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Screening of Excitons in Semiconductors

J. G. Gay
Research Laboratories, General Motors Corporation, Warren, Michigan 48090

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A theoretical study of screening of excitons in semiconductors is presented. The study was motivated by a desire to improve the understanding of the optical effects of exciton screening, particularly with regard to photoreflectance experiments. The theory is based on a dielectric-function approach to the screening and thus ignores exchange contributions to the screened electron-hole interaction. To avoid having to work with retarded interactions, the region of carrier concentration for which the plasma frequency is comparable to the exciton binding energy is not treated. Away from this region the interaction can be approximated as instantaneous, and expressions for the exciton energy can be derived. In numerical application to CdS it is found that screened exciton binding energies are comparable to those obtained with a Debye-Hückel potential for the interaction. However, because the free-carrier plasma is self-screened, the band gap is a function of carrier concentration. When this is taken into account, the absolute-energy shift of excitons under screening (which is what figures in the optical effects) is much less than the binding-energy shift. In addition to the downward shift of continuum absorption due to the self-screening, the screening modifies the continuum enhancement and reduces it to unity for very high carrier concentrations.

I. INTRODUCTION

The optical properties of a crystal are determined by ϵ_2, the imaginary part of the transverse dielectric function. In the effective-mass approximation, ϵ_2, near the direct spin-degenerate band edge of a semiconductor, is given by[1,2]

$$\epsilon_2(E) = 2\left(\frac{2\pi e\hbar}{m}\right)^2 |P_{cv}|^2\left(\sum_n \frac{F_n}{(E_{cv}-E_n)^2}\right.$$
$$\left.\times\delta[E-(E_{cv}-E_n)]+\frac{F(E)}{(E_{cv}+E)^2}\,S(E)\right), \qquad (1)$$

where the energy E is measured from the top of the valence band, E_{cv} is the gap energy, and P_{cv} is the conduction- to valence-band momentum-matrix element. The first term gives the contribution of the bound exciton states. The E_n are binding energies and the F_n are enhancement factors[2] given by

$$F_n = |\psi_n(0)|^2\,, \qquad (2)$$

where $\psi_n(r)$ is the nth relative bound-electron-hole wave function of zero angular momentum. The second term gives the continuum contribution. $S(E)$ is the joint density of states and $F(E)$ is the continuum enhancement,

$$F(E) = \lim_{r\to 0}\left|\frac{\psi_q(r)}{(2/\pi)^{1/2}\sin qr/qr}\right|^2\,, \qquad (3)$$

which involves the ratio of the zero-angular-momentum wave function with electron-hole interaction to that without. $\vec{q}$ is the wave vector corresponding to E.

Since the electron-hole interaction determines the E_n, F_n, and $F(E)$, and influences $S(E)$, changes in the interaction can produce changes in the band-edge optical properties.

Albers[3] has proposed that reflectance changes observed in modulated-reflectance experiments on crystals are in part due to screening of the electron-hole interaction produced by modulation of surface-carrier concentrations. Screening effects should be most prominent in photoreflectance experiments[4] because the modulation is a direct injection of free carriers produced by pumping with an intense light beam. Albers was able to show, on the basis of a Debye-Hückel potential for the screened interaction, that shifts in the exciton ground state due to screening could easily account for the magnitude of the photoreflectance signal of CdS, and could reproduce portions of the structure of the spectrum. More recently Stöbel *et al.*[5] have published new photoreflectance data on CdS, which they ascribe in part to screening energy shifts. Because of this apparent contribution of screening to the photoreflectance signal a theoretical study of screening was undertaken whose results are reported here.

The theoretical development is hampered by two fundamental complexities. The first complexity is that the plasma-exciton interaction includes exchange between the exciton particles and the particles of the free-carrier plasma. The other is that the screened electron-hole interaction is not instantaneous because of the inertia of the plasma. In going from weak screening of a bound-exciton state to screening sufficient to cause the state to disappear, one cannot avoid a region in which the plasmon energy and the exciton binding energy are comparable: $\hbar\omega_p \sim E_b$. In this region, particularly, one is confronted with a retarded interaction and has to deal with a Bethe-Salpeter equation in the relative coordinates rather than a Schrödinger equation.[6] Similarly for continuum states there is a velocity region between slow particles which the plasma screens, in effect, instantaneously, and fast particles which the plasma does not see, where the electron-hole interaction depends on the particles's past as well as present location. The parameter which replaces E_b is the velocity-momentum product $\hbar\vec{v}\cdot\vec{q}$.[7]

We ignore the exciton-plasma exchange problem. We treat the exciton charge density as classical and the plasma's response to it via the longitudinal dielectric function $\kappa(\omega, \vec{q})$. We get around the retarded-interaction problem by avoiding the regions $\hbar\omega_p \sim E_b$ and $\omega_p \sim \vec{v}\cdot\vec{q}$. Away from these regions the exciton charge density approaches limits in which it is static. In the no-exchange approximation the plasma response then involves only the static dielectric function $\kappa(\vec{q}) = \kappa(0, \vec{q})$, and Schrödinger equations can be constructed which approximate the actual situation at least in an idealization in which the exciton is at rest and scattering processes are not present.

Within this very simplified framework it is possible to obtain a qualitatively satisfying picture of the effects of screening which shows clearly the limitations of an instantaneous-interaction approximation, and which points up a feature of screening which has not been emphasized, namely, the self-screening of the free-carrier plasma. This effect, which causes a decrease in the band gap with increase in carrier concentration, affects the exciton energy shifts and thereby the principal contribution of screening to the photoreflectance effect.[3, 5]

The theoretical development is presented in Secs. II and III and includes numerical calculations for CdS. The results are discussed in Sec. IV.

II. SCREENING OF BOUND STATES

A static classical charge density $\rho(\vec{x})$ introduced into a crystal induces a density

$$\delta\rho(\vec{x}) = \int d^3x'\,\rho(\vec{x}')\,[1/\kappa(\vec{x}-\vec{x}') - 1] \;, \tag{4}$$

with transform

$$\delta\rho(\vec{q}) = \rho(\vec{q})\,[1/\kappa(\vec{q}) - 1] \;, \tag{5}$$

where $\kappa(\vec{q})$ is the static longitudinal dielectric function.

While the application of (4) or (5) to compute the density induced by electrons and holes has been justified by Kohn[8] and Sham and Rice[9] for weakly bound systems added to a perfect insulator, it is not correct for a semiconductor containing a free-carrier plasma. This is because to avoid exchange effects it is essential that there be an energy gap, large relative to the exciton binding energy, separating filled from empty levels. Thus if we use (4) or (5) to compute charges induced in the free-carrier plasma, we completely ignore exchange between the plasma and exciton particles.[10] Nevertheless, we use an approach based on the dielectric function because it accounts for a part of the plasma-exciton interaction in a consistent way, and leads to manageable calculations.

We assume therefore that the exciton charge density, consisting of the charge density of the electron and hole,

$$\rho(\vec{q}) = \rho_e(\vec{q}) + \rho_h(\vec{q}) \;, \tag{6}$$

induces a charge density in the free-carrier plasma according to (5). This implies that $\rho(\vec{q})$ is in some sense static. These densities give rise to potentials $\phi(\vec{q})$ and $\delta\phi(\vec{q})$, and have an energy of assembly

$$\begin{aligned} W &= \frac{1}{2}\int \frac{d^3q}{(2\pi)^3}\,[\rho(\vec{q}) + \delta\rho(\vec{q})][\phi(-\vec{q}) + \delta\phi(-\vec{q})] \\ &= \frac{1}{2\kappa_0}\int \frac{d^3q}{(2\pi)^3}\frac{4\pi}{q^2}\,[\rho(\vec{q}) + \delta\rho(\vec{q})][\rho(-\vec{q}) + \delta\rho(-\vec{q})] \;. \end{aligned} \tag{7}$$

In (7) κ_0 is the static longitudinal dielectric function of the crystal in the absence of free carriers (presumed independent of $\vec{q}$). It is present because any charge seen by the plasma is already screened by the valence electrons whose frequency response is much greater than that of the plasma. Using (6) and (5) in (7) allows us to express W in terms of $\rho_e(\vec{q})$, $\rho_h(\vec{q})$, and $\kappa(\vec{q})$, where from here on $\kappa(\vec{q})$ will mean the dielectric function of the free-carrier plasma alone,

$$\begin{aligned} W = {} & \frac{1}{2\kappa}\int \frac{d^3q}{2\pi^2}\,\frac{1}{q^2}\,[\rho_e(\vec{q})\,\rho_h(-\vec{q}) + \rho_h(\vec{q})\rho_e(-\vec{q})] \\ & \times\left[1 + 2\left(\frac{1}{\kappa(\vec{q})} - 1\right) + \left(\frac{1}{\kappa(\vec{q})} - 1\right)^2\right] \\ & + \frac{1}{2\kappa_0}\int \frac{d^3q}{2\pi^2}\,\frac{1}{q^2}\,[\rho_e(\vec{q})\,\rho_e(-\vec{q}) + \rho_h(\vec{q})\,\rho_h(-\vec{q})] \\ & \times\left[z\left(\frac{1}{\kappa(\vec{q})} - 1\right) + \left(\frac{1}{\kappa(\vec{q})} - 1\right)^2\right] . \end{aligned} \tag{8}$$

In (8) the first term represents electron-hole interactions while the second represents self-energy terms. The terms $\rho_e(\vec{q})\,\rho_e(-\vec{q})$ and $\rho_h(\vec{q})\,\rho_h(-\vec{q})$, which represent bare-particle self-energies, have been discarded.

We now examine separately the two cases in which we may treat the exciton charge density as static. First we consider the case of an exciton weakly bound relative to the plasma frequency $E_b \ll \hbar\omega_p$. Then the plasma responds so swiftly that it sees the instantaneous position of the electron and hole. Thus, we have

$$\rho_e(\vec{x}) = -e\delta(\vec{x} - \vec{r}_e) \;, \qquad \rho_h(\vec{x}) = e\delta(\vec{x} - \vec{r}_h) \;. \tag{9}$$

We can locate the center of mass at the origin and the electron and hole on the z axis for convenience. Then the transforms of (9) are

$$\begin{aligned} \rho_e(\vec{q}) &= -ee^{-i\vec{q}\cdot\vec{r}_e} = -ee^{-i\vec{q}\cdot\hat{z}m_h r/M} \;, \\ \rho_h(\vec{q}) &= ee^{-i\vec{q}\cdot\vec{r}_h} = ee^{i\vec{q}\cdot\hat{z}m_e r/M} \;. \end{aligned} \tag{10}$$

In these $r = |\vec{r}| = |\vec{r}_e - \vec{r}_h|$ is the electron-hole separation and M is the exciton mass. Using the densities (10) in (8) gives an energy of assembly

$$W(r) = -\frac{e^2}{2\kappa_0}\int \frac{d^3q}{2\pi^2}\frac{1}{q^2}\left[\left(e^{-i\vec{q}\cdot\hat{z}r} + e^{i\vec{q}\cdot\hat{z}r}\right)\frac{1}{\kappa(\vec{q})^2} - 2\left(\frac{1}{\kappa(\vec{q})^2} - 1\right)\right] , \qquad (11)$$

in which the factors involving $\kappa(\vec{q})$ have been simplified.

The first term in (11) depends on r while the second does not. Thus, we have

$$W(r) = V(r) + W_\infty . \qquad (12)$$

$V(r)$ is an electron-hole potential, so from effective-mass theory we can write a Wannier equation for the excition binding energy,

$$[p^2/2\mu + V(r)]\psi(\vec{r}) = E_b\,\psi(\vec{r}) , \qquad (13)$$

where spherical bands are assumed and μ is the reduced effective mass. W_∞ is composed of clothing energies of the electron and hole, and does not contribute to the binding energy. It does contribute to the absolute exciton energy, however, and will figure in the energy shifts which produce the photoreflectance signal.

Let us look now at the opposite limit $E_b \gg \hbar\omega_p$. Since the Coulomb interaction is instantaneous, the $\rho_e\rho_h$ terms [the "one" in the first term of (8)] are treated as before and contribute the Coulomb potential $-e^2/\kappa_0 r$. The remaining terms contain induced densities and involve the response of the plasma to the excition density. The condition $E_b \gg \hbar\omega_p$ means, however, that the plasma is too sluggish to respond to the instantaneous relative position of the excition[11] (though it still sees the instantaneous position of the center of mass). This is taken care of by using a time-average exciton charge density

$$\rho(\vec{x}) = \int d^3r_e\, d^3r_h [e\delta(\vec{x} - \vec{r}_h) - e\delta(\vec{x} - \vec{r}_e)]\, |\Psi(\vec{r}_e, \vec{r}_h)|^2 , \qquad (14)$$

where $\Psi(\vec{r}_e, \vec{r}_h)$ is the wave function of a localized exciton, i.e.,

$$|\Psi(\vec{r}_e, \vec{r}_h)|^2 = \delta(\vec{R} - \vec{R}_0)\, |\psi(\vec{r})|^2 , \qquad (15)$$

where $\vec{R}$ is the center-of-mass coordinate,

$$\vec{R} = (m_e\vec{r}_e + m_h\vec{r}_h)/M . \qquad (16)$$

Since the charge induced by $\rho(\vec{x})$ is independent of $\vec{R}_0$ we may determine the induced charge with $\vec{R}_0 = 0$, i.e., with

$$|\Psi(\vec{r}_e, \vec{r}_h)|^2 = \delta(\vec{R})\, |\psi(\vec{r})|^2 . \qquad (17)$$

Then, we have

$$\rho(\vec{x}) = e(M/m_e)^3 |\psi(M\vec{x}/m_e)|^2 - e(M/m_h)^3 |\psi(M\vec{x}/m_h)|^2$$
$$= \rho_h(\vec{x}) + \rho_e(\vec{x}) . \qquad (18)$$

The energy of assembly is

$$W_{\text{av}} = \langle \psi(\vec{r}) | \frac{-e^2}{\kappa_0 r} | \psi(\vec{r}) \rangle + \frac{1}{4\pi^2\kappa_0}\int \frac{d^3q}{q^2}\rho(\vec{q})\,\rho(-\vec{q})\left(\frac{1}{\kappa(\vec{q})^2} - 1\right) . \qquad (19)$$

If we add to W_{av} the kinetic energy

$$T = \langle \psi(\vec{r}) | (p^2/2\mu) | \psi(\vec{r}) \rangle , \qquad (20)$$

we obtain the absolute exciton energy, i.e., the energy referred to a bare separated electron and hole. To get the binding energy we must refer the energy to a clothed separated electron and hole, i.e.,

$$E_b = T + W_{\text{av}} - W_\infty , \qquad (21)$$

where W_∞ is defined by (12) and (11).

We can write (21) as a Wannier equation,

$$[p^2/2\mu + V_{\text{av}}(r)]\psi(\vec{r}) = E_b\,\psi(r) , \qquad (22)$$

where

$$V_{\text{av}}(r) = \frac{-e^2}{\kappa_0 r} + \frac{1}{4\pi^2\kappa_0}\int \frac{d^3q}{q^2}\left(\frac{1}{\kappa(\vec{q})^2} - 1\right) \times \left\{ e\int d^3x\, e^{-i\vec{q}\cdot\vec{x}}\left[\delta\left(\frac{M\vec{x}}{m\hat{e}} - \vec{r}\right) - \delta\left(\frac{M\vec{x}}{m_h} - \vec{r}\right)\right]\rho(-\vec{q}) - 2e^2 \right\} . \qquad (23)$$

The potential (23) depends on $\psi(\vec{r})$ through $\rho(-\vec{q})$ and, as a consequence, (22) must be solved self-consistently.

In order to do calculations based on the Schrödinger equations (13) and (22) it is necessary to approximate the dielectric function $\kappa(\vec{q})$. We use for $\kappa(\vec{q})$ the long-wave limit of the self-consistent-field (SCF) dielectric function of a classical plasma (see the Appendix),

$$\kappa(\vec{q}) = 1 + Q^2/q^2 , \qquad (24)$$

where Q is the Debye-Hückel screening parameter,

$$Q^2 = 4\pi N e^2/\kappa_0 kT , \qquad (25)$$

and where N is the carrier concentration. The classical plasma approximation, i.e., a Boltzmann distribution for the plasma particles, was chosen because we wish to work at moderately high temperatures (~ 80 °K), and because we were not able to express $\kappa(\vec{q})$ in terms of known functions when the Fermi distribution was used. The price paid is that exchange is eliminated even among the plasma particles. The use of the long-wave limit instead of the exact SCF $\kappa(\vec{q})$,

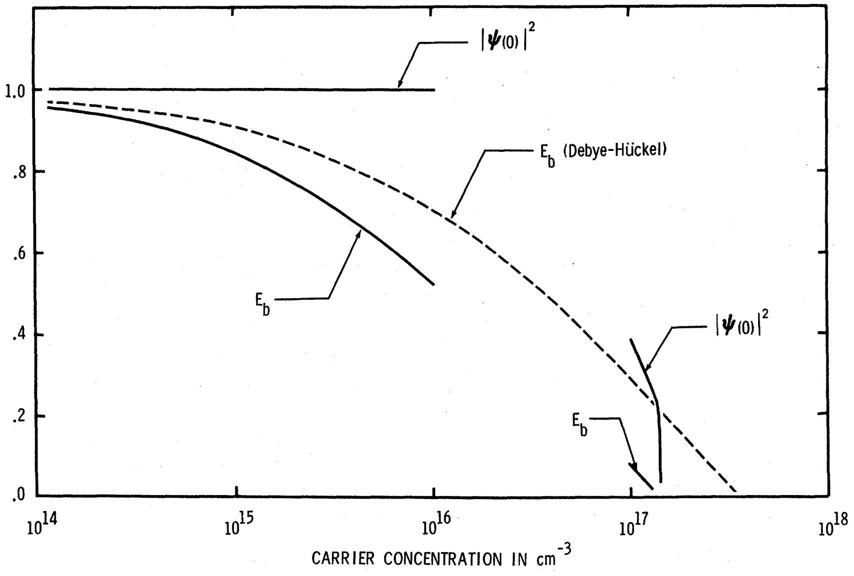

FIG. 1. Binding energy and enhancement relative to their unscreened values as a function of carrier concentration for the ground-state exciton in CdS. The Debye-Hückel binding energy is given for reference. The gap running from 10^{16} to 10^{17} represents approximately the region specified by (30) where static solutions are not applicable. To the left of the gap the curves were obtained from (22). To the right they were obtained from (13).

$$\kappa(\vec{q}) = 1 + g(q) Q^2/q^2 , \tag{26}$$

introduces some error. In (26) $g(q)$ is a cutoff function, described in the Appendix, which decreases the susceptibility at short wavelengths. This error is discussed in Sec. IV.

The approximation (24) when inserted in (11) leads to manageable integrals which yield a potential

$$V(r) = (e^2/\kappa_0)\,(-e^{-Qr}/r + \tfrac{1}{2} Q e^{-Qr}) \tag{27}$$

and a clothing energy

$$W_\infty = -3e^2 Q/2\kappa_0 . \tag{28}$$

The Schrödinger equation (13) with (27) for $V(r)$ can be solved for all its bound states by one of the standard techniques.

The nonlinear equation (22) is not so simple. Consequently we estimate only its ground state. This is done variationally using the trial function

$$\psi(r) = (\eta^3/\pi)^{1/2}\, e^{-\eta r} . \tag{29}$$

It turns out that the integrals involved in computing the expectation value of E_b with respect to (29) can all be done in closed form and give a sum of rational functions of η for the expectation value. Minimizing this sum with respect to η gives estimates of the ground-state energy and wave function.

Because we wish to keep the calculations uniform, and because estimates of the excited states or more accurate estimates of the ground state are not of much practical value, only the ground state of (13) was estimated, again variationally using the trial function (29).

The calculations were done for CdS at 80 °K. CdS was chosen because its relatively tightly bound excitons and modest intrinsic-surface electric fields favor screening effects over electric field effects.[3] The material parameters used were $m_e = 0.2m$, $m_h = 0.7m$, and $\kappa = 8.46$. These give an unscreened binding energy of the ground state of 2.96×10^{-2} eV. The results are shown in Fig. 1 as plots of E_b and $|\psi(0)|^2$ vs N relative to their unscreened values.

The region $\hbar\omega_p \sim E_b$ in which neither static solution applies was arbitrarily taken as

$$\tfrac{1}{10} < \hbar\omega_p \,|\, E_b \,| < 10 , \tag{30}$$

where ω_p was computed assuming equal numbers of electrons and holes,

$$\omega_p^2 = 4\pi N e^2/\kappa_0 \mu . \tag{31}$$

As indicated in Fig. 1, our calculations predict uniformly larger decreases in the binding energy than does the Debye-Hückel potential. This does not imply that greater energy shifts in the photon energy required to excite an exciton are predicted. This is because the screening actually decreases the band gap E_{cv}, which compensates the decrease in E_b. This will be discussed in Sec. IV.

III. SCREENING OF CONTINUUM STATES

As implied by Sec. II, slow continuum states are shifted in energy by W_∞. This will be discussed in Sec. IV. In this section we wish to estimate the effects of screening on the continuum enhancement factor (3).

For small relative velocities, i.e., when $\vec{v}\cdot\vec{q} \ll \omega_p$, the plasma reacts instantaneously to the electron-hole position, and we have the Schrödinger equation (13) to which potential scattering theory can be applied to obtain $\psi(0)$. For high relative velocities, $\vec{v}\cdot\vec{q} \gg \omega_p$, the plasma reacts only to the time-average charge density, which is zero

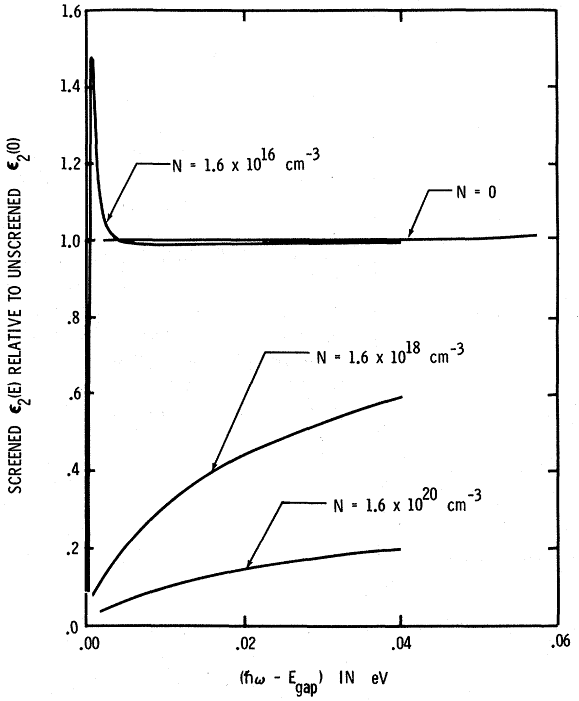

FIG. 2. Imaginary part of the transverse dielectric function due to continuum absorption as a function of energy for various carrier concentrations. Values are relative to the unscreened value at the band edge. The curves were computed assuming that the plasma response is instantaneous. Negative shifts in the energies of slow particles due to self-screening of the plasma are not incorporated.

for a continuum state. The second term of (23) vanishes and $V_{\mathrm{av}}(r)$ reduces to a Coulomb potential. Thus for fast particles the plasma has no effect on the electron-hole interaction and $\psi(0)$ is not changed from its unscreened value.

For the low-velocity limit, potential scattering theory gives for the enhancement factor (3),

$$F(E) = \lim_{r \to 0} |1/f_q(r)|^2 , \qquad (32)$$

where $f_q(r)$ is the Jost function[2] defined as the solution of the zero-angular-momentum reduced radial equation satisfying the boundary condition

$$\lim_{r \to \infty} e^{iqr} f_q(r) = 1 . \qquad (33)$$

Thus the effect of screening on the continuum enhancement for small $\vec{v} \cdot \vec{q}$ is determined by finding the Jost functions associated with the Schrödinger equation (13). Our calculations for CdS use the approximate potential (27). The Jost function is then easily found by starting at large r ($= 10/Q$) with a plane wave and numerically integrating the radial equation to the origin. The value at the origin gives the enhancement via (32). The results are shown in Fig. 2 for three carrier concentrations relative to the Coulomb enhancement,[1]

$$F_c(E) = \pi\alpha e^{\pi\alpha}/\sinh\pi\alpha , \quad \alpha^2 = R/(E - E_{cv}) , \qquad (34)$$

where R is the exciton Rydberg $\mu e^4/2\hbar^2\kappa_0^2$. For the lowest carrier concentration $N = 1.6 \times 10^{16}/\mathrm{cm}^3$ it is seen that $\epsilon_2(E)$ is essentially unchanged from its unscreened behavior except for the structure near $E = 0$. This low-energy structure is strongly Q dependent, so the particular structure shown is not characteristic of the low-N enhancement. For the larger concentrations, 1.6×10^{18} and 1.6×10^{20}, $\epsilon_2(E)$ has markedly diminished until at 1.6×10^{20} it has essentially become the dielectric function without interaction proportional to $S(E)$. The change from Coulomb behavior occurs near the point 1.35×10^{17} where the last bound state disappears.

If we adopt

$$\vec{v} \cdot \vec{q} < \tfrac{1}{10} \omega_p \qquad (35)$$

as the condition for small relative velocities and use $\hbar\vec{v} = \vec{\nabla}_{\vec{q}} E$, the condition becomes

$$E < \tfrac{1}{20} \hbar\omega_p . \qquad (36)$$

Using (32) for ω_p shows that the three calculations of Fig. 2 taken in order of increasing N are valid for E less than 2×10^{-4}, 2×10^{-3}, and 2×10^{-2} eV. Thus for all but the largest N the screening effects on the continuum enhancement are much less than indicated in Fig. 2.

IV. DISCUSSION

This work was undertaken to try to improve the understanding of the role of screening in photoreflectance experiments. Ideally one would like to develop the theory sufficiently that the changes in the transverse dielectric function due to screening are predicted quantitatively, and then use these changes to compute a theoretical photoreflectance spectrum which can be subjected to a detailed comparison with experiment.

We do not attempt such a comparison for two reasons. The first is that the screening theory developed in Secs. II and III is not quantitatively accurate. The second is that we believe that variation in the dielectric function with depth into the crystal, due both to intrinsic surface effects and to variation in pumped carrier density with depth, affects the photoreflectance signal but is not sufficiently understood to incorporate into a photoreflectance-spectrum calculation.

Consequently we confine our discussion to a more or less qualitative description of the consequences of the theory of Secs. II and III. The theory predicts quite different bound-state energy shifts than the shifts obtained by Albers using the Debye-Hückel potential. In addition the clothing of slow continuum states shifts absorption into the band

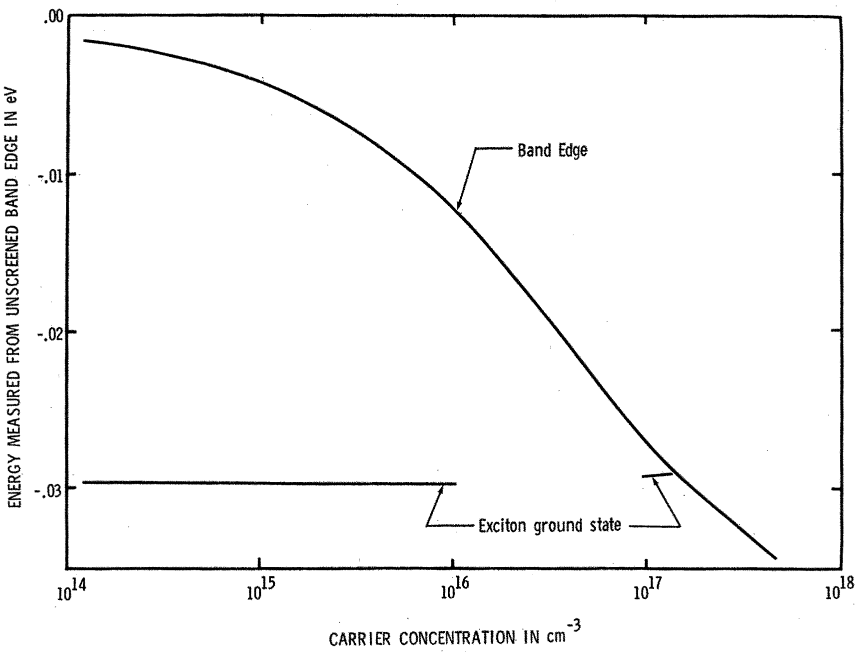

FIG. 3. Qualitative behavior of the band edge and ground-state energy as a function of carrier concentration in CdS. The nearly constant exciton energy is fortuitous (see text).

gap and provides a potential new source of photoreflectance signal.[12]

Energy shifts which contribute to the photoreflectance signal (or to any optical effect involving photons near the band-gap energy) are due to the difference between the energies required to create a screened and an unscreened electron-hole pair. Therefore, to the extent that valence electrons are not screened by the free-carrier plasma, energies are to be measured relative to the top of the valence band. In computing the exciton binding energies in Sec. II, we measured energies relative to the bottom of the conduction band. However, because of the clothing energy W_∞ the band-gap energy depends on the carrier concentration. To get absolute shifts we must refer the excition energies to the top of the valence band by taking account of this change in the band gap.

The change enters the binding-energy calculations for low and high carrier concentrations differently. At low N, where the plasma sees only the average position of the electron and hole, W_∞ does not figure in the exciton energy itself, and affects the binding energy only by lowering the continuum edge. We get the absolute excition energy by deleting W_∞ from (21). When this is done the exciton energy shows a very slight negative shift because of the electrostatic energy of its charge cloud.

At high N, where the plasma sees the instantaneous position of the electron and hole, W_∞ is contained in the absolute exciton energy. The exciton energy is obtained by adding the negative W_∞ to the positive shift caused by the decrease in the binding energy [cf. (12)]. This means that for large N we cannot hope to estimate absolute energy shifts accurately. In fact, we cannot predict the sign of the shift because it is the difference of large quantities which themselves can only be crudely calculated via the theory of Sec. II. If W_∞ is approximated by (28), the absolute shifts are negative. Provided that the observed shifts are due entirely to screening, this is contrary to experiment.[3,5] The negative shift is due in part to the use of the long-wave approximation for $\kappa(\vec{q})$. The integrands which lead to (27) for $V(r)$ and (28) for W_∞ have different large-$\vec{q}$ behavior. The integrands for $V(r)$ contain oscillatory factors of the form $\sin qr/qr$, which provide a natural cutoff. The integrands for W_∞ do not contain these factors, so W_∞ is affected more by the long-wave approximation for $\kappa(\vec{q})$. If we approximate the cutoff function of Fig. 5 by

$$g(x)=1, \quad x\leq 1 \qquad g(x)=0, \quad x>1 \tag{37}$$

the integrals for W_∞ can be done, and give

$$W_\infty=\frac{2e^2}{\kappa_0\pi}\left(-\frac{3}{2}Q\tan^{-1}\frac{q_{\max}}{Q}+\frac{Q^2}{2}\,\frac{q_{\max}}{q_{\max}^2+Q^2}\right) , \tag{38}$$

where $q_{\max}=2(2\mu kT)^{1/2}/\hbar$. However, the integrals required to obtain $V(r)$ using the cutoff (37) could not be done. Figure 3 therefore shows the shifts in the continuum-edge energy and ground-state exciton energy vs carrier concentration for CdS at 80 °K, using (27) for $V(r)$ and (38) for W_∞. The slight upward shift in the excition energy at high N is thus fortuitous. The results of Fig. 3 do show, however, that it is not correct to work with bind-

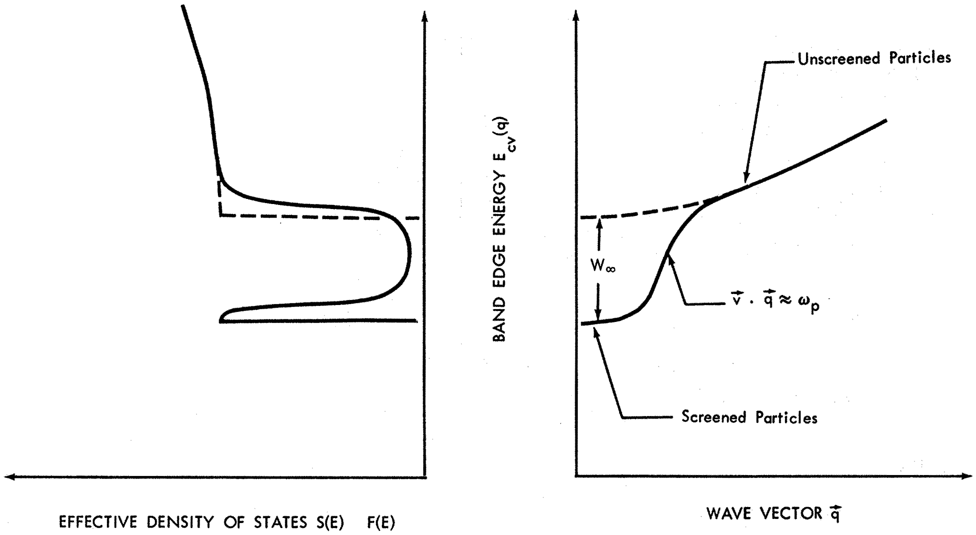

FIG. 4. Schematic showing the nipple in the $E_{cv}(q)$ curve and the consequent density of states which occur because of self-screening of slow plasma particles.

ing-energy changes alone. In view of the near cancellation of the dielectric effects it is not worthwhile to refine the calculation of the absolute exciton shifts since exchange effects[10,12] will have to be included to determine the sign of the shifts.

The continuum shift is not a rigid lowering of the $E_{cv}(\vec{q})$ curve because only slow particles are screened. The screening actually produces a nipple in $E_{cv}(\vec{q})$ at $\vec{q}=0$. This is illustrated in Fig. 4 along with a schematic of the resulting density of states. The nipple shape in the region $\vec{v}\cdot\vec{q}\sim\omega_p$ depends on the continuum solutions to a Bethe-Salpeter equation, so a determination of the shape is not a simple matter. However, one can make an order-of-magnitude estimate of the amount of absorption shifted as follows: Suppose the continuum absorption in an energy range ΔE above the edge is rigidly shifted downward. The amount of absorption involved can be estimated from (1) and expressed as a fraction of the amount contained in the ground-state exciton line. Using (36) to estimate ΔE we find that for N in the range $10^{16}-10^{17}$ per cm^3 the amount of absorption shifted is of the order of 1% of the absorption of the ground-state exciton line.

Calculation of the differential reflectance signal caused by a shift of this amount shows that it can make only a minor contribution to the photoreflectance signal. Furthermore, the absorption is reduced by blocking or hand filling.[13] Estimates which ignore the multiple valence bands of CdS show that at 80 °K W_∞ is equal to the effective Fermi level E_F at $N=2\times10^{16}$, and is several kT below at $N=10^{17}$. Thus, because the shifted states are filled, this source will not become more important at high carrier concentrations. The maximum contribution in fact occurs in the region of carrier concentration at which $W_\infty\sim E_F$.

The discussion above has covered the principal results of this paper insofar as they bear on photoreflectance experiments. These are (i) exciton energy shifts due to screening are considerably smaller than the corresponding binding-energy shifts, and (ii) screening of the continuum does not make a major contribution in the carrier concentration range ($<10^{17}$ per cm^3) which is achieved in current photoreflectance experiments on CdS. At higher concentrations the loss in continuum enhancement illustrated in Fig. 2 can be significant.

In addition to providing these results the dielectric-screening theory has value in providing a picture of the process by which excitons are screened. In summary, the picture is the following.

At low concentrations the free-carrier plasma is sluggish and responds only to the time-average charge density of the exciton. In this limit the plasma simply clothes the exciton charge cloud and lowers its energy. As its density increases the plasma becomes less sluggish and begins to respond to the relative motion of the electron and hole. Now, in addition to the clothing of the exciton charge cloud, the electron and hole become individually clothed and the electron-hole interaction begins to be screened. However, until the plasma frequency becomes much greater than the exciton binding energy, the plasma does not respond instantly to the electron and hole motion, and the screened interaction is retarded, making it necessary to describe the relative motion by means of a Bethe-Salpeter equation. Finally, as the plasma density becomes large, the plasma ceases to see the electron and hole as a charge cloud and responds essentially instantly to their relative motion. In this limit the screened electron-hole interaction becomes instantaneous and the relative motion can be described by a Schrödinger equation with a potential similar to the Debye-Hückel potential. The exciton binding energy vanishes when the plasma density becomes high enough that it is energetically favorable to clothe the exciton particles with a unit charge cloud rather than to bind them together.

It is probable that in a correct theory which incorporates exchange the details of the screening process will be altered but the basic features just described will persist.

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APPENDIX

Feix[14] gives the following expression for the longitudinal dielectric function of a classical plasma computed in the self-consistent-field approximation:

$$\kappa(\omega, q) = 1 - \frac{v(q)N}{\pi^{1/2}kT}\int_{-\infty}^{\infty} dt\left(\frac{e^{-(t+y/2)^2} - e^{-(t-y/2)^2}}{2ty - s + i\eta}\right), \tag{A1}$$

where $v(q)$ is the Fourier transform of the Coulomb potential, $y = \hbar q/(2mkT)^{1/2}$, and $s = \hbar\omega/kT$.

By manipulation this can be converted into an expression involving the integral representation of the "w" error function,[15]

$$\kappa(\omega, q) = 1 - \frac{v(q)N}{\pi^{1/2}kT}\frac{1}{y}\frac{\pi}{i} \times\left[W\left(\frac{-y^2 - s + i\eta}{2y}\right) - W\left(\frac{y^2 - s + i\eta}{2y}\right)\right]. \tag{A2}$$

$W(z)$ is an entire function defined in a region including the real axis by

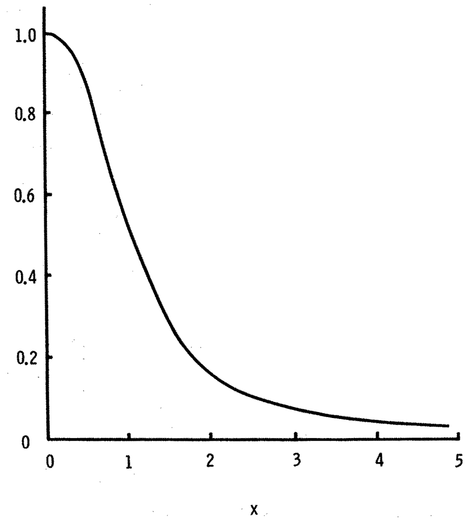

FIG. 5. The cutoff function of the classical dielectric function.

$$W(z) = e^{-z^2}\left(1 + \frac{2i}{\pi^{1/2}}\int_0^z e^{t^2} dt\right). \tag{A3}$$

Thus (A2) and (A3) permit the calculation of $\kappa(\omega, q)$ for all real values of its arguments. For $\omega = 0$ and $\eta \to 0+$, we have

$$\mathrm{Im}\,\kappa(0, q) = 0\,, \qquad \mathrm{Re}\,\kappa(0, q) = 1 + g(\tfrac{1}{2}y)\,Q^2/q^2\,, \tag{A4}$$

where

$$Q^2 = 4\pi N e^2/\kappa_0 kT \tag{A5}$$

and

$$g(x) = (1/x)\,e^{-x^2}\int_0^x e^{t^2} dt\,. \tag{A6}$$

$g(x)$ is easily evaluated using tables of Dawson's integral,[15] and is plotted in Fig. 5. It functions as a cutoff on the susceptibility at short wavelengths.

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Impact Ionization in Crossed Fields in Semiconductors

H. Reuter and K. Hübner
Institut für Angewandte Physik, Universität Heidelberg, Heidelberg, Germany

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Starting from the motion of the free electron, a model is developed for the impact ionization of electron-hole pairs in the presence of a strong transverse magnetic field. The ionization rate was found to depend only on the quotient of the effective electric field strength divided by the magnetic field E_{eff}/B. For n-InSb the ionization rate was calculated in dependence of E_{eff}/B for different values of the mean free path for optical-phonon scattering. Impact ionization begins at $E_{\mathrm{eff}}/B = 2.7\times10^5$ m sec^{-1}.

I. INTRODUCTION

The problem of impact ionization in semiconductors in crossed electric and magnetic fields was first investigated by Toda and Glicksman.[1] They suggested the "transverse breakdown," and impact ionization in the Hall direction at comparable or lower electric fields than in the absence of a magnetic field. But measurements by Ferry and Heinrich[2] showed a decrease of the ionization rate caused by the magnetic field. This result was in agreement with unpublished measurements done in our laboratory. Therefore, and because of our interest in the ionization process in the somewhat different geometric conditions of a θ pinch,[3] we developed a model for the impact ionization in crossed fields, in which the Hall field is regarded as an independent physical quantity. The decrease of the ionization rate predicted by our model therefore does not exclude the existence of a transverse breakdown, but only indicates that this effect will be caused by a nonlinear dependence of the Hall field strength on the magnetic field, as was also predicted by Schmidt and Nelson.[4]

Our model is valid for a semiconductor with the following properties: (a) moderately doped n type, (b) parabolic conduction band, (c) dominant optical-phonon scattering, (d) isotropic effective mass. Starting from the equation of motion of a free electron, we investigated (Secs. II–V) the behavior of an electron in a magnetic field. The velocity vector of such an electron is moving on a gyration circle which is not centered in the origin of the velocity plane. To get a one-dimensional (energy) description, we divided this gyration circle into a "fast" half and a "slow" one, as determined by the absolute value of the velocity. The energy of the electron was averaged separately over each half circle and the continuous motion of the velocity vector on the gyration circle was replaced by transitions between the two energy mean values. With these transitions and those caused by the scattering with acoustical and optical phonons, the Boltzmann equations and two continuity equations for the motion of the particles in the energy space are formulated (Sec. VI). In Sec. VII this system of equations is solved and the energy distribution of the electrons is determined. The ionization rate, the number of electron-hole pairs produced by one electron within unit time, is given in Sec. VIII. It was found to depend on $u=(E_z^2+E_H^2)^{1/2}/B$ only. Here E_z is the external electric field, E_H is the Hall field, and B is the magnetic field.

II. SOLUTION OF EQUATION OF MOTION

Moving in the crystal the electrons are not subject to a homogeneous friction, but lose their energy by single impacts. Between the impacts the behavior of the electrons is described by the equation of motion for free particles:

$$\frac{d\vec{v}}{dt} = -\frac{e}{m^*}(\vec{E}+\vec{v}\times\vec{B}), \tag{1}$$

where t is the time, $-e$ is the electric charge of the electron, m^* is the effective mass, $\vec{v}$ is the velocity, $\vec{B}$ is the magnetic field, and $\vec{E}$ is the electric field at the position of the particle. The electric field is the sum of the applied external electric field E_z and the Hall field E_H.

If the magnetic field is perpendicular to the elec-