

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

If the basis  $\mathbf{e}_i$  is orthonormal,  $\Delta(g_{km})$  and  $V$  are equal to one,  $\Delta(B_j)$  is equal to the volume  $V'$  of the cell built on the basis vectors  $\mathbf{e}'_i$  and

$$\Delta(g'_{ij}) = V'^2.$$

This relation is actually general and one can remove the prime index:

$$\Delta(g_{ij}) = V^2. \tag{1.1.2.21}$$

In the same way, we have for the corresponding reciprocal basis

$$\Delta(g^{ij}) = V^{*2},$$

where  $V^*$  is the volume of the reciprocal cell. Since the tables of the  $g_{ij}$ 's and of the  $g^{ij}$ 's are inverse, so are their determinants, and therefore the volumes of the unit cells of the direct and reciprocal spaces are also inverse, which is a very well known result in crystallography.

1.1.3. Mathematical notion of tensor

1.1.3.1. Definition of a tensor

For the mathematical definition of tensors, the reader may consult, for instance, Lichnerowicz (1947), Schwartz (1975) or Sands (1995).

1.1.3.1.1. Linear forms

A linear form in the space  $E_n$  is written

$$T(\mathbf{x}) = t_i x^i,$$

where  $T(\mathbf{x})$  is independent of the chosen basis and the  $t_i$ 's are the coordinates of  $T$  in the dual basis. Let us consider now a bilinear form in the product space  $E_n \otimes F_p$  of two vector spaces with  $n$  and  $p$  dimensions, respectively:

$$T(\mathbf{x}, \mathbf{y}) = t_{ij} x^i y^j.$$

The  $np$  quantities  $t_{ij}$ 's are, by definition, the components of a tensor of rank 2 and the form  $T(\mathbf{x}, \mathbf{y})$  is invariant if one changes the basis in the space  $E_n \otimes F_p$ . The tensor  $t_{ij}$  is said to be twice covariant. It is also possible to construct a bilinear form by replacing the spaces  $E_n$  and  $F_p$  by their respective conjugates  $E^n$  and  $F^p$ . Thus, one writes

$$T(\mathbf{x}, \mathbf{y}) = t_{ij} x^i y^j = t^i_j x^i y^j = t^{ij} x_i y_j,$$

where  $t^{ij}$  is the doubly contravariant form of the tensor, whereas  $t^i_j$  and  $t^j_i$  are mixed, once covariant and once contravariant.

We can generalize by defining in the same way tensors of rank 3 or higher by using trilinear or multilinear forms. A vector is a tensor of rank 1, and a scalar is a tensor of rank 0.

1.1.3.1.2. Tensor product

Let us consider two vector spaces,  $E_n$  with  $n$  dimensions and  $F_p$  with  $p$  dimensions, and let there be two linear forms,  $T(\mathbf{x})$  in  $E_n$  and  $S(\mathbf{y})$  in  $F_p$ . We shall associate with these forms a bilinear form called a tensor product which belongs to the product space with  $np$  dimensions,  $E_n \otimes F_p$ :

$$P(\mathbf{x}, \mathbf{y}) = T(\mathbf{x}) \otimes S(\mathbf{y}).$$

This correspondence possesses the following properties:

- (i) it is distributive from the right and from the left;
- (ii) it is associative for multiplication by a scalar;
- (iii) the tensor products of the vectors with a basis  $E_n$  and those with a basis  $F_p$  constitute a basis of the product space.

The analytical expression of the tensor product is then

$$\left. \begin{aligned} T(\mathbf{x}) &= t_i x^i \\ S(\mathbf{y}) &= s_j y^j \end{aligned} \right\} P(\mathbf{x}, \mathbf{y}) = p_{ij} x^i y^j = t_i s_j x^i y^j = t_i s_j x^i y^j.$$

One deduces from this that

$$p_{ij} = t_i s_j.$$

It is a tensor of rank 2. One can equally well envisage the tensor product of more than two spaces, for example,  $E_n \otimes F_p \otimes G_q$  in  $npq$  dimensions. We shall limit ourselves in this study to the case of affine tensors, which are defined in a space constructed from the product of the space  $E_n$  with itself or with its conjugate  $E^n$ . Thus, a tensor product of rank 3 will have  $n^3$  components. The tensor product can be generalized as the product of multilinear forms. One can write, for example,

$$\left. \begin{aligned} P(\mathbf{x}, \mathbf{y}, \mathbf{z}) &= T(\mathbf{x}, \mathbf{y}) \otimes S(\mathbf{z}) \\ p^j_{ik} x^i y_j z^k &= t^i x^i y_j s_k z^k. \end{aligned} \right\} \tag{1.1.3.1}$$

1.1.3.2. Behaviour under a change of basis

A multilinear form is, by definition, invariant under a change of basis. Let us consider, for example, the trilinear form (1.1.3.1). If we change the system of coordinates, the components of vectors  $\mathbf{x}, \mathbf{y}, \mathbf{z}$  become

$$x^i = B^\alpha_i x'^\alpha; \quad y_j = A^\beta_j y'_\beta; \quad z^k = B^\gamma_k z'^\gamma.$$

Let us put these expressions into the trilinear form (1.1.3.1):

$$P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p^j_{ik} B^\alpha_i x'^\alpha A^\beta_j y'_\beta B^\gamma_k z'^\gamma.$$

Now we can equally well make the components of the tensor appear in the new basis:

$$P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p'^\beta_{\alpha\gamma} x'^\alpha y'_\beta z'^\gamma.$$

As the decomposition is unique, one obtains

$$p'^\beta_{\alpha\gamma} = p^j_{ik} B^\alpha_i A^\beta_j B^\gamma_k. \tag{1.1.3.2}$$

One thus deduces the rule for transforming the components of a tensor  $q$  times covariant and  $r$  times contravariant: they transform like the product of  $q$  covariant components and  $r$  contravariant components.

This transformation rule can be taken inversely as the definition of the components of a tensor of rank  $n = q + r$ .

*Example.* The operator  $O$  representing a symmetry operation has the character of a tensor. In fact, under a change of basis,  $O$  transforms into  $O'$ :

$$O' = AOA^{-1}$$

so that

$$O'^i_j = A^i_k O^k_l (A^{-1})^l_j.$$

Now the matrices  $A$  and  $B$  are inverses of one another:

$$O^i_j = A^i_k O^k_l B^l_j.$$

The symmetry operator is a tensor of rank 2, once covariant and once contravariant.

1.1.3.3. Operations on tensors

1.1.3.3.1. Addition

It is necessary that the tensors are of the same nature (same rank and same variance).