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(M, N)-exponential model in the theory of excitons

V. N. Piskovoi

Institute of Semiconductor Physics NAS Ukraine, 45 prospekt Nauki, Kyiv, 252028, Ukraine

Ya. M. Strelniker

School of Physics and Astronomy, Raymond and Beverly Sackler Faculty of Exact Sciences, Tel Aviv University, Tel Aviv 69978, Israel

Abstract. The one- exponential excitonic model, widely used in the theory of light propagation through spatially dispersive media, is generalized in order to take into account the simultaneous existing of M exciton states and N transport mechanisms. The physical reason and possibilities of the proposed model is demonstrated on the base of the Frenkel exciton. The model essentially extends the area of the possible applications consarving at the same time the exact solubilities and other advantages of the traditional exponential-like approaches for the case of the bounded media. The model is used in the paper for deriving the balance equations of the energy density and the energy flux density as well as for studing of boundary value and some other crystal optics problems near the excitonic resonances.

Keywords: crystal optics, spatial dispersion, excitons, exponential model, additional light waves, additional boundary conditions, energy flux density.

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I. Introduction

The modern crystal optics with spatial dispersion (COSD) takes its origin from the pioneer work of Pekar [1] on the additional light waves (ALW) theory. The results of the extensive studies in this area, connected with the excitons problems, are well summarized in refs. [2–4].

In accordance with ref. [2] the generalized term *exciton* refers to any non-conducting excited state of a crystal, which is characterized by one continuous quantum number (wave vector \mathbf{k}) and that the energy is separated from the ground state by an energy gap. The definition contains all specifications essential for the description of the basic results on the spatial dispersion theory. At the same time it makes clear why the different exciton-like states are succesfully described via the system of the coupled polarization oscillators, placed at the points of a crystal lattice. Such a system is usually presented by the following dynamic equation [5]:

$$\left(\frac{\partial^2}{\partial t^2} + \omega_0^2 + 2\nu \frac{\partial}{\partial t} \right) \mathbf{p}(\mathbf{l}, t) + \sum_{\mathbf{l}'} V_{\mathbf{l}, \mathbf{l}'} \mathbf{p}(\mathbf{l}', t) = 2\omega_0 FE(\mathbf{l}, t), \quad (1.1)$$

where \mathbf{E} is the electric field, $\mathbf{p}(\mathbf{l}, t)$ the time dependent dipole moment of the oscillator located at the \mathbf{l} -th site (the lattice vector $\mathbf{l} = l_x \mathbf{a}_x + l_y \mathbf{a}_y + l_z \mathbf{a}_z$, where \mathbf{a}_i are the lattice peri-

ods and l_i are the integers); ω_0 and ν are the oscillators eigenfrequency and damping rate constant, respectively; F determines the interaction of the medium with the electrical field. Matrix $V_{\mathbf{l}, \mathbf{l}'}$ describes the nonlocal interaction between the polarization oscillators and accounts, specifically, for ALW and other *large effects of spatial dispersion* in spectral region of excitonic resonances.

In COSD there is a number of models which take into account the spatial dispersion effects of the real excitons. However, in the case of bounded crystal only few of them are exactly soluble. They correspond to the following choice of the coupling matrix:

$$V = 0, \quad \text{FB model} \quad (1.2)$$

$$V \sim \sum_i^N a_i \delta_{i, |\mathbf{l}-\mathbf{l}'|} \quad \text{NN model} \quad (1.3)$$

$$V \sim e^{-\Gamma|\mathbf{l}-\mathbf{l}'|} \quad \text{Exp model} \quad (1.4)$$

The form (1.2) corresponds to the flat band (FB) excitonic model, which is considered in the usual birefringence (BF) theory of crystal optics without spatial dispersion. The form (1.3) corresponds to the models of the N -neighbors oscillator interaction¹. The form (1.4) corresponds to the exponential model (EM) we try to modify in this paper.

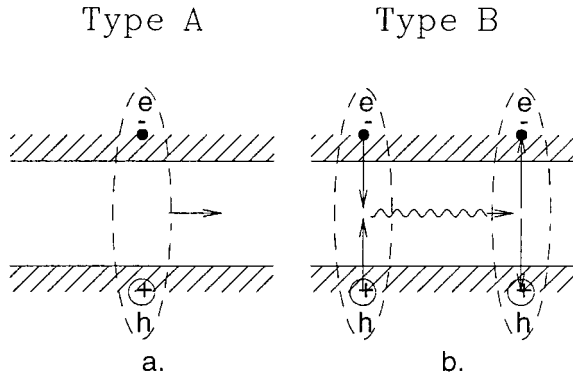


Fig. 1. A schematic diagrams for exchange (a) and resonant (b) transports of Wannier-Mott excitons.

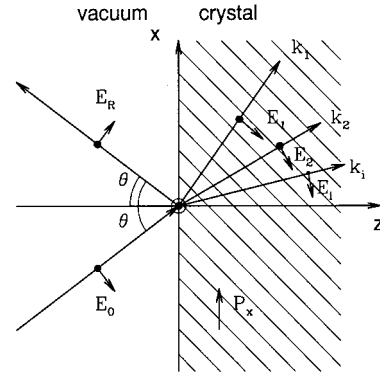


Fig. 2. A coordinate system and the directions of the *p*-polarized incident (E_0), reflected (E_R) and penetrating (E_i) electric field amplitudes. The appearance of the additional rays E_i ($i > 1$) is exclusively due to spatial dispersion phenomena.

There are, at least, three strong advantages of the using of exponential model in spatial dispersion theory. Firstly, its exact solvability. This means that for bounded media, as well as for the infinite one, the crystal polarization could be determined by the limited number of the plane waves, with

wave vectors $\mathbf{k}_j = \frac{\omega}{c} \mathbf{n}_j$, where \mathbf{n}_j are the refraction vectors (RV) [10–11]. Secondly, its natural appearance in the case of the bounded crystals [10, 12–15, 45–48]. Thirdly, because the results of many other models of the excitons could be obtained as the limit case of EM. For example, the NN-model (see (1.3)) may be obtained from (1.4) by setting $\Gamma \gg 1$, and of FB model (1.2) by tending $\Gamma \rightarrow \infty$, and so on.

Due to all these features, the EM is successfully used for solving the different problems in COSD and, in particular, for the more discussed question of the ALW-theory, connected with the problem of the additional boundary conditions (ABC)² see refs. [2, 10, 11, 16–19], etc. Nevertheless, the recent studies as well as some of unsolved problems, pointed in the previous works on ALW theory [20, 2, 14], prove that one-exponential model is insufficient to solve the problems in the case of the several excitonic energies transport canals existing simultaneously. For the case of Wannier-Mott excitons those are the resonance (annihilation) and the exchange canals [26]. The exchange

mechanism means the movement of the bounded electron and hole along each of their own band, while the resonant mechanism means the annihilation of the electron-hole pair at one point and its generation at another, see fig. 1. For the tight-binding models of excitons it may be the s.c. «A» and «B» canals, see refs. [14, 15, 19], etc.

The paper is organized as follows: In sec.II, we generalize the one-exp model by the simultaneous consideration of the many- (say M) excitonic states and N different excitonic transport mechanisms and introducing by this the (M, N) -exponential model. We demonstrate the reality of such model on the bases of Frenkel excitons. In sec III, the proposed model is used for studying the traditional aspects of ALW physics. In Sec IV, the energy transport and the behavior of the energy flux on the crystal surface as well as the form of the ABCs are analyzed in details. The Summary provides a discussion of the obtained results. In Appendixes A and B we present the detail descriptions of some technical evaluations, «the plane-wise methods» of lattice summation, etc.

II. Soluble model

In this section we propose a generalization of the one-exp excitonic model for the system with M total number of the excited states, in the vicinity of the given energy, and N energy transport canals which we call as an (M, N) -exponential excitonic model. We start with some physical justification, using Frenkel exciton model, which is explored usually for molecular crystals [23].

Let the crystal orientation be as it is shown in fig 2, with $\mathbf{a}_x, \mathbf{a}_y$ lying in crystal surface and \mathbf{a}_z being perpendicular to it, so that two lattice subscripts, $\{l_x, l_y\} \equiv \mathbf{l}_\parallel$, are the integers taking the values from $-\infty$ up to $+\infty$ and the third one, $l \equiv l_z$, takes the values 1, 2, 3 ... For simplicity, we shall consider the tetragonal symmetry of the crystal, with $|\mathbf{a}_x| = |\mathbf{a}_y| \equiv a_\parallel$, $|\mathbf{a}_z| \equiv a_\perp$ (for the cubic symmetry we have $a_\perp = a_\parallel$). This does not restrict the generality of the consideration but simplifies the evaluations.

¹ The different kind of the N -neighbors models are the most popular in COSD, especially the next nearest neighbors model [2–4]. Among them is the group of the exact solvable (for the bounded crystal) models in which the special kind of interaction between the N -nearest pairs of oscillators is taken into account [6–9].

² Under the existence of ALW, the usual Maxwell boundary conditions (MBC) are not sufficient to determine the amplitudes of all reflected and transmitted waves in a unique way. They must be supplement with additional boundary conditions (ABC), whose amount must be equal to the amount of additional waves, see refs. [1–4].

The excited states of the crystal are assumed to be Frenkel exciton states, treated in the tight-binding approximation. The appropriate many-electron state of the crystal, which describe the ground, Ψ^0 , and the m -th ($0 \leq m \leq M$) excited states, $\Phi_m(\mathbf{l})$, can be written as the product of the cells wave functions

$$\Psi^0 = \hat{s} \prod_{\mathbf{l}'} \psi(\mathbf{l}'), \quad (2.1)$$

$$\Phi_m(\mathbf{l}) = \hat{s} \phi_m(\mathbf{l}) \prod_{\mathbf{l}' \neq \mathbf{l}} \psi(\mathbf{l}'), \quad (2.2)$$

where $\psi(\mathbf{l})$ and $\phi_m(\mathbf{l})$ are the ground and the perturbed states of the \mathbf{l} -th unit cell, \hat{s} the operator of anti-symmetrization of wave functions in respect to electron coordinates. The Hamiltonian, \hat{H} , of the crystal in electromagnetic field and the operator of the specific electrical polarization of the medium, $\hat{\mathbf{P}}(\mathbf{r})$, have the form

$$\hat{H} = \hat{H}^{(0)} + \hat{H}_{int}, \quad (2.3)$$

$$\hat{H}_{int} = -\sum \hat{\mathbf{d}}_{\mathbf{l}} \cdot \mathbf{E}(\mathbf{l}, t), \quad (2.4)$$

$$\hat{\mathbf{P}}(\mathbf{r}) = \sum_{\mathbf{l}} \hat{\mathbf{d}}_{\mathbf{l}} \delta(\mathbf{r} - \mathbf{l}), \quad (2.5)$$

Here $\hat{H}^{(0)}$ is the energy operator of the non-perturbed crystal; \hat{H}_{int} is the interaction operator of the crystal with the electro-magnetic field, written in the dipole approximation; $\hat{\mathbf{d}}_{\mathbf{l}}$ is the dipole operator of the \mathbf{l} -th unit cell. The perturbed by electro-magnetic field state of the crystal could be written as follows

$$\Psi = \Psi^0 + \sum_{\mathbf{l}, m} b_m(\mathbf{l}, t) \Phi_m(\mathbf{l}), \quad (2.6)$$

In order to find the coefficients $b_m(\mathbf{l}, t)$, we substitute (2.6) into the time-dependent Schrodinger equation and for the «first order approximation» obtain

$$\begin{aligned} & -i\hbar \frac{\partial b_m(\mathbf{l}, t)}{\partial t} + H_{m\mathbf{l}, m\mathbf{l}}^{(0)} b_m(\mathbf{l}, t) + \\ & + \sum_{m', \mathbf{l}' \neq \mathbf{l}} H_{m\mathbf{l}, m'\mathbf{l}'}^{(0)} b_{m'}(\mathbf{l}', t) = \mathbf{d}_m \cdot \mathbf{E}(\mathbf{l}, t), \end{aligned} \quad (2.7)$$

where $H_{\mathbf{l}\mathbf{l}'}^{(0)} \equiv H_{\mathbf{l}\mathbf{l}'}^{(0)}$ are the known matrix elements (see [23,24]), $\mathbf{d}_m = \langle \psi | \hat{\mathbf{d}} | \phi_m \rangle$ – the dipole moment of the unit cell which is produced in the transition (real or virtual) to the m -th excited state. After the averaging of the dipole op-

erator (2.5) on the wave functions (2.6), we find the appropriate partial excitonic deposits into the total crystal specific polarization:

$$\mathbf{P}_m(\mathbf{l}, t) = \frac{\mathbf{d}_m b_m(\mathbf{l}, t)}{\nu} + \text{c.c.}, \text{ for the discrete system} \quad (2.8)$$

$$\mathbf{P}_m(z, t) = \frac{\mathbf{d}_m}{\nu} \{b_m(\mathbf{l}, t)\}_{\mathbf{l} \rightarrow z} + \text{c.c.}, \text{ in the continual limit} \quad (2.9)$$

where ν is the volume of an unit cell.

The resonance ($\mathbf{l} \neq \mathbf{l}'$) integrals in (2.7) could be represented in the form $H_{\mathbf{l}\mathbf{l}'}^{(0)} = H_{\mathbf{l}\mathbf{l}'}^{(1)} + H_{\mathbf{l}\mathbf{l}'}^{(2)}$, where the first and the second terms correspond to the direct and exchange resonance interactions, respectively. The exchange integrals decaying exponentially with the distance [23], and could be represented in the form

$$\sum_{\mathbf{l}' \neq \mathbf{l}} H_{\mathbf{l}\mathbf{l}'}^{(2)} b(\mathbf{l}', t) \approx g \sum_{\mathbf{l}' \neq \mathbf{l}} e^{-\Gamma|\mathbf{l}\mathbf{l}'|} b(\mathbf{l}', t) \text{ (for each } m). \quad (2.10)$$

The situation with $H_{\mathbf{l}\mathbf{l}'}^{(1)}$, is more complicated due to their slow decaying with the distance [24]. Nevertheless, the Coulomb interaction between the cells could be written and calculated in the multi-pole expansions [50, 51]. Note, however, that by evaluation $H^{(1)}$ only in the dipole-to-dipole interaction approximation, $H^{(d)}$, some corrections, $H^{(1)} - H^{(d)}$, need to be taken into account, which could be formally included into (2.10).

The translational symmetry along \mathbf{a}_x and \mathbf{a}_y axes allows to seek the solution of eq. (2.7) in the form $b(\mathbf{l}) = b(l) \exp(i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel})$, where $\mathbf{q}_{\parallel} \equiv \mathbf{k}_{\parallel} a_{\parallel}$ and $\mathbf{k}_{\parallel} = \{k_x, k_y\}$ are the dimensionless and dimension tangential projections of the exciton wave-vector. After summation over \mathbf{l}_{\parallel} in (2.7) we obtain (see Appendix A)

$$\begin{aligned} & \sum_{\mathbf{l}' \neq \mathbf{l}, m'} H_{m\mathbf{l}, m'\mathbf{l}'}^{(d)} b_{m'}(\mathbf{l}', t) = \\ & = \sum_{\mathbf{l}' \neq \mathbf{l}, m'} b_{m'}(\mathbf{l}', t) e^{i\mathbf{q}_{\parallel} \cdot \mathbf{l}'_{\parallel}} \left[\frac{\mathbf{d}_m \cdot \mathbf{d}_{m'}}{|\mathbf{l}\mathbf{l}'|^3} - \frac{3\mathbf{d}_m \cdot (\mathbf{l}\mathbf{l}') (\mathbf{l}\mathbf{l}') \cdot \mathbf{d}_{m'}}{|\mathbf{l}\mathbf{l}'|^5} \right] = \\ & = \frac{\xi}{\nu} \sum_{m', \mathbf{l}'} \mathbf{d}_m \cdot \hat{T}(l, l') \cdot \mathbf{d}_{m'} b_{m'}(l', t) e^{i\mathbf{q}_{\parallel} \cdot \mathbf{l}'_{\parallel}}, \end{aligned} \quad (2.11)$$

where $\xi \equiv a_{\perp}/a_{\parallel}$. For $l' \neq l$ (see Appendix A) the tensor $\hat{T}(l, l')$ has the form of the dyad-sums formed by the vectors $\mathbf{T}_{\mathbf{Q}_i}$:

$$\hat{T}(l \neq l') = 2\pi \sum_{\mathbf{Q}_i} \mathbf{T}_{\mathbf{Q}_i} \mathbf{T}_{\mathbf{Q}_i} \frac{e^{-\xi|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}|l-l'|}}{|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}|}, \quad (2.12)$$

$$\mathbf{T}_{\mathbf{Q}_i} = \left\{ (\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel})_x, (\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel})_y, i \operatorname{sign}(l - l') (\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}) \right\}. \quad (2.13)$$

In (2.12) the summation extends over sites of the corresponding reciprocal two-dimensional lattice (with vectors equal to $\mathbf{Q}_\parallel/a_\parallel$). For $l' = l$ (Appendix A), the tensor \hat{T} reduces to the form, given by (A21)–(A25). In the limit $\mathbf{q}_\parallel \ll 1$ \hat{T} could be expressed in the form of the sum of the regular and singular parts quite similar to 3D case [50, 51]:

$$\lim_{q_\parallel \rightarrow 0} \hat{T} = \text{Reg } \hat{T} + \text{Sing } \hat{T}, \quad (2.14)$$

Where

$$\text{Reg } T_{ij} = T_i^{(0)} \delta_{ij} + T_{ijl'j'}^{(1)} q_{l'} q_{j'}, \quad (2.15)$$

and the definitions «Reg» and «Sing» mean the *regular* and *singular* parts, respectively. The singular part of \hat{T} is connected in plane-wise method with the location of the vectors of the dipole moments in respect to the slab planes:

$$\text{Sing } T_{ij} = \frac{4\pi}{\xi} \delta_{iz} \delta_{jz} + O_{ij}(q_\parallel), \quad (2.16)$$

where $O_{ij}(q_\parallel)$ is the part of higher order in q . Note, that just opposite to mentioned above 3D case the singular part of T ($l' = l$) tensor contains the term linear in respect to q_\parallel already in dipole approximation. Namely, for $i, j = x, y$ $O_{ij} = 2\pi q_l q_{j'}/q_\parallel$ and $O_{zz} = -2\pi q_\parallel$. In both (2.15) and (2.16) cases $T_{xz} \equiv T_{yz} \equiv 0$.

As it follows from (A21)–(A25) and (2.12)–(2.13), for $\mathbf{Q}_\parallel \neq 0$, the Reg \hat{T} part contains the main portion of the Lorentz's local field [9]. This part of (2.11) may be formally adjoined to $H_{ml, m'l}^{(0)}$ term of (2.7), so that the last becomes the excitonic energy of the planes rather than the single-cell one. The Sing \hat{T} part of (2.14) may be adjoined to $Q_\parallel = 0$ term in (2.12) to form the macroscopic field part of the dipole-to-dipole interaction [19].

After the substitution of (2.10) and (2.11)–(2.16) into (2.7) and using (2.8), we obtain a system of M differential – difference equations for M partial crystal polarizations, \mathbf{P}_m , which are interacting one with other through the sum of exponentially decaying potentials of (1.4) type. Summarizing and comparing these results with the results obtained for one-exponential model (see Sec.I) we introduce the generalized (M, N)-exponential model for the material equations of motion of crystal polarization:

$$\begin{aligned} & \left[\frac{\partial^2}{\partial t^2} + \omega_{0m}^2 + 2\nu_m \frac{\partial}{\partial t} \right] \mathbf{P}_m(\mathbf{l}_\parallel, l, t) + \\ & + \sum_{i, m', l'}^{N, M} (\theta(l-l') \hat{g}_i^{m, m'} e^{-\gamma_{i, m}(l-l')} + \\ & + \theta(l'-l) \hat{f}_i^{m, m'} e^{-\gamma_{i, m}(l-l')} + \\ & + \hat{f}_i^{m, m'} e^{-\gamma_{i, m}(l+l')}) \cdot \mathbf{P}_{m'}(\mathbf{l}_\parallel, l', t) = \\ & = 2 \omega_{0m} F_m \cdot \mathbf{E}(\mathbf{l}_\parallel, l, t). \end{aligned} \quad (2.17)$$

Here θ is the step function, ω_{0m} the basic resonance frequencies ν_m the damping constants; the matrixes $\hat{g}_i^{m, m'}$ and $\hat{f}_i^{m, m'}$ the second-rank tensors in the usual space, that determine the intensities of the i -th mechanism (the total number of which is equal to N) of interaction between the oscillators, while the parameters $\gamma_{i, m}$ determine its spatial damping rate; tensor $r_i^{m, m'}$ describes the additional interaction between the oscillators, introduced by the possible mirror image forces arising at media interface. The second-rank tensors F_m determine the oscillator-field interaction. They are usually expressed in different but equivalent forms:

$$F_m = \omega_p^2 f_m / 8\pi \omega_{0, m} = \omega_{0, m} a_{st}^m / 2 = \varepsilon_0 \Delta_m / 4\pi = \mathbf{d}_m \mathbf{d}_m / \nu \hbar,$$

where ω_p is the plasma frequency and f_m the oscillator strength of the considered photo-transition; a_{st}^m the contribution of the given excitation to static polarizability; Δ_m the magnitude of the «transverse-longitudinal» splitting of the exciton lines (see figs. 3–6) and ε_0 the background polarizability; the last expression for F_m follows directly from (2.7). The subscript l' in (2.17) takes the values $(-\infty, +\infty)$ for infinite media (in this case $r_i \equiv 0$) and $(1, L)$ or $(1, +\infty)$ for finite and semi-infinite media, respectively. For the investigation, the physical phenomena arising from the intersection of a crystal with e.m. field the material equations should be considered together with the system of the ideal Maxwell's equations with the polarization density vector written in the form $\mathbf{P}(\mathbf{r}, t) = \sum_m \mathbf{P}_m(\mathbf{r}, t)$. The appropriate investigations form the content of the next sections.

III. (1, N)-exponential model and ALW problems

In this section we apply the (1, N)-exp model to the study of the optical properties of bounded, absorbing, and spatially dispersive dielectric crystal. As before we assume the crystal to be located in the $z \geq 0$ half space and $y = 0$ is the plane of light incidence, see fig. 2. For the given geometry the z components of RV , $n_{zj} = n_{zj}(\omega, n_x)$, can be found as the function of ω and n_x from the Maxwell-Fresnel dispersion equation, where n_x is the x component of RV , determined by Snell law, and j denotes the number of the wave.

Beforehand it is useful to perform some typical approximations, which do not take one out of reality and are well-founded by number of papers dealing with traditional (1, 1)-exp model and by general investigations on COSD [2–4]. First of all, as usual crystal optics deals with $\mathbf{k} \cdot \mathbf{a}_i \ll 1$, we restrict ourselves by the continuous media approximation and substitute (2.8) by (2.9).³ In addition, we shall ignore the near-the-surface distortion effects caused by r_i terms in (2.17), see Appendix B.

The further simplification is connected with the consideration of the resonance frequency region, $\omega \equiv \omega_0$, corresponding to the isolated non-degenerate dipole-allowed exciton absorption band (i.e. the case $M = 1$). In practice, this situation is realized in experiments for the different optical two- and uni-axis crystals [2]. Let us assume the partial vector of the polarizability being directed along the x -axis of the crystal illuminated externally by a p -polarized optical wave, that means (see (2.9), (2.11)) that $\mathbf{P}_m = \{P_x, 0, 0\}$ [with

$f_i = g_i$ in (2.17)]⁴ and electric field vector, $\mathbf{E} = \{E_x, 0, E_z\}$.

As the result of the performed above approximations and simplifications, we obtain an one-dimensional integro-differential equation for P_x :

$$\begin{aligned} & \left[\frac{\partial^2}{\partial t^2} + \omega_0^2 + 2\nu \frac{\partial}{\partial t} \right] P_x(z, \mathbf{r}_{\parallel}, t) - \\ & - 2 \sum_i^N G_i \frac{\omega_0^2}{c} \int_a^{\infty} \exp\left(-\Gamma_i \frac{\omega_0}{c} |z - z'|\right) P_x(z', \mathbf{r}_{\parallel}, t) dz' = \\ & = 2\omega_0 F E_x(z, \mathbf{r}_{\parallel}, t), \end{aligned} \quad (3.1)$$

where the lower limit, a , in the integral takes in our case two values, namely $-\infty$ for unbounded and 0 for semi-infinite crystal, respectively. All coefficients in (3.1) can be expressed as the functions of real crystal parameters for each type of excitons (for the case of the Frenkel exciton they were determined sec.II). Equation (3.1) should be considered simultaneously with the ideal Maxwell's equations and material equations, which determine the non-resonance background contribution into the crystal polarizability:

$$\nabla \times \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t}, \quad (3.2)$$

$$\nabla \times \mathbf{B} = \frac{1}{c} \frac{\partial}{\partial t} (\hat{\epsilon}_0 \cdot \mathbf{E} + 4\pi \mathbf{P}), \quad (3.3)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (3.4)$$

$$\nabla \cdot (\hat{\epsilon}_0 \cdot \mathbf{E} + 4\pi \mathbf{P}) = 0. \quad (3.5)$$

Here $\hat{\epsilon}_0$ is a tensor of the crystal background dielectric permittivity, which for the chosen symmetry has the following form: $\epsilon_{0\parallel} \equiv \epsilon_{0,xx}, \epsilon_{0\perp} \equiv \epsilon_{0,zz}, \epsilon_{0,yy}$. Therefore, for the background polarization tensor $\hat{\alpha}_0$, we have:

$$\alpha_{0\parallel} = (\epsilon_{0\parallel} - 1)/4\pi, \quad \alpha_{0\perp} = (\epsilon_{0\perp} - 1)/4\pi,$$

$\alpha_{0,yy} = (\epsilon_{0,yy} - 1)/4\pi$. In the bounded crystal the system of equations (3.2)–(3.5) is supplemented by conventional Maxwell boundary conditions, which for the geometry shown in fig. 2 have the form

$$E_x(+0) = E_x(-0), \quad (3.6)$$

³ The detailed analysis of the difference between the optical properties of dielectric crystals obtained in exp-model by continual and discrete approaches is done in ref [10] for $\nu_m = 0$. The results show that for the most of the crystal optics problems the continual approach for (2.17) is good justified. This is especially correct when $\nu_m \neq 0$.

⁴ For the arbitrary polarization $f_i \neq g_i$ (see (2.12), (2.13)) and even the known one- exponential model must be exposed to some additional mathematical treatment.

$$B_y(+0) = B_y(-0), \quad (3.7)$$

where the definitions $z = \mp 0$ correspond to near-to-the-surface area in the vacuum and in the medium, respectively. The amplitudes $E_x(+0)$ and $B_y(+0)$ are the boundary values of the total electric and magnetic fields (the sum of amplitudes of all waves in the crystal). The main purpose of the different methods used for the solution of the system of equations (3.1)–(3.7) is to formulate the appropriate «extinction theorem» for the space dispersive media (it is done traditionally in terms of either the polarization operator, or the Hertz vector or the causal Green function [2], see also the special wave-vector-space method developed recently in refs. [21, 22]). However here we shall use an advantage of the main result obtained from their studies in the framework of one- exp model [11, 18] – the final results of these complicated enough methods lead to the same results as the straightforward methods of the pioneer works on this theme (see refs. [1, 2]).

A. Unbounded medium

We solve the system of equations (3.1)–(3.5) first for unbounded medium (i.e. medium extending from «-» to «+» infinity) and then we impose boundary conditions in such a way that tends to zero the fictitious polarization outside the crystal. For spatial homogeneous in xy -plane configuration and monochromatic wave, in the frequency range $\omega \equiv \omega_0$, the equation (3.1) takes the form

$$\begin{aligned} & (\omega_0 - \omega - i\nu) P_x(z) - \\ & - \sum_{i=1}^N G_i \frac{\omega_0}{c} \int_a^{\infty} \exp\left(-\Gamma_i \frac{\omega_0}{c} |z - z'|\right) \times \\ & \times P_x(z') dz' = F E_x(z), \end{aligned} \quad (3.8)$$

where we omitted the common exponential factor,

$\exp(i \frac{\omega}{c} n_x x - i\omega t)$. Note that, in accordance with Snell law, $n_x = n_{0,x}$, where $n_{0,x} = \sin\theta$ and θ is the light incident and reflection angle (see fig. 2).

For the infinite crystal (i.e. for $a = -\infty$) we can seek the common solution of eqs.(3.2)–(3.5) and (3.8) in the form

proportional to $\exp(in_{zj} \frac{\omega}{c} z)$ for each possible wave j , the

total number of which is J . The explicit expressions for n_{zj} are determined finally in self-consistent way from the appropriate Fresnel's dispersion equation, see below (3.18)–(3.19). In the traditional BF theory, $J = 1$ for fixed light polarization. However, as it was first shown in ref. [1], the ALW can really exist in the exciton absorption region. Their total number, $J - 1$, depends on the type, degeneracy and symmetry of the exciton state. For the case of (3.8) we obtain:

$$P_x = \alpha_{xx}^{ex} E_x, \quad (3.9)$$

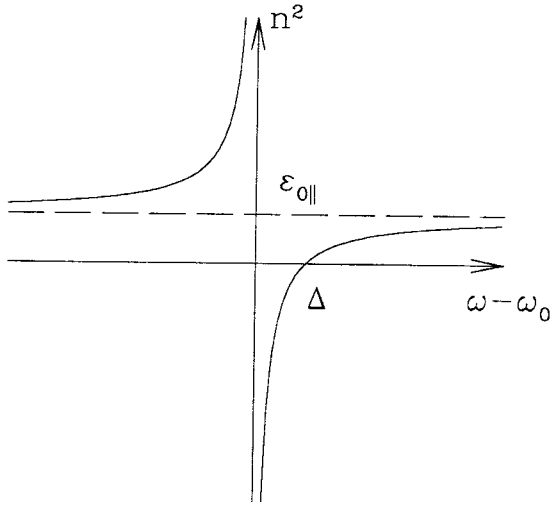


Fig. 3. The birefringence case. Dependence of the light waves refractive index, n , on the frequency difference, $\omega - \omega_0$, in the region of the insulating excitonic photo-transition with energy $\hbar\omega_0$ and zero damping. $\epsilon_{0||}$ is background dielectric permeability; Δ is the frequency of the «transverse-longitudinal» splitting. No additional waves exist.

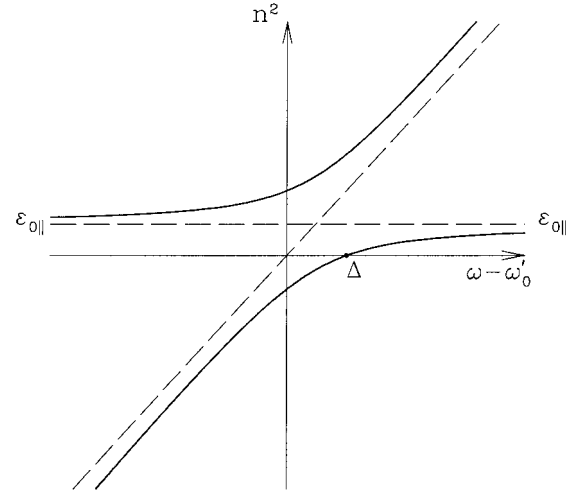


Fig. 4. The NN-excitonic model. The waves with two different n exist for each ω , i.e. the case with one additional wave in comparison with fig.3. All the definitions are the same as in fig.3. The parameters ω'_0 [see (3.24)] and m_{ex} [see (3.21)] correspond to those of refs. [10, 27]

where α_{xx}^{ex} is the excitonic part of the crystal polarizability

$$\alpha_{xx}^{ex} = F(\omega_{ex} - \omega - i\nu)^{-1}, \quad (3.10)$$

and

$$\mathcal{E}^{ex} \equiv \hbar\omega_{ex} = \hbar\omega_0 - 2\hbar \sum_{i=1}^N \frac{(\frac{\omega_0}{c})^2 G_i \Gamma_i}{(\Gamma_i \frac{\omega_0}{c})^2 + \kappa_z^2}, \quad (3.11)$$

may be interpreted as the appropriate excitonic energy with quasi-momentum $\hbar\kappa_z = \hbar \frac{\omega_0}{c} n_z$.

The tensor (3.10), together with the appropriate background polarizability tensor determines the full dielectric permittivity $\hat{\epsilon}$

$$\hat{\epsilon} = \hat{\epsilon}_0 + 4\pi\hat{\alpha}^{ex}, \quad (3.12)$$

where

$$\hat{\epsilon}_{||} \equiv \epsilon_{xx} = \epsilon_{0||} + 4\pi\alpha_{xx}^{ex}, \quad (3.13)$$

$$\epsilon_{\perp} \equiv \epsilon_{zz} = \epsilon_{0\perp}, \quad (3.14)$$

$$\epsilon_{yy} = \epsilon_{0y}. \quad (3.15)$$

At the same time, if the self consistent solution of the system (3.1)–(3.5) has the form $\exp(i\frac{\omega}{c}n_0x + i\frac{\omega}{c}n_zz - i\omega t)$, then the appropriate amplitudes of the electro-magnetic fields

are determined by the system of the homogeneous equations

$$\hat{\epsilon} \cdot \mathbf{E} = (n^2 \hat{I} - \mathbf{nn}) \cdot \mathbf{E}, \quad (3.16)$$

$$E_y = 0. \quad (3.17)$$

The nontrivial solutions of the homogeneous system (3.16)–(3.17) exist only if its determinant is equal to zero

$$|n^2 \hat{I} - \mathbf{nn} - \hat{\epsilon}| = 0, \quad (3.18)$$

In our geometry the expression (3.18) gives the following equation for possible values of n_z

$$\frac{n_z^2}{(1 - \sin^2 \theta / \epsilon_{\perp 0})} = \epsilon_{0||} + 4\pi\alpha_{xx}^{ex}, \quad (3.19)$$

From (3.10)–(3.11) it follows that for N -exp model the eq.(3.19) is of the $N+1$ order in respect to n_z^2 . So, we have $J=N+1$ different waves near the exciton resonance region (propagated in the positive direction, along the z -axis of fig. 2) and N from them are Pekar's additional light waves.

We present here for comparison four types of $n^2(\omega)$ curves for the following different cases: 1) $N=0$, which corresponds to the BF theory, see fig. 3; 2) $N=1$ with $\Gamma \gg 1$, which means the transition from EM to NN model, i.e. effective mass (e.m.) approximation, with one ALW (see fig. 4) and with

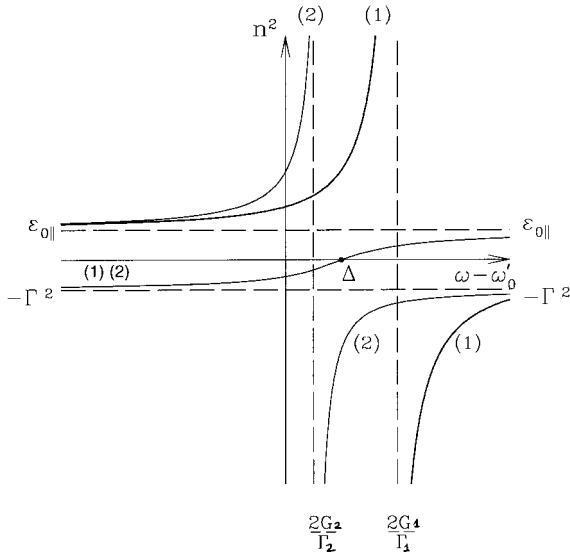


Fig. 5. The (1,1)-exp model with one additional wave as in the case of fig. 4. The curves 1 and 2 correspond to $2G_1/\Gamma_1 > \Delta$ and $2G_2/\Gamma_2 < \Delta$ cases, respectively. The model parameters G and Γ determine the intensity and the space decrement of the exp-like oscillators interaction. All the rest definitions are the same as in figs. 3 and 4 ω'_0 is determined by (3.24).

$$\mathcal{E}^{ex} = \mathcal{E}_0 + \frac{\hbar^2 k_z^2}{2m_{ex}}, \quad (3.20)$$

in (3.10) instead of (3.11), where

$$m_{ex} \cong \frac{\hbar \Gamma_1^3}{4G_1} \left(\frac{\omega_0}{c} \right)^2, \quad (3.21)$$

is the excitonic e.m.; 3) $G_1 \neq 0, \Gamma_1 \cong 1$, which is the ordinary one-exp excitonic model with one ALW, as in the previous case, see fig. 5. 4) $G_1 \neq 0, G_2 \neq 0$, which corresponds to the two-exponential ($N=2$) excitonic model with two ALWs [see fig. 6, their RVs are determined from the cubic equation (3.19)]. For simplicity, we assume here that $\nu = 0, m_{ex} > 0$, (i.e. $G_i > 0$) and consider the normal light incidence ($n_{0x} = 0$). We also take the main parameters in accordance with experimental results of the ref. [27] and the additional one (connected with EM) of the same order as in ref. [10], where the calculations like fig. 5 (for $2G/\Gamma > \Delta$) are presented. Note, that in our case the proliferation of the refractive indices in the transition from 1-EM (see fig. 5) to 2-EM (see fig. 6) is physically well-grounded and must be clear distinguished from the case of the fictive proliferation, when one passes from EM to its NN -approximation. The critical discussion of the last situation is presented in refs. [2,11]. It predicts the following transition from (1, N)-exp model to the mixed, in general case, model. For the determination of the number of the real light waves, we must

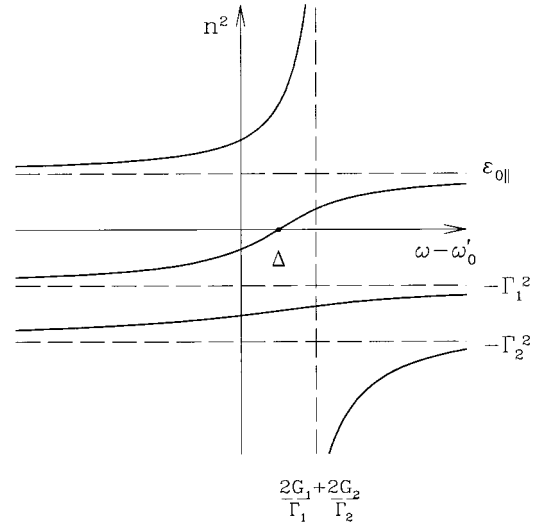


Fig. 6. The (1,2)-exp model with the double ($N=2$), in comparison with the case of fig.5, number of the parameters Γ_i and $G_i, i=1, 2$. In each frequency region two additional waves exist. ω'_0 is determined by (3.24).

single out in (3.8), (3.11) R canals of the exciton transport, for which $\Gamma_i \gg 1$. Similar to (3.20)–(3.21) we can merge them in the one canal with some effective array of the parameters such as the e.m.

$$m_{ex} = \hbar \left(\frac{\omega_0}{c} \right)^2 \left(\sum_{i=N+1-R}^N \frac{4G_i}{\Gamma_i^3} \right)^{-1}, \quad (3.22)$$

The formula (3.11) reduces then to the form

$$\mathcal{E}^{ex} = \mathcal{E}_0 + \frac{\hbar^2 k_z^2}{2m_{ex}} + \sum_{i=1}^{N-R} \frac{2G_i \hbar}{\Gamma_i} \frac{k_z^2}{\left(\Gamma_i \frac{\omega_0}{c} \right)^2 + k_z^2}, \quad (3.23)$$

where E'_0 corresponds to the bottom of the excitonic band

$$\mathcal{E}_0 \equiv \hbar \omega'_0 = \hbar \omega_0 - 2\hbar \sum_{i=1}^N \frac{G_i}{\Gamma_i}. \quad (3.24)$$

In accordance with [2, 11], for all canals of R type we should restrict ourselves only by the first non-vanishing term in the expansion of the corresponding terms in (3.11) over $(n_z/\Gamma)^2$ in order to avoid the non-physical proliferation of the refractive indices. According to (3.19), the whole totality of the R canals gives only one real ALW, the other $N - R$ canals will give $N - R$ additional solution of the dispersion equation.

B. Bounded medium

We return now to eq. (3.8) and study its solution in the case of the semi-infinite medium (i.e. for $a = 0$). Eq. (3.8) is a non-homogeneous Fredholm equation with a sum of an Hermitian and quasi-degenerate Kernels. Such an equation may be solved exactly without any additional conditions. In this sense the model proposed by us essentially extend the class of the exactly soluble excitonic models, which were described in the Introduction. The necessity of some additional conditions or ABCs and their forms depend on the specific methods chosen for solving of the discussed light propagation problems.

One of those methods is based on a transformation of the integral equation (3.8) into differential equation of order $2N$. Therefore, in order to determine the coefficients of the general solution of this equation, one should impose additional conditions, which may be as follows: eq. (3.8) has to be satisfied identically for any arbitrary value of z -coordinate, or the same should be correct for the appropriate of its z derivatives. Since even in the simple one-exponential model this approach is clumsy [17], we use here another method for solving (3.8). Namely, we substitute the truncated equation (3.8) by a non-truncated one (i.e. with $a = -\infty$) and set to zero separately (since it must be true for arbitrary value of z) all appropriate complements. This leads to the following ABCs

$$\int_{-\infty}^0 \exp\left(\Gamma_i \frac{\omega_0}{c} z\right) P_x(z) = 0, \quad \text{for } i = 1, 2, \dots, N. \quad (3.25)$$

Note that the system (3.25) represents only a new form of ABC in addition to mostly used conditions presented in refs. [2–4]. It is easy to check that (3.25) is correct for the arbitrary coordinate dependences of the electric field in r.h.s. of (3.8). For the plane waves, the conditions (3.25) transforms to the form:

$$\sum_{j=1}^J \frac{P_{x,j}(0)}{\Gamma_i + i n_{z,j}} = 0, \quad \text{for } i = 1, 2, 3 \dots N \quad (3.26)$$

where the summation is made over all transmitted waves, J , which are determined during the process of solving of dispersion equation (3.19). For our case this equation is of $N + 1$ degree in respect to n_z^2 . I.e., there are $N + 1$ different solutions, n_z , and, therefore, $N + 1$ boundary conditions: one MBC (3.6)–(3.7) and N of ABCs of the (3.26) form. This confirms that the above chosen method for solving of the system of equations (3.1)–(3.5) for the case of semi-infinite crystal may be fulfilled in self-consistence way.

For the case $\Gamma \gg |n_{z,j}|$, (which corresponds to NN (or e.m.) approximation) the ABC (3.25), (3.26) can be transformed to the wide used in ALW theory form

$$P_{ex,x}(0) = \sum_j P_{x,j}(0) = 0, \quad (3.27)$$

which means the tendency to zero at the boundary of the partial exciton contribution, P_{ex} , into the total crystal

polarizability. In ALW theory the ABC (3.27) is often called «the Pekar's boundary condition».

Let us determine now the light reflection index, $r = |r_{am}|^2$, and the complex amplitude reflection coefficient, r_{am} . For the above chosen polarization configuration (see fig. 1) after some evaluations, which follow the standard methods [2], we obtain

$$r_{am} = \frac{E_R}{E_0} = \frac{\bar{n}_0 - n_{p,z}}{\bar{n}_0 + n_{p,z}}, \quad (3.28)$$

where $\bar{n}_0 \equiv \bar{\epsilon}_0 / \epsilon_{0\parallel} \cos \theta$ and $\bar{\epsilon}_0 \equiv \epsilon_{0\parallel} (1 - \sin^2 \theta / \epsilon_{0\perp})$. The effective index of refraction, $n_{p,z}$, is determined by

$$n_{p,z} = \frac{n' + i\mu \bar{\epsilon}_0 n''}{n'' + i\mu n'}. \quad (3.29)$$

For $N = 1$, with n_{1z} , and n_{2z} corresponding to refracting indexes of two dispersive branches shown in fig. 5, we have

$$n' = n_{1z} n_{2z} + \bar{\epsilon}_0, \quad (3.30)$$

$$n'' = n_{1z} + n_{2z}, \quad (3.31)$$

$$m = \frac{1}{\Gamma}. \quad (3.32)$$

For $\Gamma \gg 1$ (i.e. $\mu \sim 0$), equation (3.29) determines the effective index of refraction for the considered geometry in NN-model, together with n_{1z}, n_{2z} , which are determined from fig. 4.

For $N = 2$ we have

$$n' = \prod_i n_{iz} + \bar{\epsilon}_0 \sum_{i=1}^3 n_{iz}, \quad (3.33)$$

$$n'' = \sum_{i>j} n_{iz} n_{jz} + \bar{\epsilon}_0, \quad (3.34)$$

$$\mu = \frac{\Gamma_2 + \Gamma_1}{\Gamma_1 \Gamma_2 - \bar{\epsilon}_0}, \quad (3.35)$$

where n_{iz} are the z components of the RVs, corresponding to three dispersion branches shown in fig. 6.

The different experimental and theoretical works dealing with ALW problems (Kramers-Kronig relations, «amplitude-phase» analysis, etc) use usually the results of refs. [9, 11]. In accordance with the latter papers, the coefficient r can be represented as a product of the appropriate partial coefficients, r_p , of all accounted waves. However, as it follows from (3.29)–(3.35), this is possible if only we does not take into account the background permittivity (i.e. for $\epsilon_{0\parallel} = \epsilon_{0\perp} = 1$). It is clear that in the most cases the later approxi-

mation essentially restricts the application of such formulae for the interpretation of the experimental data. In addition to this we note, that besides questions, connected with the possibilities of the direct and indirect experimental observations of ALW phenomena (see [2–4]), the including of each exponential-like mechanism into the oscillator-to-oscillator interaction gives two additional parameters (G_p, Γ_p), that in fact increase the approximation ability of the analytical formulae.

IV. The energy balance equation

There are many papers which analyze the energy transfer near the exciton resonance. This is explained in two courses. First, due to strong frequency and spatial dispersion, corresponding to the area of polariton spectra, the energy flux in crystal is no longer given by the ordinary Poynting vector. Second, as it was shown in [3, 28] due to the essential role of the radiation absorption in spectral region of excitonic transitions, there are no universal expressions for the energy density and the energy flux, based on the general form of dielectric permittivity for spatial dispersive media [see below the notes to (4.10)]. Only some concrete excitonic model should be used for this purpose. As we mentioned before, the EMs may be very useful in this sense, because they do not only describe the different types of real excitons but include also the different limits and approximations made for their models, such as non-spatial dispersive media [see (1.2)], low absorbed medium [with $\nu \rightarrow 0$ in (1.1), (2.17)], the NN -model (1.3), etc. However, until now, as well as it is known to authors, the studies of the corresponding questions were not performed even for the case of one-exp model. Therefore, using the introduced and developed above N -exp model (including the standard case $N=1$), we shall obtain some expressions for exciton energy and exciton energy flux density.

For obtaining the corresponding Poynting equation we multiply equation (3.2) by \mathbf{B} , and (3.3) by \mathbf{E} and deriving then one from another

$$\frac{1}{8\pi} \frac{\partial}{\partial t} (\mathbf{B} \cdot \mathbf{B} + \mathbf{E} \cdot \hat{\epsilon}_0 \cdot \mathbf{E}) + \frac{c}{4\pi} \nabla \cdot [\mathbf{E} \times \mathbf{B}] + \mathbf{E} \cdot \frac{\partial \mathbf{P}}{\partial t} = 0. \quad (4.1)$$

Let us introduce a new quantity, $\tau_{a,p}$ for each possible excitonic transport mechanism

$$\tau_{a,i} = \int_a^\infty \exp\left(-\Gamma_i \frac{\omega_0}{c} |z - z'|\right) P_x(z', \mathbf{r}_\parallel, t) dz', \quad (4.2)$$

(compare it with the «reduced polarization» of ref. [2]). For simplicity we omit for a moment the number i and will restore it after the eq.(4.8). For (4.2) one can find (by direct differentiation) the following relation

$$\frac{\partial^2 \tau_a}{\partial z^2} = \left(\frac{\omega_0}{c}\right)^2 \Gamma^2 \tau_a - 2 \frac{\omega_0}{c} \Gamma P_x. \quad (4.3)$$

Using the latter, we can write

$$P_x \frac{\partial \tau_a}{\partial t} = \left[\frac{\Gamma \omega_0}{2c} \tau_a - \frac{c}{2\Gamma \omega_0} \frac{\partial^2 \tau_a}{\partial z^2} \right] \frac{\partial \tau_a}{\partial t} = \frac{\partial}{\partial t} \left[\frac{\omega_0 \Gamma}{2c} \tau_a^2 + \frac{c}{2\Gamma \omega_0} \left(\frac{\partial \tau_a}{\partial z} \right)^2 \right] - \frac{c}{2\Gamma \omega_0} \frac{\partial}{\partial z} \left(\frac{\partial \tau_a}{\partial t} \frac{\partial \tau_a}{\partial z} \right). \quad (4.4)$$

For $a=0$ from eq.(4.2) it automatically follows that

$$\frac{\partial \tau_0}{\partial z} \Big|_{z=0} = \Gamma \frac{\omega_0}{c} \tau_0 \Big|_{z=0}. \quad (4.5)$$

The expression similar to (4.5) could be written also for $a=-\infty$, but only for ABC in the form (3.25)

$$\frac{\partial \tau_{-\infty}}{\partial z} \Big|_{z=0} = \Gamma \frac{\omega_0}{c} \tau_{-\infty} \Big|_{z=0}. \quad (4.6)$$

For the plane waves we have

$$\tau_{-\infty} = \sum_j \frac{2\Gamma c}{\omega_0 (\Gamma^2 + n_{zj}^2)} P_{xj}, \quad (4.7)$$

$$\frac{\partial \tau_{-\infty}}{\partial z} = \sum_j i \frac{2\Gamma n_{zj}}{\Gamma^2 + n_{zj}^2} P_{xj}, \quad (4.8)$$

Using equations (3.1) and (4.4), it is possible to write (4.1) in form of an energy balance equation

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{S} + Q = 0, \quad (4.9)$$

where W , \mathbf{S} and Q can be interpreted as the energy density, the vector of the energy flux density and the energy dissipation rate, respectively. For the chosen in sec. III polarization they can be written as:

$$W = \frac{B^2 + \mathbf{E} \cdot \hat{\epsilon}_0 \cdot \mathbf{E}}{8\pi} + \frac{(\partial P_x / \partial t)^2}{4\omega_0 F} + W_1, \quad (4.10)$$

$$\mathbf{S} = \frac{c}{4\pi} \mathbf{E} \times \mathbf{B} + \mathbf{S}_1, \quad (4.11)$$

$$Q = \frac{\nu}{\omega_0 F} \left(\frac{\partial P_x}{\partial t} \right)^2. \quad (4.12)$$

The terms W_1 and $\mathbf{S}_1(0, 0, S_{1z})$ are directly connected with above discussed spatial dispersion:

$$W_1 = \sum_{i=1}^N \frac{G_i \omega_0}{cF} \left[\frac{c}{4\Gamma_i \omega_0} \left(\frac{\partial \tau_{a,i}}{\partial z} \right)^2 + \frac{\Gamma_i \omega_0}{4c} \tau_{a,i}^2 - P_x \tau_{a,i} \right], \quad (4.13)$$

$$S_{1z} = - \sum_{i=1}^N \frac{G_i}{2F \Gamma_i} \frac{\partial \tau_{a,i}}{\partial t} \frac{\partial \tau_{a,i}}{\partial z}. \quad (4.14)$$

Here some comments should be made: All representations like the expression (4.9) are indefinite since it is always possible to add to both \mathbf{S} and W some mutually compensative additional parts, which represent the derivative on the time and the divergence of the arbitrary vector-function, respectively. However, for the monochromatic waves, the interesting values of the averaged over the time density flux of the energy are unique. The next comment is on the nonlocal character of different quantities in the Poynting's equation (4.9). The following two approaches to this and similar problems are known:

1. One of them combines the introduction of above mentioned quantities with the appropriate choice of the region for the averaging of the energy of particles and fields. In particular, if the long-range interactions between particles are significant then, in order to determine the energy flux density, one has to take the elementary volumes of linear size larger than the typical wavelength of polariton under consideration [2].

2. In another approach, like in ref. [29], the problem is solved by introduction of the additional local parameters, the macroscopic field \mathbf{E} in particular. In such a way the local basis of the macroscopic approach is restored. Of course, eventually the macroscopic field \mathbf{E} is partly determined by the conditions in other space regions, but this difficulty is overcome by using the Maxwell's equations which are local in their nature. In our problem, besides \mathbf{E} and in full analogy with it, the additional quantities $\tau_{ai}(z)$ are introduced [see (4.2)].

Above, we have discussed the energy fluxes without any details about the field behavior at the crystal boundary. However, such details are very important to connect the total energy fluxes inside and out the crystal. Let $S_z(\omega, -0)$ and $S_z(\omega, +0)$ be the z -components of the energy flux densities (averaged over time) near the plane boundary in vacuum and medium, respectively. To connect these quantities first we must use the conventional MBC (3.6), (3.7). Then (4.11) gives us

$$\overline{S_z(\omega, +0)} = \overline{S_z(\omega, -0)} - \sum_{i=1}^N \frac{G_i}{2F \Gamma_i} \overline{\left(\frac{\partial \tau_{ai}}{\partial z} \frac{\partial \tau_{ai}}{\partial t} \right)_{z=0}}. \quad (4.15)$$

Using the relation (4.5) it is easy to show, that the last term in (4.15) is equal to zero

$$\left[\overline{\left(\frac{\partial \tau_0}{\partial z} \frac{\partial \tau_0}{\partial t} \right)_{z=0}} \right] = \frac{\omega_0}{2c} \Gamma \overline{\left(\frac{\partial \tau_0^2}{\partial t} \right)_{z=0}} = 0.$$

Therefore, for $a = 0$ the continuity of the averaged energy flux across the medium automatically follows for EM (i.e. without any additional boundary conditions). Naturally, for $a = -\infty$, the continuity condition of \mathbf{S} on the boundary could be proved only by using the proper ABC. In EM, the latter

leads to the relation (4.6), which in the same manner as before gives the tendency to zero on the boundary of the last term in (4.15). In conclusion, we shall show that the all known before expressions for the flux density and energy density for the excitonic resonance region could be obtained as the partial (limited) case of the expressions (4.10)–(4.14).

For the case when the special dispersion is ignored, the balance equation was considered in [30]. For this case the appropriate expressions for different terms in (4.9) can be obtained directly from (4.10)–(4.14) by setting the interaction constant to zero (i.e. in $G = 0$ approximation).

For the case of the NN-model, the balance equation was in the details, studied in refs. [31, 32]. The appropriate transition to this polariton model has been made already in sec.III by substituting of the eqs. (3.11), (3.25) by the (3.20), (3.27) ones. Note in addition, that for $\Gamma \gg 1$ the quantity $\tau - \infty$ and its derivative take the forms:

$$\begin{aligned} \tau_{-\infty} &= \int_{-\infty}^z \exp\left[-\Gamma \frac{\omega_0}{c} (z - z')\right] P(z', \mathbf{r}_{\parallel}, t) dz' + \\ &+ \int_z^{\infty} \exp\left[\Gamma \frac{\omega_0}{c} (z - z')\right] P(z', \mathbf{r}_{\parallel}, t) dz' \equiv \\ &\equiv \frac{2c}{\Gamma \omega_0} P(\mathbf{r}, t) + \frac{2c^3}{\Gamma^3 \omega_0^3} \frac{\partial^2 P}{\partial z^2}, \end{aligned} \quad (4.16)$$

$$\frac{\partial \tau_{-\infty}}{\partial z} \equiv \frac{2c}{\Gamma \omega_0} \frac{\partial P}{\partial z}. \quad (4.17)$$

From (4.16) and (4.17) it follows that eq. (3.1) could be transformed for $N = 1$ into differential equation of second degree, in respect to z , which is just the starting material equation of refs. [31, 32]. In this case the values W_1 (see (4.13) and S_{1z} (see (4.14) take the form:

$$W_1 = \frac{\hbar}{4Fm_{ex}} \left(\frac{\partial P}{\partial z} \right)^2, \quad (4.18)$$

$$S_{1z} = - \frac{\hbar}{2Fm_{ex}} \frac{\partial P}{\partial t} \frac{\partial P}{\partial z}. \quad (4.19)$$

The flux continuity on the surface is determined now by boundary condition (3.27), or in a more general form by:

$$\left(P + \gamma \frac{\partial P}{\partial z} \right)_{z=0} = 0, \quad (4.20)$$

where the parameter γ should be real (see Appendix B).

For the case of zero damping (i.e. for $\nu = 0$ in (3.1) and single-wave approximation, the expression (4.14) for S_{1z} may be compared also with the similar expressions, obtained in ref. [3]. The latter is expressed through the dielectric permittivity of the medium. For the field and polarization geometry, chosen in sec.III, it has the form

$$\overline{S_{1z}} = -\frac{c}{4} \frac{\partial a_{xx}}{\partial n_z} \overline{E_x^2}. \quad (4.21)$$

Substituting (3.9)–(3.11) into (4.21), as well as (4.7)–(4.8) into (4.14), we find that (4.21) and (4.14) are completely identical and have the form

$$\overline{S_{1z}} = -\frac{4G\Gamma c}{F} \frac{n_z}{(\Gamma^2 + n_z^2)^2} \overline{P_x^2}. \quad (4.22)$$

Note that in the absence of absorption we have $\nabla \cdot \overline{\mathbf{S}} = 0$, what follows directly from (4.9). I.e. the interference flux, which may appear, in principle, due to existence of the many waves (in our case one the main wave and one additional) is absent. Only in this particular case the normal to surface part of the total energy flux (4.14) reduces to the sum of fluxes (4.22) for each wave. However, as it may be seen from the detail analysis of (4.14), for the nonzero damping, the sum of the different normal modes gives rise to the interference energy fluxes. Moreover, the interference energy fluxes along the surface exist even in non-absorbing media. Therefore, in all those cases, the expression (4.21) (or their sum over j) is inadequate and one must return to expressions (4.13), (4.14) or (4.18), (4.19).

V. Summary

Many aspects of the optical properties of the spatial dispersive media may be solved by the consideration of the system of oscillating dipoles, placed at the sites of the crystal lattice. There are only few models for which the problem of the system interaction with the electro-magnetic field could be solved *exactly*. In the present paper we essentially extend this class of the models by simultaneously taking into account the number of excitonic states and canals of the excitonic transport. The physical reason and justification of such model is demonstrated in the paper on the base of Frenkel exciton model. Nevertheless, this does not restrict the generality since the modern definition of the excitonic-like states (see sec.I) includes not only the genuine electron excitons of different models, but the varieties of other waves and their corresponding quasi-particles, such as optical phonons, vibrons, spin waves, plasmons, polaritons, etc. The studies of this type of states in the bounded crystalline media are closely attached to the definite group of the lattice-wave sums. The different methods are used for the calculation of the latter, and among them- the s.c. «plane-wise» method, by help of which the dipole-to-dipole interaction may be reduced to the exponential like coupling between the oscillators, placed in the parallel crystal planes (see Appendix A).

The advantage of the method is determined by the fact that in this case the idealized models, composed of a finite or semi-infinite crystal slab (with flat surface) and plane light waves, close to all corresponds to the real reflection and transmission experiments (see sec.III).

The similar to discussed in the present paper lattice sum often occur in some other problems of solid state physics,

such, for example, as the problem of the dipole ferromagnetism, in respect to problems of the stability of the semiconductors and antiferromagnetic lattices, etc. The exponential like models via Forster type inter-well coupling [33] find also some continuous increase in the modern studies of the different dielectric and semiconductor artificial made structures [34]. The same situation arises in the case of an array of parallel infinite planar slabs and other layered systems and systems with reduced dimensionality. So, we hope, that the generalized (M, N)-exponential model will be useful for solving of the above mentioned problems too.

We used the (1, N)-exp model in order to calculate the light reflection coefficients for the semi-infinite spatially dispersive absorbing dielectric in the vicinity of the isolated dipole-allowed excitonic transition. The frequency dependence of the RVs for $N = 0, 1, 2$ and the appropriate forms of the ABC are analyzed in details. A general expression for Poynting-Pekar vector of energy flux density is derived for this region and its connection with the boundary conditions is shown. The applications of the (M, N)-exp model to other crystal optics problems will be presented elsewhere.

The further generalization of the model in the framework of the exact soluble ones, is also straightforward: the left part of eq. (2.17) may be supplied by oscillator-to-oscillator interaction of (1.3) type, which makes it a mix of the exponential and near-neighbors models [19] [in sec. III, we pointed some other possibilities of the transition from the exponential model to the mixed one in the case of excitonic transport mechanisms with large γ_i in (2.17)]. Similarly to the discussed above we can treat the r.h.s. of (2.17), if the higher multipoles should be taken into account and, especially, for the dipole-forbidden excitonic transitions, when (2.17) should be substituted by the higher multiple moments [25], etc.

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Appendix A: evaluation of the lattice sums by the plane-wise method

In the fact, the well-known Ewald's method [29], the different variations of which are determined by the configuration-symmetrical considerations rather than by the properties of the concrete exciton-like states, lies on the basis of all known evaluations of the dipole-wave lattice sums. For the situation described in the paper-the slab or semi-infinite media-the base of the appropriate calculations was inherent in refs. [35–39] and received the name *the method of plane-wis summation* (see also [9, 12, 40, 45–48]).

As it follows from (2.11), it is possible to express all components of the tensor $\hat{T}(l', l)$ through the $\Xi(l', l; \mathbf{q}_{\parallel})$

function, and its first and second derivatives on the components of \mathbf{q}_{\parallel} vector:

$$T_{xx} = \left[2 \frac{\partial^2}{\partial q_x^2} - \frac{\partial^2}{\partial q_y^2} + \xi^2 (l-l')^2 \right] \Xi(l, l'; \mathbf{q}_{\parallel}), \quad (\text{A1})$$

$$T_{yy} = T_{xx}(q_x \leftrightarrow q_y), \quad (\text{A2})$$

$$T_{xy} = T_{yx} = 3 \frac{\partial^2 \Xi(l, l'; \mathbf{q}_{\parallel})}{\partial q_x \partial q_y}, \quad (\text{A3})$$

$$T_{xz} = T_{zx} = -3i\xi(l-l') \frac{\partial \Xi(l, l'; \mathbf{q}_{\parallel})}{\partial q_x}, \quad (\text{A4})$$

$$T_{yz} = T_{zx}(q_x \leftrightarrow q_y), \quad (\text{A5})$$

$$T_{zz} = -(T_{xx} + T_{yy}), \quad (\text{A6})$$

$$\text{where } \Xi(l', l; \mathbf{q}_{\parallel}) \equiv \sum_{\mathbf{l}_{\parallel}} \frac{\exp(i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel})}{[\mathbf{l}_{\parallel}^2 + \xi^2 (l-l')^2]^{3/2}}. \quad (\text{A7})$$

According to (2.11) the summation in (A7) is carried out at condition $\mathbf{l} \equiv \{l_x, l_y, l-l'\} \neq 0$. The latter sum could be evaluated differently in the two different cases $l' \neq l$ (a) and $l' = l$ (b).

a. The case $l' \neq l$. Using in (A7) the typical for Ewald's methods transformation

$$r^{-5} = \frac{1}{\Gamma(5/2)} \int_0^{\infty} dt t^{3/2} e^{-r^2 t}. \quad (\text{A8})$$

[where $\Gamma(5/2)$ is Gamma-function] one obtains

$$\Xi(l', l; \mathbf{l}_{\parallel}) = \frac{1}{\Gamma(5/2)} \int_0^{\infty} dt t^{3/2} \sum_{\mathbf{l}_{\parallel}} e^{-l'^2 t + i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel} - \xi^2 (l-l')^2 t}. \quad (\text{A9})$$

Using the generalized two-dimensional θ -transformation

$$\sum_{\mathbf{l}_{\parallel}} \exp(-l'^2 t + i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel}) = \frac{\pi}{t} \sum_{\mathbf{Q}_{\parallel}} \exp\left[-|\mathbf{Q}_{\parallel} + \mathbf{q}_{\parallel}|^2 / 4t\right], \quad (\text{A10})$$

and substituting it into (A9), we obtain the following expression

$$\Xi(l', l; \mathbf{l}_{\parallel}) = \frac{\pi}{\Gamma(5/2)} \sum_{\mathbf{Q}_{\parallel}} \int_0^{\infty} dt t^{1/2} e^{-|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}|^2 / 4t - \xi^2 (l-l')^2 t}. \quad (\text{A11})$$

Here $\mathbf{Q}_{\parallel} = \{2\pi Q_x, 2\pi Q_y\}$, where Q_x and Q_y are the integers taking the values from $-\infty$ up to $+\infty$. So, that $\mathbf{Q}_{\parallel}/a_{\parallel}$ can be interpreted as the vector of the appropriate plane reciprocal lattice. Taking into account the formula [41]

$$\int_0^{\infty} x^{\alpha-1} e^{-px-s/x} dx = 2(s/p)^{\alpha/2} K_{\alpha}(2\sqrt{ps}), \quad \text{Re } p, s > 0, \quad (\text{A12})$$

the expression (A11) converts to the following form

$$\begin{aligned} \Xi(l', l; \mathbf{l}_{\parallel}) &= \\ &= \frac{2\pi}{\Gamma(5/2)} \sum_{\mathbf{Q}_{\parallel}} \left(\frac{|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}|}{2\xi|l-l'|} \right)^{3/2} K_{3/2}\left(\xi|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}||l-l'|\right). \end{aligned} \quad (\text{A13})$$

Substituting the explicit form of the McDonald's function, K_a , for $a = 3/2$ (see [42])

$$K_{3/2}(z) = \left(\frac{\pi}{2z} \right)^{1/2} e^{-z} (1+z^{-1}), \quad (\text{A14})$$

and the correspondent Gamma function,

$\Gamma(5/2) = 3\sqrt{\pi}/4$, into eq. (A13), we obtain the following expression

$$\begin{aligned} \Xi(l, l', \mathbf{q}_{\parallel}) &= \\ &= \frac{2\pi}{3\xi^2|l-l'|^2} \sum_{\mathbf{Q}_{\parallel}} \left(|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}| + \frac{1}{\xi|l-l'|} \right) e^{-\xi|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}||l-l'|}. \end{aligned} \quad (\text{A15})$$

By substituting (A15) into (A1)-(A6) we are able to calculate all the components of the tensor $T(l \neq l')$ see eqs.(2.12)-(2.13).

b. The case $l' = l$. For the evaluation of the sums of the form

$$\Xi(l' = l; \mathbf{q}_{\parallel}) = \sum_{\mathbf{l}_{\parallel} \neq 0} \frac{\exp(i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel})}{l_{\parallel}^5}. \quad (\text{A16})$$

we introduce the Ewald's parameter τ , which splits the range of the integration in (A8) into two parts – from 0 up to $\tau\pi$ and from $\tau\pi$ up to ∞ . In spite that the initial sum (A16) is independent, of course, of the choice of the Ewald's parameter, the idea being to choose it in a way that gives equally rapid convergence of the sums over the direct and reciprocal lattices, connected by (A10) equality:

$$\begin{aligned} \Xi(l' = l; \mathbf{q}_{\parallel}) &= \frac{1}{\Gamma(5/2)} \int_0^{\infty} dt t^{3/2} \left(\sum_{\mathbf{l}_{\parallel}} e^{-l'^2 t + i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel}} - 1 \right) = \\ &= \frac{\pi}{\Gamma(5/2)} \int_0^{\tau\pi} dt t^{1/2} \left(\sum_{\mathbf{Q}_{\parallel}} e^{-|\mathbf{q}_{\parallel} + \mathbf{Q}_{\parallel}|^2 / 4t} - \frac{t}{\pi} \right) + \\ &+ \frac{1}{\Gamma(5/2)} \int_{\tau\pi}^{\infty} dt t^{3/2} \sum_{\mathbf{l}_{\parallel} \neq 0} e^{-l'^2 t + i\mathbf{q}_{\parallel} \cdot \mathbf{l}_{\parallel}} = \end{aligned}$$

$$= \frac{4\pi^2}{3} \tau^{3/2} \sum_{\mathbf{Q}_\parallel} \varphi_{-5/2} \left(\left| \mathbf{q}_\parallel + \mathbf{Q}_\parallel \right|^2 / 4\tau\pi \right) - \frac{8}{15} \tau^{5/2} \pi^2 + \frac{4\pi^2}{3} \tau^{5/2} \sum_{l_1 \neq 0} \varphi_{3/2} (\pi l_1^2) e^{i q_1 l_1}, \quad (\text{A17})$$

where

$$\varphi_\alpha(x) = \int_1^\infty t^\alpha e^{-tx} dt, \quad (\text{A18})$$

is the Misra's function of the order α , see their definition in ref. [49]. These functions satisfy the following recurrent formulae

$$\varphi_\alpha(x) = \varphi_0(x) + \frac{\alpha}{x} \varphi_{\alpha-1}(x), \quad (\text{A19})$$

$$\frac{\partial \varphi_\alpha(x)}{\partial x} = -\varphi_{\alpha+1}(x). \quad (\text{A20})$$

By substituting (A17) into (A1)–(A6) and using the equations (A19), (A20) and the equation of (A10) type it is possible to obtain all the components of the \hat{T} ($l' = l$) tensor presented in (2.11):

$$\begin{aligned} T_{xx} = & 2\pi \left[\frac{1}{3} - e^{-q_\parallel^2/4\pi} + \frac{q_x^2}{2\pi} \varphi_{-1/2}(q_\parallel^2/4\pi) \right] - \\ & - \pi \sum_{l_1 \neq 0} \varphi_{1/2}(\pi l_1^2) e^{i q_1 l_1} - \\ & - \pi \sum_{\mathbf{Q}_\parallel \neq 0} \varphi_{-3/2} \left(\left| \mathbf{q}_\parallel + \mathbf{Q}_\parallel \right|^2 / 4\pi \right) + \\ & + 2\pi^2 \sum_{l_1 \neq 0} (l_\parallel^2 - 2l_x^2) \varphi_{3/2}(\pi l_1^2) e^{i q_1 l_1} - \\ & - \frac{1}{2} \sum_{\mathbf{Q}_\parallel \neq 0} \left(\left| \mathbf{q}_\parallel + \mathbf{Q}_\parallel \right|^2 - 2(\mathbf{q}_\parallel + \mathbf{Q}_\parallel)_x^2 \right) \times \\ & \times \varphi_{-1/2} \left(\left| \mathbf{q}_\parallel + \mathbf{Q}_\parallel \right|^2 / 4\pi \right), \quad (\text{A21}) \end{aligned}$$

$$T_{yy} = T_{xx}(l_x \leftrightarrow l_y; (\mathbf{q}_\parallel + \mathbf{Q}_\parallel)_x \leftrightarrow (\mathbf{q}_\parallel + \mathbf{Q}_\parallel)_y), \quad (\text{A22})$$

$$T_{xz} = T_{yz} = 0, \quad (\text{A23})$$

$$T_{zz} = -(T_{zz} + T_{yy}), \quad (\text{A24})$$

$$T_{xy} = T_{yx} = q_x q_y \varphi_{-1/2}(q_\parallel^2/4\pi) -$$

$$- 4\pi^2 \sum_{l_1 \neq 0} l_x l_y \varphi_{3/2}(\pi l_1^2) e^{i q_1 l_1} +$$

$$+ \sum_{\mathbf{Q}_\parallel \neq 0} (\mathbf{q}_\parallel + \mathbf{Q}_\parallel)_x (\mathbf{q}_\parallel + \mathbf{Q}_\parallel)_y \varphi_{-1/2} \left(\left| \mathbf{q}_\parallel + \mathbf{Q}_\parallel \right|^2 / 4\pi \right). \quad (\text{A25})$$

By deriving (A21)–(A25) we choose the parameter $\tau = 1$, that gives the equal convergence ability for all considered lattice sums. Note that the first three terms in (A21) (plased into the square brackets) form in the limits $q_\parallel \rightarrow 0$ the main part of the Lorentz field and the part of the macroscopical field of the polarized medium

Appendix B

The ABC (4.20) or its limit case ($\gamma \rightarrow \infty$)

$$\partial P / \partial z |_{z=0} = 0 \quad (\text{B1})$$

are used in some of papers on ALW physics instead of Pekar's condition (3.27). However, the usefulness of such generalization is small and, even some times, dubious. It is because the term with gradient in BC (4.20) is proportional to small parameter $\mathbf{k} \cdot \mathbf{a}$, while the macroscopic crystal boundary itself is determined by the less precision. The parameter γ , presented in (4.20), sometimes serves as additional fitting parameter, but it is not connected with the more-or-less determined parameter, characterized the excitonic state. In the best case the introduction of such magnitudes does not make the fitting of the theory with the experiment more convinient. In the worst case, the attempt to use such term as a fitting parameter between experimental and theoretical data needs to use a complex value of γ , which is in contradiction with the energy conservation law [43].

Note, that the transition from ABC (3.27) to (4.20) is usually connected with the different surface distortions in the crystal, i.e. considering the case of the $r_i \neq 0$ terms in (2.17) For one-exp model the corresponding term is taken into account in ref. [17] by formal changing of the oscillator to oscillator interaction operator in eq. (3.1) by the following expression

$$\begin{aligned} - 2G \frac{\omega_0^2}{c} \int_0^\infty \left\{ \exp \left[-\Gamma \frac{\omega_0}{c} |z - z'| \right] + \right. \\ \left. + R \exp \left[-\Gamma \frac{\omega_0}{c} (z + z') \right] \right\} P(z') dz'. \quad (\text{B2}) \end{aligned}$$

In ref. [15], the appearance of the term with $R \neq 0$ [namely, $R \sim (\epsilon_0 - 1)$] is connected with the real reflection forces, which appeared by putting the system of oscillators into a medium with background dielectric permittivity ϵ_0 . Repeating the evaluations of sec. III, with (B2) in (3.1), we come to the same eqs. (3.9)–(3.11), but instead of (3.25) we have such form of ABC

$$\int_{-\infty}^0 \exp(\Gamma \frac{\omega}{c} z) P_x(z) dz - R \int_0^\infty \exp(-\Gamma \frac{\omega_0}{c} z) P_x(z) dz = 0. \quad (\text{B3})$$

The latter could be easily generalized for (N, M)-exponential model by introducing the parameters Γ_i , and R_i , for each possible canals of exciton propagation.

In the case of the ordinary NN -model (i.e. when $\Gamma \gg 1$) it is possible to obtain the condition of the form (4.20) by expanding $P_x(z)$ in (B3) into the series near the point $z = 0$, namely

$$\left[(1-R)P_x - \frac{(1+R)}{\Gamma(\omega_0/c)} \frac{\partial P_x}{\partial z} \right]_{z=0} = 0. \quad (\text{B4})$$

From (B4) it follows that for all possible R the term with the derivative in (B4) brings the negligible small contribution (of the order $\mathbf{k} \cdot \mathbf{a}$) excepting extremely narrow range of the values of R , namely $R = 1 + O(\mathbf{k} \cdot \mathbf{a})$ [let's $\gamma \rightarrow \infty$ in (4.20)]. The result is in full agreement with ref. [44], where the sufficient general excitonic model was studied. In ref. [44] this special but *extremely narrow* region of the values of R was accepted as the set of the zero mire by proving of the general theorem about the impossibility of the boundary condition (B2). Therefore, practically for each R , the Pekar's condition (3.27) is fulfilled. Taking into account the terms with $R \neq 0$ have no practical influence excepting the essential cases of the near-the-surface distortions, which lead to appearance of the «dead layer» or surface states [5, 7, 8].

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(M, N)-ЕКСПОНЕНЦІАЛЬНА МОДЕЛЬ В ТЕОРІЇ ЕКСИТОНІВ

В. М. Пісковий

Інститут фізики напівпровідників НАН України

Я. М. Стрельнікер

Тель-Авівський Університет, Факультет точних наук ім. Раймонда і Беверлі Саклера, Відділення фізики і астрономії, Ізраїль

Резюме. Побудовано узагальнену експоненціальну модель, що враховує можливість одночасного існування декількох паралельних каналів розповсюдження світлової енергії екситонами. Детальне фізичне обґрунтування моделі здійснено на базі екситонів Френкеля. Нова модель зберігає всі переваги широко вживаної одно-експоненціальної моделі екситону, як однієї з небагатьох задач в теорії розповсюдження електро-магнітних хвиль в обмежених просторово-диспергуючих середовищах, що мають точний розв'язок. В той же час вона суттєво розширює можливості досліджень нелокальних оптичних явищ в кристалах. В роботі запропонована модель використовується, зокрема, для одержання додаткових краєвих умов та рівняння балансу для потоку та густоти поляритонної енергії, а також для вирішення ряду інших проблем кристалооптики з просторовою дисперсією в спектральній області екситонних резонансів.

(M, N)-ЭКСПОНЕНЦИАЛЬНАЯ МОДЕЛЬ В ТЕОРИИ ЭКСИТОНОВ

В. Н. Писковой

Институт физики полупроводников НАН Украины

Я. М. Стрельникер

Тель-Авивский Университет, Факультет точных наук им. Раймонда и Беверли Саклера, Отделение физики и астрономии, Израиль

Резюме. Построена обобщенная экспоненциальная модель, учитывающая возможность одновременного существования нескольких параллельных каналов переноса световой энергии экситонами. Детальное физическое обоснование модели проведено на базе экситонов Френкеля. Новая модель сохраняет все преимущества одно-экспоненциальной модели экситона, как одной из немногих точно решаемых задач в теории распространения электромагнитных волн в ограниченных пространственно диспергирующих средах. Вместе с тем она существенно расширяет возможности исследования нелокальных оптических явлений в кристаллах. В работе предложенная модель используется, в частности, для вывода добавочных граничных условий и уравнения баланса для плотности и потока поляритонной энергии, а также для решения ряда других проблем кристаллооптики с пространственной дисперсией.