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

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

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

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

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,

$$\left.\begin{array}{l} P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = T(\mathbf{x}, \mathbf{y}) \otimes S(\mathbf{z}) \\ p_{ik}^j x^i y_j z^k = t_i^j x^i y_j s_k z^k. \end{array}\right\} \tag{1.1.3.1}$$

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

$$x^i = B_\alpha^i x'^\alpha; \quad y_j = A_j^\beta y'_\beta; \quad z^k = B_\gamma^k z'^\gamma.$$

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

$$P(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p_{ik}^j B_\alpha^i x'^\alpha A_j^\beta y'_\beta B_\gamma^k z'^\gamma.$$

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

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

As the decomposition is unique, one obtains

$$p_{\alpha\gamma}'^\beta = p_{ik}^j B_\alpha^i A_j^\beta B_\gamma^k. \tag{1.1.3.2}$$

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

$$O_j'^i = A_k^i O_l^k (A^{-1})_j^l.$$

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

$$O_j'^i = A_k^i O_l^k B_j^l.$$

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).

1.1.3.3.2. *Multiplication by a scalar*

This is a particular case of the tensor product.

1.1.3.3.3. *Contracted product, contraction*

Here we are concerned with an operation that only exists in the case of tensors and that is very important because of its applications in physics. In practice, it is almost always the case that tensors enter into physics through the intermediary of a contracted product.

(i) *Contraction*. Let us consider a tensor of rank 2 that is once covariant and once contravariant. Let us write its transformation in a change of coordinate system:

$$t_i^{\prime j} = A_p^j B_i^q t_q^p.$$

Now consider the quantity $t_i^{\prime i}$ derived by applying the Einstein convention ($t_i^{\prime i} = t_1^{\prime 1} + t_2^{\prime 2} + t_3^{\prime 3}$). It follows that

$$t_i^{\prime i} = A_p^i B_i^q t_q^p = \delta_p^q t_q^q$$
$$t_i^{\prime i} = t_p^p.$$

This is an invariant quantity and so is a *scalar*. This operation can be carried out on any tensor of rank higher than or equal to two, provided that it is expressed in a form such that its components are (at least) once covariant and once contravariant.

The *contraction* consists therefore of equalizing a covariant index and a contravariant index, and then in summing over this index. Let us take, for example, the tensor $t_i^{\prime jk}$. Its contracted form is $t_i^{\prime ik}$, which, with a change of basis, becomes

$$t_i^{\prime ik} = A_p^k t_q^{qp}.$$

The components t_i^{ik} are those of a vector, resulting from the contraction of the tensor t_i^{jk}. The rank of the tensor has changed from 3 to 1. In a general manner, the contraction reduces the rank of the tensor from n to $n - 2$.

Example. Let us take again the operator of symmetry O. The trace of the associated matrix is equal to

$$O_1^1 + O_2^2 + O_3^3 = O_i^i.$$

It is the resultant of the contraction of the tensor O. It is a tensor of rank 0, which is a scalar and is invariant under a change of basis.

(ii) *Contracted product*. Consider the product of two tensors of which one is contravariant at least once and the other covariant at least once:

$$p_i^{jk} = t_i^j z^k.$$

If we contract the indices i and k, it follows that

$$p_i^{ji} = t_i^j z^i.$$

The contracted product is then a tensor of rank 1 and not 3. It is an operation that is very frequent in practice.

(iii) *Scalar product*. Next consider the tensor product of two vectors:

$$t_i^j = x_i y^j.$$

After contraction, we get the scalar product:

$$t_i^i = x_i y^i.$$

1.1.3.4. *Tensor nature of physical quantities*

Let us first consider the dielectric constant. In the introduction, we remarked that for an isotropic medium

$$\mathbf{D} = \varepsilon \mathbf{E}.$$

If the medium is anisotropic, we have, for one of the components,

$$D^1 = \varepsilon_1^1 E^1 + \varepsilon_2^1 E^2 + \varepsilon_3^1 E^3.$$

This relation and the equivalent ones for the other components can also be written

$$D^i = \varepsilon_j^i E^j \qquad (1.1.3.3)$$

using the Einstein convention.

The scalar product of $\mathbf{D}$ by an arbitrary vector $\mathbf{x}$ is

$$D^i x_i = \varepsilon_j^i E^j x_i.$$

The right-hand member of this relation is a bilinear form that is invariant under a change of basis. The set of nine quantities ε_j^i constitutes therefore the set of components of a tensor of rank 2. Expression (1.1.3.3) is the contracted product of ε_j^i by E^j.

A similar demonstration may be used to show the tensor nature of the various physical properties described in Section 1.1.1, whatever the rank of the tensor. Let us for instance consider the piezoelectric effect (see Section 1.1.4.4.3). The components of the electric polarization, P^i, which appear in a medium submitted to a stress represented by the second-rank tensor T_{jk} are

$$P^i = d^{ijk} T_{jk},$$

where the tensor nature of T_{jk} will be shown in Section 1.3.2. If we take the contracted product of both sides of this equation by any vector of covariant components x_i, we obtain a linear form on the left-hand side, and a trilinear form on the right-hand side, which shows that the coefficients d^{ijk} are the components of a third-rank tensor. Let us now consider the piezo-optic (or photoelastic) effect (see Sections 1.1.4.10.5 and 1.6.7). The components of the variation $\Delta\eta^{ij}$ of the dielectric impermeability due to an applied stress are

$$\Delta\eta^{ij} = \pi^{ijkl} T_{jl}.$$

In a similar fashion, consider the contracted product of both sides of this relation by two vectors of covariant components x_i and y_j, respectively. We obtain a bilinear form on the left-hand side, and a quadrilinear form on the right-hand side, showing that the coefficients π^{ijkl} are the components of a fourth-rank tensor.

1.1.3.5. *Representation surface of a tensor*

1.1.3.5.1. *Definition*

Let us consider a tensor $t_{ijkl\dots}$ represented in an orthonormal frame where variance is not important. The value of component $t_{1111\dots}'$ in an arbitrary direction is given by

$$t_{1111\dots}' = t_{ijkl\dots} B_1^i B_1^j B_1^k B_1^l \dots,$$

where the B_1^i, B_1^j, $\dots$ are the direction cosines of that direction with respect to the axes of the orthonormal frame.

The *representation surface* of the tensor is the polar plot of $t_{1111\dots}'$.

1.1.3.5.2. *Representation surfaces of second-rank tensors*

The representation surfaces of second-rank tensors are quadrics. The directions of their principal axes are obtained as follows. Let t_{ij} be a second-rank tensor and let $\mathbf{OM} = \mathbf{r}$ be a vector with coordinates x_i. The doubly contracted product, $t_{ij} x^i x^j$, is a scalar. The locus of points M such that

$$t_{ij}x^i x^j = 1$$

is a quadric. Its principal axes are along the directions of the eigenvectors of the matrix with elements t_{ij}. They are solutions of the set of equations

$$t_{ij}x^i = \lambda x^j,$$

where the associated quantities λ are the eigenvalues.

Let us take as axes the principal axes. The equation of the quadric reduces to

$$t_{11}(x^1)^2 + t_{22}(x^2)^2 + t_{33}(x^3)^2 = 1.$$

If the eigenvalues are all of the same sign, the quadric is an ellipsoid; if two are positive and one is negative, the quadric is a hyperboloid with one sheet; if one is positive and two are negative, the quadric is a hyperboloid with two sheets (see Section 1.3.1).

Associated quadrics are very useful for the geometric representation of physical properties characterized by a tensor of rank 2, as shown by the following examples:

(i) *Index of refraction* of a medium. It is related to the dielectric constant by $n = \varepsilon^{1/2}$ and, like it, it is a tensor of rank 2. Its associated quadric is an ellipsoid, the optical indicatrix, which represents its variations with the direction in space (see Section 1.6.3.2).

(ii) *Thermal expansion*. If one cuts a sphere in a medium whose thermal expansion is anisotropic, and if one changes the temperature, the sphere becomes an ellipsoid. Thermal expansion is therefore represented by a tensor of rank 2 (see Chapter 1.4).

(iii) *Thermal conductivity*. Let us place a drop of wax on a plate of gypsum, and then apply a hot point at the centre. There appears a halo where the wax has melted: it is elliptical, indicating anisotropic conduction. Thermal conductivity is represented by a tensor of rank 2 and the elliptical halo of molten wax corresponds to the intersection of the associated ellipsoid with the plane of the plate of gypsum.

1.1.3.5.3. *Representation surfaces of higher-rank tensors*

Examples of representation surfaces of higher-rank tensors are given in Sections 1.3.3.4.4 and 1.9.4.2.

1.1.3.6. *Change of variance of the components of a tensor*

1.1.3.6.1. *Tensor nature of the metric tensor*

Equation (1.1.2.17) describing the behaviour of the quantities $g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j$ under a change of basis shows that they are the components of a tensor of rank 2, the *metric tensor*. In the same way, equation (1.1.2.19) shows that the g^{ij}'s transform under a change of basis like the product of two contravariant coordinates. The coefficients g^{ij} and g_{ij} are the components of a *unique tensor*, in one case doubly contravariant, in the other case doubly covariant. In a general way, the Euclidean tensors (constructed in a space where one has defined the scalar product) are geometrical entities that can have covariant, contravariant or mixed components.

1.1.3.6.2. *How to change the variance of the components of a tensor*

Let us take a tensor product

$$t^{ij} = x^i y^j.$$

We know that

$$x^i = g^{ik}x_k \quad \text{and} \quad y^j = g^{jl}y_l.$$

It follows that

$$t^{ij} = g^{ik}g^{jl}x_k y_l.$$

$x_k y_l$ is a tensor product of two vectors expressed in the dual space:

$$x_k y_l = t_{kl}.$$

One can thus pass from the doubly covariant form to the doubly contravariant form of the tensor by means of the relation

$$t^{ij} = g^{ik}g^{jl}t_{kl}.$$

This result is general: to change the variance of a tensor (in practice, to raise or lower an index), it is necessary to make the contracted product of this tensor using g^{ij} or g_{ij}, according to the case. For instance,

$$t^l_k = g^{jl}t_{lk}; \quad t^{ij}_k = g_{kl}t^{ijl}.$$

Remark

$$g^i_j = g^{ik}g_{kj} = \delta^i_j.$$

This is a property of the metric tensor.

1.1.3.6.3. *Examples of the use in physics of different representations of the same quantity*

Let us consider, for example, the force, $\mathbf{F}$, which is a tensor quantity (tensor of rank 1). One can define it:
(i) by the fundamental law of dynamics:

$$\mathbf{F} = m\boldsymbol{\Gamma}, \quad \text{with } F^i = m \, \mathrm{d}^2 x^i/\mathrm{d}t^2,$$

where m is the mass and $\boldsymbol{\Gamma}$ is the acceleration. The force appears here in a *contravariant* form.
(ii) as the derivative of the energy, W:

$$F_i = \partial W/\partial x^i = \partial_i W.$$

The force appears here in *covariant* form. In effect, we shall see in Section 1.1.3.8.1 that to form a derivative with respect to a variable contravariant augments the covariance by unity. The general expression of the law of dynamics is therefore written with the energy as follows:

$$m \, \mathrm{d}^2 x^i/\mathrm{d}t^2 = g^{ij}\partial_j W.$$

1.1.3.7. *Outer product*

1.1.3.7.1. *Definition*

The tensor defined by

$$\mathbf{x} \bigwedge \mathbf{y} = \mathbf{x} \otimes \mathbf{y} - \mathbf{y} \otimes \mathbf{x}$$

is called the *outer product* of vectors $\mathbf{x}$ and $\mathbf{y}$. (*Note*: The symbol is different from the symbol $\wedge$ for the vector product.) The analytical expression of this tensor of rank 2 is

$$\left.\begin{array}{l}\mathbf{x} = x^i\mathbf{e}_i \\ \mathbf{y} = y^j\mathbf{e}_j\end{array}\right\} \implies \mathbf{x}\bigwedge\mathbf{y} = (x^i y^j - y^i x^j)\mathbf{e}_i \otimes \mathbf{e}_j.$$

The components $p^{ij} = x^i y^j - y^i x^j$ of this tensor satisfy the properties

$$p^{ij} = -p^{ji}; \quad p^{ii} = 0.$$

It is an *antisymmetric* tensor of rank 2.

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

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

It is easy to check that

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

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

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

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:

$$
x'^i = A^i_j x^j.
$$

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

$$
A^i_j = \partial x'^i / \partial x^j = \partial_j x'^i.
$$

It should be noted that the covariance has been increased.

1.1.3.8.2. *Generalization*

Consider a field of tensors t^j_i that are functions of space variables. In a change of coordinate system, one has

$$
t^j_i = A^\alpha_i B^j_\beta t'^\beta_\alpha.
$$

Differentiate with respect to x^k:

$$
\frac{\partial t^j_i}{\partial x^k} = \partial_k t^j_i = A^\alpha_i B^j_\beta \frac{\partial t'^\beta_\alpha}{\partial x'^\gamma}\frac{\partial x'^\gamma}{\partial x^k}
$$

$$
\partial_k t^j_i = A^\alpha_i B^j_\beta A^\gamma_k \partial_\gamma t'^\beta_\alpha.
$$

It can be seen that the partial derivatives $\partial_k t^j_i$ 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^j_i. It is therefore possible to introduce a tensor of rank 1, ∇ (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 φ, one obtains

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

This is a covariant vector in reciprocal space.

Now let us form the tensor product of ∇ 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

$$
u^i(\mathbf{r} + \mathbf{dr}) = u^i(\mathbf{r}) + \frac{\partial u^i}{\partial x^j}\ dx^j + \tfrac{1}{2}\frac{\partial^2 u^i}{\partial x^j \partial x^k}\ dx^j\ dx^k + \ldots. \quad (1.1.3.5)
$$

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

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

$$
D^i = \varepsilon^i_j E^j + \chi^i_{jk}E^j E^k + \ldots
$$

(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), Paufler (1986), Shuvalov (1988), Sirotin & Shaskol'skaya (1982), and Wooster (1973).