International Tables for Crystallography (2006). Vol. D, Section 1.2.4, pp. 51–53.

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

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

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)

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

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

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

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. They 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

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

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

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

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

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

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.

references