

# Multiparticle description of surface excitons in semiconductors

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It is shown that a bound electron-hole state with large c.m.s. momentum exists in degenerate semiconductors. The binding energy of such a state exceeds the binding energy of an electron and a hole with zero c.m.s. momentum. The formation of the bound state is tracked in one-, three-, and quasi-two-dimensional systems. Quasi-two-dimensional systems are most convenient for the observation of the described effect.

## 1. INTRODUCTION

The existence of a bound state of an electron and a hole in three-dimensional systems against the background of a large number of free electrons was first predicted in Ref. 1. A similar effect was predicted in quasi-two-dimensional systems in Ref. 2, while in Ref. 3 were presented calculations of the binding energy of a surface exciton as a function of the carrier density. The ground-state energy was determined in Refs. 2 and 3 by using an equation whose validity for the many-particle problem had not been proved. In Ref. 3, furthermore, in an investigation of high densities it was recognized that account must be taken of the filling of  $\mathbf{k}$  space, but this account was quite rough.

All the computations described above were carried out for a case when the momentum  $\mathbf{P}$  of the exciton mass center was zero. This constraint is justified in the study of direct transitions, when transitions with  $\mathbf{P} \neq 0$  are forbidden by the momentum-conservation law.<sup>4</sup> In semiconductors with a many-valley band structure, however, the situation is different, and optical transitions proceed with participation of a third particle (phonon, impurity, etc.). In such semiconductor transitions into states with  $\mathbf{P} \neq 0$  are allowed. It is therefore of interest to find the exciton energy dispersion law  $\Omega(\mathbf{P})$ . It is necessary here to take into account the orthogonality of the exciton wave function to the wave functions of the free particles filling states with energy lower than the Fermi energy.

We obtain in this paper, using the Bethe–Salpeter (BS) equation, the binding energy of an exciton at zero temperature in degenerate one-, three-, and quasi-two-dimensional systems. The most convenient for the study of such an exciton are apparently quasi-two-dimensional systems. On the one hand, it is possible in them to get around the complexities connected with the anisotropy of the effective-mass tensor for a multivalley band, since there usually exists a surface over which the effective mass is isotropic. On the other hand, it is easy to vary the carrier density, and hence the maximum momentum of the distribution ( $k_F$ ).

We shall show that the bound state (exciton) obtained in Ref. 1 at  $P=0$  exists also at larger  $P$  of order  $k_F(m_1 + m_2)/m_1$ , where  $m_1$  and  $m_2$  are respectively the effective masses of the electron and hole (the major carriers are the electrons), and the binding energy is in this case substantially higher than for  $P=0$ . In addition, whereas at  $P=0$  the gap between the exciton energy and the energy of the free electron-hole decreases exponentially with increase of  $k_F$ , in the case of large  $P$  this gap has a complicated dependence on  $k_F$  and a section exists where the dependence of the

gap width on  $k_F$  is not exponential. We shall also derive, on the basis of these BS equation, equations that make it possible to determine in the most vital quasi-two-dimensional case the binding energy of an exciton in the limit of high and low electron densities in the channel. It will be shown that for low densities the equation obtained agrees with the equation used in Refs. 2 and 3.

In Sec. 2 we obtain an expression for the exciton from the BS equation. By way of an example that permits all the calculations to be carried through to conclusion and to understand the structure of the solution, this equation will be solved in Sec. 3 in the one-dimensional case of a  $\delta$ -like potential. In addition, approximate solutions of this equations will be obtained in Secs. 4 and 5 for a Coulomb potential in the three- and quasi-two-dimensional cases, respectively. All the calculations are made in the lowest order in the gas parameter. It is shown in the Appendix how to obtain from the result an equation that is valid in the low-density limit.

## 2. EQUATION FOR THE EXCITON SPECTRUM WITH ALLOWANCE FOR $\mathbf{k}$ -SPACE OCCUPANCY

We obtain an equation that describes an exciton in a quasi-two-dimensional electron gas, for example in an electron accumulation layer in an MIC structure. From this case it is easy to go over to others by assuming, for example, for the three-dimensional case that the motion is free along all of three coordinates. We shall not consider the complicated character of the valence band, i.e., we shall assume that the holes have an isotropic effective mass  $m_2$ . We assume that one hole was produced in the bulk of the semiconductor, and study the bound states of the hole and an electron. The Hamiltonian of the system takes in the second-quantization the form

$$H = \int d\mathbf{x} \{ -\Psi_e^+(\mathbf{x}) \hat{K}_e \Psi_e(\mathbf{x}) + \Phi_{HF^e}(\mathbf{x}) \Psi_e^+(\mathbf{x}) \Psi_e(\mathbf{x}) - \Psi_h^+(\mathbf{x}) \hat{K}_h \Psi_h(\mathbf{x}) + \Phi_{HF^h}(\mathbf{x}) \Psi_h^+(\mathbf{x}) \Psi_h(\mathbf{x}) \} + \int d\mathbf{x} d\mathbf{y} N \{ \frac{1}{2} \Psi_e^+(\mathbf{x}) \Psi_e^+(\mathbf{y}) V(\mathbf{x}-\mathbf{y}) \Psi_e(\mathbf{y}) \Psi_e(\mathbf{x}) - \Psi_e^+(\mathbf{x}) \Psi_h^+(\mathbf{y}) V(\mathbf{x}-\mathbf{y}) \Psi_h(\mathbf{y}) \Psi_e(\mathbf{x}) + \frac{1}{2} \Psi_h^+(\mathbf{x}) \Psi_h^+(\mathbf{y}) V(\mathbf{x}-\mathbf{y}) \Psi_h(\mathbf{y}) \Psi_h(\mathbf{x}) \}. \quad (1)$$

We assume that the width of the band gap  $E_g$  is much larger than all other energies, and therefore carry out all the calculations accurate to  $E_g^{-1}$ . The quantities  $\psi_e$  and  $\psi_h$  are the field operators of the electrons and the holes,  $\hat{K}_e$  and  $\hat{K}_h$  are the kinetic-energy operators of the electrons and the holes.  $N$  is the normal ordering symbol, and  $V(\mathbf{x}-\mathbf{y}) = 1/|\mathbf{x}-\mathbf{y}|$  is the Coulomb potential. We use an atomic system of units. The potentials  $\Phi_{HF}^{e,h}$  are self-consistent and obtained by solv-

ing single-particle Hartree-Fock equation; it was their separation in (1) which lead to the appearance of the symbol of normal ordering in front of the two-particle interaction operator. The Hartree-Fock equations for the inversion layer in the MDC structure have been solved, for example, in Ref. 5. In the mixed representation, the Green's functions of the electrons and holes take the form

$$G(\mathbf{k}, z_1, z_2, \omega) = \sum_{\alpha} \frac{\varphi_{\mathbf{k},\alpha}(z_1) \varphi_{\mathbf{k},\alpha}(z_2)}{e_{\alpha}(\mathbf{k}) - \omega - i0 \operatorname{sign}(e_{\alpha} - \mu)}. \quad (2)$$

Here  $\mu$  is the level of the carrier chemical potential,  $\mathbf{k}$  is the quasimomentum in the plane of the boundary, and  $z$  is the coordinate perpendicular to the boundary. In the zeroth approximation  $e_{\alpha}(\mathbf{k})$  and  $\varphi_{\mathbf{k},\alpha}(z)$  are the eigenfunction and eigenvalues corresponding to the Hartree-Fock equation.

The electron-hole binding energy is determined by the poles of the total vertex of the electron-hole interaction. To find these poles it suffices to solve a homogeneous BS equation (Fig. 1). In the limit  $k_F \gg 1$ , where the random-phase approximation can be used, one can choose for  $K$  a screened Coulomb potential  $V_{\text{eff}}$ . In the opposite case  $k_F \ll 1$   $K$  must be replaced by  $V$ . Inclusion in  $K$  of diagrams with more than one potential  $V_{\text{eff}}$  leads to corrections that are small in the gas parameter  $r_s$  (Ref. 1). (The quantity  $r_s$  is proportional to  $k_F$  at  $k_F \ll 1$  and to  $k_F^{-1}$  at  $k_F \gg 1$ .)

After simple transformations,<sup>6</sup> introducing in lieu of the total vertex a new variable  $\chi$ , we get

$$\begin{aligned} i\chi(\mathbf{k}_1, \mathbf{k}_2, z_1, z_2, \Omega, \delta) &= \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\omega}{2\pi} dz_3 dz_4 G_e\left(\mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} + \delta\right) \\ &\times G_h\left(\mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} - \delta\right) V_{\text{eff}}(\mathbf{k}, z_3, z_4, \delta - \omega) \\ &\times \chi(\mathbf{k}_1 - \mathbf{k}, \mathbf{k}_2 + \mathbf{k}, z_3, z_4, \Omega, \omega). \end{aligned} \quad (3)$$

To calculate  $V_{\text{eff}}$  in the limit of large  $k_F$  it is necessary to sum over all the loop diagrams. The entire frequency dependence in  $V_{\text{eff}}$  is then contained in the polarization operator. From the explicit form of this operator (see, e.g., Ref. 7) it is seen that its dependence on the frequency is weak and can be neglected. Moreover, allowance for a finite screening radius leads only to a correction of higher order in the gas parameter to the Fourier transform of the potential for particles on the Fermi surface. This will lead, as will be shown below, to logarithmic corrections to the exciton binding energy. Allowance for these corrections will generally speaking be an exaggeration of the accuracy of the estimates, and  $V_{\text{eff}}$

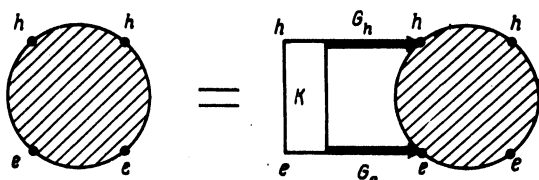


FIG. 1. Homogeneous Bethe-Salpeter equation. Hatched circle—sought total vertex, rectangle—analogue of potential, thick lines—Green's functions of particles.

can be assumed equal to  $V$  wherever it does not lead to divergence of the integral. The right-hand side of (3) can then be integrated over  $\omega$ , and the entire equation (3) over  $\delta$ , and we can put

$$\int \frac{d\omega}{2\pi} \chi(\mathbf{k}_1, \mathbf{k}_2, z_1, z_2, \Omega, \omega) = \chi(\mathbf{k}_1, \mathbf{k}_2, z_1, z_2, \Omega).$$

For the function  $\chi$ , which is the analog of the electron-hole wave function, we obtain the equation

$$\begin{aligned} i\chi(\mathbf{k}_1, \mathbf{k}_2, z_1, z_2, \Omega) &= \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\delta}{2\pi} dz_3 dz_4 G_e\left(\mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} + \delta\right) \\ &\times G_h\left(\mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} - \delta\right) V(\mathbf{k}, z_3, z_4) \chi(\mathbf{k}_1 - \mathbf{k}, \mathbf{k}_2 + \mathbf{k}, z_3, z_4, \Omega). \end{aligned} \quad (4)$$

It is shown in the Appendix that in the limit as  $k_F \rightarrow 0$  Eq. (4) reduces to the Schrödinger equation used in Refs. 2 and 3 to calculate the binding energy of a surface exciton.

As shown in Refs. 2 and 3, Eq. (4) has a bound state in the limit  $k_F \ll 1$ . It is analogous to the state obtained by Mahan<sup>1</sup> for an electron-hole pair in the bulk of a semiconductor.

In the calculation of the Green's function  $G_e$  in (4) one can disregard electron interaction with a single hole. This function can be represented by a sum of two parts, one corresponding to an electron localized in a surface potential well, and the other to a free electron in the bulk of the semiconductor (it is assumed for simplicity that there is only one filled subband in the potential well). The right-hand side of (4) is then represented as a sum of two parts, one corresponding to the surface exciton and the other to a bulk exciton. If the energies of the surface and bulk excitons differ greatly, the bulk-exciton contribution can be neglected in the calculation of the surface exciton, and vice versa. The case of close energies of the surface of bulk excitons calls for a separate analysis.

In the Green's function, account must be taken of its interaction with quasi-two-dimensional electrons. At large  $z$  this interaction reduces to the known electrostatic image forces. Allowance for these forces at small  $z$  is quite complicated, and its analysis is not part of our problem. It is assumed below that the image forces are included in the initial Hartree-Fock equation. The hole Green's function takes then the form

$$G_h(\mathbf{k}, z_1, z_2, \omega) = \sum_{\beta} \frac{\psi_{\beta}(z_1) \psi_{\beta}^*(z_2)}{e_{\beta}(\mathbf{k}) - \omega - i0}.$$

Here  $\psi_{\beta}(z)$  is obtained from the solution of a Dyson equation in which image forces are taken into account in the mass operator. It will be shown below that the form of  $\psi_{\beta}$  is not too important for the determination of the main contribution to the binding energy.

Retaining in  $G_e$  only the surface contribution, we integrate (4) with respect to  $\delta$ :

$$\begin{aligned} \chi(\mathbf{k}_1, \mathbf{k}_2, z_1, z_2, \Omega) &= \int \frac{d\mathbf{k}}{(2\pi)^2} dz_3 dz_4 \sum_{\beta} \frac{\varphi_{\mathbf{k}_1}(z_1) \varphi_{\mathbf{k}_1}(z_3) \psi_{\beta}(z_2) \psi_{\beta}^*(z_4)}{e_e(\mathbf{k}_1) + e_{\beta}(\mathbf{k}_2) - \Omega} \theta(|\mathbf{k}_1| - k_F) \\ &\times V(\mathbf{k}, z_3, z_4) \chi(\mathbf{k}_1 - \mathbf{k}, \mathbf{k}_2 + \mathbf{k}, z_3, z_4, \Omega) \end{aligned}$$

[here  $\theta(x)$  is the Heaviside step function and  $\varepsilon_c$  is the single-particle energy of an electron in the bare Green's function].

It is convenient in this equation to change to the c.m.s. system:

$$\mathbf{P} = \mathbf{k}_1 + \mathbf{k}_2, \quad \mathbf{q} = (m_2 \mathbf{k}_1 - m_1 \mathbf{k}_2) / M,$$

$$M = m_1 + m_2, \quad \mu = m_1 m_2 / M.$$

We then obtain ultimately

$$\chi(\mathbf{P}, \mathbf{q}, z_1, z_2, \Omega) = \theta\left(\left|\mathbf{q} + \frac{m_1}{M} \mathbf{P}\right| - k_F\right) \int \frac{d\mathbf{k}}{(2\pi)^2} dz_3 dz_4$$

$$\times V(\mathbf{k} - \mathbf{q}, z_3, z_4) \sum_{\beta} \frac{\varphi(z_1) \varphi(z_3) \psi_{\beta}(z_2) \psi_{\beta}^*(z_4)}{\varepsilon_c(m_1 \mathbf{P} / M + \mathbf{q}) + \varepsilon_{\beta}(m_2 \mathbf{P} / M - \mathbf{q}) - \Omega}$$

$$\times \chi(\mathbf{P}, \mathbf{k}, z_3, z_4, \Omega). \quad (5)$$

### 3. ONE-DIMENSIONAL MOTION WITH SHORT-RANGE POTENTIAL

To understand better the structure of the states that set in during the solution of (5), we consider first one-dimensional motion with short range potential  $V(x) = V_0 \delta(x)$ . In this case one starts out with the Green's functions of the free particles, and Eq. (5) is correspondingly rewritten in the form

$$\chi(P, q, \Omega)$$

$$= \theta\left(\left|q + \frac{m_1}{M} P\right| - k_F\right) \int_{-\infty}^{\infty} \frac{dk}{2\pi} V_0 \frac{\chi(P, k, \Omega)}{q^2 / 2\mu + P^2 / 2M - \Omega}.$$

(6)

(We have chosen  $P > 0$ ). Integrating this equation over  $dq/2\pi$ , we obtain an equation for the eigenvalues:

$$1 = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \theta(|q + P'| - k_F) \frac{V_0}{q^2 / 2\mu + P^2 / 2M - \Omega}, \quad P' = \frac{m_1}{M} P.$$

Equation can thus be integrated, and as a result we get for  $P^2 / 2M - \Omega < 0$  and  $\lambda^2 = 2\mu(\Omega - P^2 / 2M)$

$$1 = \frac{\mu V_0}{2\pi} \frac{1}{\lambda} \ln \left| \frac{(k_F + \lambda)^2 - P'^2}{(k_F - \lambda)^2 - P'^2} \right|, \quad (7a)$$

and for  $P^2 / 2M - \Omega > 0$  and  $\lambda^2 = 2\mu(P^2 / 2M - \Omega)$  we have

$$1 = \frac{\mu V_0}{\lambda \pi} \left( \pi - \operatorname{arctg} \frac{k_F - P'}{\lambda} - \operatorname{arctg} \frac{k_F + P'}{\lambda} \right). \quad (7b)$$

Equation (7a) goes over into (7b) at  $\lambda = 0$ , i.e., when<sup>1)</sup>

$$P'^2 - k_F^2 = -2k_F \mu V_0 / \pi.$$

In the region  $m_1 P / M < k_F$  it is easy to obtain an approximate analytic solution of Eq. (7a) as  $V_0 \rightarrow 0$ :

$$\Omega = \frac{P^2}{2M} + \frac{(k_F - P')^2}{2\mu} - \frac{k_F - P'}{\mu} \left\{ \left[ P'^2 + 4k_F(k_F - P') \right. \right.$$

$$\left. \left. \times \exp\left(-\frac{2\pi(k_F - P')}{\mu V_0}\right) \right]^{1/2} - P' \right\}, \quad (8a)$$

and a solution of Eq. (7b) in the region  $P' > k_F$ :

$$\Omega = \frac{P^2}{2M} - \frac{(\mu V_0)^2}{2\mu} \left( 1 + \frac{\mu V_0}{\pi(P' - k_F)} \right)^{-2}. \quad (8b)$$

The exact solution shown in Fig. 2 differs substantially from (8a) or (8b) only in the vicinity of the intersection point of curve  $\Omega(P)$  and the function  $P^2 / 2M$ .

Let us examine in detail the picture in Fig. 2. It shows in addition to the  $\Omega(P)$  plot also the dependence of the energy of the free electron-hole pair with electron momentum  $k_1 = k_F$  on the mass-center momentum  $P$ :

$$E_p(P) = \frac{P^2}{2M} + \frac{1}{2\mu} \left( k_F - \frac{m_1}{M} P \right)^2,$$

and a plot of the function  $P^2 / 2M$ . These parabolas are tangent at the point  $m_1 P / M = k_F$ . In this case the minimum energy of the free electron-hole pairs in which the electron occupies a state with energy higher than the Fermi energy and the hole has arbitrary energy, equal to  $E_p(P)$  ( $k_1 = k_F$ ) for  $m_1 P / M < k_F$  and to  $P^2 / 2M$  ( $k_1 = m_1 P / (m_1 + m_2)$ ) for  $m_1 P / M > k_F$ . The energy of an exciton with a given  $P$  should be lower than the free-pair energy. At the inverse ratio of these energies, the exciton state is either nonexistent or is quasistationary. The distinctive feature of the one-dimensional case is that the exciton state exists for all  $P$ . However, regardless of the dimensionality of space, the binding energy is exponentially small as  $P \rightarrow 0$  [see (8a)], and at  $m_1 P / M \sim k_F$  the binding energy has a power-law dependence on  $V_0$ . The cause of this difference is that for  $P = 0$  the electron and the hole move counter to each other, while at  $P = M k_F / m_1$  they move in parallel, and this leads to a more effective interaction between them. Note that  $P = 0$  corresponds to the local maximum of the exciton energy ( $d^2 \Omega / dP^2|_{P=0} < 0$ ).

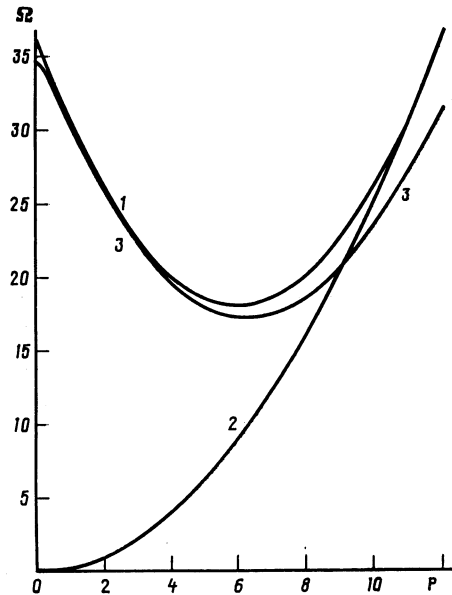


FIG. 2. Dependence of the energy  $\Omega$  of a one-dimensional exciton on the mass-center momentum  $P$  for the case  $m_1 = m_2 = 1$ ,  $k_F = 6$ ,  $V_0 = 8$  (curve 3). Curve 1 up to the point of tangency with curve 2—minimum energy of free electron-hole pair with electron momentum  $k_1 > k_F$ . Past the tangency point the minimum energy of such a pair is described by curve 2.

#### 4. DISPERSION LAW FOR BULK EXCITON

Mahan's paper<sup>1</sup> was followed by a detailed study of an exciton in a degenerate electron Fermi liquid.<sup>8</sup> We therefore consider here only the variation of the energy  $\Omega(P)$  of such an exciton in the region of large  $P(m_1P/M \sim k_F)$ . Starting again with initial free particles, we rewrite Eq. (5) (in the three-dimensional case) in the form

$$\chi(\mathbf{P}, \mathbf{q}, \Omega) = \frac{\theta(|\mathbf{P}' + \mathbf{q}| - k_F)}{P^2/2M + q^2/2\mu - \Omega} \int \frac{d\mathbf{k}}{(2\pi)^3} V(\mathbf{q} - \mathbf{k}) \chi(\mathbf{P}, \mathbf{q}, \Omega). \quad (9)$$

The function  $\chi(\mathbf{P}, \mathbf{q}, \Omega)$  satisfying Eq. (9) is spherically asymmetric. It depends on the angle  $\vartheta$  between the vectors  $\mathbf{P}$  and  $\mathbf{q}$ . It is easy to verify, however, that it becomes spherically symmetric at  $q > P' + k_F$ . The spherical symmetry is thus violated in the region  $|k_F - P'| < q < k_F + P'$ . If we introduce then the function

$$\Xi(\mathbf{P}, \mathbf{q}) = \int \frac{d\mathbf{k}}{(2\pi)^3} V(\mathbf{q} - \mathbf{k}) \chi(\mathbf{P}, \mathbf{q}, \Omega),$$

it can be regarded as approximately dependent on the angles, since the function  $\chi$  which depends on the angles in a bounded region averages out with a spherically symmetric function. Changing in (9) from  $\chi$  to  $\Xi$  and integrating the resultant equation over the angles of the vector  $\mathbf{q}$ , we obtain

$$4\pi\Xi(\mathbf{P}, \mathbf{q}) = \int_{|\mathbf{P}' + \mathbf{k}| > k_F} \frac{d\mathbf{k}}{(2\pi)^3} \frac{8\pi^2}{qk} \ln \left| \frac{q+k}{q-k} \right| \frac{\Xi(\mathbf{P}, \mathbf{k})}{k^2/2\mu + P^2/2M - \Omega}.$$

Using for  $V$  the expression  $V = 4\pi/(k^2 + q_s^2)(q_s^{-1}$  is the screening radius), for a screened potential, we can see that the main contribution is made by the region  $q \sim k \sim k_F$ . The logarithm can then be replaced by  $\ln(2k_F/q_s)$ , after which the equation can be integrated. The result is

$$\frac{2\pi\lambda}{\mu \ln(2k_F/q_s)} = \ln \left| \frac{(k_F + \lambda)^2 - P'^2}{(k_F - \lambda)^2 - P'^2} \right| + \frac{k_F^2 - P'^2}{P'\lambda} \ln \left| \frac{k_F + P'}{k_F - P'} \right| - \frac{k_F^2 - P'^2 - \lambda^2}{2P'\lambda} \ln \left| \frac{(k_F + P')^2 - \lambda^2}{(k_F - P')^2 - \lambda^2} \right| \quad (10a)$$

for  $P^2/2M - \Omega < 0$  and  $\lambda = 2\mu(\Omega - P^2/2M)$  and

$$\frac{2\pi\lambda}{\mu \ln(2k_F/q_s)} = 2 \left[ \pi - \arctg \frac{k_F + P'}{\lambda} - \arctg \frac{k_F - P'}{\lambda} + \frac{P'^2 - k_F^2}{2P'\lambda} \ln \left| \frac{k_F + P'}{k_F - P'} \right| + \frac{k_F^2 - P'^2 + \lambda^2}{4P'\lambda} \ln \left| \frac{(k_F + P')^2 + \lambda^2}{(k_F - P')^2 + \lambda^2} \right| \right] \quad (10b)$$

for  $P^2/2M - \Omega > 0$  and  $\lambda = 2\mu(P^2/2M - \Omega)$ .

The solution of Eq. (10a) goes over into the solution of Eq. (10b) at  $\lambda = 0$ .  $P$  satisfies then the equation

$$\frac{2\pi}{\ln(2k_F/q_s)} = \frac{\mu}{P'} \ln \left| \frac{k_F + P'}{k_F - P'} \right| + \frac{2\mu k_F}{k_F^2 - P'^2}.$$

At  $P = 0$  Eq. (10a) turns into the equation obtained in Ref. 1. Numerical solutions of Eqs. (10a) and (10b) are shown in Figs. 3 and 4 for different effective-mass ratios.<sup>2)</sup> Note that the quantity  $\Omega(P)$  that satisfies (10) and is shown in these figures does not exist for all  $P$ . The quantity exists at  $P = 0$ , and then vanishes for small  $P$  and reappears again in the region  $m_1P/M \sim k_F$ . The cause of the high binding energy in

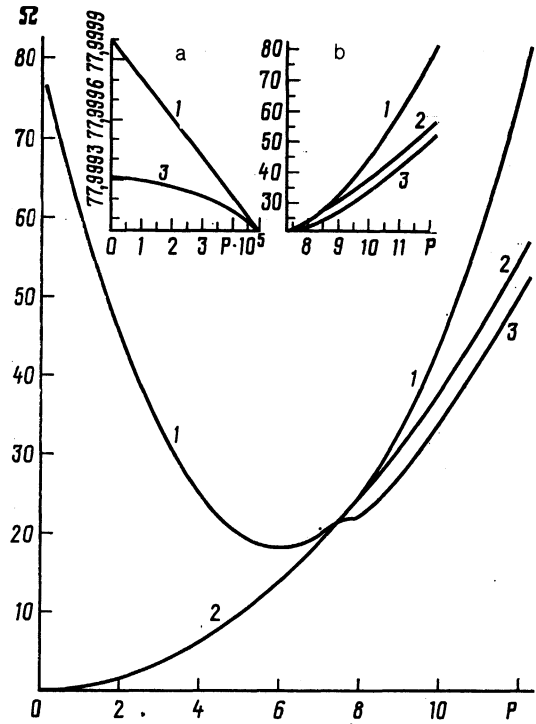


FIG. 3. Dependence of the exchange-exciton energy  $\Omega$  on the mass-center momentum  $P$  for masses  $m_1 = 1$ ,  $m_2 = 0.3$ , and  $k_F = 6$ . Curves 1-3 are similar to the one-dimensional case (see Fig. 2). The inset a shows the region of small  $P$ , and inset b the region of large  $P \sim Mk_F/M_1$ .

the region  $m_1P/M \sim k_F$  is, as before, that in this case the electron and hole move almost in parallel.

#### 5. QUASI-TWO-DIMENSIONAL SURFACE EXCITON

The energy of a quasi-two-dimensional surface exciton can be obtained by solving Eq. (5). For an exact solution of

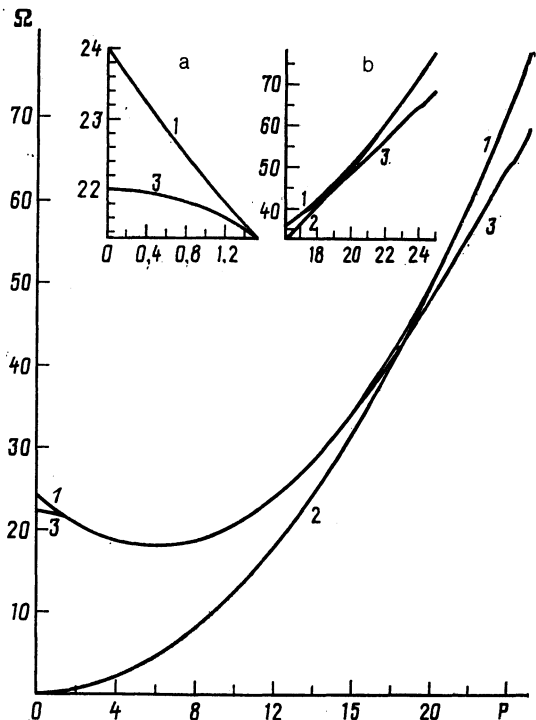


FIG. 4. The same as Fig. 3, but for  $m_1 = 1$ ,  $m_2 = 3$ , and  $k_F = 6$ .

(5) we must know the wave functions of the electrons and holes in the Hartree-Fock approximation, but these can be obtained only numerically. We can nevertheless estimate this energy without knowing the exact form of these functions. To this end we introduce, as in the three-dimensional case, the quantity

$$\Xi_{\alpha}(\mathbf{P}, \mathbf{q}, \Omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} dz_1 dz_2 V(\mathbf{k}-\mathbf{q}, z_1, z_2) \times \chi(\mathbf{P}, \mathbf{k}, z_1, z_2, \Omega) \varphi(z_1) \psi_{\alpha}^*(z_2). \quad (11)$$

(We assume, according to Ref. 5, that the Hartree-Fock wave function of the electron is practically independent of the momentum  $\mathbf{k}_1$  near the surface.) Just as in the three-dimensional case, we assume that  $\Xi$  depends weakly on the angle  $\vartheta$  between  $\mathbf{q}$  and  $\mathbf{P}$  and integrate over  $\vartheta$  neglecting this dependence. We obtain then on the left  $2\pi$ , and on the right the integral

$$V_0(\mathbf{q}, \mathbf{k}) = \int d\theta V(\mathbf{q}-\mathbf{k}, z_1, z_2) = 2\pi \int_{-\pi}^{\pi} d\theta \frac{\exp[-|z_1-z_2|(q^2+k^2-2qk \cos \theta)^{1/2}]}{(q^2+k^2-2qk \cos \theta)^{1/2}+q}. \quad (12)$$

For  $m_1 P/M < k_F$  we have  $q \gg 1$  and  $k \gg 1$ . Expanding  $|\mathbf{q}-\mathbf{k}|$  in a power series in the vicinity of the saddle point  $\vartheta = 0$  and extending the integration over the interval  $(-\infty, \infty)$ , we obtain a quantity the main contribution to which does not contain  $q$ :

$$V_0 = \frac{4\pi}{(2qk)^{1/2}} \Gamma\left(\frac{1}{2}\right) \Gamma\left(\frac{1}{2}, |z_1-z_2| |\mathbf{q}-\mathbf{k}|\right)$$

(see Ref. 9, p. 325). Here  $\Gamma(n)$  is the Euler gamma function, and  $\Gamma(n, a)$  the incomplete gamma function. Since  $q \sim k$  and  $z_1 \sim z_2$ , the second argument in the incomplete gamma function can be replaced by zero and the expression for the interaction potential assumes the simple form

$$V_0 = 4\pi^2 / (2qk)^{1/2}.$$

This quantity no longer depends on  $z_1$  and  $z_2$ , and therefore the equation for  $\Xi(P, q, \Omega)$  can be integrated over  $dz_1$  and  $dz_2$  using the normizability of the functions  $\varphi$  and the orthogonality of  $\psi$ . Excluding, as in the three-dimensional case, the quantity  $\Xi_{\alpha}$  from the equation and assuming that all the corrections to the parabolic dispersion law can be reduced to constants, we obtain

$$2^{1/2} = \int_{k_F+P'}^{\infty} \frac{dk}{k^2/2\mu + P^2/2M + \varepsilon_{\alpha} - \varepsilon_0 - \Omega} + 2 \int_{k_F-P'}^{k_F+P'} \frac{dk \arccos[(k_F^2 - P'^2 - k^2)/2P'k]}{k^2/2\mu + P^2/2M + \varepsilon_{\alpha} - \varepsilon_0 - \Omega}, \quad (13)$$

where  $\varepsilon_0$  is the energy of the bottom of the surface subband. Unfortunately, the last integral in this expression cannot be calculated in elementary functions. Nonetheless, in the important limiting cases  $P' \ll 1$  and  $P' \sim k_F$  we can estimate this integral and obtain the solutions of Eq. (13) in the lowest order in the gap parameter.

In the  $P \ll 1$  limit the bound states of the electron and hole occur at  $\varepsilon_{\alpha} - \varepsilon_0 + P^2/2M < 0$ . The first integral in (13) is then analogous to the corresponding integral in the three-dimensional case, while the second, after the change of variables

$$\lambda^2 = 2\mu(\Omega - P^2/2M - \varepsilon_{\alpha} + \varepsilon_0), \quad k = k_F + P' \sin x, \\ \lambda = k_F - P' - \eta, \quad \eta \ll 1$$

and after discarding terms of second order in  $\sin x$ ,  $P'$ , and  $\eta$  compared with  $k_F$ , reduces to a tabulated integral (see Ref. 9, p. 416). The final equation for the eigenvalue in the region  $m_1 P/M \ll 1$  takes the form

$$\frac{4\pi\mu}{k_F} \ln \frac{4k_F}{\eta + P' + (\eta^2 + 2P'\eta)^{1/2}} = 2^{1/2},$$

from which we get for  $0 < m_1 P/M < a$

$$\eta = \frac{(a-P')^2}{a}, \quad a = k_F \exp\left(-\frac{2^{1/2} k_F}{4\pi\mu}\right), \\ \Omega = \frac{k_F^2}{2\mu} + \frac{P^2}{2M} + E_g + \varepsilon_{\alpha} - \varepsilon_0 - \frac{k_F(a^2 + P^2)}{2a\mu}.$$

$\eta$  vanishes at the point  $m_1 P/M = a$ , and the exciton energy becomes equal to the free-pair energy, while at larger  $P$  the exciton state vanishes. The  $\Omega(P)$  dependence in the region of small  $P$  is similar to that shown in Figs. 3 and 4 for the three-dimensional case.

In the limiting case  $m_1 P/M \sim k_F$ , in the region  $k_F - P = p$ ,  $0 < p \ll 1$  the first term gives a value of order  $(2k_F)^{-1}$ , which can be neglected at large  $k_F$ . Using the mean-value theorem, we can estimate the second integral in (13). As a result we get

$$2^{1/2} = \frac{4\mu\gamma}{\lambda} \left( \frac{\pi}{2} - \arctg \frac{p}{\lambda} \right), \\ \lambda^2 = 2\mu \left( \frac{P^2}{2M} + \varepsilon_{\alpha} - \varepsilon_0 - \Omega \right),$$

where

$$\gamma = \arccos \frac{p^2 - k_0^2 - 2k_F p}{2k_0(k_F - p)},$$

and  $k_0$  is a number on the order of  $\lambda$ . For the value of  $p_0$  at which  $\lambda = 0$  we get

$$4\mu\gamma/p_0 = 2^{1/2}.$$

[ $p_0$  corresponds to  $P$  at which  $\Omega(P)$  crosses  $p^2/2M$ ]. In the other limiting case  $p = 0$ ,  $m_1 P/M = k_F$  we have  $2\pi\mu\gamma/\lambda = 2^{1/2}$ . More accurate estimates yield  $\pi^2\mu/\lambda = 2^{1/2}$ , i.e. again  $\gamma \sim 1$ .

The quasi-two-dimensional exciton behaves thus like the three-dimensional one. In the region  $\mathbf{P} \ll 1$  there is an exponentially small gap between the exciton energy and the energy of a pair with the same  $\mathbf{P}$ . This gap is rapidly filled with increase of  $P$ . An exciton arises anew in the region  $m_1 P/M \sim k_F$  where the electron and hole move almost parallel. In this region the gap between the exciton and free-energy energies is substantially larger than in the region  $P \sim 0$ , and it increases with increase of  $P$ . This character of

the behavior of the exciton is not greatly influenced by the specific form of the wave functions of the free electron and hole.

## 6. CONCLUSION

As already noted, the most favorable conditions for the observation of the described exciton in the case of a large momentum of the mass center occur in quasi-two-dimensional systems. Such systems were investigated in Refs. 10. The existence of an exciton can be manifested in the features of the differential luminescence spectra.

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## APPENDIX

In the limit as  $k_F \rightarrow 0$  and under the assumption that  $V_{\text{eff}}$  and the self-energy corrections to the Green's functions  $\Sigma_e$  and  $\Sigma_h$  are independent of frequency, Eq. (4) reduces to the equation obtained in Ref. 3 for a surface exciton. To prove this, it is easiest to use the operator equality of the complete Green's functions:<sup>11</sup>

$$\begin{aligned} & \left[ G_e^{-1} \left( \mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} + \delta \right) + G_h^{-1} \left( \mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} + \delta \right) \right] \\ & \times G_e \left( \mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} + \delta \right) G_h \left( \mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} - \delta \right) \\ & = \left[ \delta(z_1 - z_3) G_h \left( \mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} - \delta \right) \right. \\ & \left. + \delta(z_2 - z_4) G_e \left( \mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} + \delta \right) \right]. \end{aligned} \quad (\text{A1})$$

Since the sum  $G_e^{-1}(\Omega/2 + \delta) + G_h^{-1}(\Omega/2 - \delta)$  is the independent of the frequency  $\delta$  for all the frequency-independent self-energy parts of  $\Sigma_e$  and  $\Sigma_h$ , Eq. (A1) can be used under the integral sign in (4). As a result we get

$$\begin{aligned} & i \{ H_e^{(0)} + H_h^{(0)} - \Omega - \Sigma_e - \Sigma_h \} \chi(\mathbf{P}, \mathbf{q}, z_1, z_2, \Omega) \\ & = \int \frac{d\mathbf{k}}{(2\pi)^2} \frac{d\delta}{2\pi} V_{\text{eff}}(\mathbf{k}, z_3, z_4) \\ & \times \left[ \delta(z_1 - z_3) G_h \left( \mathbf{k}_2, z_2, z_4, \frac{\Omega}{2} + \delta \right) + \delta(z_2 - z_4) G_e \right. \\ & \left. \times \left( \mathbf{k}_1, z_1, z_3, \frac{\Omega}{2} - \delta \right) \right] \chi(\mathbf{P}, \mathbf{k} - \mathbf{q}, z_3, z_4, \Omega) dz_3 dz_4. \end{aligned}$$

It must be remembered here that since (A1) is an operator equation, the term in the square brackets in this equation (and under the integral sign) must be taken to be a single operator. This means that when integrating over  $\delta$  the inte-

gration contour must be closed on the same (arbitrary) side for  $G_e$  and  $G_h$ . Taking the last remark into account, we obtain after integrating over  $\delta, z_3$  and  $z_4$

$$\begin{aligned} & [H_e^{(0)} + H_h^{(0)} - \Omega - \Sigma_e - \Sigma_h] \chi(\mathbf{P}, \mathbf{q}, z_1, z_2, \Omega) \\ & = \theta \left( \left| \mathbf{q} + \frac{m_1}{M} \mathbf{P} \right| - k_F \right) \\ & \times \int \frac{d\mathbf{k}}{(2\pi)^2} V_{\text{eff}}(\mathbf{k}, z_1, z_2) \chi(\mathbf{P}, \mathbf{k} - \mathbf{q}, z_1, z_2, \Omega). \end{aligned} \quad (\text{A2})$$

In the limits as  $k_F \rightarrow 0$  and  $\theta \rightarrow 1$  and in the coordinate representation Eq. (A2) goes over into the Schrödinger equations with corrections for the screening of the potential and for the image forces. It can be shown that under certain assumptions the screened potential is equal in the RPA approximation to the potential obtained in Ref. 3 in the Thomas-Fermi approximation.

In the limit  $k_F \gg 1$ , in view of the theta function in the right-hand side of (A2), this equation becomes integrodifferential also in the  $\mathbf{x}$ -representation and therefore it is simpler to consider in this limit the purely integral equation (5).

- <sup>1</sup>We consider the case  $k_F \gg 1$ . For  $k_F \ll 1$  solution of Eq. (7b) yields the binding energy in a one-dimensional delta-like potential well.
- <sup>2</sup>The  $\Omega(P)$  plot shown in Fig. 3 has a weak local minimum at a value of  $P$  close to  $k_F M/m_1$ , but we do not know whether it is preserved when exact account is taken of the angular dependence of  $\chi$  in Eq. (9).

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