

Influence of valence band degeneracy on the fundamental optical absorption in direct-gap semiconductors in the region of exciton effects

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The form of the fundamental absorption spectrum is found for direct-gap cubic semiconductors in the region of exciton effects subject to an allowance for the valence band degeneracy. Calculations are made of the positions of the first few exciton peaks, their intensities, profile of the continuous spectrum at photon energies $h\nu$ exceeding the band gap E_g , and fractions of light and heavy holes as a function of $h\nu - E_g$. The absorption in the exciton peaks and in the continuous spectrum is higher than that predicted by the hydrogen-like model. The difference between the absorption calculated allowing and ignoring the Coulomb effects tends to a constant value on increase in $h\nu - E_g$. Near the edge of the continuous spectrum the fraction of light holes (relative to the total number of the generated holes) is considerably less than at high values of $h\nu - E_g$ when the Coulomb effects are unimportant. A description is given of a method for numerical calculation of the levels and wave functions of the discrete spectrum and of the orthonormalized functions of the continuous spectrum of single-particle quantum systems described by partial differential equations with nonseparable variables.

1. INTRODUCTION

The profile of the fundamental absorption edge of semiconductors is governed by exciton effects.^{1,2} The Coulomb interaction between a photoelectron and a photohole gives rise to exciton absorption peaks representing the bound states of an electron and hole at photon energies $h\nu$ smaller than the band gap E_g , and at $h\nu = E_g$ the absorption coefficient does not yet vanish (as would be expected in the absence of the Coulomb effects). The absorption spectrum has been calculated by Elliott¹ allowing for the exciton effects in the simplest hydrogen-like model of an exciton in which both the conduction and valence bands are nondegenerate and isotropic. In this case the positions of the exciton peaks relative to the edge of the continuous spectrum are the same as the positions of levels of a hydrogen-like atom, the intensities of the peaks decrease on increase in the number n as n^{-3} , and in the range $h\nu > E_g$ the absorption spectrum can be determined from the known wave functions of the continuous spectrum of the hydrogen atom. The imaginary part of the optical permittivity is

$$\varepsilon''(\omega) = \frac{8\pi |d|^2}{E_{ex} a_{ex}^3} \left[1 - \exp\left(-\frac{2\pi}{k}\right) \right]^{-1},$$

$$k = \left[\frac{2(h\nu - E_g)}{E_{ex}} \right]^{1/2} \quad (1)$$

Here, d is the matrix element of the dipole moment of a transition between the bands; E_{ex} and a_{ex} is the doubled ionization energy and the effective Bohr radius of an exciton. In the simple model of Elliott the ratio of the absorption with allowance for Coulomb interaction to the absorption calculated ignoring this interaction is equal to the familiar Sommerfeld factor

$$\frac{\varepsilon''(\omega)}{[\varepsilon''(\omega)]_0} = \frac{2\pi}{k} \left[1 - \exp\left(-\frac{2\pi}{k}\right) \right]^{-1}, \quad (2)$$

which tends to unity on increase in the energy $h\nu - E_g$.

The valence band of all cubic semiconductors is degenerate even in the relatively simple case when the spin-orbit splitting Δ of the valence bands is large compared with the exciton energies, and the Hamiltonian is a 4×4 matrix. We shall consider direct-gap semiconductors. In these materials the effective mass of an electron is isotropic and the valence band nonsphericity is usually slight, i.e., we have $\delta = (\gamma_3 - \gamma_2)/\gamma_1 \ll 1$, where γ_i are the valence band parameters introduced by Luttinger. In this spherical approximation the Hamiltonian of an exciton with zero total quasimomentum can be represented in the form analogous to the Hamiltonian of an acceptor in the spherical approximation³:

$$H = \frac{1}{2} \{ \hat{p}^2 \cdot \hat{1} - \mu_{ex} (P^{(2)} \cdot J^{(2)}) \} - \frac{1}{r} \hat{1}. \quad (3)$$

Here $\hat{1}$ is a unit 4×4 matrix; $(P^{(2)} \cdot J^{(2)})$ is a scalar product of irreducible tensors of the second rank, derived in the usual way from the components of the momentum \mathbf{p} and quasispin matrices \mathbf{J} with $J = 3/2$; $\mu_{ex} = [\gamma_1 / (\gamma_1 + \gamma_e)] \mu$; $\gamma_e = m_0 / m_e$ is the ratio of the masses of a free electron and of a conduction electron; $\mu = 2(2\gamma_2 + 3\gamma_3) / 5\gamma_1$. The units of length and energy in Eq. (3) are

$$a_{ex} = \hbar^2 (\gamma_1 + \gamma_e) \varepsilon_0 / m_0 e^2, \quad E_{ex} = m_0 e^4 / \hbar^2 \varepsilon_0^2 (\gamma_1 + \gamma_e), \quad (4)$$

where ε_0 is the static permittivity.

It is known from the solution of the problem of a shallow acceptor in the spherical approximation³⁻⁶ that the quantum-mechanical problem with the Hamiltonian (1) reduces to a solution of a system of two ordinary second-order differential equations for radial functions, and that in the general case, i.e., for an arbitrary value of μ_{ex} , an analytic solution cannot be obtained. The energies of the first two lowest discrete levels of excitons are calculated in Ref. 7 for several direct-gap semiconductors, i.e., the positions of two exciton absorption peaks are found. The calculations are made in Ref. 7 on the basis that the approximate equality of

the effective masses of an electron and a light hole in direct-gap semiconductors ensures that the value of μ_{ex} does not exceed ~ 0.3 (see Table I below), i.e., this quantity is small, so that the energy levels are calculated from perturbation theory in which the zeroth approximation is the hydrogen-like limit ($\mu_{ex} = 0$). The binding energies of the excitons, allowing for the real structure of the valence band, are calculated by a variational method in Ref. 8. However, the problem of the continuous spectrum in the fundamental optical absorption region of semiconductors ($h\nu \geq E_g$) has yet to be tackled.

We shall calculate the profile of the fundamental absorption edge of direct-gap semiconductors allowing for the exciton effects and for the valence band degeneracy. We shall obtain the final (numerical) results by a numerical calculation and we shall not apply perturbation theory in μ_{ex} . We shall adopt this approach for two reasons. Firstly, the parameter μ_{ex} in the case under discussion is no longer that small and the precision of perturbation theory in respect of μ_{ex} cannot be high. On the other hand, the exciton binding energies E_b found by calculation can be used to find most accurately the band gap E_g of semiconductors by adding the excitation energy of an exciton peak to E_b (Ref. 9). Therefore, the errors in the calculation of the discrete spectrum of excitons should be reduced as much as possible and in any case below the errors associated with the inaccuracy of the determination of the energy band parameters. Secondly, the numerical method used by us is fairly general and can be (in contrast to perturbation theory in respect of μ_{ex}) applied to solve problems far from the hydrogen-like limit, particularly to calculate the exciton effects in indirect-band semiconductors.

In the physics of semiconductors one encounters many one-particle quantum systems described by partial differential equations with nonseparable variables, viz., a hydrogen-like atom in a strong magnetic field, a hole in the Coulomb field, an electron (moving in the Coulomb field), an exciton in a many-valley semiconductor, etc. Expanding the required wave function in terms of a suitable system of functions of angular and spin variables (in terms of spherical functions in the case of a nondegenerate energy band, in terms of the L - S coupling functions in the case of a degenerate band, etc.), we can reduce partial differential equations generally to an infinite system of ordinary differential equations for radial functions. However, in the case of states with a moderately high energy, the functions with fast angular oscillations should be negligible, which makes it possible to drop them and to reduce the problem to a solution of a large but finite number N of ordinary second-order differential equations.¹⁰ The method described below is not limited to the $N = 2$ case (as is true of the spherical model of an exci-

ton) and can be used to calculate not only the energies and wave functions of the discrete spectrum of the systems mentioned above, but also to find the quantities which can be expressed in terms of the functions of the continuous spectrum, such as photoionization cross sections of acceptors and donors, non-Born scattering cross sections of electrons and holes, scattering cross sections of electrons in a strong magnetic field, etc.

This approach is completely analogous to that used in the quantum scattering theory, i.e., in problems which can be reduced to multichannel scattering with a strong coupling between the channels¹¹ (scattering by a nonspherical potential, etc.). The method which is described in the Appendix 1 generalizes the methods from the theory of multichannel scattering.

2. EXPRESSION FOR THE OPTICAL ABSORPTION AND INITIAL EQUATIONS

The imaginary part of the permittivity of a cubic semiconductor, which governs the absorption spectrum, is¹²

$$\epsilon_{\alpha\beta}''(\omega) = 4\pi^2 d_{\sigma M}^{\alpha} \sum_n \psi_M^{(n)}(0) \psi_{M'}^{(n)*}(0) d_{\sigma M}^{\beta*} \delta[E_n - (h\nu - E_g)]. \quad (5)$$

Here, $\psi_M^{(n)}(0)$ is the value at the point $r = 0$ of the wave function component with $M = \pm 1/2, \pm 3/2$ describing the n th state of an exciton and representing a spinor corresponding to the total angular momentum $J = 3/2$; E_n is the energy of this state; $\sigma = \pm 1/2$ is the spin quantum number of an electron; $d_{\sigma M}^{\alpha}$ are 2×4 matrices given in Refs. 12 and 13. These matrices contain a factor d which, if we neglect the influence of the local field on the optical response, is equal to the matrix element $\langle S | ez | Z \rangle$ of the dipole moment between the Bloch functions of the conduction and valence band edges.

The eigenstates $\psi^{(n)}$ of the Hamiltonian (3) may be selected to be the states with a specific parity P , a total angular momentum F , and its projection F_z . We then find that³⁻⁶

$$\psi^{(n)}(r) = R_L^{(E_n, P, F)}(r) |LJFF_z\rangle + R_{L+2}^{(E_n, P, F)}(r) |L+2, JFF_z\rangle. \quad (6)$$

where $|LJFF_z\rangle$ are the familiar L - S coupling functions; R_L are radial functions; $L = F - 3/2$ or $L = F - 1/2$, depending on the parity P (the parity of L is the same as the parity of the state). In a discrete spectrum the radial functions are normalized by the condition

$$\int_0^{\infty} dr r^2 \{ [R_L^{(E_n, P, F)}(r)]^2 + [R_{L+2}^{(E_n, P, F)}(r)]^2 \} = 1. \quad (7)$$

In the case of a continuous spectrum we shall show that there are N (in our case $N = 2$) different solutions satisfying the condition that they be finite at $r = 0$. We shall label these

TABLE I. Parameters of GaAs, InP, and GaSb

Semiconductor	γ_1	γ_2	γ_3	m_e/m_0	ϵ_0	μ_{ex}	E_{ex} , meV
GaAs	6,85 [17]	2,10 [17]	2,90 [17]	0,0665	12,56	0,236	7,88
InP	4,95 [18]	1,65 [18]	2,35 [18]	0,0803	12,37	0,238	10,22
GaSb	12,4 [19]	4,1 [19]	5,6 [19]	0,040	15,7	0,267	2,95

solutions by the index s :

$$\int_0^\infty dr r^2 [R_L^{(EPFs)}(r) R_L^{(E'PFs')}(r) + R_{L+2}^{(EPFs)}(r) R_{L+2}^{(E'PFs')}(r)] = \delta_{ss'} \delta(E-E'). \quad (8)$$

If $r = 0$, then only the functions $R_L^{(EPFs)}$ with $P = 1$, $F = 3/2$, and $L = 0$ differ from zero. Consequently, the intensities of the exciton lines at $h\nu = E_g - |E_n|$ [with areas $\varepsilon''(h\nu)$ under the peaks] are

$$\int_{h\nu \approx E_g - |E_n|} d(h\nu) \varepsilon''(h\nu) = \frac{4\pi}{3} \frac{|d|^2}{a_{ex}^2} |R_0^{(E_n, 1, 3/2)}(0)|^2. \quad (9)$$

In the continuous spectrum at $h\nu \geq E_g$, we have

$$\varepsilon''(\omega) = \frac{4\pi}{3} \frac{|d|^2}{a_{ex}^3 E_{ex}} \sum_s |R_0^{(E, 1, 3/2, s)}(0)|^2, \quad E = \frac{h\nu - E_g}{E_{ex}}. \quad (10)$$

The radial functions in Eqs. (7)–(10) are dimensionless.

The system of equations for R_L and R_{L+2} is given in Refs. 3–6. We can go over to the functions f_l and f_h , the asymptotes of which are (in contrast to the asymptotes of R_L and R_{L+2}) sinusoidal⁶:

$$R_L = \frac{\beta f_h + f_l}{r(1+\beta^2)^{1/2}}, \quad R_{L+2} = \frac{f_h - \beta f_l}{r(1+\beta^2)^{1/2}}, \quad (11)$$

$$\beta = 3^{L-F+1} \left(\frac{F+3/2}{F-1/2} \right)^{1/2}.$$

If $F = 3/2$ and $P = 1$ ($L = 0$), one of the equations for f_l and f_h is

$$(1+\mu_{ex}) f_l'' + 2 \left(\frac{1}{r} + E \right) f_l - \frac{3\mu_{ex}}{r} f_l' - 3 \left(1 - \frac{\mu_{ex}}{2} \right) \frac{f_l}{r^2} + 3 \left(1 + \frac{\mu_{ex}}{2} \right) \frac{f_h}{r^2} = 0, \quad (12)$$

and the second is obtained by the substitutions $l \leftrightarrow h$, $\mu_{ex} \rightarrow -\mu_{ex}$.

The asymptote of the normalized solutions of the system obtained for the case $k_{|m|} r \gg 1$ is (for energies $E > 0$)

$$f_{|m|}^{(s)} \approx a_{|m|}^{(s)} \left(\frac{2}{\pi} \frac{dk_{|m|}}{dE} \right)^{1/2} \sin(k_{|m|} r + \delta_{C|m|} + \delta_{|m|}^{(s)}). \quad (13)$$

Here, $|m| = 1/2$ refers to a light hole (l) and $|m| = 3/2$ to a heavy hole (h),

$$k_{1/2, 3/2} = [2E / (1 \pm \mu_{ex})]^{1/2},$$

$a_{|m|}^{(s)}$ are the amplitudes and $\delta_{|m|}^{(s)}$ are the phases of the solutions which are bounded at zero ($s = 1$ and $s = 2$), and

$$\delta_{C|m|} = [k_{|m|} (1 \pm \mu_{ex})]^{-1} \ln(2k_{|m|} r) \quad (14)$$

is the Coulomb phase which is the same for both solutions.

Let us assume that

$$A_{s|m|} = a_{|m|}^{(s)} \exp(i\delta_{|m|}^{(s)})$$

is a matrix of complex amplitudes. It follows from Eqs. (8) and (13) that the condition of orthonormalization of solutions of the system (12) can be expressed in the form (A^+ is the Hermitian conjugate matrix)

$$\frac{1}{2} \sum_{|m|} (A_{s|m|} A_{|m|s'}^+ + A_{s'|m|} A_{|m|s}^+) = \delta_{ss'}. \quad (15)$$

It is shown in the Appendix 2 that the amplitudes $A_{s|m|}$ of the solutions of the system (12) which are finite at zero satisfy the additional condition

$$\sum_{|m|} A_{s|m|} A_{|m|s'}^+ = \sum_{|m|} A_{s'|m|} A_{|m|s}^+. \quad (16)$$

Together with Eq. (15) this condition means that the matrix of complex amplitudes is unitary, i.e.,

$$\sum_{|m|} A_{s|m|} A_{|m|s'}^+ = \delta_{ss'}. \quad (17)$$

The method for solution of systems of ordinary differential equations of the (12) type is given in the Appendix 1.

If $E = 0$, we have to transform (as in the hydrogen atom problem) to a variable $x = (8r)^{1/2}$ and to the functions $u_{|m|} = x^{-1/2} f_{|m|}$. One of the two equations for $u_{|m|}$ is

$$(1+\mu_{ex}) u_l'' + u_l - 6\mu_{ex} \frac{1}{x} u_l' - \frac{3}{4} (17-7\mu_{ex}) \frac{1}{x^2} u_l + 3(4+\mu_{ex}) \frac{1}{x^2} u_h = 0. \quad (18)$$

The second equation is obtained by the substitutions $u_l \leftrightarrow u_h$ and $\mu_{ex} \rightarrow -\mu_{ex}$.

The asymptote of the solutions of Eqs. (18) has the following form when $x \gg 1$:

$$\sin[(1 \pm \mu_{ex})^{-1/2} x + \Delta_{|m|}].$$

The amplitudes and phases of the asymptotes $u_{|m|}$ can be related to the amplitudes and phases of the asymptotes $f_{|m|}$ in the limit $E \rightarrow 0$ if we bear in mind that for $r \gg 1$ the asymptote $f_{|m|}$ is a combination of Whittaker functions

$$W_{\pm i\alpha, |m|}(\mp 2ik_{|m|} r),$$

where

$$\alpha_{|m|} = [(1 \pm \mu_{ex}) k_{|m|}]^{-1}.$$

In the limit $E \rightarrow 0$ the combination of Whittaker functions, which for $k_{|m|} r \gg 1$ reduces to Eq. (13), has the following asymptote of $u_{|m|}$ in the case when $r \gg 1$:

$$u_{|m|}(x) \approx [4\pi^2 (1 \pm \mu_{ex})]^{-1/2} a_{|m|}^{(s)} \sin[(1 \pm \mu_{ex})^{-1/2} x + \Delta_{|m|}^{(s)}], \quad (19)$$

where the phase shift is $\Delta_{|m|}^{(1)} - \Delta_{|m|}^{(2)} = \delta_{|m|}^{(1)} - \delta_{|m|}^{(2)}$. This relationship between the asymptotes of $u_{|m|}$ and $f_{|m|}$ allows us to find the orthonormalized radial functions for $E = 0$ by solving Eq. (18) subject to Eq. (19).

3. DISTRIBUTION OF PHOTOHOLES BETWEEN BRANCHES OF THE SPECTRUM AND OF PHOTOELECTRONS BETWEEN ENERGIES

Radiation of photon energy $h\nu > E_g$ generates light holes with a quasimomentum k_l and heavy holes with the quasimomentum k_h , as well as two groups of electrons with the same quasimomenta. In the limiting case $k_{|m|} \gg 1$, when the exciton effects are weak, the ratio of the numbers of light and heavy holes is $[(1 - \mu_{ex}) / (1 + \mu_{ex})]^{3/2}$. It would be of interest to determine how this ratio is affected by the exciton effects.

We can tackle this problem by selecting in Eq. (5) for $\varepsilon''(\omega)$ the functions $\psi_{\mathbf{k}m}^{(n)}$ in the form $\psi_{\mathbf{k}m}^{(n)}$, each of them

representing a superposition of a plane wave of given momentum \mathbf{k} and given helicity $m = \pm 1/2$ and $\pm 3/2$ with waves which are purely converging at infinity. This approach is a direct generalization of that employed in dealing with the photoelectric effect of atoms. The function $\psi_{\mathbf{k}m}^{(-)}$ is related to the function $\psi_{\mathbf{k}m}^{(+)}$, which is a plane wave with a given helicity plus a function which has only diverging waves at infinity. The function $\psi_{\mathbf{k}m}^{(+)}$ is calculated in Refs. 5 and 14 using the theory of scattering of a hole by a defect. However, the problem of the scattering of a hole in a Coulomb field has not yet been solved. Formulation of this problem requires additional analysis. In view of the slow fall of the Coulomb potential the Schrödinger equation has no solutions in the form of a pure plane wave together with a converging or a diverging purely spherical wave (in contrast to the potentials that decrease more rapidly than $1/r$). There are two ways of overcoming this difficulty¹⁵: 1) the use in the derivation of $\psi_{\mathbf{k}m}^{(-)}$ of a suitably deformed plane wave (with a given helicity) so that the asymptote $\psi_{\mathbf{k}m}^{(-)}$ satisfies the Schrödinger equation with the Coulomb field; 2) the truncation of the Coulomb potential at a sufficiently distant point R . We shall adopt the second method.

We shall assume that solutions of the system (12) in the region $r < R$, which are linearly independent and finite at zero, are the functions (13) with the same amplitudes and phases. If $r > R$, i.e., in the region where the potential vanishes, we find that, to within $(k_{|m|}R)^{-1} \ll 1$,

$$f_{|m|}^{(*)} = \tilde{a}_{|m|}^{(*)} (2/\pi)^{1/2} (dk_{|m|}/dE)^{1/2} \sin(k_{|m|}r + \tilde{\delta}_{|m|}^{(*)}). \quad (20)$$

From the condition of matching of the solutions (13) and (20) at the point $r = R$ it follows that, with the same accuracy $(k_{|m|}R)^{-1} \ll 1$,

$$\tilde{a}_{|m|}^{(*)} = a_{|m|}^{(*)}, \quad \tilde{\delta}_{|m|}^{(*)} = \delta_{|m|}^{(*)} + \delta_{c|m|}(R). \quad (21)$$

Strictly speaking, the orthonormalization condition (15) applies to complex amplitudes

$$\tilde{A}_{s|m|} = \tilde{a}_{s|m|}^{(*)} \exp(i\tilde{\delta}_{s|m|}^{(*)}).$$

However, when the point of truncation of the Coulomb potential R is sufficiently far, the complex amplitudes $A_{s|m|}$ differ from $\tilde{A}_{s|m|}$ only by the constant phase $\delta_{c|m|}(R)$.

In the field with the truncated potential the asymptote of the function $\psi_{\mathbf{k}m}^{(-)}$ is a combination of a plane wave of given helicity and converging spherical waves. We shall seek $\psi_{\mathbf{k}m}^{(-)}$ in the form of a superposition of states with given values of E , P , F , and F_2 . We must include in the expansion all N solutions with given quantum numbers. Using Eqs. (6) and (11), we obtain

$$\begin{aligned} \psi_{\mathbf{k}m}^{(-)}(\mathbf{r}) = & \frac{1}{r} \sum'_{PFF_2s} C(\mathbf{k}m; PFF_2s) \\ & \times \left\{ \frac{f_l^{(EPF_2s)}(r)}{(1+\beta^2)^{1/2}} [|LJFF_2\rangle - \beta |L+2, JFF_2\rangle] \right. \\ & \left. + \frac{f_h^{(EPF_2s)}}{(1+\beta^{-2})^{1/2}} [|LJFF_2\rangle + \beta^{-1} |L+2, JFF_2\rangle] \right\}. \quad (22) \end{aligned}$$

A prime of the summation sign means that for $F = 1/2$ there

is only one term in square brackets: $L = 1$ for $P = -1$ and $L = 2$ for $P = 1$.

We shall determine the coefficient C in Eq. (22) by expanding a plane wave $\psi_{\mathbf{k}m}$ with a given helicity m in terms of the L - S coupling functions. We readily obtain^{5,14}

$$\begin{aligned} \psi_{\mathbf{k}m}(\mathbf{r}) = & \sum_{LFF_2} i^L [4\pi(2L+1)]^{1/2} \\ & \times \left[\begin{matrix} L & J & F \\ 0 & m & m \end{matrix} \right] j_L(kr) D_{F_2}^{(F)} \left(\frac{\mathbf{k}}{k} \right) |LJFF_2\rangle. \quad (23) \end{aligned}$$

The matrix in brackets is the Clebsch-Gordan coefficient¹⁶ and $D_{F_2}^{(F)}(\mathbf{k}/k)$ is a finite-rotations matrix of rank $2F + 1$.

We shall use

$$\begin{aligned} \left[\begin{matrix} L & J & F \\ 0 & m & m \end{matrix} \right] = & \left(\frac{2F+1}{2L+1} \right)^{1/2} (-1)^{2F-J+m} \left[\begin{matrix} F & J & L \\ -m & m & 0 \end{matrix} \right], \\ \left[\begin{matrix} F & J & L+2 \\ -m & m & 0 \end{matrix} \right] = & \left[\begin{matrix} F & J & L \\ -m & m & 0 \end{matrix} \right] \cdot \begin{cases} \beta^{-1}, & |m| = 3/2, \\ -\beta, & |m| = 1/2 \end{cases} \end{aligned} \quad (24)$$

and reduce Eq. (23) to

$$\begin{aligned} \psi_{\mathbf{k}m}(\mathbf{r}) = & \sum'_{PFF_2} i^L (-1)^{2F-J+m} [4\pi(2F+1)]^{1/2} \\ & \times \left[\begin{matrix} F & J & L \\ -m & m & 0 \end{matrix} \right] D_{F_2}^{(F)} \left(\frac{\mathbf{k}}{k} \right) \{ j_L(kr) |LJFF_2\rangle \\ & + (\beta \delta_{|m|, 1/2} - \beta^{-1} \delta_{|m|, 3/2}) j_{L+2}(kr) |L+2, JFF_2\rangle \}. \quad (25) \end{aligned}$$

Comparing the asymptote (22) [subject to Eq. (20)] with the asymptote (25), we obtain the required expression for the coefficients in Eq. (22) from the N conditions that the amplitudes of diverging waves should vanish:

$$\begin{aligned} C(\mathbf{k}m; PFF_2s) = & i^L (-1)^{2F-J+m} \pi [2(2F+1)]^{1/2} [1 \\ & + \beta^{2(s/2-m^2)}]^{1/2} \left(k_{|m|}^2 \frac{dk_{|m|}}{dE} \right)^{-1/2} \left[\begin{matrix} F & J & L \\ -m & m & 0 \end{matrix} \right] D_{F_2}^{(F)} \left(\frac{\mathbf{k}}{k} \right) \tilde{A}_{|m|s}^{-1}. \quad (26) \end{aligned}$$

Here, the matrix \tilde{A}^{-1} is the inverse of \tilde{A} . In view of the unitary nature of the matrix \tilde{A} [see Eqs. (17) and (21)] the functions $\psi_{\mathbf{k}m}^{(-)}$ are orthonormalized:

$$\int d^3r \psi_{\mathbf{k}m}^{(-)*}(\mathbf{r}) \psi_{\mathbf{k}'m'}^{(-)}(\mathbf{r}) = (2\pi)^3 \delta_{mm'} \delta(\mathbf{k}-\mathbf{k}'). \quad (27)$$

We shall substitute in Eq. (5) the functions $\psi_{\mathbf{k}m}^{(-)}$. Since

$$(\psi_{\mathbf{k}m}^{(-)}(0))_{\mathcal{M}} = (4\pi)^{-3/2} \sum_s C(\mathbf{k}m; 1, 3/2, Ms) R_0^{(E, 1, 3/2, s)}(0), \quad (28)$$

it follows that in the case of radiation polarized along the Z axis we have

$$\begin{aligned} \varepsilon''(\omega) = & \frac{4\pi |d|^2}{3a_{ex}^3 E_{ex}} \sum_{|m|} \left| \sum_s A_{s|m|} R_0^{(E, 1, 3/2, s)}(0) \right|^2 \\ & \times \int \frac{d^3k}{4\pi} \left(k^2 \frac{dk}{dE} \right)^{-1} \\ & \times \left[1 + \left(\frac{5}{4} - m^2 \right) P_2(\cos \theta_k) \right] \delta[E_{|m|}(k) - E]. \quad (29) \end{aligned}$$

It is clear from Eq. (29) that the fractions of light holes ($|m| = 1/2$) and of heavy holes ($|m| = 3/2$) in the total number of photoholes are given by

$$c_{|m|} = \left| \sum_s A_{s|m|} R_0^{(E, 1, 3/2, s)}(0) \right|^2 \left[\sum_s |R_0^{(E, 1, 3/2, s)}(0)|^2 \right]^{-1}. \quad (30)$$

TABLE II. Energy levels of s states of discrete exciton spectrum and corresponding intensities of exciton peaks in units of $(4\pi/3)|d|^2/a_{ex}^3$.

	GaAs	InP	GaSb
$1s$	$\begin{cases} E /E_{ex} \\ E , \text{ meV} \\ R_0^2(0) \end{cases}$	$\begin{cases} 0,526 \\ 4,145 \\ 4,72 \end{cases}$	$\begin{cases} 0,527 \\ 5,386 \\ 4,73 \end{cases}$
$2s$	$\begin{cases} E /E_{ex} \\ E , \text{ meV} \\ R_0^2(0) \end{cases}$	$\begin{cases} 0,135 \\ 1,064 \\ 0,588 \end{cases}$	$\begin{cases} 0,135 \\ 1,380 \\ 0,590 \end{cases}$
$3s$	$\begin{cases} E /E_{ex} \\ E , \text{ meV} \\ R_0^2(0) \end{cases}$	$\begin{cases} 0,0633 \\ 0,499 \\ 0,165 \end{cases}$	$\begin{cases} 0,0634 \\ 0,648 \\ 0,166 \end{cases}$
$3s'$	$\begin{cases} E /E_{ex} \\ E , \text{ meV} \\ R_0^2(0) \end{cases}$	$\begin{cases} 0,0523 \\ 0,412 \\ 0,0132 \end{cases}$	$\begin{cases} 0,0523 \\ 0,534 \\ 0,0130 \end{cases}$
$E(2s) - E(1s), \text{ meV, calculation}$	3,084	4,006	1,168
$E(2s) - E(1s), \text{ meV, experiment}$	3,15 [21]	3,84(4) [22]	—

It therefore follows that the exciton effects do not affect the distribution of the directions of the momenta of photoelectrons and photoholes, but they do affect the distribution of holes between the branches of the spectrum and, consequently, the number of electrons with the momenta k_l and k_h . As expected, the truncation of the Coulomb potential does not affect the expression for $\varepsilon''(\omega)$ or the distribution of holes between the branches of the spectrum.

4. RESULTS OF CALCULATIONS

Numerical calculations were carried out for three direct-gap semiconductors, GaAs, InP, and GaSb, for which the available experimental data are the most accurate. Table I gives the values of the parameters used in our calculations. Table II lists the energies of the first four exciton s levels found in this way. We can see that the exciton binding energy $E_b = |E(1s)|$ is higher than in the hydrogen-like limit ($\mu_{ex} = 0$) and also that the levels $2s$ and $3s$ are deeper than in this limit. The levels of the s and d type, which are degenerate for $\mu_{ex} = 0$, split for $\mu_{ex} \neq 0$ and this is manifested by the appearance of a doublet (levels $3s$ and $3s'$).

The separations between the exciton peaks can be compared directly with the experimental results. Table II gives the calculated and experimental values of the difference $E(2s) - E(1s)$. The discrepancy between them ($\approx 2\%$ in the case of GaAs and $\approx 4\%$ in the case of InP) may be attributed to errors in the determination of the energy band parameters. In fact, the Hamiltonian (1) of the spherical approximation is simplified by dropping terms of the cubic symmetry, the magnitude of which is governed by the dimensionless parameter $\delta_{ex} = (\gamma_3 - \gamma_2)/(\gamma_1 + \gamma_e)$. In the case of GaAs, this parameter is $\delta_{ex} = 3.66 \times 10^{-2}$. It is known²⁰ that the cubic symmetry terms affect the levels with $F = 3/2$ only in the second order, so that we can expect the inaccuracy of the spherical approximation to be $\sim 10^{-3}$. The numerical calculations of the energy levels are accurate to within $\sim 10^{-4}$. Hence, it follows that the $\sim 10^{-2}$ discrepancy between the calculated and experimental values of $E(2s) - E(1s)$ is most probably due to inaccuracy of the determination of the energy band parameters, and more specifically of the Luttinger parameters.

It should also be pointed out that the value $E(3s) - E(2s) = 0.565 \text{ meV}$ found for GaAs is close to the experimental 0.6 meV (Ref. 21).

The exciton binding energies $|E(1s)|$ were calculated in Refs. 17–19 using the second order of perturbation theory in μ_{ex} (Ref. 7). These energies agree with those found by us within the limits of the error given in the cited papers ($\sim 10^{-2}$).

Table II lists also the values of $R_0^2(0)$, i.e., the intensities of the exciton lines in units of $(4\pi/3)|d|^2/a_{ex}^3$. If $\mu_{ex} = 0$, this quantity is equal to $4/n^2$, where n is the level number. We can see that the intensities of the $1s - 3s$ peaks increase on increase in μ_{ex} . The $3s'$ line, which appears because of the $s-d$ splitting, is very weak and very close to $3s$ and, therefore, it is difficult to resolve.

We shall now consider the continuous spectrum. If $\varepsilon''(h\nu)$ is plotted in the range $h\nu > E_g$ in units of $(4\pi/3)|d|^2/a_{ex}^3 E_{ex}$ and the difference $h\nu - E_g$ in units of E_{ex} , then similar curves are obtained for GaAs, InP, and GaSb because of the similarity of the corresponding values of μ_{ex} . Figure 1 shows the dependence $\varepsilon''(h\nu)$ for GaAs. It is qualitatively the same as in the hydrogen-like limit: we have $\varepsilon''(E_g) \neq 0$ and the difference $\varepsilon''(h\nu) - [\varepsilon''(h\nu)]_0$, where $[\varepsilon''(h\nu)]_0$ is the value of $\varepsilon''(h\nu)$ obtained ignoring the exciton effects, tends to a constant value on increase in $h\nu - E_g$.

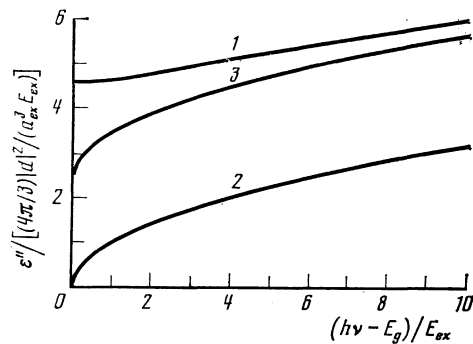


FIG. 1. Frequency dependences of the imaginary part of the permittivity calculated for $\mu_{ex} = 0.236$ (GaAs): 1) allowing for the exciton effects and the valence band degeneracy; 2) ignoring the exciton effects; 3) curve 2 shifted by the asymptotic difference $\varepsilon'' - [\varepsilon'']_0$ (see Table III).

TABLE III. Parameters of optical absorption spectra at photon energies $h\nu > E_g$: $\varepsilon''(E_g)$, asymptotic value of difference $\varepsilon''(h\nu) - [\varepsilon''(h\nu)]_0$ at $h\nu - E_g \gg E_{ex}$ in units $(4\pi/3)|d|^2/a_{ex}^3 E_{ex}$ (see text), and fraction of light holes $c_{1/2}$ for $h\nu = E_g$ and $h\nu - E_g \gg E_{ex}$

Semiconductor	$\varepsilon''(E_g)$	$\varepsilon''(h\nu) - [\varepsilon''(h\nu)]_0$	$c_{1/2}(E_g)$	$c_{1/2}(\infty)$
GaAs	4,546	2,46	0,075	0,327
InP	4,555	2,46	0,074	0,326
GaSb	4,718	2,58	0,061	0,306

Table III lists both the values of $\varepsilon''(E_g)$ and the asymptotic values of the difference $\varepsilon'' - [\varepsilon'']_0$. If $\mu_{ex} = 0$, these quantities amount to (in the units given above) 4 and 2, respectively. We can see that when μ_{ex} is increased, both quantities rise and their ratio changes.

Comparison of the calculated value of $\varepsilon''(E_g)$ with that deduced from the measured absorption coefficient,

$$\alpha(E_g) = \varepsilon''(E_g) E_g / \hbar c e^{\frac{1}{2}} \text{opt.}$$

allows us to find $|d|$. In the case of GaAs, InP, and GaSb, we have $\alpha(E_g) = 9.3 \times 10^3 \text{ cm}^{-1}$ (Ref. 23), $10.7 \times 10^3 \text{ cm}^{-1}$ (Ref. 24), and $4.0 \times 10^3 \text{ cm}^{-1}$ (Ref. 25). This comparison shows that the value of $|d|$ for these semiconductors is, respectively, 16.7, 13.3, and 16.2 (in atomic units of $\hbar^2/m_0 e$).

On the other hand, the value of d found by the one-electron theory ignoring the correction for the local field is equal to the matrix element of the dipole moment between the Bloch functions of the energy band edges (see Sec. 2 above). In this case we have $d = dP/E_g$, where $P = \hbar \langle S | p_z | Z \rangle / m_0$. The value of P is known from the $\mathbf{k} \cdot \mathbf{p}$ variant of perturbation theory and, according to Ref. 26, it amounts to 0.73, 0.62, and 0.71 for GaAs, InP, and GaSb, respectively (in atomic units of e^2). The corresponding values of $|d|$ expressed in atomic units are 13.0, 11.8 and 24.0. We can see that the values of $|d|$ found from the optical absorption spectra and from the $\mathbf{k} \cdot \mathbf{p}$ perturbation theory do not agree. The difference is due to the fact that the optical response includes a contribution not only of the macroscopic field, but also of the local field with wave vectors close to the reciprocal lattice vectors (for a discussion of this point see Ref. 27).

It is interesting to consider the spectral dependence of the fraction of light $c_{1/2}$ and heavy $c_{3/2} = 1 - c_{1/2}$ holes in the total number of holes generated by light of $h\nu > E_g$ photon energy. It is known that if $h\nu - E_g \gg E_{ex}$, when the Coulomb effects are negligible, we find that

$$c_{1/2} = \left\{ 1 + \left(\frac{1 + \mu_{ex}}{1 - \mu_{ex}} \right)^{1/2} \right\}^{-1}, \quad h\nu - E_g \gg E_{ex}. \quad (31)$$

Lowering of the photon energy $h\nu$ reduces rapidly the fraction of light holes and increases that of heavy holes (Fig. 2), so that at $h\nu = E_g$ the former is approximately a quarter of the value obtained from Eq. (31) (see Table III). This effect becomes rapidly stronger on increase in μ_{ex} .

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APPENDIX 1

We shall consider a system of N ordinary second-order differential equations of the (12) type. We shall denote the required functions by y_2, \dots, y_N and we shall assume that $y_{i+N} = ry'_i$. The system of equations in question assumes the form of a system of $2N$ ordinary first-order equations:

$$y'_i = \hat{A}_{ij}(r) y_j, \quad (\text{A.1.1})$$

where \hat{A} is a square matrix of the order of $2N$.

In the problem of an exciton under consideration, as well as in the problems of shallow impurities or scattering in the Coulomb field in the absence of a magnetic field, we have

$$\hat{A}(r) = r^{-1} \hat{A}_0 + \hat{A}_1 + r \hat{A}_2, \quad (\text{A.1.2})$$

where \hat{A}_0 , \hat{A}_1 , and \hat{A}_2 are independent of r .

The matrix \hat{A}_0 is Hermitian-like (all its eigenvalues are real) and, therefore, it can be represented in the form

$$(\hat{A}_0)_{ij} = T_{in} \lambda_n T_{nj}^{-1}, \quad (\text{A.1.3})$$

where T is a $2N \times 2N$ transformable matrix; the index n labels the eigenvalues λ_n ($n = 1, \dots, 2N$). In the case of equations for the functions f with the sinusoidal asymptote, these eigenvalues are $\lambda_n = \dots, -L-2, -L, L+1, L+3, \dots$ [in the case of the equations for the radial functions it follows from Eq. (11) that the eigenvalues λ_n are smaller by unity].

If we change over from the functions y_i to $z_n = T_{nj}^{-1} y_j$, we find that in the matrix of the coefficients on the right-hand side the term with the lowest degree is λ_n/r . Hence, it follows that the condition specifying finite solutions at $r = 0$ represents vanishing of those N of the quantities $z_n(0)$ which correspond to $\lambda_n < 1$ [when equations for the radial functions $R_L(r)$ are solved, the condition becomes $\lambda_n < 0$]:

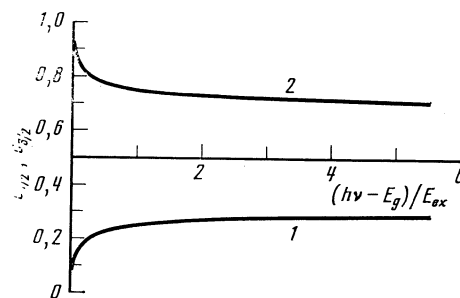


FIG. 2. Frequency dependences of the fractions of light (curve 1) and heavy (curve 2) holes in the total number of holes generated optically for $\mu_{ex} = 0.236$ (GaAs).

$$T_{nj}^{-1}y_j(0)=0, \quad \lambda_n < 1. \quad (\text{A.1.4})$$

We thus have N solutions for $2N$ quantities.

The condition that (A.1.4) be bounded at the point $r=0$ can be applied at a finite point r (such transfer of the boundary conditions is discussed in the review in Ref. 28 and also in Refs. 29 and 30), where it becomes

$$\varphi_{nj}(r)y_j(r)=0. \quad (\text{A.1.5})$$

The matrix $\varphi(r)$, which in our case has N rows and $2N$ columns, satisfies the matrix system of equations²⁸

$$\varphi' + \varphi A - \varphi A \varphi^+ (\varphi \varphi^+)^{-1} \varphi = 0 \quad (\text{A.1.6})$$

and the initial condition (A.1.4):

$$\varphi_{ni}(0) \equiv (\varphi_0)_{ni} = T_{ni}^{-1}. \quad (\text{A.1.7})$$

It is important to note that $\varphi(r)$ can be expanded near the point $r=0$ as a power series,²⁸ in contrast to individual solutions of the system (A.1.1). In particular, if r_0 is sufficiently small, then

$$\varphi(r_0) = \varphi_0 + r_0 \varphi_1. \quad (\text{A.1.8})$$

The matrix φ_1 found by substituting Eq. (A.1.8) into Eq. (A.1.6) and equating to zero the sum of all the terms on the left-hand side that do not depend on r_0 . The matrix $\varphi(r)$ specified at near-zero but finite point r_0 can be transferred by means of Eq. (A.1.6) to an arbitrary point $r_1 \geq 1$.

Let us assume that $y^{(q)}(r)$ ($q=1, \dots, 2N$) are such vector solutions of Eq. (A.1.1.) for which in the limit $r \rightarrow \infty$ only one function (f_l or f_h) differs from zero and it is given either by

$$[(2/\pi)(dk/dE)]^{1/2} \sin(kr + \delta_c)$$

or by

$$[(2/\pi)(dk/dE)]^{1/2} \cos(kr + \delta_c),$$

where $k = k_l$ or k_h , and δ_c is the Coulomb phase of Eq. (14). These $2N$ solutions (N sinusoidal and N cosinusoidal) are orthonormalized, but they do not satisfy the condition at zero.

The method of asymptotic expansions of solutions of ordinary differential equations (see, for example, Ref. 31) can be used readily to obtain a correction $\sim r_\infty^{-1}$ to asymptotic solutions $y^{(q)}(r)$ at a sufficiently distant point r_∞ . This makes it possible to solve $2N$ Cauchy problems starting from the finite point r_∞ and then obtain $2N$ vectors $y^{(q)}(r_1)$ at the same point r_1 to which the matrix $\varphi(r)$ specifying the finite nature of the solutions at zero is transferred. We shall seek solutions in the form

$$y_i(r) = \sum_q a_q y_i^{(q)}(r), \quad (\text{A.1.9})$$

where a_q are the amplitudes. Substituting Eq. (A.1.9) into the finite solution condition (A.1.5) taken at an intermediate point r_1 , we obtain N homogeneous equations for $2N$ amplitudes a_q :

$$\sum_q a_q \sum_i \varphi_{ni}(r_1) y_i^{(q)}(r_1) = 0, \quad n=1, \dots, N. \quad (\text{A.1.10})$$

This system has N linearly independent solutions $a_q^{(s)}$ ($s=1, \dots, N$), which should be orthonormalized:

$$\sum_q a_q^{(s)} a_q^{(s')} = \delta_{ss'}. \quad (\text{A.1.11})$$

Knowing the amplitudes, we can find N orthonormalized solutions for the radial functions at any point $r > r_0$.

We can obtain the eigenvalues of the energy E and the eigenfunctions of a discrete spectrum by writing down at a sufficiently distant point r_∞ the condition for finite solutions at infinity^{29,32} [N conditions for $2N$ quantities $y_i(r_\infty)$] and then use Eq. (A.1.6) to transfer this condition from r_∞ to an intermediate point r_1 . At this point we obtain $2N$ homogeneous solutions for $2N$ quantities $y_i(r_1)$ (N conditions for finite solutions at zero and N conditions for finite solutions at infinity). The eigenvalues are found by equating to zero the determinant of the system.

APPENDIX 2.

Unitarity of a matrix of complex amplitudes

We shall multiply term-by-term the first equation in the system (12) for the first solution $f_{|m|}^{(1)}$ by the function $f_i^{(2)}(r)$ and the second equation by $f_h^{(2)}$. We can similarly multiply equations for $f_{|m|}^{(2)}$ by $f_l^{(1)}$ and $f_h^{(1)}$, and subtract from the first equation of the first system the first equation of the second system, and then from the second equation of the first system the second equation of the second system, and then we shall add the results. This shows that $dW/dr = 0$, where

$$W(r) = (1 + \mu_{ex}) \left[f_l^{(2)} \frac{df_l^{(1)}}{dr} - f_l^{(1)} \frac{df_l^{(2)}}{dr} \right] + (1 - \mu_{ex}) \left[f_h^{(2)} \frac{df_h^{(1)}}{dr} - f_h^{(1)} \frac{df_h^{(2)}}{dr} \right] + \frac{3\mu_{ex}}{r} (f_l^{(1)} f_h^{(2)} - f_l^{(2)} f_h^{(1)}). \quad (\text{A.2.1})$$

For those solutions which are finite at zero, we find that $f_{|m|} \rightarrow 0$ in the limit $r \rightarrow 0$ and this variation is not slower than r , so that $W(0) = 0$ and, therefore, for all values of r , we have

$$W(r) = 0. \quad (\text{A.2.2})$$

Similar relationships [with $W(r)$ without the last term] are well known from the quantum theory of multichannel scattering¹¹ and they follow from the Hermitian nature of the problem.

Substituting in Eq. (A.2.2) the asymptotic expression (13) for the functions $f_{|m|}^{(s)}$ in the limit $k_{|m|} r \rightarrow \infty$, we obtain

$$\sum_{|m|} a_{|m|}^{(1)} a_{|m|}^{(2)} \sin(\delta_{|m|}^{(1)} - \delta_{|m|}^{(2)}) = 0. \quad (\text{A.2.3})$$

This can be written in the form (16) and hence [allowing for the orthonormalization condition (15)] we find that the matrix of complex amplitudes (17) is unitary.

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