

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

(i) The submatrices associated with the principal properties are symmetric with respect to interchange of the indices related to the causes and to the effects: these properties are represented by symmetric tensors. For instance, the dielectric constant and the elastic constants are represented by symmetric tensors of rank 2 and 4, respectively (see Section 1.1.3.4).

(ii) The submatrices associated with terms that are symmetric with respect to the main diagonal of matrices (C) and (R) and that represent cross effects are transpose to one another. For instance, matrix (C_S^E) representing the converse piezoelectric effect is the transpose of matrix (C_P^T) representing the piezoelectric effect. It will be shown in Section 1.1.3.4 that they are the components of tensors of rank 3.

1.1.1.5. Onsager relations

Let us now consider systems that are in steady state and not in thermodynamic equilibrium. The intensive and extensive parameters are time dependent and relation (1.1.1.3) can be written

$$J_m = L_{mn}X_n,$$

where the intensive parameters X_n are, for instance, a temperature gradient, a concentration gradient, a gradient of electric potential. The corresponding extensive parameters J_m are the heat flow, the diffusion of matter and the current density. The diagonal terms of matrix L_{mn} correspond to thermal conductivity (Fourier's law), diffusion coefficients (Fick's law) and electric conductivity (Ohm's law), respectively. Non-diagonal terms correspond to cross effects such as the thermoelectric effect, thermal diffusion etc. All the properties corresponding to these examples are represented by tensors of rank 2. The case of second-rank axial tensors where the symmetrical part of the tensors changes sign on time reversal was discussed by Zheludev (1986).

The Onsager reciprocity relations (Onsager, 1931a,b)

$$L_{mn} = L_{nm}$$

express the symmetry of matrix L_{mn} . They are justified by considerations of statistical thermodynamics and are not as obvious as those expressing the symmetry of matrix (C_P^Q). For instance, the symmetry of the tensor of rank 2 representing thermal conductivity is associated with the fact that a circulating flow is undetectable.

Transport properties are described in Chapter 1.8 of this volume.

1.1.2. Basic properties of vector spaces

[The reader may also refer to Section 1.1.4 of Volume B of International Tables for Crystallography (2000).]

1.1.2.1. Change of basis

Let us consider a vector space spanned by the set of n basis vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3, \dots, \mathbf{e}_n$. The decomposition of a vector using this basis is written

$$\mathbf{x} = x^i \mathbf{e}_i \tag{1.1.2.1}$$

using the Einstein convention. The interpretation of the position of the indices is given below. For the present, we shall use the simple rules:

- (i) the index is a subscript when attached to basis vectors;
- (ii) the index is a superscript when attached to the components. The components are numerical coordinates and are therefore dimensionless numbers.

Let us now consider a second basis, \mathbf{e}'_j . The vector \mathbf{x} is independent of the choice of basis and it can be decomposed also in the second basis:

$$\mathbf{x} = x'^i \mathbf{e}'_i. \tag{1.1.2.2}$$

If A_i^j and B_j^i are the transformation matrices between the bases \mathbf{e}_i and \mathbf{e}'_j , the following relations hold between the two bases:

$$\left. \begin{aligned} \mathbf{e}_i &= A_i^j \mathbf{e}'_j; & \mathbf{e}'_j &= B_j^i \mathbf{e}_i \\ x^i &= B_j^i x'^j; & x'^j &= A_j^i x^i \end{aligned} \right\} \tag{1.1.2.3}$$

(summations over j and i , respectively). The matrices A_i^j and B_j^i are inverse matrices:

$$A_i^j B_j^k = \delta_i^k \tag{1.1.2.4}$$

(Kronecker symbol: $\delta_i^k = 0$ if $i \neq k$, $= 1$ if $i = k$).

Important Remark. The behaviour of the basis vectors and of the components of the vectors in a transformation are different. The roles of the matrices A_i^j and B_j^i are opposite in each case. The components are said to be *contravariant*. Everything that transforms like a basis vector is *covariant* and is characterized by an *inferior* index. Everything that transforms like a component is *contravariant* and is characterized by a *superior* index. The property describing the way a mathematical body transforms under a change of basis is called *variance*.

1.1.2.2. Metric tensor

We shall limit ourselves to a *Euclidean* space for which we have defined the scalar product. The analytical expression of the scalar product of two vectors $\mathbf{x} = x^i \mathbf{e}_i$ and $\mathbf{y} = y^j \mathbf{e}_j$ is

$$\mathbf{x} \cdot \mathbf{y} = x^i \mathbf{e}_i \cdot y^j \mathbf{e}_j.$$

Let us put

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij}. \tag{1.1.2.5}$$

The nine components g_{ij} are called the components of the *metric tensor*. Its tensor nature will be shown in Section 1.1.3.6.1. Owing to the commutativity of the scalar product, we have

$$g_{ij} = \mathbf{e}_i \cdot \mathbf{e}_j = \mathbf{e}_j \cdot \mathbf{e}_i = g_{ji}.$$

The table of the components g_{ij} is therefore symmetrical. One of the definition properties of the scalar product is that if $\mathbf{x} \cdot \mathbf{y} = 0$ for all \mathbf{x} , then $\mathbf{y} = \mathbf{0}$. This is translated as

$$x^i y^j g_{ij} = 0 \quad \forall x^i \implies y^j g_{ij} = 0.$$

In order that only the trivial solution ($y^j = 0$) exists, it is necessary that the determinant constructed from the g_{ij} 's is different from zero:

$$\Delta(g_{ij}) \neq 0.$$

This important property will be used in Section 1.1.2.4.1.

1.1.2.3. Orthonormal frames of coordinates – rotation matrix

An orthonormal coordinate frame is characterized by the fact that

$$g_{ij} = \delta_{ij} \quad (= 0 \text{ if } i \neq j \text{ and } = 1 \text{ if } i = j). \tag{1.1.2.6}$$

One deduces from this that the scalar product is written simply as

$$\mathbf{x} \cdot \mathbf{y} = x^i y^j g_{ij} = x^i y^i.$$

Let us consider a change of basis between two orthonormal systems of coordinates:

$$\mathbf{e}_i = A_i^j \mathbf{e}'_j.$$

Multiplying the two sides of this relation by \mathbf{e}'_p , it follows that

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$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \mathbf{e}'_k \cdot \mathbf{e}'_j = A_i^j g'_{kj} = A_i^j \delta_{kj} \quad (\text{written correctly}),$$

which can also be written, if one notes that variance is not apparent in an orthonormal frame of coordinates and that the position of indices is therefore not important, as

$$\mathbf{e}_i \cdot \mathbf{e}'_j = A_i^j \quad (\text{written incorrectly}).$$

The matrix coefficients, A_i^j , are the direction cosines of \mathbf{e}'_j with respect to the \mathbf{e}_i basis vectors. Similarly, we have

$$B_j^i = \mathbf{e}_i \cdot \mathbf{e}'_j$$

so that

$$A_i^j = B_j^i \quad \text{or} \quad A = B^T,$$

where T indicates transpose. It follows that

$$A = B^T \quad \text{and} \quad A = B^{-1}$$

so that

$$\left. \begin{aligned} A^T &= A^{-1} &\Rightarrow & A^T A = I \\ B^T &= B^{-1} &\Rightarrow & B^T B = I. \end{aligned} \right\} \quad (1.1.2.7)$$

The matrices A and B are unitary matrices or matrices of rotation and

$$\Delta(A)^2 = \Delta(B)^2 = 1 \Rightarrow \Delta(A) = \pm 1. \quad (1.1.2.8)$$

If $\Delta(A) = 1$ the senses of the axes are not changed – *proper* rotation.

If $\Delta(A) = -1$ the senses of the axes are changed – *improper* rotation. (The right hand is transformed into a left hand.)

One can write for the coefficients A_i^j

$$A_i^j B_j^k = \delta_i^k; \quad A_i^j A_j^k = \delta_i^k,$$

giving six relations between the nine coefficients A_i^j . There are thus *three* independent coefficients of the 3×3 matrix A .

1.1.2.4. Covariant coordinates – dual or reciprocal space

1.1.2.4.1. Covariant coordinates

Using the developments (1.1.2.1) and (1.1.2.5), the scalar products of a vector \mathbf{x} and of the basis vectors \mathbf{e}_i can be written

$$x_i = \mathbf{x} \cdot \mathbf{e}_i = x^j \mathbf{e}_j \cdot \mathbf{e}_i = x^j g_{ij}. \quad (1.1.2.9)$$

The n quantities x_i are called *covariant* components, and we shall see the reason for this a little later. The relations (1.1.2.9) can be considered as a system of equations of which the components x^j are the unknowns. One can solve it since $\Delta(g_{ij}) \neq 0$ (see the end of Section 1.1.2.2). It follows that

$$x^j = x_i g^{ij} \quad (1.1.2.10)$$

with

$$g^{ij} g_{jk} = \delta_k^i. \quad (1.1.2.11)$$

The table of the g^{ij} 's is the inverse of the table of the g_{ij} 's. Let us now take up the development of \mathbf{x} with respect to the basis \mathbf{e}_i :

$$\mathbf{x} = x^i \mathbf{e}_i.$$

Let us replace x^i by the expression (1.1.2.10):

$$\mathbf{x} = x_j g^{ji} \mathbf{e}_i, \quad (1.1.2.12)$$

and let us introduce the set of n vectors

$$\mathbf{e}^j = g^{ji} \mathbf{e}_i \quad (1.1.2.13)$$

which span the space E^n ($j = 1, \dots, n$). This set of n vectors forms a *basis* since (1.1.2.12) can be written with the aid of (1.1.2.13) as

$$\mathbf{x} = x_j \mathbf{e}^j. \quad (1.1.2.14)$$

The x_j 's are the components of \mathbf{x} in the basis \mathbf{e}^j . This basis is called the *dual basis*. By using (1.1.2.11) and (1.1.2.13), one can show in the same way that

$$\mathbf{e}_j = g_{ij} \mathbf{e}^i. \quad (1.1.2.15)$$

It can be shown that the basis vectors \mathbf{e}^j transform in a change of basis like the components x^j of the physical space. They are therefore *contravariant*. In a similar way, the components x_j of a vector \mathbf{x} with respect to the basis \mathbf{e}^j transform in a change of basis like the basis vectors in direct space, \mathbf{e}_j ; they are therefore *covariant*:

$$\left. \begin{aligned} \mathbf{e}^j &= B_k^j \mathbf{e}^k; & \mathbf{e}^k &= A_j^k \mathbf{e}^j \\ x_i &= A_i^j x'_j; & x'_j &= B_j^i x_i. \end{aligned} \right\} \quad (1.1.2.16)$$

1.1.2.4.2. Reciprocal space

Let us take the scalar products of a covariant vector \mathbf{e}_i and a contravariant vector \mathbf{e}^j :

$$\mathbf{e}_i \cdot \mathbf{e}^j = \mathbf{e}_i \cdot g^{jk} \mathbf{e}_k = \mathbf{e}_i \cdot \mathbf{e}_k g^{jk} = g_{ik} g^{jk} = \delta_i^j$$

[using expressions (1.1.2.5), (1.1.2.11) and (1.1.2.13)].

The relation we obtain, $\mathbf{e}_i \cdot \mathbf{e}^j = \delta_i^j$, is identical to the relations defining the reciprocal lattice in crystallography; *the reciprocal basis then is identical to the dual basis \mathbf{e}^i .*

1.1.2.4.3. Properties of the metric tensor

In a change of basis, following (1.1.2.3) and (1.1.2.5), the g_{ij} 's transform according to

$$\left. \begin{aligned} g_{ij} &= A_i^k A_j^m g'_{km} \\ g'_{ij} &= B_i^k B_j^m g_{km}. \end{aligned} \right\} \quad (1.1.2.17)$$

Let us now consider the scalar products, $\mathbf{e}^i \cdot \mathbf{e}^j$, of two contravariant basis vectors. Using (1.1.2.11) and (1.1.2.13), it can be shown that

$$\mathbf{e}^i \cdot \mathbf{e}^j = g^{ij}. \quad (1.1.2.18)$$

In a change of basis, following (1.1.2.16), the g^{ij} 's transform according to

$$\left. \begin{aligned} g^{ij} &= B_k^i B_m^j g'^{km} \\ g'^{ij} &= A_k^i A_m^j g^{km}. \end{aligned} \right\} \quad (1.1.2.19)$$

The volumes V' and V of the cells built on the basis vectors \mathbf{e}'_i and \mathbf{e}_i , respectively, are given by the triple scalar products of these two sets of basis vectors and are related by

$$\begin{aligned} V' &= (\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3) \\ &= \Delta(B_j^i) (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3) \\ &= \Delta(B_j^i) V, \end{aligned} \quad (1.1.2.20)$$

where $\Delta(B_j^i)$ is the determinant associated with the transformation matrix between the two bases. From (1.1.2.17) and (1.1.2.20), we can write

$$\Delta(g'_{ij}) = \Delta(B_j^i) \Delta(B_j^m) \Delta(g_{km}).$$

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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}'_j and

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

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

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

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,

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

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

$$x^i = B^i_{\alpha} x'^{\alpha}; \quad y_j = A^{\beta}_j y'_{\beta}; \quad z^k = B^k_{\gamma} z'^{\gamma}.$$

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

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

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

$$p'^{\beta}_{\alpha\gamma} = p^j_{ik} B^i_{\alpha} A^{\beta}_j B^k_{\gamma}. \quad (1.1.3.2)$$

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' :

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

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).