International Tables for Crystallography (2013). Vol. D, Section 1.2.7.4.6, pp. 68–70.

$$P\Omega QQ^{-1}v = DQ^{-1}v = 0,$$

where $D_{ij} = d_i\delta_{ij}$. The dimension of the solution space is the number of elements d_i that are equal to zero. The corresponding rows of Q form a basis for the solution space. (See example further on.)

1.2.7.4.4. *Determination of the vector representation*

For a point group G, its isomorphism class and its character table are known. For each conjugacy class, a representative element is given as word $A_1A_2\ldots$ where the A_i's correspond to generators. Replacing the letters by the generating matrices, one obtains as product a matrix for which the trace is the character of the vector representation in the conjugacy class. The characters of all conjugacy classes being known, the representation can be decomposed into irreducible components by means of

$$m_\alpha = (1/|G|)\sum_i n_i\chi_\alpha^*(i)\chi(i),$$

where α labels the irreducible representations (the row number in the character table), m_α the number of times the representation α occurs, $|G|$ the order of the group G, n_i the number of elements in the ith conjugacy class (given as the second row in the character table), $\chi_\alpha(i)$ the cyclotomic in the ith row and αth column of the character table, and $\chi(i)$ the calculated character in the ith conjugacy class.

1.2.7.4.5. *Determination of tensor products and their decomposition*

Given a character (for an irreducible representation from the character table, or for the vector representation, for example), the character of the standard rank n tensor is the nth power of the character and can be decomposed with the multiplicity formula for m_α given above.

Fully symmetrized or antisymmetrized tensor products have characters given by

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

From this follows immediately the dimension of the subspaces of symmetric and antisymmetric tensors:

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

The general expression for arbitrary rank can be determined as follows. (See also Section 1.2.2.7)

(1) If n is the rank, the first step is to determine all possible decompositions

$$n = \sum_{i=1}^n f_i$$

with non-negative integers f_i satisfying $f_i \le f_{i-1}$.

(2) For each such decomposition $m = 1,\ldots n_{\rm tot}$ there is a term

$$P_m = \prod_{i=1}^p \binom{N_i}{f_i}(f_i-1)!,$$

where $N_1 = n$, $N_i = N_{i-1} - f_{i-1}$ $(i > 1)$ and p is the number of nonzero integers f_i.

(3) If there are equal values of f_i in the mth decomposition, P_m should be divided by $t!$ for each t-tuple of equal values $(f_{k+1} = \ldots = f_{k+t})$.

(4) The sign of the term P_m is $+1$ for a symmetrized power and

$$\prod_{i=1}^p (-1)^{(f_i-1)}$$

for an antisymmetrized power.

(5) The expression for the character of the (anti)symmetrized power then is

$$\chi^\pm(R) = (1/M!)\sum_{m=1}^{n_{\rm tot}} {\rm sign}_m P_m \prod_{i=1}^p \chi(R^{f_i}).$$

1.2.7.4.6. *Invariant tensors*

Once one has the character of the properly symmetrized tensor, the number of invariants is just m_1, the number of times the trivial representation occurs in the decomposition.

Example (1). Dimension 3, rank 3, symmetry type (123), group 3. Basis: *xxx*, *xxy*, *xxz*, *xyy*, *xyz*, *xzz*, *yyy*, *yyz*, *yzz*, *zzz*. Under

$$\begin{pmatrix} 0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{pmatrix}$$

the basis elements go to *yyy*, *yyz*, *yyx*, *yzz*, *yzx*, *yxx*, *zzz*, *zzx*, *zxx*, *xxx*, respectively, and these are equivalent to *yyy*, *yyz*, *xyy*, *yzz*, *xyz*, *xxy*, *zzz*, *xzz*, *xxz*, *xxx*, respectively. This gives the ten-dimensional matrix

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

Then $P(M-E)Q=D$, with D diagonal. There are four diagonal elements of D which are zero, and the invariant tensors correspond to the corresponding four columns of the matrix Q. The invariant polynomials are

$$xxx+yyy+zzz,\quad xxy+xzz+yyz,\quad xxz+yzz+xyy,\quad xyz.$$

Example (2). Dimension 2, rank 2, symmetry type (12). Group generated by

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

Basis xx, xy, yy goes to yy, $-xy+yy$, $xx-2xy+yy$. This gives

$$M=\begin{pmatrix}0&0&1\\0&-1&-2\\1&1&1\end{pmatrix}.$$

Because

$$\begin{pmatrix}1&0&0\\2&1&2\\1&0&1\end{pmatrix}(M-E)\begin{pmatrix}1&-1&1\\0&1&0\\0&-1&1\end{pmatrix}=\begin{pmatrix}-1&0&0\\0&0&0\\0&0&2\end{pmatrix},$$

the invariant tensor corresponds to the second column of Q, which as a polynomial reads $-xx+xy-yy$. This can be written with the tensor T_{ij} as

$$-xx+xy-yy=-\sum_{i,j}T_{ij}x_ix_j,\qquad T_{ij}=\begin{pmatrix}1&-\frac{1}{2}\\-\frac{1}{2}&1\end{pmatrix}.$$

This tensor T is invariant under the group.

Example (3). Dimension 3, rank 2, tensor type (12). Group generated by matrix([[0 −1 0][1 0 0][0 0 1]]). The basis xx, xy, xz, yy, yz, zz goes under the generator to yy, $-xy$, $-yz$, xx, xz, zz. The solution of $(M-E)v=0$ is

$$\alpha_1(xx+yy)+\alpha_2 zz.$$

The matrix D has two zeros on the diagonal.

Example (4). Dimension 3, rank 3, type (123). Same group as in Example (3). Basis xxx, xxy, xxz, xyy, xyz, xzz, yyy, yyz, yzz, zzz. The solution

$$\alpha_1(xxz+yyz)+\alpha_2 zzz$$

corresponds to a tensor with relations $T_{113}=T_{223}$, $T_{111}=T_{112}=T_{122}=T_{123}=T_{133}=T_{222}=T_{233}=0$.

Example (5). Dimension 3, rank 4, type ((12)(34)). Not only $i_1\le i_2$ and $i_3\le i_4$, but also (i_1i_2), should come lexicographically before (i_3i_4). Basis $xxxx$, $xxxy$, $xxxz$, $xxyy$, $xxyz$, $xxzz$, $xyxy$, $xyxz$, $xyyy$, $xyyz$, $xyzz$, $xzxz$, $xzyy$, $xzyz$, $xzzz$, $yyyy$, $yyyz$, $yyzz$, $yzyz$, $yzzz$, $zzzz$. Under the same group as in example (3), there are seven invariants. Invariant polynomial:

$$\alpha_1(xxxx+yyyy)+\alpha_2(xxxy-xyyy)+\alpha_3 xxyy+\alpha_4 xyxy$$
$$+\alpha_5 zzzz+\alpha_6(xxzz+yyzz)+\alpha_7(xzxz+yzyz).$$

Table 1.2.7.2. *Calculation with characters*

Generator	Composite character	Characters				Decomposition
$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	3	0	0		
	$\chi(R)^3$	27	0	0		
	$\chi(R^2)$	3	0	0		
	$\chi(R^2)\chi(R)$	9	0	0		
	$\chi(R^3)$	3	3	3		
Example (1)	$\frac{1}{6}(\chi(R)^3+3\chi(R^2)\chi(R)+2\chi(R^3))$	10	1	1		$4D_1+3D_2+3D_3$
$\begin{pmatrix}0&-1\\1&-1\end{pmatrix}$	R	E	A	AA		
	$\chi(R)$	2	−1	−1		
	$\chi(R)^2$	4	1	1		
	$\chi(R^2)$	2	−1	−1		
Example (2)	$\frac{1}{2}(\chi(R)^2+\chi(R^2))$	3	0	0		$D_1+D_2+D_3$
$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$	R	E	A	AA	AAA	
	$\chi(R)$	3	1	−1	1	
	$\chi(R)^2$	9	1	1	1	
	$\chi(R^2)$	3	−1	3	−1	
Example (3)	$\frac{1}{2}(\chi(R)^2+\chi(R^2))$	6	0	2	0	$2D_1+D_2+2D_3+D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (4)	$\chi(R)^3$	27	1	−1	1	
	$\chi(R^2)$	3	−1	3	−1	
	$\chi(R^2)\chi(R)$	9	−1	−3	−1	
	$\chi(R^3)$	3	1	−1	1	
	$\frac{1}{6}(\chi(R)^3+3\chi(R^2)\chi(R)+2\chi(R^3))$	10	0	−2	0	$2D_1+3D_2+2D_3+3D_4$
As above	$\chi(R)$	3	1	−1	1	
Example (5)	$\frac{1}{2}(\chi(R)^2+\chi(R^2))=\chi_s(R)$	6	0	2	0	
	$\chi_s(R)^2$	36	0	4	0	
	$\chi_s(R^2)$	6	2	6	2	
	((12)(34))	21	1	5	1	$7D_1+4D_2+6D_3+4D_4$
As above, example (6)	$\frac{1}{2}(\chi(R)^2-\chi(R^2))$	3	1	−1	1	$D_1+D_2+D_4$
As above, example (7)	$\frac{1}{6}(\chi(R)^3-3\chi(R^2)\chi(R)+2\chi(R^3))$	1	1	1	1	D_1

This corresponds to the tensor relations

$$\begin{array}{lll} \mathrm{T}_{xxxx} = -\mathrm{T}_{yyyy} & \mathrm{T}_{xxxy} = \mathrm{T}_{xyyy} & \mathrm{T}_{xxxz} = 0 \\ \mathrm{T}_{xxyz} = 0 & \mathrm{T}_{xxzz} = \mathrm{T}_{yyzz} & \mathrm{T}_{xyxz} = 0 \\ \mathrm{T}_{xyyz} = 0 & \mathrm{T}_{xyzz} = 0 & \mathrm{T}_{xzxz} = \mathrm{T}_{yzyz} \\ \mathrm{T}_{xzyy} = 0 & \mathrm{T}_{xzyz} = 0 & \mathrm{T}_{xzzz} = 0 \\ \mathrm{T}_{yyyz} = 0 & \mathrm{T}_{yzzz} = 0 & \end{array}$$

$$\rightarrow \begin{pmatrix} \alpha_1 & \alpha_3 & \alpha_6 & 0 & 0 & \alpha_2 \\ \alpha_3 & \alpha_1 & \alpha_6 & 0 & 0 & -\alpha_2 \\ \alpha_6 & \alpha_6 & \alpha_5 & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & \alpha_7 & 0 \\ \alpha_2 & -\alpha_2 & 0 & 0 & 0 & \alpha_4 \end{pmatrix}.$$

The latter form is that of an elastic tensor with the usual convention $1 = xx$, $2 = yy$, $3 = zz$, $4 = yz$, $5 = xz$, $6 = xy$.

Example (6). Dimension 3, rank 2, type [12]. The same group as in example (3). Basis $xy, xz, yz \rightarrow -yx, -yz, xz$, which are equivalent to xy, $-yz$, xz. The transformation in the tensor space is

$$M = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & -1 & -1 \end{pmatrix} v = 0:$$

$$v = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \sim xy.$$

There is just one invariant antisymmetric polynomial $xy = -yx$ corresponding to the tensor

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

Example (7). Dimension 3, rank 3, type [123]. Basis xyz invariant under the group: $xyz \rightarrow -yxz \sim xyz$. The corresponding tensor is the fully antisymmetric rank 3 tensor: $\mathrm{T}_{ijk} = 1$ if ijk is an even permutation of 123, $= -1$ if ijk is an odd permutation, and $= 0$ if two or three indices are equal (permutation tensor, see Section 1.1.3.7.2).

Example (8). Calculation with characters. See Table 1.2.7.2.

Example (9). The action matrix for a pseudotensor.

Take the group $4/m$ with generators

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

Consider the rank 3 pseudotensor (123). The action matrix is determined from the action of the generators A and B on the basis:

	A	B
xxx	$-yyy$	$-xxx$
xxy	xyy	$-xxy$
xxz	yyz	xxz
xyy	$-xxy$	$-xyy$
xyz	$-xyz$	xyz
xzz	$-yzz$	$-xzz$
yyy	xxx	$-yyy$
yyz	xxz	yyz
yzz	xzz	$-yzz$
zzz	zzz	zzz

Therefore, the action matrix becomes

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

After diagonalization, one finds two nonzero elements on the diagonal:

$$zzz = a; \quad xxz = yyz = b;$$

$$xxx = xxy = xyy = xyz = xzz = yyy = yzz = 0.$$

1.2.8. Glossary

$\mathrm{T}_{i_1 \ldots i_n}$	tensor of rank n
$O(n)$	orthogonal group
$\mathbb{Z}$	ring of integers
$\mathbf{e}_i$	basis vectors
g	metric tensor
K	point group
R	orthogonal transformation
C_m	cyclic group of order m
$SO(n)$	special orthogonal group
$\mathbb{Z}^+$	positive integers
D_n	dihedral group of order n
E	unit transformation, matrix or element
I	inversion
$D(K)$	representation of K
$\Gamma(K)$	matrix representation of K
$\lvert K \rvert$	order of K
$\oplus$	sum of spaces or operators
$\otimes$	tensor product
$\in$	element of
$\mathbf{a}_i$	basis of space or lattice