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1991 J. Phys.: Condens. Matter 3 2561

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Conservation laws in electrically polarizable spatially dispersive media: II. Additional boundary condition

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Received 10 August 1990

Abstract. The additional boundary condition (ABC) is considered from the point of view of the angular momentum conservation law. This ABC is shown to be representable as a continuity condition for the macroscopic flux of internal angular momentum and is proved to be consistent with the ABC used previously by various authors, which reveal the physical reasons that lie behind the very existence of the ABC problem in macroscopic crystal optics.

1. Introduction

In part I of this work (Bar'yakhtar *et al* 1991) we have substantiated the possibility of obtaining a macroscopic additional boundary condition (ABC) as a continuity condition for the macroscopic flux density of internal angular momentum (IAM). It was shown that to solve this problem one must study conservation laws describing the spatially dispersive (SD) medium with excitonic polarization within the scope of the general approach, where mechanical vibrational, polarization and electromagnetic degrees of freedom are considered together.

The set of equations (21)–(24), (29) and (32) obtained in part I within the scope of such a general approach enables us to study these conservation laws and to obtain balance equations for constants of motion by applying the variational formalism presented, for example, in the monograph by Bogolubov and Shirkov (1980). We give some basic principles of this formalism in section 2. The balance equations are derived in sections 3–5. The statement of boundary conditions (BC) and an analysis of them are given in sections 6 and 7. Finally, in section 8 we summarize our conclusions.

2. Basic principles

To begin with, let us consider a closed system consisting of the material body and its own electromagnetic fields \mathbf{E} and \mathbf{B} with the external fields \mathfrak{E} and \mathfrak{B} being absent. In this case, in accordance with the Nöther theorem, we may find the mathematical representation of the conservation laws and obtain an explicit form of the constants of motion by setting to zero the variation of action integral A , which is due to variations of coordinates \mathbf{x} , of time t and also of the field variables \mathbf{u} , \mathbf{p} , \mathbf{A} and Φ . The aforesaid variations, which all

are concerned with infinitesimal space and time displacements or with infinitesimal space rotations, are given as

$$\begin{aligned} x_k &\rightarrow x'_k = x_k + \delta x_k \\ t &\rightarrow t' = t + \delta t \\ \Psi_n(x, t) &\rightarrow \Psi'_n(x', t') = \Psi_n(x, t) + \delta \Psi_n(x, t). \end{aligned} \tag{1}$$

Here δ denotes the variation holding material coordinates X fixed, and Ψ_n runs over all field variables and their space and time derivatives as the subscript n runs through the set of integers. Using relations (1) we may write

$$\begin{aligned} \delta A &= \int_{\Delta} [\delta \mathcal{L} + \mathcal{L}(J_0 - 1)] d^3x dt \\ &= \int_{\Delta} \left(\frac{\partial \mathcal{L}}{\partial \Psi_n} \bar{\delta} \Psi_n + (\mathcal{L} \delta \dot{x}_k)_{,k} + \partial_t(\mathcal{L} \delta t) \right) d^3x d^3t = 0 \end{aligned} \tag{2}$$

where $\bar{\delta}$ denotes the variation holding x and t fixed, but J_0 is the Jacobian of the transformation (1),

$$J_0 = 1 + (\delta x_k)_{,k} + \partial_t(\delta t). \tag{3}$$

Note that the variation $\bar{\delta}$ commutes with the operations $\partial/\partial x$ and $\partial/\partial t$, but the variation δ does not.

Equation (2) reflects the fact that Lagrangian density \mathcal{L} and the space-time volume element $d^3x dt$ are invariant under space and time displacements and under space rotations; therefore in equation (2) one should understand Δ to be an arbitrary space-time region.

For the case of Lagrangian density \mathcal{L} constructed in I we may rewrite equation (2) as

$$\delta A = \int_{\Delta} (\partial_t \mathcal{L} + \mathfrak{y}_{k,k}) d^3x dt = 0 \tag{4}$$

where

$$\mathcal{L} = \frac{\partial \mathcal{L}}{\partial v_m} x_{m,A} \bar{\delta} u_A - \gamma_m \bar{\delta} p_m + \frac{\partial \mathcal{L}}{\partial (\partial_t A_m)} \bar{\delta} A_m + \mathcal{L} \delta t \tag{5}$$

and

$$\begin{aligned} \mathfrak{y}_k &= \left(\frac{\partial \mathcal{L}}{\partial u_{A,k}} + \frac{\partial \mathcal{L}}{\partial v_m} x_{m,A} v_k \right) \bar{\delta} u_A - \pi_{mk} \bar{\delta} p_m - \pi_{mkl} (\bar{\delta} p_m)_{,l} + \pi_{mkl,l} \bar{\delta} p_m \\ &\quad - v_k \gamma_m \bar{\delta} p_m + \frac{\partial \mathcal{L}}{\partial A_{m,k}} \bar{\delta} A_m + \frac{\partial \mathcal{L}}{\partial \Phi_{,k}} \bar{\delta} \Phi + \mathcal{L} \delta x_k. \end{aligned} \tag{6}$$

Above we used the notation defined in I. Hereafter to avoid repetition we shall use them without notice and ask the reader to refer to part I of this work.

To derive equations (4)–(6) we used Lagrangian equations (21)–(24) of I. Keeping in mind that Δ is arbitrary, we may reduce equation (4) to

$$\partial_t \mathcal{L} + \mathfrak{y}_{k,k} = 0. \tag{7}$$

Thus, substituting specific expressions for the variations of field variables in equations

(5)–(7) one can find the constants of motion in explicit form. Then assuming external fields to be non-zero and using equations (21)–(25), (29) and (32) of I, one can derive balance equations for these constants of motion.

Now let us study the conservation laws of linear momentum, angular momentum (AM) and energy in detail.

3. Momentum conservation

To find a mathematical representation of the conservation law of linear momentum we use the transformation (1) where

$$\begin{aligned} \delta x &\equiv \text{const} & \delta t &\equiv 0 \\ \delta u &= \delta x & \delta \chi &\equiv 0. \end{aligned} \tag{8}$$

Here, for short, the symbol χ denotes a number of field variables $\{p, A, \Phi\}$. Then the expressions for the variations of the field variables assume the following form

$$\bar{\delta} u_A = X_{A,j} \delta x_j \quad \bar{\delta} \chi = -\delta x_j \chi_{,j}. \tag{9}$$

Substituting the foregoing expressions in relations (5) and (6), and dropping an insignificant coefficient δx_j we get

$$\begin{aligned} \mathfrak{L} &= \rho v_j + \frac{1}{c} [\mathbf{B} \times \rho \mathbf{p}]_j + \frac{1}{4\pi c} D_m A_{m,j} \\ \mathfrak{y}_k &= \frac{\partial \mathfrak{L}}{\partial u_{A,k}} X_{A,j} + v_k \left(\rho v_j + \frac{1}{c} [\mathbf{B} \times \rho \mathbf{p}]_j \right) + p_{m,j} \pi_{mk} + 2p_{m,lj} \pi_{mkl} - (p_{m,j} \pi_{mkl})_{,l} \\ &\quad + \frac{1}{4\pi} (H_m \varepsilon_{mkl} A_{l,j} + D_k \Phi_{,j}) + \mathfrak{L} \delta_{kj} \end{aligned} \tag{10}$$

where D and H are conventionally the electric induction and the magnetic field strength, respectively,

$$\mathbf{D} = \mathbf{E} + 4\pi \mathbf{p} \quad \mathbf{H} = \mathbf{B} - 4\pi \rho \mathbf{m} \tag{11}$$

and c denotes the velocity of light in vacuum. To derive relations (10) we used equations (6), (10) and (14) of part I and also the identity (A1.1) from part I.

In order to derive expressions (10) in the gauge-invariant form we must add to equation (7), with \mathfrak{L} and \mathfrak{y}_k being defined by relations (10), the following identity, which is the corollary of the Maxwell equations:

$$-\partial_t \left(\frac{1}{4\pi c} D_m A_{j,m} \right) + \frac{1}{4\pi} \left(\frac{1}{c} D_k \partial_t A_j - H_m \varepsilon_{mkl} A_{j,l} \right)_{,k} = 0. \tag{12}$$

Then, using relation (A1.9) of part I we may rewrite equation (7) as

$$\partial_t g_j + \sigma_{jk,k} = 0 \tag{13}$$

where g_j is the momentum density in the Abraham form

$$g_j = \rho v_j + (1/4\pi c) [\mathbf{E} \times \mathbf{B}]_j \tag{14}$$

and σ_{jk} is momentum flux density

$$\sigma_{jk} = \rho v_j v_k + t_{jk} + \mu_{jk}. \tag{15}$$

Here tensor t_{jk} is defined by equation (33) of part I, and the tensor μ_{jk} is

$$\mu_{jk} = - (1/4\pi) (D_k E_j + B_k H_j) + (1/8\pi) (E^2 + B^2) \delta_{jk} - \rho m_l B_l \delta_{jk}. \tag{16}$$

As is seen from equation (14) the momentum density g consists of the mechanical

momentum density ρv and that for the electromagnetic field generated by the material body, $(1/4\pi c)[E \times B]$. By using the mass conservation law (A1.2) and equations (32) of I, and also by using Maxwell's equations, we get balance equations in the form

$$\partial_i(\rho v_j) + (\rho v_j v_k + t_{jk}),k = f_j \tag{17a}$$

$$\partial_i((1/4\pi c)[E \times B]_j) + \mu_{jk,k} = -f_j \tag{17b}$$

where f_j is given as

$$f_j = \rho p_m E_{m,j} + \rho m_l B_{l,j} + \partial_i((1/c)[\rho p \times B]_j). \tag{18}$$

The last term on the right-hand side of equation (18) is the so-called Abraham force. It is important that this term arises not only in equation (17b) but also in equation (17a). This is the reason why one must interpret this term as a force (Abraham's point of view) and not as a portion of the electromagnetic field momentum (Minkowski's point of view). Confusion like this is concerned with the problem of making a choice in macroscopic electrodynamics between Abraham's energy-momentum tensor and that in Minkowski's form. Details may be found, for example, in monographs of Møller (1972) and Ginzburg (1981).

As is seen from equations (17) the cause of confusion is the incompleteness of description. Had investigators described the medium within the scope of the general approach, the aforesaid problem would have not arisen at all.

To turn to the case when external fields are non-zero, it is sufficient in equations (14)–(18) to substitute quantities \mathcal{E} and \mathcal{B} for E and B , which reflects the fact that the following transformation

$$E \rightarrow \mathcal{E} = E + \mathcal{E} \quad B \rightarrow \mathcal{B} = B + \mathcal{B} \tag{19}$$

does not break the validity of any relation used to derive equations (14)–(18).

4. Angular momentum conservation

To find a mathematical representation of the conservation law of AM we use the transformation (1) with

$$\begin{aligned} \bar{\delta}x_i &= \varepsilon_{ijk}x_j \delta\varphi_k & \bar{\delta}u_A &= X_{A,i} \delta x_i & \bar{\delta}\Phi &= -\Phi_{,i} \delta x_i \\ \bar{\delta}p_i &= \varepsilon_{ijk}p_j \delta\varphi_k - p_{i,l} \delta x_l & \bar{\delta}A_i &= \varepsilon_{ijk}A_j \delta\varphi_k - A_{i,l} \delta x_l. \end{aligned} \tag{20}$$

Here vector $\delta\varphi$ denotes an arbitrary infinitesimal angle of space rotation.

Let us pay attention, first of all, to the restraints that rotational invariance imposes on the Lagrangian density \mathcal{L} . By substituting relations (20) in equation (2), one may get, keeping in mind that in equation (2) Δ is arbitrary, the condition of rotational invariance in the following form

$$\varepsilon_{kji}(\sigma_{ji} - \eta_{ji}) = 0 \tag{21}$$

with

$$\eta_{ji} = (\pi_j + \rho[E_j]p_i + \pi_{jm}p_{i,m} + \pi_{jmi}p_{i,mi} - (\pi_{mli}p_{m,j}),l + \gamma_j d_l p_i) \tag{22}$$

where

$$[E_j] = E_j + (1/c)(v \times B)_j. \tag{23}$$

To be convinced of the validity of equation (21), one should substitute (15) in (21) and then use equation (40) of I.

By substituting relations (20) in equations (5)–(7), we get after some algebra (omitted here since it is similar to that employed in the previous section) the AM conservation statement of the form

$$\partial_t J_i + T_{ik,k} = 0 \tag{24}$$

where J is the AM density vector

$$J = L + l \tag{25a}$$

with

$$L_i = \varepsilon_{ijk} x_j g_k \tag{25b}$$

$$l_i = \varepsilon_{ijk} \gamma_j p_k \tag{25c}$$

and T_{ik} is the AM flux density tensor

$$T_{ik} = T_{ik}^{(L)} + T_{ik}^{(l)} \tag{26a}$$

with

$$T_{ik}^{(L)} = \varepsilon_{ijl} x_j \sigma_{lk} \tag{26b}$$

$$T_{ik}^{(l)} = l_i v_k + \varepsilon_{ijl} \mathfrak{T}_{jlk} \tag{26c}$$

Here the following notation was used

$$\mathfrak{T}_{jlk} = \pi_{jk} p_l + \pi_{jnk} p_{l,n} + \pi_{nkj} p_{n,l} - \pi_{jkn,n} p_l \tag{26d}$$

As seen from equation (25a), the total AM density consists of the orbital component L , which depends directly on the centre-of-mass coordinates x , and the *internal* one l , which is non-zero only for the case of *polarized* media. Relations (26b, c) define corresponding components of the AM flux density.

The key point in relation (26c) is that IAM may be transferred through the crystal provided that spatial dispersion is the case. Moreover, as is seen from equation (26d), inclusion of the terms dependent on second-order space derivatives of p as the components of the Lagrangian density gives rise to three additional terms in the expression for $T_{ik}^{(l)}$ in comparison with results of the work by Lam and Lax (1978).

By using equations (25b, c) and also by using equation of motion (22) for p from part I, one may get balance equations of the orbital AM component and of the IAM. The former is

$$\partial_t L_i + T_{ik,k}^{(L)} + \varepsilon_{ijk} \sigma_{jk} = 0. \tag{27a}$$

The latter should be decomposed in a way such that the last term on the left-hand side of equation (27a) be different from a corresponding term of the IAM balance equation in sign only. Keeping this in mind we use equation (21) and get

$$\partial_t l_i + T_{ik,k}^{(l)} - \varepsilon_{ijk} \eta_{jk} = 0. \tag{27b}$$

It is the method with the aid of which one might derive the expression for $T_{ik}^{(l)}$ from the IAM balance equation (27b) (with the latter being the corollary of the equation of motion for p only); but to follow this procedure it is necessary that the expression for σ_{jk} be at hand. In other words, it is impossible to obtain the expression for the IAM flux density solely from the equation of motion for p ; just like the case mentioned above in which it

was insufficient that (17b) be used solely to resolve the disagreement between Abraham and Minkowski. That is why the general approach was necessary from the very beginning.

Besides, it is appropriate to note the following important fact. In the limiting case $u \rightarrow 0$, dealt with by ordinary crystal optics, the terms (18) and (19) of part I, which describe spatial dispersion, become

$$\frac{1}{2}p_{i,k}B_{ijkl}^{(0)}p_{j,l} - \frac{1}{2}p_iB_{ijkl}^{(1)}p_{j,kl}. \tag{28}$$

Here $\hat{B}^{(0)}$ and $\hat{B}^{(1)}$ possess the following symmetry upon interchange of tensor indices:

$$B_{ijkl}^{(0)} = B_{jilk}^{(0)} \quad \text{and} \quad B_{ijkl}^{(1)} = B_{ijlk}^{(1)}. \tag{29}$$

Meanwhile, the equation of motion for p involves only symmetric portions, $\hat{\beta}^{(0)}$ and $\hat{\beta}^{(1)}$, of these tensors:

$$\hat{\beta}_{ijkl}^{(n)} = \frac{1}{4}(B_{ijkl}^{(n)} + B_{jilk}^{(n)} + B_{ijlk}^{(n)} + B_{jilk}^{(n)}) \quad n = 0, 1. \tag{30}$$

That is why, on considering the problem within the scope of ordinary crystal optics, investigators confine themselves to a description of the spatial dispersion in terms of $\hat{\beta}^{(0)}$ only. As is seen from equation (26d), restrictions (30) do not hold for the expression of the IAM flux density, which reflects the fact that the three terms on the right-hand side of equation (22) from I are involved in the expression (26d), having been multiplied by different factors. Thus, we may infer that the equation of motion for p , or, in other words, the k -dependent dielectric permittivity tensor $\hat{\epsilon}(k)$, in general contains incomplete information on spatial dispersion.

5. Energy conservation

To consider mathematical formulation of energy conservation we use transformation (1) where

$$\begin{aligned} \delta t &= \text{const} & \delta x &= 0 \\ \delta \chi &= -\partial_t \chi \delta t & \chi &= \{u, p, A, \Phi\}. \end{aligned} \tag{31}$$

Following the procedure described above and again omitting the algebra we get energy balance equations as

$$\begin{aligned} \partial_t W_f + (c/4\pi)[E \times H]_{l,l} + q &= 0 \\ \partial_t W_m + \{S_l - (c/4\pi)[E \times H]_{l,l}\} - q &= 0 \\ q &= E \cdot \partial_t(\rho p) - \rho m \cdot \partial_t B. \end{aligned} \tag{32}$$

Here energy density W is resolved into components associated with the electromagnetic field W_f and the medium W_m by

$$\begin{aligned} W_f &= (E^2 + B^2)/8\pi \\ W_m &= \frac{1}{2}\rho v^2 + \frac{1}{2}\rho(d_t p)^* \hat{f}^{-1}(d_t p)^* + \rho \Sigma \end{aligned} \tag{33}$$

and S is the vector of energy flux density in the form

$$\begin{aligned} S_l &= \frac{c}{4\pi} [E \times H]_l + v_l(W_m - \rho p \cdot E) + \rho \frac{\partial(\mathcal{L}^{(0)}/\rho)}{\partial u_{A,l}} X_{A,k} v_k \\ &\quad - \partial_i p_m \pi_{ml} + 2\partial_i p_m \pi_{mln,n} - (\partial_i p_m \pi_{mln})_{,n}. \end{aligned} \tag{34}$$

If transformation (19) is employed, equations (24)–(27) and (32)–(34) will hold for the case of non-zero external fields. Let us note that formulae (33) and (34) are the generalization of the results obtained by Lax and Nelson (1976), Lam and Lax (1978), Agranovich and Ginzburg (1966), Bishop and Maradudin (1976) and Selkin (1977).

6. Boundary conditions

Letting N represent the inward normal to the crystal surface we may write BC for the case of a boundary surface moving with velocity v as

$$[\sigma_{jk} - g_j v_k]_{in}^{out} N_k = 0 \tag{35a}$$

$$[T_{jk} - J_j v_k]_{in}^{out} N_k = 0 \tag{35b}$$

$$[S_k - W v_k]_{in}^{out} N_k = 0 \tag{35c}$$

where the square bracket notation indicates the jump at the boundary in the enclosed quantity and is given by

$$[\dots]_{in}^{out} = (\dots)^{out} - (\dots)_{in}$$

Relations (35) should conventionally be completed with BC for the electromagnetic field. We give below these BC obtained in work by Bar'yakhtar *et al* (1987) which hold true for the case of a moving boundary surface:

$$\begin{aligned} [\mathfrak{B}_\perp]_{in}^{out} &= 0 & [\mathfrak{B}_\parallel]_{in}^{out} &= [N \times (v/c)] \mathfrak{P} \\ [\mathfrak{E}_\perp]_{in}^{out} &= -4\pi[\rho p_\perp]_{in}^{out} & [\mathfrak{E}_\parallel]_{in}^{out} &= (N \cdot v/c) \cdot (v_\parallel/c) \mathfrak{P}. \end{aligned} \tag{36}$$

Here

$$\mathfrak{P} = 4\pi(N \cdot [\rho p]_{in}^{out})/[1 - (v_\perp/c)^2].$$

Symbols \perp and \parallel denote vector components normal and parallel to the surface element plane, that is

$$\mathfrak{B}_\perp = N \cdot (N \cdot \mathfrak{B}) \quad \mathfrak{B}_\parallel = [N \times [\mathfrak{B} \times N]].$$

Note that BC (36) are consistent with those obtained by Lax and Nelson (1976) but, in contrast, the right-hand sides of equations (36) are expressed in terms of polarization p in an explicit way.

By substituting expressions (25)–(26) for T_{jk} and for J_j in equation (35b) and by assuming the BC (35a) to be satisfied, one may rewrite (35b) as

$$\epsilon_{ij} [\mathfrak{E}_{jlk}]_{in}^{out} N_k = 0. \tag{37a}$$

It is the BC we suppose to be used as an ABC. Notice that this ABC, in contrast with others obtained till now, is non-linear in quantity p . Just as expected, in the absence of spatial dispersion, equation (37a) degenerates into a trivial identity.

By using equations (36) we may, after some rather tedious algebra, reduce BC (35a, c) to the form

$$[\mathcal{G}_{kj} + \delta_{kj} 2\pi(\rho p_{\perp})^2]_{\text{in}}^{\text{out}} N_k = 0 \tag{37b}$$

$$[\mathcal{G}_k]_{\text{in}}^{\text{out}} N_k = 0 \tag{37c}$$

where the following notation was introduced:

$$\mathcal{G}_{kj} = \rho \frac{\partial(\mathcal{L}^{(0)}/\rho)}{\partial u_{A,k}} X_{A,j} + p_{m,j} \pi_{mk} + p_{m,ij} \pi_{mkl} - p_{m,j} \pi_{mkl,i} \tag{38a}$$

$$\mathcal{G}_k = \pi_{mk} d_i p_m + \pi_{mkn} d_i p_{m,n} - \pi_{mkn,n} d_i p_m \tag{38b}$$

In equation (37b) terms of the order of $(v/c)^2$ or weaker were omitted.

As for the ABC problem, BC (37a) and (37c) are of particular interest. One can generalize them to the case of N isolated exciton levels by employing the transformation (2) of part I, so that the aforesaid equations will assume the form of a sum over N exciton modes. However, since conditions like these are to be satisfied not at a single frequency point but over some frequency range, they will happen to be split into a number of independent equations, where each one looks like (37). Thus, on considering the ' N exciton levels' approximation one may use equations (37) as BC for each isolated exciton mode.

7. Analysis of boundary conditions

In order to demonstrate how the obtained BC works, let us consider a well studied example, when a π -polarized plane electromagnetic wave is incident on a boundary surface of a crystal with $43m$ point group symmetry. The geometry of the experiment is as follows:

$$\begin{aligned} N &= (0; 1; 0) & c &= (0; 0; 1) \\ k \perp c & & \mathcal{E} \perp c. & \end{aligned} \tag{39}$$

Here c denotes the vector of crystalline uniaxial anisotropy and k is the wavevector of an incident ray. For the sake of simplicity, let us confine ourselves to a consideration of one single exciton mode, with which the following stored energy per unit mass is associated:

$$\Delta \Sigma = \frac{1}{2} p_i K_{ij} p_j + \frac{1}{2} p_{i,k} B_{ijkl}^{(0)} p_{j,l} - \frac{1}{2} p_i B_{ijkl}^{(1)} p_{j,kl} \tag{40}$$

Substituting (40) into equations (37a, c) and taking conventionally an average over a time period and also over a space period along the surface plane (i.e. over the x coordinate) we get

$$\begin{aligned} p_x (\nabla \cdot p) \beta_{11}^{(3)} + p_y [\nabla \times p]_z \beta_{12}^{(3)} &= 0 \\ \partial_i p_y (\nabla \cdot p) \beta_{11}^{(2)} - \partial_i p_x [\nabla \times p]_z \beta_{12}^{(2)} &= 0 \end{aligned} \tag{41}$$

with $p = (p_x; p_y; 0)$. Here the following notation was used:

$$\begin{aligned} \beta_{11}^{(2)} &= \beta_{xxxx}^{(0)} + \beta_{xxx}^{(1)} & \beta_{11}^{(3)} &= \beta_{xxxx}^{(0)} + \frac{1}{4}(\beta_{xxx}^{(1)} + \beta_{xyy}^{(1)}) \\ \beta_{12}^{(2)} &= \beta_{xyy}^{(0)} + \beta_{xyy}^{(1)} & \beta_{12}^{(3)} &= \beta_{xyy}^{(0)} + \frac{1}{4}(3\beta_{xyy}^{(1)} - \beta_{xxx}^{(1)}) \end{aligned}$$

where tensor quantities $\hat{\beta}^{(0)}$ and $\hat{\beta}^{(1)}$ have already been defined in (30). Conditions (41) were written in a way such that the contributions of longitudinal and transverse modes be resolved. Notice that equations (41) are BC for excitons rather than for polaritons. So the set of equations (41) makes it possible to obtain exciton reflectivity without going beyond the frame of the macroscopic approach.

Converting from $p(t, x)$ to Fourier transforms by substituting

$$p(t, x) = \text{Re} \left(\sum_{a=1}^3 p(\omega, k^{(a)}) \exp(-i\omega t + ik^{(a)} \cdot x) \right) \tag{42}$$

with

$$k_x^{(1)} = k_x^{(2)} = k_x^{(3)} \quad k_y^{(a)} > 0 \quad k_z^{(a)} = 0 \quad a = 1, 2, 3$$

into equations (41) we get

$$\text{Im} \sum_{\substack{a=1 \\ b=1}}^3 \{ p_x^*(\omega, k^{(a)}) (k^{(b)} \cdot p(\omega, k^{(b)})) \beta_{11}^{(3)} + p_y^*(\omega, k^{(a)}) [k^{(b)} \times p(\omega, k^{(b)})]_z \beta_{12}^{(3)} \} = 0 \tag{43a}$$

and

$$\text{Re} \sum_{\substack{a=1 \\ b=1}}^3 \{ p_y^*(\omega, k^{(a)}) (k^{(b)} \cdot p(\omega, k^{(b)})) \beta_{11}^{(2)} + p_x^*(\omega, k^{(a)}) [k^{(b)} \times p(\omega, k^{(b)})]_z \beta_{12}^{(2)} \} = 0. \tag{43b}$$

Here by summing over a and over b we take into account contributions of three exciton modes, two transverse ($a = 1, 2$) and one longitudinal ($a = 3$), which are inherent for the case of geometry (39). Asterisk denotes complex conjugation†.

Supposing $\sum_a p_x(\omega, k^{(a)})$ and $\sum_a p_y(\omega, k^{(a)})$ to be independent quantities one may linearize (43) as

$$\begin{bmatrix} \sum_a (k^a \cdot p(\omega, k^{(a)})) \\ \sum_a [k^{(a)} \times p(\omega, k^{(a)})]_z \end{bmatrix} = \frac{\omega}{c\lambda} \begin{bmatrix} \psi^{(2)}\xi & i\psi^{(3)} \\ -i & -\xi \end{bmatrix} \begin{bmatrix} \sum_a p_x(\omega, k^{(a)}) \\ \sum_a p_y(\omega, k^{(a)}) \end{bmatrix} \tag{44}$$

where the following notation was introduced

$$\psi^{(2)} = \beta_{12}^{(2)} / \beta_{11}^{(2)} \quad \psi^{(3)} = \beta_{12}^{(3)} / \beta_{11}^{(3)}$$

and λ and ξ are some arbitrary dimensionless real parameters.

† Note that equations (43a) and (43b) originate from AM conservation and energy conservation laws, respectively.

In order to complete the set of equations (44), one must add to them BC (36), which for the case of a stationary crystal surface assumes the form

$$(1/4\pi\rho)E^{(0)}(1 - R)\varepsilon_0 \cos \theta = - \sum_a p_x(\omega, k^{(a)}) - \sum_a [k^{(a)} \times p(\omega, k^{(a)})]_z k_y^{(a)} / \mathfrak{D}^{(a)} \quad (45)$$

$$(1/4\pi\rho)E^{(0)}(1 + R) = -(\omega/c) \sum_a [k^{(a)} \times p(\omega, k^{(a)})]_z / \mathfrak{D}^{(a)}$$

with

$$\mathfrak{D}^{(a)} = (k^{(a)})^2 - \varepsilon_0 \omega^2 / c^2.$$

Here ε_0 is the background permittivity, ρ is the crystal density, θ is the angle of incidence, $E^{(0)}$ is incident wave amplitude, and R denotes amplitude reflectivity, that is

$$R = E^{(R)} / E^{(0)}$$

where $E^{(R)}$ is reflection amplitude.

To make an interface between this theory and results obtained earlier by different authors, let us consider the most simple limiting case of normal incidence. Solving the set of equations (44) and (45) for R gives

$$R = (\bar{n} - 1) / (\bar{n} + 1) \quad (46a)$$

with efficient index of refraction, \bar{n} , being expressed as

$$\bar{n} = n \frac{(\bar{n}_0 + n)\phi + (\bar{n}_0 - n)}{(\bar{n}_0 + n)\phi - (\bar{n}_0 - n)} \quad (46b)$$

where $n = \varepsilon_0^{1/2}$ and

$$\bar{n}_0 = (n_m + \varepsilon_0) / n_a.$$

Here $n_a = n^{(1)} + n^{(2)}$ and $n_m = n^{(1)}n^{(2)} = n^{(3)}\varepsilon_0^{1/2}$, where $n^{(a)}$ with $a = 1, 2$ denote indices of refraction for two transverse modes (polaritons), but $n^{(3)}$ denotes that for longitudinal mode. Quantity ϕ in (46b) may be expressed as

$$\phi = (\kappa - i\lambda n) / (\kappa + i\lambda n) \quad (47a)$$

where

$$\kappa = 1 + i\lambda n_a + \psi^{(2)}\xi^2 / (\psi^{(3)} + i\lambda n^{(3)}). \quad (47b)$$

The ABC obtained by Hopfield and Thomas (1963) gives a result that looks like (46) provided

$$\phi = \exp(-2inl\omega/c). \quad (48)$$

Here l is the thickness of an exciton-free surface layer. For the case of $ln\omega/c \ll 1$ and $(ln_a\omega/c)^2 \ll 1$ relation (47a) is consistent with (48) provided that for λ the following expression is substituted

$$\lambda = (1 + \psi^{(2)}\xi^2 / \psi^{(3)})l\omega/c.$$

Thus, one may conclude that in terms of Hopfield and Thomas' (1963) theory λ is a

measure of the exciton-free layer thickness. If $\lambda = 0$, we get from (44) Pekar's (1957, 1983) ABC in the form

$$\sum_a p(\omega, \mathbf{k}^{(a)}) = 0. \tag{49}$$

As for the quantity ξ , its physical meaning will be realized if one notices that even for the case of normal incidence the amplitude of a longitudinal wave does not equal zero and is proportional to $\xi\lambda$. Consequently, ξ is a measure of the crystal point group symmetry breaking that occurs within the surface layer. However, to consider a contribution like that to reflectivity, so far as we know, has not been customary until now. So, keeping in mind that the purpose of this section is to compare the results shown above with those obtained previously by various authors, we shall hereafter set $\xi = 0$ without notice.

The ABC (44) may be readily converted to coordinate representation in the form

$$[\hat{\mathbf{M}}\mathbf{p} + l_{\text{eff}}(\partial\mathbf{p}/\partial y)]|_{y=0} = 0 \tag{50}$$

where notation $l_{\text{eff}} = \lambda/k_0$ was used (here k_0 denotes the wavevector of electromagnetic waves in vacuum), and

$$\hat{\mathbf{M}} = \begin{bmatrix} M_{xx} & M_{xy} \\ M_{yx} & M_{yy} \end{bmatrix} = \begin{bmatrix} 1 & -ik_{\parallel}l_{\text{eff}} \\ ik_{\parallel}l_{\text{eff}} & \psi^{(3)} \end{bmatrix} \quad k_{\parallel} = k_0 \sin \theta \tag{51}$$

is a matrix with real diagonal elements.

Thus, one may conclude that relation (50) is the generalized ABC, which depends on a single phenomenological parameter, l_{eff} , where l_{eff} is an integrated characteristic that describes the influence of the boundary layer on the exciton reflectivity through the difference between optical properties of the layer (spatial dispersion properties in particular) and those of the bulk crystal. For the particular case, when we stay within the frame of the dead-layer model approximation proposed by Hopfield and Thomas (1963) with electromagnetic waves falling normally on the *sd* medium from the vacuum, the effective length of the boundary layer, l_{eff} , agrees with the thickness of the dead layer, l . Meanwhile the realm of application of the generalized ABC (50) seems to be much wider than that for the dead-layer approximation. For example, on making use of ABC (50) one may even treat the surface layer, which is essentially inhomogeneous in the direction normal to the crystal surface; the only limitation is that the effective thickness of this layer must be sufficiently small ($k_0l_{\text{eff}} \ll 1$) that making use of BC for the electromagnetic field in the form (36) be justified. Moreover it seems that there is no obstruction whatever preventing us from considering as a boundary layer in ABC (50) not only the surface layer of the crystal but also, say, a thin film.

For the case of normal incidence, as was to be expected, the ABC (50) may be readily reduced to the commonly used form

$$[a_i p_i + b_i(\partial p_i/\partial y)]|_{y=0} = 0 \quad i = x, y \tag{52}$$

where ratios a_i/b_i ($i = x, y$) are real, which in accord with Bishop and Maradudin (1976) and with Selkin (1977) is a consequence of making use of the energy conservation law.

Since, according to the works by Birman and Zeyher (1974), Birman (1982) and Halevi and Fuchs (1984), the form of the ABC in its coordinate representation is directly related to the exciton reflectivities, we may now turn to deriving explicit expressions for these reflectivities. Unfortunately, we could not immediately apply the formulae given

in the works just mentioned above to the physical situation under consideration. First, for the case of oblique incidence, the ABC (50) may not be reduced to the form (52). Secondly, the medium being considered is assumed to be anisotropic. So we are to derive expressions for exciton reflectivities ourselves.

To begin with, we must show dispersion relations for exciton modes. After some algebra one may get

$$(k^{(l)})^2 = (\omega^2 - \omega_T^2)/(\beta_{xx}^{(2)} f_{xx}) \tag{53a}$$

$$(k^{(t)})^2 = (k^{(l)})^2/\psi^{(2)} \tag{53b}$$

with $\text{Re}(k^{(\alpha)}) \geq 0, \text{Im}(k^{(\alpha)}) \geq 0, \alpha = l, t$, and

$$k_{\perp}^{(l)} = k^{(l)}\Gamma^{(l)} \tag{53c}$$

$$k_{\perp}^{(t)} = k^{(t)}\Gamma^{(t)} \tag{53d}$$

and where

$$\omega_T^2 = K_{xx}f_{xx} \tag{54a}$$

$$\Gamma^{(l)} = (1 - q^2)^{1/2} \tag{54b}$$

$$\Gamma^{(t)} = (1/\psi^{(2)} - q^2)^{1/2} \tag{54c}$$

$$q = k_{\parallel}/k^{(l)}. \tag{54d}$$

In formulae (53) $k^{(l)}$ and $k^{(t)}$ are wavevectors for longitudinal and transverse excitons, respectively, but $k_{\perp}^{(l)}$ and $k_{\perp}^{(t)}$ are corresponding components normal to the surface plane.

Note that for the geometry (39), no matter what the quantity q equals, every exciton mode may be resolved into longitudinal and transverse components with the corresponding unit eigenvectors for exciton polarization being representable as

$$\langle l+ | = (q; \Gamma^{(l)}) \quad \langle l- | = (q; \Gamma^{(l)}) \tag{55a}$$

$$\langle t+ | = (\Gamma^{(t)}; -q)(\psi^{(2)})^{1/2} \quad \langle t- | = (\Gamma^{(t)}; q)(\psi^{(2)})^{1/2}. \tag{55b}$$

For the sake of convenience we use here 'bra-ket' notation, but '+' and '-' denote that the corresponding exciton waves propagate along the y axis and in the opposite direction, respectively. Thus, for the case when exciton waves fall on the crystal surface and reflect inwards, we may express the excitonic polarization $|p^{ex}\rangle$ as

$$|p^{ex}\rangle \sim [|\alpha-\rangle G_{\alpha\beta}(y - y_0) + |\alpha+\rangle G_{\alpha\gamma}(y)r_{\gamma\epsilon}^{ex}G_{\epsilon\beta}(-y_0)]s_{\beta} \tag{56a}$$

where the Green function for excitons is

$$G_{\alpha\beta}(y) = \delta_{\alpha\beta} \exp(ik_{\perp}^{(\alpha)}|y|). \tag{56b}$$

Hereafter summation over all repeated Greek subscripts is implied. Quantities s_{β} ($\beta = l, t$) characterize the source of exciton waves, which is assumed to be located at the point y_0 inside the crystal and far away from the boundary surface, $y < y_0$. In relation (56a) $r_{\gamma\epsilon}^{ex}$ is the exciton reflectivity tensor in polarization eigenvectors representation. Keeping

in mind that $|l+\rangle$ and $|t+\rangle$ compose a complete basis in the (x, y) plane, one may express matrix \mathbf{M} from equation (51) in a similar way as

$$m_{\alpha\beta} = T_{\alpha\gamma} \langle \gamma+ | \hat{\mathbf{M}} | \beta+ \rangle \tag{57a}$$

where

$$T_{\alpha\gamma} \langle \gamma+ | \beta+ \rangle = \delta_{\alpha\beta}. \tag{57b}$$

In formulae (57) the fact that eigenvectors $\langle l+ |$ and $\langle t+ |$ are not orthogonal was taken into account.

Now let us note that ABC (50), as has already been emphasized above, are the ABC for excitons rather than those for polaritons. So, there is no need to consider polariton modes to obtain reflectivities $r_{\alpha\beta}^{\text{ex}}$, but we must only substitute relations (56) into (50). By using again the fact that $|l+\rangle$ and $|t+\rangle$ compose a complete basis one may get, after some algebra, the following relation

$$r_{\alpha\beta}^{\text{ex}} = (ik_{\perp}^{(\beta)} l_{\text{eff}} \hat{\mathbf{l}} + \hat{\mathbf{m}})^{-1} (ik_{\perp}^{(\beta)} l_{\text{eff}} \hat{\mathbf{l}} - \hat{\mathbf{m}})_{\gamma\epsilon} C_{\epsilon\beta} \quad \alpha = l, t; \beta = l, t \tag{58}$$

which completes the derivation of exciton reflectivities.

Here we used the notation

$$\begin{aligned} |\alpha-\rangle &= |\beta+\rangle C_{\beta\alpha} \\ C_{\beta\alpha} &= T_{\beta\gamma} \langle \gamma+ | \alpha-\rangle \end{aligned} \quad \alpha = l, t; \beta = l, t.$$

When normal incidence is the case, formula (58) may be substantially simplified as

$$\hat{\mathbf{r}}^{\text{ex}} = \begin{bmatrix} r_{ll}^{\text{ex}} & r_{lt}^{\text{ex}} \\ r_{tl}^{\text{ex}} & r_{tt}^{\text{ex}} \end{bmatrix} = \begin{bmatrix} \frac{ik_{\perp}^{(l)} l_{\text{eff}} - \psi^{(3)}}{ik_{\perp}^{(l)} l_{\text{eff}} + \psi^{(3)}} & 0 \\ 0 & \frac{ik_{\perp}^{(t)} l_{\text{eff}} - 1}{ik_{\perp}^{(t)} l_{\text{eff}} + 1} \end{bmatrix}. \tag{59}$$

The key point in equations (58) and (59) is that $\psi^{(3)}$ is not an arbitrary parameter but is the *specified* constant that describes properties of exciton modes within the bulk of the crystal. For example, in the case when $\beta^{(1)} = 0$ that ordinary crystal optics deals with†, one may, by comparing macroscopic dispersion relations (53) with those used in microscopic theory, express $\psi^{(3)}$ and $\psi^{(2)}$ as

$$\psi^{(3)} = \psi^{(2)} = \beta_{l2}^{(2)} / \beta_{l1}^{(2)} = M_{\parallel} / M_{\perp}.$$

Here M_{\parallel} and M_{\perp} denote effective mass for longitudinal exciton and that for transverse exciton, respectively.

In the light of the foregoing reasoning it is obvious that our approach differs in essence from the approach proposed by Forstmann (1979). In his work Forstmann split up the condition of energy flux continuity at the surface into two separate BC, which in terms of this work would mean that two different components on the left-hand side of equation (43b) should be set zero separately with equation (43a) being omitted. Had we followed this method, the ABC would look like (44) with $\xi = 0$ provided that quantity $\psi^{(3)}$ be an *arbitrary* parameter. Consequently, Forstmann's method being applied to SD media with excitonic polarization is equivalent to treating l_{eff} and $\psi^{(3)}$ in equations (58)

† It is appropriate to note that, when one considers an experimental geometry like (39), approximation $\beta^{(1)} = 0$ is certainly justified.

Table 1. Conditions of consistency between formulae (59) and values of r_{ii}^{ex} and r_{ii}^{ex} by which the ABC used previously by various authors are characterized. The case of normal incidence ($q = 0$) is considered. Condition $k_0 l_{eff} \ll 1$ is assumed to be satisfied.

ABC	r_{ii}^{ex}	r_{ii}^{ex}	Consistency conditions
Pekar (1957)	-1	-1	$k_{\perp}^{(l)} l_{eff} \ll 1, \quad k_{\perp}^{(l)} l_{eff} \ll \psi^{(3)}$
Rimbey and Mahan (1974)	-1	1	$k_{\perp}^{(l)} l_{eff} \ll 1, \quad k_{\perp}^{(l)} l_{eff} \gg \psi^{(3)}$
Fuchs and Kliever (1968)	1	-1	$k_{\perp}^{(l)} l_{eff} \gg 1, \quad k_{\perp}^{(l)} l_{eff} \ll \psi^{(3)}$
Ting et al (1975)	1	1	$k_{\perp}^{(l)} l_{eff} \gg 1, \quad k_{\perp}^{(l)} l_{eff} \gg \psi^{(3)}$

and (59) as arbitrary parameters, which for the case of normal incidence does not differ from treating quantities r_{ii}^{ex} and r_{ii}^{ex} themselves as arbitrary parameters, thereby adding nothing new in comparison with, say, the approach proposed by Halevi and Fuchs (1984).

It is appropriate to note also that Forstmann removed the indeterminacy mentioned above by making use of BC for the electromagnetic field which were chosen to be much more restrictive than BC (36) in this work, with justification being hardly convincing. In our opinion, an approach like that is certainly equivalent to *postulating*, consciously or otherwise, the new ABC, say, in the form

$$j_{\perp}(0) - \langle j_{\perp}(0) \rangle_t = 0$$

where j_{\perp} is electric current normal component (or $j_{\perp} = \rho \delta p_{\perp} / \delta t$ in terms of this work), and angle brackets $\langle . . . \rangle_t$ denote averaging over time.

It is the condition of IAM flux continuity (43a) that enables us to express two quantities, r_{ii}^{ex} and r_{ii}^{ex} , in equation (59) (or even four quantities $r_{\alpha\beta}^{ex}$ in equation (58)) as being governed by one single parameter, l_{eff} . In turn, l_{eff} is certainly determined by the specific physical state of the crystal sample under study.

When one deals with some non-dissipative SD medium, where there are no transverse excitons ($\psi^{(2)} = 0, \psi^{(3)} = 0$) but longitudinal modes (say, plasmons) only are considered, the reflectivity tensor $r_{\alpha\beta}^{ex}$ tends to be the unit matrix

$$r_{\alpha\beta}^{ex} \rightarrow \delta_{\alpha\beta} \tag{60}$$

no matter what the quantities q and l_{eff} equal. For the particular case of normal incidence ($q = 0$) this result might easily be derived from relation (59) by setting

$$\psi^{(3)} \rightarrow 0 \quad k_{\perp}^{(l)} \rightarrow \infty.$$

As is seen from equation (60), to describe, say, metallic media with negligible energy dissipation there is no need to introduce boundary layer thickness, l_{eff} , or any other arbitrary parameter.

It is important to note that the conclusion mentioned above is distinct from one made by Forstmann and Stenschke (1977). The definiteness in equation (60) was achieved by making use of equation (43a), while Forstmann and Stenschke achieved this by imposing restrictions on BC for the electromagnetic field.

Finally we may compare formulae (59) with the corresponding values of the parameters r_{ii}^{ex} and r_{ii}^{ex} by which the ABC used previously by various authors are characterized. We show results of this comparison in table 1 in the way Halevi and Fuchs (1984) did.

Since for $q = 0$ the following equation holds

$$k_{\perp}^{(1)} = k_{\perp}^{(1)}(\psi^{(2)})^{-1/2}$$

then we may conclude that the Rimbey–Mahan (Fuchs–Kliewer) ABC would be consistent with formulae (59) if $\psi^{(2)} \ll 1$ ($\psi^{(2)} \gg 1$). Meanwhile for most cases with which crystal optics deals we have $\psi^{(2)} \gg 1$. Then as frequency ω tunes away from ω_T the specification of ABC runs through the sequence shown below:

$k_{\perp}^{(1)} I_{\text{eff}} \ll 1$	$k_{\perp}^{(1)} I_{\text{eff}} \ll 1$	$k_{\perp}^{(1)} I_{\text{eff}} \gg 1$
Pekar (1957)	Hopfield and Thomas (1963)	Ting <i>et al</i> (1975).

8. Conclusions

From the above we may conclude that taking the law of angular momentum conservation into account enables us to solve the ABC problem consistently within the frame of the macroscopic approach. In particular, reflectivity for excitons may be found by applying macroscopic methods only. In addition, the relation between angular momentum conservation and ABC reveals the physical reasons behind the very existence of the ABC problem in macroscopic crystal optics.

The ABC obtained above is not free from some disadvantages, among which we should mention its limited degree of detail, but this is the cost we pay for its generality. Moreover, for some simple experimental geometries the ABC degenerates into a trivial identity. However, a disadvantage like this seems to be surmountable by means of applying the method of ‘perturbed’ geometries and of letting these perturbations decrease towards zero.

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