ELECTROMAGNETIC WAVES IN A MEDIUM POSSESSING A CONTINUOUS ENERGY SPECTRUM. III

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The theory of electromagnetic waves in a crystal in the presence of spatial dispersion due to exciton states, developed in previous papers, [1,2] is applied to the analysis of a number of problems. Double refraction in a cubic crystal as the result of spatial dispersion is considered. The transmission of a wave through a plane-parallel plate at an arbitrary angle of incidence is discussed. A generalization of the Fresnel formulas is given. The results obtained are compared with the corresponding results of the Pekar theory [9] and a critical discussion of the latter is given.

A scheme was given in [1] for the solution of the Maxwell equations in a nonconducting, spatially dispersive medium. The solenoidal part of the electric field is determined by the equation

$$\Delta\mathscr{E}^{\perp}_{x'}(\mathbf{r}) + \gamma\,[\mathscr{E}^{\perp}_{x'}(\mathbf{r}) + 4\pi P^{\perp}_{x'}(\mathbf{r})] = 0, \qquad (1)$$

where $P^{\perp}$ is the solenoidal part of the polarization

$$P_{x'}(\mathbf{r}) = \int K_{x'y'}(\mathbf{r}, \mathbf{r}')\,\mathscr{E}^{\perp}_{y'}(\mathbf{r}')\,d\mathbf{r}', \qquad (2)$$

$\gamma = \mu\omega^2/c^2$. The irrotational part of the electric field is determined by the expression

$$\mathscr{E}^{\parallel}_{x'}(\mathbf{r}) = -4\pi P^{\parallel}_{x'}(\mathbf{r}),$$

where $P^{\parallel}$ is the irrotational part of the polarization.

In [2] (in subsequent citations—II) the polarizability kernel was obtained for a plane-parallel plate in the case in which the spatial dispersion is due to the exciton states of the crystal:

$$K = K^{+} + K^{-},$$

$$K^{\pm}_{x'y'} = [L^2/(2\pi)^2 2\hbar\omega] \sum_{\alpha} \sum_{k_3=-k_N}^{k_N} \int \Gamma^{\pm}(\mathbf{k}, \alpha) \sum_{\mathbf{b}\mathbf{b}'} \exp\{\mp i\,[k_3 b_{3z} z + k_x(x-x') + k_y(y-y') + (k_1 b_{1z} + k_2 b_{2z})(z-z') + 2\pi(\mathbf{b}\mathbf{r} - \mathbf{b}'\mathbf{r}')]\}\,[g^{\pm}_{x'y'}(\mathbf{b}, \mathbf{b}', \mathbf{k}, \mathbf{k}, \alpha)\exp(\pm i k_3 b_{3z} z') - g^{\pm}_{x'y'}(\mathbf{b}, \mathbf{b}', \mathbf{k}, \tilde{\mathbf{k}}, \alpha)\exp(\mp i k_3 b_{3z} z')]\,dk_x dk_y. \qquad (3)$$

Here L measures the dimensions of the principal region; α is the number of the exciton band;

$$k_{1,2} = \mathbf{k}\mathbf{a}_{1,2} = \tilde{\mathbf{k}}\mathbf{a}_{1,2}, \quad k_3 = \mathbf{k}\mathbf{a}_3 = -\tilde{\mathbf{k}}\mathbf{a}_3 = \pi\nu/(N+1), \quad \nu = 1, \ldots, N, \quad k_N = \pi N/(N+1);$$

$\mathbf{a}_i$ ($i = 1, 2, 3$) are the unit lattice vectors, where $\mathbf{a}_{1,2}$ are parallel to the surfaces of the plate; N is the number of elementary cells contained within the thickness l of the plate; $\mathbf{b}_i$ ($i = 1, 2, 3$) are the unit vectors of the reciprocal lattice;

$$\Gamma^{\pm}(\mathbf{k}, \alpha) = \mp \frac{E(\mathbf{k},\alpha) - E_0}{E(\mathbf{k}, \alpha) \pm i\varepsilon(\mathbf{k}, \alpha, \mp\omega) - E_0 \pm \hbar\omega},$$

$E(\mathbf{k}, \alpha)$ is the energy of the exciton, E_0 the energy of the ground state, ϵ is determined by the finiteness of the lifetime of the exciton state;

$$g^{+}_{x'y'}(\mathbf{b}, \mathbf{b}', \mathbf{k}, \mathbf{k}', \alpha) = g^{*}_{x'}(\mathbf{b}, \mathbf{k}, \alpha)\,g_{y'}(\mathbf{b}', \mathbf{k}', \alpha), \quad g^{-} = g^{+*},$$

$g(\mathbf{b}, \mathbf{k}, \alpha)$ are the expansion coefficients of the polarization matrix element in the vectors of the reciprocal lattice $\mathbf{b}$; the z axis is perpendicular to the plate, i.e., $z = 0, l$ on the surfaces of the plate.

The transmission of a normally incident wave through a slab or plate of a cubic crystal was considered in II, but the double refraction which can be produced by spatial dispersion was not taken into account. In the present paper, we investigate this effect. Furthermore, we consider the case of an arbitrary angle of incidence; finally, we find the longitudinal component of the electric field of the wave.

1. DOUBLE REFRACTION

The possibility of optical anisotropy of a cubic crystal due to the finite wavelength was suggested by Lorentz in 1878. [3] Calculation of double refraction for single crystals of the NaCl type was given in [4], and for crystals of the diamond type in [5]. From the phenomenological point of view, the calculations mentioned were based on an expansion of the dielectric constant ϵ in powers of $\mathbf{k}$. The effect is shown to be very small in this case; for example, for crystals of the diamond type the difference in the indices of refraction for the two polarizations is $\sim 10^{-4}$.

Again from the phenomenological viewpoint, one must distinguish the spatial dispersion described by expansions of the quantities ϵ and $1/\epsilon$ in powers of $\mathbf{k}$.[6] We shall speak, respectively, of direct and reciprocal spatial dispersion. From the viewpoint of II and the present paper, direct and reciprocal dispersion are described by expansions (in powers of $\mathbf{k}$) of the numerator and denominator of the polarizability kernel, respectively. The double refraction studied in [4,5] is due to direct spatial dispersion. Here we consider double refraction that results from reciprocal dispersion. We emphasize that by double refraction we mean here not the effect of increase in the number of waves, but the difference in the propagation of waves with different polarizations.

For small $\mathbf{k}$, a cubic crystal contains pairs of almost transverse exciton bands in which the polarization matrix element $P_{\alpha\perp}$ is perpendicular to $\mathbf{k}$ in the zeroth approximation (in k). Neglecting direct dispersion, we restrict ourselves to the zeroth approximation in $\mathbf{P}_{\alpha\perp}$; here[7] $|\mathbf{P}_{\alpha_1^\perp}| = |\mathbf{P}_{\alpha_2^\perp}|$ and $\mathbf{P}_{\alpha_1^\perp}\cdot\mathbf{P}_{\alpha_2^\perp} = 0$. We consider normal incidence on the plate of a wave whose electric vector is parallel to one of the $\mathbf{P}_{\alpha_n^\perp}$. Let k_0 be the wave vector and $\mathscr{E}_n$, R_n, D_n the amplitudes of the incident, reflected, and transmitted waves. By the method developed in II, we get

$$R_n = \mathscr{E}_n \frac{1 - G_n^2 + F_n^2}{G_n^2 + (1 + iF_n)^2}, \qquad D_n = \mathscr{E}_n \frac{i2G_n \exp(-ik_0 l)}{G_n^2 + (1 + iF_n)^2}. \quad (4)$$

Here*

$$F_n = f_{n1} \operatorname{ctg} \varkappa_{n1} l + f_{n2} \operatorname{ctg} \varkappa_{n2} l,$$

$$G_n = f_{n1} / \sin \varkappa_{n1} l + f_{n2} / \sin \varkappa_{n2} l,$$

$$f_{n1} = \frac{\varkappa_{n2} / k_0}{1 - (\varkappa_{n2}^2 - k_n^2) / (\varkappa_{n1}^2 - k_n^2)},$$

f_{n2} is obtained from f_{n1} by interchange of the indices 1, 2; $\kappa_{n1,2}^2$ are the roots of the equation

$$-\varkappa^2 + \gamma(1 + 4\pi\beta) + B/(\xi_n \varkappa^2 - i\varepsilon_n - \zeta) = 0,$$

$$B = 4\pi\gamma L^2 l |\mathbf{P}_{\alpha\perp}|^2 [E(0, \alpha\perp) - E_0] / \hbar\omega,$$

$$\xi_n = \hbar^2 / 2m_n^*, \quad \zeta = E_0 + \hbar\omega - E(0, \alpha\perp),$$

where m_n^* is the effective mass for the direction of $\mathbf{k}$ perpendicular to the plate, and β takes into account the local part of the polarization; k_n is the root of the equation

$$\xi_n k^2 - i\varepsilon_n - \zeta = 0.$$

*ctg = cot.

In accord with II, the indicated results agree with the corresponding results of [8,9] in the absence of double refraction (for $m_1^* = m_2^*$). Inasmuch as m_1^* and m_2^* can be appreciably different from one another, it is clear from [4] that the double refraction due to reciprocal spatial dispersion can be very large. Reciprocal dispersion should apparently give a significant contribution also in the case of a non-cubic crystal.

2. INCIDENCE OF A WAVE ON A PLATE AT AN ARBITRARY ANGLE

We take the yz plane as the plane of incidence and seek a solution of (1) in the form

$$\mathscr{E}_{x'}^{\perp}(\mathbf{r}) = \sum_s c_{sx'} \exp(i\mathbf{k}_s\mathbf{r}), \quad (5)$$

$$\mathbf{k}_s\mathbf{c}_s = 0, \quad (6)$$

where $\mathbf{k}_0$ is the wave vector in the outer medium, the components of $\mathbf{k}_s$ are 0, k_{0y}, κ_s, while the smoothness of the field is guaranteed by the condition $|\kappa_s| d \ll 1$ (d is the lattice diameter). As was done in II, one can separate in (2) the local part of the polarization $\mathbf{P}_l(\mathbf{r})$ which occurs because of K^+, and those components in K^- for which $E(0, \alpha) - E_0 - \hbar\omega$ is sufficiently large. The nonlocal part of the polarization $\mathbf{P}_n(\mathbf{r})$ comes about as the result of the remaining components of K^- and can be calculated by the method developed in II. In the integration and summation over the components of k in (3), the principal contribution to $\mathbf{P}_n(\mathbf{r})$ is made by the region around the points $\mathbf{k}_s$ and $\mathbf{k}_{\alpha q}$, where the components of the latter vector are 0, k_{0y}, $k_{\alpha q}$, and

$$E(\mathbf{k}_{\alpha q}, \alpha) - i\varepsilon(\mathbf{k}_{\alpha q}, \alpha, \omega) - E_0 - \hbar\omega = 0.$$

As a result of the calculation, we get

$$P_{nx'}(\mathbf{r}) = \sum_s c_{sy'} [p_{sx'y'}^{(1)}(\mathbf{r}) + p_{sx'y'}^{(2)}(\mathbf{r})], \quad (7)$$

where $p^{(1)}$ and $p^{(2)}$ are the contributions made by the points $\mathbf{k}_s$ and $\mathbf{k}_{\alpha q}$, respectively. Without writing down the very cumbersome expressions for $p^{(1)}$ and $p^{(2)}$, we note that $p_s^{(1)} \sim \exp(i\mathbf{k}_s\cdot\mathbf{r})$, while $p_s^{(2)}$ contains an exponential with a different exponent. In order to get the solution of (1) in the form (5), it is obviously necessary to equate to zero the part of $\mathbf{P}_n^\perp$ which comes about as the result of $p^{(2)}$. This leads to the additional conditions for $\mathbf{c}_s$:

$$\sum_s c_{sy'} \sum_b [G_{sy'}(b, \mathbf{k}_{\alpha q}^+, \alpha) - G_{sy'}(b, \widetilde{\mathbf{k}}_{\alpha q}^+, \alpha)] = 0,$$

$$\sum_s c_{sy'}^{\pm} \exp(i\varkappa_s l) \sum_b \exp(-i2\pi bl) [G_{sy'}(b, \mathbf{k}_{\alpha q}^-, \alpha) - G_{sy'}(b, \widetilde{\mathbf{k}}_{\alpha q}^-, \alpha)] = 0. \quad (8)$$

Here

$$G_s(b, k^{\pm}_{\alpha q}, \alpha) = g^*(b_0, k^{\pm *}_{\alpha q}, \alpha)/(\varkappa_s - 2\pi b - k^{\pm}_{\alpha q});$$

only the component along b_3 in b_0 differs from zero; it is denoted by b; the signs ± on k indicate the sign of the imaginary part. Now, substituting (5), $\mathbf{P}_l$ and the remaining part of (7) in (1), we get the equation for κ_S and $\mathbf{c}_S$:

$$(-k^2 + \gamma) c_{x'} + 4\pi\gamma (lL^2/\hbar\omega) \times\Big[\sum_\alpha \Gamma^-(\mathbf{k},\alpha) g^{\perp}_{x'}(0, \mathbf{k}, \alpha) g^{\perp}_{y'}(0, \mathbf{k}^*, \alpha) + \sum_\alpha \Gamma^+(-\mathbf{k}, \alpha)\, g^{\perp *}_{x'}(0, -\mathbf{k}^*, \alpha)\, g^{\perp}_{y'}(0, -\mathbf{k}, \alpha)\Big] c_{y'} = 0, \quad (9)$$

where the components of $\mathbf{k}$ are 0, k_{0y}, κ; $\mathbf{g}^{\perp}(\mathbf{b},\mathbf{k},\alpha)$ are the components of $\mathbf{g}(\mathbf{b},\mathbf{k},\alpha)$ along $\mathbf{k} + 2\pi\mathbf{b}$. It is easy to see that there are three independent equations in (9) and (6). By the method developed in II, it is possible to show that the number of solutions of the system (9) and (6) exceeds the number of additional conditions (8) by four, so that (5) has precisely four independent solutions.

The longitudinal field far from the surface is determined by the formula

$$\mathscr{E}^{\parallel}_{x'}(\mathbf{r}) = -4\pi\, [P^{\parallel}_{lx'}(\mathbf{r}) + P^{\parallel}_{nx'}(\mathbf{r})], \quad (10)$$

where only the part due to $p^{(1)}$ enters into $P^{\parallel}_n$.

The amplitudes of the reflected wave and the wave transmitted through the plate can be expressed in terms of the amplitude of the incident wave from the usual Maxwell boundary conditions and the additional conditions (8).

3. CUBIC CRYSTAL

Even in the absence of spatial dispersion, it is rather difficult to obtain a solution of the problem of a doubly refracting plate in explicit form for the case of oblique incidence. Therefore, in the application of the results of the preceding section, we limit ourselves to a cubic crystal when there is no double refraction due to the reciprocal spatial dispersion. As was shown above, this takes place for $m^*_{\alpha_1^\perp} = m^*_{\alpha_2^\perp}$.

A longitudinal band, which we shall designate $\alpha^{\parallel}$, is associated with the pair of transverse exciton bands in the cubic crystal. To be specific, we consider a crystal without a center of symmetry, when linear terms are present in the expansion of $\mathbf{g}(0,\mathbf{k},\alpha)$ in terms of $\mathbf{k}$. In first approximation,

$$\mathbf{g}(0, \mathbf{k}, \alpha_n^{\perp}) = \mathbf{l}_n (ak) P_\alpha + [\mathbf{k}, \mathbf{q}^{\perp}(ak, \alpha_n^{\perp})] + \mathbf{k} q^{\parallel}(ak, \alpha_n^{\perp}),$$
$$\mathbf{g}(0, \mathbf{k}, \alpha^{\parallel}) = (\mathbf{k}/k) P_\alpha + [\mathbf{k}, \mathbf{q}^{\perp}(ak, \alpha^{\parallel})] + \mathbf{k} q^{\parallel}(ak, \alpha^{\parallel}). \quad (11)^*$$

Here and in what follows, $a \to +0$; $\mathbf{l}_{1,2}$ are unit vectors perpendicular to one another and to $\mathbf{k}$; let $\mathbf{l}_1$ be perpendicular to the plane of incidence and let $\mathbf{l}_2$ lie in it. To simplify the notation we assume the effective masses to be isotropic. Making use of [7], it is easy to obtain (for small k)

$$E(\mathbf{k}, \alpha) = E(0, \alpha^{\perp}) + 4\pi l L^2 |P_\alpha|^2 \delta_{\alpha\alpha^{\parallel}} + \xi_\alpha k^2 + \ldots,$$

where $\xi_{\alpha_1^\perp} = \xi_{\alpha_2^\perp} = \xi_{\alpha^\parallel}$.

It is easy to see that $\mathscr{E}^{\parallel} \sim k_S$; we shall consider in $\mathscr{E}^{\perp}$ the terms of zero order and in $\mathscr{E}^{\parallel}$ the terms of first order in k_S. In the zeroth approximation, the components referring to longitudinal bands do not enter into (9). Let the resonance condition $E(0,\alpha) - E_0 - \hbar\omega \approx 0$ be satisfied only for one value of α (isolated triplet of bands). The most interesting case is the one in which $|k_{\alpha q}| d \ll 1$; here, under the additional conditions (8), we can neglect the components with $b \neq 0$.

Taking into account all that has been said, we can obtain the following results. Let the transverse field lie in the plane of incidence, $\mathscr{E}^0_{2x'}$, $R_{2x'}$, $D_{2x'}$ are the amplitudes of the incident, reflected, and transmitted waves. Then

$$\mathscr{E}^{\perp}_{2x'} = \exp(ik_{0y}y) \sum_{s=1}^{4} c_{sx'} \exp(i\varkappa_s z), \quad x' = y, z, \quad \mathscr{E}^{\perp}_{2x} = 0; \quad (12)$$

$$R_{2y} = \mathscr{E}^0_{2y} \frac{\Delta_2 - q_0(\Delta_3 + \Delta_4) + q_0^2 \Delta_5}{-\Delta_2 + q_0(\Delta_3 - \Delta_4) + q_0^2 \Delta_5},$$
$$D_{2y} = -\mathscr{E}^0_{2y} \frac{2q_0 \exp(-ik_{0z} l)\, \Delta_1}{-\Delta_2 + q_0(\Delta_3 - \Delta_4) + q_0^2 \Delta_5}. \quad (13)$$

Here

$$\Delta_1 = \begin{vmatrix} \gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\ q_1\gamma_1 & q_2\gamma_2 & q_3\gamma_3 & q_4\gamma_4 \\ p_1^+ & p_2^+ & p_3^+ & p_4^+ \\ p_1^-\gamma_1 & p_2^-\gamma_2 & p_3^-\gamma_3 & p_4^-\gamma_4 \end{vmatrix},$$

Δ_2 is obtained from Δ_1 by substitution of q for γ in the first line, Δ_3 by substitution of q for γ in the first row, and of γ for $q\gamma$ in the second, Δ_4 by substitution of unity for γ in the first row, Δ_0 by substitution of unity for γ in the first row and of γ for $q\gamma$ in the second;

$$p_s^{\pm} = (\tilde{k}^{\pm} + k_{0y}^2/\varkappa_s)\, r_s(\tilde{k}^{\pm}) - (k^{\pm} + k_{0y}^2/\varkappa_s)\, \bar{r}_s(k^{\pm}),$$
$$q_s = (\varkappa_s + k_{0y}^2/\varkappa_s)/\mu, \qquad q_0 = k_{0z} + k_{0y}^2/k_{0z},$$
$$\gamma_s = \exp(i\varkappa_s l), \qquad r_s(k) = 1/(\varkappa_s - k)\,(k_{0y}^2 + k^2)^{1/2},$$
$$k^{\pm} = k^0 + \tau^{\pm}, \quad \tilde{k}^{\pm} = k^0 - \tau^{\pm}, \quad \tau^{\pm} \equiv \tau^{\pm}_{\alpha\perp},$$
$$\tau^{\pm}_{\alpha q} = (k^{\pm}_{\alpha q})_3 b_{3z} = k^{\pm}_{\alpha q} - k^0, \qquad k^0 = k_1^0 b_{1z} + k_2^0 b_{2z},$$

k_1^0, k_2^0 are determined from

$$k_1^0 b_{1x} + k_2^0 b_{2x} = 0, \quad b_1^0 k_{1y} + k_2^0 b_{2y} = k_{0y}.$$

Now let the transverse field be perpendicular to the plane of incidence. The field inside the plate

* $[\mathbf{k}, \mathbf{g}] = \mathbf{k} \times \mathbf{q}$.

is described by Eq. (12). One must replace the index 2 by the index 1 and set $x' = x$. Equations for the amplitudes are obtained from (13) by replacement of 2 by 1, y by x, q_s by κ_s/μ, q_0 by k_{0z}, and p_s by $[(\kappa_s - k^0)^2 - (\tau^{\pm})^2]^{-1}$.

4. GENERALIZATION OF THE FRESNEL FORMULAS. TOTAL INTERNAL REFLECTION OF A SINGLE WAVE

Let us consider the case of a semi-infinite crystal. Let $\mathrm{Im}(\kappa_{1,2}) < 0$, $\mathrm{Im}(\kappa_{3,4}) > 0$. As $l \to \infty$ we have $\gamma_{1,2} \to \infty$ and $\gamma_{3,4} \to 0$, and (13) reduces to

$$D_{2y} = 0, \quad R_{2y} = \mathscr{E}^0_{2y} \frac{p_4^+ (q_0 - q_1) - p_3^+ (q_0 - q_4)}{p_4^+ (q_0 + q_3) - p_3^+ (q_0 + q_4)}.$$

R_{1x} is obtained from R_{2y} by the substitutions shown at the end of the previous section. The results shown give a generalization of the Fresnel formulas to the case where spatial dispersion is taken into account.

In the case of a semi-infinite crystal, only two components remain in (12), with $s = 3$ and 4. It is interesting to establish the conditions for which one (and only one) of these two waves undergoes total internal reflection if in the case of normal incidence this does not occur for either. (For a purely imaginary index of refraction, total reflection takes place for normal incidence, too.) It is shown that for realization of the case outlined it is necessary and sufficient that

$$(k^2)_j = \{(-1)^j \sqrt{(\zeta + \xi_{\alpha\perp}\bar{\gamma})^2 - 4\xi_{\alpha\perp}(\bar{\gamma}\zeta - B)}$$
$$+ \zeta + \xi_{\alpha\perp}\bar{\gamma}\}/2\xi_{\alpha\perp} > 0, \quad j = 1, 2,$$

where

$$\bar{\gamma} = \gamma \Big\{1 + 4\pi (lL^2/\hbar\omega) \Big[\sum_{\alpha} \Gamma^+ (0, \alpha\perp) |P_\alpha|^2$$
$$+ \sum_{\alpha'}^{\alpha' \neq \alpha} \Gamma^- (0, \alpha'\perp) |P_{\alpha'}|^2\Big]\Big\},$$

and that k_{0y}^2 lie between the values $(k^2)_1$ and $(k^2)_2$. If the smallest of the k_j is larger than the wave vector in the vacuum, then it is necessary that the wave be incident not from a vacuum but from a medium with a sufficiently large index of refraction. Having accomplished an experiment of this type, we can investigate the separate transmission through the plate of a wave with a large value of k_j; this would be very useful in the determination of parameters relating to the separate waves. We shall set down the relevant formulas. Let $\kappa_1^2 = \kappa_3^2 < 0$ and $\kappa_2^2 = \kappa_4^2 > 0$. Then, for a sufficiently thick plate, we find from (13)

$$R_{2y} = \mathscr{E}^0_{2y} \frac{f_{12}^{--} f_{43}^{+-} - \exp(i2\varkappa_4 l) f_{14}^{--} f_{23}^{+-}}{-f_{12}^{--} f_{43}^{++} + \exp(i2\varkappa_4 l) f_{14}^{--} f_{23}^{++}},$$

$$D_{2y} = -\mathscr{E}^0_{2y} 2q_0 p_3^+ \begin{vmatrix} 1 & 1 & 1 \\ q_1 & q_2 & q_4 \\ p_1^- & p_2^- & p_4^- \end{vmatrix} \exp[i(\varkappa_4 - k_{0z}) l]$$
$$\times [-f_{12}^{--} f_{42}^{++} + \exp(2i\varkappa_4 l) f_{14}^{--} f_{23}^{++}]^{-1}, \qquad (14)$$

where $f_{ik}^{\pm\pm} = p_i^{\pm}(q_k \pm q_0) - p_k^{\pm}(q_i \pm q_0)$, in which the first ± signs on f are identical with the sign on p, and the second with the sign in front of q_0. R_{1x} and D_{1x} are obtained from (14) by the substitutions shown at the end of the previous section. The dependence on plate thickness in (14) is the same as in the absence of spatial dispersion,[10] which corresponds to total internal reflection of one of the waves.

5. LONGITUDINAL FIELD

The longitudinal component of the electric field of the wave is determined by (10), whence we find

$$\mathscr{E}^{\parallel}_{2x'}(\mathbf{r}) = -4\pi (lL^2/\hbar\omega) \sum_s \exp(i\mathbf{k}_s\mathbf{r}) k_{sx'} (k_{0y}^2 + \varkappa_s^2)^{-1/2}$$
$$\times \sum_\alpha \{\Gamma^- (\mathbf{k}_s, \alpha\parallel) [\mathbf{k}_s, \mathbf{q}^{\perp *}(a\mathbf{k}_s^*, \alpha\parallel)] \mathbf{c}_s P_\alpha$$
$$+ \Gamma^- (\mathbf{k}_s, \alpha\perp)(k_{0y}c_{sz} - \varkappa_s c_{sy}) q^{\parallel}(a\mathbf{k}_s, \alpha_2^{\perp}) P_\alpha^*$$
$$+ \Gamma^+ (0, \alpha\parallel) [\mathbf{k}_s, \mathbf{q}^{\perp}(-a\mathbf{k}_s, \alpha\parallel)] \mathbf{c}_s P_\alpha$$
$$+ \Gamma^+ (0, \alpha\perp)(k_{0y}c_{sz} - \varkappa_s c_{sy}) q^{\parallel *}(-a\mathbf{k}_s^*, \alpha_2^{\perp}) P_\alpha\}$$

(the transverse field is in the plane of incidence),

$$\mathscr{E}^{\parallel}_{1x'}(\mathbf{r}) = -4\pi (lL^2/\hbar\omega) \sum_s \exp(i\mathbf{k}_s\mathbf{r}) k_{sx'} c_{sx} \sum_\alpha \Big\{\Gamma^- (\mathbf{k}_s, \alpha\parallel)$$
$$\times [\mathbf{k}_s, \mathbf{q}^{\perp *}(a\mathbf{k}_s^*, \alpha\parallel)]_x (k_{0y}^2 + \varkappa_s^2)^{-1/2} P_\alpha$$
$$+ \Gamma^- (\mathbf{k}_s, \alpha\perp) q^{\parallel}(a\mathbf{k}_s, \alpha_1^{\perp}) P_\alpha^*$$
$$+ \Gamma^+ (0, \alpha\parallel) [\mathbf{k}_s, q^{\perp}(-a\mathbf{k}_s, \alpha\parallel)]_x (k_{0y}^2 + \varkappa_s^2)^{-1/2} P_\alpha^*$$
$$- \Gamma^+ (0, \alpha\perp) q^{\parallel *}(-a\mathbf{k}_s^*, \alpha_1^{\perp}) P_\alpha\Big\}$$

(the transverse field is perpendicular to the plane of incidence). The principal contribution to $\mathscr{E}^{\parallel}_{x'}$ is made by components from Γ^-. For small ϵ_α, the longitudinal field can reach large values if the expression obtained from the denominator of Γ^- vanishes as $\epsilon_\alpha \to 0$. It is not difficult to show that this is possible only for $\alpha = \alpha^{\parallel}$. Thus the large values of the longitudinal field are obtained as a consequence of the longitudinal bands. The ratio of the maximum value of the longitudinal field to the transverse is of the order of $4\pi k_s d l L^2 |P_\alpha|^2/\epsilon_\alpha$ and can be very large if ϵ_α is sufficiently small. If we take into account the contribution of the longitudinal bands in the transverse field, then we get (for the given ratio),

$$4\pi k_s dlL^2 |P_\alpha|^2 (\varepsilon_\alpha + 4\pi k_s^2 d^2 lL^2 | P_\alpha |^2)^{-1}.$$

If $4\pi k_s^2 d^2 l L^2 |P_\alpha|^2 \ll \epsilon_\alpha$, the previous result is obtained. For the opposite inequality we have $\mathscr{E}^{\parallel}/\mathscr{E}^{\perp} \approx 1/k_s d \gg 1$. Thus, in the case of a limitingly small ϵ_α, $\mathscr{E}^{\parallel}$ can exceed $\mathscr{E}^{\perp}$ appreciably. We emphasize that the anomalously large values of the longitudinal field are possible only in the presence of longitudinal bands in the crystal, for which the transverse part of the polarization matrix element tends to zero as $k \rightarrow 0$.

In the preceding sections, the analysis was carried out under the assumption that the longitudinal field is limitingly small in comparison with the transverse one. If this condition is violated, then it is necessary to take $\mathscr{E}^{\parallel}_{x'}$ into account in the Maxwell boundary conditions (for oblique incidence of the wave). We shall not write out the cumbersome formulas obtained in this case, but shall limit ourselves to a qualitative consideration. The longitudinal field lies in the plane of incidence; therefore, if the transverse field lies in the plane of incidence, the same holds for the total field also. In this case, account of $\mathscr{E}^{\parallel}_{x'}$ in the boundary conditions leads only to a quantitative change in the expression for the amplitudes of the reflected and transmitted waves. If the field in the incident wave is perpendicular to the plane of incidence, then a component due to $\mathscr{E}^{\parallel}_{x'}$ appears in the refracted waves; it lies in the plane of incidence. The corresponding component appears also in the reflected and transmitted waves, leading to a depolarization of the reflected and transmitted waves. The indicated effect is absent at normal incidence; in this way, it differs considerably from the optical activity. Moreover, it is not connected with double refraction. In this regard, it differs from depolarization upon reflection from an anisotropic medium in the absence of spatial dispersion.

In conclusion, we note that the presence of the transverse part in the polarization matrix element for the longitudinal band should lead to absorption of light in the vicinity of the frequency $[E(0, \alpha^{\parallel}) - E_0]/\hbar$. In view of the fact that there is only one longitudinal band (in an isolated triplet of bands), this absorption must possess complete dichroism.

An experimental test of the results obtained in this research appears to us to be highly desirable.

6. COMPARISON WITH THE PEKAR THEORY

We shall compare our results with the corresponding results of the Pekar theory.[8,9,11] These results, which pertain to double refraction in the case of normal incidence, correspond to those which appear in [11]. In [9] the incidence of a wave on a semi-infinite crystal was considered, and the reflected and transmitted waves were found. In that case the results were significantly different from ours (although, as noted in II, we used the wave functions of the exciton states as set forth by Pekar[8]). The difference can be traced to the following points: in the first place, for the case in which the transverse field is perpendicular to the plane of incidence, $\mathscr{E}^{\parallel} = 0$ in [9]; in the second, for the case in which the transverse field lies in the plane of incidence, $\mathscr{E}^{\parallel}_{x'}$ is given in [9] by an expression that is proportional to the longitudinal component of that part of (7) which take place because of $p^{(2)}$ and, in accord with the second section of the present paper, is equal to zero; in the third place, the Fresnel formula in [9] for this case differs from that obtained here.

The first point is connected with the fact that Pekar's theory takes into account only the zeroth approximation in $\mathbf{k}$ in the polarization matrix elements, in which approximation $\mathscr{E}^{\parallel} = 0$. However, as shown in the previous section, $\mathscr{E}^{\parallel}$ can even exceed $\mathscr{E}^{\perp}$, so that it is impossible to restrict oneself to the zeroth approximation.

The second and third points are connected with a difference in the methods used in the Pekar theory and in the present research. The equation for the $\mathbf{k}_s$ in the Pekar theory is equivalent to our (9). However, while we obtained (9) as the result of an approximate solution of (1), so that the additional conditions (8) automatically arise in the process of solution, an equation similar to (9) appears in [8] at the beginning and requires the independent introduction of additional conditions. In other words, our integral equation (2), which connects the polarization and the field, has already been solved with respect to the polarization, while the corresponding Eq. (17) in [8] is a differential equation and requires additional conditions. As such, Pekar uses boundary conditions which require the vanishing of the exciton part of the polarization on the surface of the crystal. If we neglect components with $\mathbf{b} \neq 0$, then we can write $P_1(r)$ in our notation in the form

$$\mathbf{P}_1(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}} \exp [i(k_x x + k_y y)] [\mathbf{g}(0, \mathbf{k}, \alpha) \exp(ik_z z) - \mathbf{g}(0, \tilde{\mathbf{k}}, \alpha) \exp(-ik_z z)],$$

where the $c_{\mathbf{k}}$ are expansion coefficients of the perturbed wave function in terms of the exciton functions. Assuming that the $c_{\mathbf{k}}$ fall off sufficiently rapidly with increase in $\mathbf{k}$, Pekar assumes that

$g(0, \mathbf{k}, \alpha) = g(0, \tilde{\mathbf{k}}, \alpha) = g(0, 0, \alpha)$; in this case he gets $\mathbf{P}_1 = 0$ for $z = 0, l$. However, according to (11), as $\mathbf{k} \to 0$, $\mathbf{g}$ depends on the direction of $\mathbf{k}$, as a consequence of which, generally speaking, $\mathbf{g}(0, a\mathbf{k}, \alpha) \neq \mathbf{g}(0, a\tilde{\mathbf{k}}, \alpha)$ $(a \to +0)$. It is easy to prove that the equality holds only when the transverse field is perpendicular to the plane of incidence. In the case in which the transverse field lies in the plane of incidence, the use of the condition $\mathbf{P}_1 = 0$ seems unsubstantiated to us. Furthermore, the longitudinal component of the field that appears in [9] is introduced specially to satisfy this condition; however, as was noted above, it is equal to zero. The longitudinal polarization waves considered in [8,9] cannot be excited by electromagnetic waves. This is connected simply with the fact that the indicated waves possess different $\mathbf{k}$ for the same frequency. The longitudinal field which figures in the present work has the same $\mathbf{k} = \mathbf{k}_s$ as the transverse field.

On the strength of the above result, the Pekar theory appears to us to be invalid, so far as it concerns the longitudinal field, and also the transverse field in the case of oblique incidence of the wave.

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