

EXCHANGE INTERACTION IN EXCITONS IN SEMICONDUCTORS

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We consider the question of exchange interaction in Wannier-Mott excitons, for an arbitrary band structure, both in the effective-mass approximation and with allowance for the corrections, considered first by Elliott^[2], connected with the short-range potential. In addition, we calculate the corrections to the non-exchange terms, which arise in the third approximation of the *kp* method, and also the corrections connected with the short-range potential. The results of the calculation show that, in agreement with the results of Rashba^[3], allowance for exchange interaction in the effective-mass approximation is equivalent to allowance for the long-range forces, and refute the results of subsequent investigations^[5,6], whose authors reached opposite conclusions. Comparison of the results of the calculations of the exchange terms in the effective-mass approximation with conclusions of the phenomenological theory^[18-20] and of the calculation of the terms connected with the short-range forces with the conclusions of the theory of invariants^[10,15,16] show that these phenomenological methods are equivalent to the microscopic approach.

INTRODUCTION

THE question of exchange interaction in Wannier-Mott excitons was discussed in a number of papers. Dresselhaus^[1], who first considered excitons in semiconductors with a complex band structure, pointed out that there is no exchange interaction in excitons in the effective-mass approximation. In a subsequent paper, Elliott^[2] noted that such an interaction does take place if account is taken, in the effective-mass approximation, of the corrections connected with the short-range part of the potential. Rashba^[3], who used, unlike Dresselhaus^[1], not the Bloch but the node representation, has shown that for shallow excitons in the effective-mass approximation, the contribution made to the energy by the exchange interaction depends, in the case of a simple band, on the direction of the exciton wave vector **K**, in analogy with the contribution that appears when long-range forces are taken into account in Frenkel excitons^[4,11]. Subsequent papers, however, gave other different formulas for the exchange splitting in the effective-mass approximation, formulas that did not agree with the Rashba formula. Thus, Dos et al.^[5] give for exchange splitting an expression that diverges at small values of **K**:

$$\Delta E_{\text{exch}} \sim 1/K^2.$$

Makarov^[6] presented, for exchange splitting of the ground state of an exciton in the effective-mass approximation, an expression that actually coincides with the formula describing the annihilation interaction in positronium (Eq. 83.24 of^[7]), has a contact character, and does not depend on the magnitude or direction of **K**.

Since at the present time exchange splitting of exci-

ton lines has become an object of experimental study and has been observed in a number of crystals^[8-11], we analyze in the present paper in detail the question of exchange interaction in excitons in semiconductors with arbitrary band structure, and consider also other corrections to the exciton energy, which, like the exchange terms, appear in higher orders of the *kp* method (concerning this method see^[12]).

EXCHANGE INTERACTION IN THE EFFECTIVE-MASS APPROXIMATION

We present first the Hamiltonian describing, in the effective-mass approximation, the interaction of two electrons, one of which is in the conduction band *m* near an extremum **k_C**, and the other in the valence band *n* near **k_V**, the bands having an arbitrary structure near the extrema. The initial Schrödinger equation describing these electrons has the usual form

$$(\mathcal{H}_0(x_1) + \mathcal{H}_0(x_2) + V(r_1 - r_2) - E)\Psi(x_1, x_2) = 0, \tag{1}$$

where $V(r) = e^2/\kappa r$, and **x** includes both the coordinate and time variables **r** and α . The dielectric constant κ , generally speaking, depends here on **r**. In the *kp* method, the wave function $\psi(x)$ is expanded in terms of the functions

$$\varphi_{s,\mathbf{k}}(x) = \psi_{s,\mathbf{k}_0}(x) e^{i\mathbf{k}x},$$

where ψ_{s,\mathbf{k}_0} are the eigenfunctions of the Hamiltonian \mathcal{H}_0 at the point **k₀** of band *s*:

$$\psi_{s,\mathbf{k}_0}(x) = e^{i\mathbf{k}_0 x} u_{s,\mathbf{k}_0}(x).$$

Let us consider first a direct exciton, when **k_C** = **k_V** = **k₀**. The function $\Psi(x_1, x_2)$ will be written in the form

$$\Psi(x_1, x_2) = \sum_{st} F_{st}(r_1, r_2) \psi_{s,\mathbf{k}_0}(x_1) \psi_{t,\mathbf{k}_0}(x_2), \tag{2}$$

and we expand the smooth function $F_{st}(r_1, r_2)$ in a series

$$F_{st}(r_1, r_2) = \sum_{\mathbf{k}_1, \mathbf{k}_2} C_{s,\mathbf{k}_1, \mathbf{k}_2} e^{i(\mathbf{k}_1 r_1 + \mathbf{k}_2 r_2)}, \tag{3}$$

¹In Frenkel excitons, this mechanism is called resonant, since it can be regarded as the result of virtual recombination and generation of excitons. In positronium theory, the same mechanism is called annihilation. The difference in the names is connected, in particular, with the fact that the definition of the exchange terms is not unique and depends on the chosen representation.

and then

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \sum_{s\mathbf{k}_1, t\mathbf{k}_2} C_{s\mathbf{k}_1, t\mathbf{k}_2} \varphi_{s\mathbf{k}_1}(\mathbf{x}_1) \varphi_{t\mathbf{k}_2}(\mathbf{x}_2). \quad (4)$$

From the antisymmetry condition $\Psi(\mathbf{x}_1, \mathbf{x}_2) = -\Psi(\mathbf{x}_2, \mathbf{x}_1)$ it follows that

$$F_{st}(\mathbf{r}_1, \mathbf{r}_2) = -F_{ts}(\mathbf{r}_2, \mathbf{r}_1), \quad C_{s\mathbf{k}_1, t\mathbf{k}_2} = -C_{t\mathbf{k}_2, s\mathbf{k}_1}. \quad (5)$$

Further, substituting (4) in (1), we multiply from the left by $\varphi_{s'\mathbf{k}_1'}^*(\mathbf{x}_1)\varphi_{t'\mathbf{k}_2'}^*(\mathbf{x}_2)$ and integrate with respect to \mathbf{x}_1 and \mathbf{x}_2 . As a result we obtain a system of equations for the coefficients $C_{s\mathbf{k}_1, t\mathbf{k}_2}$:

$$\sum_{s\mathbf{k}_1, t\mathbf{k}_2} \langle s'\mathbf{k}_1' t'\mathbf{k}_2' | \mathcal{H} | s\mathbf{k}_1 t\mathbf{k}_2 \rangle C_{s\mathbf{k}_1, t\mathbf{k}_2} = EC_{s'\mathbf{k}_1' t'\mathbf{k}_2'} \quad (6)$$

The matrix $\langle s'\mathbf{k}_1' t'\mathbf{k}_2' | \mathcal{H} | s\mathbf{k}_1 t\mathbf{k}_2 \rangle$ contains the diagonal terms

$$\langle s'\mathbf{k}_1' t'\mathbf{k}_2' | \mathcal{H}_0 | s\mathbf{k}_1 t\mathbf{k}_2 \rangle = \left(E_s(\mathbf{k}_0) + E_t(\mathbf{k}_0) + \frac{\hbar^2}{2m} (k_1^2 + k_2^2) \right) \delta_{s's} \delta_{t't} \delta_{\mathbf{k}_1, \mathbf{k}_1'} \delta_{\mathbf{k}_2, \mathbf{k}_2'}, \quad (6a)$$

the intraband non-diagonal (Coulomb) terms

$$\langle s'\mathbf{k}_1' t'\mathbf{k}_2' | \mathcal{H}_1 | s\mathbf{k}_1 t\mathbf{k}_2 \rangle = V_{\mathbf{k}_1' - \mathbf{k}_1} \delta_{s's} \delta_{t't} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'}, \quad (6b)$$

interband Coulomb terms, which we shall consider in detail below, and interband $\mathbf{k}\mathbf{p}$ terms

$$\langle s'\mathbf{k}_1' t'\mathbf{k}_2' | \mathcal{H}_2 | s\mathbf{k}_1 t\mathbf{k}_2 \rangle = \frac{\hbar^2}{m} [(k_1 p_{s's}) \delta_{t't} + (k_2 p_{t't}) \delta_{s's}] \delta_{\mathbf{k}_1, \mathbf{k}_1'} \delta_{\mathbf{k}_2, \mathbf{k}_2'}, \quad (6c)$$

where $p_{s's}$ are the matrix elements of the momentum operator on the functions $\psi_{s\mathbf{k}_0}$, and

$$V_{\mathbf{q}} = \frac{1}{V} \int V(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}.$$

Further, as usual, it is necessary to obtain the equation of the effective-mass method, containing only the coefficients $C_{m\mathbf{k}_1, n\mathbf{k}_2}$ and $C_{n\mathbf{k}_2, m\mathbf{k}_1}$, where m, m', \dots are the conduction bands under consideration, and n, n', \dots the valence bands, eliminating the remaining interband matrix elements \mathcal{H}_2 by means of the transformation $S^{[12]}$:

$$\tilde{\mathcal{H}} = e^{-S} \mathcal{H} e^S.$$

As a result we obtain a system of equations with dimensionality $2N_c N_v$, where N_c and N_v are the multiplicities of the degeneracy of the conduction and valence bands at the extremum point \mathbf{k}_0 . However, taking the condition (5) into account, we obtain from these $2N_c N_v$ equations a system of equations with dimensionality $N_c N_v$ only for the coefficients $C_{m\mathbf{k}_1, n\mathbf{k}_2}$:

$$\sum_{m\mathbf{k}_1, n\mathbf{k}_2} (\langle m'\mathbf{k}_1' n'\mathbf{k}_2' | \tilde{\mathcal{H}} | m\mathbf{k}_1 n\mathbf{k}_2 \rangle - \langle m'\mathbf{k}_1' n'\mathbf{k}_2' | \tilde{\mathcal{H}} | n\mathbf{k}_2 m\mathbf{k}_1 \rangle) \times C_{m\mathbf{k}_1, n\mathbf{k}_2} = EC_{m'\mathbf{k}_1' n'\mathbf{k}_2'}, \quad (7)$$

containing exchange terms—the second term of (7).

The first nonzero contribution to the exchange terms is made by the terms of third order—second in \mathcal{H}_2 and first in \mathcal{H}_1 . A contribution of the same order is contained also in the first term of (7).

The terms of fourth order in \mathcal{H}_2 , i.e., in \mathbf{k} , allowance for which is equivalent to allowance for the nonparabolicity of the bands, make a contribution of the same order to the energy, i.e., on the order of E_0^2/E_g , but since they make no contribution to the exchange energy,

we shall not write them out explicitly²⁾. Terms of higher order, as can be readily shown, contain the additional small parameter E_0/E_g or $\hbar^2 \mathcal{H}^2/2mE_g$. Here E_g is the width of the forbidden band and E_0 is the exciton binding energy.

If we retain only the terms of first order in \mathcal{H}_1 and of second in \mathcal{H}_2 , then we obtain

$$\langle m'\mathbf{k}_1' n'\mathbf{k}_2' | \tilde{\mathcal{H}}^{(1,2)} | m\mathbf{k}_1 n\mathbf{k}_2 \rangle = (\mathcal{H}(\mathbf{k}_1)_{m'm} \delta_{n'n} + \mathcal{H}(\mathbf{k}_2)_{n'n} \delta_{m'm}) \delta_{\mathbf{k}_1, \mathbf{k}_1'} \delta_{\mathbf{k}_2, \mathbf{k}_2'} + V_{\mathbf{k}_1' - \mathbf{k}_1} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'} \delta_{m'm} \delta_{n'n}, \quad (8)$$

where $\mathcal{H}(\mathbf{k})$ is the single-band Hamiltonian of the effective-mass method, equal to

$$\mathcal{H}(\mathbf{k})_{m'm} = \frac{\hbar^2 k^2}{2m} \delta_{m'm} + \frac{\hbar^2}{m^2} \sum_{\alpha\beta} k_\alpha k_\beta \{ p_{m'm}^\alpha p_{m'm}^\beta \} / (E_m - E_s). \quad (9)$$

Here E_s is the energy in the band s at the point \mathbf{k}_0 .

In the third-order approximation, the non-exchange terms in (7) contain the contribution

$$\langle m'\mathbf{k}_1' n'\mathbf{k}_2' | \tilde{\mathcal{H}}^{(3)} | m\mathbf{k}_1 n\mathbf{k}_2 \rangle = (\langle m'\mathbf{k}_1' | \Delta \mathcal{H} | m\mathbf{k}_1 \rangle \delta_{n'n} + \langle n'\mathbf{k}_2' | \Delta \mathcal{H} | n\mathbf{k}_2 \rangle \delta_{m'm}) \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'}, \quad (10)$$

where

$$\langle m'\mathbf{k}' | \Delta \mathcal{H} | m\mathbf{k} \rangle = - \left[\sum_{\alpha\beta} (k_\alpha' - k_\alpha) (k_\beta' - k_\beta) G_{m'm}^{\alpha\beta} + (g_{m'm}[\mathbf{k}'\mathbf{k}]) \right] V_{\mathbf{k}' - \mathbf{k}}, \quad (11)$$

here

$$G_{m'm}^{\alpha\beta} = \frac{1}{2} \frac{\hbar^2}{m^2} \sum_i \{ p_{m'm}^\alpha p_{m'm}^\beta \} / (E_s - E_m)^2, \quad (12)$$

$$g_{m'm}^\gamma = \frac{1}{2} \frac{\hbar^2}{m^2} \sum_{\alpha\beta\gamma} \delta_{\alpha\beta\gamma} \frac{p_{m'm}^\alpha p_{m'm}^\beta}{(E_s - E_m)^2}.$$

In (9) and (12), the curly brackets denote a symmetrized product, and $\delta_{\alpha\beta\gamma}$ is a unit antisymmetrical tensor.

The exchange term in (7) differs from zero only if the matrix elements of the operator p_{mn} are not equal to zero, and is equal in third approximation to

$$\langle m'\mathbf{k}_1' n'\mathbf{k}_2' | \tilde{\mathcal{H}}^{(3)} | n\mathbf{k}_2 m\mathbf{k}_1 \rangle = \sum_{\alpha\beta} Q_{m'n', nm}^{\alpha\beta} (k_{1\alpha} - k_{2\alpha}') (k_{1\beta} - k_{2\beta}') \times V_{\mathbf{k}_1' - \mathbf{k}_2} \delta_{\mathbf{k}_1 + \mathbf{k}_2, \mathbf{k}_1' + \mathbf{k}_2'}, \quad (13)$$

where

$$Q_{m'n', nm}^{\alpha\beta} = \frac{\hbar^2}{m^2} \frac{p_{m'n'}^\alpha p_{n'm}^\beta}{(E_m - E_n)^2}.$$

If all $p_{mn} = 0$, then the exchange terms appear only when account is taken of terms of higher order in \mathcal{H}_2 , and contain an additional small quantity.

In order to change over to the \mathbf{r} -representation it is necessary to multiply Eq. (7) by $\exp[i(\mathbf{k}_1' \cdot \mathbf{r}_1 + \mathbf{k}_2' \cdot \mathbf{r}_2)]$ and sum over \mathbf{k}_1' and \mathbf{k}_2' . Taking into account the smallness of \mathbf{k} and \mathbf{k}' it is possible to replace summation over \mathbf{k}_1 and \mathbf{k}_1' or \mathbf{k}_2 and \mathbf{k}_2' by separate summations

²⁾We note that allowance for the dispersion of the dielectric constant κ in (1) can lead to corrections to the non-exchange terms of the order E_0^2/E_g . As noted by Moskalenko [13], all such terms, as well as the term (31) (see below), which is connected with the short-range forces, lead to a splitting of the s and p states which are degenerate in the case of spherical bands, similar to the splitting of the s and p levels of the hydrogen atom in relativistic theory [7].

over $\mathbf{q} = \mathbf{k}'_1 - \mathbf{k}_1 = \mathbf{k}_2 - \mathbf{k}'_2$, and in the last term, i.e., in (13), by summation over $\mathbf{q} = \mathbf{k}'_1 - \mathbf{k}_2 = \mathbf{k}_1 - \mathbf{k}'_2$. The exchange term (13) will then contain the sum

$$\sum_{\mathbf{k}_1, \mathbf{k}_2} C_{m, \mathbf{k}_1, \mathbf{k}_2} \exp[i(\mathbf{k}_1 \mathbf{r}_2 + \mathbf{k}_2 \mathbf{r}_1)] = F_{mn}(\mathbf{r}_2, \mathbf{r}_1)$$

unlike the non-exchange terms containing $F_{mn}(\mathbf{r}_1, \mathbf{r}_2)$. As a result, we obtain a system of equations for the functions $F_{mn}(\mathbf{r}_1, \mathbf{r}_2)$:

$$\begin{aligned} \sum_{mn} \int d\mathbf{r}_1 d\mathbf{r}_2 \{ [\mathcal{H}_{m'm}(-i\nabla_{\mathbf{r}_1}) \delta_{n'n} + \mathcal{H}_{n'n}(-i\nabla_{\mathbf{r}_2}) \delta_{m'm} \\ + \mathcal{H}_{m'n', m'n}(\mathbf{r}_1, \mathbf{r}_2)] \delta(\mathbf{r}'_1 - \mathbf{r}_1) \delta(\mathbf{r}'_2 - \mathbf{r}_2) \\ - \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) \} F_{mn}(\mathbf{r}_1, \mathbf{r}_2) = EF_{m'n'}(\mathbf{r}'_1, \mathbf{r}'_2). \end{aligned} \quad (14)$$

Here

$$\begin{aligned} \mathcal{H}_{m'n', m'n}(\mathbf{r}_1, \mathbf{r}_2) &= V(r) \delta_{m'm} \delta_{n'n} \\ &+ \Delta \mathcal{H}_{m'm}(\mathbf{r}_1, \mathbf{r}_2) \delta_{n'n} + \Delta \mathcal{H}_{n'n}(\mathbf{r}_1, \mathbf{r}_2) \delta_{m'm}, \quad (15) \\ \Delta \mathcal{H}_{m'm}(\mathbf{r}_1, \mathbf{r}_2) &= -\frac{e^2}{\kappa} \left[\sum_{\alpha\beta} \left(G_{m'm}^{\alpha\beta} - \frac{1}{3} \text{Sp } G_{m'm} \delta_{\alpha\beta} \right) \right. \\ &\times \left. 3 \frac{r_{\alpha} r_{\beta}}{r^5} - \frac{4\pi}{3} \text{Sp } G_{m'm} \delta(r) + \frac{1}{r^3} (g_{m'm} [r \nabla_{\mathbf{r}_1}) \right], \quad (16) \\ \text{Sp } G_{m'm} &= \sum_{\alpha} G_{m'm}^{\alpha\alpha}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2. \end{aligned}$$

The last term in (14), which describes the exchange interaction, is equal to

$$\begin{aligned} \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) \\ = - \sum_{\alpha\beta} Q_{m'n', m'n}^{\alpha\beta} \frac{\partial^2 V(\mathbf{r}_1 - \mathbf{r}_2)}{\partial r_{1\alpha} \partial r_{1\beta}} \delta(\mathbf{r}_1 - \mathbf{r}'_2) \delta(\mathbf{r}_2 - \mathbf{r}_1). \end{aligned} \quad (17)$$

The operator (14) determines the interaction of two electrons that are in different bands m and n . Landau and Berestetskii, in positronium theory, derived rules for transforming the Hamiltonian describing the interaction of two electrons in empty and filled bands, into a Hamiltonian that describes the interaction of an electron and a positron^[14]. Similar rules are valid also on going from electron-electron to electron-hole interaction in semiconductors, namely, to obtain the Hamiltonian describing the interaction of an electron m and a hole n it is necessary, first, to reverse the sign of that term of $\mathcal{H}_{n'n}(\mathbf{k}_2)$ which defines the energy of the electron in filled band, and in the operators $\langle m'n' | \mathcal{H} | mn \rangle$ and $\mathcal{H}^{\text{exch}}$, which determine the interaction of the electron and the hole; second, it is necessary to replace ψ_n by $\mathcal{X} \psi_n$ and to reverse the sequence of the indices of the valence band, since creation of an electron denotes annihilation of a hole and vice-versa. According to these rules, the transition from electron-electron to electron-hole interaction is effected by the transformations

$$\begin{aligned} \mathcal{H}_{n'n}^h(\mathbf{r}_2, \mathbf{r}'_2) &= -\mathcal{H}_{n'n}^e(\mathbf{r}_2, \mathbf{r}'_2), \\ \mathcal{H}_{m'n', m'n}^h(\mathbf{r}_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) &= -\mathcal{H}_{m'n', m'n}^e(\mathbf{r}_1, \mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2). \end{aligned} \quad (18)$$

Here \mathcal{X} is the time-inversion operation. The symbol $\mathcal{H}_{n'n}^h$ denotes that if we choose as the basis the wave functions of the holes ψ_n^h , then the matrix elements must be calculated with the wave functions of the "missing" electron $\mathcal{X} \psi_n^h$. It is necessary to bear in mind here that $p_{ns}^{\alpha} = -p_{s'n}^{\alpha}$, and therefore for the matrix $\mathcal{H}_{n'n}^h(9)$, just for $G_{n'n}(12)$, we have $\mathcal{H}_{n'n}^h = \mathcal{X} \mathcal{H}_{n'n}^e \mathcal{X}^{-1}$.

$= G_{n'n}$, and for the matrix $g_{n'n}(12)$ we have $g_{n'n}^h = -g_{n'n}^e$. Here the term $\mathcal{H}_{n'n}^h(\mathbf{k}_2) = -\mathcal{H}_{n'n}^e(\mathbf{k}_2)$ is the usual Hamiltonian defining the hole spectrum in the effective-mass approximation.

As a result of the indicated transformations, the electron-hole interaction operator takes the form

$$\begin{aligned} \mathcal{H}_{m'n', m'n}^{\text{eh}}(\mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) &= \left[\mathcal{H}_{m'm}^e(-i\nabla_{\mathbf{r}_1}) \delta_{n'n} \right. \\ &+ \left. \mathcal{H}_{n'n}^h(-i\nabla_{\mathbf{r}_2}) \delta_{m'm} - \frac{e^2}{\kappa |\mathbf{r}_1 - \mathbf{r}_2|} + \Delta \mathcal{H}_{m'n', m'n}^{\text{eh}}(\mathbf{r}_1, \mathbf{r}_2) \right] \\ &\times \delta(\mathbf{r}'_1 - \mathbf{r}_1) \delta(\mathbf{r}'_2 - \mathbf{r}_2) + \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2), \end{aligned} \quad (19)$$

where

$$\begin{aligned} \Delta \mathcal{H}_{m'n', m'n}^{\text{eh}}(\mathbf{r}_1, \mathbf{r}_2) &= -\frac{e^2}{\kappa} \left\{ \sum_{\alpha\beta} \frac{3r_{\alpha} r_{\beta}}{r^5} \left[\left(G_{m'm}^{\alpha\beta} - \frac{1}{3} \text{Sp } G_{m'm} \delta_{\alpha\beta} \right) \delta_{n'n} \right. \right. \\ &+ \left. \left. \left(G_{n'n}^{\alpha\beta} - \frac{1}{3} \text{Sp } G_{n'n} \delta_{\alpha\beta} \right) \delta_{m'm} \right] - \frac{4\pi}{3} \delta(r) (\text{Sp } G_{m'm} \delta_{n'n} \right. \\ &+ \left. \text{Sp } G_{n'n} \delta_{m'm}) + r^{-3} [(g_{m'm} [r \nabla_{\mathbf{r}_1}) \delta_{n'n} - (g_{n'n} [r \nabla_{\mathbf{r}_2}) \delta_{m'm}] \right\}. \end{aligned} \quad (20)$$

The first three terms in (19) give the equation derived by Dresselhaus^[1] for the exciton in the effective-mass approximation. The term (20) describes corrections to the Coulomb potential.

The first two terms in $\Delta \mathcal{H}^{\text{eh}}$ correspond to the effective dipole-dipole and to the contact interactions, respectively. The matrix $G^{\alpha\beta}$ defining it is similar to the matrix (9) defining the spectrum. The last term in $\Delta \mathcal{H}^{\text{eh}}$ (20) describes the interaction of the orbital angular momenta of the slow and fast functions; the matrix $g^{\alpha\beta}$ defining it is similar to the matrix defining the magnetic moment of the electron, which is connected with the orbital motion^[15]. The last term in (19) is due to the exchange term (17):

$$\begin{aligned} \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) &= \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}'_2, \mathbf{r}_1, \mathbf{r}_2) \\ &= - \sum_{\alpha\beta} Q_{m'n', m'n}^{\alpha\beta} \frac{\partial^2 V(\mathbf{r}_1 - \mathbf{r}_2)}{\partial r_{1\alpha} \partial r_{1\beta}} \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}'_2). \end{aligned} \quad (21)$$

If we introduce new variables³⁾

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{R} = a\mathbf{r}_1 + b\mathbf{r}_2, \\ \mathbf{K} &= \mathbf{k}_1 + \mathbf{k}_2, \quad \mathbf{k} = \tilde{b}\mathbf{k}_1 - \tilde{a}\mathbf{k}_2, \end{aligned} \quad (22)$$

then in terms of the variables (22) the operator (21) will be of the form

$$\begin{aligned} \mathcal{H}_{m'n', m'n}^{\text{exch}}(\mathbf{r}'\mathbf{R}, \mathbf{r}\mathbf{R}) &= \\ &= - \sum_{\alpha\beta} Q_{m'n', m'n}^{\alpha\beta} \frac{\partial^2 V(\mathbf{R} - \mathbf{R}')}{\partial R_{\alpha} \partial R_{\beta}} \delta(\mathbf{r}) \delta(\mathbf{r}'), \end{aligned} \quad (23)$$

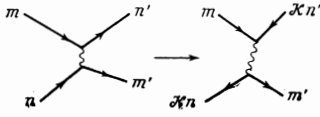
where

$$Q_{m'n', m'n}^{\alpha\beta} = \frac{\hbar^2}{m^2 E_g^2} P_{m'n'}^{\alpha} P_{n'm}^{\beta}. \quad (24)$$

The wave function of the exciton $\Psi_{\mathbf{K}}^j$ can be written in the effective-mass method in the form

$$\Psi_{\mathbf{K}}^j(\mathbf{r}, \mathbf{R}) = \frac{1}{\sqrt{\mathcal{V}^2}} e^{i\mathbf{K}\mathbf{R}} \begin{vmatrix} f_{\mathbf{K}m, n_1}^j \\ f_{\mathbf{K}m, n_2}^j \\ \vdots \\ f_{\mathbf{K}m, n_{N_0}}^j \\ \vdots \\ f_{\mathbf{K}n, N_0}^j \end{vmatrix} \quad (25)$$

³⁾The matrices a and b can be chosen in arbitrary fashion, but in such a way that they satisfy the condition $a + b = I$, so that the Jacobian of the transformation is $|\partial(\mathbf{r}_1, \mathbf{r}_2) / \partial(\mathbf{r}, \mathbf{R})| = 1$. In this case we have $\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2 = \mathbf{k} \cdot \mathbf{r} + \mathbf{K} \cdot \mathbf{R}$.



The matrix element of the operator (23), calculated with the functions (25), is

$$\langle j'K' | \mathcal{H}^a | jK \rangle = \frac{4\pi e^2}{\kappa} \sum_{mnm'n'a\beta} Q_{m'n'a\beta}^{a\beta} \frac{K_\alpha K_\beta}{K^2} \cdot f_{km'n'}^*(0) f_{kmn}(0) \delta_{KK'}. \quad (26)$$

Formula (23) and formula (26) (for a simple band) differ from the corresponding formulas given by Rashba only in that account is taken of the dielectric constant. The derivation presented above shows that formula (23) is valid for all the exciton states at an arbitrary band structure.

We note that although the term \mathcal{H}^a is the result of allowance for the exchange interaction of the electrons in the valence band and in the conduction band, it describes a long-range electron-hole interaction, which can be regarded as the result of virtual recombination and generation of an exciton.

The figure shows clearly that on going over from the electron-electron to the electron-hole interaction in accordance with the rules indicated above, the diagram of the exchange interaction is transformed into the diagram of the annihilation interaction.

It is seen from (26) that the quantity \mathcal{H}^a depends significantly on the direction of the vector \mathbf{K}^a .

ALLOWANCE FOR SHORT-RANGE FORCES (DIRECT EXCITONS)

The matrix element of the interaction potential in Eq. (4) is equal to

$$\langle s'k_1't'k_2' | V | sk_1tk_2 \rangle = \gamma^2 \sum_{ML} B_M^{s's} B_L^{t't} V_{\mathbf{b}_M+\mathbf{q}_1, \mathbf{b}_M+\mathbf{q}_1, -\mathbf{b}_L, -\mathbf{q}_2}, \quad (27)$$

where $\mathbf{q}_1 = \mathbf{k}'_1 - \mathbf{k}_1$, $\mathbf{q}_2 = \mathbf{k}'_2 - \mathbf{k}_2$, and $B_M^{S'S'}$ are the Fourier-expansion coefficients of the periodic function

$$\sum_{\mathbf{x}} \psi_{s'k_2}^*(\mathbf{x}) \psi_{sk_1}(\mathbf{x}) = \sum_{\mathbf{m}} B_M^{s's} e^{-i\mathbf{m}\cdot\mathbf{x}},$$

in terms of the reciprocal-lattice vectors \mathbf{b}_M .

For a slowly varying potential, the main contribution to the sum (27) is made by terms with $\mathbf{b}_M = 0$, since \mathbf{k}_1 and \mathbf{k}_2 are small compared with the dimensions of the Brillouin zone. Then

$$\delta_{\mathbf{b}_M+\mathbf{q}_1, -\mathbf{b}_L-\mathbf{q}_2} = \delta_{\mathbf{b}_M, -\mathbf{b}_L} \delta_{\mathbf{q}_1, -\mathbf{q}_2}.$$

We have therefore retained in (6b) only one term from (27), the one with $\mathbf{b}_M = \mathbf{b}_L = 0$. We took into account here the fact that $B_0^{S'S} = \gamma^{-1} \delta_{S'S}$.

We now take account in (27) of the terms with $\mathbf{b}_M \neq 0$

⁴As indicated above, for positronium, the equation for which in second approximation of perturbation theory coincides, apart from some constants, with the equation for the exciton in the case of simple bands, the annihilation term, unlike (26), has the contact form. The reason for this difference is that for an exciton the wavelength of the light λ , corresponding to the exciton excitation energy, i.e., E_g , greatly exceeds the Bohr radius of the exciton a_e , whereas for positronium, to the contrary, $\lambda \approx \hbar/2mc \ll a_p = 2\hbar^2/me^2$. Therefore for the exciton we can neglect retardation, which plays the major role for the positronium [14,7].

and $\mathbf{b}_L \neq 0$. It suffices here to consider the matrix elements of the operator V between the valence bands and the conduction bands.

We consider first the non-exchange terms. At small \mathbf{k} , we can neglect the dependence of $V_{\mathbf{b}_M+\mathbf{q}_1}$ on \mathbf{q}_1 for $\mathbf{b}_M \neq 0$, and from (27) we obtain

$$\begin{aligned} \langle m'k_1'n'k_2' | \delta V | mk_1nk_2 \rangle &= \gamma^2 \sum_{M \neq 0, L \neq 0} B_M^{m'm} B_L^{n'n} V_{\mathbf{b}_M} \delta_{\mathbf{b}_M, -\mathbf{b}_L} \delta_{\mathbf{q}_1, -\mathbf{q}_2} \\ &= (\langle m'n' | V | mn \rangle - V_0 \delta_{m'm} \delta_{n'n}) \delta_{\mathbf{q}_1, -\mathbf{q}_2}, \end{aligned} \quad (28)$$

where

$$\begin{aligned} \langle m'n' | V | mn \rangle &= \gamma^2 \sum_{ML} B_M^{m'm} B_L^{n'n} V_{\mathbf{b}_M} \delta_{\mathbf{b}_M, -\mathbf{b}_L} \\ &= \int \psi_{m'k_2}^*(\mathbf{x}_1) \psi_{mk_1}(\mathbf{x}_1) V(\mathbf{r}_1 - \mathbf{r}_2) \psi_{nk_2}(\mathbf{x}_2) \psi_{n'k_1}(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2 \\ &= \int u_{m'k_2}^*(\mathbf{x}_1) u_{mk_1}(\mathbf{x}_1) V(\mathbf{r}_1 - \mathbf{r}_2) u_{nk_2}(\mathbf{x}_2) u_{n'k_1}(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2, \end{aligned} \quad (29)$$

$$V_0 = \frac{1}{\gamma} \int V(\mathbf{r}) d\mathbf{r}.$$

Changing over to the \mathbf{r} representation, i.e., multiplying δV by $\exp[i(\mathbf{q}_1 \cdot \mathbf{r}_1 + \mathbf{q}_2 \cdot \mathbf{r}_2)]$, and summing over \mathbf{q}_1 and \mathbf{q}_2 , we obtain

$$\delta V_{m'n', mn}(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2') = \gamma^2 (\langle m'n' | V | mn \rangle - V_0 \delta_{m'm} \delta_{n'n}) \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1' - \mathbf{r}_1) \delta(\mathbf{r}_2' - \mathbf{r}_2). \quad (30)$$

Changing over now, in accordance with (18), from the electron-electron interaction to the electron-hole interaction, we obtain

$$\delta V_{m'n', mn}^{eh}(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2') = -\gamma^2 (\langle m'n' | V | mn \rangle - V_0 \delta_{m'm} \delta_{n'n}) \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1' - \mathbf{r}_1) \delta(\mathbf{r}_2' - \mathbf{r}_2), \quad (31)$$

since $\langle m' \mathcal{X} | V | m \mathcal{X}' \rangle = \langle m'n' | V | mn \rangle$.

We consider now the exchange term

$$\begin{aligned} \langle m'k_1'n'k_2' | \delta V | nk_2mk_1 \rangle &= \int d\mathbf{x}_1 d\mathbf{x}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \varphi_{m'k_1'}(\mathbf{x}_1) \\ &\quad \varphi_{n'k_2'}^*(\mathbf{x}_2) \varphi_{nk_2}(\mathbf{x}_2) \varphi_{mk_1}(\mathbf{x}_1) = \\ &= \gamma^2 \sum_{ML} B_M^{m'n} B_L^{n'm} V_{\mathbf{b}_L+\mathbf{k}_2'-\mathbf{k}_1, \mathbf{b}_L+\mathbf{k}_2'-\mathbf{k}_1, -\mathbf{b}_M+\mathbf{k}_2-\mathbf{k}_1}. \end{aligned} \quad (32)$$

Here the term with $\mathbf{b}_L = \mathbf{b}_M = 0$ vanishes. In the remaining terms, as before, we can neglect the dependence of $V_{\mathbf{b}_L+\mathbf{k}_2'-\mathbf{k}_1}$ on $\mathbf{k}_2' - \mathbf{k}_1$, and then we obtain an expression similar to (28):

$$\langle m'k_1'n'k_2' | \delta V | nk_2mk_1 \rangle = \langle m'n' | V | nm \rangle \delta_{\mathbf{k}_1'+\mathbf{k}_2', \mathbf{k}_1+\mathbf{k}_2}, \quad (33)$$

where

$$\begin{aligned} \langle m'n' | V | nm \rangle &= \int d\mathbf{x}_1 d\mathbf{x}_2 \psi_{m'k_2}^*(\mathbf{x}_1) \psi_{nk_1}(\mathbf{x}_1) V(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad \times \psi_{n'k_2}(\mathbf{x}_2) \psi_{mk_1}(\mathbf{x}_2). \end{aligned} \quad (34)$$

In the coordinate representation

$$\begin{aligned} \delta V_{m'n', mn}^{\text{exch}}(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2') &= \gamma^2 \langle m'n' | V | nm \rangle \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(\mathbf{r}_2 - \mathbf{r}_2'). \end{aligned} \quad (35)$$

On going from the electron-electron to the electron-hole interaction, in accordance with (18), the operator δV^{exch} , like δV (30), retains a local character

$$\begin{aligned} \delta V_{m'n', mn}^{\text{exch}}(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2') &= \gamma^2 \langle m' \mathcal{X} | V | \mathcal{X}' n' m \rangle \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ &\quad \times \delta(\mathbf{r}_1 - \mathbf{r}_1') \delta(\mathbf{r}_2 - \mathbf{r}_2'), \end{aligned} \quad (36)$$

where $\langle m' \mathcal{X} | V | \mathcal{X}' n' m \rangle$, according to (34), is equal to

$$\langle m' \mathcal{H} n | V | \mathcal{H} n' m \rangle = \int d\mathbf{x}_1 d\mathbf{x}_2 u_{m'k_c}^*(\mathbf{x}_1) \mathcal{H} u_{n'k_c}(\mathbf{x}_1) \times V(\mathbf{r}_1 - \mathbf{r}_2) u_{m k_c}(\mathbf{x}_2) (\mathcal{H} u_{n k_c}(\mathbf{x}_2))^* \quad (37)$$

We include $\delta V^{\text{eh exc}}$, as well as (21), in the Hamiltonian \mathcal{H}^{eh} with positive sign. Formula (36) differs from that given by Elliott^[2] in that u_{nk_0} is replaced by $\mathcal{H} u_{nk_0}$.

INDIRECT EXCITONS

For an indirect exciton, when $\mathbf{k}_C \neq \mathbf{k}_V$, the wave function $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ must be expanded in terms of the product of the functions

$$\begin{aligned} \varphi_{s\mathbf{k}} &= \psi_{s\mathbf{k}_c} e^{i\mathbf{k}\mathbf{r}} = u_{s\mathbf{k}_c} e^{i(\mathbf{k}_c + \mathbf{k})\mathbf{r}}, \\ \varphi_{t\mathbf{k}} &= \psi_{t\mathbf{k}_v} e^{i\mathbf{k}\mathbf{r}} = u_{t\mathbf{k}_v} e^{i(\mathbf{k}_v + \mathbf{k})\mathbf{r}}, \end{aligned} \quad (38)$$

where $\psi_{s\mathbf{k}_c}$ and $\psi_{t\mathbf{k}_v}$ are the eigenfunctions of H_0 at the points \mathbf{k}_c and \mathbf{k}_v , respectively, for all bands.

The function $\Psi(\mathbf{x}_1, \mathbf{x}_2)$, satisfying the antisymmetry condition, takes the form

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \frac{1}{\sqrt{2}} \sum_{st} F_{st}(\mathbf{r}_1, \mathbf{r}_2) \psi_{s\mathbf{k}_c}(\mathbf{x}_1) \psi_{t\mathbf{k}_v}(\mathbf{x}_2) - F_{st}(\mathbf{r}_2, \mathbf{r}_1) \psi_{s\mathbf{k}_c}(\mathbf{x}_2) \psi_{t\mathbf{k}_v}(\mathbf{x}_1). \quad (39)$$

If we now write $F_{st}(\mathbf{r}_1, \mathbf{r}_2)$ in the form (3), we obtain in place of (4)

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \sum_{s\mathbf{k}_1 t\mathbf{k}_2} C_{s\mathbf{k}_1 t\mathbf{k}_2} \varphi_{s\mathbf{k}_1}(\mathbf{x}_1) \varphi_{t\mathbf{k}_2}(\mathbf{x}_2), \quad (40)$$

where

$$\varphi_{s\mathbf{k}_1 t\mathbf{k}_2}^2 = \frac{1}{\sqrt{2}} (\varphi_{s\mathbf{k}_1}(\mathbf{x}_1) \varphi_{t\mathbf{k}_2}(\mathbf{x}_2) - \varphi_{s\mathbf{k}_1}(\mathbf{x}_2) \varphi_{t\mathbf{k}_2}(\mathbf{x}_1)). \quad (41)$$

We substitute (40) into (1), multiply from the left by $\varphi_{s'\mathbf{k}'_1 t'\mathbf{k}'_2}^* (\mathbf{x}_1, \mathbf{x}_2)$ and integrate with respect to \mathbf{x}_1 and \mathbf{x}_2 . As a result we obtain a system of equations for $C_{s\mathbf{k}_1 t\mathbf{k}_2}$, similar to (6), in which the diagonal terms H_0 and the interband terms H_2 , just as for direct excitons, are determined respectively by Eqs. (6a) and (6c). If we neglect the short-range forces, i.e., neglect all the components of $v_{\mathbf{k}}$ with \mathbf{k} containing either the vectors of the reciprocal lattice \mathbf{b}_M or the difference $\mathbf{k}_C - \mathbf{k}_V$, then we likewise obtain for \mathcal{H}_1 an expression coinciding with (6b). In contrast, however, to the direct excitons, where it is necessary to retain in (7) the coefficients C_{st} with $s = m$ and $t = n$ and with $s = n$ and $t = m$, here the conduction band functions $\psi_{m\mathbf{k}}$ are contained only among the functions $\psi_{s\mathbf{k}_c}$, and the valence-band functions $\psi_{n\mathbf{k}_v}$ among the functions $\psi_{t\mathbf{k}_v}$. Therefore in the effective-mass approximation there are no exchange terms for the direct excitons, and the non-exchange terms are determined by the same formulas (19), (9), and (20) as for the direct exciton. If account is taken of the short-range forces, i.e., if we retain in \mathcal{H} all the components $V_{\mathbf{k}}$ with large \mathbf{k} , neglecting, just as in (28) and (33), their dependence on the small quantities \mathbf{k}_1 , \mathbf{k}'_1 , \mathbf{k}_2 , and \mathbf{k}'_2 , then we obtain as a result for the non-exchange terms a formula that coincides with (31), and for the indirect excitons, in analogy with (29), we get

$$\langle m' n' | V | m n \rangle = \int u_{m'k_c}^*(\mathbf{x}_1) u_{m k_c}(\mathbf{x}_1) V(\mathbf{r}_1 - \mathbf{r}_2) \times u_{n'k_v}^*(\mathbf{x}_2) u_{n k_v}(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2. \quad (42)$$

Since the functions of the expansion (40) constitute antisymmetrized products, when account is taken of the short range, \mathcal{H}^{eh} will include also exchange terms deter-

mined by (36), where for the indirect excitons, in analogy with (37), we have

$$\langle m' \mathcal{H} n | V | \mathcal{H} n' m \rangle = \int d\mathbf{x}_1 d\mathbf{x}_2 u_{m'k_c}^*(\mathbf{x}_1) \mathcal{H} u_{n'k_v}(\mathbf{x}_1) \times V(\mathbf{r}_1 - \mathbf{r}_2) u_{m k_c}(\mathbf{x}_2) (\mathcal{H} u_{n k_v}(\mathbf{x}_2))^* e^{i(\mathbf{k}_v - \mathbf{k}_c)\mathbf{r}(\mathbf{r}_1 - \mathbf{r}_2)}. \quad (43)$$

CONCLUSION

Thus, allowance for the exchange interaction of the conduction electrons and the valence electrons leads to electron-hole interactions of two types for the exciton: annihilation or resonant interaction (26), which depends strongly on the direction of the vector \mathbf{K} of the exciton, and exchange interaction (36), which does not depend in first approximation on the wave vector of the exciton.

The interaction (26) is connected with the slowly varying ("macroscopic") part of the interaction potential $V(\mathbf{r}_1 - \mathbf{r}_2)$, and its contribution to the energy is of the order of E_0^2/E_g , where E_0 is the exciton binding energy and E_g is the width of the forbidden band.

The contribution of the exchange interaction (36) to the energy is of the order of $E_a(a_0/a_e)^3$, where E_a is the atomic energy $\sim e^2/a_0$, and a_0 is the lattice constant, since the main contribution to the integral (39) is made by regions of small $r = |\mathbf{r}_1 - \mathbf{r}_2| \sim a_0$, for which $V(r) \sim e^2/r$.

The Hamiltonian (36) describing the exchange interaction can be written out, apart from the constants, by using the method of invariants^[15,16].

In the case when both bands are only spin-degenerate, the exchange energy for the ground state of the exciton depends only on the spins $\mathbf{s}_1 = \sigma_1/2$ and $\mathbf{s}_2 = \sigma_2/2$ of the electron and of the hole, respectively. For a cubic crystal, in the case when the extrema of both bands lie at the point $\mathbf{k}_C = \mathbf{k}_V = 0$, we can write $\delta V^{\text{eh exc}}$ in the form

$$\delta V^{\text{eh exc}} = \Delta_0 + \Delta_1(\sigma_1 \sigma_2) = \Delta_0 - 3\Delta_1 + 2\Delta_1 S^2, \quad (44)$$

where $S = \mathbf{s}_1 + \mathbf{s}_2$ is the total spin of the system. If the wave functions of the valence band $u_{n\mathbf{k}_0}$ transform at the point of the extremum like

$$Y_{\frac{3}{2}}^{\frac{3}{2}} = -\frac{i}{\sqrt{3}}[(X + iY)\beta + Z\alpha], \quad Y_{-\frac{3}{2}}^{\frac{3}{2}} = -\frac{i}{\sqrt{3}}[(X - iY)\alpha - Z\beta],$$

and those of the valence band like $R\alpha$ and $R\beta$, where α and β are spin functions and R is a function that transforms in accordance with the unity representation, and if the potential $V(r)$ has spherical symmetry, then

$$\Delta_0 = 3\Delta_1 = \frac{1}{2} |f(0)|^2 \int V(\mathbf{r}_1 - \mathbf{r}_2) \mathcal{R}^*(\mathbf{r}_1) X(\mathbf{r}_1) \mathcal{R}(\mathbf{r}_2) X^*(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (45)$$

On the other hand, if the valence band is quadruply degenerate and the basis functions $u_{n\mathbf{k}_0}$ transform like⁵⁾

$$\begin{aligned} Y_{\frac{3}{2}}^{\frac{3}{2}} &= -\frac{i}{\sqrt{2}}(X + iY)\alpha, & Y_{-\frac{3}{2}}^{\frac{3}{2}} &= \frac{i}{\sqrt{6}}[(X - iY)\alpha + 2Z\beta], \\ Y_{\frac{1}{2}}^{\frac{3}{2}} &= -\frac{i}{\sqrt{6}}[(X + iY)\beta - 2Z\alpha], & Y_{-\frac{1}{2}}^{\frac{3}{2}} &= \frac{i}{\sqrt{2}}(X - iY)\beta, \end{aligned}$$

⁵⁾The functions $Y_m^{3/2}$ and $Y_m^{3/2}$ are given here in a canonical basis [17], which differs from the Luttinger-Kohn (LK) basis used in [12] by phase factors. The matrices J_{LK} (and σ_{LK}) in the LK basis are connected with the matrices J in the canonical basis by the relations $J_{xLK} = J_y$, $J_{yLK} = J_x$, $J_{zLK} = J_z$.

then we can write the matrix $\delta V^{\text{eh exch}}$ for the ground state in the form^[10]

$$\delta V^{\text{eh exch}} = \Delta_0 + \Delta_1(\mathbf{J}\sigma) + \Delta_2 \sum_{\mathbf{j}} J_j^2 \sigma_{\mathbf{j}}, \quad (46)$$

where J_j is the matrix of the angular momentum operator J_j with $j = 3/2$.

In the case of spherical symmetry of $V(\mathbf{r})$, $\Delta_2 = 0$, and

$$\Delta_0 = \frac{3}{2} \Delta_1 = \frac{1}{2} |f_1(0)|^2 \int \mathcal{R}^*(\mathbf{r}_1) X(\mathbf{r}_1) \mathcal{R}(\mathbf{r}_2) X^*(\mathbf{r}_2) \cdot V(\mathbf{r}_1 - \mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2. \quad (47)$$

Here $f_1(\mathbf{r})$ is a smooth function that transforms in accordance with the unity representation and enters in (25) for basis functions $u_{\mu k_0}$ transforming just like $\psi_{\mu}^{[10]}$; for the remaining functions $f_{mn}(0) = 0$ ($n \neq m$).

We shall show now that allowance for the annihilation interaction (26) is completely equivalent to allowance for the interaction in the phenomenological theory^[17-19]. The spectrum of the excitons with allowance for the annihilation interaction (26) is determined by the secular equation

$$|E_j \delta_{ij} + \mathcal{H}_{ij}^e - E \delta_{ij}| = 0. \quad (48)$$

Here the exchange interaction (36) is contained in the Hamiltonian H^{eh} and the values of the energy E_j and of the function ψ_j (25) are the eigenvalues and eigenfunctions of this Hamiltonian.

As $\mathbf{K} \rightarrow 0$, according to (26), the matrix elements \mathcal{H}_{ij}^e can be written in the form of the product

$$\mathcal{H}_{ij}^e = A_i^* A_j,$$

where

$$A_j = \frac{2\hbar}{mE_g} \frac{\sqrt{\pi} e}{\sqrt{\kappa} K} \sum_{mna} f_{mn}^j(0) p_{\mathcal{X}nm}^a K^a, \quad (49)$$

and the determinant with terms of this type is equal to

$$|C_i \delta_{ij} + A_i B_j| = \prod_i C_i \left(1 + \sum_i \frac{A_i B_i}{C_i} \right). \quad (50)$$

Therefore the eigenvalues of (48) are determined by the equation

$$\prod_i (E_i - E) \left[1 + \frac{4\pi e^2}{\kappa K^2} \frac{\hbar^2}{m^2 E_g^2} \cdot \sum_{\substack{am'n'}} K^a f_{m'n'}^i(0) p_{m'n'}^a \sum_{\beta mn} f_{mn}^i(0) p_{\mathcal{X}nm}^{\beta} K^{\beta} \right]. \quad (51)$$

For optically inactive terms, for which

$$\sum_{mn} f_{mn}^i(0) p_{\mathcal{X}nm}^a = 0$$

for all α , the roots of Eq. (51) are $E_{\nu} = E_i$; in exactly the same way, for N -fold degenerate optically active terms $N-1$ roots E_{ν} become equal to E_i . The remaining roots are determined by the equation

$$\kappa + \frac{4\pi e^2}{K^2} \frac{\hbar^2}{m^2 E_g^2} \sum_i (E_i - E)^{-1} \times \sum_{am'n'} f_{m'n'}^i(0) p_{m'n'}^a K^a \sum_{\beta mn} f_{mn}^i(0) p_{\mathcal{X}nm}^{\beta} K^{\beta} = 0. \quad (52)$$

As indicated by Born and Kung Huang^[18], Pekar^[19], and Agranovich and Ginzburg^[20], the contribution of the interaction can be determined from the phenomenological equation

$$\sum_{\alpha\beta} \kappa_{\alpha\beta} K^{\alpha} K^{\beta} = 0, \quad (53)$$

if we include in κ the contribution made to the dielectric constant of the crystal $\Delta\kappa^e$ connected with the excitation of the excitons. Equation (53) follows from the equation

$$\text{div } \mathbf{D} = \sum_{\alpha\beta} K_{\alpha} K_{\beta} \kappa_{\alpha\beta} \varphi_{\alpha} = 0,$$

to which Maxwell's equation reduces if retardation is neglected.

As shown in^[20,21]

$$\Delta\kappa^e = -\frac{4\pi}{\hbar\omega^2 \mathcal{V}^e} \sum_i \frac{j_i^{\alpha} j_i^{\beta}}{\omega - \omega_i}. \quad (54)$$

It is easy to show that for an exciton described by a wave function (25), the matrix element of the current operator is

$$j_i^{\alpha} = \sqrt{\mathcal{V}^e} \sum_{mn} f_{mn}^i(0) j_{m\mathcal{X}n} = \sqrt{\mathcal{V}^e} \frac{e}{m} \sum_{mn} f_{mn}^i(0) p_{m\mathcal{X}n}^{\alpha}. \quad (55)$$

Substituting (55) and (54) in (53), we obtain an equation that coincides with (55) (recognizing that in the approximation under consideration $\hbar\omega = E_g$). This shows that formula (23) takes full account of the long-range contribution in the dipole approximation, i.e., without allowance for the dependence of the matrix elements $p_{m\mathcal{X}n}$ on \mathbf{K} . If it is necessary to take this dependence into account, then it is necessary to include in (13) terms of higher order in \mathcal{K}_2 .

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