

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

This corresponds to the tensor relations

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

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

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 → -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 → -yxz ~ xyz. The corresponding tensor is the fully antisymmetric rank 3 tensor: 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
xyy	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:

$$\begin{aligned}
 zzz &= a; & xxz &= yyz = b; \\
 xxx &= xxy = xyy = xyz = xzz = yyy = yzz = 0.
 \end{aligned}$$

1.2.8. Glossary

T _{i₁...i_n}	tensor of rank n
O(n)	orthogonal group
Z	ring of integers
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
Z ⁺	positive integers
D _n	dihedral group of order n
E	unit transformation, matrix or element
I	inversion
D(K)	representation of K
Γ(K)	matrix representation of K
K	order of K
⊕	sum of spaces or operators
⊗	tensor product
∈	element of
a _i	basis of space or lattice

1.2. REPRESENTATIONS OF CRYSTALLOGRAPHIC GROUPS

V^*	dual space	ω	factor system
S	basis transformation	$\text{Det}(R)$	determinant of R
χ	character	$\left(\begin{array}{cc cc} \alpha & \beta & \gamma & \\ i & j & k & \ell \end{array} \right)$	Clebsch–Gordan coefficients
$\chi(R)$	value of χ at R		
C_i	conjugacy class		
χ_α	irreducible character	θ	time-reversal operator
m_α	multiplicity		
N	order of K		
d_α	dimension of irreducible representation α		
n_i	order of class C_i		
c_{ijk}	class multiplication constants		
T	tetrahedral group		
O	octahedral group		
I	icosahedral group		
$P(K)$	projective representation		
$W_i(A_1, \dots, A_p)$	word in generators A_j		
K^d	double group		
$E(n)$	Euclidean group		
$g = \{R \mathbf{a}\}$	element of $E(n)$		
$T(n)$	translation group in n dimensions		
Λ	lattice		
Λ^*	reciprocal lattice		
$\mathbf{a}(R)$	translation vector system		
\mathbf{k}	vector in dual space		
$G_{\mathbf{k}}$	group of \mathbf{k}		
$K_{\mathbf{k}}$	point group of $G_{\mathbf{k}}$		

References

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