aligned} S\Gamma_2(R) &= \sum_{R' \in K} \Gamma_1(R') M \Gamma_2^{-1}(R') \Gamma_2(R) \\ &= \Gamma_1(R) \sum_{R' \in K} \Gamma_1^{-1}(R) \Gamma_1(R') M \Gamma_2^{-1}(R') \Gamma_2(R) \\ &= \Gamma_1(R) \sum_{R' \in K} \Gamma_1(R^{-1}R') M \Gamma_2^{-1}(R^{-1}R') = \Gamma_1(R) S. \end{aligned}$$

Because $\Gamma_1(K)$ and $\Gamma_2(K)$ are supposed to be irreducible, it follows from Schur's lemma that either Γ_1 and Γ_2 are not equivalent and S is the null matrix, or they are equivalent. If they are not equivalent one has

$$0 = S_{ij} = \sum_{R \in K} \sum_{kl} \Gamma_1(R)_{ik} M_{kl} \Gamma_2(R^{-1})_{lj}. \quad (1.2.2.23)$$

Because we have taken an arbitrary matrix M, this implies that

$$\sum_{R \in K} \Gamma_1(R)_{ik} \Gamma_2(R^{-1})_{lj} = 0 \quad (1.2.2.24)$$

whenever $\Gamma_1(K)$ and $\Gamma_2(K)$ are not equivalent.

When the two irreducible representations are equivalent we assume them to be identical. Then S commutes with all matrices $\Gamma_1(K)$ of an irreducible representation and is thus a multiple of the identity (in case one considers complex representations). Its trace is then $d\lambda$ if the dimension of the representation is denoted by d, but on the other hand it is

$$\mathrm{Tr}(S) = \sum_{R \in K} \mathrm{Tr}\big(\Gamma_1(R) M \Gamma_1(R^{-1})\big) = N\mathrm{Tr}(M).$$

Therefore,

$$S_{ij} = (N/d)\mathrm{Tr}(M)\delta_{ij} = \sum_{R \in K} \sum_{kl} \Gamma_1(R)_{ik} M_{kl} \Gamma_1(R^{-1})_{lj}. \quad (1.2.2.25)$$

Hence

$$\sum_{R\in K}\Gamma_1(R)_{ik}\Gamma_1(R^{-1})_{lj}=(N/d)\delta_{ij}\delta_{kl}. \qquad (1.2.2.26)$$

This leads to the following proposition.

Proposition. If $\Gamma_\alpha(K)$ and $\Gamma_\beta(K)$ are irreducible complex representations of the finite group K one has

$$\sum_{R\in K}\Gamma_\alpha(R)_{ik}\Gamma_\beta(R^{-1})_{lj}=(N/d)\delta_{ij}\delta_{kl}\delta'_{\alpha\beta}, \qquad (1.2.2.27)$$

where $\delta'_{\alpha\beta}$ is zero if the representations are not equivalent, unity if they are identical and undefined if they are equivalent but not identical.

For unitary representations the orthogonality relations can be written as

$$\sum_{R\in K}\Gamma_\alpha(R)_{ik}\Gamma_\beta(R)^*_{jl}=(N/d)\delta_{ij}\delta_{kl}\delta'_{\alpha\beta}. \qquad (1.2.2.28)$$

According to Section 1.2.2.2 for finite groups K, there is always an equivalent unitary representation.

1.2.2.5. *Characters*

Two equivalent representations of a group K are conjugate subgroups in the group of nonsingular linear transformations. Corresponding matrices therefore have the same invariants. It is a remarkable fact that one of these invariants suffices for characterizing the equivalence class of a representation, namely the trace. The *character* of an element $R\in K$ in a representation $D(K)$ is the trace $\chi(R)=\mathrm{Tr}(D(R))$. It is a complex function on the group: for every $R\in K$ there is a complex number $\chi(R)$.

The character only depends on the conjugacy class: if two elements R and R' belong to the same class there is an element $T\in K$ such that $R'=TRT^{-1}$. Hence $\chi(R')=\mathrm{Tr}(D(TRT^{-1}))=\mathrm{Tr}(D(R))=\chi(R)$. Notice that for the identity element one has $D(E)=$ the d-dimensional unit matrix and $\chi(E)=d$. For the same reason, the character for two equivalent representations is the same.

From the orthogonality relations for the matrix elements of two irreducible representations follow those for characters.

Proposition. For two irreducible complex representations of a finite group K, one has

$$\sum_{R\in K}\chi_\alpha(R)\chi^*_\beta(R)=N\delta_{\alpha\beta}. \qquad (1.2.2.29)$$

Here one can use the Kronecker delta because characters of equivalent representations are equal, even if they are not identical.

The character of the sum of two representations is the sum of the characters. More generally, the character of the sum of irreducible representations D_α, each with multiplicity m_α, is

$$\chi(R)=\sum_\alpha m_\alpha\chi_\alpha(R).$$

This gives a *formula for the multiplicity* of an irreducible component:

$$\begin{aligned}m_\alpha=\sum_\beta m_\beta\delta_{\alpha\beta}&=(1/N)\sum_{R\in K}\sum_\beta m_\beta\chi_\beta(R)\chi^*_\alpha(R)\\&=(1/N)\sum_{R\in K}\chi(R)\chi^*_\alpha(R).\end{aligned} \qquad (1.2.2.30)$$

From the expression for the multiplicities follows:

Proposition. The representations $D_1(K)$ and $D_2(K)$ are equivalent if and only if their characters are the same: $\chi_1(R)=\chi_2(R)$. Two equivalent representations obviously have the same character. Nonequivalent irreducible representations have different characters because of the orthogonality relations and the multiplicities and irreducible components are uniquely determined by the formula (1.2.2.30).

Because the character is constant on a conjugacy class, (1.2.2.30) can also be written as

$$m_\alpha=(1/N)\sum_{i=1}^k n_i\chi(C_i)\chi^*_\alpha(C_i), \qquad (1.2.2.31)$$

where C_i denotes the ith conjugacy class ($i=1,2,\ldots k$) and n_i the number of its elements.

Proposition. The representation $D(K)$ is irreducible if and only if

$$(1/N)\sum_{i=1}^k n_i|\chi(C_i)|^2=1.$$

Proof: For a representation that is equivalent to the sum of irreducible representations with multiplicities m_α one has

$$\begin{aligned}(1/N)\sum_{i=1}^k n_i|\chi(C_i)|^2&=(1/N)\sum_{i=1}^k\sum_{\alpha\beta}n_im_\alpha m_\beta\chi_\alpha(C_i)\chi^*_\beta(C_i)\\&=\sum_{\alpha\beta}m_\alpha m_\beta\delta_{\alpha\beta}=\sum_\alpha m_\alpha^2.\end{aligned} \qquad (1.2.2.32)$$

If the representation is irreducible, there is exactly one value of α for which $m_\alpha=1$, whereas all other multiplicities vanish. If the representation is reducible, $\sum_\alpha m_\alpha^2>1$.

Proposition. (Burnside's theorem.) The sum of the squares of the dimensions of all nonequivalent irreducible representations is equal to the order of the group.

Proof: Consider the regular representation. The value of its character in an element R is given by the number of elements $R_i\in K$ for which $RR_i=R_i$. Therefore,

$$\chi(R)=\begin{cases}0 & \text{for } R\neq E;\\ N & \text{for } R=E.\end{cases}$$

The multiplicity formula (1.2.2.30) then gives

$$m_\alpha=(1/N)\sum_{R\in K}\chi(R)\chi^*_\alpha(R)=(1/N)\chi(E)\chi^*_\alpha(E)=d_\alpha.$$

Each irreducible representation occurs in the regular representation with a multiplicity equal to its dimension. Therefore,

$$N=\chi(E)=\sum_\alpha m_\alpha\chi_\alpha(E)=\sum_\alpha d_\alpha^2.$$

Proposition. The number of nonequivalent irreducible representations of a finite group K is equal to the number of its conjugacy classes.

Proof: Take from each equivalence class of irreducible representations of K one unitary representative $\Gamma_\alpha(K)$. The matrix elements $\Gamma_\alpha(R)_{ij}$ are complex functions on the group. The number of these functions is the sum over α of d_α^2 and that is equal to the order of the group according to Burnside's theorem. The number of independent functions on K is, of course, also equal to the order N of the group. If one considers the usual scalar product of functions on the group,

$$f_1\cdot f_2\equiv\sum_{R\in K}f_1^*(R)f_2(R),$$

the scalar product of two of the N functions is

$$\sum_{R\in K}\Gamma^*_\alpha(R)_{ij}\Gamma_\beta(R)_{kl}=(N/d_\alpha)\delta_{\alpha\beta}\delta_{ik}\delta_{jl} \qquad (1.2.2.33)$$

according to the orthogonality relations. This means that the N functions indeed form an orthogonal basis in the space of all functions on the group. In particular, consider a function $f(K)$ that is constant on conjugacy classes. This function can be expanded in the basis functions.

$$\begin{aligned} f(R) &= \sum_{\alpha ij} f_{\alpha ij}\Gamma_\alpha(R)_{ij} \\ &= \sum_{\alpha ij} f_{\alpha ij}(1/N)\sum_{T\in K}\Gamma_\alpha(TRT^{-1})_{ij} \\ &= (1/N)\sum_{\alpha ijkl}\sum_{T\in K} f_{\alpha ij}\Gamma_\alpha(T)_{ik}\Gamma_\alpha(R)_{kl}\Gamma_\alpha(T^{-1})_{lj} \\ &= (1/N)\sum_{\alpha ijkl} f_{\alpha ij}\Gamma_\alpha(R)_{kl}(N/d_\alpha)\delta_{ij}\delta_{kl} \\ &= \sum_\alpha \sum_{i=1}^{d_\alpha}(f_{\alpha ii}/d_\alpha)\chi_\alpha(R). \end{aligned}$$

This implies that every class function can be written as a linear combination of the character functions. Therefore, the number of such character functions must be equal to or larger than the number of conjugacy classes. On the other hand, the number of dimensions of the space of class functions is k, the number of conjugacy classes. For the scalar product in this space given by

$$f_1\cdot f_2 \equiv \sum_{i=1}^{k}(n_i/N)f_1^*(C_i)f_2(C_i)$$

the character functions are orthogonal:

$$\sum_{i=1}^{k}(n_i/N)\chi_\alpha^*(C_i)\chi_\beta(C_i) = (1/N)\sum_{R\in K}\chi_\alpha^*(R)\chi_\beta(R) = \delta_{\alpha\beta}. \quad (1.2.2.34)$$

There are at most k mutually orthogonal functions, and consequently the number of nonequivalent irreducible characters $\chi_\alpha(K)$ is exactly equal to the number of conjugacy classes.

As additional result one has the following proposition.

Proposition. The functions $\Gamma_\alpha(R)_{ij}$ with $\alpha = 1, 2, \ldots, k$ and $i, j = 1, 2, \ldots, d_\alpha$ form an orthogonal basis in the space of complex functions on the group K. The characters χ_α form an orthogonal basis for the space of all class functions.

The characters of a group K can be combined into a square matrix, the *character table*, with entries $\chi_\alpha(C_i)$. Besides the orthogonality relations mentioned above, there are also relations connected with *class multiplication constants*. Consider the conjugacy classes C_i of the group K. Formally one can introduce the sum of all elements of a class:

$$M_i = \sum_{R\in C_i} R.$$

It can be proven that the multiplication of two such class sums is the sum of class sums, where such a class sum may occur more than once:

$$M_iM_j = \sum_k c_{ijk}M_k, \quad c_{ijk}\in\mathbb{Z}.$$

The coefficients c_{ijk} are called the *class multiplication constants*. The elements of the character table then have the following properties.

$$(1/N)\sum_{i=1}^{k} n_i\chi_\alpha(C_i)\chi_\beta^*(C_i) = \delta_{\alpha\beta}; \quad (1.2.2.35)$$

$$(1/N)\sum_{\alpha=1}^{k}\chi_\alpha(C_i)\chi_\alpha^*(C_j) = (1/n_i)\delta_{ij}; \quad (1.2.2.36)$$

$$n_i\chi_\alpha(C_i)n_j\chi_\alpha(C_j) = d_\alpha\sum_{l=1}^{k}c_{ijl}n_l\chi_\alpha(C_l). \quad (1.2.2.37)$$

As an example, consider the permutation group on three letters S_3. It consists of six permutations. It is a group that is isomorphic with the point group 32. The character table is a 3×3 array, because there are three conjugacy classes (C_i, $i = 1, 2, 3$), and consequently three irreducible representations (Γ_i, $i = 1, 2, 3$) (see Table 1.2.2.1).

The two one-dimensional representations are equal to their character. A representative representation for the third character is generated by matrices

$$\Gamma_3(A) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \Gamma_3(B) = \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$$

and the group of matrices is equivalent to an orthogonal group with generators

$$\Gamma_3(A)' = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}, \quad \Gamma_3(B)' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The character table is in agreement with the class multiplication table

$$\begin{array}{lll} C_1C_1 = C_1 & C_2C_1 = C_2 & C_3C_1 = C_3 \\ C_1C_2 = C_2 & C_2C_2 = 2C_1 + C_2 & C_3C_2 = 2C_3 \\ C_1C_3 = C_3 & C_2C_3 = 2C_3 & C_3C_3 = 3C_1 + 3C_2. \end{array}$$

1.2.2.6. *The representations for point groups in one, two and three dimensions*

For the irreducible representations of the point groups, it is necessary to know something about the structure of these groups. Since the representations of isomorphic groups are the same, one can restrict oneself to representatives of the isomorphism classes. In the following, we give a brief description of the structure of the point groups in spaces up to three dimensions. The character tables are given in Section 1.2.6. For the infinite series of groups (C_n and D_n), the crystallographic members are given explicitly separately.

(i) C_n. Cyclic groups are Abelian. Therefore, each element is a conjugacy class on itself. Irreducible representations are one-dimensional. The representation is determined by its value on a generator. Since $A^n = E$, the character $\chi(A)$ of an irreducible representation is an nth root of unity. There are n one-dimensional representations. For the pth irreducible representation, one has $\chi^{(p)}(A) = \exp(2\pi ip/n)$.

(ii) D_n. From the defining relations, it follows that A^p and A^{-p} ($p = 1, 2, \ldots, n$) form a conjugacy class and that A^pB and $A^{p+2}B$ belong to the same class. Therefore, one has to distinguish the

Table 1.2.2.1. *Character table for $S_3 \sim D_3$*

Elements Symbols	(1) E	(123) A	(132) A^2	(23) B	(13) A^2B	(12) AB
Class Order	C_1 1	C_2 3		C_3 2		
Γ_1	1	1		1		
Γ_2	1	1		−1		
Γ_3	2	−1		0		

cases of even n from those of odd n. For odd n, one has a class consisting of E (order 1), $(n-1)/2$ classes with elements $A^{\pm p}$, and one class with all elements A^pB (order 2). For even n, there is a class consisting of E (order 1), one with $A^{n/2}$, and $(n-2)/2$ classes with $A^{\pm p}$. The other elements form two classes of order 2 elements, one with the elements A^pB for p odd, the other with A^pB for p even.

The number of one-dimensional irreducible representations is the order of the group (N) divided by the order of the *commutator group*, which is the group generated by all elements $aba^{-1}b^{-1}$ ($a, b \in K$). For n odd this number is 2, for n even it is 4. In addition there are two-dimensional irreducible representations: $(n-1)/2$ for odd n, $n/2-1$ for even n.

(iii) T, O, I. The conjugacy classes of the tetrahedral, the octahedral and the icosahedral groups T, O and I, respectively, are given in the tables in Section 1.2.6.

(iv) $K \times C_2$. Because the generator of C_2 commutes with all elements of the group, the number of conjugacy classes of the direct product $K \times C_2$ is twice that for K. If A is the generator of C_2 and C_i are the classes of K, then the classes of the direct product are C_i and C_iA. The element A, which commutes with all elements of the direct product, is in an irreducible representation represented by a multiple of the identity. Because A is of order 2, the factor is ±1. Therefore, the character table looks like

$$\chi(K \times C_2) = \begin{pmatrix} \chi(K) & \chi(K) \\ \chi(K) & -\chi(K) \end{pmatrix}.$$

The n irreducible representations where A is represented by $+E$ are called *gerade* representations, the other, where A is represented by $-E$, are called *ungerade*.

In general, if K and H are finite groups with irreducible representations $D_{1\alpha}(K)$ and $D_{2\beta}(H)$, the *outer tensor product* acts on the tensor product $V_1 \otimes V_2$ of representation spaces as

$$(D_{1\alpha}(R) \otimes D_{2\beta}(R'))\mathbf{a} \otimes \mathbf{b} = (D_{1\alpha}(R)\mathbf{a}) \otimes (D_{2\beta}(R')\mathbf{b}), \quad \mathbf{a} \in V_1, \mathbf{b} \in V_2. \qquad (1.2.2.38)$$

With the irreducibility criterion, one checks that this is an irreducible representation of $K \times H$. Moreover, $D_{1\alpha} \otimes D_{2\beta}$ is equivalent with $D_{1\alpha'} \otimes D_{2\beta'}$ if and only if $\alpha = \alpha'$ and $\beta = \beta'$. This means that one obtains all nonequivalent irreducible representations of $K \times H$ from the outer tensor products of the irreducible representations of K and H. If the group H is C_2, there are two irreducible representations of C_2, both one-dimensional. That means that the tensor product simplifies to a normal product. If $H = C_2$ and $D_{2\beta}(H)$ is the trivial representation, one has from (1.2.2.38)

$$D_{\alpha g}(R) = D_\alpha(R), \quad D_{\alpha g}(RA) = D_\alpha(R), \quad R \in K$$
$$D_{\alpha u}(R) = D_\alpha(R), \quad D_{\alpha u}(RA) = -D_\alpha(R).$$

The letters g and u come from the German *gerade* (even) and *ungerade* (odd). They indicate the sign of the operator associated with the generator A of C_2: $+1$ for g representations, -1 for u representations. The number of nonequivalent irreducible representations of $K \otimes C_2$ is twice that of K.

Schur's lemma and the orthogonality relations and theorems derived above are formulated for complex representations and are, generally, not valid for integer or real representations. Nevertheless, many physical properties can be described using representation theory, but being real quantities they sometimes require a slightly different treatment. Here we shall discuss the relation between the complex representations and *physical or real representations*. Consider a real matrix representation $\Gamma(K)$. If it is reducible over complex numbers, it can be fully reduced. When is an irreducible component itself real? A first condition is clearly that its character is real. This is, however, not sufficient. A real representation can by a complex basis transformation be put into a complex form and such a transformation does not change the character. Therefore, a better question is: which complex irreducible representations can be brought into real form? Consider a complex irreducible representation with a real character. Then it is equivalent with its complex conjugate *via* a matrix S:

$$\Gamma(R) = S\Gamma^*(R)S^{-1}, \quad R \in K.$$

Here one has to distinguish two different cases. To make the distinction between the two cases one has the following:

Proposition. Suppose that $\Gamma(K)$ is a complex irreducible representation with real character, and S a matrix intertwining $\Gamma(K)$ and its complex conjugate. Then S satisfies either $SS^* = E$ or $SS^* = -E$. In the former case, there exists a basis transformation that brings $\Gamma(K)$ into real form, in the latter case there is no such basis transformation.

Proposition. If $\Gamma(K)$ is a complex irreducible representation with real character $\chi(K)$, the latter satisfies

$$(1/N) \sum_{R \in K} \chi(R^2) = \pm1.$$

If the right-hand side is $+1$, the representation can be put into real form, if it is -1 it cannot. (Proofs are given in Section 1.2.5.5.)

Consequently, a complex irreducible representation $\Gamma(K)$ is equivalent with a real one if $\chi(R) = \chi^*(R)$ and $\sum_R \chi(R^2) = N$. If that is not the case, a real representation containing $\Gamma(K)$ as irreducible component is the matrix representation

$$\tfrac{1}{2}\begin{pmatrix} \Gamma(R) + \Gamma^*(R) & i(\Gamma(R) - \Gamma^*(R)) \\ -i(\Gamma(R) - \Gamma^*(R)) & \Gamma(R) + \Gamma^*(R) \end{pmatrix} \sim \begin{pmatrix} \Gamma(R) & 0 \\ 0 & \Gamma^*(R) \end{pmatrix}. \qquad (1.2.2.39)$$

The basis transformation is given by

$$S = \begin{pmatrix} E & E \\ -iE & iE \end{pmatrix}.$$

The dimension of the physically irreducible representation is $2d$, if d is the dimension of the complex irreducible representation $\Gamma(K)$. In summary, there are three types of irreducible representation:

(1) First kind: $\chi(K) = \chi^*(K)$, $\sum_{R \in K} \chi(R^2) = +N$, dimension of real representation d;

(2) Second kind: $\chi(K) = \chi^*(K)$, $\sum_{R \in K} \chi(R^2) = -N$, dimension of real representation $2d$;

(3) Third kind: $\chi(R) \neq \chi(R)^*$, $\sum_{R \in K} \chi(R^2) = 0$, dimension of real representation $2d$.

Examples of the three cases:

(1) The matrices

$$D(A) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \text{ and } D(B) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

generate a group that forms a faithful representation of the dihedral group $D_4 = 422$, for which the character table is given in Table 1.2.6.5. If one uses the same numbering of conjugacy classes, its character is $\chi(C_i) = 2, 0, -2, 0, 0$. It is an irreducible representation ($2^2 + 2^2 = N = 8$) with real character. The sum of the characters of the squares of the elements is $2 + 2 \times (-2) + 2 + 2 \times 2 + 2 \times 2 = 8 = N$. Therefore, it is equivalent to a real matrix representation, *e.g.* with

$$D'(A) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \text{ and } D'(B) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

(2) The matrices

$$D(A) = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \text{ and } D(B) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

generate a group that is a faithful representation of the quaternion group of order 8. This group has five classes: E, $\{A, A^3\}$, $\{B, B^3\}$, $\{BA, AB\}$ and A^2. The character of the elements is $\chi(R) = 2, 0, 0, 0, -2$ for the five classes. Then

$$(1/8)\sum_R \chi(R^2) = -1,$$

which means that the representation is essentially complex. A real physically irreducible representation of the group is generated by

$$\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

and the generated group is a crystallographic group in four dimensions.

(3) The complex number $\exp(2\pi i/n)$ generates a representation of the cyclic group C_n. For $n > 2$ the representation is not equivalent with its complex conjugate. Therefore, it is not a physical representation. The physically irreducible representation that contains this complex irreducible component is generated by

$$\begin{pmatrix} \cos(2\pi/n) & -\sin(2\pi/n) \\ \sin(2\pi/n) & \cos(2\pi/n) \end{pmatrix} \simeq \begin{pmatrix} \exp(2\pi i/n) & 0 \\ 0 & \exp(-2\pi i/n) \end{pmatrix}.$$

All complex irreducible representations of the finite point groups in up to three dimensions with real character can be put into a real form. This is not true for higher dimensions, as we have seen in the example of the quaternion group.

1.2.2.7. *Tensor representations*

When $V_1, \ldots, V_n$ are linear vector spaces, one may construct tensor products of these spaces. There are many examples in physics where this notion plays a role. Take the example of a particle with spin. The wave function of the particle has two components, one in the usual three-dimensional space and one in spin space. The proper way to describe this situation is *via* the tensor product. In normal space, a basis is formed by spherical harmonics Y_{lm}, in spin space by the states $|ss_z\rangle$. Spin–orbit interaction then plays in the $(2l+1)(2s+1)$-dimensional space with basis $|lm\rangle \otimes |ss_z\rangle$. Another example is a physical tensor, *e.g.* the dielectric tensor ε_{ij} of rank 2. It is a symmetric tensor that transforms under orthogonal transformations exactly like a symmetric bi-vector with components $v_iw_j + v_jw_i$, where v_i and w_i $(i = 1, 2, 3)$ are the components of vectors $\mathbf{v}$ and $\mathbf{w}$. A basis for the space of symmetric bi-vectors is given by the six vectors $(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i)$ $(i \leq j)$. The space of symmetric rank 2 tensors has the same transformation properties.

A basis for the tensor space $V_1 \otimes V_2 \otimes \ldots \otimes V_n$ is given by $\mathbf{e}_{1i} \otimes \mathbf{e}_{2j} \otimes \ldots \otimes \mathbf{e}_{nk}$, where $i = 1, 2, \ldots, d_1$; $j = 1, 2, \ldots d_2$; ... ; $k = 1, 2, \ldots, d_n$. Therefore the dimension of the tensor product is the product of the dimensions of the spaces V_i (see also Section 1.1.3.1.2). The tensor space consists of all linear combinations with real or complex coefficients of the basis vectors. In the summation one has the multilinear property

$$\left(\sum_{i=1}^{d_1} c_{1i}\mathbf{e}_{1i}\right) \otimes \left(\sum_{j=1}^{d_2} c_{2j}\mathbf{e}_{2j}\right) \otimes \ldots = \sum_{ij\ldots} c_{1i}c_{2j}\ldots \mathbf{e}_{1i} \otimes \mathbf{e}_{2j} \otimes \ldots . \quad (1.2.2.40)$$

In many cases in practice, the spaces V_i are all identical and then the dimension of the tensor product $V^{\otimes n}$ is simply d^n.

The tensor product of n identical spaces carries in an obvious way a representation of the permutation group S_n of n elements. A permutation of n elements is always the product of pair exchanges. The action of the permutation (12), that interchanges spaces 1 and 2, is given by

$$P_{12}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \ldots = \mathbf{e}_j \otimes \mathbf{e}_i \otimes \mathbf{e}_k \otimes \ldots . \quad (1.2.2.41)$$

Two subspaces are then of particular interest, that of the tensors that are invariant under all elements of S_n and those that get a minus sign under pair exchanges. These spaces are the spaces of fully *symmetric and antisymmetric tensors*, respectively.

If the spaces $V_1, \ldots, V_n$ carry a representation of a finite group K, the tensor product space carries the product representation.

$$\mathbf{e}_{1j_1} \otimes \mathbf{e}_{2j_2} \otimes \ldots = \bigotimes_{i=1}^{n} \mathbf{e}_{ij_i} \rightarrow \sum_{k_1k_2\ldots} \Gamma_1(R)_{k_1j_1}\Gamma_2(R)_{k_2j_2}\ldots \mathbf{e}_{1k_1} \otimes \mathbf{e}_{2k_2} \otimes \ldots . \quad (1.2.2.42)$$

The matrix $\Gamma(R)$ of the tensor representation is the tensor product of the matrices $\Gamma_i(R)$. In general, this representation is reducible, even if the representations Γ_i are irreducible. The special case of $n = 2$ has already been discussed in Section 1.2.2.3.

From the definition of the action of $R \in K$ on vectors in the tensor product space, it is easily seen that the character of R in the tensor product representation is the product of the characters of R in the representations Γ_i:

$$\chi(R) = \prod_{i=1}^{n} \chi_i(R). \quad (1.2.2.43)$$

The reduction in irreducible components then occurs with the multiplicity formula.

$$m_\alpha = (1/N)\sum_{R\in K} \chi_\alpha^*(R)\prod_{i=1}^{n} \chi_i(R). \quad (1.2.2.44)$$

If the tensor product representation is a real representation, the physically irreducible components can be found by first determining the complex irreducible components, and then combining with their complex conjugates the components that cannot be brought into real form.

The tensor product of the representation space V with itself has a basis $\mathbf{e}_i \otimes \mathbf{e}_j$ $(i, j = 1, 2, \ldots, d)$. The permutation (12) transforms this into $\mathbf{e}_j \otimes \mathbf{e}_i$. This action of the permutation becomes diagonal if one takes as basis $\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i$ $(1 \leq i \leq j \leq d$, spanning the space $V_s^{\otimes 2})$ and $\mathbf{e}_i \otimes \mathbf{e}_j - \mathbf{e}_j \otimes \mathbf{e}_i$ $(1 \leq i < j \leq d$, spanning the space $V_a^{\otimes 2})$. If one considers the action of K, one has with respect to the first basis $\chi(R) = \chi_\alpha(R)^2$ if V carries the representation with character $\chi_\alpha(K)$. With respect to the second basis, one sees that the character of the permutation $P = (12)$ is given by $\frac{1}{2}d(d+1) - \frac{1}{2}d(d-1) = d$. The action of the element $R \in K$ on the second basis is

$$R\big(\mathbf{e}_i \otimes \mathbf{e}_j \pm \mathbf{e}_j \otimes \mathbf{e}_i\big) = \sum_{kl}(\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,ij}\big(\mathbf{e}_i \otimes \mathbf{e}_j \pm \mathbf{e}_j \otimes \mathbf{e}_i\big).$$

This implies that both $V_s^{\otimes 2}$ and $V_a^{\otimes 2}$ are invariant under R. The character in the subspace is

$$\chi^+(R) = \sum_{k\leq l}(\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,kl} \quad (1.2.2.45)$$

for the symmetric subspace and

$$\chi^-(R) = \sum_{k<l}(\Gamma_\alpha \otimes \Gamma_\alpha)(R)_{kl,kl} \quad (1.2.2.46)$$

for the antisymmetric one. Consequently one has

$$\chi^{\pm}(R) = \tfrac{1}{2}(\chi_\alpha(R)^2 \pm \chi_\alpha(R^2)); \quad d^{\pm} = \tfrac{1}{2}d_\alpha(d_\alpha \pm 1). \quad (1.2.2.47)$$

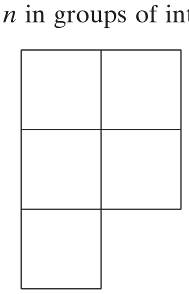
For $n > 2$, the tensor product space does not carry just a symmetric and an antisymmetric subspace, but also higher-dimensional representations of the permutation group S_n. The derivation of the character of the fully symmetric and fully antisymmetric subspaces remains rather similar. The formulae for the character of the representation of K carried by the fully symmetric (+) and fully antisymmetric (−) subspace, respectively, for $n = 1, 2, 3, 4, 5, 6$ are

$$\begin{aligned}
n = 2: \chi^{\pm}(R) &= \frac{1}{2!}\big(\chi(R)^2 \pm \chi(R^2)\big)\\
n = 3: \chi^{\pm}(R) &= \frac{1}{3!}\big(\chi(R)^3 \pm 3\chi(R^2)\chi(R) + 2\chi(R^3)\big)\\
n = 4: \chi^{\pm}(R) &= \frac{1}{4!}\big(\chi(R)^4 \pm 6\chi(R^2)\chi(R)^2 + 3\chi(R^2)^2\\
&\quad + 8\chi(R^3)\chi(R) \pm 6\chi(R^4)\big)\\
n = 5: \chi^{\pm}(R) &= \frac{1}{5!}\big(\chi(R)^5 \pm 10\chi(R^2)\chi(R)^3 + 15\chi(R^2)^2\chi(R)\\
&\quad + 20\chi(R^3)\chi(R)^2 \pm 20\chi(R^3)\chi(R^2)\\
&\quad \pm 30\chi(R^4)\chi(R) + 24\chi(R^5)\big)\\
n = 6: \chi^{\pm}(R) &= \frac{1}{6!}\big(\chi(R)^6 \pm 15\chi(R^2)\chi(R)^4 + 45\chi(R^2)^2\chi(R)^2\\
&\quad + 40\chi(R^3)^2 \pm 15\chi(R^2)^3 + 40\chi(R^3)\chi(R)^3\\
&\quad \pm 120\chi(R^3)\chi(R^2)\chi(R) \pm 90\chi(R^4)\chi(R)^2\\
&\quad + 90\chi(R^4)\chi(R^2) + 144\chi(R^5)\chi(R)\\
&\quad \pm 120\chi(R^6)\big)
\end{aligned}$$

From this follows immediately the dimension of the two subspaces:

$$\begin{aligned}
n = 2&: \frac{1}{2}(d^2 \pm d)\\
n = 3&: \frac{1}{6}(d^3 \pm 3d^2 + 2d)\\
n = 4&: \frac{1}{24}(d^4 \pm 6d^3 + 11d^2 \pm 6d)\\
n = 5&: \frac{1}{120}(d^5 \pm 10d^4 + 35d^3 \pm 50d^2 + 24d)\\
n = 6&: \frac{1}{720}(d^6 \pm 15d^5 + 85d^4 \pm 225d^3 + 274d^2 \pm 120d).
\end{aligned}$$

These expressions are based on Young diagrams. The procedure will be exemplified for the case of $n = 5$. In the expression for $\chi^{\pm}$ occur the partitions of n in groups of integers:



$5 = 4 + 1 = 3 + 2 = 3 + 1 + 1 = 2 + 2 + 1 = 2 + 1 + 1 + 1 = 1 + 1 + 1 + 1 + 1$. Each partition corresponds with a Young diagram with as many rows as there are terms in the sum, and in each row the corresponding number of boxes. The total number of boxes is n. Each partition corresponds with a term $\chi(R^{i_1})\chi(R^{i_2})\ldots$ such that $\sum_j i_j = n$. Here i_1 is the number of boxes in the first row *etc*. The prefactor then is the number of possible permutations compatible with the partition. For example, the partition $2 + 2 + 1$ allows the permutations

(12)(34)(5) (13)(24)(5) (14)(23)(5) (12)(35)(4) (13)(25)(4)
(15)(23)(4) (12)(45)(3) (14)(25)(3) (15)(24)(3) (13)(45)(2)
(14)(35)(2) (15)(34)(2) (23)(45)(1) (24)(35)(1) (25)(34)(1)

The sign of all these permutations is even: they are the product of an even number of pair interchanges. The prefactor for the term $\chi(R^2)\chi(R^2)\chi(R)$ is then $+15/5!$.

1.2.2.8. *Projective representations*

It is useful to consider a more general type of representation, one that gives only a homomorphism from a group to linear transformations up to a factor. In quantum mechanics, the relevance of such representations is a consequence of the freedom of the phase of the wave function, but they also occur in classical physics. In particular, we shall need this generalized concept for the determination of representations of crystallographic space groups.

A *projective representation* of a group K is a mapping from K to the group of nonsingular linear transformations of a vector space V such that

$$D(R)D(R') = \omega(R, R')D(RR') \quad \forall\ R, R' \in K,$$

where $\omega(R, R')$ is a nonzero real or complex number. The name stems from the fact that the mapping is a homomorphism if one identifies linear transformations that differ by a factor. Then one looks at the transformations of the lines through the origin, and these form a projective space. Other names are *multiplier* or *ray representations*. The mapping ω from $K \times K$ to the real or complex numbers is called the *factor system* of the projective representation. An ordinary representation is a projective representation with a trivial factor system that has only the value unity. A projective representation that can be identified with $D(H)$ is one with $D'(R) = u(R)D(R)$ for some real or complex function u on the group. It gives the same transformations of projective space. The projective representations $D(H)$ and $D'(H)$ are called *associated*. Their factor systems are related by

$$\omega'(R, R') = \frac{u(R)u(R')}{u(RR')}\omega(R, R'), \quad (1.2.2.48)$$

as one can check easily. Two factor systems that are related in this way are also called *associated*.

Not every mapping $\omega : K \times K \to$ complex numbers can be considered as a factor system. There is the following proposition:

Proposition. A mapping ω from $K \times K$ to the complex numbers can occur as factor system for a projective representation if and only if one has

$$\omega(R_1, R_2)\omega(R_1R_2, R_3) = \omega(R_1, R_2R_3)\omega(R_2, R_3) \quad \forall\ R_1, R_2, R_3 \in K. \quad (1.2.2.49)$$

If one has two mappings ω_1 and ω_2 satisfying this relation, the product $\omega(R, R') = \omega_1(R, R')\omega_2(R, R')$ also satisfies the relation. Therefore, factor systems form an Abelian multiplicative group. A subgroup is formed by all factor systems that are associated with the trivial one:

$$\omega(R, R') = \frac{u(R)u(R')}{u(RR')}$$

for some function u on the group. These form another Abelian group and the factor group consists of all essentially different factor systems. This factor group is called *Schur's multiplicator group*.

A projective representation is called *reducible* if there is a proper invariant subspace. It is fully reducible if there is a basis on which the representation matrices form the direct sum of two representations. This is exactly as for ordinary representations. Equivalence of projective representations is slightly more subtle. Two projective representations are called *associated* if their factor systems are associated. They are *weakly equivalent* if there is a complex function $u(R)$ on the group and a nonsingular linear transformation S such that

$$D_2(R) = u(R)SD_1(R)S^{-1} \quad \forall\, R \in K. \tag{1.2.2.50}$$

This implies that their factor systems are associated. Two projective representations are *strongly equivalent* if their factor systems are identical and there exists a nonsingular linear transformation S such that $D_2(R)S = SD_1(R)$. Therefore, strong equivalence implies weak equivalence, which in turn implies association. The reason for this distinction will soon become clear.

For projective representations with identical factor systems there exist *orthogonality relations* for matrix elements and for characters. It is important to notice that for projective representations the character is generally not a class function, because one can multiply every operator with a separate constant.

Proposition. For given factor system ω there is a finite number r of strong equivalence classes of irreducible projective representations. The dimensions of the nonequivalent irreducible representations satisfy

$$\sum_{\alpha=1}^{r} d_\alpha^2 = N. \tag{1.2.2.51}$$

Proposition. For two irreducible projective matrix representations with the same factor system, the following holds:

$$\sum_{R\in K} \Gamma_\alpha(R)_{ij}\Gamma_\beta^{-1}(R)_{kl} = (N/d_\alpha)\delta'_{\alpha\beta}\delta_{il}\delta_{jk}. \tag{1.2.2.52}$$

Notice that, in general, for projective representations $\Gamma(R^{-1}) \neq \Gamma(R)^{-1}$! Every projective representation of a finite group is strongly equivalent with a unitary representation, for which one has

$$\sum_{R\in K} \Gamma_\alpha(R)_{ij}\Gamma_\beta(R)_{ik}^{*} = (N/d_\alpha)\delta'_{\alpha\beta}\delta_{il}\delta_{jk}, \tag{1.2.2.53}$$

and for the characters

$$\sum_{R\in K} \chi_\alpha(R)\chi_\beta^{*}(R) = N\delta_{\alpha\beta}. \tag{1.2.2.54}$$

For projective representations with the same factor system, one can construct the sum representation, which still has the same factor system: $(\Gamma_1 \oplus \Gamma_2)(R) = \Gamma_1(R) \oplus \Gamma_2(R)$. On the other hand, a reducible projective representation can be decomposed into irreducible components with the same factor system and multiplicities

$$m_\alpha = (1/N)\sum_{R\in K} \chi(R)\chi_\alpha^{*}(R), \tag{1.2.2.55}$$

as follows directly from the orthogonality conditions.

Projective representations of a group K may be constructed from the ordinary representations of a larger group R. Suppose that R has a subgroup A in the centre, which means that all its elements commute with all elements of R. Suppose furthermore that the factor group R/A is isomorphic with K. Therefore, the order of R is the product of the orders of A and K. Because K is the factor group, each element of R corresponds to a unique element of K and the elements of the subgroup A correspond to the unit element in K. Then consider an irreducible representation D of R. For two elements r_1 and r_2 of R there are elements k_1 and k_2 in K. Define linear operators $P(k_i) = D(r_i)$. Then k_1k_2 corresponds to r_1r_2 up to an element $a \in A$. This means

$$P(k_1)P(k_2) = D(a)P(k_1k_2).$$

Because a commutes with all elements of R, the operator $D(a)$ commutes with all the operators of the irreducible representation $D(R)$. From Schur's lemma it follows that it is a multiple of the unit operator. Moreover, this multiple depends on k_1 and k_2: $D(a) = \omega(k_1, k_2)E$. Therefore, an irreducible representation of R gives a projective representation of K. It has been shown by Schur that one obtains all projective representations of K, *i.e.* one representative from each strong equivalence class for each class of non-associated factor systems, in the way presented if one takes for the group A the multiplicator group. The way to find all projective representations of K is then: determine the multiplicator group, determine R, determine the ordinary irreducible representations of R. We shall not go into detail, but only present a way to characterize projective representations (Janssen, 1973).

First we consider an example, the group $K = 2mm$, isomorphic to D_2. It can be shown that the multiplicator group is the group of two elements. Therefore, the representation group R has eight elements and one can show that it is isomorphic to D_4 or to the quaternion group (in general there is not a unique R). The character table of D_4 is given in Table 1.2.2.2.

The centre is generated by A^2. If the elements of the factor group are e, a, b and ab, then E and A^2 correspond to e, A and A^3 to a, B and A^2B to b, and AB and A^3B to ab. Because A^2 is represented by the unit element for the four one-dimensional representations, each element of the factor group corresponds to a unique element of the representation. $P(a)$ can be chosen to be $D(A)$ or $D(A^3)$, but because $D(A^2) = E$ for the one-dimensional representations these are equal. Therefore, the one-dimensional representations of $K = D_2$ have a trivial factor system. For the two-dimensional representation one may choose

$$P(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad P(a) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$
$$P(b) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad P(ab) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

It is easily checked that this forms a projective representation with a nontrivial factor system. One can characterize the projective representation starting from the defining relations $a^2 = b^2 = (ab)^2 = e$. One has $P(a)^2 = -E$, $P(b)^2 = E$, $(P(a)P(b))^2 = E$. It is easily seen that one cannot achieve a trivial factor system by multiplication of the P matrices by suitably chosen factors. Therefore, the factor system is not associated with the trivial one either. This is the general situation. The ordinary representations of R can be partitioned into groups, each group corresponding with one class of associated factor systems, and within each group one finds representatives of each strong equivalence class. For the example above, there is only one such class for the nontrivial factor system as one sees from $d^2 = 4 = N = |D_2|$.

The general procedure then is to characterize a factor system with expressions stemming from defining relations for the group K. Defining relations are expressions (words) in the generators that fix the isomorphism class of the group. They are of the form

Table 1.2.2.2. *Character table of D_4*

	E	A, A^3	A^2	B, A^2B	AB, A^3B
Γ_1	1	1	1	1	1
Γ_2	1	−1	1	1	−1
Γ_3	1	1	1	−1	−1
Γ_4	1	−1	1	−1	1
Γ_5	2	0	−2	0	0

$$W_i(A_1, A_2, \ldots, A_p) = E, \quad i = 1, 2, \ldots, s \qquad (1.2.2.56)$$

if the A_i are the generators. For a projective representation the corresponding product

$$W_i(D(A_1), D(A_2), \ldots, D(A_p)) = \lambda_i E$$

is a multiple of the identity operator. The defining relations are not unique for a group. Therefore, there is arbitrariness here. The complex numbers λ_i that correspond to the defining relations may be changed by multiplying the operators $D(R)$ by factors $u(R)$. This changes the factor system to an associated one. If in a table the factor systems are given by the numbers λ_i, one can identify the class of a given factor system by calculating the corresponding words and solving the problem of finding the table values by taking into account additional factors $u(R)$. For example, the factor system that gives the values of λ_i for D_2 above is associated with one that gives $\lambda_{1,2,3} = 1, 1, -1$, if one multiplies $P(a)$ by i.

1.2.2.9. *Double groups and their representations*

Three-dimensional rotation point groups are subgroups of $SO(3)$. In quantum mechanics, rotations act according to some representation of $SO(3)$. Because wave functions can be multiplied by an arbitrary phase factor, in principle projective representations play a role here. The projective representations of $SO(3)$ can be obtained from the ordinary representations of the representation group, which is $SU(2)$, the group of all 2×2 matrices

$$\begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} \quad \text{with } |a|^2 + |b|^2 = 1.$$

For example, in spin space for a particle with spin $\frac{1}{2}$, a rotation over φ along the z axis acts according to

$$\begin{pmatrix} \exp(i\varphi/2) & 0 \\ 0 & \exp(-i\varphi/2) \end{pmatrix},$$

and in general the representation for a rotation over φ along an axis $\hat{n}$ is

$$\cos(\varphi/2)E + i\sin(\varphi/2)(\boldsymbol{\sigma} \cdot \hat{n}),$$

where $\boldsymbol{\sigma}$ is a vector with the three Pauli spin matrices as components. Because the matrices for $\varphi = 2\pi$ become $-E$, the representation has a nontrivial factor system. As a representation of $SU(2)$, however, it is an ordinary representation.

To each rotation ($R \in SO(3)$) correspond two elements $\pm U(R) \in SU(2)$. To a point group $K \subset SO(3)$ corresponds a subset of $SU(2)$ which is in fact a subgroup, because $U(R)U(R') = \pm U(RR')$. This group is the *double group* K^d. It contains both E and $-E$, which are both mapped to the unit element of $SO(3)$ under the homomorphism $SU(2) \to SO(3)$. Because $\pm E$ commute with all elements of K^d, this group C_2 is an invariant subgroup and the factor group K^d/C_2 is isomorphic to K. Therefore, every representation of K is a representation of K^d, but in general there are other representations as well, the *extra representations*. Notice that the double group of K does not only depend on the isomorphism class of K, but also on the geometric class, because the realization as subgroup of $O(3)$ comes in.

As an example, we take the group $222 \subset SO(3)$. The two generators 2_x and 2_y correspond, respectively, to the matrices

$$\pm\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \pm\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

These matrices generate a group of order eight, which can also be presented by

$$A = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad A^4 = B^2 = (AB)^2 = E.$$

This group is isomorphic with D_4, a group with five irreducible representations: four one-dimensional and one two-dimensional. The former are the four ordinary representations of D_2 because both E and $-E$ are represented by the unit matrix. The two-dimensional representation has $\Gamma(-E) = -\Gamma(E)$ and is, therefore, not an ordinary representation for 222. It is an extra representation for the double group 222^d, or a projective representation of 222. Choosing one element from $SU(2)$ for each generator of 222 one obtains

$$\Gamma(2_x) = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \Gamma(2_y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\Gamma(2_x)^2 = \Gamma(2_y)^2 = E, \quad (\Gamma(2_x)\Gamma(2_y))^2 = -E.$$

The factor system fixed in this way is not associated to a trivial one (otherwise the irreducible representation could not be two-dimensional). The extra representation of the double group corresponds to a nontrivial projective representation of the point group itself.

To construct the character table of the double group, it is worthwhile to note that the elements of K^d mapped on one class of K form two classes, except when the class in K consists of 180° rotations and there exists for one element of this class another 180° rotation in K with its axis perpendicular to that of the former element. The example above illustrates this: there are four classes in $K = 222$ and five classes in K^d. The identity in K corresponds to $\pm E$ in K^d, and these form two classes. The other pairs $\pm A$, $\pm B$ and $\pm AB$ are mapped each on one class. This is, however, not the most general case. $\pm u(R)$ only belong to the same class if there is an element $S \in K$ such that $u(R)u(S) = -u(S)u(R)$. If one brings $u(R)$ into diagonal form, one sees that this is only possible if the diagonal elements are $\pm i$, *i.e.* when the rotation angle of R is π. In this case one has

$$u(S)\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = -\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}u(S),$$

then

$$u(S) = \begin{pmatrix} 0 & \exp(i\varphi) \\ -\exp(-i\varphi) & 0 \end{pmatrix},$$

which is a twofold rotation with axis perpendicular to the z axis. Therefore, in general, if a class in K of 180° rotations does not exist or if there is not a perpendicular 180° rotation, the class in K corresponds to two classes in K^d.

As a second example, we consider the group $K = 32$ of order six. It is generated by a threefold rotation along the z axis and a twofold rotation perpendicular to the first one. Corresponding elements of $SU(2)$ are

$$A = \begin{pmatrix} \frac{1}{2} + \frac{1}{2}i\sqrt{3} & 0 \\ 0 & \frac{1}{2} - \frac{1}{2}i\sqrt{3} \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

The group K^d generated by these elements is of order 12 with six classes: E, $-E$, (A, A^5), (A^2, A^4), (B, A^2B, A^4B) and (AB, A^3B, A^5B), which are mapped on the three classes of $K = 32$. Therefore, there are six irreducible representations for K^d: four one-dimensional ones and two two-dimensional ones. Two one-dimensional and one two-dimensional representations are the ordinary representations of K, the other ones are extra representations and have $\Gamma(-E) = -\Gamma(E)$. As projective representations of $K = 32$, they are associated with ordinary representations: for the one-dimensional ones this is obvious; for the two-dimensional one, generated by A and B, one can find an associated one $\Gamma(A) = -A$, $\Gamma(B) = iB$ such that

$$\Gamma(A)^3 = \Gamma(B)^2 = (\Gamma(A)\Gamma(B))^2 = E$$

and, consequently, this representation has a trivial factor system. This shows that, although 32^d has three extra representations, there are no nontrivial projective representations.

The characters for the double point groups are given in Table 1.2.6.7.

1.2.3. Space groups

1.2.3.1. *Structure of space groups*

The Euclidean group $E(n)$ in n dimensions is the group of all distance-preserving inhomogeneous linear transformations. In Euclidean space, an element is denoted by

$$g = \{R|\mathbf{a}\}$$

where $R \in O(n)$ and $\mathbf{a}$ is an n-dimensional translation. On a point $\mathbf{r}$ in n-dimensional space, g acts according to

$$\{R|\mathbf{a}\}\mathbf{r} = R\mathbf{r} + \mathbf{a}. \qquad (1.2.3.1)$$

Therefore, $|g\mathbf{r}_1 - g\mathbf{r}_2| = |\mathbf{r}_1 - \mathbf{r}_2|$. The group multiplication law is given by

$$\{R|\mathbf{a}\}\{R'|\mathbf{a}'\} = \{RR'|\mathbf{a} + R\mathbf{a}'\}. \qquad (1.2.3.2)$$

The elements $\{E|\mathbf{a}\}$ form an Abelian subgroup, the group of n-dimensional translations $T(n)$.

An n-dimensional space group is a subgroup of $E(n)$ such that its intersection with $T(n)$ is generated by n linearly independent basis translations. This means that this *lattice translation subgroup* A is isomorphic to the group of n-tuples of integers: each translation in A can be written as

$$\{E|\mathbf{a}\} = \prod_{i=1}^{n} \{E|\mathbf{e}_i\}^{n_i} = \{E|\sum_{i=1}^{n} n_i\mathbf{e}_i\}. \qquad (1.2.3.3)$$

The lattice translation subgroup A is an invariant subgroup because

$$g\{E|\mathbf{a}\}g^{-1} = \{R|\mathbf{b}\}\{E|\mathbf{a}\}\{R|\mathbf{b}\}^{-1} = \{E|R\mathbf{a}\} \in A.$$

The factor group G/A, of the space group G and the lattice translation group A, is isomorphic to the group K formed by all elements R occurring in the elements $\{R|\mathbf{a}\} \in G$. This group is the *point group* of the space group G. It is a subgroup of $O(n)$.

The *unit cell* of the space group is a domain in n-dimensional space such that every point in space differs by a lattice translation from some point in the unit cell, and such that between any two points in the unit cell the difference is not a lattice translation. The unit cell is not unique. One choice is the n-dimensional parallelepiped spanned by the n basis vectors. The points in this unit cell have coordinates between 0 (inclusive) and 1. Another choice is not basis dependent: consider all points generated by the lattice translation group from an origin. This produces a lattice of points Λ. Consider now all points that are closer to the origin than to any other lattice point. This domain is a unit cell, if one takes care which part of the boundary belongs to it and which part not, and is called the *Wigner–Seitz cell*. In mathematics it is called the *Voronoi cell* or *Dirichlet domain* (or region).

Because the point group leaves the lattice of points invariant, it transforms the Wigner–Seitz cell into itself. This implies that points inside the unit cell may be related by a point-group element. Similarly, space-group elements may connect points inside the unit cell, up to lattice translations. A *fundamental region* or *asymmetric unit* is a part of the unit cell such that no points of the fundamental region are connected by a space-group element, and simultaneously that any point in space can be related to a point in the fundamental region by a space-group transformation.

Because $\{E|R\mathbf{a}\}$ belongs to the lattice translation group for every $R \in K$ and every lattice translation $\{E|\mathbf{a}\}$, the lattice Λ generated by the vectors $\mathbf{e}_i$ ($i = 1, 2, \ldots, n$) is invariant under the point group K. Therefore, the latter is a crystallographic point group. On a basis of the lattice Λ, the point group corresponds to a group $\Gamma(K)$ of integer matrices. One has the following situation. The space group G has an invariant subgroup A isomorphic to $\mathbb{Z}^n$, the factor group G/A is a crystallographic point group K which acts according to the integer representation $\Gamma(K)$ on A. In mathematical terms, G is an *extension* of K by A with homomorphism Γ from K to the group of automorphisms of A.

The vectors $\mathbf{a}$ occurring in the elements $\{E|\mathbf{a}\} \in G$ are called primitive translations. They have integer coefficients with respect to the basis $\mathbf{e}_1, \ldots, \mathbf{e}_n$. However, not all vectors $\mathbf{a}$ in the space-group elements are necessarily primitive. One can decompose the space group G according to

$$G = A + g_2A + g_3A + \ldots + g_NA. \qquad (1.2.3.4)$$

To every element $R \in K$ there is a coset g_iA with $g_i = \{R|\mathbf{a}(R)\}$ as representative. Such a representative is unique up to a lattice translation. Instead of $\mathbf{a}(R)$, one could as well have $\mathbf{a}(R) + \mathbf{n}$ as representative for any lattice translation $\mathbf{n}$. For a particular choice, the function $\mathbf{a}(R)$ from the point group to the group $T(n)$ is called the *system of nonprimitive translations* or *translation vector system*. It is a mapping from the point group K to $T(n)$, modulo A. Such a system of nonprimitive translations satisfies the relations

$$\mathbf{a}(R) + R\mathbf{a}(S) = \mathbf{a}(RS) \bmod A \quad \forall\ R, S \in K. \qquad (1.2.3.5)$$

This follows immediately from the product of two representatives g_i.

If the lattice translation subgroup A acts on a point $\mathbf{r}$, one obtains the set $\Lambda + \mathbf{r}$. One can describe the elements of G as well as combinations of an orthogonal transformation with $\mathbf{r}$ as centre and a translation. This can be seen from

$$\{R|\mathbf{a}\} = \{E|\mathbf{a} - \mathbf{r} + R\mathbf{r}\}\{R|\mathbf{r} - R\mathbf{r}\}, \qquad (1.2.3.6)$$

where now $\{R|\mathbf{r} - R\mathbf{r}\}$ leaves the point $\mathbf{r}$ invariant. The new system of nonprimitive translations is given by

$$\mathbf{a}'(R) = \mathbf{a}(R) + (R - E)\mathbf{r}. \qquad (1.2.3.7)$$

This is the effect of a *change of origin*. Therefore, for a space group, the systems of nonprimitive translations are only determined up to a primitive translation and up to a change of origin.

It is often convenient to describe a space group on another basis, the conventional lattice basis. This is the basis for a sublattice with the same, or higher, symmetry and with the same number of free parameters. Therefore, the sublattice is also invariant under K and with respect to the conventional basis, which is obtained from the original one *via* a basis transformation S, the point group has the form

$$\Gamma_{\text{conventional}}(R) = S\Gamma_{\text{primitive}}(R)S^{-1}, \qquad (1.2.3.8)$$

where S is the *centring matrix*. It is a matrix with determinant equal to the inverse of the number of lattice points of the primitive lattice inside the unit cell of the conventional lattice. As an example, consider the primitive and centred rectangular lattices in two dimensions. Both have symmetry $2mm$, and two parameters a and b. The transformation from a basis of the conventional lattice $[(2a, 0)$ and $(0, 2b)]$ to a basis of the primitive lattice $[(a, -b)$ and $(a, b)]$ is given by S, and the relations between the generators of the point groups are

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = S\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}S^{-1}, \quad S = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$
$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = S\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}S^{-1}.$$

1.2.3.2. *Irreducible representations of lattice translation groups*

The lattice translation group A is isomorphic to the group $\mathbb{Z}^n$ of n-tuples of integers. This is an infinite group and, therefore, the usual techniques for finite groups cannot be applied. A way past this is the following. If $\mathbf{a}_i$ are the basis vectors of the lattice Λ, the lattice translation group generated by the translations $\{E|N\mathbf{a}_i\}$ forms an Abelian subgroup A^N of A. The factor group A/A^N is a finite group isomorphic to the direct product of n cyclic groups of order N. Each representation of this group is a representation of A with the property that the elements of A^N are represented by the unit operator. This procedure is in fact that of periodic boundary conditions in solid-state physics. In the following, we shall consider only the representations of A that satisfy this condition.

The irreducible representations of the direct product of n cyclic groups of order N are all one-dimensional. According to Section 1.2.2.6 they can be characterized by n integers and read

$$\Gamma^{\{p_j\}}\left(\{E|\sum_{i=1}^{n} n_i\mathbf{e}_i\}\right) = \exp[2\pi i(n_1p_1 + n_2p_2 + \ldots + n_np_n)/N], \tag{1.2.3.9}$$

because a representation of the cyclic group C_N is determined by its value on the basis translations:

$$\Gamma^p(\{E|\mathbf{e}\}) = \exp(2\pi i p/N), \quad 0 \le p < N.$$

There are exactly N^n nonequivalent irreducible representations.

If $\mathbf{a}_i$ are basis vectors of the lattice Λ, its dual basis consists of vectors $\mathbf{b}_j$ defined by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}. \tag{1.2.3.10}$$

These vectors $\mathbf{b}_j$ span the *reciprocal lattice* Λ^*. The scalar product of an arbitrary lattice vector $\mathbf{a}$ and a reciprocal-lattice vectors $\mathbf{K}$ is then

$$\mathbf{K}\cdot\mathbf{a} = \left(\sum_{i=1}^{n} m_i\mathbf{b}_i\right)\cdot\left(\sum_{j=1}^{n} n_j\mathbf{a}_j\right) = 2\pi\sum_{i=1}^{n} n_im_i. \tag{1.2.3.11}$$

The expression (1.2.3.9) then can be written more concisely if one introduces an n-dimensional vector $\mathbf{k}$:

$$\mathbf{k} = (1/N)\sum_{i=1}^{n} p_i\mathbf{b}_i. \tag{1.2.3.12}$$

Then (1.2.3.9) simplifies to

$$\Gamma^{\{\mathbf{k}\}}(\{E|\mathbf{a}\}) = \exp(i\mathbf{k}\cdot\mathbf{a}). \tag{1.2.3.13}$$

Because $0 \le p_i/N < 1$, the vector $\mathbf{k}$ belongs to the unit cell of the reciprocal lattice. If one chooses that unit cell as the Voronoi cell for the reciprocal lattice, which in direct space would be the Wigner–Seitz cell, it is called the *Brillouin zone*. Therefore, representations of the lattice translation subgroup are characterized by a vector in the Brillouin zone. In fact, the vectors $\mathbf{k}$ form a mesh inside the Brillouin zone, but this mesh becomes finer if N increases. In the limit of N going to ∞, the wavevectors $\mathbf{k}$ fill the Brillouin zone.

Just like the direct lattice, the reciprocal lattice is invariant under the point group K. The Brillouin zone, or at least its interior, is invariant under K as well. A *fundamental domain* in the Brillouin zone is a part of the zone such that no two points of the fundamental region are related by a point-group transformation from K and that any point in the Brillouin zone can be obtained from a point in the fundamental region by a point-group transformation.

1.2.3.3. *Irreducible representations of space groups*

For representations of space groups, we use the same argumentation as for the lattice translation subgroup. Notice that the group A^N generated by the vectors $\{E|N\mathbf{e}_i\}$ is an invariant Abelian subgroup of the space group G as well.

$$\{R|\mathbf{a}\}\{E|N\mathbf{e}_i\}\{R^{-1}|-R^{-1}\mathbf{a}\} = \{E|NR\mathbf{e}_i\} \in A^N.$$

The factor group G/A^N is a finite group of order N^n times the order of the point group K. Representations of this factor group are representations of G with the property that all elements of A^N are mapped on the unit operator. We shall consider here only such space-group representations.

Suppose that $\Gamma(G)$ is an irreducible representation of the space group G. Its restriction $\Gamma(A)$ to the lattice translation subgroup is then reducible, unless it is one-dimensional. Each irreducible representation of A is characterized by a vector $\mathbf{k}$ in the Brillouin zone. Therefore,

$$\Gamma(\{E|\mathbf{a}\}) = \begin{pmatrix} \exp(i\mathbf{k}_1\cdot\mathbf{a}) & 0 & 0 & \ldots & 0 & 0 \\ 0 & \exp(i\mathbf{k}_2\cdot\mathbf{a}) & 0 & \ldots & 0 & 0 \\ 0 & 0 & \exp(i\mathbf{k}_3\cdot\mathbf{a}) & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & \ldots & 0 \\ 0 & 0 & 0 & \ldots & 0 & \exp(i\mathbf{k}_n\cdot\mathbf{a}) \end{pmatrix}. \tag{1.2.3.14}$$

Some of the vectors $\mathbf{k}_i$ may be identical. Therefore, the matrix representation can be written as

$$\Gamma(\{E|\mathbf{a}\}) = \begin{pmatrix} \exp(i\mathbf{k}_1\cdot\mathbf{a})E & 0 & 0 & \ldots & 0 & 0 \\ 0 & \exp(i\mathbf{k}_2\cdot\mathbf{a})E & 0 & \ldots & 0 & 0 \\ 0 & 0 & \exp(i\mathbf{k}_3\cdot\mathbf{a})E & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & \exp(i\mathbf{k}_s\cdot\mathbf{a})E \end{pmatrix}. \tag{1.2.3.15}$$

It can be shown that the dimensions of the unit matrices E are all the same (and equal to d). Then

$$n = s \cdot d.$$

With respect to the basis on which the translation is of this form, every basis vector in the pth block is multiplied by a factor $\exp(i\mathbf{k}_p\cdot\mathbf{a})$.

Suppose that $\{R|\mathbf{u}\}$ is an element of the space group G. Consider a basis vector v of the representation space that gets a factor $\exp(i\mathbf{k}\cdot\mathbf{a})$ under the translation $\{E|\mathbf{a}\}$. Then one has

$$\begin{aligned} D(\{E|\mathbf{a}\})v &= \exp(i\mathbf{k}\cdot\mathbf{a})v \\ D(\{E|\mathbf{a}\})D(\{R|\mathbf{u}\})v &= D(\{R|\mathbf{u}\})D(\{E|R^{-1}\mathbf{a}\})v \\ &= \exp(iR\mathbf{k}\cdot\mathbf{a})D(\{R|\mathbf{u}\})v, \end{aligned}$$

and because $D(\{R|\mathbf{u}\})v$ also belongs to the representation space there are vectors that transform with the vector $R\mathbf{k}$ as well as vectors that transform with $\mathbf{k}$. This means that for every vector $\mathbf{k}$ occurring in a block in (1.2.3.5), there is also a block for each vector $R\mathbf{k}$ as R runs over the point group K. The vectors $\{R\mathbf{k}|R \in K\}$ form *the star of* $\mathbf{k}$. Vectors $R\mathbf{k}$ that differ by a reciprocal-lattice vector ($\mathbf{k}' = \mathbf{k} + \mathbf{K}$ with $K \in \Lambda^*$) correspond to the same representation and are therefore considered to be the same. Generally, a vector $\mathbf{k}$ may be left invariant by a subgroup of the point group K. This point group $K_{\mathbf{k}}$ is the *point group of* $\mathbf{k}$.

$$K_{\mathbf{k}} \equiv \{R|R\mathbf{k} \equiv \mathbf{k} \bmod \Lambda^*\}. \quad (1.2.3.16)$$

Then there are s point-group elements R_i such that

$$K = K_{\mathbf{k}} \cup R_2K_{\mathbf{k}} \cup \ldots \cup R_sK_{\mathbf{k}} \quad (1.2.3.17)$$

and each element R_i corresponds to a vector in the star:

$$\mathbf{k}_i = R_i\mathbf{k}_1; \quad \mathbf{k}_1 = \mathbf{k}, \quad i = 1, 2, \ldots, s.$$

Therefore, the blocks in (1.2.3.15) for an irreducible representation of the space group G correspond to the s branches of the star of $\mathbf{k}$. They are all of the same dimension d. If the vectors $\mathbf{k}_i$ in (1.2.3.15) belonged to two or more different stars, the representation would be reducible.

To the point group of $\mathbf{k}$ corresponds a subgroup of the space group G that has $K_{\mathbf{k}}$ as point group. It is called *the group of* $\mathbf{k}$ and is defined by

$$G_{\mathbf{k}} \equiv \{g = \{R|\mathbf{a}\} \in G|R \in K_{\mathbf{k}}\}. \quad (1.2.3.18)$$

Analogously to (1.2.3.17), one can write

$$G = G_{\mathbf{k}} \cup g_2G_{\mathbf{k}} \cup \ldots \cup g_sG_{\mathbf{k}} \quad (1.2.3.19)$$

for elements $g_i = \{R_i|\mathbf{a}_i\}$ of the space group G.

As one sees from (1.2.3.15), there is a subspace of vectors v that get a factor $\exp(i\mathbf{k} \cdot \mathbf{a})$ for any lattice translation $\mathbf{a}$. If one considers the action of $D(g)$ with $g \in G_{\mathbf{k}}$, it follows immediately that a vector from this space is transformed into a vector of the same space: the subspace corresponding to a vector $\mathbf{k}$ is invariant under $G_{\mathbf{k}}$. Therefore this space $V_{\mathbf{k}}$ carries a representation of $G_{\mathbf{k}}$. It can be seen as follows that one may construct the irreducible representation of the whole group G as soon as one knows the representation $D_{\mathbf{k}}$ of $G_{\mathbf{k}}$ in $V_{\mathbf{k}}$. To that end, consider a basis $\mathbf{e}_1, \ldots, \mathbf{e}_d$ in $V_{\mathbf{k}}$. The vectors

$$\boldsymbol{\psi}_{i\mu} = D(g_i)\mathbf{e}_\mu \quad (i = 1, 2, \ldots, s;\ \mu = 1, 2, \ldots, d), \quad (1.2.3.20)$$

form a basis of the whole representation space. Under a lattice-translation vector $\mathbf{a}$, the vector $\boldsymbol{\psi}_{i\mu}$ gets a factor $\exp(i\mathbf{k}_i \cdot \mathbf{a})$. On this basis, one can determine the matrix representation $\Gamma(G)$. Take an element $\{R|\mathbf{u}\} \in G$. It belongs to a certain coset $g_mG_{\mathbf{k}}$ in the decomposition of G. In addition, the element $\{R|\mathbf{u}\}g_i$ belongs to a well defined $g_jG_{\mathbf{k}}$. This means that there is an element $\{S|\mathbf{v}\}$ in the group $G_{\mathbf{k}}$ such that

$$\{R|\mathbf{u}\}g_i = g_j\{S|\mathbf{v}\} \quad (i = 1, 2, \ldots, s;\ \{S|\mathbf{v}\} \in G_{\mathbf{k}}).$$

Then one can write

$$\begin{aligned} D(\{R|\mathbf{u}\})\psi_{i\mu} &= D(\{R|\mathbf{u}\})D(g_i)\mathbf{e}_\mu \\ &= D(g_j)D(\{S|\mathbf{v}\})\mathbf{e}_\mu \\ &= D(g_j)\sum_{\nu=1}^{d}\Gamma_{\mathbf{k}}(\{S|\mathbf{v}\})_{\nu\mu}\mathbf{e}_\mu \\ &= \sum_{\nu=1}^{d}\Gamma_{\mathbf{k}}(\{S|\mathbf{v}\})_{\nu\mu}\psi_{j\nu} \\ &= \sum_{j=1}^{s}\sum_{\nu=1}^{d}\Gamma(\{R|\mathbf{u}\})_{j\nu,i\mu}\psi_{j\nu}. \end{aligned}$$

This means that the representation matrix $\Gamma(\{R|\mathbf{u}\})$ can be decomposed into $s \times s$ blocks of dimension d. In each row of blocks there is exactly one that is not a block of zeros, and the same is true for each column of blocks. Moreover, the only nonzero block in the ith column and in the jth row is

$$D_{\mathbf{k}}(\{S|\mathbf{v}\}) = D_{\mathbf{k}}(g_j^{-1}\{R|\mathbf{u}\}g_i), \quad (1.2.3.21)$$

where i and j are uniquely related by

$$\{R|\mathbf{u}\}g_i \in g_jG_{\mathbf{k}}. \quad (1.2.3.22)$$

It can be shown that $\Gamma(G)$ is irreducible if and only if $D_{\mathbf{k}}(G_{\mathbf{k}})$ is irreducible. From the construction, it is obvious that one may obtain all irreducible representations of G in this way. Moreover, one obtains all representations of G if one takes for the construction all stars and for each star all irreducible representations of $G_{\mathbf{k}}$.

So the final step is to determine all nonequivalent irreducible representations of $G_{\mathbf{k}}$. Notice that the lattice translation subgroup is a subgroup of $G_{\mathbf{k}}$. Therefore,

$$D_{\mathbf{k}}(\{E|\mathbf{a}\}) = \exp(i\mathbf{k} \cdot \mathbf{a})E.$$

If one makes a choice for the system of nonprimitive translations $\mathbf{u}(R)$, every element $g = \{S|\mathbf{v}\} \in G_{\mathbf{k}}$ can be written uniquely as

$$g = \{E|\mathbf{a}\}\{S|\mathbf{u}(S)\},$$

for a lattice translation $\mathbf{a}$. Therefore, one has

$$D_{\mathbf{k}}(\{S|\mathbf{v}\}) = \exp(i\mathbf{k} \cdot \mathbf{a})D_{\mathbf{k}}(\{S|\mathbf{u}(S)\}) \equiv \exp\{i\mathbf{k} \cdot [\mathbf{a} + \mathbf{u}(S)]\}\Gamma(S) \quad (1.2.3.23)$$

if one defines

$$\Gamma(S) = \exp[-i\mathbf{k} \cdot \mathbf{u}(S)]D_{\mathbf{k}}(\{S|\mathbf{u}(S)\}). \quad (1.2.3.24)$$

It is important to notice that this definition of Γ does not depend on the choice of the system of nonprimitive translations. If one takes $\mathbf{u}'(S) = \mathbf{u}(S) + \mathbf{b}$ ($\mathbf{b} \in A$), the result for $\Gamma(S)$ is the same. The product of two matrices $\Gamma(S)$ and $\Gamma(S')$ then becomes

$$\begin{aligned} \Gamma(S)\Gamma(S') &= \exp\big\{-i\mathbf{k} \cdot [\mathbf{u}(S) + \mathbf{u}(S')]\big\}D_{\mathbf{k}}(\{SS'|\mathbf{u}(S) + S\mathbf{u}(S')\}) \\ &= \exp\big\{-i\mathbf{k} \cdot [\mathbf{u}(S') - S\mathbf{u}(S')]\big\}\Gamma(SS'). \end{aligned} \quad (1.2.3.25)$$

One sees that the matrices $\Gamma(R)$ form a projective representation of the point group of $\mathbf{k}$. The factor system is given by

$$\begin{aligned} \omega(S, S') &= \exp\{-i\mathbf{k} \cdot [\mathbf{u}(S') - S\mathbf{u}(S')]\} \\ &= \exp[-i(\mathbf{k} - S^{-1}) \cdot \mathbf{u}(S')]. \end{aligned} \quad (1.2.3.26)$$

Such a factor system may, however, be equivalent to a trivial one.

If the space group $G_{\mathbf{k}}$ is symmorphic, one may choose the system of nonprimitive translations to be zero. Consequently, in this case the factor system $\omega(S, S')$ is unity and the matrices $\Gamma(S)$ form an ordinary representation of the space group $G_{\mathbf{k}}$. This is also the case if $\mathbf{k}$ is not on the Brillouin-zone boundary. If $\mathbf{k}$ is inside the Brillouin zone and $S \in K_{\mathbf{k}}$, one has $S\mathbf{k} = \mathbf{k} + \mathbf{K}$ only for $\mathbf{K} = 0$. So inside the Brillouin zone one has $S\mathbf{k} = \mathbf{k}$ for all $S \in K_{\mathbf{k}}$. This implies that

$$\exp\{-i\mathbf{k} \cdot [\mathbf{u}(S') - S\mathbf{u}(S')]\} = \exp[-i(\mathbf{k} - S^{-1}\mathbf{k}) \cdot \mathbf{u}(S')] = 1.$$

A nontrivial factor system $\omega(S, S')$ can therefore only occur for a nonsymmorphic group $G_{\mathbf{k}}$ and for a $\mathbf{k}$ on the Brillouin-zone boundary. But even then, it is possible that one may redefine the matrices $\Gamma(S)$ with an appropriate phase factor such that they form an ordinary representation. This is, for example, always the case if $K_{\mathbf{k}}$ is cyclic, because cyclic groups do not have genuine projective representations. These are always associated with an ordinary representation.

If the factor system $\omega(S, S')$ is not associated with a trivial one, one has to find the irreducible projective representations with the given factor system. As seen in the previous section, one may do this by using the defining relation for the point group $K_{\mathbf{k}}$. If these are words $W_i(A_1, \ldots, A_r)$ in the generators $A_1, \ldots, A_r$, the corresponding expressions in the representation

$$W_i(D_{\mathbf{k}}(A_1), \ldots, D_{\mathbf{k}}(A_r)) = \lambda_iE$$

are multiples of the unit operator. The values of λ_i fix the class of the factor system completely. By multiplying the operators $D_{\mathbf{k}}(A_j)$ by proper phase factors, the values of λ_i can be trans-

Table 1.2.3.1. *Choices of* **k** *in the fundamental domain of Pmmm and the elements of* $K_{\mathbf{k}}$

k	Wyckoff position	$K_{\mathbf{k}}$	Elements							
000	*a*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}00$	*b*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$0\frac{1}{2}0$	*e*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$00\frac{1}{2}$	*c*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$0\frac{1}{2}\frac{1}{2}$	*g*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}0\frac{1}{2}$	*d*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}\frac{1}{2}0$	*f*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	*h*	*mmm*	*E*	m_x	m_y	m_z	$\bar{1}$	2_x	2_y	2_z
$\xi00$	*i*	2*mm*	*E*	m_y	m_z	2_x				
$\xi\frac{1}{2}0$	*k*	2*mm*	*E*	m_y	m_z	2_x				
$\xi0\frac{1}{2}$	*j*	2*mm*	*E*	m_y	m_z	2_x				
$\xi\frac{1}{2}\frac{1}{2}$	*l*	2*mm*	*E*	m_y	m_z	2_x				
$0\eta0$	*m*	*m*2*m*	*E*	m_x	m_z	2_y				
$\frac{1}{2}\eta0$	*o*	*m*2*m*	*E*	m_x	m_z	2_y				
$0\eta\frac{1}{2}$	*n*	*m*2*m*	*E*	m_x	m_z	2_y				
$\frac{1}{2}\eta\frac{1}{2}$	*p*	*m*2*m*	*E*	m_x	m_z	2_y				
00ζ	*q*	*mm*2	*E*	m_x	m_y	2_z				
$\frac{1}{2}0\zeta$	*s*	*mm*2	*E*	m_x	m_y	2_z				
$0\frac{1}{2}\zeta$	*r*	*mm*2	*E*	m_x	m_y	2_z				
$\frac{1}{2}\frac{1}{2}\zeta$	*t*	*mm*2	*E*	m_x	m_y	2_z				
$0\eta\zeta$	*u*	*m*11	*E*	m_x						
$\frac{1}{2}\eta\zeta$	*v*	*m*11	*E*	m_x						
$\xi0\zeta$	*w*	1*m*1	*E*	m_y						
$\xi\frac{1}{2}\zeta$	*x*	1*m*1	*E*	m_y						
$\xi\eta0$	*y*	11*m*	*E*	m_z						
$\xi\eta\frac{1}{2}$	*z*	11*m*	*E*	m_z						
$\xi\eta\zeta$	α	1	*E*							

formed into those tabulated. Then the tables give all irreducible representations for this factor system.

In summary, the procedure for finding all irreducible representations of a space group G is as follows.

(1) Consider all stars of **k** with respect to G. This means that one takes all vectors **k** in a *fundamental region* of the Brillouin zone.

(2) For each star, one determines the group $K_{\mathbf{k}}$.

(3) For each $K_{\mathbf{k}}$, one determines the factor system $\omega(S, S')$.

(4) For this factor system, one looks for all nonequivalent irreducible (projective) representations.

(5) From the representations $D_{\mathbf{k}}(K_{\mathbf{k}})$, one determines the representations $\Gamma_{\mathbf{k}}(G_{\mathbf{k}})$ and $\Gamma(G)$ according to the procedure given above.

1.2.3.4. *Characterization of space-group representations*

The irreducible representations of space groups are characterized by a star of vectors in the Brillouin zone, and by the irreducible, possibly projective, representations of the point group of one point from that star.

The stars are sets of vectors in the Brillouin zone related mutually by transformations from the point group K of the space group G modulo reciprocal-lattice vectors. To obtain all stars, it is sufficient to take all vectors in the fundamental domain of the Brillouin zone, *i.e.* a part of the Brillouin zone such that no vectors in the domain are related by point-group elements (modulo Λ^*) and such that every point in the Brillouin zone is related to a vector in the fundamental domain by a point-group operation.

From each star one takes one point **k** and determines the nonequivalent irreducible representations of the point group $K_{\mathbf{k}}$, the ordinary representations if the group $G_{\mathbf{k}}$ is symmorphic or **k** is inside the Brillouin zone, or the projective representations with factor system ω [equation (1.2.3.26)] otherwise. These representations are labelled μ. There are several conventions for the choice of this label, but an irreducible representation of G is always characterized by a pair $(\mathbf{k}, \mu)$, where **k** fixes the star and μ the irreducible point-group representation.

The projective representations of the group of **k**, *i.e.* of $K_{\mathbf{k}}$, can be obtained from the ordinary representations of a larger group. If the factor system $\omega(R, R')$ is of order m [$\omega^m(R, R') = 1$ for all R, R'], the order of this larger group $\hat{K}_{\mathbf{k}\omega}$ is m times the order of $K_{\mathbf{k}}$. Then the irreducible representations of the space group are labelled by the vector **k** in the Brillouin zone and an irreducible ordinary representation of $\hat{K}_{\mathbf{k}\omega}$, where ω follows from (1.2.3.26).

Two stars such that one branch of the first one has the same $K_{\mathbf{k}}$ as one branch of the other determine representations that are quite similar. The only difference is the numerical value of the factors $\exp(i\mathbf{k}\cdot\mathbf{a})$, the form of the representation matrices being the same. Such irreducible representations of the space group are said to belong to the same *stratum*. Strata are denoted by a symbol for one vector **k** in the Brillouin zone. For example, the origin, conventionally denoted by Γ, belongs to one stratum that corresponds to the ordinary representations of the point group K. For a simple cubic space group, the point $[\frac{1}{2}, 0, 0]$ is denoted by X. Its $K_{\mathbf{k}}$ is the tetragonal group $4/mmm$. All points $[\xi, 0, 0]$ with $\xi \neq 0$ and $-\frac{1}{2} < \xi < \frac{1}{2}$ form one stratum with point group $4mm$. This stratum is denoted by Δ *etc.* The strata can be compared with the Wyckoff positions in direct space. There a Wyckoff position is a manifold in the unit cell for which all points have the same site symmetry, modulo the lattice translations. Here it is a manifold of k vectors with the same symmetry group modulo the reciprocal lattice. The action of $G_{\mathbf{k}}$ does not involve the nonprimitive translations. Therefore, the strata correspond to Wyckoff positions of the corresponding symmorphic space group. The stratum symbols for the various three-dimensional Bravais classes are given in Table 1.2.6.11.

As an example, we consider here the orthorhombic space group *Pnma*. The orthorhombic Brillouin zone has a fundamental domain with volume that is one-eighth of that of the Brillouin zone. The various choices of **k** in this fundamental domain, together with the corresponding point groups $K_{\mathbf{k}}$, are given in Table 1.2.3.1. The vectors **k** correspond to Wyckoff positions of the group *Pmmm*.

In the tables, the vectors **k** and their corresponding Wyckoff positions are given for the holohedral space groups. In general, the number of different strata is smaller for the other groups. One can still use the same symbols for these groups, or take the symbols for the Wyckoff positions for the groups that are not holohedral. Consider as an example the group *Pmm*2. Its holohedral space group is *Pmmm*. The strata of irreducible representations can be labelled by the symbols for Wyckoff positions of *Pmm*2 as well as those of *Pmmm*. This is shown in Table 1.2.3.2.

Table 1.2.3.2. *Strata of irreducible representations of Pmm*2 *and Pmmm*

k	Wyckoff position in *Pmm*2	Wyckoff positions in *Pmmm*	$K_{\mathbf{k}}$
00ζ	*a*	*a*, *c*, *q*	*mm*2
$0\frac{1}{2}\zeta$	*b*	*e*, *g*, *r*	*mm*2
$\frac{1}{2}0\zeta$	*c*	*b*, *d*, *s*	*mm*2
$\frac{1}{2}\frac{1}{2}\zeta$	*d*	*f*, *h*, *t*	*mm*2
$\xi0\zeta$	*e*	*i*, *j*, *w*	1*m*1
$\xi\frac{1}{2}\zeta$	*f*	*k*, *l*, *x*	1*m*1
$0\eta\zeta$	*g*	*m*, *n*, *u*	*m*11
$\frac{1}{2}\eta\zeta$	*h*	*o*, *p*, *v*	*m*11
$\xi\eta\zeta$	*i*	*y*, *z*, α	1

The defining relations for the point group *mmm* are

$$A^2 = B^2 = (AB)^2 = C^2 = E, \quad AC = CA, \quad BC = CB.$$

Table 1.2.3.3. *Characteristic values of λ_i for the projective irreps of $K_{\mathbf{k}}$ for the point group mmm*

k	A^2 λ_1	B^2 λ_2	$(AB)^2$ λ_3	C^2 λ_4	$AC = CA$ λ_5	$BC = CB$ λ_6	Representations Number	Dimension
000	1	1	1	1	1	1	8	1
$\frac{1}{2}00$	−1	1	−1	1	−1	1	2	2
$0\frac{1}{2}0$	1	−1	1	1	1	1	2	2
$00\frac{1}{2}$	1	1	1	−1	−1	1	2	2
$0\frac{1}{2}\frac{1}{2}$	1	−1	1	−1	−1	1	2	2
$\frac{1}{2}0\frac{1}{2}$	−1	1	−1	−1	1	1	8	1
$\frac{1}{2}\frac{1}{2}0$	−1	−1	−1	1	−1	1	2	2
$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	−1	−1	−1	−1	1	1	2	2
$\xi00$	1	1	1				4	1
$\xi\frac{1}{2}0$	−1	1	−1				4	1
$\xi0\frac{1}{2}$	1	−1	−1				4	1
$\xi\frac{1}{2}\frac{1}{2}$	−1	−1	1				4	1
$0\eta0$	1	1	1				4	1
$\frac{1}{2}\eta0$	−1	1	1				1	2
$0\eta\frac{1}{2}$	1	−1	1				1	2
$\frac{1}{2}\eta\frac{1}{2}$	−1	−1	1				4	1
00ζ	1	1	1				4	1
$\frac{1}{2}0\zeta$	−1	1	−1				1	2
$0\frac{1}{2}\zeta$	1	−1	1				1	2
$\frac{1}{2}\frac{1}{2}\zeta$	−1	−1	−1				1	2
$0\eta\zeta$	1						2	1
$\frac{1}{2}\eta\zeta$	−1						2	1
$\xi0\zeta$	1						2	1
$\xi\frac{1}{2}\zeta$	−1						2	1
$\xi\eta0$	1						2	1
$\xi\eta\frac{1}{2}$	−1						2	1
$\xi\eta\zeta$							1	1

For the subgroups, the defining relations follow from these. The corresponding expressions in the representation matrices $\Gamma(A_i)$ for the generators of the point groups give expressions

$$W_i^{\rm left}(A_1,\ldots,A_r) = \lambda_i W_i^{\rm right}(A_1,\ldots,A_r), \quad i = 1,\ldots.$$

In the example one has

$$\begin{array}{ll}\Gamma(A)^2 = \lambda_1 E & \Gamma(B)^2 = \lambda_2 E \\ (\Gamma(A)\Gamma(B))^2 = \lambda_3 E & \Gamma(C)^2 = \lambda_4 E \\ \Gamma(A)\Gamma(C) = \lambda_5 \Gamma(C)\Gamma(A) & \Gamma(B)\Gamma(C) = \lambda_6\Gamma(C)\Gamma(B).\end{array}$$

The values for λ_i characterize the projective representation factor system and are given in Table 1.2.3.3. They are unity for ordinary representations.

By putting factors i in front of the representation matrices in the appropriate places, some of the values of λ_i can be changed from −1 to +1. In this way, one obtains either ordinary representations, which are necessarily one-dimensional for these Abelian groups, or projective representations, which are in this case two-dimensional. This is indicated as well in Table 1.2.3.3. The one-dimensional irreducible representations are ordinary representations of the group $K_{\mathbf{k}}$. The two-dimensional ones are projective representations, but correspond to ordinary representations of the larger groups isomorphic to $D_4 \times C_2$ and D_4.

1.2.3.5. *Double space groups and their representations*

In Section 1.2.2.9, it was mentioned that the transformation properties of spin-$\frac{1}{2}$ particles under rotations are not given by the orthogonal group $O(3)$, but by the covering group $SU(2)$. Hence, the transformation of a spinor field under a Euclidean transformation g is given by

$$g\Psi(\mathbf{r}) = \pm U(R)\Psi(R^{-1}(\mathbf{r}-\mathbf{a})) \quad \forall\ g = \{R|\mathbf{a}\} \in E(3), \quad (1.2.3.27)$$

where the $SU(2)$ operator $U(R)$ is given by

$$U(R) = E\cos(\varphi/2) + (\boldsymbol{\sigma}\cdot\mathbf{n})\sin(\varphi/2) \quad (1.2.3.28)$$

when the rotation R has angle φ and axis $\mathbf{n}$. When R does not belong to $SO(3)$ one has to take $U(-R)$.

For an ordinary space group, one can construct the double space group by

$$\{R|\mathbf{a}\} \rightarrow \{\pm U(R)|\mathbf{a}\} \quad (1.2.3.29)$$

with multiplication rule

$$\{U(R)|\mathbf{a}\}\{U(S)|\mathbf{b}\} = \{U(R)U(S)|\mathbf{a} + R\mathbf{b}\}. \quad (1.2.3.30)$$

An invariant subgroup of the double space group is the translation group A. The factor group is the double point group K^d of the point group K.

The representations of the double space groups can be constructed in the same way as those of ordinary space groups. They are characterized by a vector $\mathbf{k}$ in the Brillouin zone and a label for an irreducible, generally projective, representation of the (double) point group $K^d_{\mathbf{k}}$ of $\mathbf{k}$, which is the double group of $K_{\mathbf{k}}$. Again, for nonsymmorphic space groups or wavevectors $\mathbf{k}$ inside the Brillouin zone, the relevant irreducible representations of $K^d_{\mathbf{k}}$ are ordinary representations with a trivial factor system.

For an element g of the space group G, there are two elements of the double space group G^d. If one considers an irreducible representation $D(G^d)$ for the double space group and takes for each $g \in G$ one of the two corresponding elements in G^d, the resulting set of linear operators forms a projective representation of the space group. It is also characterized by a vector $\mathbf{k}$ in the Brillouin zone and a projective representation of the point group (not its double) $K_{\mathbf{k}}$. This projective representation does not have the same factor system as discussed in Section 1.2.3.3, because the factor system now stems partly from the nonprimitive translations and partly from the fact that a double point group gives a projective representation of the ordinary point group $K_{\mathbf{k}}$.

The projective representations of a space group corresponding to ordinary representations of the double space group again are characterized by the star of a vector $\mathbf{k}$. The projective representation of the group $G_{\mathbf{k}}$ then is given by

$$P_{\mathbf{k}}(\{R|\mathbf{a}\}) = \exp(i\mathbf{k}\cdot\mathbf{a})\Gamma(R), \quad (1.2.3.31)$$

where the projective representation $\Gamma(K_{\mathbf{k}})$ has the factor system

$$\begin{aligned}\Gamma(R)\Gamma(S) &= \omega_s(R,S)\exp[-i(\mathbf{k} - R^{-1}\mathbf{k})\cdot\mathbf{a}(S)]\Gamma(RS)\\ &= \omega(R,S)\Gamma(RS),\end{aligned} \quad (1.2.3.32)$$

where ω_s is the spin factor system for $K_{\mathbf{k}}$ and $\mathbf{a}(S)$ is the nonprimitive translation of the space-group element with orthogonal part S. The factor system ω can be characterized by the defining relations of $K_{\mathbf{k}}$. If these are the words

$$W_i(A_1,\ldots,A_p) = E,$$

then the factor system ω is characterized by the factors λ_i in

$$W_i(\Gamma(A_1),\ldots,\Gamma(A_p)) = \lambda_i E. \quad (1.2.3.33)$$

The factors λ_i are the product of the values found from the spin factor system ω_s and those corresponding to the factor system for an ordinary representation [equation (1.2.3.26)].

1.2.4. Tensors

1.2.4.1. *Transformation properties of tensors*

A vector is an element of an N-dimensional vector space that transforms under an orthogonal transformation, an element of $O(n)$, as

$$x = \sum_{i=1}^{n} \xi_i \mathbf{a}_i \to x' = \sum_{i=1}^{n} \xi'_i \mathbf{a}_i = \sum_{ij} R_{ij} \xi_j \mathbf{a}_i, \quad \{R_{ij}\} \in O(n).$$

A tensor of rank r under $O(n)$ is an object with components $T_{i_1 \ldots i_r}$ ($i_j = 1, 2, \ldots, n$) that transforms as (see Section 1.1.3.2)

$$T_{i_1 \ldots i_r} \to T'_{i_1 \ldots i_r} = \sum_{j_1=1}^{n} \ldots \sum_{j_r=1}^{n} R_{i_1 j_1} \ldots R_{i_r j_r} T_{j_1 \ldots j_r}.$$

A rank-zero tensor is a scalar, which is invariant under $O(n)$. A pseudovector (or axial vector) has components x_i and transforms according to

$$x_i \to x'_i = \mathrm{Det}(R) \sum_j R_{ij} \xi_j$$

and analogously for pseudotensors (or axial tensors – see Section 1.1.4.5.3).

A vector field is a vector-valued function in n-dimensional space. Under an orthogonal transformation it transforms according to

$$F_i(\mathbf{r})' = \sum_{j=1}^{n} R_{ij} F_j(R^{-1}\mathbf{r}). \qquad (1.2.4.1)$$

Under a Euclidean transformation, the function transforms according to

$$F_i(\mathbf{r})' = \sum_{j=1}^{n} R_{ij} F_j(R^{-1}(\mathbf{r} - \mathbf{a})), \quad \{R|\mathbf{a}\} \in E(n). \qquad (1.2.4.2)$$

In a similar way, one has (pseudo)tensor functions under the orthogonal group or the Euclidean group. So it is important to specify under what group an object is a tensor, unless no confusion is possible.

The n-dimensional vectors form a vector space that carries a representation of the group $O(n)$. Moreover, it is an irreducible representation space. To stress this fact, one could speak of *irreducible tensors and vectors*. Vectors are here just rank-one tensors. The three-dimensional Euclidean vector space carries in this way an irreducible representation of $O(3)$. Such representations are characterized by an integer l and are $(2l+1)$-dimensional. The usual three-dimensional space is therefore an irreducible $l = 1$ space for $O(3)$.

Since point groups are subgroups of the orthogonal group and space groups are subgroups of the Euclidean group, tensors inherit their transformation properties from their supergroups. As we have seen in Sections 1.2.2.3 and 1.2.2.7, one can also define tensors in a quite abstract way. Irreducible tensors under a group are then elements of a vector space that carries an irreducible representation of that group. Generally, tensors are elements of a vector space that carries a tensor product representation and (anti)symmetric tensors belong to a space with an (anti)symmetrized tensor product representation.

Because the point groups one usually considers in physics are subgroups of $O(2)$ or $O(3)$, it is useful to consider the irreducible representations of these groups. The groups $O(2)$ and $O(3)$ are not finite, but they are compact, and for compact groups most of the theorems for finite groups are still valid if one replaces sums over group elements by integration over the group.

The group $O(3)$ is the direct product $SO(3) \times C_2$. Therefore, there are even and odd representations. They have the property

$$D^{\pm}(R) = \Delta(R), \quad D^{\pm}(-R) = \pm\Delta(R), \quad R \in SO(3).$$

The irreducible representations are labelled by non-negative integers ℓ and have character

$$\chi_\ell(R) = \frac{\sin(\ell + \frac{1}{2})\varphi}{\sin \frac{1}{2}\varphi} \qquad (1.2.4.3)$$

if R is a rotation with rotation angle φ. From the character it follows that the dimension of the representation D_ℓ is equal to $(2\ell + 1)$.

The tensor product of two irreducible representations of $SO(3)$ is generally reducible:

$$D_\ell \otimes D_m = \bigoplus_{j=|\ell-m|}^{\ell+m} D_j \qquad (1.2.4.4)$$

and the symmetrized and antisymmetrized tensor products are

$$(D_m \otimes D_m)_s = \bigoplus_{j=0}^{m} D_{2j}, \qquad (1.2.4.5)$$

$$(D_m \otimes D_m)_a = \bigoplus_{j=1}^{m} D_{2j-1}. \qquad (1.2.4.6)$$

If the components of the tensor $T_{i_1 \ldots i_r}$ are taken with respect to an orthonormal basis, the tensor is called a *Cartesian tensor*. The orthogonal transformation R then is represented by an orthogonal matrix R_{ij}. Cartesian tensors of higher rank than one are generally no longer irreducible for the group $O(n)$. For example, the rank-two tensors in three dimensions have nine components T_{ij}. Under $SO(3)$, they transform according to the tensor product of two $\ell = 1$ representations. Because

$$D_1 \otimes D_1 = D_0 \oplus D_1 \oplus D_2,$$

the space of rank 2 Cartesian tensors is the direct sum of three invariant subspaces. This corresponds to the fact that a general rank 2 tensor can be written as the sum of a diagonal tensor, an antisymmetric tensor and a symmetric tensor with trace zero. These three tensors are irreducible tensors, in this case also called *spherical tensors*, *i.e.* irreducible tensors for the orthogonal group.

An irreducible tensor with respect to the group $O(3)$ transforms, in general, according to some reducible representation of a point group $K \in O(3)$. If the group K is a symmetry of the physical system, the tensor should be invariant under K, *i.e.* it should transform according to the identity representation of K.

Consider, for example, a symmetric second-rank tensor under $O(3)$. This means that it belongs to the space that transforms according to the representation

$$D_0 \oplus D_2$$

[see (1.2.4.6)]. If the symmetry group of the system is the point group $K = 432$, the representation

$$D_0(K) \oplus D_2(K)$$

has character

R:	ε	$\beta = C_3$	$\alpha^2 = C_{4z}^2$	$\alpha = C_{4z}$	$\alpha\beta = C_2$
$\chi(R)$:	6	0	2	0	2

and is equivalent to the direct sum

$$\Gamma_1 \oplus \Gamma_3 \oplus \Gamma_5.$$

The multiplicity of Γ_1 is one. Therefore, the space of tensors invariant under K is one-dimensional. Consequently, there is only one parameter left to describe such a symmetric second-rank tensor invariant under the cubic group $K = 432$. Noninvariant symmetric second-rank tensors are sums of tensors which transform according to the Γ_3 and Γ_5 representations. Here we are especially interested in invariant tensors.

1.2.4.2. *Invariants*

The dimension of the space of tensors of a certain type which are invariant under a point group K is equal to the number of free parameters in such a tensor. This number can be found as the multiplicity of the identity representation in the tensor space. For the 32 three-dimensional point groups this number is given in Table 1.2.6.9 for general second-rank tensors, symmetric second-rank tensors and a number of higher-rank tensors.

Invariant tensors, *i.e.* tensors of a certain type left invariant by a given group, may be constructed in several ways. The first way is a direct calculation. Take as an example again a second-rank symmetric tensor invariant under the cubic group 432. This means that

$$Rf = f \quad \forall\ R \in K,$$

which is a concise notation for

$$(Rf)_{ij} = \sum_{kl} R_{ik} R_{jl} f_{kl} = f_{ij}.$$

The group has two generators. Because each element of K is the product of generators, a tensor is left invariant under a group if it is left invariant by the generators. Therefore, one has in this case for

$$f = \begin{pmatrix} a_1 & a_2 & a_3 \\ a_2 & a_4 & a_5 \\ a_3 & a_5 & a_6 \end{pmatrix}$$

the equation

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} f \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} f \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = f.$$

These equations form a system of 12 linear algebraic equations for the coefficients of f with the solution

$$a_1 = a_4 = a_6; \quad a_2 = a_3 = a_5 = 0.$$

Up to a factor there is only one such tensor:

$$f = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix},$$

in agreement with the finding that the space of invariant second-rank symmetric tensors is one-dimensional. An overview of these relations for the 32 point groups can be found in Section 1.1.4 in this volume.

This method can always be used for groups with a finite number of generators. Another method for determining invariant tensors is using projection operators.

If a group, for example a point group, acts in some linear vector space, for example the space of tensors of a certain type, this space carries a representation. Then it is possible to construct a basis such that the representation corresponds to a choice of matrix representation. In particular, if the representation is reducible, it is possible to construct a basis such that the matrix representation is in reduced form. This can be achieved with *projection operators*.

Suppose the element $R \in K$ acts in a space as an operator $D(R)$ such that the representation $D(K)$ is equivalent with a matrix representation $\Gamma(K)$ which has irreducible components $\Gamma_\alpha(K)$. Then choose a vector v in the representation space and construct the d_α vectors

$$v_i = (1/N) \sum_{R\in K} \Gamma_\alpha(R)^*_{ji} D(R) v \qquad (1.2.4.7)$$

with j fixed. If v does not have a component in the invariant space of the irreducible representation D_α, these vectors are all zero, but for a sufficiently general vector the d_α vectors form a basis for the irreducible representation. This property follows from the orthogonality relations.

Using this relation one can write for an invariant symmetric second-rank tensor

$$f = (1/N) \sum_{R\in K} D(R) f' = (1/N) \sum_{R\in K} \Gamma(R) f' \Gamma(R)^T$$

for an arbitrary symmetric second-rank tensor f'. For the group $K = 432$ this would give a tensor with components $f_{ij} = a\delta_{ij}$. Of course, this is a rather impractical method if the order of the group is large. A simple example for a very small group is the construction of the symmetrical and antisymmetrical components of a function: $f_\pm(x) = [f(x) \pm f(-x)]/2$.

1.2.4.3. *Clebsch–Gordan coefficients*

The tensor product of two irreducible representations of a group K is, in general, reducible. If $\mathbf{a}_i$ is a basis for the irreducible representation Γ_α $(i = 1, \ldots, d_\alpha)$ and $\mathbf{b}_j$ one for Γ_β $(j = 1, \ldots, d_\beta)$, a basis for the tensor product space is given by

$$\mathbf{e}_{ij} = \mathbf{a}_i \otimes \mathbf{b}_j.$$

On this basis, the matrix representation is, in general, not in reduced form, even if the product representation is reducible. Suppose that

$$\Gamma_\alpha \otimes \Gamma_\beta \sim \sum_\gamma{}^{\oplus} m_\gamma \Gamma_\gamma.$$

This means that there is a basis

$$\psi_{\gamma\ell k} \quad (\ell = 1, \ldots, m_\gamma;\ k = 1, \ldots, d_\gamma),$$

on which the representation is in reduced form. The multiplicity m_γ gives the number of times the irreducible component Γ_γ occurs in the tensor product. The basis transformation is given by

$$\psi_{\gamma\ell k} = \sum_{ij} \left(\begin{array}{cc|cc} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{array} \right) \mathbf{a}_i \otimes \mathbf{b}_j. \qquad (1.2.4.8)$$

The basis transformation is unitary if one starts with orthonormal bases and has coefficients

$$\left(\begin{array}{cc|cc} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{array} \right) \qquad (1.2.4.9)$$

called *Clebsch–Gordan coefficients*. For the group $O(3)$ they are the original Clebsch–Gordan coefficients; for bases $|\ell m\rangle$ and $|\ell' m'\rangle$ of the $(2\ell + 1)$- and $(2\ell' + 1)$-dimensional representations D_ℓ and $D_{\ell'}$, respectively, of $O(3)$ one has

$$|JM\rangle = \sum_{mm'} \begin{pmatrix} \ell & \ell' & J \\ m & m' & M \end{pmatrix} |\ell m\rangle \otimes |\ell' m'\rangle,$$
$$(J = |\ell - \ell'|, \ldots, \ell + \ell'). \qquad (1.2.4.10)$$

The multiplicity here is always zero or unity, which is the reason why one leaves out the number ℓ in the notation.

If the multiplicity m_γ is unity, the coefficients for given α, β, γ are unique up to a common factor for all i, j, k. This is no longer the case if the multiplicity is larger, because then one can make linear combinations of the basis vectors belonging to Γ_γ. Anyway, one has to follow certain conventions. In the case of $O(3)$, for example, there are the Condon–Shortley phase conventions. The degree of freedom of the Clebsch–Gordan coefficients for given matrix representations Γ_α can be seen as follows. Suppose that there are two basis transformations, S and S', in the tensor product space which give the same reduced form:

$$S(D_\alpha \otimes D_\beta)S^{-1} = S'(D_\alpha \otimes D_\beta)S'^{-1} = D = \bigoplus m_\gamma D_\gamma. \qquad (1.2.4.11)$$

Then the matrix $S'S^{-1}$ commutes with every matrix $D(R)$ ($R \in K$). If all multiplicities are zero or unity, it follows from Schur's lemma that $S'S^{-1}$ is the direct sum of unit matrices of dimension d_γ. If the multiplicities are larger, the matrix $S'S^{-1}$ is a direct sum of blocks which are of the form

$$\begin{pmatrix} \lambda_{11}E & \lambda_{12}E & \ldots & \lambda_{1m_\gamma}E \\ \lambda_{21}E & \lambda_{22}E & \ldots & \lambda_{2m_\gamma}E \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_{m_\gamma 1}E & \ldots & \ldots & \lambda_{m_\gamma m_\gamma}E \end{pmatrix},$$

such that $\mathrm{Det}(\lambda_{ij}) = 1$, and the E's are d_γ-dimensional unit matrices. This means that for multiplicity-free ($m_\gamma \le 1$) cases, the Clebsch–Gordan coefficients are unique up to a common factor for all coefficients involving one value of γ.

The Clebsch–Gordan coefficients satisfy the following rules:

$$\begin{pmatrix} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{pmatrix} = \begin{pmatrix} \beta & \alpha & \gamma & \\ j & i & k & \ell \end{pmatrix}$$

$$\begin{pmatrix} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{pmatrix} = 0, \text{ if } D_\alpha \otimes D_\beta \text{ does not contain } D_\gamma$$

$$\sum_{k\ell} \begin{pmatrix} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{pmatrix}^* \begin{pmatrix} \alpha & \beta & \gamma & \\ i' & j' & k & \ell \end{pmatrix} = \delta_{ii'}\delta_{jj'}$$

$$\sum_{ij} \begin{pmatrix} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{pmatrix}^* \begin{pmatrix} \alpha & \beta & \gamma & \\ i & j & k' & \ell' \end{pmatrix} = \delta_{kk'}\delta_{\ell\ell'}.$$

For the basis vectors of the invariant space belonging to the identity representation Γ_1, one has $\gamma = d_\gamma = 1$. Consequently,

$$\psi_\ell = \sum_{ij} \begin{pmatrix} \alpha & \beta & 1 & \\ i & j & 1 & \ell \end{pmatrix} \mathbf{a}_i \otimes \mathbf{b}_j.$$

1.2.5. Magnetic symmetry

1.2.5.1. *Magnetic point groups*

Until now, the symmetry transformations we have considered affect only spatial variables. In physics, however, time coordinates are also often essential, and time reversal is a very important transformation as well.

The time-reversal operation generates a group of order 2 with as elements the unit operator E and the time-reversal operator T. This transformation commutes with transformations of spatial variables. One can consider the combined operation of T and a Euclidean transformation. In other words, we consider the direct product of the Euclidean group $E(d)$ and the time-reversal group of order 2. Elements of this direct product that belong to $E(d)$ are called *orthochronous*, whereas the elements of the coset which are combinations of a Euclidean transformation with T are called *antichronous*. We shall start by considering combinations of T and orthogonal transformations in the physical d-dimensional space. Such combinations generate a subgroup of the direct product of $O(d)$ and the time-reversal group.

There are three types of such groups. First, one can have a group that is already a subgroup of $O(d)$. This group does not have time-reversing elements. A second type of group contains the operator T and is, therefore, the direct product of a subgroup of $O(d)$ with the time-reversal group. The third type of group contains antichronous elements but not T itself. This means that the group contains a subgroup of index 2 that belongs to $O(d)$ and one coset of this subgroup, all elements of which can be obtained from those of the subgroup by multiplication with one fixed time-reversing element which is not T. If one then multiplies all elements of the coset by T, one obtains a group that belongs to $O(d)$ and is isomorphic to the original group. This is the same situation as for subgroups of $O(3)$, which is the direct product of $SO(3)$ with space inversion I. Here also all subgroups of $O(d) \times \mathbb{Z}_2$ are isomorphic to point groups or to the direct product of a point group and $\mathbb{Z}_2$. Magnetic groups can be used to characterize spin arrangements. Because spin inverses sign under time reversal, a spin arrangement is never invariant under T. Therefore, the point groups of the second type are also called *nonmagnetic point groups*. Because time reversal does not play a role in groups of the first type, these are called *trivial magnetic point groups*, whereas the groups of the third type are called *nontrivial magnetic point groups*.

Magnetic point groups are discussed in Chapter 1.5. Orthochronous magnetic point groups (trivial magnetic groups) are denoted by their symbol as a normal point group. Magnetic point groups containing T are denoted by the symbol for the orthochronous subgroup, which is a trivial magnetic group, to which the symbol $1'$ is added. Magnetic point groups that are neither trivial nor contain T are isomorphic to a trivial magnetic point group. They are denoted by the symbol of the latter in which all symbols for antichronous elements are marked with a prime ($'$). For example, $\bar{1}$ is the trivial magnetic group generated by I, $\bar{1}1'$ is the group of four elements generated by I and T, and $\bar{1}'$ is the magnetic group of order 2 generated by the product IT.

Two magnetic point groups are called equivalent if they are conjugated in $O(d) \times \mathbb{Z}_2$ by an element in $O(d)$. This means that under the conjugation antichronous elements go to antichronous elements. The equivalence classes of magnetic point groups are the magnetic crystal classes. There are 32 classes of trivial crystallographic magnetic point groups, 32 classes of direct products with the time-reversal group and 58 classes of nontrivial magnetic crystallographic point groups. They are given in Table 1.2.6.12.

1.2.5.2. *Magnetic space groups*

Magnetic space groups are subgroups of the direct product of the Euclidean group $E(d)$ with the time-reversal group (this direct product is sometimes called the *Shubnikov group*) such that the orthochronous elements together with the products of the antichronous elements and T form a space group in d dimensions. As in the case of magnetic point groups, one can distinguish trivial magnetic groups, which are subgroups of $E(d)$, direct products of a trivial group with the time-reversal group (nonmagnetic) and nontrivial magnetic space groups with antichronous elements but without T. The groups of the third type can be transformed into groups of the first type by multiplication of all antichronous elements by T.

The translation subgroup U of a magnetic space group G is the intersection of G and $T(d) \times \{E, T\}$. The factor group G/U is (isomorphic to) a subgroup of $O(d) \times \{E, T\}$. For trivial magnetic space groups, the point group is a subgroup of $O(d)$. For direct products with $\{E, T\}$, the translation group is the direct product of an orthochronous lattice with $\{E, T\}$ and the point group is a subgroup of $O(d)$. Magnetic space groups with antichronous elements but without T have either a translation subgroup consisting of orthochronous elements or one with antichronous elements as well. In the first case, the point group is a subgroup of $O(d) \times \{E, T\}$ and contains antichronous elements; in the second case, one may always choose orthochronous elements for the coset representatives with respect to the translation group, and the point group is a subgroup of $O(d)$. Therefore, nontrivial magnetic space groups without T have either the same lattice or the same point group as the space group of orthochronous elements.

Two magnetic space groups are equivalent if they are affine conjugated *via* a transformation with positive determinant that maps antichronous elements on antichronous elements. Then there are 1651 equivalence classes: 230 classes of trivial groups with only orthochronous elements, 230 classes of direct products with $\{E, T\}$ and 1191 classes with nontrivial magnetic groups.

1.2.5.3. *Transformation of tensors*

Vectors and tensors transforming in the same way under Euclidean transformations may behave differently when time reversal is taken into account. As an example, both the electric field **E** and magnetic field **B** transform under a rotation as a position vector. Under time reversal, the former is invariant, but the latter changes sign. Therefore, the magnetic field is called a pseudovector field under time reversal. Under spatial inversion, the field **E** changes sign, as does a position vector, but the field **B** does not. Therefore, the magnetic field is also a pseudovector under central inversion. The electric polarization induced by an electric field is given by the electric susceptibility, a magnetic moment induced by a magnetic field is given by the magnetic susceptibility and in some crystals a magnetic moment is induced by an electric field *via* the magneto-electric susceptibility. Under the four elements of the group generated by $T = 1'$ and $I = \bar{1}$, the fields and susceptibility tensors transform according to

	E	$\bar{1}$	$1'$	$\bar{1}'$
E	1	−1	1	−1
B	1	1	−1	−1
χ_{ee}	1	1	1	1
χ_{mm}	1	1	1	1
χ_{me}	1	−1	−1	1

Here $\bar{1}' = \bar{1}1'$.

In general, a vector transforms as the position vector **r** under rotations and changes sign under $\bar{1}$, but not under $1'$. A pseudovector under $\bar{1}$ or (respectively and) $1'$ gets an additional minus sign. The generalization to tensors is straightforward.

$$gT_{i_1 \ldots i_n} = \varepsilon_P \varepsilon_T \sum_{j_1 \ldots j_n} \left(\prod_{k=1}^{n} R_{i_k j_k} \right) T_{j_1 \ldots j_n}, \qquad (1.2.5.1)$$

where ε_P and ε_T are ± 1, depending on the pseudotensor character with respect to space and time reversal, respectively.

Under a rotation $[R \in SO(d)]$, a vector transforms according to a representation characterized by the character $\chi(R)$ of the representation. In two dimensions $\chi = 2\cos\varphi$ and in three dimensions $\chi = 1 + 2\cos\varphi$, if φ is the rotation angle. Under IR the character gets an additional minus sign, under RT it is the same, and under RIT there is again an additional minus sign. For pseudovectors, either under I or T or both, there are the extra factors ε_P, ε_T and $\varepsilon_P \varepsilon_T$, respectively. As an example, the character of the representations corresponding to the electric and magnetic fields in two orthorhombic point groups (222, $2'2'2$ and $2'mm'$) are given in Table 1.2.5.1.

Table 1.2.5.1. *Character of the representations corresponding to the electric and magnetic fields in point groups 222, $2'2'2$ and $2'mm'$*

n_i is the number of invariants.

Point group	**E**				n_i	**B**				n_i
222	3	−1	−1	−1	0	3	−1	−1	−1	0
$2'2'2$	3	−1	−1	−1	0	3	1	1	−1	1
$2'mm'$	3	−1	1	1	1	3	1	−1	1	1

The number of invariant components is the multiplicity of the trivial representation in the representation to which the tensor belongs. The nonzero invariant field components are B_z for $2'2'2$, E_x and B_y for $2'mm'$. These components can be constructed by means of projection-operator techniques, or more simply by solving the linear equations representing the invariance of the tensor under the generators of the point group. For example, the magnetic field vector B transforms to $(-B_x, B_y, -B_z)$ under m_y and to $(B_x, B_y, -B_z)$ under m_z', and this gives the result that for $2'mm'$ all components are zero except B_y.

1.2.5.4. *Time-reversal operators*

In quantum mechanics, symmetry transformations act on state vectors as unitary or anti-unitary operators. For the Schrödinger equation for one particle without spin,

$$\hbar i \frac{\partial}{\partial t} \Psi(\mathbf{r}, t) = H\Psi(\mathbf{r}, t), \qquad (1.2.5.2)$$

the operator that reverses time is the complex conjugation operator θ with

$$\theta\Psi(\mathbf{r}, t) = \Psi^*(\mathbf{r}, t) \qquad (1.2.5.3)$$

satisfying

$$\hbar i \frac{\partial}{\partial t} \Psi^*(\mathbf{r}, -t) = H\Psi^*(\mathbf{r}, -t),$$

which is the time-reversed equation.

This operator is *anti-linear* $[\theta(\alpha\Psi + \beta\Phi) = \alpha^*\theta\Psi + \beta^*\Phi]$ and has the following commutation relations with the operators **r** and **p** for position and momentum:

$$\theta\mathbf{r}\theta^{-1} = \mathbf{r}, \quad \theta\mathbf{p}\theta^{-1} = -\mathbf{p}. \qquad (1.2.5.4)$$

For a Euclidean transformation $g = \{R|\mathbf{a}\}$, the operation on the state vector is given by the unitary operator

$$T_g\Psi(\mathbf{r}) = \Psi(g^{-1}\mathbf{r}) = \Psi(R^{-1}(\mathbf{r} - \mathbf{a})). \qquad (1.2.5.5)$$

The two operators θ and T_g commute. Therefore, if g is an orthochronous element of the symmetry group, the corresponding operator is T_g, and if gT is an antichronous element the operator is θT_g. The operator θT_g is also *anti-unitary*: it is anti-linear and conserves the absolute value of the Hermitian scalar product: $|\langle\theta T_g\Psi|\theta T_g\Phi\rangle| = |\langle\Psi|\Phi\rangle|$.

If the particle has a spin, the time-reversal operator has to have the commutation relation

$$\theta\mathbf{S}\theta^{-1} = -\mathbf{S} \qquad (1.2.5.6)$$

with the spin operator **S**. For a spin-$\frac{1}{2}$ particle, the spin operators are $S_i = \hbar\sigma_i/2$ in terms of the Pauli matrices. Then the time-reversal operator is

$$T_T = \sigma_2\theta. \qquad (1.2.5.7)$$

The operators corresponding to the elements of a magnetic symmetry group are generally (anti-)unitary operators on the state vectors. These operators form a representation of the magnetic symmetry group.

$$T_g T_{g'} = T_{gg'}. \qquad (1.2.5.8)$$

In principle, they even form a projective representation, but as discussed before for particles without spin the factor system is trivial, and for particles with spin one can take as the symmetry group the double group of the symmetry group.

1.2.5.5. *Co-representations*

Suppose the magnetic point group G has an orthochronous subgroup H and an antichronous coset $H' = aH$ for some antichronous element a. The elements of H are represented by unitary operators, those of H' by anti-unitary operators. These operators correspond to matrices in the following way. Suppose Φ_j are the elements of a basis of the state vector space. Then

$$T_g \Phi_j = \sum_k M(g)_{kj} \Phi_k, \quad g \in G. \qquad (1.2.5.9)$$

The matrices M do not form a matrix representation in the usual sense. They satisfy the relations

$$\begin{aligned} M(g_1 g_2) &= M(g_1) M(g_2) \quad g_1 \in H \\ &= M(g_1) M^*(g_2) \quad g_1 \in H', \end{aligned} \qquad (1.2.5.10)$$

as one verifies easily. Matrices satisfying these relations are called *co-representations* of the group G.

A co-representation is irreducible if there is no proper invariant subspace. If a co-representation is reducible, there is a basis transformation S that brings the matrices into a block form. For co-representations, a basis transformation S with

$$S\Phi_i = \sum_{j=1}^{m} S_{ji} \Phi_j \qquad (1.2.5.11)$$

transforms the matrices according to

$$M(h) \to S^{-1} M(h) S, \quad M(ah) \to S^{-1} M(ah) S^*, \quad (h \in H). \qquad (1.2.5.12)$$

Here a is the coset representative of the antichronous elements. The co-representation restricted to the orthochronous subgroup H gives an ordinary representation of H which is not necessarily irreducible even if the co-representation is irreducible. Suppose that $\Phi_1 \ldots \Phi_m$ form a basis for the irreducible co-representation of G and that the restriction to H is also irreducible. The elements $T_a\Phi_1, \ldots, T_a\Phi_m$ form another basis for the space, and on this basis the representation matrices of H follow from

$$T_h T_a \Phi_i = T_a T_{a^{-1}ha} \Phi_i = \sum_{j=1}^{m} M(a^{-1}ha)^*_{ji} T_a \Phi_j. \qquad (1.2.5.13)$$

Because both bases are bases for the same irreducible space, it means that the (ordinary) representations $M(H)$ and $M(a^{-1}Ha)^*$ are equivalent.

If the representation $M(H)$ is reducible, there is a basis $\varphi_1, \ldots, \varphi_d$ for the irreducible representation $D(H)$. A basis for the whole space then is given by

$$\varphi_1, \ldots, \varphi_d, T_a\varphi_1, \ldots, T_a\varphi_d,$$

because the co-representation of G would be reducible if the last d vectors were dependent on the first d. On this basis, the matrices for the co-representation become

$$\begin{aligned} M(h) &= \begin{pmatrix} D(h) & 0 \\ 0 & D(a^{-1}ha)^* \end{pmatrix}, \\ M(ah) &= \begin{pmatrix} 0 & D(aha) \\ D(h)^* & 0 \end{pmatrix}, \quad h \in H, a \in H' \end{aligned} \qquad (1.2.5.14)$$

because

$$\begin{aligned} T_a h \varphi_i &= T_a \sum_j D(h)_{ji} \varphi_j = \sum_j D(h)^*_{ji} T_a \varphi_j \\ T_a h T_a \varphi_i &= T_a ha \varphi_i = \sum_j D(aha)_{ji} \varphi_j. \end{aligned}$$

The two irreducible components for $M(H)$ can be either equivalent or non-equivalent. If they are not equivalent the co-representation is indeed irreducible, because a basis transformation S that leaves the matrices $M(h)$ the same is necessarily of the form $\lambda E \oplus \mu E$ because of Schur's lemma, and such a matrix cannot bring the matrices $D(ah)$ into a reduced form. In this case, the co-representation $M(G)$ is irreducible, in agreement with the starting assumption, and the dimension m is twice the dimension of the representation $D(H)$: $m = 2d$.

If the two irreducible components $D(H)$ and $D(a^{-1}Ha)^*$ are equivalent, there is a basis transformation U such that

$$D(a^{-1}ha)^* = U^{-1} D(h) U \quad \forall\, h \in H.$$

The basis transformation

$$T = \begin{pmatrix} 1 & 0 \\ 0 & U^{-1} \end{pmatrix}$$

then gives a new matrix co-representation for G:

$$\begin{aligned} M(h) \to T^{-1} M(h) T &= \begin{pmatrix} D(h) & 0 \\ 0 & D(h) \end{pmatrix}, \\ M(ah) \to T^{-1} M(ah) T^* &= \begin{pmatrix} 0 & D(aha) U^{*-1} \\ UD(h)^* & 0 \end{pmatrix}. \end{aligned}$$

The most general basis transformation S that leaves $M(h)$ in the same form is then

$$S = \begin{pmatrix} \lambda E & \mu E \\ \rho E & \sigma E \end{pmatrix}. \qquad (1.2.5.15)$$

Under this basis transformation, the matrices $M(ah)$ become

$$S^{-1} M(ah) S^* = \frac{1}{(\lambda\sigma - \mu\rho)} \mathcal{M}$$

with

$$\begin{aligned} \mathcal{M}_{11} &= -\lambda^* \mu UD(h)^* + \rho^* \sigma D(aha) U^{*-1} \\ \mathcal{M}_{12} &= |\sigma|^2 D(aha) U^{*-1} - |\mu|^2 UD(h)^* \\ \mathcal{M}_{21} &= |\lambda|^2 UD(h)^* - |\rho|^2 D(aha) U^{*-1} \\ \mathcal{M}_{22} &= \lambda\mu^* UD(h)^* - \rho\sigma^* D(aha) U^{*-1}. \end{aligned}$$

This is block diagonal if

$$|\mu|^2 UU^* D(a^{-1}ha) U^{*-1} U^* = |\sigma|^2 D(aha)$$

and analogous expressions for $|\lambda|^2$ and $|\rho|^2$ also hold.

The transformation matrix U satisfies $UU^* = \pm D(a^2)$, as one can show as follows. From the definition

$$D(a^{-1}ha)^* = U^{-1} D(h) U$$

follow the two relations

$$D(a^{-2}ha^2) = U^{*-1}U^{-1}D(h)UU^*$$
$$D(a^{-2}ha^2) = D(a^2)^{-1}D(h)D(a^2).$$

(Notice that $a^2 \in H$.) Because $D(H)$ is irreducible, it follows that $UU^*D(a^{-2})$ is a multiple of the identity: $UU^* = \chi D(a^2)$. The factor χ is real because

$$D(a^2)^* = U^{-1}D(a^2)U = U^{-1}UU^*U/\chi$$

and

$$D(a^2)^* = U^*U/\chi^*.$$

Hence $\chi = \chi^* = \pm 1$.

The conditions for the transformed matrix $M(ah)$ to be block diagonal then read

$$\pm|\mu|^2 D(a^2)D(a^{-1}ha) = |\sigma|^2 D(aha), \qquad (1.2.5.16)$$

with the corresponding expressions for λ and ρ. If χ is equal to -1, these equations do not have a solution. However, when $\chi = +1$ there is a solution, which means that the co-representation is reducible, contrary to the assumption. Therefore, this situation can not occur.

One can summarize these considerations in the following theorem.

Theorem 1. If the restriction of an irreducible co-representation to the orthochronous subgroup is reducible, then either the (two) irreducible components are non-equivalent, or they are equivalent and connected by a basis transformation U for which $UU^* = -D(a^2)$. If the restriction $M(H)$ is irreducible, it is equivalent to $M(a^{-1}Ha)^*$.

In the former case, the dimension of the co-representation is twice that of the restriction, in the latter case they are equal. Therefore, one has the following corollary.

Corollary. A d-dimensional irreducible representation of the orthochronous subgroup H can occur as irreducible component of the restriction of an irreducible co-representation of G with dimension m with

$m = 2d$ if $D(H)$ nonequivalent to $D(a^{-1}Ha)^*$

$m = 2d$ if $D(H)$ equivalent to $D(a^{-1}Ha)^*$ and $UU^* = -D(a^2)$

$m = d$ if $D(H)$ equivalent to $D(a^{-1}Ha)^*$ and $UU^* = +D(a^2)$.

The three cases from theorem (1) can be distinguished by the following theorem:

Theorem 2. The irreducible representation $D(H)$ with character $\chi(H)$ belongs to the respective cases of theorem (1) if

$$\sum_{h\in H}\chi(ahah) = \begin{cases} 0 & \text{for the first case} \\ -N & \text{for the second case} \\ N & \text{for the third case.}\end{cases} \qquad (1.2.5.17)$$

The proof of theorem (2) goes as follows. We have

$$\sum_{h\in H}\chi(ahah) = \sum_{h\in H}\sum_{i=1}^{d} D(ahah)_{ii} = \sum_{i,k,l} D(a^2)_{ik}\sum_{h\in H} D(a^{-1}ha)_{kl}D(h)_{li}, \qquad (1.2.5.18)$$

and this gives zero if $D(H)$ and $D(a^{-1}Ha)^*$ are non-equivalent, because of the orthogonality relations. If the two representations are equivalent, we take for convenience unitary representations. Then there is a unitary matrix U with

$$D(a^{-1}ha)^* = U^{-1}D(h)U.$$

Then we have

$$\begin{aligned}\sum_{h\in H}\chi(ahah) &= \sum_{ik\ell mn} D(a^2)_{ik}(U^{*-1})_{km}\sum_{h\in H} D(h)^*_{mn}U_{n\ell}D(h)_{\ell i} \\ &= (N/d)\sum_{i,k,\ell} D(a^2)_{ik}(U^{*-1})_{k\ell}U^*_{i\ell} \\ &= (N/d)\sum_{i,k} D(a^2)_{ik}(U^*U)_{ik} \\ &= \pm(N/d)\sum_{i,k} D(a^2)_{ik}D(a^{-2})_{ki} = \pm N.\end{aligned}$$

This proves theorem (2).

In the special case of a group G in which the time reversal $1'$ occurs as element, one may choose $a = 1'$. In this case, a^2 is the identity and the expressions simplify. Theorem (1) now states that an irreducible d-dimensional representation $D(H)$ of an orthochronous group can occur as irreducible component in the restriction of an irreducible m-dimensional co-representation of $H \times \{E, 1'\}$, with

$m = 2d$ if $D(H)$ nonequivalent to $D(H)^*$

$m = 2d$ if $D(H) = UD(H)^*U^{-1}$ and $UU^* = -E$

$m = d$ if $D(H) = UD(H)^*U^{-1}$ and $UU^* = +E$,

which correspond to, respectively, [*cf.* theorem (2)]

$$\sum_{h\in H}\chi(h^2) = \begin{cases} 0 \\ -N \\ +N \end{cases}. \qquad (1.2.5.19)$$

For a spinless particle, the time-reversal operator is the complex conjugation θ. This generates a co-representation of the group $\mathbb{Z}_2$. The symmetry group is the direct product of the point group H and $\mathbb{Z}_2$. Compared to the degeneracy d of a state characterized by the irreducible representation $D(H)$, the degeneracy is double ($m = 2d$) for the first two cases and the same for the third case. When it is a particle with spin $\frac{1}{2}$, the time-reversal operator is $\sigma_2\theta$, which is of order 4. If one takes for the coset representative a the time reversal, one has $D(a^2) = -E$. Therefore, the degeneracy is now doubled in the first and third case, and the same for the second. This is Kramer's degeneracy.

1.2.6. Tables

In the following, a short description of the tables is given in order to facilitate consultation without reading the introductory theoretical Sections 1.2.2 to 1.2.5.

Table 1.2.6.1. Finite point groups in three dimensions. The point groups are grouped by isomorphism class. There are four infinite families and six other isomorphism classes. (Notation: C_n for the cyclic group of order n, D_n for the dihedral group of order $2n$, T, O and I the tetrahedral, octahedral and icosahedral groups, respectively). Point groups of the first class are subgroups of $SO(3)$, those of the second class contain $-E$, and those of the third class are not subgroups of $SO(3)$, but do not contain $-E$ either. The families C_n and D_n are also isomorphism classes of two-dimensional finite point groups.

Table 1.2.6.2. Among the infinite number of finite three-dimensional point groups, 32 are crystallographic.

Table 1.2.6.3. Character table for the cyclic groups C_n. The generator is denoted by α. The number of elements in the conjugacy classes (n_i) is one for each class. The order is the smallest nonnegative power p for which $A^p = E$. The n irreducible representations are denoted by Γ_i.

Table 1.2.6.4. Character tables for the dihedral groups D_n of order $2n$. n_i is the number of elements in the conjugacy class C_i. The irreducible representations are denoted by Γ_i.

Table 1.2.6.1. *Finite point groups in three dimensions*

Isomorphism class	First class with determinants > 0	Second class with $-E$	Third class without $-E$	Order
C_n	n		$\bar{n}$ (n even, >2) m ($n=2$)	n
D_n	$n22$ (n even) $n2$ (n odd, >1)		nmm (n even) $\bar{n}2m$ (n even) nm (n odd)	$2n$
$C_n \times C_2$		$\bar{n}$ (n odd) n/m (n even)		$2n$
$D_n \times C_2$		n/mmm (n even, ≥ 4) mmm ($n=2$) $\bar{n}m$ (n odd, >0)		$4n$
T	23			12
O	432		$\bar{4}3m$	24
I	532			60
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48
$I \times C_2$		$\bar{5}\bar{3}m$		120

Table 1.2.6.5. The character tables for the 32 three-dimensional crystallographic point groups. The groups are grouped by isomorphism class (there are 18 isomorphism classes).

For each isomorphism class, the character table is given, including the symbol for the isomorphism class, the number n of elements per conjugacy class and the order of the elements in each such class. The conjugation classes are specified by representative elements expressed in terms of the generators $\alpha, \beta, \ldots$. The irreps are denoted by Γ_i, where i takes as many values as there are conjugation classes. In each isomorphism class for each point group, given by its international symbol and its Schoenflies symbol, identification is made between the generators of the abstract group (α, β) and the generating orthogonal transformations. Notation: C_{nx} is a rotation of $2\pi/n$ along the x axis, σ_x is a reflection from a plane perpendicular to the x axis, S_{nz} is a rotation over $2\pi/n$ along the z axis multiplied by $-E$ and σ_v is a reflection from a plane through the unique axis.

The notation for the irreducible representations can be given as Γ_i, but other systems have been used as well. Indicated below are the relations between Γ_i and a system that uses a characterization according to the dimension of the representation and (for groups of the second kind) the sign of the representative of $-E$. This nomenclature is often used by spectroscopists.

A, A_1, A_2, A', A''	one-dimensional
B, B_1, B_2, B_3	one-dimensional
E	two-dimensional
T, T_1, T_2	three-dimensional
A_g, B_g *etc.*	*gerade*
A_u, B_u *etc.*	*ungerade*

The other notation for which the relation with the present notation is indicated is that of Kopský, and is used in the accompanying software.

The three functions x, y and z transform according to the vector representation of the point group, which is generally reducible. The reduction into irreducible components of this three-dimensional vector representation is indicated.

The six bilinear functions x^2, xy, xz, y^2, yz, z^2 transform according to the symmetrized product of the vector representation. The basis functions of the irreducible components are indicated. Because the basis functions are real, one should consider the physically irreducible representations.

Table 1.2.6.6. The point groups of the second class containing $-E$ are obtained from those of the first class by taking the direct product with the group generated by $\bar{1}$. From the point groups, one obtains nonmagnetic point groups by the direct product with the group generated by the time reversal $1'$. The relation between the characters of a point group and its direct products with

Table 1.2.6.2. *Crystallographic point groups in three dimensions*

Isomorphism class	First class	Second class with $-E$	Third class without $-E$	Order
C_1	1			1
C_2	2	$\bar{1}$	m	2
C_3	3			3
C_4	4		$\bar{4}$	4
D_2	222	$2/m$	$2mm$	4
C_6	6	$\bar{3}$	$\bar{6}$	6
D_3	32		$3m$	6
$C_4 \times C_2$		$4/m$		8
D_4	422		$4mm$, $\bar{4}2m$	8
$D_2 \times C_2$		mmm		8
D_6	622	$\bar{3}m$	$6mm$, $\bar{6}2m$	12
T	23			12
$C_6 \times C_2$		$6/m$		12
$D_4 \times C_2$		$4/mmm$		16
O	432		$\bar{4}3m$	24
$D_6 \times C_2$		$6/mmm$		24
$T \times C_2$		$m\bar{3}$		24
$O \times C_2$		$m\bar{3}m$		48

Table 1.2.6.3. *Irreducible representations for cyclic groups* C_n

$\omega = \exp(2\pi i/n)$, l.c.d. = largest common divisor.

	ε	α	α^2	α^3	$\ldots$	α^{n-1}
n_i	1	1	1	1	$\ldots$	1
Order	1	n	n/l.c.d.$(n, 2)$	n/l.c.d.$(n, 3)$	$\ldots$	n
Γ_1	1	1	1	1	$\ldots$	1
Γ_2	1	ω	ω^2	ω^3	$\ldots$	ω^{-1}
$\vdots$	1	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
Γ_n	1	ω^{-1}	ω^{-2}	ω^{-3}	$\ldots$	ω

Table 1.2.6.4. *Irreducible representations for dihedral groups* D_n

(a) n odd. $m = 1, \ldots, (n-1)/2$; $j = 1, \ldots, (n-1)/2$, l.c.d. = largest common divisor.

	ε	α^j	$\ldots$	β
n_i	1	1	2	n
Order	1	n/l.c.d.(n, j)	$\ldots$	2
Γ_1	1	1	$\ldots$	1
Γ_2	1	1	$\ldots$	-1
Γ_{2+m}	2	$2\cos(2\pi mj/n)$	$\ldots$	0

(b) n even. $m = 1, \ldots, (n/2-1)$; $j = 1, \ldots, (n/2-1)$, l.c.d. = largest common divisor.

	ε	$\alpha^{n/2}$	α^j	$\ldots$	β	$\alpha\beta$
n_i	1	1	2	$\ldots$	$n/2$	$n/2$
Order	1	2	n/l.c.d.(n, j)	$\ldots$	2	2
Γ_1	1	1	1	$\ldots$	1	1
Γ_2	1	1	1	$\ldots$	-1	-1
Γ_3	1	$(-1)^{n/2}$	$(-1)^j$	$\ldots$	1	-1
Γ_4	1	$(-1)^{n/2}$	$(-1)^j$	$\ldots$	-1	1
Γ_{4+m}	2	$(-1)^m 2$	$2\cos(2\pi mj/n)$	$\ldots$	0	0

Table 1.2.6.5. *Irreducible representations and character tables for the 32 crystallographic point groups in three dimensions*

(*a*) C_1

C_1	ε
n	1
Order	1
Γ_1	1

1 C_1	$\Gamma_1 : A = \chi_1$	x, y, z	$x^2, y^2, z^2, yz, xz, xy$

(*b*) C_2

C_2	ε	α
n	1	1
Order	1	2
Γ_1	1	1
Γ_2	1	-1

2 C_2	$\alpha = C_{2z}$	$\Gamma_1 : A = \chi_1$ $\Gamma_2 : B = \chi_3$	z x, y	x^2, y^2, z^2, xy yz, xz
m C_s	$\alpha = \sigma_z$	$\Gamma_1 : A' = \chi_1$ $\Gamma_2 : A'' = \chi_3$	x, y z	x^2, y^2, z^2, xy yz, xz
$\bar{1}$ C_i	$\alpha = I$	$\Gamma_1 : A_g = \chi_1^+$ $\Gamma_2 : A_u = \chi_1^-$	 x, y, z	$x^2, y^2, z^2, yz, xz, xy$

(*c*) C_3 $[\omega = \exp(2\pi i/3)]$.

C_3	ε	α	α^2
n	1	1	1
Order	1	3	3
Γ_1	1	1	1
Γ_2	1	ω	ω^2
Γ_3	1	ω^2	ω

Matrices of the real two-dimensional representation:

	ε	α	α^2
$\Gamma_2 \oplus \Gamma_3$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$

3 C_3	$\alpha = C_{3z}$	$\Gamma_1 : A = \chi_1$ $\Gamma_2 \oplus \Gamma_3 : E = \chi_{1c} + \chi_{1c}^*$	z x, y	$x^2 + y^2, z^2$ $x^2 - y^2, xz, yz, xy$

(*d*) C_4

C_4	ε	α	α^2	α^3
n	1	1	1	1
Order	1	4	2	4
Γ_1	1	1	1	1
Γ_2	1	i	-1	$-i$
Γ_3	1	-1	1	-1
Γ_4	1	$-i$	-1	i

Matrices of the real two-dimensional representation:

	ε	α	α^2	α^3
$\Gamma_2 \oplus \Gamma_4$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$

4 C_4	$\alpha = C_{4z}$	$\Gamma_1 : A = \chi_1$ $\Gamma_3 : B = \chi_3$ $\Gamma_2 \oplus \Gamma_4 : E = \chi_{1c} + \chi_{1c}^*$	z x, y	$x^2 + y^2, z^2$ $x^2 - y^2, xy$ yz, xz
$\bar{4}$ S_4	$\alpha = S_4$	$\Gamma_1 : A = \chi_1$ $\Gamma_3 : B = \chi_3$ $\Gamma_2 \oplus \Gamma_4 : E = \chi_{1c} + \chi_{1c}^*$	 z x, y	$x^2 + y^2, z^2$ $x^2 - y^2, xy$ yz, xz

(*e*) C_6 $[\omega = \exp(\pi i/3)]$.

C_6	ε	α	α^2	α^3	α^4	α^5
n	1	1	1	1	1	1
Order	1	6	3	2	3	6
Γ_1	1	1	1	1	1	1
Γ_2	1	ω	ω^2	-1	$-\omega$	$-\omega^2$
Γ_3	1	ω^2	$-\omega$	1	ω^2	$-\omega$
Γ_4	1	-1	1	-1	1	-1
Γ_5	1	$-\omega$	ω^2	1	$-\omega$	ω^2
Γ_6	1	$-\omega^2$	$-\omega$	-1	ω^2	ω

Matrices of the real representations:

	$\Gamma_2 \oplus \Gamma_6$	$\Gamma_3 \oplus \Gamma_5$
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
α^2	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$
α^3	$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
α^4	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$
α^5	$\begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$

6 C_6	$\alpha = C_{6z}$	$\Gamma_1 : A = \chi_1$ $\Gamma_4 : B = \chi_3$ $\Gamma_2 \oplus \Gamma_6$: $E_1 = \chi_{1c} + \chi_{1c}^*$ $\Gamma_3 \oplus \Gamma_5$: $E_2 = \chi_{2c} + \chi_{2c}^*$	z x, y 	$x^2 + y^2, z^2$ xz, yz $x^2 - y^2, xy$
$\bar{3}$ S_6	$\alpha = S_{3z}$	$\Gamma_1 : A_g = \chi_1^+$ $\Gamma_4 : A_u = \chi_1^-$ $\Gamma_2 \oplus \Gamma_6$: $E_u = \chi_{1c}^- + \chi_{1c}^{-*}$ $\Gamma_3 \oplus \Gamma_5$: $E_g = \chi_{1c}^+ + \chi_{1c}^{+*}$	 z x, y $x^2 - y^2, xy, xz, yz$	$x^2 + y^2, z^2$
$\bar{6}$ C_{3h}	$\alpha = S_{6z}$	$\Gamma_1 : A' = \chi_1$ $\Gamma_4 : A'' = \chi_3$ $\Gamma_2 \oplus \Gamma_6$: $E' = \chi_{2c} + \chi_{2c}^*$ $\Gamma_3 \oplus \Gamma_5$: $E'' = \chi_{1c} + \chi_{1c}^*$	 z x, y	$x^2 + y^2, z^2$ xz, yz $x^2 - y^2, xy$

(*f*) D_2

D_2	ε	α	β	$\alpha\beta$
n	1	1	1	1
Order	1	2	2	2
Γ_1	1	1	1	1
Γ_2	1	1	-1	-1
Γ_3	1	-1	1	-1
Γ_4	1	-1	-1	1

222 D_2	$\alpha = C_{2x}$ $\beta = C_{2y}$ $\alpha\beta = C_{2z}$	$\Gamma_1 : A_1 = \chi_1$ $\Gamma_2 : B_3 = \chi_3$ $\Gamma_3 : B_2 = \chi_4$ $\Gamma_4 : B_1 = \chi_2$	 x y z	x^2, y^2, z^2 yz xz xz
$mm2$ C_{2v}	$\alpha = C_{2z}$ $\beta = \sigma_x$ $\alpha\beta = \sigma_y$	$\Gamma_1 : A_1 = \chi_1$ $\Gamma_2 : A_2 = \chi_2$ $\Gamma_3 : B_2 = \chi_3$ $\Gamma_4 : B_1 = \chi_4$	z y x	x^2, y^2, z^2 xy yz xz
$2/m$ C_{2h}	$\alpha = C_{2z}$ $\beta = \sigma_z$ $\alpha\beta = I$	$\Gamma_1 : A_g = \chi_1^+$ $\Gamma_2 : A_u = \chi_1^-$ $\Gamma_3 : B_u = \chi_3^-$ $\Gamma_4 : B_g = \chi_3^+$	 z x, y 	x^2, y^2, z^2, xy z

Table 1.2.6.5 (*cont.*)

(*g*) D_3

D_3	ε	α	β
n	1	2	3
Order	1	3	2
Γ_1	1	1	1
Γ_2	1	1	−1
Γ_3	2	−1	0

Matrices of the two-dimensional representation:

	ε	α	β
Γ_3	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&-1\end{pmatrix}$	$\begin{pmatrix}-1&1\\0&1\end{pmatrix}$

32 D_3	$\alpha = C_{3z}$ $\beta = C_{2x}$	$\Gamma_1 : A_1 = \chi_1$		x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$	z	
		$\Gamma_3 : E = \chi_1$	x, y	xz, yz, xy, x^2-y^2
$3m$ C_{3v}	$\alpha = C_{3z}$ $\beta = \sigma_v$	$\Gamma_1 : A_1 = \chi_1$	z	x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$		
		$\Gamma_3 : E = \chi_1$	x, y	xz, yz, xy, x^2-y^2

(*h*) D_4

D_4	ε	α	α^2	β	$\alpha\beta$
n	1	2	1	2	2
Order	1	4	2	2	2
Γ_1	1	1	1	1	1
Γ_2	1	1	1	−1	−1
Γ_3	1	−1	1	1	−1
Γ_4	1	−1	1	−1	1
Γ_5	2	0	−2	0	0

Matrices of the two-dimensional representation:

	Γ_5
ε	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$
α	$\begin{pmatrix}0&-1\\1&0\end{pmatrix}$
α^2	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$
β	$\begin{pmatrix}-1&0\\0&1\end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$

422 D_4	$\alpha = C_{4z}$ $\beta = C_{2x}$	$\Gamma_1 : A_1 = \chi_1$		x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$	z	
		$\Gamma_3 : B_1 = \chi_3$		x^2-y^2
		$\Gamma_4 : B_2 = \chi_4$		xy
		$\Gamma_5 : E = \chi_1$	x, y	xz, yz
$4mm$ C_{4v}	$\alpha = C_{4z}$ $\beta = \sigma_v$	$\Gamma_1 : A_1 = \chi_1$	z	x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$		
		$\Gamma_3 : B_1 = \chi_3$		x^2-y^2
		$\Gamma_4 : B_2 = \chi_4$		xy
		$\Gamma_5 : E = \chi_1$	x, y	xz, yz
$\bar{4}2m$ D_{2d}	$\alpha = S_{4z}$ $\beta = C_{2v}$ $\alpha\beta = \sigma_d$	$\Gamma_1 : A_1 = \chi_1$		x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$		
		$\Gamma_3 : B_1 = \chi_3$		x^2-y^2
		$\Gamma_4 : B_2 = \chi_4$	z	xy
		$\Gamma_5 : E = \chi_1$	x, y	xz, yz

(*i*) D_6

D_6	ε	α	α^2	α^3	β	$\alpha\beta$
n	1	2	2	1	3	3
Order	1	6	3	2	2	2
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	1	−1	−1
Γ_3	1	−1	1	−1	1	−1
Γ_4	1	−1	1	−1	−1	1
Γ_5	2	1	−1	−2	0	0
Γ_6	2	−1	−1	2	0	0

Matrices of the two-dimensional representations:

	Γ_5	Γ_6
ε	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$
α	$\begin{pmatrix}1&-1\\1&0\end{pmatrix}$	$\begin{pmatrix}0&-1\\1&-1\end{pmatrix}$
α^2	$\begin{pmatrix}0&-1\\1&-1\end{pmatrix}$	$\begin{pmatrix}-1&1\\-1&0\end{pmatrix}$
α^3	$\begin{pmatrix}-1&0\\0&-1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&1\end{pmatrix}$
β	$\begin{pmatrix}-1&1\\0&1\end{pmatrix}$	$\begin{pmatrix}-1&1\\0&1\end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix}-1&0\\-1&1\end{pmatrix}$	$\begin{pmatrix}0&-1\\-1&0\end{pmatrix}$

622 D_6	$\alpha = C_{6z}$ $\beta = C_{2x}$	$\Gamma_1 : A_1 = \chi_1$		x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$	z	
		$\Gamma_3 : B_1 = \chi_3$		x^2-y^2
		$\Gamma_4 : B_2 = \chi_4$		xy
		$\Gamma_5 : E_1 = \chi_1$	x, y	xz, yz
		$\Gamma_6 : E_2 = \chi_2$		
$6mm$ C_{6v}	$\alpha = C_{6z}$ $\beta = \sigma_v$	$\Gamma_1 : A_1 = \chi_1$	z	x^2+y^2, z^2
		$\Gamma_2 : A_2 = \chi_2$		
		$\Gamma_3 : B_1 = \chi_3$		x^2-y^2
		$\Gamma_4 : B_2 = \chi_4$		xy
		$\Gamma_5 : E_1 = \chi_1$	x, y	xz, yz
		$\Gamma_6 : E_2 = \chi_2$		
$\bar{6}2m$ D_{3h}	$\alpha = S_{6z}$ $\beta = C_{2v}$ $\alpha\beta = \sigma_d$	$\Gamma_1 : A_1' = \chi_1$		x^2+y^2, z^2
		$\Gamma_2 : A_2' = \chi_2$		
		$\Gamma_3 : A_1'' = \chi_3$		x^2-y^2
		$\Gamma_4 : A_2'' = \chi_4$	z	xy
		$\Gamma_5 : E' = \chi_2$		xz, yz
		$\Gamma_6 : E'' = \chi_1$	x, y	
$\bar{3}m$ D_{3v}	$\alpha = S_{3z}$ $\beta = \sigma_d$	$\Gamma_1 : A_{1g} = \chi_1^+$		x^2+y^2, z^2
		$\Gamma_2 : A_{2g} = \chi_2^+$		
		$\Gamma_3 : A_{1u} = \chi_1^-$	z	
		$\Gamma_4 : A_{2u} = \chi_2^-$		
		$\Gamma_5 : E_u = \chi_1^-$	x, y	
		$\Gamma_6 : E_g = \chi_1^+$		$xz.yz, xy, x^2-y^2$

(*j*) T [$\omega = \exp(2\pi i/3)$].

T	ε	α	α^2	β
n	1	4	4	3
Order	1	3	3	2
Γ_1	1	1	1	1
Γ_2	1	ω	ω^2	1
Γ_3	1	ω^2	ω	1
Γ_4	3	0	0	−1

Table 1.2.6.5 (*cont.*)

Real representations of dimension $d > 1$:

	$\Gamma_2 \oplus \Gamma_3$	Γ_4
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$
α^2	$\begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
β	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

23	$\alpha = C_{3d}$	$\Gamma_1 : A = \chi_1$		$x^2 + y^2 + z^2$
T	$\beta = C_{2z}$	$\Gamma_2 \oplus \Gamma_3 : E = \chi_{3c} + \chi_{3c}^*$		$x^2 - y^2, x^2 - z^2$
		$\Gamma_4 : T = \chi_1$	x, y, z	xy, xz, yz

(*k*) O

O	ε	β	α^2	α	$\alpha\beta$
n	1	8	3	6	6
Order	1	3	2	4	2
Γ_1	1	1	1	1	1
Γ_2	1	1	1	-1	-1
Γ_3	2	-1	2	0	0
Γ_4	3	0	-1	1	-1
Γ_5	3	0	-1	-1	1

Higher-dimensional representations:

	Γ_3	Γ_4	Γ_5
ε	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
β	$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
α^2	$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
α	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
$\alpha\beta$	$\begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix}$	$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}$

432	$\alpha = C_{4z}$	$\Gamma_1 : A_1 = \chi_1$		$x^2 + y^2 + z^2$
O	$\beta = C_{3d}$	$\Gamma_2 : A_2 = \chi_2$		
	$\alpha\beta = C_2$	$\Gamma_3 : E = \chi_3$		$x^2 - y^2, y^2 - z^2$
		$\Gamma_4 : T_1 = \chi_1$	x, y, z	
		$\Gamma_5 : T_2 = \chi_2$		xy, xz, yz
$\bar{4}3m$	$\alpha = S_{4z}$	$\Gamma_1 : A_1 = \chi_1$		$x^2 + y^2 + z^2$
T_d	$\beta = C_{3d}$	$\Gamma_2 : A_2 = \chi_2$		
	$\alpha\beta = \sigma_d$	$\Gamma_3 : E = \chi_3$		$x^2 - y^2, y^2 - z^2$
		$\Gamma_4 : T_1 = \chi_1$		
		$\Gamma_5 : T_2 = \chi_2$	x, y, z	xy, yz, xz

Other point groups which are of second class and contain $-E$. See Table 1.2.6.6(*a*).

Group	Isomorphism class	Rotation subgroup
$4/m$	$C_4 \times \mathbb{Z}_2$	4
$6/m$	$C_6 \times \mathbb{Z}_2$	6
mmm	$D_2 \times \mathbb{Z}_2$	222
$4/mmm$	$D_4 \times \mathbb{Z}_2$	422
$6/mmm$	$D_6 \times \mathbb{Z}_2$	622
$m\bar{3}$	$T \times \mathbb{Z}_2$	23
$m\bar{3}m$	$O \times \mathbb{Z}_2$	432

Table 1.2.6.6. *Direct products with* $\{E, \bar{1}\}$ *and* $\{E, 1'\}$

(*a*) With $\{E, \bar{1}\}$.

$K \times \mathbb{Z}_2$	$R \in K$	$\bar{R}$
Γ_g	$\chi(R)$	$\chi(R)$
Γ_u	$\chi(R)$	$-\chi(R)$

$4/m$	$C_4 \times \mathbb{Z}_2$	*cf.* 4
$6/m$	$C_6 \times \mathbb{Z}_2$	*cf.* 6
mmm	$D_2 \times \mathbb{Z}_2$	*cf.* 222
$4/mmm$	$D_4 \times \mathbb{Z}_2$	*cf.* 422
$6/mmm$	$D_6 \times \mathbb{Z}_2$	*cf.* 622
$m\bar{3}$	$T \times \mathbb{Z}_2$	*cf.* 23
$m\bar{3}m$	$O \times \mathbb{Z}_2$	*cf.* 432

(*b*) With $\{E, 1'\}$.

$K \times \mathbb{Z}_2$	$R \in K$	R'
Γ_+	$\chi(R)$	$\chi(R)$
Γ_-	$\chi(R)$	$-\chi(R)$

$1'$	$C_1 \times \mathbb{Z}_2$	*cf.* 1
$21'$	$C_2 \times \mathbb{Z}_2$	*cf.* 2
$m1'$	$C_2 \times \mathbb{Z}_2$	*cf.* m
$2221'$	$D_2 \times \mathbb{Z}_2$	*cf.* 222
$2mm1'$	$D_2 \times \mathbb{Z}_2$	*cf.* $2mm$
$41'$	$C_4 \times \mathbb{Z}_2$	*cf.* 4
$\bar{4}1'$	$C_4 \times \mathbb{Z}_2$	*cf.* $\bar{4}$
$4mm1'$	$D_4 \times \mathbb{Z}_2$	*cf.* $4mm$
$4221'$	$D_4 \times \mathbb{Z}_2$	*cf.* 422
$\bar{4}2m1'$	$D_4 \times \mathbb{Z}_2$	*cf.* $\bar{4}2m$
$31'$	$C_3 \times \mathbb{Z}_2$	*cf.* 3
$321'$	$D_3 \times \mathbb{Z}_2$	*cf.* 32
$\bar{3}1'$	$C_6 \times \mathbb{Z}_2$	*cf.* $\bar{3}$
$3m1'$	$D_3 \times \mathbb{Z}_2$	*cf.* $3m$
$6mm1'$	$D_6 \times \mathbb{Z}_2$	*cf.* $6mm$
$61'$	$C_6 \times \mathbb{Z}_2$	*cf.* 6
$\bar{6}1'$	$C_6 \times \mathbb{Z}_2$	*cf.* $\bar{6}$
$6221'$	$D_6 \times \mathbb{Z}_2$	*cf.* 622
$\bar{6}2m1'$	$D_6 \times \mathbb{Z}_2$	*cf.* $\bar{6}2m$
$231'$	$T \times \mathbb{Z}_2$	*cf.* 23
$4321'$	$O \times \mathbb{Z}_2$	*cf.* 432
$\bar{4}3m1'$	$O \times \mathbb{Z}_2$	*cf.* $\bar{4}3m$

(*c*) With $\{E, \bar{1}\}$ and $\{E, 1'\}$.

$K \times \mathbb{Z}_2 \times \mathbb{Z}_2$	$R \in K$	$\bar{R}$	R'	$\bar{R}'$
Γ_{g+}	$\chi(R)$	$\chi(R)$	$\chi(R)$	$\chi(R)$
Γ_{u+}	$\chi(R)$	$-\chi(R)$	$\chi(R)$	$-\chi(R)$
Γ_{g-}	$\chi(R)$	$\chi(R)$	$-\chi(R)$	$-\chi(R)$
Γ_{u-}	$\chi(R)$	$-\chi(R)$	$-\chi(R)$	$\chi(R)$

$\bar{1}'$	$C_1 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 1
$21'/m$	$C_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 2
$4/m1'$	$C_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 4
$6/m1'$	$C_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 6
$mmm1'$	$D_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 222
$4/mmm1'$	$D_4 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 422
$\bar{3}m1'$	$D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* $3m$
$6/mmm1'$	$D_6 \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 622
$m\bar{3}1'$	$T \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 23
$m(\bar{3})m1'$	$O \times \mathbb{Z}_2 \times \mathbb{Z}_2$	*cf.* 432

groups generated by $\bar{1}$, $1'$ and $\{\bar{1}, 1'\}$ are given in Tables 1.2.6.6(*a*), (*b*) and (*c*), respectively.

Table 1.2.6.7. The representations of a point group are also representations of their double groups. In addition, there are extra representations which give projective representations of the point groups. For several cases, these are associated with an ordinary representation. As extra representations, those irreducible representations of the double point groups that give rise to projective representations of the point groups with a factor system that is not associated with the trivial one are given. These do not correspond to ordinary representations of the single group.

Table 1.2.6.8. If one chooses for each element of a point group one of the two corresponding $SU(2)$ elements, the latter form a projective representation of the point group. If one selects for the rotation $R \in K \subset SO(3)$ the element

$$u(R) = E\cos(\varphi/2) + i(\boldsymbol{\sigma}\cdot\mathbf{n})\sin(\varphi/2),$$

where φ is the rotation angle and $\mathbf{n}$ the rotation axis, and for $R \in K \subset O(3)\backslash SO(3)$ the element

$$u(R) = E\cos(\psi/2) + i(\boldsymbol{\sigma}\cdot\mathbf{n})\sin(\psi/2),$$

where ψ and $\mathbf{n}$ are the rotation angle and axis of the rotation $-R$, the matrices $u(R)$ form a projective representation:

$$u(R)u(R') = \omega_s(R, R')u(RR').$$

The factor system ω_s is the spin factor system. It is determined *via* the generators and defining relations

$$W_i(A_1, \ldots, A_p) = E$$

of the point group K. Then

$$W_i(u(A_1), \ldots, u(A_p)) = \lambda_i E,$$

and the factors λ_i fix uniquely the class of the factor system ω_s. These factors are given in the table.

Because $\bar{1}$ is represented by the unit matrix in spin space, the double groups of two isomorphic point groups obtained from each other by replacing the elements $R \in O(3)\backslash SO(3)$ by $-R$ are the same.

The projective representations with factor system ω_s may sometimes be associated with one with a trivial factor system. If this is the case, there are actually no extra representations of the

Table 1.2.6.7. *Extra representations of double point groups*

222^d	E	$-E$	$\pm A$	$\pm B$	$\pm AB$				
Γ_5'	2	-2	0	0	0				
422^d	E	$-E$	$\pm A^2$	A	$-A$	$\pm B$	$\pm AB$		
Γ_6'	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0		
Γ_7'	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0		
622^d	E	$-E$	A^2	$-A^2$	$\pm B$	$\pm A^3$	A^5	$-A^5$	$\pm A^3B$
Γ_8'	2	-2	1	-1	0	0	$\sqrt{3}$	$-\sqrt{3}$	0
Γ_9'	2	-2	1	-1	0	0	$-\sqrt{3}$	$\sqrt{3}$	0
Γ_7'	2	-2	-2	2	0	0	0	0	0
23^d	E	$-E$	A	$-A$	A^2	$-A^2$	$\pm B$		
Γ_5'	2	-2	1	-1	1	-1	0		
Γ_6'	2	-2	ω	ω^4	ω^2	ω^5	0		
Γ_7'	2	-2	ω^5	ω^2	ω^4	ω	0		
432^d	E	$-E$	B	$-B$	$\pm A^2$	A	$-A$	$\pm AB$	
Γ_6'	2	-2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	
Γ_7'	2	-2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	
Γ_8'	4	-4	-1	1	0	0	0	0	

Table 1.2.6.8. *Projective spin representations of the 32 crystallographic point groups*

Point group	Relations giving λ_i	Double group	Extra representations
1 $\bar{1}$	$A = E$ $A^2 = E$	1^d	No No
2, *m* 2/*m*	$A^2 = -E$ $A^2 = B^2 = -E$, $(AB)^2 = E$	2^d	No
222, 2*mm* *mmm*	$A^2 = B^2 = (AB)^2 = -E$ $A^2 = B^2 = (AB)^2 = -E$ $C^2 = E$, $AC = CA$, $BC = CB$	222^d	Yes
4, $\bar{4}$ 4/*m*	$A^4 = -E$ $A^4 = B^2 = -E$, $AB = BA$	4^d	No
422, 4*mm*, $\bar{4}2m$ 4/*mmm*	$A^4 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E$, $AC = CA$, $BC = CB$	422^d	Yes
3 $\bar{3}$	$A^3 = -E$ $A^6 = E$	3^d	No
32, 3*m* $\bar{3}m$	$A^3 = B^2 = (AB)^2 = -E$ $A^6 = E$, $B^2 = (AB)^2 = -E$	32^d	No
6, $\bar{6}$ 6/*m*	$A^6 = -E$ $A^6 = B^2 = -E$, $AB = BA$	6^d	No
622, 6*mm*, $\bar{6}2m$ 6/*mmm*	$A^6 = B^2 = (AB)^2 = -E$ As above, plus $C^2 = E$, $AC = CA$, $BC = CB$	622^d	Yes
23 *m*3	$A^3 = B^2 = (AB)^3 = -E$ As above, plus $C^2 = E$, $AC = CA$, $BC = CB$	23^d	Yes
432, $\bar{4}3m$ $m\bar{3}m$	$A^4 = B^3 = (AB)^2 = -E$ As above, plus $C^2 = E$, $AC = CA$, $BC = CB$	432^d	Yes

double group. If there are extra representations, these are irreducible representations of the double group: see Table 1.2.6.7.

Table 1.2.6.9. For the 32 three-dimensional crystallographic point groups, the character of the vector representation Γ and the number of times the identity representation occurs in a number of tensor products of this vector representation are given. This is identical to the number of free parameters in a tensor of the corresponding type. For the direct products $K \times C_2$, the character is equal to that of K on the rotation subgroup, and its opposite $[\chi(-R) = -\chi(R)]$ for the coset $-K$.

Table 1.2.6.10. The irreducible projective representations of the 32 three-dimensional crystallographic point groups that have a factor system that is not associated to a trivial one. In three (and two) dimensions all factor systems are of order two.

Table 1.2.6.11. The special points in the Brillouin zones. Strata of irreducible representations of the space groups are characterized by the wavevector **k** of such a point and a (possibly projective) irreducible representation of the point group $K_{\mathbf{k}}$. The latter is the intersection of the symmetry group of **k** (the group of **k** for the holohedral point group) and the point group of the space group. For each Bravais class the special points for the holohedry are given. These are given by their coordinates with respect to a basis of the reciprocal lattice of the conventional cell. These points correspond to Wyckoff positions in the corresponding dual lattice. The symbols for these Wyckoff positions and their site symmetry are given. A well known notation for the special points is that of Kovalev, as used in his book on representations of space groups. Correspondence with the notation in Kovalev (1987) is given.

Table 1.2.6.12. The three-dimensional crystallographic magnetic and nonmagnetic point groups of type I (trivial magnetic, no antichronous elements), type II (nonmagnetic, containing time reversal as an element) and type III (nontrivial magnetic, without time reversal itself, but with antichronous elements).

1.2.7. Introduction to the accompanying software *Tenχar*

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1.2.7.1. *Overview*

The determination of tensors with specified properties often requires long calculations. In principle the algorithms are simple, but in complicated cases errors can be made. This is therefore a situation in which it is best to rely on computer calculations. For this reason, this volume is accompanied by two software packages. Here we shall give a short introduction to the *Tenχar* package that deals with tensors with specific symmetry properties in the first module, and with characters of representations of point groups in the second module. The latter play a role when determining the number of independent elements of a tensor invariant under a given point group, but they are much more widely applicable.

The software package has a graphical interface with windows and buttons. When the program is started, a window opens up in which a choice may be made between the tensor part or the character part of the program.

Within each of the two sections of the program, the results of the calculations are given in numbered windows. It is possible to browse through the various pages. Each page may be sent to a separate window (by the command 'to window'), or to a file (by the command 'to file'). Opened windows may be closed again using a 'close' button.

Special features of the package are that it is dimension- and rank-independent, and that it performs the calculations in an exact way. The number of dimensions and the rank are only limited by the computer memory and by the time the program needs for higher dimensions and ranks. The calculations are exact in the sense of the computer algebra software. Here this is achieved by performing the calculations with integers and

Table 1.2.6.9. *Number of free parameters of some tensors*

Group	Isomorphism class	Character of the vector representation	Multiplicity identity representation in				
			$\Gamma^{\otimes 2}$	$\Gamma_s^{\otimes 2}$	$\Gamma^{\otimes 3}$	$\Gamma \otimes \Gamma_s^{\otimes 2}$	$(\Gamma_s^{\otimes 2})_s^{\otimes 2}$
1	C_1	3	9	6	27	18	21
$\bar{1}$	C_2	3, −3	9	6	0	0	21
2	C_2	3, −1	5	4	13	8	13
m	C_2	3, 1	5	4	14	10	13
$2/m$	$C_2 \times C_2$		5	4	0	0	13
222	D_2	3, −1, −1, −1	3	3	6	3	9
$2mm$	D_2	3, 1, 1, −1	3	3	7	5	9
mmm	$D_2 \times C_2$		3	3	0	0	9
3	C_3	3, 0, 0	3	2	9	6	9
$\bar{3}$	$C_3 \times C_2$		3	2	0	0	9
32	D_3	3, 0, −1	2	2	4	2	6
$3m$	D_3	3, 0, 1	2	2	5	4	6
$\bar{3}m$	$D_3 \times C_2$		2	2	0	0	6
6	C_6	3, 2, 0, −1, 0, 2	3	2	7	4	5
$\bar{6}$	C_6	3, 2, 0, 1, 0, −2	3	2	2	2	5
$6/m$	$C_6 \times C_2$		3	2	0	0	5
622	D_6	3, 2, 0, −1, −1, −1	2	2	3	1	5
$6mm$	D_6	3, 2, 0, −1, 1, 1	2	2	4	3	5
$\bar{6}2m$	D_6	3, −2, 0, 1, −1, 1	2	2	1	1	5
$6/mmm$	$D_6 \times C_2$		2	2	0	0	5
4	C_4	3, 1, −1, 1	3	2	7	4	7
$\bar{4}$	C_4	3, −1, −1, −1	3	2	6	4	7
$4/m$	$C_4 \times C_2$		3	2	0	0	7
422	D_4	3, 1, −1, −1, −1	2	2	3	1	6
$4mm$	D_4	3, 1, −1, 1, 1	2	2	4	3	6
$\bar{4}2m$	D_4	3, −1, −1, −1, 1	2	2	3	2	6
$4/mmm$	$D_4 \times C_2$		2	2	0	0	6
23	T	3, 0, 0, −1	1	1	2	1	3
$m3$	$T \times C_2$		1	1	0	0	3
432	O	3, 0, −1, 1, −1	1	1	1	0	3
$\bar{4}3m$	O	3, 0, −1, −1, 1	1	1	1	1	3
$m3m$	$O \times C_2$		1	1	0	0	3

Table 1.2.6.10. *Irreducible projective representations of the 32 crystallographic point groups*

(*a*) D_2

$A^2 = B^2 = E, (AB)^2 = -E$				
Elements	E	A	B	AB
Γ'_5	2	0	0	0

(*b*) D_4

$A^4 = -E, B^2 = (AB)^2 = E$								
Elements	E	A^2	A	A^3	B	A^2B	AB	A^3B
Γ'_6	2	0	$i\sqrt{2}$	$i\sqrt{2}$	0	0	0	0
Γ'_7	2	0	$-i\sqrt{2}$	$-i\sqrt{2}$	0	0	0	0

(*c*) D_6

$A^6 = B^2 = E, (AB)^2 = -E$												
Elements	E	A^2	A^4	B	A^2B	A^4B	A^3	A	A^5	AB	A^3B	A^5B
Γ'_7	2	2	2	0	0	0	0	0	0	0	0	0
Γ'_8	2	−1	−1	0	0	0	0	$i\sqrt{3}$	$-i\sqrt{3}$	0	0	0
Γ'_9	2	−1	−1	0	0	0	0	$-i\sqrt{3}$	$i\sqrt{3}$	0	0	0

(*d*) T [$\omega = \exp(2\pi i/3)$].

$A^3 = E, B^2 = (AB)^3 = -E$						
Elements	E	A	BAB	BA	AB	A^2
Γ'_5	2	−1	1	1	1	−1
Γ'_6	2	ω^5	ω^2	ω^2	ω^2	ω^5
Γ'_7	2	ω	ω^4	ω^4	ω^4	ω
Elements	ABA	A^2B	BA^2	B	ABA^2	A^2BA
Γ'_5	−1	−1	−1	0	0	0
Γ'_6	ω^5	ω^5	ω^5	0	0	0
Γ'_7	ω	ω	ω	0	0	0

(*e*) O

$A^4 = -E, B^3 = (AB)^2 = E$						
Elements	E	B	AB^2A	A^2B	BA^2	B^2
Γ'_6	2	−1	1	−1	−1	−1
Γ'_7	2	−1	1	−1	−1	−1
Γ'_8	4	1	−1	1	1	1
Elements	BA^2B	ABA^3	A^2B^2	A^2	BA^2B^2	B^2A^2B
Γ'_6	1	1	1	0	0	0
Γ'_7	1	1	1	0	0	0
Γ'_8	−1	−1	−1	0	0	0
Elements	A	A^3	A^3B	BA^3	B^2A	AB^2
Γ'_6	$i\sqrt{2}$	$i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$	$-i\sqrt{2}$
Γ'_7	$-i\sqrt{2}$	$-i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$	$i\sqrt{2}$
Γ'_8	0	0	0	0	0	0
Elements	A^2B^2A	BA	AB	AB^2A^2	AB^2A^2B	B^2AB^2
Γ'_6	0	0	0	0	0	0
Γ'_7	0	0	0	0	0	0
Γ'_8	0	0	0	0	0	0

(*f*) $C_4 \times C_2$

$A^4 = B^2 = E, AB = -BA$								
Elements	E	A	A^2	A^3	B	AB	A^2B	A^3B
Γ'_9	2	0	2	0	0	0	0	0
Γ'_{10}	2	0	−2	0	0	0	0	0

(*g*) $C_6 \times C_2$

$A^6 = B^2 = E, AB = -BA$												
Elements	E	A	A^2	A^3	A^4	A^5	B	AB	A^2B	A^3B	A^4B	A^5B
Γ'_{13}	2	0	2	0	2	0	0	0	0	0	0	0
Γ'_{14}	2	0	$2\omega^2$	0	$2\omega^4$	0	0	0	0	0	0	0
Γ'_{15}	2	0	$2\omega^4$	0	$2\omega^4$	0	0	0	0	0	0	0

Table 1.2.6.10 (*cont.*)

(*h*) $D_2 \times C_2$

$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_9	2	0	0	0	2	0	0	0
Γ'_{10}	2	0	0	0	−2	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{11}	2	0	2	0	0	0	0	0
Γ'_{12}	2	0	−2	0	0	0	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{13}	2	$2i$	0	0	0	0	0	0
Γ'_{14}	2	$-2i$	0	0	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{15}	2	0	0	0	0	0	2	0
Γ'_{16}	2	0	0	0	0	0	−2	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{17}	2	0	0	0	0	$2i$	0	0
Γ'_{18}	2	0	0	0	0	$-2i$	0	0
$A^2 = E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{19}	2	0	0	$2i$	0	0	0	0
Γ'_{20}	2	0	0	$-2i$	0	0	0	0
$A^2 = -E, B^2 = C^2 = (AB)^2 = E, AC = -CA, BC = -CB$								
Elements	E	A	B	AB	C	AC	BC	ABC
Γ'_{21}	2	0	0	0	0	0	0	$2i$
Γ'_{22}	2	0	0	0	0	0	0	$-2i$

cyclotomics. Use of arbitrary real numbers would imply a finite precision.

Detailed instructions for the use of the program, together with a guided tour (*QuickStart*), can be found in the manual for the program.

1.2.7.2. *Tensors*

The tensor module of *Tenχar* determines the number of independent elements and the relations between the elements of tensors and pseudotensors invariant under a chosen point group and with specified permutation symmetry of the indices. Although the list of point groups provided in a database is limited to dimensions two and three, the program runs for arbitrary dimensions. Similarly, the choice of index permutation symmetry is limited to rank smaller than or equal to four. This is also not a restriction of the program, which works for arbitrary rank. For higher dimensions and higher ranks, the user needs to provide additional information. The limiting factors are in fact the speed, which becomes low for higher dimensions and/or higher rank, and the available memory, which must be sufficient to store the tensor elements.

When the program is started and the tensor part is chosen *via* a button, a selection box opens. The user can specify dimension and rank in open fields. A field without a coloured border has a formally correct content, but the user should check whether the pregiven numbers correspond to his wishes. In open fields with a coloured border, additional information must be given. Clicking on the button 'point group' results in the opening of a new selection window. A specific two- or three-dimensional point group may be chosen *via* geometric crystal classes. This point group may be viewed if wished. The chosen point group is given by generating matrices and is the one under which the (pseudo)tensor is invariant.

The second symmetry is the index permutation symmetry. For tensors and pseudotensors up to rank four, all possible symmetries are tabulated after clicking 'permutation symmetry'. The indices are numbered from 0 to $r - 1$, where r is the rank. The symbol for a tensor symmetric in the indices 2 and 3 is (2 3), and it is [2 3] if the tensor gets a minus sign under permutation. Arbitrary combinations of symmetric and antisymmetric series can be made. For example, (0 1) 2 [3 4] is a rank-five tensor which is symmetric in the first two indices and antisymmetric in the last two indices. The symbol (0 1 2) characterizes a rank-three tensor that is fully symmetric in all indices. For (pseudo)tensors of rank five and higher, the user needs to specify the permutation symmetry using parentheses in this way. Symmetrization of other pairs is similar. For example, if the rank-three tensor T is symmetric in the first and last indices, the symbol for its permutation character is (0 2) 1. Then $T_{xyz} = T_{zyx}$.

Different settings of the point group may be specified. The standard setting of a point group as given in *International Tables for Crystallography* Volume A may be different from the one to be specified. In this case, the user may perform a basis transformation which transforms the standard setting to the desired setting. This is done *via* the button 'basis transformation'. The standard setting is chosen with 'no transformation'. The transformation from a hexagonal to an orthogonal (Cartesian) basis is performed by selecting 'hC transformation'.

Finally, the tensor or pseudotensor with the specified point group and permutation symmetry is calculated and displayed in a (numbered) window. The command for this is given by clicking on the button 'tensor' or 'pseudotensor', respectively. In the window appear the input data, such as the point group, the

Table 1.2.6.11. *Special points in the Brillouin zones in three dimensions*

(*a*) Triclinic

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{1}$	k_8
b	$00\frac{1}{2}$	$\bar{1}$	k_7
c	$0\frac{1}{2}0$	$\bar{1}$	k_6
d	$\frac{1}{2}00$	$\bar{1}$	k_5
e	$\frac{1}{2}\frac{1}{2}0$	$\bar{1}$	k_4
f	$\frac{1}{2}0\frac{1}{2}$	$\bar{1}$	k_3
g	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_2
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_1

(*b*) Monoclinic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_7
b	$00\frac{1}{2}$	$2/m$	k_{11}
c	$\frac{1}{2}00$	$2/m$	k_{12}
d	$0\frac{1}{2}0$	$2/m$	k_{13}
e	$0\frac{1}{2}\frac{1}{2}$	$2/m$	k_9
f	$\frac{1}{2}0\frac{1}{2}$	$2/m$	k_8
g	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{14}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{10}
i	00γ	2	k_3
j	$0\frac{1}{2}\gamma$	2	k_5
k	$\frac{1}{2}0\gamma$	2	k_4
l	$\frac{1}{2}\frac{1}{2}\gamma$	2	k_6
m	$\alpha\beta0$	m	k_1
n	$\alpha\beta\frac{1}{2}$	m	k_2

(*c*) Monoclinic *A*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$2/m$	k_6
b	010	$2/m$	k_8
c	$\frac{1}{2}00$	$2/m$	k_7
d	$\frac{1}{2}10$	$2/m$	k_9
e	$0\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_4
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_5
g	00γ	2	k_2
h	$\frac{1}{2}0\gamma$	2	k_3
i	$\alpha\beta0$	m	k_1

(*d*) Orthorhombic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{19}
b	$\frac{1}{2}00$	mmm	k_{20}
c	$00\frac{1}{2}$	mmm	k_{22}
d	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{24}
e	$0\frac{1}{2}0$	mmm	k_{21}
f	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{25}
g	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{23}
h	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	mmm	k_{26}
i	$\alpha00$	$2mm$	k_7
j	$\alpha0\frac{1}{2}$	$2mm$	k_{12}
k	$\alpha\frac{1}{2}0$	$2mm$	k_{10}
l	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_{11}
m	$0\beta0$	$m2m$	k_8
n	$0\beta\frac{1}{2}$	$m2m$	k_{15}
o	$\frac{1}{2}\beta0$	$m2m$	k_{13}
p	$\frac{1}{2}\beta\frac{1}{2}$	$m2m$	k_{14}
q	00γ	$mm2$	k_9
r	$0\frac{1}{2}\gamma$	$mm2$	k_{18}
s	$\frac{1}{2}0\gamma$	$mm2$	k_{16}
t	$\frac{1}{2}\frac{1}{2}\gamma$	$mm2$	k_{17}
u	$0\beta\gamma$	m	k_1
v	$\frac{1}{2}\beta\gamma$	$m11$	k_2
w	$\alpha0\gamma$	$1m1$	k_3
x	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4
y	$\alpha\beta0$	$11m$	k_5
z	$\alpha\beta\frac{1}{2}$	$11m$	k_6

(*e*) Orthorhombic *C*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	010	mmm	k_{15}
c	$01\frac{1}{2}$	mmm	k_{17}
d	$00\frac{1}{2}$	mmm	k_{16}
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$2/m$	k_{13}
g	$\alpha00$	$2mm$	k_8
h	$\alpha0\frac{1}{2}$	$2mm$	k_9
i	$0\beta0$	$m2m$	k_{10}
j	$0\beta\frac{1}{2}$	$m2m$	k_{11}
k	00γ	$mm2$	k_6
l	01γ	$mm2$	k_7
m	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_5
n	$0\beta\gamma$	$m11$	k_1
o	$\alpha0\gamma$	$1m1$	k_2
p	$\alpha\beta0$	$11m$	k_3
q	$\alpha\beta\frac{1}{2}$	$11m$	k_4

(*f*) Orthorhombic *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{17}
b	001	mmm	k_{18}
c	$0\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{13}
	$1\frac{1}{2}\frac{1}{2}$	$2/m11$	k_{10}
d	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{14}
	$\frac{1}{2}1\frac{1}{2}$	$12/m1$	k_{11}
e	$\frac{1}{2}\frac{1}{2}0$	$112/m$	k_{15}
	$\frac{1}{2}\frac{1}{2}1$	$112/m$	k_{12}
f	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	222	k_{16}
g	$\alpha00$	$2mm$	k_7
h	$0\beta0$	$m2m$	k_8
i	00γ	$mm2$	k_9
j	$\frac{1}{2}\frac{1}{2}\gamma$	112	k_6
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\frac{1}{2}\frac{1}{2}$	211	k_4
m	$0\beta\gamma$	$m11$	k_1
n	$\alpha0\gamma$	$1m1$	k_2
o	$\alpha\beta0$	$11m$	k_3

(*g*) Orthorhombic *F*

k		$K_{\mathbf{k}}$	Kovalev
a	000	mmm	k_{14}
b	100	mmm	k_{15}
c	010	mmm	k_{16}
d	001	mmm	k_{17}
e	$\alpha00$	$2mm$	k_4
f	$\alpha10$	$2mm$	k_5
g	$0\beta0$	$m2m$	k_6
h	$1\beta0$	$m2m$	k_7
i	00γ	$mm2$	k_8
j	01γ	$mm2$	k_9
k	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{10}
	$-\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{11}
	$\frac{1}{2}-\frac{1}{2}\frac{1}{2}$	$\bar{1}$	k_{12}
	$\frac{1}{2}\frac{1}{2}-\frac{1}{2}$	$\bar{1}$	k_{13}
l	$0\beta\gamma$	$m11$	k_1
m	$\alpha0\gamma$	$1m1$	k_2
n	$\alpha\beta0$	$11m$	k_3

(*h*) Tetragonal *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{17}
b	$00\frac{1}{2}$	$4/mmm$	k_{19}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{18}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$4/mmm$	k_{20}
e	$0\frac{1}{2}\frac{1}{2}$	mmm	k_{16}
f	$0\frac{1}{2}0$	mmm	k_{15}
g	00γ	$4mm$	k_{13}
h	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_{14}
i	$0\frac{1}{2}\gamma$	$mm2$	k_{12}
j	$\alpha\alpha0$	$2mm$	k_{10}
k	$\alpha\alpha\frac{1}{2}$	$2mm$	k_{11}
l	$0\beta0$	$m2m$	k_8
m	$0\beta\frac{1}{2}$	$m2m$	k_9
n	$\alpha\frac{1}{2}0$	$2mm$	k_6
o	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_7
p	$\alpha\beta0$	$11m$	k_1
q	$\alpha\beta\frac{1}{2}$	$11m$	k_2
r	$\alpha\alpha\gamma$	m	k_5
s	$0\beta\gamma$	$m11$	k_3
t	$\alpha\frac{1}{2}\gamma$	$1m1$	k_4

(*i*) Tetragonal *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$4/mmm$	k_{14}
b	001	$4/mmm$	k_{15}
c	$\frac{1}{2}\frac{1}{2}0$	mmm	k_{13}
d	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}m2$	k_{12}
e	00γ	$4mm$	k_{10}
f	$\frac{1}{2}0\frac{1}{2}$	$12/m1$	k_{11}
g	$\frac{1}{2}\frac{1}{2}\gamma$	$2mm$	k_9
h	$\alpha\alpha0$	$2mm$	k_7
i	$\alpha00$	$2mm$	k_7
j	$\alpha(1-\alpha)0$	$2mm$	k_8
k	$\frac{1}{2}\beta\frac{1}{2}$	121	k_5
l	$\alpha\beta0$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3
	$\alpha(1-\alpha)\gamma$	m	k_4
n	$\alpha0\gamma$	$1m1$	k_1

(*j*) Trigonal *R* (rhombohedral axes)

k		$K_{\mathbf{k}}$	Kovalev
a	000	$\bar{3}m$	k_7
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_8
c	$\alpha\alpha\alpha$	$3m$	k_6
d	$00\frac{1}{2}$	$2/m$	k_4
e	$\frac{1}{2}\frac{1}{2}0$	$2/m$	k_5
f	$\alpha(-\alpha)0$	2	k_2
g	$\alpha(-\alpha)\frac{1}{2}$	2	k_2
h	$\alpha\beta\beta$	m	k_1

Table 1.2.6.11 (*cont.*)

(*k*) Hexagonal *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$6/mmm$	k_{16}
b	$00\frac{1}{2}$	$6/mmm$	k_{17}
c	$\frac{1}{3}\frac{1}{3}0$	$\bar{6}m2$	k_{13}
d	$\frac{1}{3}\frac{1}{3}\frac{1}{2}$	$\bar{6}m2$	k_{15}
e	00γ	$6mm$	k_{11}
f	$\frac{1}{2}00$	mmm	k_{12}
g	$\frac{1}{2}0\frac{1}{2}$	mmm	k_{14}
h	$\frac{1}{3}\frac{1}{3}\gamma$	$3m$	k_{10}
i	$\frac{1}{2}0\gamma$	$2mm$	k_9
j	$\alpha 00$	$2mm$	k_5
k	$\alpha 0\frac{1}{2}$	$2mm$	k_7
l	$\alpha\alpha 0$	$2mm$	k_6
m	$\alpha\alpha\frac{1}{2}$	$2mm$	k_8
n	$\alpha 0\gamma$	m	k_3
o	$\alpha\alpha\gamma$	m	k_4
p	$\alpha\beta 0$	m	k_1
q	$\alpha\beta\frac{1}{2}$	m	k_2

(*l*) Cubic *P*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{12}
b	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$m\bar{3}m$	k_{13}
c	$\frac{1}{2}\frac{1}{2}0$	$4/mmm$	k_{11}
d	$00\frac{1}{2}$	$4/mmm$	k_{10}
e	00γ	$4mm$	k_8
f	$\frac{1}{2}\frac{1}{2}\gamma$	$4mm$	k_7
g	$\alpha\alpha\alpha$	$3m$	k_9
h	$\frac{1}{2}0\gamma$	$mm2$	k_6
i	$\alpha\alpha 0$	$2mm$	k_4
j	$\alpha\alpha\frac{1}{2}$	$2mm$	k_5
k	$\alpha\beta 0$	$11m$	k_1
l	$\alpha\beta\frac{1}{2}$	$11m$	k_2
m	$\alpha\alpha\gamma$	m	k_3

(*m*) Cubic *F*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$4/mmm$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{3}m$	k_9
d	$10\frac{1}{2}$	$\bar{4}m2$	k_8
e	$\alpha 00$	$4mm$	k_6
f	$\alpha\alpha\alpha$	$3m$	k_5
g	$\alpha 01$	$2mm$	k_7
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)\frac{1}{2}$	2	k_3
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2

(*n*) Cubic *I*

k		$K_{\mathbf{k}}$	Kovalev
a	000	$m\bar{3}m$	k_{11}
b	001	$m\bar{3}m$	k_{10}
c	$\frac{1}{2}\frac{1}{2}\frac{1}{2}$	$\bar{4}3m$	k_{10}
d	$\frac{1}{2}\frac{1}{2}0$	mmm	k_9
e	$\alpha 00$	$4mm$	k_8
f	$\alpha\alpha\alpha$	$3m$	k_7
g	$\alpha\frac{1}{2}\frac{1}{2}$	$2mm$	k_6
h	$\alpha\alpha 0$	$2mm$	k_4
i	$\alpha(1-\alpha)0$	$2mm$	k_9
j	$\alpha\beta$	$11m$	k_1
k	$\alpha\alpha\gamma$	m	k_2
	$\alpha(1-\alpha)\gamma$	m	k_3

Table 1.2.6.12. *Magnetic point groups*

Type I	Type II	Type III
1	$1'$	
$\bar{1}$	$\bar{1}1'$	$\bar{1}'$
2	$21'$	$2'$
m	$m1'$	m'
$2/m$	$21'/m$	$2'/m$, $2/m'$, $2'/m'$,
222	$2221'$	$2'2'$
$2mm$	$2mm1'$	$2'mm'$, $2m'm'$
mmm	$mmm1'$	$m'mm$, $m'm'm$, $m'm'm'$
4	$41'$	$4'$
$\bar{4}$	$\bar{4}1'$	$\bar{4}'$
$4/m$	$41'/m$	$4'/m$, $4/m'$, $4'/m'$
422	$4221'$	$4'22'$, $42'2'$
$4mm$	$4mm1'$	$4'mm'$, $4m'm'$
$\bar{4}2m$	$\bar{4}2m1'$	$\bar{4}'2'm$, $\bar{4}'2m'$, $\bar{4}2'm'$
$4/mmm$	$4/mmm1'$	$4/m'mm$, $4'/mm'm$, $4'/m'm'm$, $4/mm'm'$, $4/m'm'm'$
3	$31'$	
$\bar{3}$	$\bar{3}1'$	$\bar{3}'$
32	$321'$	$32'$
$3m$	$3m1'$	$3m'$
$\bar{3}m$	$\bar{3}m1'$	$\bar{3}'m$, $\bar{3}'m'$, $\bar{3}m'$
6	$61'$	$6'$
$\bar{6}$	$\bar{6}1'$	$\bar{6}'$
$6/m$	$61'/m$	$6'/m$, $6/m'$, $6'/m'$
622	$6221'$	$6'22'$, $62'2'$
$6mm$	$6mm1'$	$6'mm'$, $6m'm'$
$\bar{6}2m$	$\bar{6}2m1'$	$\bar{6}'2'm$, $\bar{6}'2m'$, $\bar{6}2'm'$
$6/mmm$	$6/mmm1'$	$6/m'mm$, $6'/mm'm$, $6'/m'm'm$, $6/mm'm'$, $6/m'm'm'$
23	$231'$	
$m\bar{3}$	$m\bar{3}1'$	$m'\bar{3}$
432	$4321'$	$4'32'$
$\bar{4}3m$	$\bar{4}3m1'$	$\bar{4}'3m'$
$m\bar{3}m$	$m\bar{3}m1'$	$m'\bar{3}m$, $m\bar{3}m'$, $m'\bar{3}m'$

dimension, the rank, the permutation symmetry and the setting basis transformation, and the calculated data: the number of independent elements (f) and the relations of these elements. They are either zero or expressed in terms of the free parameters $a_0, \ldots, a_{f-1}$. The tensor elements are given by sequences $x, y, z, \ldots$. The four elements of a general rank-two tensor in two dimensions are xx, xy, yx, yy, corresponding to T_{11}, T_{12}, T_{21} and T_{22}, respectively.

1.2.7.3. *Characters*

Calculations with characters of representations of point groups can be done in the character module of the program. It is selected in the main window by clicking 'character'. A selection window opens in which a point group may be selected just as in the tensor module. The point groups are organized according to dimension and geometric crystal class. Selection of a point group leads to the display of the character table if one asks for it by selecting 'view character table'.

The character table consists of a square array of (complex) numbers. The number of rows is the number of nonequivalent irreducible representations and is equal to the number of columns, which is the number of conjugacy classes of the group. For crystallographic groups, the complex numbers that form the entries of the character table are cyclotomic numbers. These are linear combinations with fractions as coefficients of complex numbers of the form $\exp(2\pi i n/m)$. For example, the square root of -1 (i) can be written as $\exp(2\pi i 1/4)$. A real number like $\sqrt{2}$ can be written as

$$\sqrt{2} = \tfrac{1}{2}\sqrt{2}(1 + i + 1 - i) = \exp(2\pi i \tfrac{1}{8}) + \exp(2\pi i \tfrac{7}{8}).$$

Another example is

$$\sqrt{5} = 1 + 2\exp(2\pi i \tfrac{1}{5}) + 2\exp(2\pi i \tfrac{4}{5}).$$

However, many entries for the three-dimensional point groups are simply integers.

The program provides the following information as rows above the characters of the irreducible representation:

(1) Representative elements of the conjugacy classes expressed in terms of the generators $a, b, \ldots$.

(2) The number of elements of each class.

(3) The order of the elements of the classes: the lowest positive power of an element that equals the identity.

Below the character table, the following information is displayed:

(1) In the mth row after the square character table, the class to which the $(m+1)$th powers of the elements from this column belong is given. If a conjugacy class has elements of order p, then only the $p-1$ first entries are given, because in the column there exists p periodicity.

(2) The determinant of the three-dimensional matrix for the element of the point group (or the elements of the conjugacy class). This is the character of an irreducible representation.

(3) Finally, the character of the vector representation is given.

As an example, the generalized character table for the three-dimensional point group $4mm$ is given in Table 1.2.7.1.

The data connected with a character table can be seen by choosing 'view character table'. The characters of the irreducible representations, the determinant representation and the vector representation are shown in the main window after selection of 'accept character table'. From the character of these representations, characters of other representations may be calculated. The results are added as rows to the table, which is shown after each calculation.

Calculations using rows from the table may have one or more arguments. Operations with one argument will produce, for example, the decomposition into irreducible components, the character of the pth power, the symmetrized or antisymmetrized square, or the character of the corresponding physical (real) representation. Operations with two or more arguments yield products and sums of characters. The arguments of a unitary, binary or multiple operation are selected by clicking on the button in front of the corresponding characters. If the result is a new character (*e.g.* the product of two characters), it is added as a row to the list of characters. If the result is not a character (*e.g.* the decomposition into irreducible components), the result is given on the worksheet.

Suppose one wants to determine the number of elastic constants for a material with cubic 432 symmetry. After selecting the character table for the group 432, one clicks on the button in front of 'vector representation' in the character table. This yields the character of the three-dimensional vector representation of the group. The character of the symmetrized square is obtained by selecting 'symmetrized square'. This gives the character of a six-dimensional representation. Determining the number of times the trivial representation occurs by selecting 'decompose' gives the number of free parameters in the metric tensor, *i.e.* 1. Clicking on 'symmetrized square' for the character of the six-dimensional representation gives the character of a 21-dimensional representation. Decomposition yields the multiplicity 3 for the trivial representation, which means that there are three independent tensor elements for a tensor of symmetry type ((0 1)(2 3)), which in turn means that there are three elastic constants for the group 432 (see Table 1.2.6.9). For the explicit determination of the independent tensor elements, the tensor module of the program should be used.

Table 1.2.7.1. *Data connected with the character table for point group* $4mm$

e	a	a^2	b	ab
1	2	1	2	2
1	4	2	2	2
1	1	1	1	1
1	1	1	−1	−1
1	−1	1	1	−1
1	−1	1	−1	1
2	0	−2	0	0
1	3	1	1	1
	2			
	1			
1	1	1	−1	−1
3	1	−1	1	1

Of course, many kinds of calculations unrelated to tensors can be carried out using the character module. Examples include the calculation of selection rules in spectroscopy or the splitting of energy levels under a symmetry-breaking perturbation.

1.2.7.4. *Algorithms*

1.2.7.4.1. *Construction of a basis*

As a basis for a tensor space without permutation symmetry, one may choose one consisting of non-commutative monomials. It has d^r elements, where d is the dimension and r is the rank. In two dimensions, these are x, y for $r=1$, xx, xy, yx, yy for $r=2$ and $xxx, xxy, xyx, xyy, yxx, yxy, yyx, yyy$ for $r=3$. Note that $xy \neq yx$.

If there is permutation symmetry among the indices $i_1, \ldots, i_p$, only polynomials $x_{i_1}x_{i_2}\ldots x_r$ occur in the basis for which $i_1 \leq i_2 \leq \ldots \leq i_p$. Then $x_{i_1}x_{i_2} = x_{i_2}x_{i_1}$. If there is antisymmetry among these indices, one has the condition $i_1 < i_2 < \ldots < i_p$ and $x_{i_1}x_{i_2} = -x_{i_2}x_{i_1}$. Therefore, in two dimensions, the basis for tensors of type (1 3)2 is $xxx, xxy, xyx, xyy, yxy, yyy$ and for those of type [1 3]2 it is xxy, xyy. These bases can be obtained from the general basis by elimination.

1.2.7.4.2. *Action of the generators of the point group G on the basis*

The transformation of the monomial $x_ix_j\ldots$ under the matrix $g \in G$ is given by the polynomial

$$\left[\sum_{m=1}^{d} g_{im}x_m\right] \times \left[\sum_{n=1}^{d} g_{jn}x_n\right] \ldots,$$

which is in principle non-commutative. This polynomial can be written as a sum of the monomials in the basis taking into account the eventual (anti)symmetry of xy and yx. In this way, basis element (a monomial) e_i is transformed to

$$ge_i = \sum_{j=1}^{d} M(g)_{ji}e_j.$$

To each generator of G corresponds such an action matrix M.

The action matrix changes if one considers pseudotensors. In the case of pseudotensors, the previous equation changes to

$$ge_i = \mathrm{Det}(g)\sum_{j=1}^{d} M(g)_{ji}e_j.$$

The function $\mathrm{Det}(g)$ is just a one-dimensional representation of the group G. The determinant is either $+1$ or -1.

1.2.7.4.3. *Diagonalization of the action matrix and determination of the invariant tensor*

An invariant element of the tensor space under the group G is a vector v that is left invariant under each generator:

$$\begin{pmatrix} M_1 - E \\ M_2 - E \\ \vdots \\ M_s - E \end{pmatrix} v = \Omega v = 0.$$

If the number of generators is one, $\Omega = M - E$. This equation is solved by diagonalization:

$$P\Omega QQ^{-1}v = DQ^{-1}v = 0,$$

where $D_{ij} = d_i\delta_{ij}$. The dimension of the solution space is the number of elements d_i that are equal to zero. The corresponding rows of Q form a basis for the solution space. (See example further on.)

1.2.7.4.4. *Determination of the vector representation*

For a point group G, its isomorphism class and its character table are known. For each conjugacy class, a representative element is given as word $A_1A_2\ldots$ where the A_i's correspond to generators. Replacing the letters by the generating matrices, one obtains as product a matrix for which the trace is the character of the vector representation in the conjugacy class. The characters of all conjugacy classes being known, the representation can be decomposed into irreducible components by means of

$$m_\alpha = (1/|G|)\sum_i n_i\chi_\alpha^*(i)\chi(i),$$

where α labels the irreducible representations (the row number in the character table), m_α the number of times the representation α occurs, $|G|$ the order of the group G, n_i the number of elements in the ith conjugacy class (given as the second row in the character table), $\chi_\alpha(i)$ the cyclotomic in the ith row and αth column of the character table, and $\chi(i)$ the calculated character in the ith conjugacy class.

1.2.7.4.5. *Determination of tensor products and their decomposition*

Given a character (for an irreducible representation from the character table, or for the vector representation, for example), the character of the standard rank n tensor is the nth power of the character and can be decomposed with the multiplicity formula for m_α given above.

Fully symmetrized or antisymmetrized tensor products have characters given by

$$\begin{aligned}
n=2:\ \chi^\pm(R) &= \frac{1}{2!}\big(\chi(R)^2 \pm \chi(R^2)\big)\\
n=3:\ \chi^\pm(R) &= \frac{1}{3!}\big(\chi(R)^3 \pm 3\chi(R^2)\chi(R) + 2\chi(R^3)\big)\\
n=4:\ \chi^\pm(R) &= \frac{1}{4!}\big(\chi(R)^4 \pm 6\chi(R^2)\chi(R)^2 + 3\chi(R^2)^2\\
&\quad + 8\chi(R^3)\chi(R) \pm 6\chi(R^4)\big)\\
n=5:\ \chi^\pm(R) &= \frac{1}{5!}\big(\chi(R)^5 \pm 10\chi(R^2)\chi(R)^3 + 15\chi(R^2)^2\chi(R)\\
&\quad + 20\chi(R^3)\chi(R)^2 \pm 20\chi(R^3)\chi(R^2)\\
&\quad \pm 30\chi(R^4)\chi(R) + 24\chi(R^5)\big)\\
n=6:\ \chi^\pm(R) &= \frac{1}{6!}\big(\chi(R)^6 \pm 15\chi(R^2)\chi(R)^4 + 45\chi(R^2)^2\chi(R)^2\\
&\quad + 40\chi(R^3)^2 \pm 15\chi(R^2)^3 + 40\chi(R^3)\chi(R)^3\\
&\quad \pm 120\chi(R^3)\chi(R^2)\chi(R) \pm 90\chi(R^4)\chi(R)^2\\
&\quad + 90\chi(R^4)\chi(R^2) + 144\chi(R^5)\chi(R)\\
&\quad \pm 120\chi(R^6)\big).
\end{aligned}$$

From this follows immediately the dimension of the subspaces of symmetric and antisymmetric tensors:

$$\begin{aligned}
n=2 &: \frac{1}{2}(d^2 \pm d)\\
n=3 &: \frac{1}{6}(d^3 \pm 3d^2 + 2d)\\
n=4 &: \frac{1}{24}(d^4 \pm 6d^3 + 11d^2 \pm 6d)\\
n=5 &: \frac{1}{120}(d^5 \pm 10d^4 + 35d^3 \pm 50d^2 + 24d)\\
n=6 &: \frac{1}{720}(d^6 \pm 15d^5 + 85d^4 \pm 225d^3 + 274d^2 \pm 120d).
\end{aligned}$$

The general expression for arbitrary rank can be determined as follows. (See also Section 1.2.2.7)

(1) If n is the rank, the first step is to determine all possible decompositions

$$n = \sum_{i=1}^n f_i$$

with non-negative integers f_i satisfying $f_i \le f_{i-1}$.

(2) For each such decomposition $m = 1, \ldots n_{\rm tot}$ there is a term

$$P_m = \prod_{i=1}^p \binom{N_i}{f_i}(f_i - 1)!,$$

where $N_1 = n$, $N_i = N_{i-1} - f_{i-1}$ $(i > 1)$ and p is the number of nonzero integers f_i.

(3) If there are equal values of f_i in the mth decomposition, P_m should be divided by $t!$ for each t-tuple of equal values $(f_{k+1} = \ldots = f_{k+t})$.

(4) The sign of the term P_m is $+1$ for a symmetrized power and

$$\prod_{i=1}^p (-1)^{(f_i-1)}$$

for an antisymmetrized power.

(5) The expression for the character of the (anti)symmetrized power then is

$$\chi^\pm(R) = (1/M!)\sum_{m=1}^{n_{\rm tot}} {\rm sign}_m P_m \prod_{i=1}^p \chi(R^{f_i}).$$

1.2.7.4.6. *Invariant tensors*

Once one has the character of the properly symmetrized tensor, the number of invariants is just m_1, the number of times the trivial representation occurs in the decomposition.

Example (1). Dimension 3, rank 3, symmetry type (123), group 3. Basis: *xxx*, *xxy*, *xxz*, *xyy*, *xyz*, *xzz*, *yyy*, *yyz*, *yzz*, *zzz*. Under

$$\begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{pmatrix}$$

the basis elements go to *yyy*, *yyz*, *yyx*, *yzz*, *yzx*, *yxx*, *zzz*, *zzx*, *zxx*, *xxx*, respectively, and these are equivalent to *yyy*, *yyz*, *xyy*, *yzz*, *xyz*, *xxy*, *zzz*, *xzz*, *xxz*, *xxx*, respectively. This gives the ten-dimensional matrix

$$M = \begin{pmatrix} 0&0&0&0&0&0&0&0&0&1\\ 0&0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&1&0\\ 0&0&1&0&0&0&0&0&0&0\\ 0&0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&0&0&1&0&0\\ 1&0&0&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0&0&0\\ 0&0&0&0&0&0&1&0&0&0 \end{pmatrix}.$$

Then $P(M-E)Q = D$, with D diagonal. There are four diagonal elements of D which are zero, and the invariant tensors correspond to the corresponding four columns of the matrix Q. The invariant polynomials are

$$xxx + yyy + zzz, \quad xxy + xzz + yyz, \quad xxz + yzz + xyy, \quad xyz.$$

Example (2). Dimension 2, rank 2, symmetry type (12). Group generated by

$$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

Basis xx, xy, yy goes to yy, $-xy+yy$, $xx-2xy+yy$. This gives

$$M = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & -2 \\ 1 & 1 & 1 \end{pmatrix}.$$

Because

$$\begin{pmatrix} 1&0&0\\ 2&1&2\\ 1&0&1 \end{pmatrix} (M-E) \begin{pmatrix} 1&-1&1\\ 0&1&0\\ 0&-1&1 \end{pmatrix} = \begin{pmatrix} -1&0&0\\ 0&0&0\\ 0&0&2 \end{pmatrix},$$

the invariant tensor corresponds to the second column of Q, which as a polynomial reads $-xx+xy-yy$. This can be written with the tensor T_{ij} as

$$-xx + xy - yy = -\sum_{i,j} T_{ij} x_i x_j, \quad T_{ij} = \begin{pmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{pmatrix}.$$

This tensor T is invariant under the group.

Example (3). Dimension 3, rank 2, tensor type (12). Group generated by matrix([[0 −1 0][1 0 0][0 0 1]]). The basis xx, xy, xz, yy, yz, zz goes under the generator to yy, $-xy$, $-yz$, xx, xz, zz. The solution of $(M-E)v = 0$ is

$$\alpha_1(xx+yy) + \alpha_2 zz.$$

The matrix D has two zeros on the diagonal.

Example (4). Dimension 3, rank 3, type (123). Same group as in Example (3). Basis xxx, xxy, xxz, xyy, xyz, xzz, yyy, yyz, yzz, zzz. The solution

$$\alpha_1(xxz+yyz) + \alpha_2 zzz$$

corresponds to a tensor with relations $T_{113} = T_{223}$, $T_{111} = T_{112} = T_{122} = T_{123} = T_{133} = T_{222} = T_{233} = 0$.

Example (5). Dimension 3, rank 4, type ((12)(34)). Not only $i_1 \le i_2$ and $i_3 \le i_4$, but also $(i_1 i_2)$, should come lexicographically before $(i_3 i_4)$. Basis $xxxx$, $xxxy$, $xxxz$, $xxyy$, $xxyz$, $xxzz$, $xyxy$, $xyxz$, $xyyy$, $xyyz$, $xyzz$, $xzxz$, $xzyy$, $xzyz$, $xzzz$, $yyyy$, $yyyz$, $yyzz$, $yzyz$, $yzzz$, $zzzz$. Under the same group as in example (3), there are seven invariants. Invariant polynomial:

$$\alpha_1(xxxx+yyyy) + \alpha_2(xxxy - xyyy) + \alpha_3 xxyy + \alpha_4 xyxy + \alpha_5 zzzz + \alpha_6(xxzz+yyzz) + \alpha_7(xzxz+yzyz).$$

Table 1.2.7.2. *Calculation with characters*

Generator	Composite character	Characters				Decomposition
$\begin{pmatrix} 0&1&0\\ 0&0&1\\ 1&0&0 \end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	3	0	0		
	$\chi(R)^3$	27	0	0		
	$\chi(R^2)$	3	0	0		
	$\chi(R^2)\chi(R)$	9	0	0		
	$\chi(R^3)$	3	3	3		
Example (1)	$\frac{1}{6}(\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3))$	10	1	1		$4D_1 + 3D_2 + 3D_3$
$\begin{pmatrix} 0&-1\\ 1&-1 \end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	2	−1	−1		
	$\chi(R)^2$	4	1	1		
	$\chi(R^2)$	2	−1	−1		
Example (2)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	3	0	0		$D_1 + D_2 + D_3$
$\begin{pmatrix} 0&-1&0\\ 1&0&0\\ 0&0&1 \end{pmatrix}$	R	E	A	AA	AAA	
	$\chi(R)$	3	1	−1	1	
	$\chi(R)^2$	9	1	1	1	
	$\chi(R^2)$	3	−1	3	−1	
Example (3)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	6	0	2	0	$2D_1 + D_2 + 2D_3 + D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (4)	$\chi(R)^3$	27	1	−1	1	
	$\chi(R^2)$	3	−1	3	−1	
	$\chi(R^2)\chi(R)$	9	−1	−3	−1	
	$\chi(R^3)$	3	1	−1	1	
	$\frac{1}{6}(\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3))$	10	0	−2	0	$2D_1 + 3D_2 + 2D_3 + 3D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (5)	$\frac{1}{2}(\chi(R)^2 + \chi(R^2)) = \chi_s(R)$	6	0	2	0	
	$\chi_s(R)^2$	36	0	4	0	
	$\chi_s(R^2)$	6	2	6	2	
	((12)(34))	21	1	5	1	$7D_1 + 4D_2 + 6D_3 + 4D_4$
As above, example (6)	$\frac{1}{2}(\chi(R)^2 - \chi(R^2))$	3	1	−1	1	$D_1 + D_2 + D_4$
As above, example (7)	$\frac{1}{6}(\chi(R)^3 - 3\chi(R^2)\chi(R) + 2\chi(R^3))$	1	1	1	1	D_1

This corresponds to the tensor relations

$$\begin{array}{lll} \mathrm{T}_{xxxx} = -\mathrm{T}_{yyyy} & \mathrm{T}_{xxxy} = \mathrm{T}_{xyyy} & \mathrm{T}_{xxxz} = 0 \\ \mathrm{T}_{xxyz} = 0 & \mathrm{T}_{xxzz} = \mathrm{T}_{yyzz} & \mathrm{T}_{xyxz} = 0 \\ \mathrm{T}_{xyyz} = 0 & \mathrm{T}_{xyzz} = 0 & \mathrm{T}_{xzxz} = \mathrm{T}_{yzyz} \\ \mathrm{T}_{xzyy} = 0 & \mathrm{T}_{xzyz} = 0 & \mathrm{T}_{xzzz} = 0 \\ \mathrm{T}_{yyyz} = 0 & \mathrm{T}_{yzzz} = 0 & \end{array}$$

$$\rightarrow \begin{pmatrix} \alpha_1 & \alpha_3 & \alpha_6 & 0 & 0 & \alpha_2 \\ \alpha_3 & \alpha_1 & \alpha_6 & 0 & 0 & -\alpha_2 \\ \alpha_6 & \alpha_6 & \alpha_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & \alpha_7 & 0 \\ \alpha_2 & -\alpha_2 & 0 & 0 & 0 & \alpha_4 \end{pmatrix}.$$

The latter form is that of an elastic tensor with the usual convention $1 = xx$, $2 = yy$, $3 = zz$, $4 = yz$, $5 = xz$, $6 = xy$.

Example (6). Dimension 3, rank 2, type [12]. The same group as in example (3). Basis $xy, xz, yz \rightarrow -yx, -yz, xz$, which are equivalent to $xy, -yz, xz$. The transformation in the tensor space is

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \end{pmatrix} v = 0:$$

$$v = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \sim xy.$$

There is just one invariant antisymmetric polynomial $xy = -yx$ corresponding to the tensor

$$T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

Example (7). Dimension 3, rank 3, type [123]. Basis xyz invariant under the group: $xyz \rightarrow -yxz \sim xyz$. The corresponding tensor is the fully antisymmetric rank 3 tensor: $\mathrm{T}_{ijk} = 1$ if ijk is an even permutation of 123, $= -1$ if ijk is an odd permutation, and $= 0$ if two or three indices are equal (permutation tensor, see Section 1.1.3.7.2).

Example (8). Calculation with characters. See Table 1.2.7.2.

Example (9). The action matrix for a pseudotensor.

Take the group $4/m$ with generators

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Consider the rank 3 pseudotensor (123). The action matrix is determined from the action of the generators A and B on the basis:

	A	B
xxx	$-yyy$	$-xxx$
xxy	xyy	$-xxy$
xxz	yyz	xxz
xyy	$-xxy$	$-xyy$
xyz	$-xyz$	xyz
xzz	$-yzz$	$-xzz$
yyy	xxx	$-yyy$
yyz	xxz	yyz
yzz	xzz	$-yzz$
zzz	zzz	zzz

Therefore, the action matrix becomes

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

After diagonalization, one finds two nonzero elements on the diagonal:

$$zzz = a; \quad xxz = yyz = b;$$

$$xxx = xxy = xyy = xyz = xzz = yyy = yzz = 0.$$

1.2.8. Glossary

$\mathrm{T}_{i_1 \ldots i_n}$	tensor of rank n
$O(n)$	orthogonal group
$\mathbb{Z}$	ring of integers
$\mathbf{e}_i$	basis vectors
g	metric tensor
K	point group
R	orthogonal transformation
C_m	cyclic group of order m
$SO(n)$	special orthogonal group
$\mathbb{Z}^+$	positive integers
D_n	dihedral group of order n
E	unit transformation, matrix or element
I	inversion
$D(K)$	representation of K
$\Gamma(K)$	matrix representation of K
$\|K\|$	order of K
$\oplus$	sum of spaces or operators
$\otimes$	tensor product
$\in$	element of
$\mathbf{a}_i$	basis of space or lattice

V^*	dual space
S	basis transformation
χ	character
$\chi(R)$	value of χ at R
C_i	conjugacy class
χ_α	irreducible character
m_α	multiplicity
N	order of K
d_α	dimension of irreducible representation α
n_i	order of class C_i
c_{ijk}	class multiplication constants
T	tetrahedral group
O	octahedral group
I	icosahedral group
$P(K)$	projective representation
$W_i(A_1, \ldots, A_p)$	word in generators A_j
K^d	double group
$E(n)$	Euclidean group
$g = \{R\|\mathbf{a}\}$	element of $E(n)$
$T(n)$	translation group in n dimensions
Λ	lattice
Λ^*	reciprocal lattice
$\mathbf{a}(R)$	translation vector system
$\mathbf{k}$	vector in dual space
$G_\mathbf{k}$	group of $\mathbf{k}$
$K_\mathbf{k}$	point group of $G_\mathbf{k}$
ω	factor system
$\mathrm{Det}(R)$	determinant of R
$\left(\begin{matrix}\alpha & \beta \\ i & j\end{matrix}\middle\vert\begin{matrix}\gamma & \\ k & \ell\end{matrix}\right)$	Clebsch–Gordan coefficients
θ	time-reversal operator

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