9
Group Algebra; Projection Operators

In this section we will become familiar with a method allowing us to carry out symmetry reduction of tensors, discussed in Section 3.8.2, by means of group theory, whereby the existence of the individual tensor components can be directly checked by a certain computational procedure. First, we introduce the concept of the linear operator $\boldsymbol{A}$, which generates from each vector $\boldsymbol{x}$ of an n-dimensional linear vector space V exactly one vector $\boldsymbol{y}$ in V according to $\boldsymbol{Ax} = \boldsymbol{y}$, whereby the following linearity relations hold:

$$\boldsymbol{A}(\boldsymbol{u}+\boldsymbol{v}) = \boldsymbol{Au}+\boldsymbol{Av} \quad \text{and} \quad \boldsymbol{A}(q\boldsymbol{u}) = q(\boldsymbol{Au}). \quad q \text{ is an arbitrary number.}$$

The symmetry operations are linear operators. In a system of n-multiple differentiable functions $f_i(\boldsymbol{x})$, all differential operators $\partial/\partial x_j$ and correspondingly higher differential operators are linear operators.

For two linear operators $\boldsymbol{A}$ and $\boldsymbol{B}$ one can define a sum and a product, namely $(\boldsymbol{A}+\boldsymbol{B})\boldsymbol{x} = \boldsymbol{Ax}+\boldsymbol{Bx}$ and $(\boldsymbol{AB})\boldsymbol{x} = \boldsymbol{A}(\boldsymbol{Bx})$. Similar to matrix multiplication $\boldsymbol{A}(\boldsymbol{Bx})$ means that the operator $\boldsymbol{B}$ operates on $\boldsymbol{x}$ and then the operator $\boldsymbol{A}$ operates on s$(\boldsymbol{Bx})$. It is clear that the operators so combined are also linear operators.

If one now constructs arbitrary linear combinations of the type

$$\boldsymbol{g} = x_i \boldsymbol{g}_i,$$

with the elements g_i of a group, taken as linear operators, then all such $\boldsymbol{g}$ represent a linear vector space of dimension h of the group. In this vector space, multiplication is defined in the way introduced above, namely

$$(x_i \boldsymbol{g}_i)(y_j \boldsymbol{g}_j) = x_i y_j (\boldsymbol{g}_i \boldsymbol{g}_j),$$

since $(\boldsymbol{g}_i \boldsymbol{g}_j)$ also represent group elements. A vector space in which multiplication is defined is called an algebra. The vector space $\bar{G}$ constructed from the elements G of a group is called *group algebra*.

We also require the notion of the *center* Z of a group G: All elements of a group, which commute with all other elements with respect to operations, form the center of the group. The center of a group possess the property of a

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subgroup, as is easily checked. Accordingly, we can introduce the center $\bar{Z}$ of the group algebra $\bar{G}$, whose elements commute with all other elements of $\bar{G}$. $\bar{Z}$ forms a subgroup of $\bar{G}$, as one sees from the subgroup properties of Z. We now come to the important theorem: The sum of the elements of each class represent a complete basis of the center $\boldsymbol{Z}$ of the group algebra. Let the sum of the classes be specified by ${}^iK$, hence, ${}^iK = {}^ig_1 + {}^ig_2 + \ldots$, where ${}^ig_j$ is the jth element of the ith class. The proof is as follows: if q is an arbitrary element taken of G, then the element $q^{-1\,i}g_jq$ also belongs to the ith class. If one lets ${}^ig_j$ run through all the elements of the class then this generates different elements in each case. If $q^{-1\,i}g_jq = q^{-1\,i}g_kq$, then we would have ${}^ig_j = {}^ig_k$, contrary to the assumption. This means, however, that the ith class sum can also be written as

$$^iK = q^{-1\,i}g_1q + q^{-1\,i}g_2q + \cdots .$$

Therefore,

$$^iK = q^{-1\,i}Kq, \qquad \text{hence} \quad q\,{}^iK = {}^iKq,$$

thus ${}^iK$ lies in $\bar{Z}$. Since the class sums are different, we obtain a basis for the linear vector space of the center of the group algebra, whose dimension is equal to the class number S. In particular, each arbitrary element taken from the center can be represented as a linear combination of the class sums.

Among these linear combinations there exists several especially interesting elements p given the name *Idempotent*, which have the property $p^2 = p$. Furthermore, if for two idempotents p_i and p_j one has $p_ip_j = 0$ for $i \neq j$, then the idempotents are orthogonal. A system of orthogonal idempotents is always linearly independent, i.e., the equation $\sum_i a_ip_i = 0$ exists only when all $a_i = 0$. In fact multiplying with p_i gives for each i: $a_ip_i^2 = a_ip_i = 0$, thus $a_i = 0$. Moreover, one finds that the sum of orthogonal idempotents is always an indempotent:

$$p = \sum_i p_i, \quad p^2 = \sum_{i,j} p_ip_j = \sum_i p_i^2 = \sum_i p_i = p.$$

There always exists a maximal set of orthogonal idempotents p_i from the center of the group algebra possessing the following properties:

1. $\sum_i^s p_i = e$ (identity element of the group)

2. Each p_i is indivisible, i.e., no orthogonal idempotents exist in $\bar{Z}$ with $p_i = p_i' + p_i''$.

3. All other idempotents can be represented as the sum of a few idempotents.

4. The maximal set is uniquely determined.

To prove 1. we form $(e - p')$ with $p' = \sum_{i=1}^{s} p_i$. This quantity is a new idempotent if it is different from zero, as one can easily check. If p' is complete, however, then a further idempotent cannot exist, i.e., $(e - p') = 0$.

Furthermore, from $p_i = p_i' + p_i''$ we would get by multiplication $p_i' = p_i' p_i$ and $p_i'' = p_i'' p_i$, and consequently $p_i' p_j = p_i' p_i p_j = 0$ and $p_i'' p_j = p_i'' p_i p_j = 0$. This means, p_i' and p_i'' would be two other orthogonal idempotents, which could take the place of p_i, contrary to the assumption that the system is maximal. The other two assertions can be easily proved by the reader. The orthogonal idempotents can now be constructed from the rules just discussed. It is seen, however, that they can also be found directly with the help of the character table, then

$$p_i = \frac{l_i}{h} \sum_{j=1}^{h} \chi_i^{\text{irr}}(g_j^{-1}) g_j,$$

where l_i is the dimension of the ith representation and h is the order of the group. For unitary matrices $\chi(g^{-1}) = \chi(g)$! The most important idempotent for our purposes is $p_1 = \frac{1}{h} \sum_{j=1}^{h} g_j$. The proof that we are dealing with an idempotent results simply from $p_1^2 = \frac{1}{h^2} \sum_{j,k}^{h} g_j g_k$.

The sum represents nothing else as the sum of all elements of the group table, hence, $\sum_{j,k}^{h} g_j g_k = h \sum_j g_j$, because each element is found once in each row. Therefore, $p_1^2 = p_1$. According to the above formula p_1 corresponds to the totally symmetric representation Γ_1. The general proof for the validity of this relationship is found, for example, with the help of the orthogonality relations of the characters.

As an example, let us again consider the PSG 3m. According to the character table (see Table 8.3)

$$p_1 = \frac{1}{6}(e + 3^1 + 3^2 + m_1 + m_2 + m_3)$$
$$p_2 = \frac{1}{6}(e + 3^1 + 3^2 - m_1 - m_2 - m_3)$$
$$p_3 = \frac{2}{6}(2e - 3^1 - 3^2).$$

The same result is obtained by using the relations

$$p_i p_j = \delta_{ij} p_i \quad \text{with} \quad p_i = k_{il} g_l \quad \text{and} \quad p_j = k_{jl} g_l.$$

The operators p_i decompose the linear vector space V in linear subspaces V_i, which in turn carry over into themselves through the respective elements of the group (G-invariant subspaces). The vectors ${}^i\boldsymbol{x}$ are called of the ith symmetry type when $p_i {}^i\boldsymbol{x} = {}^i\boldsymbol{x}$. The set of all these ith symmetry type vectors from V span the subspace V_i. Consequently, V_i is assigned the ith irreducible representation.

We now consider an important theorem: Each vector $\boldsymbol{x}$ of the vector space V is uniquely decomposed in a sum of vectors ${}^i\boldsymbol{x}$ from the subspaces V_i according to

$$\boldsymbol{x} = {}^1\boldsymbol{x} + {}^2\boldsymbol{x} + {}^3\boldsymbol{x} + \ldots {}^s\boldsymbol{x}.$$

This is recognized as follows: With $\sum_i p_i = e$ one obtains

$$\boldsymbol{x} = e\boldsymbol{x} = \left(\sum_i^s p_i\right) x = p_1 x + p_2 x + \ldots p_s x.$$

Due to this property, these idempotents are also referred to as *projection operators*. According to Neumann's principle, the following is true for the transformation in a symmetry equivalent system

$$t'_{ij\ldots s} = u_{ii^*} u_{jj^*} \cdots u_{ss^*} t_{i^*j^*\ldots s^*} = t_{ij\ldots s}.$$

The transformation matrices in the respective linear vector space are therefore equal to (1) and the associated irreducible representation is $\Gamma_1 = (1, 1, \ldots, 1)$. Thus, one obtains with the help of p_1, operating on arbitrary vectors $\boldsymbol{t}$ of the linear vector space spanned by the tensor components, those components lying in V_1 which construct the tensor.

We can directly employ this property for the symmetry reduction of tensors. For this purpose p_1 is applied to the vectors $\boldsymbol{t}$ of the linear vector space spanned by the tensor components. Thus

$$\boldsymbol{t}' = p_1(\boldsymbol{t}) = \frac{1}{h}\sum_{l=1}^{h} g_l(\boldsymbol{t}) = \boldsymbol{t}.$$

This is explained using the first- to third-rank tensors of the PSG 3m as examples. For each g_l we write the Kronecker product of the respective transformation matrices. In the case of the first-rank tensor we use the three-dimensional vector representation $\Gamma'_3 = \Gamma_3 + \Gamma_1$. Thus with Γ'_3:

$$g_1 = e = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_2 = 3^1 = \begin{pmatrix} -1/2 & \sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$
$$g_3 = 3^2 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_4 = \mathrm{m}_1 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{9.1}$$
$$g_5 = \mathrm{m}_2 = \begin{pmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ -\sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g_6 = \mathrm{m}_3 = \begin{pmatrix} 1/2 & \sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

(see 8.2)

$$
\begin{aligned}
p_1(\boldsymbol{t}) &= \frac{1}{6}\Big(g_1(\boldsymbol{t}) + g_2(\boldsymbol{t}) + g_3(\boldsymbol{t}) + g_4(\boldsymbol{t}) + g_5(\boldsymbol{t}) + g_6(\boldsymbol{t})\Big) \\
&= \frac{1}{6}\left\{ (t_1, t_2, t_3) + \left(\frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2, -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2, t_3\right)\right. \\
&\qquad\qquad + \left(-\frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2, \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2, t_3\right) \\
&\qquad + (-t_1, t_2, t_3) + \left(\frac{1}{2}t_1 - \frac{\sqrt{3}}{2}t_2, -\frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2, 0\right) \\
&\qquad\qquad \left. + \left(\frac{1}{2}t_1 + \frac{\sqrt{3}}{2}t_2, \frac{\sqrt{3}}{2}t_1 - \frac{1}{2}t_2, t_3\right) \right\} \\
&= (0, 0, t_3) = t.
\end{aligned}
$$

This means that only the component t_3 exists.

If the components $t_{ij\ldots s}$ are independent of one another, then p_1 can be applied to vectors only exhibiting one component, respectively. However, if relations exist among the components as in the case of degeneracy (in trigonal crystals, for example, $t_{11} = t_{22}$), then it is convenient to apply the projection on the complete vector $\boldsymbol{t}$ of the given linear vector space. This situation is recognized by the fact that the projection p_1, applied to certain vectors with only one component leads to a vector with several components. This is illustrated by the second-rank tensor of the PSG 3m. We have, for example,

$$
p_1(t_{11}, 0, 0 \ldots 0) = \left(\frac{1}{2}t_{11}, \frac{1}{2}t_{11}, 0, 0, 0, 0, 0, 0, 0\right),
$$

when the vector $\boldsymbol{t}$ has the form

$$
\boldsymbol{t} = (t_{11}, t_{22}, t_{33}, t_{23}, t_{31}, t_{12}, t_{32}, t_{13}, t_{21}).
$$

From this, it would follow that $t_{11} = t_{22} = 0$, which would be correct in the case of $t_{22} = 0$. If we now construct $p_1(\boldsymbol{t})$, we find

$$
p_1(\boldsymbol{t}) = \left(\frac{1}{2}(t_{11} + t_{22}), \frac{1}{2}(t_{11} + t_{22}), t_{33}, 0, 0, 0, 0, 0, 0\right).
$$

The existence of the independent components $t_{11} = t_{22}$ and t_{33} follows from the fact that $p_1(\boldsymbol{t}) = \boldsymbol{t}$. In practice, in has proved useful, as a first step, to calculate projections with only one component, respectively. We can then determine which tensor components vanish and which components are coupled with others. The projections carried out in a second step with the complete vector $\boldsymbol{t}$ are then easier to calculate, because the vanished components need no longer be taken into consideration.

This is again illustrated by the third-rank tensor of the PSG 3m.

1. Step: Calculating the projection of vectors $\boldsymbol{t}$ with only one component respectively. For this one requires the factors $u_{ii}u_{jj}u_{kk}$ (for $i = i^*, j = j^*, k = k^*$) appearing in the transformation $t'_{ijk} = u_{ii^*}u_{jj^*}u_{kk^*}t_{i^*j^*k^*}$, in other words, the products of the diagonal coefficients of g_i in the three-dimensional representation Γ'_3 (see above).

$$\begin{aligned}
p_1(t_{111}, 0, 0\ldots) &= 0;\\
p_1(0, t_{222}, 0, 0\ldots) &= (0, \frac{1}{4}t_{222}, \ldots),\\
p_1(\ldots 0\ldots, t_{112}, \ldots 0\ldots) &= (\ldots, \frac{1}{4}t_{112}, \ldots),\\
p_1(\ldots 0\ldots, t_{113}, \ldots 0\ldots) &= (\ldots, \frac{1}{2}t_{113}, \ldots),\\
p_1(\ldots 0\ldots, t_{123}, \ldots 0\ldots) &= 0,\\
p_1(\ldots 0\ldots, t_{223}, \ldots 0\ldots) &= (\ldots, \frac{1}{2}t_{223}, \ldots),\\
p_1(\ldots 0\ldots, t_{133}, \ldots 0\ldots) &= 0,\\
p_1(\ldots 0\ldots, t_{233}, \ldots 0\ldots) &= 0,\\
p_1(\ldots 0\ldots, t_{333}) &= (\ldots 0\ldots, t_{333}).
\end{aligned}$$

Similar projections apply to t_{121}, t_{211}, t_{131}, t_{311}, t_{232}, t_{322}. Consequently, the following tensor components vanish: t_{111}, t_{123}, t_{231}, t_{312}, t_{132}, t_{321}, t_{213}, t_{133}, t_{313}, t_{331}, t_{233}, t_{323}, t_{332}. Those remaining are: t_{222}, t_{112}, t_{121}, t_{211}, t_{113}, t_{131}, t_{311}, t_{223}, t_{232}, t_{322} and t_{333}.

2. Step: One lets p_1 act on a vector containing only the nonvanishing components. Because $p_1(\boldsymbol{t}) = \boldsymbol{t}$ we obtain the following relations:

$$\begin{aligned}
&t_{112} = t_{121} = t_{211} = -t_{222} = \frac{1}{4}(t_{112} + t_{121} + t_{211} - t_{222}),\\
&t_{113} = t_{223} = \frac{1}{2}(t_{113} + t_{223}),\\
&t_{131} = t_{232} = \frac{1}{2}(t_{131} + t_{232}),\\
&t_{311} = t_{322} = \frac{1}{2}(t_{311} + t_{322}),\\
&t_{333} = t_{333}.
\end{aligned}$$

Accordingly, the components of this tensor span a five-dimensional space. This result is identical with that derived in Section 4.4.

The question now arises, when is the projection procedure, discussed here, preferred to that discussed in Section 4.2.1. With respect to the projection method, the calculation procedure shows that the projection method deals with a stringent prescription, which in the form presented can be easily transferred to a computer program. Thus, in many cases, in particular, with higher rank tensors, one can attain complete symmetry reduction more quickly than with the method of the transformation of the components in symmetry equivalent reference systems. Special emphasis is placed on the possibility of checking the existence of individual tensor components with the help of the projections. A substantial contraction of the calculation procedure is achieved when one uses the following conditions taken from symmetry operations as, for example, in the case of a two-fold axis parallel $\boldsymbol{e}_i$ or a symmetry plane perpendicular $\boldsymbol{e}_i$ (index i an odd number of times or an even number of times with odd-rank tensors and an even number of times or odd number of times with even-rank tensors). In particular, the cyclic permutability of the indices in cubic crystals should be noted. The projection method represents an extremely useful instrument for many other applications including the analysis of the vibrational states in molecules and crystals as well as in the classification of phase transformations and the interactions resulting from these (normal coordinate analysis, symmetry types of the interactions).