International Tables for Crystallography (2006). Vol. D, Section 1.2.2, pp. 35–46.

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* (2002). 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

$$g = \begin{pmatrix} a & -a/2 \\ -a/2 & a \end{pmatrix}.$$

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

$$n_1n'_1a - n_1n'_2a/2 - n_2n'_1a/2 + n_2n'_2a.$$

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

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

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

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

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

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

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) 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) 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 $\mathbf{a}_i$:

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

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

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

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

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

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

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

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

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

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

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

One has

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

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

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

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:

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

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

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

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

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

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,

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

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 above.

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

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

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, $\sum_\alpha m^2_\alpha>1$.

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,

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

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^2_α 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:

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

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.

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

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

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

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

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

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

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

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

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

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 $v_i w_j + v_j w_i$, 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 $(\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i)$ $(i \le j)$. 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 $i = 1, 2, \ldots, d_1$; $j = 1, 2, \ldots d_2$; $\ldots$; $k = 1, 2, \ldots, d_n$. 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

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

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

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

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.

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

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:

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

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

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

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 $\mathbf{e}_i \otimes \mathbf{e}_j + \mathbf{e}_j \otimes \mathbf{e}_i$ $(1 \le i \le j \le d$, spanning the space $V_s^{\otimes 2})$ and $\mathbf{e}_i \otimes \mathbf{e}_j - \mathbf{e}_j \otimes \mathbf{e}_i$ $(1 \le i < j \le d$, 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

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

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

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

for the symmetric subspace and

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

for the antisymmetric one. Consequently one has

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

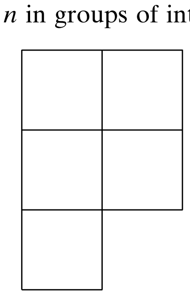
For $n > 2$, the tensor product space does not carry just a symmetric and an antisymmetric subspace, but also higher-dimensional representations of the permutation group S_n. The derivation of the character of the fully symmetric and fully antisymmetric subspaces remains rather similar. The formulae 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

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

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.

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 $\mathbf{r}$ different from the origin, 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

references