# Theory of excitons in semiconductor quantum wells containing degenerate electrons or holes

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A variational theory is presented for the binding energy and optical strength of the quasi-twodimensional excitons created optically at low temperature in a quantum well containing degenerate carriers of one type (electrons or holes). Both screening and the exclusion principle are taken into account. Radiative recombination is also considered, and it is shown that either no exciton is involved in the radiation, or the radiation is from an exciton identical to the one created optically. It is shown that when the exclusion principle applies, binding is not obtained for arbitrarily large carrier density. It is shown that the binding energy can be very small while the optical strength is still significant. Calculations are presented showing the binding energy and optical strength versus density for GaAs wells of various widths and electron and hole densities  $0 < N < 2 \times 10^{11}$  cm<sup>-2</sup>.

## I. INTRODUCTION

The importance of excitons in understanding the optical spectra of quantum wells can hardly be overemphasized, because nearly every feature seen is due to an exciton.<sup>1</sup> This remains true even when the wells contain a degenerate population of carriers,<sup>1</sup> either electrons or holes introduced by doping. Several papers $^{2-5}$  have given calculations of the exciton binding energy B as a function of well width L [the "quasi-two-dimensional (2D) exciton"] in the absence of carriers. There is some experimental confirmation of these calculations<sup>2</sup> in that the observed and calculated exciton term values 2S-1S have been shown to be in good agreement. For quantum wells containing carriers calculations on the effect of screening on the binding energy of Coulombic impurities have been reported.<sup>6</sup> It has been emphasized<sup>6</sup> that in the limit of high carrier density N, B becomes independent of N and retains a substantial part of its unscreened value. The effect of free-carrier screening on bound states, mobility, and transport effective masses at metal-oxide-semiconductor (MOS) interfaces has been extensively studied theoretical- $1y.^7$ 

None of these previous papers directly addresses the problems considered here: (a) An electron-hole pair is created by photon absorption in a quantum well containing a degenerate population of electrons or holes-does the spectrum for this process have at least one discrete transition to an excitonic bound state? (b) The system just described relaxes to its ground state and ultimately decays radiatively with the destruction of an electron-hole pair-does the spectrum for this process have any structure or energy shift due to the Coulomb interaction of the pair? There are, of course, many excitons possible in a quantum-well spectrum corresponding to the various subbands available to the electron and hole. The equilibrium carriers are in the lowest electron or hole subband, and we shall assume that no higher subbands are occupied. If neither the electron nor hole of the pair in question (a) is in a subband occupied by carriers the only effect of the carriers is screening described by a dielectric function. In this case it is known<sup>8</sup> that an excitonic bound state exists regardless of the size of N. If either the electron or the hole is in a subband occupied by carriers the exclusion principle restricts the phase space available for the electron-hole pair and it is not clear that a bound state exists. Question (b) concerns the nature of the ground state of a system of, say, a hole and a population of electrons at low temperature. Do the annihilating electron and hole occupy initially plane-wave states, an exciton state, or a superposition of the two types of state? The answers to both questions are required for the proper interpretation of the excitation and luminescence spectra of quantum wells containing carriers.

We have attempted to answer (a) by carrying out variational calculations of *B* using a momentum-space variational wave function with one parameter. This parameter is directly related to the optical strength *S* of the exciton transition. Both *B* and *S* are reported as functions of *N* for GaAs quantum wells of thickness L = 72, 109, 130, 230, and 630 Å for both holes and electrons and for excitons requiring and not requiring the exclusion principle. The calculations assume parabolic energy subbands, carriers in only one subband, and the random-phase approximation (RPA) dielectric function at zero frequency (static screening with spatial dispersion). For a typical case with  $L \sim 100$  Å, this limits the density to  $N_h < 3 \times 10^{11}$  cm<sup>-2</sup> for holes and  $N_e < 2 \times 10^{12}$  cm<sup>-2</sup> for electrons; the validity limits are smaller for larger *L*.

The answer to (b) is obtained theoretically by two different approaches which lead to the same conclusion about the radiating state. If the exciton binding energy *B* is greater than the combined Fermi level  $E_F$ , the exciton ground state is stable against relaxation and radiation occurs from this exciton; if  $B < E_F$  the exciton relaxes to plane-wave states for the electron and hole from which radiation occurs at the (renormalized) gap energy. In the first case Coulomb effects are manifest in the radiation, in the second case they are not. However there is always one Coulomb effect, the band-gap renormalization due to the carriers which has been treated in another paper.<sup>9</sup>

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#### **II. EXCITONS IN THE FERMI SEA**

We consider the ground quasi-2D excitonic state of an electron and heavy hole in the presence of a degenerate population of electrons or heavy holes in the lowest quantum-well subband. The exciton created by the absorption of a photon of zero momentum is described by a wave function of the form

$$\Psi(\mathbf{r}) = \sum_{q} \Psi(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} / \sqrt{A} ,$$

$$\Psi(\mathbf{q}) = 0 \quad \text{for } |q| < k_{F} ,$$
(1)

where  $k_F$  is the Fermi wave number, **r** is the 2D relative coordinate, and **q** the corresponding wave vector, and A is an arbitrary normalization area. Since the total momentum is zero, the separate electron and hole wave vectors are **q**, -**q**, respectively. Note that  $\Psi(r)$  contains only Fourier components outside the Fermi sea to satisfy the exclusion principle. The Schrödinger equation for  $\Psi(\mathbf{q})$ for parabolic electron and heavy-hole bands is

$$q^{2}\Psi(\mathbf{q}) - 2(2\pi)^{-2} \int v(\mathbf{q} - \mathbf{k})\Psi(\mathbf{k})d\mathbf{k} = E\Psi(\mathbf{q}) , \qquad (2)$$

where the units of length and energy are the Bohr radius  $a_B = \epsilon_0 \hbar^2 / (e^2 \mu)$  and Rydberg  $R = e^2 / (2\epsilon_0 a_B)$ , respectively ( $\mu$  = reduced mass), and the potential

$$v(\mathbf{k}) = [\epsilon(k)/\epsilon_0]^{-1} \int v(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$$
(3)

includes screening by the carriers through the dielectric function  $\epsilon(k)/\epsilon_0$ . As we have written (2), positive  $v(\mathbf{k})$  corresponds to an attractive interaction. The zero of energy corresponds to the separated particles at rest.

For the interaction we choose the model potential,<sup>10</sup>

$$v(r) = (1 - e^{-\gamma r})/r , \qquad (4)$$

$$v(k) = \left[ c - (c(k)) \right] 2\pi \left[ k^{-1} - (k^2 + \alpha^2)^{-1/2} \right] \qquad (5)$$

used previously for the biexciton. A calibration of 
$$\gamma^{-1}$$

against the well width has been obtained by comparison of accurate variational calculations using the true Coulomb potential with variational calculations using Eq. (4). Note that in absolute units,  $\gamma$  (cm<sup>-1</sup>) depends only on L; in dimensionless units it depends also on the appropriate  $a_B$ . For  $\epsilon(k)/\epsilon_0$  we use the 2D RPA result<sup>11</sup> specialized to the interaction Eq. (4) and zero frequency,

$$\epsilon(k)/\epsilon_0 = 1 + (2m_s/\mu)[k^{-1} - (k^2 + \gamma^2)^{-1/2}] \times [1 - (1 - 4k_F^2/k^2)^{1/2}], \qquad (6)$$

where  $m_s$  is the screening carrier mass,  $\mu$  the exciton reduced mass, and  $(x)^{1/2}$  is considered zero when x < 0. In using Eq. (6) we are treating the exciton lifetime as infinite.

If  $\Psi(\mathbf{q}) = \Psi(\mathbf{q})$  is isotropic and normalized such that

$$\int_{k_{F}}^{\infty} \Psi(q)^{2} q \, dq = 1 ,$$
  

$$\Psi(\mathbf{r}) = \Psi(r) = (2\pi)^{-1/2} \int_{k_{F}}^{\infty} \Psi(q) J_{0}(qr) q \, dq , \qquad (7)$$
  

$$\int [\Psi(r)]^{2} dr = 1 ,$$

the energy functional is

$$E[\Psi] = \int_{k_F}^{\infty} k^2 [\Psi(k)]^2 k \, dk$$
  
-2(2\pi)^{-2}  $\int_{\Gamma} v(g) g \, dg \, d\theta \int_{k_F}^{\infty} \Psi(k) \Psi(\tau) k \, dk,$   
 $\tau = (k^2 + g^2 - 2kg \cos\theta)^{1/2},$  (8)

 $k > k_F$ ,  $\tau > k_F$  (in region  $\Gamma$ ).

An example of  $\Psi(r)$  is plotted in Fig. 1. When  $\Psi$  and E satisfy Eq. (2),  $E[\Psi] = E$ , and E is the minimum value of  $E[\Psi]$  with respect to variations of  $\Psi$ . We obtain an approximation to E from Eq. (8) using the variational function

$$\Psi(q) = \begin{cases} 2b^2/(q^2 + b^2 - f^2)^{3/2}, & q > k_F \\ 0, & q < k_F. \end{cases}$$
(9)

When  $k_F = 0$  this corresponds to the function  $b(2/\pi)^{1/2}e^{-br}$  often used in exciton calculations. The parameter b is chosen to minimize  $E[\Psi] \equiv E(b)$  and the binding energy of the exciton relative to the combined Fermi level  $E_F = k_F^2$  is

$$B = k_F^2 - (E[\Psi])_{\min} .$$
 (10)

Note that  $k_F^2$  includes both electron and hole energies at the Fermi momentum  $k_F$ . If B > 0 the exciton is stable and has an optical strength proportional to<sup>12</sup>

$$S \propto |p_{cv}|^2 a_B^{-2} |\Psi(r=0)|^2 ,$$

$$|\Psi(r=0)|^2 = (2/\pi)b^2 ,$$
(11)

where  $p_{cv}$  is the interband momentum matrix element.

The formalism given above applies to the heavy-hole exciton in a Fermi sea of either electrons or heavy holes all in the lowest quantum-well subband. The density is assumed sufficiently low that the parabolic approximation for the subband may be used. This formalism also applies to a screened Coulombic impurity state if the bound carrier is the same as the screening carriers, providing the appropriate values of  $\mu$ ,  $a_B$ , and  $\gamma$  are used. If neither bound particle is the same as the screening carriers (e.g., the light-hole exciton in a sea of heavy holes) the ex-



FIG. 1. Wave function Eq. (9) in r space for  $b = k_F/3$ , the optimum value for electrons with L = 130 Å. Plotted is  $Y = \Psi(r)/\Psi(0)$  vs X = br.

clusion principle must be removed from (7)–(10), by setting  $k_F = 0$  while retaining  $k_F$  in Eq. (6).

The above formulation applies to the production of an exciton by absorption of a photon. Subsequently the system *electron* + *hole* + *Fermi sea* relaxes to its ground state from which a photon can be emitted by radiative recombination. We ask what if any Coulomb effects are present in the radiating state. Without Coulomb interaction the lowest electron-hole state is the electron-heavy-hole plane wave  $\chi(\mathbf{q}) = \delta_{q,0}$ ; with interaction we may plausibly write the more general state

$$\chi(\mathbf{q}) = \alpha \delta_{q,0} + \beta (2\pi/A)^{1/2} \Psi(q) ,$$
  

$$|\alpha|^{2} + |\beta|^{2} = 1 ,$$
  

$$\sum_{q} |\chi(\mathbf{q})|^{2} = 1 ,$$
(12)

where  $\Psi(q)$  is approximated by Eq. (9), and  $\beta$  is to be determined along with b by minimizing the energy functional. It is easy to show that the mixed term in the functional involving both terms of Eq. (12) vanishes as  $A \rightarrow \infty$ . This means that the exciton parameter b is independent of  $\beta$ , and has the same value as for photon absorption with production of a heavy-hole exciton. The energy functional for  $\chi(\mathbf{q})$  reduces to

$$E[\chi] = |\beta|^2 E[\Psi] . \tag{13}$$

It follows that  $\beta = 1$  if  $(E[\Psi])_{\min} < 0$  corresponding to the same heavy-hole exciton involved in absorption, or to  $\beta = 0$  if  $(E[\Psi])_{\min} > 0$  corresponding to a plane wave (i.e., no Coulomb effects in emission). The crossover occurs when the exciton binding energy  $B = k_F^2$ , the combined Fermi level. This conclusion does not depend on the particular form Eq. (9) for  $\Psi(q)$ ;  $\Psi(q)$  could be the exact exciton wave function satisfying Eq. (2).

These conclusions may seem surprising because it is well known<sup>8</sup> that an attractive interaction in 2D always produces for particles unrestricted by exclusion at least one bound state. Our argument above has led to the conclusion that this is not necessarily so in the presence of exclusion. However, there could be two weaknesses in the argument just given: (a) it depends on the variation of an energy functional which can only give an upper bound on the energy, and (b) the form Eq. (12) may not be correct even if  $\Psi(\mathbf{q})$  is an exact solution of Eq. (2). Therefore we consider a special case which is exactly solvable.

Consider the Schrödinger equation for  $\chi(\mathbf{q})$  in the form (Bethe-Goldstone equation<sup>13</sup>)

$$\begin{split} \chi(\mathbf{q}) &= \delta_{q,0} + (E - E_q)^{-1} \Gamma(q) A^{-1} \sum_{\mathbf{k}} \lambda V(\mathbf{q}, \mathbf{k}) \chi(\mathbf{k}) ,\\ \Gamma(q) &= \begin{cases} 1, & q > k_F \\ 0, & q < k_F \end{cases} \\ E - E_0 &= A^{-1} \sum_{\mathbf{k}} \lambda V(0, \mathbf{k}) \chi(\mathbf{k}) , \end{split}$$
(14)

where  $V(\mathbf{q}, \mathbf{k})$  is an unspecified interaction that includes screening, and  $\lambda < 0$  corresponds to attraction. If  $V(\mathbf{q}, \mathbf{k})$ is assumed to be separable, which is to say

$$V(\mathbf{q},\mathbf{k}) = u(\mathbf{q})u(\mathbf{k})^* , \qquad (15)$$

an equation can be obtained for  $\sum_{\mathbf{k}} u(\mathbf{k})^* \chi(\mathbf{k})$ , from which it follows that the eigenvalue E is a root of the equation

$$\frac{\lambda |u(0)|^2}{A(E-E_0)} + \frac{\lambda}{A} \sum_{\mathbf{k}} \Gamma(k) \frac{|u(k)|^2}{E-E_k} = 1 , \qquad (16)$$

where  $E_0=0$  in the present case. As  $A \to \infty$  the first term on the left is nonzero only at E=0 corresponding to the plane wave  $\chi(\mathbf{q})=\delta_{q,0}$ . If  $\lambda < 0$  the second term gives a root  $E_x < k_F^2$  corresponding to the exciton state,

$$\chi(\mathbf{q})_{\mathbf{x}} = C\Gamma(q)u(q)/(E_{\mathbf{x}} - E_{q}) , \qquad (17)$$

with C a normalization constant. The larger  $|\lambda|$  is, the larger  $k_F^2 - E_x = B$  is. At sufficiently large  $|\lambda|$  the exciton is stable  $(B > k_F^2)$ ; otherwise the plane wave is stable, in complete agreement with our previous conclusions.

### **III. CALCULATIONS**

We write the energy functional Eq. (8) as

$$E[\Psi] \equiv E(b) = I(b) + U(b) ,$$

$$T = b^{2} + k_{F}^{2} ,$$

$$U(b) = -\frac{4b^{4}}{\pi^{2}} \int_{k_{F}}^{\infty} dk \frac{k}{(k^{2} + b^{2} - k_{F}^{2})^{3/2}} \times \int_{0}^{\infty} dg \frac{v(g)gF(\rho,\phi)}{(k^{2} + b^{2} + g^{2} - k_{F}^{2})^{3/2}} ,$$

$$\rho = 2kg/(k^{2} + b^{2} + g^{2} - k_{F}^{2}) ,$$

$$\begin{bmatrix} 0, \ g < k - k_{F} \\ . \ k^{2} + g^{2} - k_{F}^{2} \end{bmatrix} ,$$
(18)

$$\phi = \begin{cases} \cos^{-1} \left[ \frac{\kappa + g - \kappa_F}{2kg} \right], & k - k_F < g < k + k_F \\ 0, & g > k + k_F \end{cases}$$

$$F(\rho, \phi) = \frac{1}{1 - \rho^2} \left[ \int_{\phi}^{\pi} d\theta (1 - \rho \cos\phi)^{1/2} - \frac{2\rho \sin\phi}{(1 - \rho \cos\phi)^{1/2}} \right],$$

where T and U are the kinetic and potential energies, respectively. The region  $\Gamma$  in Eq. (8) is contained in the definition of  $\phi$ . Singularities (discontinuous slope) in the integrand occur at  $k = k_F^2$  from Eq. (6) and at  $g = k \pm k_F$ from the kinks in  $\phi$ ; the former causes no difficulty but the latter require a transformation of variable to achieve adequate numerical accuracy. Also the limits on the kand g integrations were transformed to 0 to 1, and the integrations performed using the Gauss-Legendre quadrature (8 points for k and 24 points for g). In trying to optimize b numerical "jitter" was encountered in E(b), making it difficult for small binding energies B < 0.1. To remove this jitter a least-squares parabolic fit to 5-10points near the optimum was computed and the optimum b and E(b) determined from this parabola. The result was considered significant if B was at least three times larger than the rms deviation. For the no-screening case  $[\epsilon(k) \equiv 1]$ ,  $v(|\mathbf{q} - \mathbf{k}|)$  can be integrated over the angle  $\angle(\mathbf{q},\mathbf{k})$  in terms of complete elliptic integrals. The resulting double integral is quite different from the one in Eq. (18), although the value should be the same. This check

indicated that our values for *B* are accurate to about  $\Delta B \sim 2 \times 10^{-3}$ , although some additional error is introduced by the singularity at  $k=2k_F$ . For the case of screening without exclusion we have compared our calculations with previous work<sup>6</sup> on Coulombic impurity bound states. Despite the fact that this work uses a different form of model potential than Eq. (5) we find very close agreement over the whole range of interest of  $k_F$ .

For all cases having an electron Fermi sea that we have studied the energy E(b) has a single minimum as shown in Fig. 2. However, for a hole Fermi sea there are sometimes two minima, and as  $k_F$  is increased the lower energy belongs first to the one at larger b and then to the one at smaller b. This is shown in Fig. 3. When this occurs we take the deeper minimum as E and the corresponding b as the optimized parameter to be used in Eq. (11), although Eq. (9) is probably a poor approximation to the wave function when the two minima are nearly equal. We do not find binding (B > 0) for arbitrarily large  $k_F$  when exclusion is included, although failing numerical accuracy made it impossible to determine the critical value of  $k_F$ .

Qualitatively the behavior of B versus  $k_F$  is the same for an electron or hole Fermi sea. In Fig. 4 we present our results for  $B(k_F)$  for four values of GaAs well width for the heavy-hole exciton in an electron Fermi sea. The density,

$$N(k_F) = k_F^2 / (2\pi a_B^2) , \qquad (19)$$

is also plotted versus  $k_F$ . Even though *B* and  $k_F$  are dimensionless the calculation is specific to GaAs because of the dielectric function Eq. (6). The calculation of  $\gamma$  is given in Fig. 1 of Ref. 10, and the material constants used for GaAs were the same as in Ref. 10:



FIG. 2. Energy functional E(b) given by Eq. (18) for electrons,  $k_F=0.5$ , L=72 Å ( $\gamma=13.9$ ), showing the combined Fermi level  $k_F^2$ . In this case, E(b) has the desirable form with a single minimum.



FIG. 3. Energy functional  $E(b)-k_F^2$ , where E(b) is given by Eq. (18), for holes,  $k_F=1.0$  and 1.1, L=109 Å ( $\gamma=10$ ), showing two extrema, an undesirable form. The deeper minimum is chosen as the optimum giving b and B.

$$m_{+} = 0.099, m_{-} = 0.19, m_{e} = 0.067,$$
  
 $a_{B_{+}} = 160 \text{ Å}, a_{B_{-}} = 130 \text{ Å},$   
 $R_{+} = 3.7 \text{ meV}, R_{-} = 4.6 \text{ meV},$   
 $\epsilon_{0} = 12.2,$ 
(20)

where masses are in units of the free-electron mass and +, - refer to the heavy hole and light hole, respectively, for transverse motion along the well. The curves labeled 1-4 in Fig. 4 are for four different well widths as follows:



FIG. 4. Binding energy of heavy-hole exciton B (units  $R_{+}=3.7 \text{ meV}$ ) given by Eq. (10) and electron density N (cm<sup>-2</sup>) given by Eq. (19) vs Fermi momentum  $k_F$  for (1) L=72 Å ( $\gamma=13.9$ ), (2) L=130 Å ( $\gamma=8.5$ ), (3) L=230 Å ( $\gamma=5.1$ ), and (4) L=630 Å ( $\gamma=2.2$ ). Dashed line shows critical condition  $B=k_F^2$ ; above this line the exciton is observed in radiative recombination as well as absorption.

(1) L=72 Å ( $\gamma=13.9$ ); (2) L=130 Å ( $\gamma=8.5$ ); (3) L=230 Å ( $\gamma=5.1$ ); (4) L=630 Å ( $\gamma=2.2$ ). The dashed line in Fig. 4 indicates the condition  $B=k_F^2$  which is critical for the exciton stability against relaxation in the Fermi sea; above this line the same exciton is observed in both absorption and emission. Figure 5 shows the corresponding curves for  $b^2$  which according to Eq. (11) is a measure of the optical strength. The relevant length and energy units in Figs. 4 and 5 are  $a_{B+}$  and  $R_+$ . In Fig. 6 we show B and  $b^2$  along with N for a GaAs

In Fig. 6 we show B and  $b^2$  along with N for a GaAs well L = 109 Å ( $\gamma = 10$ ) containing heavy holes. For other values of L the behavior can be deduced quite closely from the dependence on  $\gamma$  shown in Fig. 5. Again  $a_{B_+}$ and  $R_+$  are the relevant units. In Fig. 7 we show a case where the exclusion principle is omitted, the lowest lighthole exciton in a sea of heavy holes. In this case the units are  $a_{B_-}$  and  $R_-$ , and L=107 Å ( $\gamma=8.3$ ). Note the asymptotic approach to constant limits as  $k_F \rightarrow \infty$ . The limit corresponds to density-independent Thomas-Fermi screening.<sup>6</sup>

#### **IV. DISCUSSION**

Returning to the questions (a) and (b) posed in the Introduction, we can summarize our findings this way: (a) If N is not overly large there is an excitonic bound state, but in the case of the lowest heavy-hole exciton not for arbitrarily large N. The optical strength lags behind the binding energy in falling off with increasing N, falling by a factor  $\sim 2$  while the binding energy is falling by a factor  $\sim 10$ , but eventually falls off even faster than the binding energy, both apparently going to zero at some critical value of N which depends on L. (b) At low density the exciton is stable in the Fermi sea (region above dashed line in Fig. 4), at high density  $k_F > B$  it relaxes to a completely dissociated plane-wave state. We have answered (a) by calculations and (b) by theoretical arguments.

The calculations employ a model potential Eq. (4) which is calibrated<sup>10</sup> to the well thickness by requiring



FIG. 5. Variational parameter  $b^2$  for the heavy-hole exciton vs Fermi momentum  $k_F$  for electrons and the same L values as in Fig. 4. Dashed line shows condition  $B = k_F^2$ . According to Eq. (11),  $b^2$  is proportional to the optical strength of the exciton.



FIG. 6. Binding energy (solid curve) of heavy-hole exciton B (units  $R_{+}=3.7$  meV), variational parameter (dashed curve)  $b^{2}$ , and hole density N (cm<sup>-2</sup>) for L=109 Å ( $\gamma=10$ ). Optical strength Eq. (11) is proportional to  $b^{2}$ .

that the commonly used variational function  $b(2/\pi)^{1/2}e^{-br}$  give the same exciton binding energy as an accurate calculation based on the true Coulomb potential. Thus in the limit  $k_F \rightarrow 0$ , the variational function Eq. (9) has a reasonable form and is guaranteed to give a good value of B. The form of Eq. (9) is therefore quite reasonable in general, so we propose that when  $b^2$  is optimized it represents at least an approximate measure of the optical strength through the relation Eq. (11). For  $k_F > 0$  the function Eq. (9) in r space has an oscillatory form as shown in Fig. 1 due to cutting off all  $q < k_F$ .

In a variational calculation one hopes that the energy functional, being minimized, has a single sharp minimum making the choice of optimum b unambiguous and reasonably precise. This is the case when the functional behaves as in Fig. 2 which is typical of most of the calculations. However, for holes, we sometimes observed the behavior shown in Fig. 3. When the two extrema are of nearly the same depth the choice of b becomes ambiguous. Figure 3 illustrates this situation for the well calcu-



FIG. 7. Binding energy (solid curve) of light-hole exciton B (units  $R_{-}=4.6$  meV), variational parameter (dashed curve)  $b^2$ , and hole density N (cm<sup>-2</sup>) vs Fermi momentum  $k_F$  for L=107 Å ( $\gamma=8.3$ ). Optical strength Eq. (11) is proportional to  $b^2$ .

lated in Fig. 6. The ambiguous region lies in the range  $1 < k_F < 1.1$ , which is a very small range in Fig. 6 and therefore not very important. Presumably this behavior means that the true wave function makes a rather rapid transition with increasing  $k_F$  from being dominated by the dielectric function at small  $k_F$  to being dominated by the Fermi cutoff at large  $k_F$ . It is interesting to note that in Fig. 7, where the Fermi cutoff is absent, both B and  $b^2$  start to saturate with increasing  $k_F$  around the same region  $k_F \sim 1$ .

We have not offered any experimental evidence to compare with the theory. Exciton binding energies are not easy to measure experimentally. The optical strength is more accessible to measurement than the binding energy. It has been observed<sup>1</sup> that hole doping to about  $5 \times 10^{10}$ cm<sup>-2</sup> in a sample with  $L \sim 100$  Å causes the normally stronger heavy-hole exciton to be weaker than the light-hole exciton, and at  $3 \times 10^{11}$  cm<sup>-2</sup> the heavy-hole exciton has disappeared. This is in agreement with our Figs. 5 and 6, for about the same L, which show that  $[b(hh)]^2 < [b(lh)]^2$  for densities  $N > 3 \times 10^{10}$  cm<sup>-2</sup>, and  $[b(hh)]^2$  seems to be vanishing at about  $3 \times 10^{11}$  cm<sup>-2</sup>. Even though not confirmed by experiment the calcula-

<sup>1</sup>R. C. Miller and D. A. Kleinman, J. Lumin. **30**, 520 (1985).

- <sup>2</sup>R. C. Miller, D. A. Kleinman, W. T. Tsang, and A. C. Gossard, Phys. Rev. B 24, 1134 (1981).
- <sup>3</sup>G. Bastard, E. Mendez, L. Chang, and L. Esaki, Phys. Rev. B **26**, 1974 (1982).
- <sup>4</sup>R. L. Greene, K. K. Bajaj, and D. E. Phelps, Phys. Rev. B 29, 1807 (1984).
- <sup>5</sup>Tsen-Fu Jiang, Solid State Commun. **50**, 589 (1984).
- <sup>6</sup>J. A. Brum, G. Bastard, and C. Guillemot, Phys. Rev. B 30, 905 (1984).
- <sup>7</sup>For a review see T. Ando, A. B. Fowler, and F. Stern, Rev.

tions of B should prove useful in understanding the spectra, especially the Stokes shift between the hh exciton seen in excitation and the luminescence peak. In good quality undoped samples the Stokes shift due to imperfections is usually < 1 meV. With doping the Stokes shift increases<sup>1</sup> but sometimes considerably less than the expected combined Fermi level. Figure 4 shows for the case of electrons with L = 72 Å that the dashed line intersects curve (1) at  $N_e \sim 2.5 \times 10^{10}$  cm<sup>-2</sup>; at this and lower densities no Stokes shift should be expected. At higher densities the Stokes shift should be  $k_F - B$  which is essentially  $k_F$  for  $N > 10^{11}$  cm<sup>-2</sup>. It is interesting to note comparing Fig. 4 (electrons) and Fig. 6 (holes) that holes extinguish B with increasing N faster than electrons. For static screening holes are more effective than electrons because of their larger mass, as seen in Eq. (6).

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- Mod. Phys. 54, 438 (1982), especially Secs. II C, II E, and II F.
- <sup>8</sup>F. Stern and W. E. Howard, Phys. Rev. **163**, 816 (1967).
- <sup>9</sup>D. A. Kleinman and R. C. Miller, Phys. Rev. B 32, 2266 (1985).
- <sup>10</sup>D. A. Kleinman, Phys. Rev. B 28, 871 (1983).
- <sup>11</sup>Y. Kuramoto and H. Kamimura, J. Phys. Soc. Jpn. **37**, 716 (1974).
- <sup>12</sup>R. J. Elliott, Phys. Rev. 108, 1384 (1957).
- <sup>13</sup>H. A. Bethe and J. Goldstone, Proc. R. Soc. London, Ser. A 238, 551 (1957).