Exciton-phonon coupling functions in uniaxial crystals

Nicolas Grigorchuk*
Bogolyubov Institute for Theoretical Physics, 14b Metrologichna str., Kiev 252143, Ukraine
(Received 28 June 1996)

Explicit expressions are found for the coupling functions of Wannier excitons interacting with both the longitudinal and transverse lattice vibrations in uniaxial crystals. The anisotropy in the effective mass of an electron and a hole, static and high frequency dielectric constants, deformation-potential constants, and the sound velocity in the crystal are all taken into consideration. [S0163-1829(97)05301-0]

I. INTRODUCTION

Recently, there has been considerable interest in anisotropic and layered structures where exciton motion essentially differs from that in isotropic and bulk systems.[1,2] These structures are expected to have improved optical and transport properties with a large potential for future device applications. A number of effects, as it seems, are directly connected with anisotropy. It was shown, for instance, in Ref. 3 that crystal anisotropy of 6H-SiC is the reason for the new line in the reflectivity spectrum. Giant energy splitting of the $2P$ exciton states of up to 7 meV due to anisotropy of the crystal was observed in Ref. 4. Many other interesting effects had been investigated in earlier publications (see, e.g., Refs. 5–9).

In many studies of exciton-phonon interaction in crystals the coupling function is used in a simplest form applicable only for qualitative estimates. To study the structure of light absorption bands and its dependence on temperature, to calculate the exciton lifetime, free path, etc., it is necessary to know the explicit form of the coupling function.[10] Some details of this problem were reviewed in Refs. 11 and 12.

A general expression for the exciton-phonon coupling functions of the isotropic ionic crystal was derived by Ansel'm and Firsov[13,14] and also by Toyozawa.[15] This problem for anisotropic crystals was considered most thoroughly by Fock, Kramer, and Bütner[16] for excitons interacting with optical phonons. An isotropic effective potential with averaged material parameters has been found.

In the present paper we will obtain the explicit expressions for the coupling functions of Wannier excitons with both the longitudinal and transverse optical and acoustic phonons, taking into consideration the anisotropy in the effective mass, dielectric and deformation potential constants, and the sound velocity in the crystal. We limit ourselves to the case of cylindrical symmetry.

The paper is organized as follows. Section II develops the formalism for determining the coupling function of exciton with the optical vibrations in uniaxial crystal. In Section III the coupling functions of exciton with the acoustic vibrations are derived using the deformation potential approach. Section IV contains our summary.

II. EXCITON COUPLING WITH OPTICAL PHONONS

Exciton interaction with optical vibrations of the anisotropic polar lattice will be considered as an independent interaction of an electron and a hole with longitudinal optical (LO) and transverse optical (TO) phonons. This interaction is realized by means of an electric field of the polarization wave. The energy operator of such interaction may be presented as[17]

$$\hat{H}(\mathbf{r}_e,\mathbf{r}_h) = -e\hat{\varphi}(\boldsymbol{\rho}_e,z_e) + e\hat{\varphi}(\boldsymbol{\rho}_h,z_h), \tag{1}$$

where $\{\boldsymbol{\rho}_i,z_i\}\equiv\mathbf{r}_i$ are the cylindrical coordinates of the electron ($i=e$) or of the hole ($i=h$) with the cylinder axis along z, and $\hat{\varphi}$ is electrostatistical potential operator of the polarization field which can be expanded in Bloch series as follows

$$\hat{\varphi}(\boldsymbol{\rho}_i,z_i) = \frac{1}{\sqrt{V}}\sum_{\mathbf{q}_\parallel\mathbf{q}_\perp} (\hat{\varphi}_{\mathbf{q}_\parallel\mathbf{q}_\perp} e^{i(\mathbf{q}_\perp\boldsymbol{\rho}_i + q_\parallel z_i)} + \hat{\varphi}^+_{\mathbf{q}_\parallel\mathbf{q}_\perp} e^{-i(\mathbf{q}_\perp\boldsymbol{\rho}_i + q_\parallel z_i)}), \tag{2}$$

where V is the volume of the crystal. The summations in (2) have to be performed over all possible values of both longitudinal and transverse components of the vibration wave vector $\mathbf{q}$. The operators $\hat{\varphi}^+_{\mathbf{q}_\parallel\mathbf{q}_\perp}$, $\hat{\varphi}_{\mathbf{q}_\parallel\mathbf{q}_\perp}$ may be expressed in terms of Bose operators of creation $\hat{b}^+$ and annihilation $\hat{b}$ of the vibration quanta. Proportional to the amplitude of the vibrations there arises a polarization field that for nonmagnetic medium without electrical currents is given by

$$\mathbf{P}(\boldsymbol{\rho}_i,z_i) = \frac{1}{\sqrt{V}}\sum_{\mathbf{q}_\parallel\mathbf{q}_\perp} (F_\parallel\boldsymbol{\epsilon}^\parallel_{\mathbf{q}_\parallel} + F_\perp\boldsymbol{\epsilon}^\perp_{\mathbf{q}_\perp})(\hat{b}_{\mathbf{q}_\parallel\mathbf{q}_\perp} e^{i(\mathbf{q}_\perp\boldsymbol{\rho}_i + q_\parallel z_i)} + \hat{b}^+_{\mathbf{q}_\parallel\mathbf{q}_\perp} e^{-i(\mathbf{q}_\perp\boldsymbol{\rho}_i + q_\parallel z_i)}), \tag{3}$$

where $\boldsymbol{\epsilon}^\parallel$, $\boldsymbol{\epsilon}^\perp$ are unit polarization vectors of phonons, and $F_\parallel, F_\perp$ represent certain parameters to be defined. To do that we start from the relationship

$$\mathbf{P}(\boldsymbol{\rho}_i,z_i) = \frac{1}{4\pi}\mathrm{grad}\varphi(\boldsymbol{\rho}_i,z_i). \tag{4}$$

Substituting Eqs. (2), (3) in Eq. (4) yields

$$\hat{\varphi}_{\mathbf{q}_\parallel\mathbf{q}_\perp} = -4\pi i\frac{F_{\parallel\perp}}{\sqrt{q_\perp^2+q_\parallel^2}}\hat{b}_{\mathbf{q}_\parallel\mathbf{q}_\perp}. \tag{5}$$

Further, we will make use of the expression for the energy of Coulomb interaction of two charges in anisotropic crystalline media. In order to account for the uniaxial symmetry of the

media under consideration, we introduce anisotropic dielectric constants $\varepsilon_j^{\parallel}$, $\varepsilon_j^{\perp}$ $(j=0,\infty)$, whose components are parallel and perpendicular to the main axis of the crystal (or to the z axis). Then in accordance with Fresnel equations we have for a uniaxial crystal the solutions

$$\varepsilon_j=\varepsilon_j^{\perp}, \tag{6}$$

that corresponds to the ordinary ray, and

$$\frac{1}{\varepsilon_j}=\frac{\sin^2\theta}{\varepsilon_j^{\parallel}}+\frac{\cos^2\theta}{\varepsilon_j^{\perp}}, \tag{7}$$

for the extraordinary ray, where $\sin\theta=q_{\perp}/|\mathbf{q}|$, $\cos\theta=q_{\parallel}/|\mathbf{q}|$, $|\mathbf{q}|=\sqrt{q_{\parallel}^2+q_{\perp}^2}$. Equation (7) may be rewritten otherwise as

$$\frac{1}{\varepsilon_j}=\frac{1}{|\mathbf{q}|^2}\left(\frac{q_{\perp}^2}{\varepsilon_j^{\parallel}}+\frac{q_{\parallel}^2}{\varepsilon_j^{\perp}}\right). \tag{8}$$

This allows us to specify the mean value of ε_j as

$$\overline{\varepsilon_j}=\frac{\varepsilon_j^{\parallel}\varepsilon_j^{\perp}}{\varepsilon_j}=\frac{1}{|\mathbf{q}|^2}(\varepsilon_j^{\perp}q_{\perp}^2+\varepsilon_j^{\parallel}q_{\parallel}^2). \tag{9}$$

Such form of ε_j is convenient in applications and has been used by Fock, Kramer, and Bütner[16] for the effective potential of exciton-phonon interaction. We will take ε_j in the form of Eq. (8).

In the case when the lattice vibrations vector $\boldsymbol{\epsilon}$ is directed transversely to the wave propagation vector $\mathbf{q}$ one can represent Eq. (8) as follows:[18]

$$\frac{1}{\varepsilon_j}=\frac{q_{\perp}q_{\parallel}}{|\mathbf{q}|^2}\left(\frac{1}{\varepsilon_j^{\perp}}-\frac{1}{\varepsilon_j^{\parallel}}\right). \tag{10}$$

As the static dielectric constants $(\varepsilon_0^{\parallel},\varepsilon_0^{\perp})$ are due to both the electronic and ionic polarizations, while the dynamic (high-frequency) dielectric constants $(\varepsilon_{\infty}^{\parallel},\varepsilon_{\infty}^{\perp})$ are caused by the electronic polarization only, one may suppose that the difference in the energy of Coulomb interaction of two charges in dielectric media with ε_0 and ε_{∞}

$$-\frac{e^2}{\varepsilon_0|\delta\mathbf{r}|}+\frac{e^2}{\varepsilon_{\infty}|\delta\mathbf{r}|}=E, \tag{11}$$

where

$$|\delta\mathbf{r}|=\sqrt{|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|^2+|z_e-z_h|^2}, \tag{12}$$

will coincide with the energy of polar displacement of ions E_{ion},[19] which is represented above by the operator $\hat{H}(\mathbf{r}_e,\mathbf{r}_h)$ of Eq. (1). Owing to the small displacement of ions one may estimate this energy by means of the perturbation theory

$$E_{\text{ion}}=E^{(1)}+E^{(2)}+\cdots. \tag{13}$$

Obviously, the first-order correction to the energy $E^{(1)}$ that goes from the average of the operator (1) over the wave functions of phonon vacuum, is equal to zero. The second order one is determined by

$$E^{(2)}=\sum_{\mathbf{q}_{\parallel}\mathbf{q}_{\perp}}\frac{\langle 0|\hat{H}(\boldsymbol{\rho}_e z_e,\boldsymbol{\rho}_h z_h)|\mathbf{q}_{\parallel}\mathbf{q}_{\perp}\rangle\langle\mathbf{q}_{\parallel}\mathbf{q}_{\perp}|\hat{H}^{+}(\boldsymbol{\rho}_e z_e,\boldsymbol{\rho}_h z_h)|0\rangle}{\omega(\mathbf{q}_{\parallel},\mathbf{q}_{\perp})-0}, \tag{14}$$

where $|0\rangle$ corresponds to the wave function of the phonon vacuum, $|\mathbf{q}_{\parallel},\mathbf{q}_{\perp}\rangle$ refers to the wave function of the state of one virtually excited phonon with components of wave vector $(\mathbf{q}_{\parallel},\mathbf{q}_{\perp})$ and with the energy $\omega(\mathbf{q}_{\parallel},\mathbf{q}_{\perp})$. Substituting Eq. (5) into Eq. (2), Eq. (2) into Eq. (1) and supposing the nondispersiveness of the optical modes (Holstein model)

$$\omega(\mathbf{q}_{\parallel},\mathbf{q}_{\perp})\equiv\Omega_{\parallel,\perp}, \tag{15}$$

one obtains

$$E_{\parallel,\perp}^{(2)}=-\frac{(4\pi eF_{\parallel,\perp})^2}{V\Omega_{\parallel,\perp}}\sum_{\mathbf{q}_{\parallel}\mathbf{q}_{\perp}}\frac{1}{q_{\parallel}^2+q_{\perp}^2}(2-e^{i\mathbf{q}_{\perp}(\boldsymbol{\rho}_e-\boldsymbol{\rho}_h)+iq_{\parallel}(z_e-z_h)}-e^{i\mathbf{q}_{\perp}(\boldsymbol{\rho}_h-\boldsymbol{\rho}_e)+iq_{\parallel}(z_h-z_e)}). \tag{16}$$

Here $E^{(2)}$ tends to zero, when $z_e\Rightarrow z_h$ and $\boldsymbol{\rho}_e\Rightarrow\boldsymbol{\rho}_h$ simultaneously.

In a more general case, when $z_e\neq z_h$ and $\boldsymbol{\rho}_e\neq\boldsymbol{\rho}_h$, changing the coordinates of the electron and hole in Eq. (16), and making use of

$$\int_0^{\infty}q_{\perp}dq_{\perp}\int_{-\infty}^{\infty}dq_{\parallel}\int_0^{2\pi}d\varphi\frac{e^{iq_{\perp}|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|\cos\varphi+iq_{\parallel}|z_e-z_h|}}{q_{\parallel}^2+q_{\perp}^2}=\frac{2\pi^2}{\sqrt{|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|^2+|z_e-z_h|^2}}, \tag{17}$$

one can find $E_{\parallel,\perp}^{(2)}$ to be

$$E_{\parallel,\perp}^{(2)}=\frac{8\pi e^2F_{\parallel,\perp}^2}{\Omega_{\parallel,\perp}\sqrt{|\boldsymbol{\rho}_e-\boldsymbol{\rho}_h|^2+|z_e-z_h|^2}}. \tag{18}$$

Taking into account Eq. (8) in Eq. (11), as well as Eq. (18) on the right-hand side of Eq. (11), one arrives at the final form for $F=\sqrt{F_{\parallel}^2+F_{\perp}^2}$:

$$F=\frac{1}{|\mathbf{q}|}\sqrt{\frac{1}{8\pi}\left[\Omega_{\parallel}q_{\perp}^2\left(\frac{1}{\varepsilon_{\infty}^{\parallel}}-\frac{1}{\varepsilon_0^{\parallel}}\right)+\Omega_{\perp}q_{\parallel}^2\left(\frac{1}{\varepsilon_{\infty}^{\perp}}-\frac{1}{\varepsilon_0^{\perp}}\right)\right]}\equiv F_{q_{\parallel}q_{\perp}}^{L}. \tag{19}$$

This form of F is valid for the longitudinal lattice vibration. Substituting Eq. (10) in Eq. (11) in an analogous manner it is easy to show that for transverse vibrations mode one gets

$$F=\frac{1}{|\mathbf{q}|}\sqrt{\frac{q_{\perp}q_{\parallel}}{8\pi}\left[\Omega_{\perp}\left(\frac{1}{\varepsilon_{\infty}^{\perp}}-\frac{1}{\varepsilon_0^{\perp}}\right)-\Omega_{\parallel}\left(\frac{1}{\varepsilon_{\infty}^{\parallel}}-\frac{1}{\varepsilon_0^{\parallel}}\right)\right]}\equiv F_{q_{\parallel}q_{\perp}}^{T}. \tag{20}$$

Now, when all the parameters of Eq. (1) are defined, let us crossover in Eq. (1) to the second quantization picture with respect to exciton variables. To do this, it is convenient to

introduce, at first, the center-of-mass and relative coordinates for the system with cylindrical symmetry:

$$\mathbf{R}_{\parallel,\perp}=\frac{m_e^{\parallel,\perp}\mathbf{r}_e^{\parallel,\perp}+m_h^{\parallel,\perp}\mathbf{r}_h^{\parallel,\perp}}{m_e^{\parallel,\perp}+m_h^{\parallel,\perp}},\quad \mathbf{r}_i^{\perp}=\boldsymbol{\rho}_i,\quad r_i^{\parallel}=z_i,\quad (i=e,h)$$

$$\boldsymbol{\rho}_\perp=\boldsymbol{\rho}_e-\boldsymbol{\rho}_h,\quad \rho_\parallel=z_e-z_h. \tag{21}$$

Then the electron and hole coordinates may be expressed as

$$\mathbf{r}_{\binom{e}{h}}^{\parallel,\perp}=\mathbf{R}_{\parallel,\perp}\pm\frac{m_{\binom{h}{e}}}{M^{\parallel,\perp}}\boldsymbol{\rho}_{\parallel,\perp}, \tag{22}$$

$$M=m_e+m_h,$$

where m_e refers to the electron and m_h the hole mass. Here and below the upper (lower) symbol in parentheses on the left-hand side of the equation corresponds with the upper (lower) sign on the right-hand side of the equation. Substituting Eqs. (20), (18), (5), (4) into Eq. (1) we come to the Hamiltonian

$$\begin{aligned}\hat{H}(\mathbf{R},\boldsymbol{\rho})=&\frac{4\pi ie}{\sqrt{V}}\sum_{\mathbf{q}_\parallel\mathbf{q}_\perp}\frac{F_{q_\parallel q_\perp}^{L,T}}{\sqrt{q_\parallel^2+q_\perp^2}}(\hat{b}_{q_\parallel q_\perp}\\&+\hat{b}^{+}_{-q_\parallel-q_\perp})e^{i(\mathbf{q}_\perp\mathbf{R}_\perp+\mathbf{q}_\parallel\mathbf{R}_\parallel)}\\&\times[e^{i\mathbf{q}_\perp\boldsymbol{\rho}_\perp(m_h^\perp/M^\perp)+i\mathbf{q}_\parallel\boldsymbol{\rho}_\parallel(m_h^\parallel/M^\parallel)}\\&-e^{-i\mathbf{q}_\perp\boldsymbol{\rho}_\perp(m_e^\perp/M^\perp)-i\mathbf{q}_\parallel\boldsymbol{\rho}_\parallel(m_e^\parallel/M^\parallel)}].\end{aligned} \tag{23}$$

The wave function of the Wannier exciton corresponding to the hydrogenlike model for the uniaxial crystal with the analogy to the one used in Refs. 13, 20 we choose the form

$$|\mathbf{k}_\perp,\mathbf{k}_\parallel\rangle=\frac{1}{\sqrt{\pi a_{\rm ex}^2 b_{\rm ex}}}e^{-\sqrt{\rho_\perp^2/a_{\rm ex}^2+\rho_\parallel^2/b_{\rm ex}^2}}\frac{1}{\sqrt{V}}e^{i(\mathbf{k}_\perp\mathbf{R}_\perp+\mathbf{k}_\parallel\mathbf{R}_\parallel)}. \tag{24}$$

Here $a_{\rm ex}$ and $\mathbf{k}_\perp$ are the exciton Bohr radius and the exciton quasimomentum in the plane (x,y), respectively, $b_{\rm ex}$ and $\mathbf{k}_\parallel$ refer to the same parameters in the z direction.

Thus, the operator of exciton-phonon interaction in the second quantization representation accounting for linear operators only will be read as

$$\hat{V}_{\text{ex-ph}}=\sum_{\substack{\mathbf{k}_\parallel\mathbf{k}_\perp\\ \mathbf{k}'_\parallel\mathbf{k}'_\perp}}\langle\mathbf{k}_\parallel\mathbf{k}_\perp|\hat{H}(\mathbf{R},\boldsymbol{\rho})|\mathbf{k}'_\parallel\mathbf{k}'_\perp\rangle\hat{a}^{+}_{\mathbf{k}_\parallel\mathbf{k}_\perp}\hat{a}_{\mathbf{k}'_\parallel\mathbf{k}'_\perp}, \tag{25}$$

where $a^{+}_{\mathbf{k}_\perp\mathbf{k}_\parallel}(a_{\mathbf{k}_\perp\mathbf{k}_\parallel})$ are creation (annihilation) operators of exciton with quasimomentum components $\mathbf{k}_\perp,\mathbf{k}_\parallel$. Using Eqs. (23), (24) in Eq. (25) and carrying out the integration in cylindrical coordinate system over all the possible values of parameters $\rho_\parallel$, $\rho_\perp$, $R_\parallel$, $R_\perp$, as over angles between vectors $(\mathbf{q}_\perp\wedge\boldsymbol{\rho}_\perp)$ and $(\mathbf{R}_\perp\wedge\mathbf{q}_\perp+\mathbf{k}_\perp+\mathbf{k}'_\perp)$ (Ref. 21), we obtain

$$\begin{aligned}\hat{V}_{\text{ex-ph}}=&-i\frac{(2\pi)^3}{V}\sum_{\substack{\mathbf{q}_\parallel\mathbf{q}_\perp\\ \mathbf{k}_\parallel\mathbf{k}_\perp}}\Phi^{L,T}(\mathbf{q}_\parallel,\mathbf{q}_\perp)\hat{a}^{+}_{\mathbf{k}_\perp\mathbf{k}_\parallel}\hat{a}_{\mathbf{k}_\perp+\mathbf{q}_\perp,\mathbf{k}_\parallel+\mathbf{q}_\parallel}\\&\times(\hat{b}_{\mathbf{q}_\parallel\mathbf{q}_\perp}+\hat{b}^{+}_{-\mathbf{q}_\parallel,-\mathbf{q}_\perp}),\end{aligned} \tag{26}$$

with

$$\Phi_{op}^{L}(q_\parallel,q_\perp)=\sqrt{\frac{2\pi e^2}{V}}\frac{\sqrt{\Omega_\perp q_\parallel^2\left(\frac{1}{\varepsilon_\infty^\perp}-\frac{1}{\varepsilon_0^\perp}\right)+\Omega_\parallel q_\perp^2\left(\frac{1}{\varepsilon_\infty^\parallel}-\frac{1}{\varepsilon_0^\parallel}\right)}}{q_\parallel^2+q_\perp^2}\left\{\frac{1}{Z_e^2(q_\perp,q_\parallel)}-\frac{1}{Z_h^2(q_\perp,q_\parallel)}\right\} \tag{27}$$

for exciton coupling with longitudinal optical phonons, and

$$\Phi_{op}^{T}(q_\parallel,q_\perp)=\sqrt{\frac{2\pi e^2}{V}}\sqrt{\Omega_\perp\left(\frac{1}{\varepsilon_\infty^\perp}-\frac{1}{\varepsilon_0^\perp}\right)-\Omega_\parallel\left(\frac{1}{\varepsilon_\infty^\parallel}-\frac{1}{\varepsilon_0^\parallel}\right)}\frac{\sqrt{q_\perp q_\parallel}}{q_\parallel^2+q_\perp^2}\left\{\frac{1}{Z_e^2(q_\perp,q_\parallel)}-\frac{1}{Z_h^2(q_\perp,q_\parallel)}\right\} \tag{28}$$

for exciton coupling with transverse optical phonons, where

$$Z_{\binom{e}{h}}(q_\perp,q_\parallel)=1+\left(\frac{a_{\rm ex}}{2}q_\perp\frac{m_{\binom{e}{h}}^\perp}{M^\perp}\right)^2+\left(\frac{b_{\rm ex}}{2}q_\parallel\frac{m_{\binom{e}{h}}^\parallel}{M^\parallel}\right)^2. \tag{29}$$

The exciton-phonon interaction operator (26) describes the elastic and inelastic scattering of excitons with the emission or absorption of phonons in uniaxial crystals. As in isotropic crystals[10] the number of excitons remains unchanged while the number of phonons changes. The functions $\Phi^L(q_\parallel,q_\perp)$ and $\Phi^T(q_\parallel,q_\perp)$ represent the exciton LO- and exciton TO-phonon coupling functions for anisotropic ionic crystals in explicit form. This function tends to zero with $\mathbf{q}_\parallel,\mathbf{q}_\perp\to 0$, and has a maximum at small values of $\mathbf{q}_\parallel,\mathbf{q}_\perp$. It does not depend on the quasimomenta of excitons as well as on the exciton band width. In the absence of the anisotropy of crystal ($m_i^\parallel=m_i^\perp$, $\varepsilon_j^\parallel=\varepsilon_j^\perp$, $a_{\rm ex}=b_{\rm ex}$, and $\Omega_\parallel=\Omega_\perp$) the coupling function (27) coincides with the one found in Refs. 13 and 15 for isotropic crystals. The energy coupling of exciton with the transverse optical phonons, as it is seen from Eq. (28), tends to zero for isotropic crystal.

III. EXCITON COUPLING WITH ACOUSTIC PHONONS

A general expression for the exciton-phonon coupling function of an isotropic nonpolar crystal was derived by

Ansel'm and Firsov[14] as well as by Toyozawa.[15] Below we will obtain the explicit expression for the coupling function of Wannier excitons with acoustic phonons taking into consideration the anisotropy in the effective mass, deformation potential constants, and sound velocity in crystal. We limit ourselves to the case of cylindrical symmetry.

Exciton interaction with vibrations of the anisotropic nonpolar lattice will be treated as an independent interaction of an electron and a hole with longitudinal and transverse acoustic phonons. We shall apply the deformation-potential method[22] to write the energy of interaction of excitons with acoustic vibrations. The fundamental idea of the deformation-potential approach introduced by Shockley and Bardeen[23] consists in calculating the electron scattering by lattice waves by taking as the interaction potential, $V(\mathbf{r})$, the shift in energy band $E_1(\mathbf{r})$ resulting from dilation. The justification for this assumption can be easily generalized for anisotropic nonpolar crystals to include scattering of an exciton by transverse as well as longitudinal acoustical modes. When the dilation of the band-edge points is expressed with help of the field of displacement $\mathbf{U}(\mathbf{r})$, the Hamiltonian of exciton-phonon interaction then becomes

$$\hat{H}(\mathbf{r}_e,\mathbf{r}_h) = -Sp C_e^{\nu\mu}\epsilon_{\nu\mu}(\boldsymbol{\rho}_j,z_j) + Sp C_h^{\nu\mu}\epsilon_{\nu\mu}(\boldsymbol{\rho}_j,z_j), \tag{30}$$

where $C_j^{\nu\mu}$ is the tensor of the deformation potential for an electron ($j=e$) or of the hole ($j=h$), $\epsilon_{\nu\mu}$ refers to the tensor function of the mechanical strain, $\{\boldsymbol{\rho}_j,z_j\}=\mathbf{r}_j$ are the cylindrical coordinates of the charge j with cylinder axis along z. Above, repeated indexes are to be summed on. The symbol Sp means that summation is carried out over diagonal elements of matrices product. For the case of cylindrical symmetry these matrices are written as

$$\mathbf{C_j}=\begin{pmatrix} C_j^{\perp} & 0 \\ 0 & C_j^{\parallel} \end{pmatrix}, \quad \boldsymbol{\epsilon}=\begin{pmatrix} \epsilon_{\perp} & 0 \\ 0 & \epsilon_{\parallel} \end{pmatrix}. \tag{31}$$

Instead of deformation potential components $C^{\perp}$, $C^{\perp}$ often has been used as the components $\Xi_d=C^{\perp}$ and $\Xi_u=C^{\parallel}-C^{\perp}$.

The strain tensor components for the case of low deformation are given by

$$\epsilon_{\perp}(\boldsymbol{\rho}_j,z_j)=\frac{\partial \mathbf{U}_{\perp}(\boldsymbol{\rho}_j,z_j)}{\partial \boldsymbol{\rho}}, \quad \epsilon_{\parallel}(\boldsymbol{\rho}_i,z_i)=\frac{\partial \mathbf{U}_{\parallel}(\boldsymbol{\rho}_j,z_j)}{\partial z}, \tag{32}$$

where $\mathbf{U}_{\perp}$, $\mathbf{U}_{\parallel}$ are the $\perp$ and $\parallel$ components of the vector field of displacement, which in quantum representation may be expanded as follows

$$\mathbf{U}(\boldsymbol{\rho}_j,z_j) = \sqrt{\frac{\hbar}{2\rho V}}\sum_{\mathbf{q}_{\perp}\mathbf{q}_{\parallel}} \frac{1}{(q_{\perp}^2+q_{\parallel}^2)^{1/4}} e^{i(\mathbf{q}_{\perp}\boldsymbol{\rho}_j+q_{\parallel}z_j)} \times\left(\frac{\mathbf{e}_{\mathbf{q}_{\perp}}}{\sqrt{S_{\perp}}}+\frac{\mathbf{e}_{\mathbf{q}_{\parallel}}}{\sqrt{S_{\parallel}}}\right)(\hat{b}_{\mathbf{q}_{\parallel}\mathbf{q}_{\perp}}+\hat{b}^{+}_{-\mathbf{q}_{\parallel},-\mathbf{q}_{\perp}}), \tag{33}$$

where $\mathbf{e}_{\mathbf{q}_{\perp}}$ and $\mathbf{e}_{\mathbf{q}_{\parallel}}$ are the unit vectors of displacement in $\perp$ and $\parallel$ to the crystal axis directions, $S_{\perp}$ and $S_{\parallel}$ refers to transverse and longitudinal sound velocity in the crystal, correspondingly, ρ is the density of the material, $b^{+}_{q_{\perp}q_{\parallel}}(b_{q_{\perp}q_{\parallel}})$ means the same as in Sec. II, the operator of the creation (annihilation) of a phonon with quasimomentum components $\{\mathbf{q}_{\perp},\mathbf{q}_{\parallel}\}=\mathbf{q}$. Here we suppose that the frequency dependence of an acoustic phonon of σth branch on the wave vector may be represented as

$$\omega_{\sigma}(\mathbf{q})=\mathbf{S}_{\sigma}|\mathbf{q}|. \tag{34}$$

Using Eqs. (32), (33) the Hamiltonian (30) for the deformation potential can be rewritten in the form

$$\hat{H}(\mathbf{r}_e,\mathbf{r}_h) = -i\sqrt{\frac{\hbar}{2\rho V}}\sum_{q_{\perp}q_{\parallel}}\frac{1}{(q_{\perp}^2+q_{\parallel}^2)^{1/4}} \times[e^{i(\mathbf{q}_{\perp}\boldsymbol{\rho}_e+q_{\parallel}z_e)}w_e(\mathbf{q}_{\perp},\mathbf{q}_{\parallel}) - e^{i(\mathbf{q}_{\perp}\boldsymbol{\rho}_h+q_{\parallel}z_h)}w_h(\mathbf{q}_{\perp},\mathbf{q}_{\parallel})](\hat{b}_{\mathbf{q}_{\parallel}\mathbf{q}_{\perp}}+\hat{b}^{+}_{-\mathbf{q}_{\parallel},-\mathbf{q}_{\perp}}). \tag{35}$$

Here

$$w_j(\mathbf{q}_{\perp},\mathbf{q}_{\parallel})=\frac{C_j^{\perp}}{\sqrt{S_{\perp}}}(\mathbf{e}_{\mathbf{q}_{\perp}}\mathbf{q}_{\perp})+\frac{C_j^{\parallel}}{\sqrt{S_{\parallel}}}(\mathbf{e}_{\mathbf{q}_{\parallel}}\mathbf{q}_{\parallel}). \tag{36}$$

As usual, the product of unit vectors obeys the following equation:

$$\mathbf{e}_{\mathbf{q}_{\perp}}\mathbf{e}_{\mathbf{q}_{\parallel}}=\delta_{\perp,\parallel}, \tag{37}$$

where $\delta_{\perp,\parallel}$ denotes Kronecker symbol. We should expect that scattering of excitons will occur due to longitudinal and transverse waves. For purely longitudinal modes (the direction of displacement $\mathbf{e}$ which coincides with the direction of wave propagation $\mathbf{q}$) the components of the unit vector can be determined as

$$\mathbf{e}_{\mathbf{q},L}=\frac{1}{\sqrt{q_{\perp}^2+q_{\parallel}^2}}\begin{cases} q_{\perp} \\ q_{\parallel}. \end{cases} \tag{38}$$

Equation (36) for longitudinal vibrations then reads

$$w_{j,L}(q_{\perp},q_{\parallel})=\frac{1}{\sqrt{q_{\perp}^2+q_{\parallel}^2}}\left(\frac{C_j^{\perp}q_{\perp}^2}{\sqrt{S_{\perp}}}+\frac{C_j^{\parallel}q_{\parallel}^2}{\sqrt{S_{\parallel}}}\right). \tag{39}$$

For purely transverse modes ($\mathbf{e}\perp\mathbf{q}$), obviously, the equality must hold that

$$e_{q_{\perp}}q_{\perp}+e_{q_{\parallel}}q_{\parallel}=0. \tag{40}$$

Hence, the components of the unit vector for the transverse mode are

$$\mathbf{e}_{\mathbf{q},T}=\frac{1}{\sqrt{q_{\perp}^2+q_{\parallel}^2}}\begin{cases} +q_{\parallel} \\ -q_{\perp}. \end{cases} \tag{41}$$

Inserting Eq. (41) in Eq. (36) the value of w for a transverse modes becomes

$$w_{j,T}(q_{\perp},q_{\parallel})=\frac{q_{\perp}q_{\parallel}}{\sqrt{q_{\perp}^2+q_{\parallel}^2}}\left(\frac{C_j^{\perp}}{\sqrt{S_{\perp}}}-\frac{C_j^{\parallel}}{\sqrt{S_{\parallel}}}\right). \tag{42}$$

It should be noted here that if the difference of modules of terms in parentheses of Eq. (42) is negative, then it becomes necessary to change the signs of the values of $q_\perp$ and $q_\parallel$ in Eq. (41).

To define the operator of the exciton-acoustic-phonon interaction for uniaxial crystal it is convenient to introduce the center-mass $\mathbf{R}$ and relative $\boldsymbol{\rho}$ coordinates in the system with cylindrical symmetry as it was done in the previous section by Eq. (21). Hence, substituting Eq. (21) into Eq. (35) we obtain

$$\begin{aligned}\hat{H}_{ac}(\mathbf{R},\boldsymbol{\rho}) - i\sqrt{\frac{\hbar}{2\rho V}}\sum_{\mathbf{q}_\perp \mathbf{q}_\parallel} \frac{1}{(q_\perp^2+q_\parallel^2)^{1/4}} e^{i(\mathbf{q}_\perp \mathbf{R}_\perp + \mathbf{q}_\parallel \mathbf{R}_\parallel)} \\ \times [e^{i\mathbf{q}_\perp \boldsymbol{\rho}_\perp (m_h^\perp/M^\perp) + iq_\parallel \rho_\parallel (m_h^\parallel/M^\parallel)} w_e(q_\perp, q_\parallel) \\ - e^{-i\mathbf{q}_\perp \boldsymbol{\rho}_\perp (m_e^\perp/M^\perp) - iq_\parallel \rho_\parallel (m_e^\parallel/M^\parallel)} \\ \times w_h(\mathbf{q}_\perp, \mathbf{q}_\parallel)](\hat{b}_{\mathbf{q}_\parallel \mathbf{q}_\perp} + \hat{b}^+_{-\mathbf{q}_\parallel, -\mathbf{q}_\perp}). \end{aligned} \tag{43}$$

This is a quite general expression for the deformation potential coupling.

Now, using the wave function given by Eq. (24), we can average Hamiltonian (43) upon exciton variables. Accounting only for the linear terms in the operator upon exciton-phonon variables, the matrix element [on the right-hand side of Eq. (25)], which is taken between the anisotropic exciton states, can be written as

$$\begin{aligned}\langle \mathbf{k}_\perp \mathbf{k}_\parallel | \hat{H}_{ac}(\mathbf{R},\boldsymbol{\rho}) | \mathbf{k}'_\perp \mathbf{k}'_\parallel \rangle \\ = -i\sqrt{\frac{\hbar}{2\rho V}} \frac{1}{\pi a_{\mathrm{ex}}^2 b_{\mathrm{ex}}} \frac{1}{V} \sum_{\mathbf{q}_\perp \mathbf{q}_\parallel} \frac{1}{(q_\perp^2+q_\parallel^2)^{1/4}} \\ \times I_R (I_\rho^e w_e - I_\rho^h w_h)(\hat{b}_{\mathbf{q}_\parallel \mathbf{q}_\perp} + \hat{b}^+_{-\mathbf{q}_\parallel, -\mathbf{q}_\perp}), \end{aligned} \tag{44}$$

where the parameters I_R and I_ρ in cylindrical system are represented as

$$\begin{aligned} I_R = \int_{-\infty}^{\infty} dR_\parallel \int_0^\infty R_\perp dR_\perp \int_0^{2\pi} d\theta \exp[iR_\perp (q_\perp + k_\perp - k'_\perp)\cos\theta \\ + iR_\parallel (q_\parallel + k_\parallel - k'_\parallel)], \end{aligned} \tag{45}$$

$$\begin{aligned} I_\rho^{\binom{e}{h}} = \int_{-\infty}^{\infty} d\rho_\parallel \int_0^\infty \rho_\perp d\rho_\perp \int_0^{2\pi} d\varphi e^{-2\sqrt{\rho_\perp^2/a_{\mathrm{ex}}^2 + \rho_\parallel^2/b_{\mathrm{ex}}^2}} \\ \times \exp\left(iq_\perp \rho_\perp \frac{m_{\binom{e}{h}}^\perp}{M^\perp} \cos\varphi - iq_\parallel \rho_\parallel \frac{m_{\binom{h}{e}}^\parallel}{M^\parallel} \right). \end{aligned} \tag{46}$$

Performing integrations, one gets the explicit expressions for these triple integrals

$$I_R = (2\pi)^3 \delta(\mathbf{q}_\perp + \mathbf{k}_\perp - \mathbf{k}'_\perp)\,\delta(q_\parallel + k_\parallel - k'_\parallel), \tag{47}$$

$$I_\rho^{\binom{e}{h}} = 16\pi a_{\mathrm{ex}}^2 b_{\mathrm{ex}} \left[4 + \left(a_{\mathrm{ex}} q_\perp \frac{m_{\binom{e}{h}}^\perp}{M^\perp} \right)^2 + \left(b_{\mathrm{ex}} q_\parallel \frac{m_{\binom{e}{h}}^\parallel}{M^\parallel} \right)^2 \right]^{-2}, \tag{48}$$

where δ is the Dirac delta function. Inserting Eqs. (47) and (48) into Eq. (44) and Eq. (44) into Eq. (25) we can obtain the operator of exciton-phonon interaction (26) with

$$\begin{aligned} \Phi_{ac}^L(q_\perp, q_\parallel) = \sqrt{\frac{\hbar}{2\rho V}} \frac{1}{(q_\perp^2+q_\parallel^2)^{3/4}} \left(\frac{q_\perp^2 \dfrac{C_e^\perp}{\sqrt{S_\perp}} + q_\parallel^2 \dfrac{C_e^\parallel}{\sqrt{S_\parallel}}}{Z_e^2(q_\perp, q_\parallel)} \right. \\ \left. - \frac{q_\perp^2 \dfrac{C_h^\perp}{\sqrt{S_\perp}} + q_\parallel^2 \dfrac{C_h^\parallel}{\sqrt{S_\parallel}}}{Z_h^2(q_\perp, q_\parallel)} \right), \end{aligned} \tag{49}$$

for exciton coupling with longitudinal acoustic vibrations and

$$\begin{aligned} \Phi_{ac}^T(q_\perp, q_\parallel) = \sqrt{\frac{\hbar}{2\rho V}} \frac{q_\perp q_\parallel}{(q_\perp^2+q_\parallel^2)^{3/4}} \left(\frac{\dfrac{C_e^\perp}{\sqrt{S_\perp}} - \dfrac{C_e^\parallel}{\sqrt{S_\parallel}}}{Z_e^2(q_\perp, q_\parallel)} \right. \\ \left. - \frac{\dfrac{C_h^\perp}{\sqrt{S_\perp}} - \dfrac{C_h^\parallel}{\sqrt{S_\parallel}}}{Z_h^2(q_\perp, q_\parallel)} \right), \end{aligned} \tag{50}$$

for exciton coupling with transverse acoustic vibrations. In Eqs. (49) and (50) the function Z is presented above by Eq. (29). The function $\Phi^{L,T}(q_{\parallel\perp} q_\parallel)$ represents in explicit form the exciton-phonon coupling function for excitons interacting with longitudinal (L) and transverse (T) acoustic phonons in uniaxial nonpolar crystals. These functions tend to zero with $\mathbf{q}_\perp, \mathbf{q}_\parallel \to 0$, simultaneously, and have maxima at small values of both $\mathbf{q}_\parallel$ and $\mathbf{q}_\perp$. The functions Φ_L and Φ_T do not depend on quasimomenta of excitons as well as on the exciton band width. In the absence of the anisotropy of crystal ($m_i^\perp = m_i^\parallel$, $C_j^\perp = C_j^\parallel$, $S_\perp = S_\parallel$, and $a_{\mathrm{ex}} = b_{\mathrm{ex}}$) the coupling function (49) coincide with the one found in Refs. 14 and 15 for isotropic crystals. There may be a discrepancy by the factor of 2/3, because in these papers the deformation potential constant is chosen to be $2/3C$ instead of C. For the case of coupling with transverse vibrations this function, as it is seen from (50), is equal to zero.

IV. SUMMARY

The exciton-phonon interaction in the anisotropic semiconductor has been extensively investigated because of interest in their fundamental physical properties as well as in their device applications. A number of effects are directly connected with the anisotropy of this interaction.[3–8] To study the structure of light absorption bands, its dependence on temperature, and to calculate the exciton lifetime, free path, etc., it is necessary to know the explicit form of the interaction energy of excitons with phonons in an anisotropic crystal, rather than one which usually has been used in simplest form. In this paper we have obtained the coupling functions for excitons interacting with both the longitudinal and transverse optical and acoustic phonons.

*Mailing address: P.B. 66, Kiev-143, 252143, Ukraine.

[1] P.V. Santos, A. Cantarero, M. Cardona, R. Nötzel, and K. Ploog, Phys. Rev. B **52**, 1970 (1995).
[2] P.M. Young, E. Runge, M. Ziegler, and H. Ehrenreich, Phys. Rev. B **49**, 7424 (1994).
[3] F. Engelbrecht and R. Helbig, Phys. Rev. B **48**, 15 698 (1993).
[4] D. Fröhlich *et al.*, Phys. Rev. B **49**, 10 337 (1994).
[5] G. Harbeke, Phys. Status Solidi **27**, 9 (1968).
[6] K. Nakao, H. Kamimura, and Y. Nishina, Nuovo Cimento **63B**, 45 (1969).
[7] A. Baldereschi and M.G. Diaz, Nuovo Cimento **68B**, 217 (1970).
[8] T. Takagahara, Phys. Rev. B **31**, 6552 (1985).
[9] J. Lee, E.S. Koteles, and M.O. Vassell, Phys. Rev. B **33**, 5512 (1986).
[10] A.S. Davydov, Phys. Status. Solidi B **20**, 143 (1967).
[11] K.J. Nash and D.J. Mowbray, J. Lumin. **44**, 315 (1989).
[12] T. Takagahara, J. Lumin. **44**, 347 (1988).
[13] A.I. Ansel'm and Yu.A. Firsov, Zh. Eksp. Teor. Fiz. **30**, 719 (1955).
[14] A.I. Ansel'm and Yu.A. Firsov, Zh. Eksp. Teor. Fiz. **28**, 151 (1955).
[15] Y. Toyozawa, Prog. Theor. Phys. **20**, 53 (1958).
[16] H. Fook, B. Kramer, and H. Büttner, Phys. Status Solidi B **67**, 199 (1975); **72**, 155 (1975).
[17] H. Haken, *Quantum Field Theory of Solids* (North-Holland, Amsterdam, 1976).
[18] L.D. Landau and E.M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, New York, 1986).
[19] C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963).
[20] P. Gomes de Costa and E.M. Conwell, Phys. Rev. B **48**, 1993 (1993).
[21] M. Abramovitz and I.A. Stegun, *Handbook of Mathematical Functions*, 10th ed. (Dover, New York, 1972).
[22] G.L. Bir and G.E. Pikus, *Symmetry and Strain-Induced Effects in Semiconductors* (Wiley, New York, 1974).
[23] W. Shockley and J. Bardeen, Phys. Rev. **77**, 407 (1950).