On the Elastic Properties of Lattices

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(Received August 13, 1946)

The potential energy of a deformed lattice can be written in the form

$$V = V_0 + V_1 + V_2,$$

where V_0 is a constant (the energy of the undeformed lattice), V_1 the part linear in the displacements of the lattice points from their normal positions, V_2 the part quadratic in the displacements. The terms of higher order are neglected. In view of the requirement that the normal position of each lattice point be a position of equilibrium the linear part vanishes ($V_1 = 0$) so that the energy is simply equal to V_2 (apart from the constant V_0). As the energy must be invariant with respect to rotations of the system, W. Voigt postulated the invariance of V_2 and derived from this assumption the so-called *Cauchy relations* between the elastic coefficients. A closer analysis shows that this conclusion is open to objection. The term V_2 represents the energy only because of the subsidiary condition $V_1 = 0$ which, upon investigation, turns out to be not invariant with respect to rotations. Hence, V_2 is not invariant either: a fact which removes the theoretical basis of the Cauchy relations.

1. INTRODUCTION

IN recent years the problem of elastic oscillations of crystalline solids (conceived as atomic lattices) was the subject of papers by Blackman,[1] Kellermann,[2] Fine,[3] Montroll,[4] and others. Considerable progress has been achieved by these authors in the study of these oscillations and in devising numerical methods for calculating the frequency distribution. It seems, nevertheless, that some of the more fundamental questions are not yet very well understood and need further elucidation. We refer, in particular, to the relations between the coefficients of the quadratic form representing the potential energy of the lattice, on one hand, and the measurable coefficients of elasticity, on the other.

It is usually stated that, in the case of central forces between the atoms of the lattice, the symmetry of the lattice coefficients is such that it involves the so-called *Cauchy relations* between the coefficients of elasticity. In mentioning the Cauchy relations all modern writers on the subject refer to W. Voigt.[5] Although these relations are admittedly in contradiction to observed facts, nobody seems to have thoroughly re-examined their derivation or the conditions under which they are supposed to be valid. We shall show in this paper that Voigt's proof contains a serious flaw which invalidates his results: *as far as measurable elasticity coefficients are concerned, no relations of the Cauchy type exist between them, even in the case of central forces.*

This fact is not only of theoretical interest but has also some bearing on practical problems. Indeed, in some of the above mentioned papers, the Cauchy relations were used as a means for determining the numerical values of the lattice coefficients. In the light of our results these numerical estimates are no longer reliable and will have to be revised.

2. EXPRESSION FOR THE POTENTIAL ENERGY

Let an atom (or point) of the lattice be labeled by the Greek index μ, and let the three cartesian coordinates of its normal position be denoted by $x_{\mu i}$ ($i = 1, 2, 3$), so that the latin subscript i refers to the three orthogonal directions of space. When the lattice is deformed, all the points get slightly displaced, and their coordinates assume the new values $x_{\mu i} + s_{\mu i}$, where $s_{\mu i}$ is called the i-component of the displacement of the point μ.

As our primary purpose is to investigate the validity of the Cauchy relations, which are

[1] M. Blackman, Proc. Roy. Soc. **A148**, 384 (1935); **149**, 126 (1935); **159**, 416 (1937); **164**, 62 (1938).
[2] E. W. Kellermann, Phil. Trans. **238**, 519 (1940).
[3] P. Chs. Fine, Phys. Rev. **56**, 355 (1939).
[4] E. W. Montroll *et al.*, J. Chem. Phys. **10**, 218 (1942); **11**, 481 (1943); **12**, 98 (1944).
[5] W. Voigt, *Lehrbuch der Kristallphysik* (Leipzig, 1910), Sections 297, 298.

claimed only for central forces between the atoms, it will save space if we restrict ourselves to the case of such forces. We assume, therefore, that the mutual energy of the pair of lattice points μ and ν is given by the function

$$\Phi(\bar{r}_{\mu\nu}),$$

symmetric in the pair of indices μ, ν.

$$\bar{r}_{\mu\nu}^2 = (a_{\mu\nu 1} + s_{\mu 1} - s_{\nu 1})^2$$
$$+ (a_{\mu\nu 2} + s_{\mu 2} - s_{\nu 2})^2 + (a_{\mu\nu 3} + s_{\mu 3} - s_{\nu 3})^2,$$

where $a_{\mu\nu i} = -a_{\nu\mu i} = x_{\mu i} - x_{\nu i}$ is the i-component of the distance between the points μ and ν. Hence, the normal distance between these points is $r_{\mu\nu}$,

$$r_{\mu\nu}^2 = a_{\mu\nu 1}^2 + a_{\mu\nu 2}^2 + a_{\mu\nu 3}^2.$$

Thus the total potential energy of the lattice can be written in the form

$$V = \tfrac{1}{2} \sum_{\mu\nu} \Phi_{\mu\nu}(\bar{r}_{\mu\nu})_0 \qquad (1)$$

where the factor $\tfrac{1}{2}$ insures that each term $\Phi_{\mu\nu}$ occurs in the expression only once.

Expanding the expression with respect to the small differences $s_{\mu i} - s_{\nu i}$ up to terms of the second order, we obtain

$$V = V_0 + V_1 + V_2, \qquad (2)$$

where V_0 is the energy of the undeformed lattice, while the terms of first and second order can be written as follows, using Einstein's convention with respect to the latin indices:

$$V_1 = \sum_{\mu\nu} A_{\mu\nu} a_{\mu\nu j}(s_{\mu j} - s_{\nu j}), \qquad (3)$$

$$V_2 = \sum_{\mu\nu} [(B_{\mu\nu j} - C_{\mu\nu} a_{\mu\nu j}^2)(s_{\mu j} - s_{\nu j})^2$$
$$+ C_{\mu\nu} a_{\mu\nu i} a_{\mu\nu j}(s_{\mu i} - s_{\nu i})(s_{\mu j} - s_{\nu j})]. \qquad (4)$$

In introducing these notations we anticipate to some extent the results of Section 5 where it will be shown that the meaning of the coefficients is as follows:

$$A_{\mu\nu} a_{\mu\nu j} = \tfrac{1}{2}(\partial\Phi_{\mu\nu}/\partial a_{\mu\nu j})_0,$$
$$B_{\mu\nu j} = \tfrac{1}{2}(\partial^2\Phi_{\mu\nu}/\partial a_{\mu\nu j}^2)_0,$$
$$C_{\mu\nu} a_{\mu\nu i} a_{\mu\nu j} = \tfrac{1}{2}(\partial^2\Phi_{\mu\nu}/\partial a_{\mu\nu i}\partial a_{\mu\nu j})_0,$$
$$\text{for } i \neq j. \qquad (5)$$

The notations are chosen so as to bring out the symmetry character in the subscripts μ and ν since it can be inferred from the Eqs. (5) that $A_{\mu\nu}$, $B_{\mu\nu j}$, $C_{\mu\nu}$ are all symmetric in μ, ν.

However, for the present, we shall not make use of the relations (5) and shall regard the coefficients simply as empirically given constants whose dependence on i, j, and symmetry character in μ, ν could be established in a different way. Indeed, it is possible to proceed as follows. Instead of introducing explicitly Eq. (1), the theory can be built up on the following two postulates:

(1) The potential energy can be represented as the sum of mutual potential energies of pairs of points (without introducing from the start the dependence on $\bar{r}_{\mu\nu}$).

(2) The potential energy is invariant with respect to translations and rotations (law of action and reaction).

The dependence on the differences $s_{\mu i} - s_{\nu i}$, only, is then obtained from the invariance with respect to translations, the symmetry character of the coefficients from the invariance with respect to rotations. In particular we wish to underline that the independence of the coefficients $A_{\mu\nu}$ and $C_{\mu\nu}$ of the directional subscripts i, j, is a necessary consequence of the rotational invariance. We shall briefly return to this question in Section 4.

3. TRANSFORMATION TO STRAIN COMPONENTS

We shall define the first-order strain components as the matrix

$$e_{ij}^{(0)} = \frac{1}{2}\left(\frac{\partial s_j}{\partial x_i} + \frac{\partial s_i}{\partial x_j}\right), \quad (i, j = 1, 2, 3). \qquad (6)$$

It should be noted that this definition is slightly different from that used in some textbooks in that the element off the diagonal $(i \neq j)$ is supplied with a factor $\tfrac{1}{2}$. In addition we shall need the components of the rotations in their usual expression

$$\omega_{ij} = \frac{1}{2}\left(\frac{\partial s_j}{\partial x_i} - \frac{\partial s_i}{\partial x_j}\right). \qquad (7)$$

Adding the two formulas

$$\partial s_j/\partial x_i = e_{ij}^{(0)} + \omega_{ii}. \qquad (8)$$

Integrating this over a region in which $e_{ij}{}^{(0)}$ and ω_{ij} are uniform, s_j is obtained as a linear function in $e_{ij}{}^{(0)}$. The substitution into the energy expressions (3), (4) gives the energy as a function of the strain components. There is, however, one difficulty: the significant terms are those of second order in the strain components; these are incomplete as calculated by the above formulas, because $e_{ij}{}^{(0)}$ is only an approximate expression neglecting second order terms. It is sufficient for substitution into V_2 where the lowest terms are of the second order, but it is not sufficient to be used in V_1 since the error introduced by this approximation is of the same order as V_2 itself. It is therefore necessary to express the displacement of s_j as a function of the strain components up to terms of the second order. This fact was overlooked by Voigt who uses only the linear approximation. This is the point from which our theory begins to differ from his.

I do not know whether the creators of the theory of elasticity were familiar with the more accurate expression of the strain tensor. The earliest reference which is at my disposal is in the third volume of P. Appell's treatise on mechanics.[6] The formula is in our notations as follows:

$$e_{ij} = \frac{1}{2}\left(\frac{\partial s_j}{\partial x_i} + \frac{\partial s_i}{\partial x_j}\right) + \frac{1}{2}\frac{\partial s_k}{\partial x_i}\frac{\partial s_k}{\partial x_j}, \qquad (9)$$

where Einstein's convention applies to the index k appearing twice. As we are interested only in terms of first and second order, it is permissible to substitute into those of the second order the first approximation (8) and even to omit in this approximation the superscript 0 (i.e., replace in these terms $e_{ij}{}^{(0)}$ by e_{ij}). Hence,

$$\frac{1}{2}\left(\frac{\partial s_j}{\partial x_i} + \frac{\partial s_i}{\partial x_j}\right) = e_{ij} - \frac{1}{2}(e_{ik}+\omega_{ik})(e_{jk}+\omega_{jk}). \quad (10)$$

It is useful to abbreviate the writing by introducing the symbol

$$f_{ij} = e_{ij} + \omega_{ij}; \qquad (11)$$

this symbol is, however, non-symmetric $(f_{ij} \neq f_{ji})$

6 Paul Appell, "Traité de Mécanique Rationelle" (Gautier-Villars, Paris, 1901), Vol. 3, p. 243.

because e_{ij} is symmetric and ω_{ij} antisymmetric.

$$e_{ij} = e_{ji}, \qquad \omega_{ij} = -\omega_{ji}. \qquad (12)$$

Adding ω_{ij} to the Eq. (10), we find

$$\partial s_j/\partial s_i = f_{ij} - \tfrac{1}{2}f_{ik}f_{jk}. \qquad (13)$$

This can be readily integrated over a region where f_{ij} can be considered as constant, with the result

$$s_j = f_{ik}x_l - \tfrac{1}{2}f_{ik}f_{jk}x_l. \qquad (14)$$

Actually, the expression could be written in a slightly more general form by adding a constant of integration $s_j{}^{(0)}$ which represents the possible translation. However, the invariance of our energy expressions with respect to translations is a matter of course so that we simplify the case by putting $s_j{}^{(0)} = 0$.

We need to substitute into Eq. (4) only the first term of the formula (14). On the other hand, the second-order part of Eq. (3) entirely depends on the second term of (14). Indeed, it is easy to see that the part of second order of $V_1 = V_1' + V_2''$ takes the form

$$V_1'' = -\tfrac{1}{2}\sum_{\mu\nu} A_{\mu\nu}f_{jk}f_{ik}a_{\mu\nu j}a_{\mu\nu l},$$

which can be also written as

$$V_1'' = -\tfrac{1}{2}\sum_{\mu\nu} A_{\mu\nu}f_{kj}f_{lj}a_{\mu\nu k}a_{\mu\nu l}. \qquad (15)$$

On the other hand, the function V_2 becomes

$$V_2 = \tfrac{1}{2}\sum_{\mu\nu}\{(B_{\mu\nu j} - C_{\mu\nu}a_{\mu\nu j}{}^2)f_{kj}f_{lj}$$
$$+ C_{\mu\nu}a_{\mu\nu i}a_{\mu\nu j}f_{ki}f_{lj}\}a_{\mu\nu k}a_{\mu\nu l}. \quad (16)$$

The complete second-order part of the energy is thus

$$V_1'' + V_2 = \tfrac{1}{2}\sum_{\mu\nu}\{(B_{\mu\nu j} - C_{\mu\nu}a_{\mu\nu j}{}^2 - A_{\mu\nu})f_{kj}f_{lj}$$
$$\times C_{\mu\nu}a_{\mu\nu i}a_{\mu\nu j}f_{ki}f_{lj}\}a_{\mu\nu k}a_{\mu\nu l}. \quad (17)$$

The writing of the last two equations is not quite orthodox with respect to Einstein's convention. What is meant here is that the summation over an index is implied if the index occurs in the term *two or more times*. (According to the strict Einstein rule it must occur just *two times*.)

4. RELATIONS BETWEEN COEFFICIENTS

Since the energy V is invariant with respect to rotations all coefficients of the expansion of V with respect to the powers and products of ω_{ij} must vanish. The first-order part V_1' contains only linear terms, while $V_1'' + V_2$ contains either terms of second order in ω_{ij} or terms in which components of ω_{ij} are multiplied by components of e_{ij}. As the rotations are independent of the strain, the two functions V_1' and $V_1'' + V_2$ must be invariant each for itself. This involves certain relations between the coefficients $A_{\mu\nu}$, $B_{\mu\nu j}$, and $C_{\mu\nu}$. It will be necessary to write out our quadratic form explicitly:

$$V_1'' + V_2 = \tfrac{1}{2} \sum_{\mu\nu} \{ (B_{\mu\nu 1} - A_{\mu\nu})a_{\mu\nu 1}{}^2 f_{11}{}^2 + [(B_{\mu\nu 3} - A_{\mu\nu})a_{\mu\nu 2}{}^2 f_{23}{}^2 + (B_{\mu\nu 2} - A_{\mu\nu})a_{\mu\nu 3}{}^2 f_{32}{}^2 + 2C_{\mu\nu}a_{\mu\nu 2}{}^2 a_{\mu\nu 3}{}^2 f_{23}f_{32}]$$

$$+ 2C_{\mu\nu}a_{\mu\nu 2}{}^2 a_{\mu\nu 3}{}^2 f_{22}f_{33} + 2C_{\mu\nu}a_{\mu\nu 1}{}^2 a_{\mu\nu 2}a_{\mu\nu 3}(f_{23}+f_{32})f_{11}$$

$$+ 2[(B_{\mu\nu 1} - A_{\mu\nu})f_{31} + C_{\mu\nu}a_{\mu\nu 1}{}^2 f_{13}]f_{11}a_{\mu\nu 1}a_{\mu\nu 3} + 2[(B_{\mu\nu 1} - A_{\mu\nu})f_{21} + C_{\mu\nu}a_{\mu\nu 1}{}^2 f_{12}]f_{11}a_{\mu\nu 1}a_{\mu\nu 2}$$

$$+ 2[(B_{\mu\nu 1} - A_{\mu\nu})f_{21}f_{31} + C_{\mu\nu}(f_{12}f_{13} + f_{13}f_{21} + f_{31}f_{12})a_{\mu\nu 1}{}^2]a_{\mu\nu 2}a_{\mu\nu 3} + \text{etc.} \}. \quad (18)$$

By "etc." are meant additional terms which result from those written out by cyclic substitution of the indices (other than μ, ν). If we replace the symbols f_{ij} by their definitions (11), the invariance with respect to rotations requires the vanishing of all terms containing components ω_{ij} or their squares and products. This affects only the components ω_{ij} with $i \neq j$ because ω_{ii} is identically zero. The square and product terms entail the following relations,

$$\left.\begin{array}{c} \sum_{\mu\nu} [(B_{\mu\nu 3} - A_{\mu\nu})a_{\mu\nu 2}{}^2 + (B_{\mu\nu 2} - A_{\mu\nu})a_{\mu\nu 3}{}^2 - C_{\mu\nu}a_{\mu\nu 2}{}^2 a_{\mu\nu 3}{}^2] = 0, \\[2mm] \sum_{\mu\nu} (B_{\mu\nu 1} - A_{\mu\nu} - C_{\mu\nu}a_{\mu\nu 1}{}^2)a_{\mu\nu 2}a_{\mu\nu 3} = 0, \end{array}\right\} \quad (19)$$

while the linear terms lead to

$$\left.\begin{array}{c} \sum_{\mu\nu} [(B_{\mu\nu 3} - A_{\mu\nu})a_{\mu\nu 2}{}^2 - (B_{\mu\nu 2} - A_{\mu\nu})a_{\mu\nu 3}{}^2] = 0, \\[2mm] \sum_{\mu\nu} (B_{\mu\nu 1} - A_{\mu\nu} - C_{\mu\nu}a_{\mu\nu 1}{}^2)a_{\mu\nu 3}a_{\mu\nu 1} = 0, \\[2mm] \sum_{\mu\nu} (B_{\mu\nu 1} - A_{\mu\nu} - C_{\mu\nu}a_{\mu\nu 1}{}^2)a_{\mu\nu 1}a_{\mu\nu 2} = 0, \end{array}\right\} \quad (19')$$

and again to another relation already listed. Further, the relations must be added which result from these by cyclic substitution.

These relations can be used to reduce to a simpler form the remaining terms, which depend only on e_{ij}, namely,

$$V_1'' + V_2 = \tfrac{1}{2} \sum_{\mu\nu} \{ (B_{\mu\nu 1} - A_{\mu\nu})a_{\mu\nu 1}{}^2 e_{11}{}^2 + 2C_{\mu\nu}a_{\mu\nu 2}{}^2 a_{\mu\nu 3}{}^2(2e_{23}{}^2 + e_{22}e_{33})$$

$$+ 4C_{\mu\nu}a_{\mu\nu 1}{}^3(a_{\mu\nu 2}e_{12} + a_{\mu\nu 3}e_{13})e_{11} + 4C_{\mu\nu}a_{\mu\nu 1}{}^2 a_{\mu\nu 2}a_{\mu\nu 3}(e_{11}e_{23} + 2e_{12}e_{13}) + \text{etc.} \}. \quad (20)$$

Returning to the remark about the symmetry of the coefficients made at the end of Section 2, we may make here the following statement. If we had not postulated in Eqs. (5) the independence of $A_{\mu\nu}$ and $C_{\mu\nu}$ on the directions but had written more generally $A_{\mu\nu j}$, $C_{\mu\nu ij}$, then the requirement of rotational invariance would have given us a much larger number of conditions than the set (19), (19'). The burden of those additional conditions is precisely that $A_{\mu\nu j}$, $C_{\mu\nu ij}$ are the same for all subscripts i, j. Thus our assumptions (5) do not represent a loss of generality but only a more concise way of writing.

5. ANALOGS TO THE CAUCHY RELATIONS

Owing to Voigt's influence it has become customary to write quadratic forms of the type (20) in a manner which with our definition of e_{ij} is as follows

$$V_1'' + V_2 = \{\tfrac{1}{2}b_{11}e_{11}^2 + 2b_{44}e_{23}^2 + b_{23}e_{22}e_{33}$$
$$+ 2(b_{14}e_{23} + b_{15}e_{31} + b_{16}e_{12})e_{11}$$
$$+ 4b_{56}e_{12}e_{13} + \text{etc.}\}. \quad (21)$$

All the coefficients b_{ij} are symmetric in i, j. By "etc.," again, are meant terms which result by cyclic substitution from those written out. In these permutations the subscripts 1, 2, 3 and 4, 5, 6 form two separate permutation groups: for instance, the term derived from $4b_{56}e_{12}e_{13}$ is $4b_{64}e_{23}e_{21}$.

By comparing with the form (20) it will be seen that taking care of the rotational invariance leads to the following symmetry relations:

$$b_{23} = b_{44}, \quad b_{14} = b_{56}, \quad (22)$$

to which must be added those following by cyclic permutation,

$$\begin{matrix} b_{31} = b_{55}, & b_{25} = b_{64}, \\ b_{12} = b_{66}, & b_{36} = b_{45}. \end{matrix} \quad (22')$$

These relations form the analogs to Voigt's Cauchy relations and we shall refer to them by that name. We shall first show that these relations are indeed identically satisfied when we have central forces. Carrying out the differentiations indicated in the Eqs. (5) we easily find

$$\left.\begin{matrix} A_{\mu\nu} = \Phi_{\mu\nu}'/2r_{\mu\nu}, \\ B_{\mu\nu j} = \tfrac{1}{2}(a_{\mu\nu j}/r_{\mu\nu})^2\Phi_{\mu\nu}'' \\ \quad + [1 - (a_{\mu\nu j}/r_{\mu\nu})^2]\Phi_{\mu\nu}'/2r_{\mu\nu}, \\ C_{\mu\nu} = [\Phi_{\mu\nu}'' - \Phi_{\mu\nu}'/r_{\mu\nu}]/2r_{\mu\nu}^2. \end{matrix}\right\} (23)$$

The accent and double accent denote here, respectively, the first and second derivatives of $\Phi_{\mu\nu}(r_{\mu\nu})$ with respect to the argument $r_{\mu\nu}$.

We have seen that the Cauchy relations (22), (22') are an immediate consequence of the conditions (19), (19') and of their cyclic permutations. It is, however, obvious that all these conditions can be satisfied by the single relation

$$B_{\mu\nu j} - A_{\mu\nu} = C_{\mu\nu}a_{\mu\nu j}^2, \quad (24)$$

holding not only for the double sum but for each term separately. Now we find, indeed, from the Eqs. (23)

$$B_{\mu\nu j} - A_{\mu\nu} = \tfrac{1}{2}(a_{\mu\nu j}/r_{\mu\nu})^2[\Phi'' - \Phi'/r_{\mu\nu}]$$
$$= C_{\mu\nu}a_{\mu\nu j}^2. \quad (25)$$

We shall now go back to Voigt's work and see in what it differs from ours. It was mentioned in Section 3 that Voigt overlooked the second order terms (in e_{ij}) contained in V_1 of Eq. (3); this led him to attribute rotational invariance to the energy term V_2 alone. Such a contention is clearly untenable. Indeed, Voigt's theory differs from our formulas of Section 4 only in one point: the terms with $A_{\mu\nu}$ are left out in all the equations. Thus Voigt arrives at conditions equivalent to our conditions (19), (19') with the $A_{\mu\nu}$ terms crossed off. For instance, the first condition is, according to him,

$$\sum_{\mu\nu} [B_{\mu\nu3}a_{\mu\nu2}^2 + B_{\mu\nu2}a_{\mu\nu3}^2 - C_{\mu\nu}a_{\mu\nu2}^2a_{\mu\nu3}^2] = 0. \quad (26)$$

However, we have just verified that in the case of central forces the condition is satisfied in our form. Hence, the left side of Voigt's Eq. (26) is not equal to zero but to the negative of the missing terms, namely, to

$$\sum_{\mu\nu} A_{\mu\nu}(a_{\mu\nu2}^2 + a_{\mu\nu3}^2).$$

This expression does not, in general, vanish but is often of the same order magnitude as the other sums entering into the Eqs. (19). In fact, it is possible to supply examples of lattices in which it can be explicitly calculated. However, it is well to remember that the simplest possible model in which each atom interacts only with its nearest neighbors is not suitable for the purpose, since in such models $A_{\mu\nu} = 0$. Thus the deviations from the Cauchy relations are caused by interactions between points which are not nearest neighbors.

Voigt wrote the quadratic form V_2 in the form (21) with the only difference that he designated the coefficients by c_{ij} (instead of b_{ij} in our form $V_1'' + V_2$). He claimed for them the Cauchy relations

$$c_{23} = c_{44}, \quad c_{14} = c_{56}, \quad \text{etc.} \quad (27)$$

It follows from our discussion that this claim was unfounded. If Voigt or the many authors

who repeated his claim had gone to the trouble to substitute into his relations of the type (26) the actual values of $B_{\mu\nu j}$ and $C_{\mu\nu}$, as they result from the assumption of central forces, they would have noticed that these relations are not satisfied. Some authors seem to regard the Cauchy relations as additional restrictive conditions imposed upon the coefficients $A_{\mu\nu}$, $B_{\mu\nu j}$, $C_{\mu\nu}$. This. is, however, a misconception. In quadratic forms which are invariant with respect to rotations these conditions are merely a manifestation of the symmetry inherent in this invariance, they are satisfied identically and do not impose any further restrictions. In quadratic forms which are not rotationally invariant the Cauchy relations are not satisfied.

6. MEASUREMENT OF STRAINS

So far our discussion has been purely mathematical. We have now to tackle the physical question whether the actually measured elasticity coefficients are of the type satisfying the Cauchy relations. It is shown in the theory of elasticity that the deformation energy of an elastic body can be represented as a quadratic form in the strains e_{ij}. This quadratic form may be written out in the manner of formula (21). Following the customary notations, we shall designate the coefficients by c_{kl}, and we shall restrict ourselves in what follows to crystals and lattices of orthorhombic symmetry. This is done exclusively for the purpose of making the writing less cumbersome: all the arguments and conclusions apply just as well to the general case. The orthorombic symmetry requires the vanishing of all the terms which are linear or bilinear in e_{23}, e_{31}, e_{12}. Thus the energy expression becomes,

$$V=[\tfrac{1}{2}c_{11}e_{11}{}^2+2c_{44}e_{23}{}^2+c_{23}e_{22}e_{33}+\text{etc.}]. \quad (28)$$

If this energy is referred to a crystal cube of the volume 1 cm^3, the components of the stresses can be obtained from it by differentiation,

$$p_{11}=\partial V/\partial e_{11}=c_{11}e_{11}+c_{12}e_{22}+c_{13}e_{33},$$
$$p_{23}=\tfrac{1}{2}\partial V/\partial e_{23}=c_{44}e_{23}, \quad (29)$$

and so on, by cyclic permutation. As the components of the deformation e_{ij} and the stress components p_{ij} are both observable, it is possible to infer from direct measurements the coefficients

of elasticity c_{kl} by means of the Eqs. (29). The question which we have to answer is as follows: with which of the two quadratic forms of the lattice must the form V be identified?

In going back to the expressions (2)–(4) of the lattice energy in terms of the displacements, it is important to point out that $V_1=0$. In fact, the j-component of the force acting on the point ν is given by $-\partial V/\partial s_{\nu j}$. For the undistorted lattice we get thus

$$\sum_\mu A_{\mu\nu}a_{\mu\nu j}=0,$$

because in the undeformed lattice every point is in an equilibrium position, so that the force on it vanishes. Multiplying this by $s_{\nu j}$ and summing with respect to ν, we find that the second term with $s_{\nu j}$ in the expression (3) vanishes. This implies, however, that the term with $s_{\mu j}$ also vanishes because it is equal to the other term, $A_{\mu\nu}$ being symmetric and $a_{\mu\nu}$ antisymmetric in μ, ν. Consequently, $V_1=0$; from the mathematical point of view it is important that this is not an identical relation but an additional condition imposed on the variables of the system. At any event, there follows,

$$V=V_2. \quad (30)$$

Therefore, the two quadratic forms in e_{ij} discussed in the preceding section have the following properties. (1) The form V_2 represents the energy of the lattice, but it is not invariant with respect to rotations and does not satisfy the Cauchy relations. (2) The form $V_1''+V_2$ is rotationally invariant and satisfied Cauchy's relations, but it is not equal to the energy. The mathematical reason for this behavior lies in the fact that the Eq. (30) results from the subsidiary condition $V_1=0$ which is not invariant with respect to rotations. Thus it comes about that the physical requirement of the invariance of the energy with respect to rotations is mathematically satisfied only when the energy is represented by the sums of a linear and a quadratic form and not by a quadratic form alone.

Since the function V which is used in the Eqs. (28) and (29) for the determination of the coefficients of elasticity must represent the energy, it is obvious that it must be identified with the form V_2. Hence, *the coefficients of elasticity do not satisfy the Cauchy relations.*

Since the whole burden of our argument hinges on this identification, it will not be amiss if we make it more cogent by calculating the stresses in a quite different way. This method has the further advantage that it works with linear relations only and is, therefore, independent of the second-order corrections to the strain expressions (as far as the stress-strain relations are concerned). Since the choice is only between the forms V_2 and $V_1'' + V_2$, one single experimentum crucis is sufficient to decide the question: we need only to calculate one stress component in one particular kind of lattice.

Let us consider an orthorombic lattice whose principal directions coincide with the coordinate axes $j = 1, 2, 3$. Let it have the shape of a prism with a square cross section of 1 cm^2 area and with its axis in the direction $j = 1$. We imagine the prism divided into two halves by an ideal plane normal to the axis and lying between two lattice-net planes. We wish to calculate the forces exerted in the axial direction by one half of the prism upon the other half.

For this purpose we shall use the representation of the lattice energy by the sums (3) and (4) in which each term refers to the mutual energy of two lattice points labelled μ and ν, respectively. The force on the point ν exerted by the point μ in the axial direction is equal to the negative derivative with respect to $s_{\nu 1}$ of their mutual energy, namely, to

$$A_{\mu\nu}a_{\mu\nu 1} + 2(B_{\mu\nu 1} - C_{\mu\nu}a_{\mu\nu 1}{}^2)(s_{\mu 1} - s_{\nu 1})$$
$$+ 2C_{\mu\nu}a_{\mu\nu 1}a_{\mu\nu k}(s_{\mu k} - s_{\nu k}).$$

Let now the points in the positive half be denoted by μ and those in the negative half by ν. The force of interaction of the two halves is then obtained by taking the double sum of the expression, where μ is extended over the positive half and ν over the negative half. We see that the first term of the double sum is a constant and independent of the displacements: it represents the force holding together the two halves of the undeformed crystal, and it is of no interest to us. The second and third terms of the double sums are the force due to the existing deformation, in other words, they represent the normal stress

$$p_{11} = 2 \sum_{\mu_{1+}\nu_{1-}} \{ (B_{\mu\nu 1} - C_{\mu\nu}a_{\mu\nu 1}{}^2)(s_{\mu 1} - s_{\nu 1})$$
$$+ C_{\mu\nu}a_{\mu\nu 1}a_{\mu\nu k}(s_{\mu k} - s_{\nu k}) \}.$$

To explain the symbols at the sign of the sum we must make the following remark. The subscripts μ and ν are abbreviations each for three indices μ_1, μ_2, μ_3 and ν_1, ν_2, ν_3 labeling the coordinates of the points. Thus the sum is actually sixfold. We do not bring in evidence the summations with respect to μ_2, μ_3, ν_2, ν_3 because they extend over the complete cross dimensions of the lattice. But it is necessary to keep in mind that μ_1 extends over the positive half and ν_1 over the negative half in the axial direction.

We make now the transition to strain components by means of the relation (14). As we need only linear terms and as rotations are inessential to us, this relation simplifies into

$$s_j = e_{ij}x_i.$$

After substituting this into our sums, all the terms with odd powers of $a_{\mu\nu 2}$ or $a_{\mu\nu 3}$ will disappear because the summations in the 2,3 directions extend over the whole crystal whose dimensions are supposed to be extremely large compared with the lattice constant. The result is

$$p_{11} = \sum_{\mu_{1+}\nu_{1-}} [B_{\mu\nu 1}e_{11} + C_{\mu\nu}(a_{\mu\nu 2}{}^2 e_{22} + a_{\mu\nu 3}{}^2 e_{33})]a_{\mu\nu 1}.$$
$$(31)$$

It is possible to get rid of the summation with respect to ν_1 in a way which we shall carry through in detail only for the case of a simple orthorhombic lattice with only one point in every fundamental region. Let us consider all the points of the ν half which lie in a straight line parallel to the axis and are, therefore, characterized by the same fixed parameters ν_2, ν_3. All these points are acted on by forces originating in points of the μ-half. In particular let us consider their interactions with the points lying in a straight line parallel to the axis in the μ-half and labeled by the common fixed parameters μ_2, μ_3. With respect to the paramaters μ_1 and ν_1 (which change along the two straight lines) we can divide all these interacting pairs of points into groups such that the axial component of the mutual distance $a_{\mu\nu 1}$ of two points is constant within a group and equal to a, $2a$, $3a$, $\cdots$, respectively, in the different groups (where a is the lattice constant in the axial direction). The number of point pairs in the group $a_{\mu\nu 1} = na$ can be readily inferred from the fact that the coordinate ν_1 can assume the values $-\delta$, $-\delta - a$, $\cdots$

$-\delta-(n-1)a$, where δ is a fraction of a. These are, altogether, n different values, whence the number of pairs within a group is also $n=a_{\mu\nu1}/a$. Now in the sums (31) the terms relating to point pairs of the same group are all identical, because $B_{\mu\nu1}$, $C_{\mu\nu}$, $a_{\mu\nu1}$ are all the same within the group. Hence, we can omit the summation with respect to ν_1 if, instead, we multiply each term of the sum by $a_{\mu\nu1}/a$. Thus we find

$$p_{11}=(2/a)\sum_{\mu_{1+}}[B_{\mu\nu1}e_{11}+C_{\mu\nu}(a_{\mu\nu2}{}^2e_{22}+a_{\mu\nu3}{}^2e_{33})]a_{\mu\nu1}{}^2.$$

In this sum ν_1 has a constant value. Since all terms are symmetric in μ, ν (including symmetry in μ_1, ν_1) the summation could be extended, instead, over the negative half of the crystal (μ_1-) without changing p_{11}. Hence, it can be also extended over the whole crystal, provided that the sum is supplied with the factor $\frac{1}{2}$. In practice the coefficients $B_{\mu\nu1}$, $C_{\mu\nu}$ decrease very rapidly with the distance between μ and ν. Hence, very few net planes of the lattice to both sides of the plane ν_1 appreciably contribute to the sum. Therefore, the plane ν_1 can be taken anywhere, within the crystal with the exception of two negligible layers at the borders. As the sum is independent of the choice of ν_1, we may sum with respect to ν_1 over the whole crystal and at the same time divide by the number N of values which ν_1 assumes within it, i.e., by the number of net planes in the direction $j=1$. To make the case comparable with that treated above, we must have a cubical crystal of 1-cm edge. Hence its length in the direction 1 is 1 cm, and the number of the net planes is $N=1/a$. Therefore, we arrive at

$$p_{11}=\sum_{\mu\nu}[B_{\mu\nu1}e_{11}+C_{\mu\nu}(a_{\mu\nu2}{}^2e_{22}+a_{\mu\nu3}{}^2e_{33})]a_{\mu\nu1}{}^2, \quad (32)$$

where the summation symbol denotes the ordinary double sum over the whole crystal.

Although the special case of the simple lattice is entirely sufficient for our purpose, we remark that this method of calculating the normal stress can be applied (with but slight changes) also to the general case when each fundamental region contains several points, possibly, of different physical properties. The result is identical with (32) in the general case also. On the other hand, the method must be modified to a greater degree in calculating the shearing stresses, because then not only the magnitudes of the individual interaction forces are significant, but also their points of attack.

Let us now see what form our general expression (18) of $V_1''+V_2$ assumes in the special case of orthorhombic symmetry. Because of the relation $a_{\mu\nu j}=-a_{\nu\mu j}$ all the terms disappear which contain odd powers of one of these parameters. Using the notation of the coefficients given by the formula (21), we find for $V_1''+V_2$

$$\left.\begin{aligned} b_{11}&=\sum_{\mu\nu}(B_{\mu\nu1}-A_{\mu\nu})a_{\mu\nu1}{}^2, \\ b_{44}&=\tfrac{1}{4}\sum_{\mu\nu}[(B_{\mu\nu3}-A_{\mu\nu})a_{\mu\nu2}{}^2 \\ &\quad +(B_{\mu\nu2}-A_{\mu\nu})a_{\mu\nu3}{}^2+2C_{\mu\nu}a_{\mu\nu2}{}^2a_{\mu\nu3}{}^2], \\ b_{23}&=\sum_{\mu\nu}C_{\mu\nu}a_{\mu\nu2}{}^2a_{\mu\nu3}{}^2. \end{aligned}\right\}(33)$$

On the other hand, the quadratic form V_2 differs from this only in that the quantities $A_{\mu\nu}$ are left out. In particular, we shall write out explicitly the following coefficients

$$\left.\begin{aligned} c_{11}&=\sum_{\mu\nu}B_{\mu\nu\cdot\mu\nu1}{}^2, \quad c_{12}=\sum_{\mu\nu}C_{\mu\nu}a_{\mu\nu1}{}^2a_{\mu\nu2}{}^2, \\ c_{13}&=\sum_{\mu\nu}C_{\mu\nu}a_{\mu\nu1}{}^2a_{\mu\nu3}{}^2. \end{aligned}\right\}(34)$$

From these results it is clear that we obtain the Eq. (32) only when we substitute $V=V_2$ into the first relation (29), while the assumption $V=V_1''+V_2$ lead to an entirely incorrect result. Hence, we obtain another confirmation that the quadratic form (28) fundamental in elasticity must be identified with the function V_2 which is not invariant with respect to rotations and which does not satisfy the Cauchy relations.