International Tables for Crystallography (2006). Vol. D, Section 1.1.3.7, pp. 9–10.

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

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, **F**, which is a tensor quantity (tensor of rank 1). One can define it:

(i) by the fundamental law of dynamics:

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

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:

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

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

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

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

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

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

$$u^i(\mathbf{r} + \mathrm{d}\mathbf{r}) = u^i(\mathbf{r}) + \frac{\partial u^i}{\partial x^j}\,\mathrm{d}x^j + \tfrac{1}{2}\frac{\partial^2 u^i}{\partial x^j \partial x^k}\,\mathrm{d}x^j\,\mathrm{d}x^k + \ldots. \qquad (1.1.3.5)$$

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).

references