

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

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

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

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

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

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

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

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

Because

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

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

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

This tensor T is invariant under the group.

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

$$\alpha_1(xx + yy) + \alpha_2zz.$$

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

$$\alpha_1(xxz + yyz) + \alpha_2zzz$$

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 $i_1 \leq i_2$ and $i_3 \leq i_4$, but also $(i_1 i_2)$, should come lexicographically before $(i_3 i_4)$. Basis $xxxx, xxxy, xxxz, xxyy, xxyz, xxzz, xyxy, xyxz, xyyy, xyyz, xyzx, xzxx, xzyy, xzyz, xzzz, yyyy, yyyz, yzzz, yzyz, yzzz, zzzz$. Under the same group as in example (3), there are seven invariants. Invariant polynomial:

$$\alpha_1(xxxx + yyyy) + \alpha_2(xxyy - xyyy) + \alpha_3(xxyy + \alpha_4xyxy + \alpha_5zzzz + \alpha_6(xxzz + yyzx) + \alpha_7(xzxx + yzyz).$$

Table 1.2.7.2. Calculation with characters

Generator	Composite character	Characters				Decomposition
$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ Example (1)	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		
	$\frac{1}{6}(\chi(R)^3 + 3\chi(R^2)\chi(R) + 2\chi(R^3))$	10	1	1		
					$4D_1 + 3D_2 + 3D_3$	
$\begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}$ Example (2)	R	E	A	AA		
	$\chi(R)$	2	-1	-1		
	$\chi(R)^2$	4	1	1		
	$\chi(R^2)$	2	-1	-1		
	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	3	0	0		
					$D_1 + D_2 + D_3$	
$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ Example (3)	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	
	$\frac{1}{2}(\chi(R)^2 + \chi(R^2))$	6	0	2	0	
					$2D_1 + D_2 + 2D_3 + D_4$	
As above Example (4)	$\chi(R)$	3	1	-1	1	
	$\chi(R)^3$	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 Example (5)	$\chi(R)$	3	1	-1	1	
	$\frac{1}{2}(\chi(R)^2 + \chi(R^2)) = \chi_s(R)$	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	
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	