

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

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

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 $A_1A_2 \dots$ 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 i th conjugacy class (given as the second row in the character table), $\chi_\alpha(i)$ the cyclotomic in the i th row and α th column of the character table, and $\chi(i)$ the calculated character in the i th 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 n th 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

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

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 $f_i \leq f_{i-1}$.

(2) For each such decomposition $m = 1, \dots, n_{\text{tot}}$ 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 m th decomposition, P_m should be divided by $t!$ for each t -tuple of equal values ($f_{k+1} = \dots = f_{k+t}$).

(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

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

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