

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

1.1.4.3.2. Symmetry of magnetic induction

The determination of the symmetry of magnetic quantities is more delicate. Considered as an effect, magnetic induction may be obtained by passing an electric current in a loop (Fig. 1.1.4.2). The corresponding symmetry is that of a cylinder rotating around its axis, $(A_\infty/M)C$. Conversely, the variation of the flux of magnetic induction through a loop induces an electric current in the loop. If the magnetic induction is considered as a cause, its effect has the same symmetry. The symmetry associated with the magnetic induction is therefore $(A_\infty/M)C$.

This symmetry is completely different from that of the electric field. This difference can be understood by reference to Maxwell's equations, which relate electric and magnetic quantities:

$$\text{curl } \mathbf{E} = \nabla \wedge \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}; \quad \text{curl } \mathbf{H} = \nabla \wedge \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}.$$

It was seen in Section 1.1.3.8.3 that the curl is an axial vector because it is a vector product. Maxwell's equations thus show that if the electric quantities (\mathbf{E} , \mathbf{D}) are polar vectors, the magnetic quantities (\mathbf{B} , \mathbf{H}) are axial vectors and *vice versa*; the equations of Maxwell are, in effect, perfectly symmetrical on this point. Indeed, one could have been tempted to determine the symmetry of the magnetic field by considering interactions between magnets, which would have led to the symmetry $A_\infty \infty M$ for the magnetic quantities. However, in the world where we live and where the origin of magnetism is in the spin of the electron, the magnetic field is an axial vector of symmetry $(A_\infty/M)C$ while the electric field is a polar vector of symmetry $A_\infty \infty M$.

1.1.4.4. Superposition of several causes in the same medium – pyroelectricity and piezoelectricity

1.1.4.4.1. Introduction

Let us now consider a phenomenon resulting from the superposition of several causes in the same medium. The symmetry of the global cause is the intersection of the groups of symmetry of the various causes: the asymmetries add up (Curie, 1894). This remark can be applied to the determination of the point groups where physical properties such as pyroelectricity or piezoelectricity are possible.

1.1.4.4.2. Pyroelectricity

Pyroelectricity is the property presented by certain materials that exhibit electric polarization when the temperature is changed uniformly. Actually, this property appears in crystals for which the centres of gravity of the positive and negative charges do not coincide in the unit cell. They present therefore a spontaneous polarization that varies with temperature because, owing to thermal expansion, the distances between these centres of gravity are temperature dependent. A very important case is that of the ferroelectric crystals where the direction of the polarization can be changed under the application of an external electric field.

From the viewpoint of symmetry, pyroelectricity can be considered as the superposition of two causes, namely the crystal

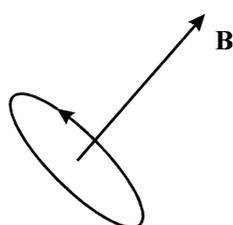


Fig. 1.1.4.2. Symmetry of magnetic induction.

with its symmetry on one hand and the increase of temperature, which is isotropic, on the other. The intersection of the groups of symmetry of the two causes is in this case identical to the group of symmetry of the crystal. The symmetry associated with the effect is that of the electric polarization that is produced, $A_\infty \infty M$. Since the asymmetry of the cause must pre-exist in the causes, the latter may not possess more than one axis of symmetry nor mirrors other than those parallel to the single axis. The only crystal point groups compatible with this condition are

$$1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm.$$

There are therefore only ten crystallographic groups that are compatible with the pyroelectric effect. For instance, tourmaline, in which the effect was first observed, belongs to $3m$.

1.1.4.4.3. Piezoelectricity

Piezoelectricity, discovered by the Curie brothers (Curie & Curie, 1880), is the property presented by certain materials that exhibit an electric polarization when submitted to an applied mechanical stress such as a uniaxial compression (see, for instance, Cady, 1964; Ikeda, 1990). Conversely, their shape changes when they are submitted to an external electric field; this is the converse piezoelectric effect. The physical interpretation of piezoelectricity is the following: under the action of the applied stress, the centres of gravity of negative and positive charges move to different positions in the unit cell, which produces an electric polarization.

From the viewpoint of symmetry, piezoelectricity can be considered as the superposition of two causes, the crystal with its own symmetry and the applied stress. The symmetry associated with a uniaxial compression is that of two equal and opposite forces, namely $A_\infty/M \infty A_2/\infty MC$. The effect is an electric polarization, of symmetry $A_\infty \infty M$, which must be higher than or equal to the intersection of the symmetries of the two causes:

$$\frac{A_\infty \infty A_2}{M \infty M} C \cap S_{\text{crystal}} \leq A_\infty \infty M,$$

where S_{crystal} denotes the symmetry of the crystal.

It may be noted that the effect does not possess a centre of symmetry. The crystal point groups compatible with the property of piezoelectricity are therefore among the 21 noncentrosymmetric point groups. More elaborate symmetry considerations show further that group 432 is also not compatible with piezoelectricity. This will be proved in Section 1.1.4.10.4 using the symmetry properties of tensors. There are therefore 20 point groups compatible with piezoelectricity:

$$1, 2, m, 222, 2mm, \\ 3, 32, 3m, 4, \bar{4}, 422, 4mm, \bar{4}2m, 6, \bar{6}, 622, 6mm, \bar{6}2m \\ 23, \bar{4}3m.$$

The intersection of the symmetries of the crystal and of the applied stress depend of course on the orientation of this stress relative to the crystallographic axes. Let us take, for instance, a crystal of quartz, which belongs to group $32 = A_33A_2$. The above condition becomes

$$\frac{A_\infty \infty A_2}{M \infty M} C \cap A_33A_2 \leq A_\infty \infty M.$$

If the applied compression is parallel to the threefold axis, the intersection is identical to the symmetry of the crystal, A_33A_2 , which possesses symmetry elements that do not exist in the effect, and piezoelectricity cannot appear. This is of course obvious because the threefold axis is not polar. For all other directions, piezoelectricity may appear.

1.1. INTRODUCTION TO THE PROPERTIES OF TENSORS

1.1.4.5. Intrinsic symmetry of tensors

1.1.4.5.1. Introduction

The symmetry of a tensor representing a physical property or a physical quantity may be due either to its own nature or to the symmetry of the medium. The former case is called intrinsic symmetry. It is a property that can be exhibited both by physical property tensors or by field tensors. The latter case is the consequence of Neumann's principle and will be discussed in Section 1.1.4.6. It applies to physical property tensors.

1.1.4.5.2. Symmetric tensors

1.1.4.5.2.1. Tensors of rank 2

A bilinear form is symmetric if

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

Its components satisfy the relations

$$t_{ij} = t_{ji}.$$

The associated matrix, T , is therefore equal to its transpose T^T :

$$T = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} = T^T = \begin{pmatrix} t_{11} & t_{21} & t_{31} \\ t_{12} & t_{22} & t_{32} \\ t_{13} & t_{23} & t_{33} \end{pmatrix}.$$

In a space with n dimensions, the number of independent components is equal to

$$(n^2 - n)/2 + n = (n^2 + n)/2.$$

Examples

(1) The metric tensor (Section 1.1.2.2) is symmetric because the scalar product is commutative.

(2) The tensors representing one of the physical properties associated with the leading diagonal of the matrix of physical properties (Section 1.1.1.4), such as the dielectric constant. Let us take up again the demonstration of this case and consider a capacitor being charged. The variation of the stored energy per unit volume for a variation $d\mathbf{D}$ of the displacement is

$$dW = \mathbf{E} \cdot d\mathbf{D},$$

where [equation (1.1.3.3)]

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

Since both D^i and E^j are expressed through contravariant components, the expression for the energy should be written

$$dW = g_{ij} E^j dD^i.$$

If we replace D^i by its expression, we obtain

$$dW = g_{ij} \varepsilon_k^i E^j dE^k = \varepsilon_{jk} E^j dE^k,$$

where we have introduced the doubly covariant form of the dielectric constant tensor, ε_{jk} . Differentiating twice gives

$$\frac{\partial^2 W}{\partial E^k \partial E^j} = \varepsilon_{jk}.$$

If one can assume, as one usually does in physics, that the energy is a 'good' function and that the order of the derivatives is of little importance, then one can write

$$\frac{\partial^2 W}{\partial E^k \partial E^j} = \frac{\partial^2 W}{\partial E^j \partial E^k}.$$

As one can exchange the role of the dummy indices, one has

$$\partial^2 W / (\partial E^j \partial E^k) = \varepsilon_{kj}.$$

Hence one deduces that

$$\varepsilon_{jk} = \varepsilon_{kj}.$$

The dielectric constant tensor is therefore symmetric. One notes that the symmetry is conveyed on two indices of the same variance. One could show in a similar way that the tensor representing magnetic susceptibility is symmetric.

(3) There are other possible causes for the symmetry of a tensor of rank 2. The strain tensor (Section 1.3.1), which is a field tensor, is symmetric because one does not take into account the rotative part of the deformation; the stress tensor, also a field tensor (Section 1.3.1), is symmetric because one neglects body torques (couples per unit volume); the thermal conductivity tensor is symmetric because circulating flows do not produce any detectable effects *etc.*

1.1.4.5.2.2. Tensors of higher rank

A tensor of rank higher than 2 may be symmetric with respect to the indices of one or more couples of indices. For instance, by its very nature, the demonstration given in Section 1.1.1.4 shows that the tensors representing principal physical properties are of even rank. If n is the rank of the associated square matrix, the number of independent components is equal to $(n^2 + n)/2$. In the case of a tensor of rank 4, such as the tensor of elastic constants relating the strain and stress tensors (Section 1.3.3.2.1), the number of components of the tensor is $3^4 = 81$. The associated matrix is a 9×9 one, and the number of independent components is equal to 45.

1.1.4.5.3. Antisymmetric tensors – axial tensors

1.1.4.5.3.1. Tensors of rank 2

A bilinear form is said to be antisymmetric if

$$T(\mathbf{x}, \mathbf{y}) = -T(\mathbf{y}, \mathbf{x}).$$

Its components satisfy the relations

$$t_{ij} = -t_{ji}.$$

The associated matrix, T , is therefore also antisymmetric:

$$T = -T^T = \begin{pmatrix} 0 & t_{12} & t_{13} \\ -t_{12} & 0 & t_{23} \\ -t_{13} & -t_{23} & 0 \end{pmatrix}.$$

The number of independent components is equal to $(n^2 - n)/2$, where n is the number of dimensions of the space. It is equal to 3 in a three-dimensional space, and one can consider these components as those of a *pseudovector* or *axial* vector. It must never be forgotten that under a change of basis the components of an axial vector transform like those of a tensor of rank 2.

Every tensor can be decomposed into the sum of two tensors, one symmetric and the other one antisymmetric:

$$T = S + A,$$

with $S = (T + T^T)/2$ and $A = (T - T^T)/2$.

Example. As shown in Section 1.1.3.7.2, the components of the vector product of two vectors, \mathbf{x} and \mathbf{y} ,

$$z_k = \varepsilon_{ijk} x^i y^j,$$

are really the independent components of an antisymmetric tensor of rank 2. The magnetic quantities, \mathbf{B} , \mathbf{H} (Section 1.1.4.3.2), the tensor representing the pyromagnetic effect (Section 1.1.1.3) *etc.* are axial tensors.

1. TENSORIAL ASPECTS OF PHYSICAL PROPERTIES

1.1.4.5.3.2. Tensors of higher rank

If the rank of the tensor is higher than 2, the tensor may be antisymmetric with respect to the indices of one or several couples of indices.

(i) *Tensors of rank 3 antisymmetric with respect to every couple of indices.* A trilinear form $T(\mathbf{x}, \mathbf{y}, \mathbf{z}) = t_{ijk}x^i y^j z^k$ is said to be antisymmetric if it satisfies the relations

$$\left. \begin{aligned} T(\mathbf{x}, \mathbf{y}, \mathbf{z}) &= -T(\mathbf{y}, \mathbf{x}, \mathbf{z}) \\ &= -T(\mathbf{x}, \mathbf{z}, \mathbf{y}) \\ &= -T(\mathbf{z}, \mathbf{y}, \mathbf{x}). \end{aligned} \right\}$$

Tensor t_{ijk} has 27 components. It is found that all of them are equal to zero, except

$$t_{123} = t_{231} = t_{312} = -t_{213} = -t_{132} = -t_{321}.$$

The three-times contracted product with the permutations tensor (Section 1.1.3.7.2), $(1/6)\varepsilon_{ijk}t_{ijk}$, is a *pseudoscalar* or *axial scalar*. It is not a usual scalar: the sign of this product changes when one changes the hand of the reference axes, change of basis represented by the matrix

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

Form $T(\mathbf{x}, \mathbf{y}, \mathbf{z})$ can also be written

$$T(\mathbf{x}, \mathbf{y}, \mathbf{z}) = P t_{123},$$

where

$$P = \varepsilon_{ijk}x^i y^j z^k = \begin{vmatrix} x^1 & x^2 & x^3 \\ y^1 & y^2 & y^3 \\ z^1 & z^2 & z^3 \end{vmatrix}$$

is the triple scalar product of the three vectors $\mathbf{x}, \mathbf{y}, \mathbf{z}$:

$$P = (\mathbf{x}, \mathbf{y}, \mathbf{z}) = (\mathbf{x} \wedge \mathbf{y} \cdot \mathbf{z}).$$

It is also a pseudoscalar. The permutation tensor is not a real tensor of rank 3: if the hand of the axes is changed, the sign of P also changes; P is therefore not a trilinear form.

Another example of a pseudoscalar is given by the rotatory power of an optically active medium, which is expressed through the relation (see Section 1.6.5.4)

$$\theta = \rho d,$$

where θ is the rotation angle of the light wave, d the distance traversed in the material and ρ is a pseudoscalar: if one takes the mirror image of this medium, the sign of the rotation of the light wave also changes.

(ii) *Tensor of rank 3 antisymmetric with respect to one couple of indices.* Let us consider a trilinear form such that

$$T(\mathbf{x}, \mathbf{y}, \mathbf{z}) = -T(\mathbf{y}, \mathbf{x}, \mathbf{z}).$$

Its components satisfy the relation

$$t^{iil} = 0; \quad t^{ijl} = -t^{jil}.$$

The twice contracted product

$$t_k^l = \frac{1}{2}\varepsilon_{ijk}t^{ijl}$$

is an *axial* tensor of rank 2 whose components are the independent components of the antisymmetric tensor of rank 3, t^{ijl} .

Examples

(1) *Hall constant.* The Hall effect is observed in semiconductors. If one takes a semiconductor crystal and applies a

magnetic induction \mathbf{B} and at the same time imposes a current density \mathbf{j} at right angles to it, one observes an electric field \mathbf{E} at right angles to the other two fields (see Section 1.8.3.4). The expression for the field can be written

$$E_i = R_H \varepsilon_{ikl} j_k B_l,$$

where $R_H \varepsilon_{ikl}$ is the Hall constant, which is a tensor of rank 3. However, because the direction of the current density is imposed by the physical law (the set of vectors $\mathbf{B}, \mathbf{j}, \mathbf{E}$ constitutes a right-handed frame), one has

$$R_H \varepsilon_{ikl} = -R_H \varepsilon_{kil},$$

which shows that $R_H \varepsilon_{ikl}$ is an antisymmetric (axial) tensor of rank 3. As can be seen from its physical properties, only the components such that $i \neq k \neq l$ are different from zero. These are

$$R_H \varepsilon_{123} = -R_H \varepsilon_{213}; \quad R_H \varepsilon_{132} = -R_H \varepsilon_{312}; \quad R_H \varepsilon_{312}; \quad R_H \varepsilon_{321}.$$

(2) *Optical rotation.* The gyration tensor used to describe the property of optical rotation presented by gyrotropic materials (see Section 1.6.5.4) is an axial tensor of rank 2, which is actually an antisymmetric tensor of rank 3.

(3) *Acoustic activity.* The acoustic gyrotropic tensor describes the rotation of the polarization plane of a transverse acoustic wave propagating along the acoustic axis (see for instance Kumaraswamy & Krishnamurthy, 1980). The elastic constants may be expanded as

$$c_{ijkl}(\omega, \mathbf{k}) = c_{ijkl}(\omega) + id_{ijklm}(\omega)k_m + \dots,$$

where d_{ijklm} is a fifth-rank tensor. Time-reversal invariance requires that $d_{ijklm} = -d_{jiklm}$, which shows that it is an antisymmetric (axial) tensor.

1.1.4.5.3.3. Properties of axial tensors

The two preceding sections have shown examples of axial tensors of ranks 0 (pseudoscalar), 1 (pseudovector) and 2. They have in common that all their components change sign when the sign of the basis is changed, and this can be taken as the definition of an axial tensor. Their components are the components of an antisymmetric tensor of higher rank. It is important to bear in mind that in order to obtain their behaviour in a change of basis, one should first determine the behaviour of the components of this antisymmetric tensor.

1.1.4.6. Symmetry of tensors imposed by the crystalline medium

Many papers have been devoted to the derivation of the invariant components of physical property tensors under the influence of the symmetry elements of the crystallographic point groups: see, for instance, Fumi (1951, 1952*a,b,c*, 1987), Fumi & Ripamonti (1980*a,b*), Nowick (1995), Nye (1957, 1985), Sands (1995), Sirotnin & Shaskol'skaya (1982), and Wooster (1973). There are three main methods for this derivation: the matrix method (described in Section 1.1.4.6.1), the direct inspection method (described in Section 1.1.4.6.3) and the group-theoretical method (described in Section 1.2.4 and used in the accompanying software, see Section 1.2.7.4).

1.1.4.6.1. Matrix method – application of Neumann's principle

An operation of symmetry turns back the crystalline edifice on itself; it allows the physical properties of the crystal and the tensors representing them to be invariant. An operation of symmetry is equivalent to a change of coordinate system. In a change of system, a tensor becomes

$$t_{\gamma\delta}^{\alpha\beta} = t_{kl}^{ij} A_i^\alpha A_j^\beta B_\gamma^k B_\delta^l.$$

If A represents a symmetry operation, it is a unitary matrix: