

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

1.1.3.7.2. Vector product

Consider the so-called permutation tensor of rank 3 (it is actually an axial tensor – see Section 1.1.4.5.3) defined by

$$\begin{cases} \varepsilon_{ijk} = +1 & \text{if the permutation } ijk \text{ is even} \\ \varepsilon_{ijk} = -1 & \text{if the permutation } ijk \text{ is odd} \\ \varepsilon_{ijk} = 0 & \text{if at least two of the three indices are equal} \end{cases}$$

and let us form the contracted product

$$z_k = \frac{1}{2} \varepsilon_{ijk} p^{ij} = \varepsilon_{ijk} x^i y^j. \quad (1.1.3.4)$$

It is easy to check that

$$\begin{cases} z_1 = x^2 y^3 - y^2 x^3 \\ z_2 = x^3 y^1 - y^3 x^1 \\ z_3 = x^1 y^2 - y^1 x^2 \end{cases}$$

One recognizes the coordinates of the vector product.

1.1.3.7.3. Properties of the vector product

Expression (1.1.3.4) of the vector product shows that it is of a covariant nature. This is indeed correct, and it is well known that the vector product of two vectors of the direct lattice is a vector of the reciprocal lattice [see Section 1.1.4 of Volume B of *International Tables for Crystallography* (2000)].

The vector product is a very particular vector which it is better not to call a vector: sometimes it is called a *pseudovector* or an *axial* vector in contrast to normal vectors or *polar* vectors. The components of the vector product are the independent components of the antisymmetric tensor  $p_{ij}$ . In the space of  $n$  dimensions, one would write

$$v_{i_3 i_4 \dots i_n} = \frac{1}{2} \varepsilon_{i_1 i_2 \dots i_n} p^{i_1 i_2}.$$

The number of independent components of  $p^{ij}$  is equal to  $(n^2 - n)/2$  or 3 in the space of three dimensions and 6 in the space of four dimensions, and the independent components of  $p^{ij}$  are not the components of a vector in the space of four dimensions.

Let us also consider the behaviour of the vector product under the change of axes represented by the matrix

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

This is a symmetry with respect to a point that transforms a right-handed set of axes into a left-handed set and reciprocally. In such a change, the components of a normal vector change sign. Those of the vector product, on the contrary, remain unchanged, indicating – as one well knows – that the orientation of the vector product has changed and that it is not, therefore, a vector in the normal sense, *i.e.* independent of the system of axes.

1.1.3.8. Tensor derivatives

1.1.3.8.1. Interpretation of the coefficients of the matrix – change of coordinates

We have under a change of axes:

$$x^i = A_j^i x^j.$$

This shows that the new components,  $x^i$ , can be considered linear functions of the old components,  $x^j$ , and one can write

$$A_j^i = \partial x^i / \partial x^j = \partial_j x^i.$$

It should be noted that the covariance has been increased.

1.1.3.8.2. Generalization

Consider a field of tensors  $t_i^j$  that are functions of space variables. In a change of coordinate system, one has

$$t_i^j = A_i^\alpha B_\beta^j t'_\alpha{}^\beta.$$

Differentiate with respect to  $x^k$ :

$$\begin{aligned} \frac{\partial t_i^j}{\partial x^k} &= \partial_k t_i^j = A_i^\alpha B_\beta^j \frac{\partial t'_\alpha{}^\beta}{\partial x'^\gamma} \frac{\partial x'^\gamma}{\partial x^k} \\ \partial_k t_i^j &= A_i^\alpha B_\beta^j A_k^\gamma \partial_\gamma t'_\alpha{}^\beta. \end{aligned}$$

It can be seen that the partial derivatives  $\partial_k t_i^j$  behave under a change of axes like a tensor of rank 3 whose covariance has been increased by 1 with respect to that of the tensor  $t_i^j$ . It is therefore possible to introduce a tensor of rank 1,  $\nabla$  (nabla), of which the components are the operators given by the partial derivatives  $\partial/\partial x^i$ .

1.1.3.8.3. Differential operators

If one applies the operator nabla to a scalar  $\varphi$ , one obtains

$$\text{grad } \varphi = \nabla \varphi.$$

This is a covariant vector in reciprocal space.

Now let us form the tensor product of  $\nabla$  by a vector  $\mathbf{v}$  of variable components. We then have

$$\nabla \otimes \mathbf{v} = \frac{\partial v^j}{\partial x^i} \mathbf{e}_i \otimes \mathbf{e}^j.$$

The quantities  $\partial_i v^j$  form a tensor of rank 2. If we contract it, we obtain the divergence of  $\mathbf{v}$ :

$$\text{div } \mathbf{v} = \partial_i v^i.$$

Taking the vector product, we get

$$\text{curl } \mathbf{v} = \nabla \wedge \mathbf{v}.$$

The curl is then an axial vector.

1.1.3.8.4. Development of a vector function in a Taylor series

Let  $\mathbf{u}(\mathbf{r})$  be a vector function. Its development as a Taylor series is written

$$u^i(\mathbf{r} + d\mathbf{r}) = u^i(\mathbf{r}) + \frac{\partial u^i}{\partial x^j} dx^j + \frac{1}{2} \frac{\partial^2 u^i}{\partial x^j \partial x^k} dx^j dx^k + \dots \quad (1.1.3.5)$$

The coefficients of the expansion,  $\partial u^i / \partial x^j$ ,  $\partial^2 u^i / \partial x^j \partial x^k$ , ... are tensors of rank 2, 3, ...

An example is given by the relation between displacement and electric field:

$$D^i = \varepsilon_j^i E^j + \chi_{jk}^i E^j E^k + \dots$$

(see Sections 1.6.2 and 1.7.2).

We see that the linear relation usually employed is in reality a development that is arrested at the first term. The second term corresponds to nonlinear optics. In general, it is very small but is not negligible in ferroelectric crystals in the neighbourhood of the ferroelectric–paraelectric transition. Nonlinear optics are studied in Chapter 1.7.

1.1.4. Symmetry properties

For the symmetry properties of the tensors used in physics, the reader may also consult Bhagavantam (1966), Billings (1969), Mason (1966), Nowick (1995), Nye (1985), Pauffer (1986), Shuvalov (1988), Sirotn & Shaskol'skaya (1982), and Wooster (1973).