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F. I. Fedorov. The Theory of the Optical Activity of Crystals. Optical activity is the most important manifestation of spatial dispersion, i.e., of the dependence of the permittivity tensor on the wave vector. Optical activity has for a long time been inseparably linked with the phenomenon of the rotation of the plane of polarization of linearly polarized light passing through a medium in an arbitrary direction (for active isotropic media and cubic crystals), or in the direction of the optical axes (for active uniaxial and biaxial crystals) with which another name, gyrotropy, is associated. On this basis, crystals of the planar classes of the intermediate syngonies, in which rotation of the polarization plane is impossible for any direction, belonged to the set of crystals which could not be optically active[1-4]. A different point of view was expounded in[5,6], and in[7] a plan for an experiment is proposed which allows the detection of the manifestation of optical activity in the planar crystals of the intermediate syngonies.

The electrodynamics of gyrotropic media is characterized by the following matter equations:

$$D_i = \varepsilon_{ik}E_k + \alpha_{ikl}\nabla_k E_l, \quad B_i = \mu_{ik}H_k + \beta_{ihl}\nabla_k H_l; \tag{1}$$

here the third-rank tensors α_{ikl} and β_{ikl} are responsible for the gyrotropy and, according to[5,6] (see also[8]), the nonvanishing of at least one of them is necessary and sufficient for the medium to be optically active. In the book[8] it was assumed that $\beta_{ikl} = 0$, and, on the basis of the symmetry principle for kinetic coefficients, α_{ikl} was found to obey the condition

$$\alpha_{ikl} = -\alpha_{lki} = e_{ilm}\alpha_{mk} \tag{2}$$

(e_{ilm} is the Levi-Civita symbol), as a result of which Eqs. (1) assume the form

$$D = \varepsilon E + [\alpha\nabla, E], \quad B = \mu H. \tag{3}*$$

In[5] this problem is considered from other angles. The restrictions on the tensors α_{ikl} and β_{ikl} are derived from the requirement that from the constitutive equations (1) and the Maxwell equations

$$\text{rot } E = -c^{-1}\dot{B}, \quad \text{div } B = 0, \tag{4a}$$
$$\text{rot } H = c^{-1}\dot{D}, \quad \text{div } D = 0 \tag{4b}$$

should follow the energy conservation law in the usual form

$$\text{div } S + \dot{w} = 0, \tag{5}$$

where **S** is the energy current density vector and w is the energy density. The condition (2) is again obtained for the activity tensor, on account of which (1) assumes the form

$$D = \varepsilon E + [\alpha\nabla, E], \quad B = \mu H + [\beta\nabla, H]; \tag{6}$$

in this case

$$S = \frac{c}{4\pi}[EH] - \frac{1}{8\pi}(\widetilde{\alpha}[E\dot{E}] + \widetilde{\beta}[H\dot{H}]), \quad w = \frac{1}{8\pi}(ED + HB), \tag{7}$$

*$[\alpha\nabla, E] \equiv \alpha\nabla \times E.$

where $\widetilde{\alpha}_{ik} = \alpha_{ki}$. The role of the vector **S** in electrodynamics is well known; therefore the new expression (7) (it differs from the standard expression $c[E \times H]/4\pi$), obtained for it in[5], is of definite interest. Note that the energy relations are not considered in[8] at all, while the expression (7) for $\beta = 0$ is used in the book[9]. In[10] the method expounded in[5] is applied to the case of moving optically active media.

It subsequently becomes clear, however, that the relations (6) and (7) together with the standard boundary conditions (continuity at the boundary of the tangential components of **E** and **H** and the normal components of **D** and **B**) do not guarantee energy-flux balance when light is reflected and refracted at the boundary of a gyrotropic medium[1].

Thus arose the necessity to change either the relations (6) and (7), or the boundary conditions, or both. Hence it is clear that we encounter in the theory of gyrotropic media a number of fundamental problems connected with the generalization of the basic electrodynamic relations.

A more detailed investigation shows that for the constitutive equations (1) the energy conservation law in the form (5) can be satisfied in more than one way. For this purpose the relations (1) were used in their original form in[5]. At the same time, we can, by decomposing the tensors α_{ikl} and β_{ikl} into their symmetric and antisymmetric parts with respect to the indices kl, separate out the curl operation and use the Maxwell equations (4) in (1). By applying such procedure to Eqs. (1) and (4), the authors of[11] obtained the relations[2]

$$D = \varepsilon (E + \alpha \text{ rot } E), \quad B = \mu (H + \widetilde{\alpha} \text{ rot } H), \tag{8}$$

for the case when the energy conservation law (5) in which

$$S = (c/4\pi)[EH], \quad w = (1/8\pi)(D\varepsilon^{-1}D + B\mu^{-1}B). \tag{9}$$

is fulfilled. In this case the energy-flux balance for light incident at the boundary of a gyrotropic medium is fulfilled when the standard boundary conditions

$$[E_1 - E_2, n] = 0, \quad (B_1 - B_2) n = 0, \tag{10}$$
$$[H_1 - H_2, n] = 0, \quad (D_1 - D_2) n = 0, \tag{11}$$

where **n** is the normal to the interface, are used.

In the constitutive equations (8), as in (3), the gyrotropy properties are determined in the most general case of a crystal of arbitrary symmetry by the single tensor α, i.e., by nine parameters. It was shown in[13] that a mutual correspondence can be established between the formulas (3) and (8), at least up to terms of first order in the small quantities α.

In this connection let us emphasize particularly the known fact that the Maxwell equations (4) alone certainly cannot uniquely determine the vectors **E**, **B**, **H**, and **D**. Indeed, it is easy to see that the vectors

$$E' = E + c^{-1}\dot{P}, \quad B' = B - \text{rot } P, \quad H' = H + c^{-1}\dot{Q}, \quad D' = D + \text{rot } Q \tag{12}$$

[1]Naturally, this difficulty pertains in full measure to the theory expounded in the book [9], since the latter is based on the relations (6) and (7).

[2]Similar results were obtained simultaneously and independently by a more complicated method in [12].

will satisfy the same equations (4) satisfied by **E**, **B**, **H**, and **D**, for completely arbitrary vector fields **P** and **Q**. Thus, until the constitutive equations are given, we cannot, strictly speaking, ascribe an entirely definite meaning to the field vectors entering into the Maxwell equations (4). Let us, following[13], set in the relations (12) **P** = 0 and **Q** = $\tilde{\alpha}$**D**. Using (8) and neglecting terms quadratic in α, we can solve (12) for the unprimed quantities and obtain, after substituting in (8)—(11), the constitutive equations, the energy conservation law and the boundary conditions expressed in terms of **E**′, **B**′, **H**′, and **D**′.[3] In consequence we obtain

$$\mathbf{D}' = \varepsilon\mathbf{E}' + \tilde{\beta}\,\text{rot}\,\mathbf{E}' + \text{rot}\,\beta\mathbf{E}', \quad \mathbf{B}' = \mu\mathbf{H}' \quad (\beta = \tilde{\alpha}\varepsilon), \tag{13}$$

$$\mathbf{S} = \frac{c}{4\pi}\left[\mathbf{E}', \mathbf{H}' - \frac{1}{c}\beta\dot{\mathbf{E}}'\right], \quad w = \frac{1}{8\pi}\left\{\mathbf{E}'\left(\varepsilon\mathbf{E}' - \frac{2}{c}\beta\dot{\mathbf{B}}'\right) + \mathbf{H}'\mathbf{B}'\right\}, \tag{14}$$

$$[\mathbf{E}'_1 - \mathbf{E}'_2, \mathbf{n}] = 0, \quad (\mathbf{B}'_1 - \mathbf{B}'_2)\mathbf{n} = 0, \tag{15}$$

$$[\mathbf{H}'_1 - \mathbf{H}'_2, \mathbf{n}] = \frac{1}{c}[\beta_1\dot{\mathbf{E}}'_1 - \beta_2\dot{\mathbf{E}}'_2, \mathbf{n}], \quad \mathbf{n}(\mathbf{D}'_1 - \mathbf{D}'_2) = \mathbf{n}\,\text{rot}\,(\beta_1\mathbf{E}_1 - \beta_2\mathbf{E}_2). \tag{16}$$

It can be shown that if in place of β another tensor γ: $\gamma = \text{Tr}\,\beta - \beta$ is introduced, then the first of the equations (13) assumes the form $\mathbf{D}' = \epsilon\mathbf{E}' + [\gamma\triangle\times\mathbf{E}']$, i.e., we obtain the constitutive equations (3). Thus, according to[13] we can go over from (8)[11] to (3)[8] through a redefinition of the vectors **H** and **D**. On redefining **E** and **B**[13], we obtain another variant of the relations (13)—(16); we can construct as many of such variants as we please.

It is shown in[14] that the relations (13)—(16) can also be arrived at not through a redefinition of Eqs. (8)—(11), but directly, on the basis of the energy conservation law (5) and the constitutive equations in the form $\mathbf{D}_i = \epsilon_{ik}\mathbf{E}_k + \alpha_{ikl}\nabla_k\mathbf{E}_l + \nabla_k\beta_{ikl}\mathbf{E}_l$, $\mathbf{B} = \mu\mathbf{H}$, using the same method as in[11]. The boundary conditions (15) and (16) may then be obtained with the aid of the standard procedure—integration around a contour close to the interface. These computations conclusively confirm once again the consistency and interconnectedness of the above-cited relations, as well as the fact that the energy conservation condition in the standard form (5), which was first used in[5], plays the major role in the phenomenological construction of the electrodynamics of gyrotropic media. This role will apparently remain in other generalizations of electrodynamics.

It was noted above that by redefining the field vectors, we can derive a multiplicity of variants of the electrodynamics of gyrotropic media, the variants differing in the form of the constitutive equations, in the corresponding expressions for **S** and w, and in the form of the boundary conditions. The meaning of the field vectors entering into the principal Maxwell equations (4) may then be different. Phenomenology does not enable us to make an unequivocal choice out of the various formulations, but in view of the simplicity and symmetry, we should in the phenomenological framework prefer the relations (8)—(11), which are characterized by the standard form of the boundary conditions and the vector **S** (and, formally, w). A very important feature of this formulation is the fact that the gyrotropy enters on equal footing into the electric and magnetic constitutive equations. In other words, if it is present, then the

corresponding terms should certainly be taken into account in both **D** and **B**. Furthermore, it was shown in[15] on the basis of a detailed microscopic quantum-mechanical analysis that the constitutive equations should have the form (8)[4]. The relations (8)—(11) are thereby conclusively justified and, it seems to us, the problem of the basic equations of the electrodynamics of gyrotropic media apparently can now be considered to have been to a considerable extent clarified.

In the report[16] V. L. Ginzburg proposes a somewhat different version of the constitutive equations. V. L. Ginzburg used a slightly modified form of the general equation (13) obtained in[13] for the particular case of an isotropic medium, writing the equation in the form $\mathbf{D} = \epsilon\mathbf{E} + \delta_\mathrm{I}\,\text{curl}\,\mathbf{E} + \text{curl}\,\delta_\mathrm{II}\mathbf{E}$. In the case of an isotropic medium it follows from Eq. (13) that $\delta_\mathrm{I} = \delta_\mathrm{II}$. The energy conservation condition then has the standard form (5). V. L. Ginzburg suggests we assume $\delta_\mathrm{I} \neq \delta_\mathrm{II}$, in which case in the energy equation appears an additional term which is of unknown nature and which we must associate with energy liberation at the boundary. No physical justification for such energy evolution (which has never been observed in transparent gyrotropic media) at a surface is not presented. Notice that if such a procedure is applied to the case of crystals, then instead of one tensor β, we shall have to use two: β_1 and β_2, i.e., 18 constants instead of 9. V. L. Ginzburg's assumption is at variance with[8], as well as the results of the microtheory[15]. The reasons inspiring such an artificial and quite considerable complication of an already existing theory, which satisfies all the basic requirements, remains completely vague.

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[3] For example, the equation $\mathbf{D}' = (1 + \nabla^\times\tilde{\alpha})\mathbf{D}$ can then be solved in the form $\mathbf{D} = (1 - \nabla^\times\tilde{\alpha})\mathbf{D}'$, etc. ($\nabla^\times\mathbf{F} = \text{curl}\,\mathbf{F}$).

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[4] We became acquainted with the work [15] only after the publication of [11]. It is worth noting that the comparatively cumbersome, but necessary, analysis in [15] yields the same results, which are derived in [11] from phenomenological considerations in only about 15 lines.

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N. N. Sirota. Electron and Spin Density Distribution and the Physical Properties of Crystals. The report dealt mainly with the structure and physical properties of crystals, including semiconductors and semimetals. The structure and physical properties of these bodies are determined by the nature and energy of the interatomic interaction. The widespread solid-state band theory can, in this connection, only be considered as an element of the general theory of the chemical bond. We must apparently agree with Coulson that the determination of the bonds in any molecule and in a crystal simply consists in the description of the electron distribution in them.

The most direct methods for determining the electron density distribution functions in a crystal are the methods used in the study of x-ray, electron, and neutron scattering. Since the value of the electron density $\rho(x, y, z)$ at a given point in a crystal is numerically equal to the square of the modulus of the wave function $|\psi(x, y, z)|^2$, it is clear that the experimentally determined electron density distribution function is at the same time a function of the square of the eigenfunctions.

The experimentally determined electron and spin density distribution functions allow us, when using the methods of quantum mechanics, to determine more accurately the form of the eigenfunctions, to partially separate the wave functions according to the orbitals of the atoms, and find with the aid of the tools of quantum mechanics the correlations between the wave and spin density distribution functions and a number of physical properties, and even carry out quantitative computations of the magnitudes of some of these properties.

The possibility of finding the electron density distribution functions in a crystal from x-ray scattering was pointed out by Bragg. The first systematic experiments and computations were carried out in our country by N. V. Ageev and likewise by V. E. Loshkarev.

In recent years experimental methods have been developed which allow us to increase considerably the accuracy of the measurements and computations.

Investigations have been carried out at the BSSR Academy of Sciences Institute of Solid-State and Semiconductor Physics on the experimental determination of x-ray, electron, and neutron scattering form factors, of structure factors, and electron and spin density distribution functions on the basis of the measurements of the absolute, Bragg-scattering intensities. The magni-

tudes of the temperature factors and the root-mean-square displacements of various sorts of ions were also determined, and the anisotropy of the ion oscillations were taken into account. As a rule, the space of the ion oscillations in a crystal had the shape of a sphere or an ellipsoid. The electron and spin density distribution functions in a crystal were computed from the experimentally determined atomic scattering functions (form factors), which were scaled to absolute zero temperature and to the state of stationary atoms when eliminating the zero-point oscillations.

The electron density distribution functions were in this case found by means of a subtractive three-dimensional Fourier synthesis—summation of three-dimensional Fourier series comprising of the differences between the structure amplitudes which had been rigorously computed for a given known distribution function for largely inner-shell electrons (it is possible this distribution was close to the real one), and for experimentally determined structure amplitudes. In such a computational method one sums up small differences which form comparatively rapidly converging series, and series-cutoff effects are completely eliminated. The experimental measurement procedures and the computational methods developed at the Institute yield relatively high degrees of accuracy. The errors are of the order of 2—3%, or, expressed in absolute quantities, of the order 0.1—0.05 el/Å^3. Electron density distribution charts were constructed for crystals of the group IV elements and for compounds of the type $A^{III}B^V$ with the diamond, sphalerite, and wurtzite structures. The experimental methods developed have enabled us to distinguish comparatively clearly bridges of sp^3-couplings in crystals with the diamond and sphalerite structures, and to find in crystals regions with depressed electron density.

For a number of substances, e.g., C, Si, Ge, and certain compounds of the type $A^{III}B^V$; potential distribution functions have been found for the lattice, and potential distribution charts have been constructed for different planes. The values of the mean potential, which are proportional to the diamagnetic susceptibilities, are in good agreement with independent magnetic measurements.

The effective charges of the ions were determined by integrating the electron density over the volume of the ions within the boundaries constructed from the electron density charts by comparing the theoretical structure amplitudes for neutral atoms with the experimentally determined amplitudes for neutral atoms with the experimentally determined amplitudes, as well as by determining the ionicity coefficient λ, assuming that the wave function comprises of component functions: $\psi = \psi_A + \lambda\psi_B$. The results of the estimates obtained by the three indicated methods are close to each other and coincide in sign. The magnitudes of the effective charges of the ions have been determined for the majority of the $A^{III}B^V$-type compounds. It has been established in this case that the A^{III} ions are always positive. For the $A^{III}B^V$-type compounds which have been investigated the values of the ionicity λ lie between the limits 0.745—0.715. A method has been developed for determining from x-ray patterns (from experimentally determined form factors f) the dia- and paramagnetic