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1994 J. Phys.: Condens. Matter 6 9335

(http://iopscience.iop.org/0953-8984/6/44/014)

J. Phys.: Condens. Matter 6 (1994) 9335–9348. Printed in the UK

Dynamical screening of excitons in a semiconductor electron–hole plasma

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Received 27 April 994

Abstract. A single-particle Hamiltonian approach is used for describing dynamical screening of excitons in optically excited semiconductors. Upon considering a particular electron–hole pair, the excitation spectrum of all the other electrons and holes is replaced by a single plasmon mode $\omega(q)$. From a Fröhlich-type Hamiltonian, 1s exciton binding energy and wavefunctions are calculated variationally with a generalization of the Lee–Low–Pines transformation. The advantage of the method, beside the simplicity, is that bandgap renormalization is accounted for within the same Hamiltonian so that a consistent comparison with experimental data is possible. In particular, our model reproduces both the remarkable persistence of the 1s GaAs exciton line under strong optical excitation and the measured transition density from bound to unbound states.

1. Introduction

There has been continuous interest in the non-linear optical properties of highly excited semiconductors, either bulk or quantum wells, particularly for potential application in the design of optoelectronic devices [1, 2, 3]. From a theoretical point of view, even more interesting is the ionization of excitons, that is, the disappearance of the exciton line due to screening and phase space occupation [4–8]. An intriguing feature observed in the optical spectra of optically excited bulk GaAs is the constancy of the exciton line over a wide range of free carrier densities. It has been recognized that this feature is due to a compensation between the variation of the exciton binding energy due to the screening action of photogenerated free carriers (electrons and holes) and the band-gap renormalization. A further increase in free-carrier density leads to the ionization of the exciton and therefore to strong non-linearities in the absorption spectra and refractive index [1, 5, 9, 10].

A theory addressing the problem of exciton in highly excited semiconductors cannot ignore bandgap renormalization effects. It is indeed necessary to treat the dynamical screening of excitons and bandgap renormalizations within the same theoretical scheme, that is, at the same level of approximation. Several many-body approaches [2, 4, 7, 8] and simplified models [11] have been proposed based on the calculation of the complex optical dielectric function from the numerical solution of the Bethe–Salpeter equation in k space. The knowledge of such a dielectric function leads directly to the absorption spectra and refractive index.

With this paper we wish to present a study of the dynamical screening of exciton using an Hamiltonian approach which has the advantage to yield closed and easily evaluable variational expression for the 1s exciton ground state energy and wavefunction. In particular, the model we propose comprises a single electron–hole pair which, besides the direct

0953-8984/94/449335+14$19.50

Coulomb potential, interacts with plasma excitations. By singling out of an electron–hole gas two particles, we attempt to reduce the many particle problem to a two particles one where the action of the electron–hole gas is taken into account in terms of plasmon dressing between and around the singled out particles. In doing this we are dealing with a sort of mean-field approximation in which the long range part of the electron–electron interaction is correctly represented [12]. We shall see that assuming a particle–gas interaction of Fröhlich type, a variational procedure, widely used in the context of polaron and bipolaron theory [13–16], is able to give both the pair self-energy and the exciton 1s binding energy.

There is one variational parameter γ in the problem to which the exciton average radius depends ($\langle r \rangle \sim \gamma^{-1}$). The exciton total energy as a function of this parameter has either one or two minima depending on the free carriers density n. In GaAs at zero temperature and for $n > 2.43 \times 10^{15}$ ($r_s < 4.0$ where $r_s = (3/4\pi n a_0^3)$ with a_0 the effective Bohr radius) the exciton total energy has just one minimum at $\gamma = 0.0$ which corresponds to $\langle r \rangle \to \infty$. In this case the exciton total energy and the free particles self-energy are the same thing and accounts for the gap renormalization. For $n < 2.43 \times 10^{15}$ ($r_s > 4.0$) the exciton total energy has two minima one of which at $\gamma = 0.0$ and the other at finite γ with the latter lower than the former. In this situation an electron–hole pair is unstable against the exciton bound state formation. A complete study of the exciton dimensions, oscillator strengths and polarization clouds is presented to clarify all the aspects of the problem.

Our variational scheme allows the determination of an effective electron–hole potential which includes dynamical screening effects. We have studied a number of properties related to this potential going from a static approximation [11, 17] where all the recoil effects due to plasmon emission and reabsorption are neglected to a dynamical description where recoil is fully accounted for. One of the properties that we can anticipate is its long range behaviour.

Depending on the actual value of the variational parameter γ one can either have or not have a screened Coulombic tail. We shall see that this result has a purely dynamical origin and is related to the way the electron–hole gas responds to the exciton.

2. Hamiltonian

In a direct semiconductor with a population of electrons and holes sustained by a laser beam, we assume that these particles are in quasi-equilibrium, that is, the pair excitation lifetimes are long compared with the relevant inter-particle scattering times. It is therefore reasonable to assume the Fermi–Dirac expression for the equilibrium distribution. At zero temperature the electron–hole gas is characterized by a plasma frequency

$$\omega_p^2 = \frac{4\pi e^2}{\epsilon_0} \sum_{i=e,h} \frac{n_i}{m_i} \tag{1}$$

and the screening wavevector

$$Q_{TF}^2 = \frac{4e^2 k_F M}{\pi \epsilon_0 \hbar^2} \qquad M = m_e + m_h \qquad k_F = \left(3\pi^2 n\right)^{1/3} \tag{2}$$

where k_F is the Fermi momentum, m_e and m_h the electron and hole band masses and $n_e = n_h = n$ the electron and hole densities.

For the plasma dispersion $\omega(q)$ a possible choice is [18]

$$\omega^2(q) = \omega_p^2 \frac{\epsilon(q)}{\epsilon(q) - \epsilon_0} \tag{3}$$

where for $\epsilon(q)$ we can either use the Thomas–Fermi expression

$$\epsilon(q) = \epsilon_0\left(1 + \frac{Q_{\mathrm{TF}}^2}{q^2}\right) \tag{4}$$

or the Lindhard expression

$$\epsilon(q) = \epsilon_0\left[1 + \frac{Q_{\mathrm{TF}}^2}{2q^2}\left(1 + \frac{1-x^2}{2x}\ln\left|\frac{1+x}{1-x}\right|\right)\right] \text{ with } x = \frac{q}{2k_{\mathrm{F}}}. \tag{5}$$

Following Overhauser [18], let us consider the Hamiltonian describing a particle interacting with a boson field

$$H = \frac{P^2}{2m} + \sum_q \hbar\omega(q)a_q^\dagger a_q + \sum_q C(q)\mathrm{e}^{\mathrm{i}q\cdot r}\left(a_q + a_q^\dagger\right) \tag{6}$$

where $C(q)$ and $\omega(q)$ are the particle–boson coupling and the boson frequency dispersion respectively. Indicating with $\rho(r)$ the electron–hole gas charge density fluctuation, the interaction energy with an electron is

$$H_{\mathrm{I}} = \int \frac{-e\rho(r)}{\epsilon_0|r - r_{\mathrm{e}}|}\,\mathrm{d}^3r = \sum_q \frac{-4\pi e}{\epsilon_0 \nu q^2}\rho(q)\mathrm{e}^{\mathrm{i}q\cdot r_{\mathrm{e}}} \tag{7}$$

where r_{e} is the electron position, $\rho(q)$ the Fourier transform of $\rho(r)$, ν the normalization volume and ϵ_0 the background static dielectric constant. By direct comparison between (6) and (7) we can define the charge density operator

$$\hat{\rho}(q) = -\frac{\epsilon_0 \nu q^2}{4\pi e}C(q)\left(a_q + a_{-q}^\dagger\right) \tag{8}$$

The f-sum for an electron–hole gas [12] reads

$$\sum_n \hbar\omega_{n0}|\langle n|\hat{\rho}(q)|0\rangle|^2 = \frac{N\hbar^2q^2}{2\mu} \text{ with } \frac{1}{\mu} = \frac{1}{m_{\mathrm{e}}} + \frac{1}{m_{\mathrm{h}}} \tag{9}$$

where $\hbar\omega_{n0}$ are the energy difference between the exact excited $|n\rangle$ and ground $|0\rangle$ states and N is the total number of particles contained in the volume ν. Since we are thinking to a plasmon model where, for a given q, there is just one mode $\omega(q)$, from (8) and (9) we have

$$C(q) = \left(\frac{2\pi e^2\hbar\omega_{\mathrm{p}}^2}{\epsilon_0 \nu q^2 \omega(q)}\right)^{1/2} \text{ where } \omega_{\mathrm{p}}^2 = \frac{4\pi e^2 n}{\mu\epsilon_0} \tag{10}$$

with $n = N/\nu$ the equilibrium density.

The above derivation can be repeated for the case of a hole so that the electron(hole)–plasmon coupling coefficient reads

$$C_{\mathrm{i}}(q) = -e_{\mathrm{i}}\left(\frac{2\pi\hbar\omega_{\mathrm{p}}^2}{\epsilon_0 \nu q^2 \omega(q)}\right)^{1/2} \quad e_{\mathrm{e}} = -|e| \qquad e_{\mathrm{h}} = |e|. \tag{11}$$

We are now ready to write the complete Hamiltonian of a electron–hole pair interacting each other through the Coulomb potential and each with the electron–hole gas

$$H = \sum_{\mathrm{i=e,h}} \frac{P_{\mathrm{i}}^2}{2m_{\mathrm{i}}} - \frac{e^2}{\epsilon_0 r} + \sum_q \hbar\omega(q)\left(a_q^\dagger a_q + \frac{1}{2}\right) + \sum_q \sum_{\mathrm{i=e,h}} C_{\mathrm{i}}(q)\left(a_q\mathrm{e}^{\mathrm{i}q\cdot r_{\mathrm{i}}} + a_q^\dagger\mathrm{e}^{-\mathrm{i}q\cdot r_{\mathrm{i}}}\right). \tag{12}$$

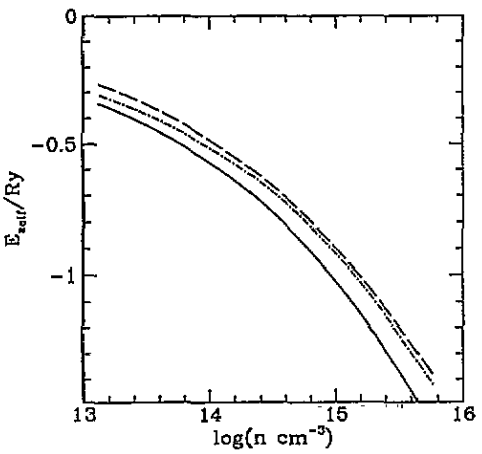

Figure 1. *Pair self-energy as a function of free* electron–hole density for GaAs. The full line is calculated from equation (14), the dot-dashed line from [23] and the dashed line from [21]. The energy is in units of effective Rydbergs.

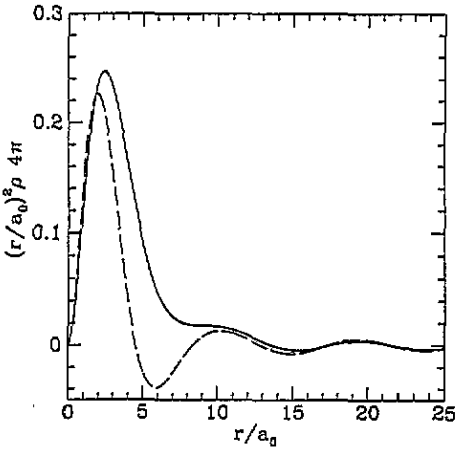

Figure 2. *Modulus of the induced charge density* ρ *as* a function of r (units of the effective Bohr radius). The full line refers to the electron and the dashed line to the hole. Material parameters are those of GaAs.

3. Free electron–hole pair interacting with a plasmon mode

Before starting our analysis of the exciton ground state from Hamiltonian (12) it is interesting to look at some results concerning the case of a free pair embedded in the electron–hole gas. One of the problems one has to face in dealing with highly excited semiconductors is the gap renormalization, that is, the energy a particle gains because of the interaction with all the other particles. Traditionally, this self-energies are calculated splitting the contribution to the single particle self-energies into a screened-exchange term, calculated with the screened Coulomb potential, and a Coulomb-hole term which accounts for the charge density fluctuations around the test charge [7, 8, 18]. From the point of view of our Hamiltonian formulation, the exchange correlation is, at this stage, neglected whereas the Coulomb-hole is fully accounted for. The pair self-energy can easily be calculated from Hamiltonian (12) *dropping the direct electron–hole Coulomb interaction*

$$H = \sum_{i=e,h} \frac{P_i^2}{2m_i} + \sum_q \hbar\omega(1)\left(a_q^\dagger a_q + \frac{1}{2}\right) + \sum_q \sum_{i=e,h} C_i(q)\left(a_q e^{iq\cdot r_i} + a_q^\dagger e^{-iq\cdot r_i}\right). \tag{13}$$

Since this Hamiltonian is formally identical to the one of the polaron problem, we may use the Lee–Low–Pines variational scheme [19, 20] and get

$$E_{self} = -\frac{e^2}{\pi\epsilon_0}\hbar\omega_p^2 \sum_{i=e,h} \int_0^\infty \frac{dq}{\omega(q)}\left(\hbar\omega(q) + \frac{\hbar^2 q^2}{2m_i}\right)^{-1}. \tag{14}$$

In figure 1, we present a comparison between the gap-renormalization numerically calculated from equation (14) and from both the universal formula of Vashishta and Kalia [21] and Zimmermann [23] for the case of GaAs. These formulae provide a good interpolation of experimental results [22]. In making this comparison we have used equation (3) for the plasma dispersion, the Lindhard expression (5) for $\epsilon(q)$ and the following material parameters [24]: $m_e = 0.067$, $m_h = 0.62$, $\epsilon_0 = 13.18$. Considering that there are no adjustable parameters in the density range considered, the agreement is satisfactory.

A point of interest for a deeper physical understanding of the problem is the calculation of the induced charge density fluctuation. From (8) and (10) the charge density operator for an electron embedded in a electron–hole gas is

$$\hat{\rho}(q) = -\left(\frac{\epsilon_0 v q^2 \hbar \omega_p^2}{8\pi\omega(q)}\right)^{1/2}\left(a_q + a_{-q}^{\dagger}\right). \tag{15}$$

The expectation value of this operator on the Lee–Low–Pines [19, 20] variational ground state wavefunction leads to

$$\rho(|r - r_e|) = -\frac{e\hbar^2\omega_p^2}{2\pi^2}\frac{1}{|r - r_e|}\int_0^\infty \frac{q\,dq}{\hbar\omega(q)}\frac{1}{\hbar\omega(q) + \hbar^2 q^2/2m_e}\sin(q|r - r_e|) \tag{16}$$

where, having taken the average with respect to the plasmon variables only, the induced charge depends on the position of r_e of the inducing electron. A feeling on the general properties of $\rho(r)$ can be gained by solving the above integral taking equation (4) for the plasmon dispersion and neglecting the kinetic term $\hbar^2 q^2/2m_e$, that is, assuming the inducing electron at rest, for instance at $r_e = 0$. We have

$$\rho(r) = \frac{e}{4\pi} Q_{TF}^2 \frac{e^{-rQ_{TF}}}{r}. \tag{17}$$

This simple result indicates that the induced charge density is exponentially decaying with r and proportional to the square of the Thomas–Fermi wavevector Q_{TF}. The total induced charge is

$$\int \rho(r)\,dr^3 = e. \tag{18}$$

From the Poisson equation

$$\nabla^2 v(r) = -\frac{4\pi\rho(r)}{\epsilon_0} \tag{19}$$

it is immediately apparent that the electrostatic potential is

$$v(r) = \frac{e}{\epsilon_0 r}\left(1 - e^{rQ_{TF}}\right). \tag{20}$$

The potential energy $V(r)$ for the presence of an hole is therefore

$$V(r) = E_{self} + ev(r) = -\frac{e^2 Q_{TF}}{\epsilon_0} + \frac{e^2}{\epsilon_0 r}\left(1 - e^{rQ_{TF}}\right) \tag{21}$$

where the first term is the self-energy (14) (gap renormalization) of a charge at rest. By adding to equation (21) the attractive Coulomb potential energy relative to an electron–hole pair $-e^2/\epsilon_0 r$ we get

$$V(r) = -\frac{e^2 Q_{TF}}{\epsilon_0} - \frac{e^2}{\epsilon_0 r}e^{-Q_{TF}} \tag{22}$$

that is, exactly the potential which comes from static screening theory [17]. It is worth stressing the way in which the static screening results from our theory. Apart of the Thomas–Fermi approximation which is not crucial for what we are going to state, the static screening is a direct result of neglecting the kinetic term $\hbar^2 q^2/2m_e$ with respect to ω_p. In other words, the plasma responds so swiftly to the electron that it sees its instantaneous positions. The above arguments can be repeated as they are to the case where the inducing particle is a hole.

In figure 2, the modulus of the electron (hole) induced particle densities are shown as calculated from (16) including both the kinetic terms and the Lindhard expression for the dielectric function. There are two interesting features. First, the total induced charge is still $\pm e$ indicating that the electron–hole interaction is again short range (the total charge is zero). Second, apart from the oscillations typical of the Lindhard dielectric function, the induced charge density has a different behaviour for the electron and the hole due to the different band mass and ultimately to a different dynamics.

4. Exciton ground state and effective potential

In this section we are going to describe a variational procedure for the Hamiltonian of equation (12). The first step is the reduction to the centre of mass and relative coordinates for the electron–hole pair

$$\begin{aligned} R &= s_1 r_e + s_2 r_h \\ r &= r_e - r_h \end{aligned} \tag{23}$$

with

$$s_1 = m_e/M \qquad s_2 = m_h/M \qquad M = m_e + m_h. \tag{24}$$

The transformed Hamiltonian reads

$$\begin{aligned} H = \frac{P^2}{2M} + \frac{p^2}{2\mu} - \frac{e^2}{\epsilon_o r} + \sum_q \hbar\omega(q)\left(a_q^\dagger a_q + \frac{1}{2}\right) \\ + \sum_q c(q)\left(\eta_q(r) a_q e^{iq\cdot R} + \eta_q^*(r) a_q^\dagger e^{-iq\cdot R}\right) \end{aligned} \tag{25}$$

where $C(q)$ is defined in (10), $\omega(q)$ is given in equation (3) and

$$\eta_q(r) = \exp(is_2 q\cdot r) - \exp(-is_1 q\cdot r). \tag{26}$$

Since the total linear momentum of the system

$$\mathcal{P} = P + \sum_q \hbar q a_q^\dagger a_q \tag{27}$$

commutes with the above Hamiltonian, the operator

$$U(R, Q) = \exp\left[i\left(Q - \sum_q q a_q^\dagger a_q\right)\cdot R\right] \tag{28}$$

clears the Hamiltonian from the centre of mass coordinate $\boldsymbol{R}$. It is in fact easy to show that

$$\tilde{H} \equiv U^{-1}HU = \frac{\hbar^2}{2M}\left(Q - \sum_q q a_q^\dagger a_q\right)^2 + \frac{p^2}{2\mu} - \frac{e^2}{\epsilon_0 r} + \sum_q \hbar\omega(q)\left(a_q^\dagger a_q + \frac{1}{2}\right) + \sum_q C(q)\left(\eta_q(r)a_q + \eta_q^*(r)a_q^\dagger\right) \tag{29}$$

where $\hbar Q$ is the eigenvalue of $\boldsymbol{P}$. Our aim is the variational calculation of the total ground state energy. The trial ground state wavefunction is chosen to be

$$|\Psi\rangle = U_{\mathrm{F}}(r)|0\rangle\phi(r) \tag{30}$$

where

$$U_{\mathrm{F}} = \exp\left[\sum_q \left(f_q(r)a_q - f_q^*(r)a_q^\dagger\right)\right] \tag{31}$$

is a generalization of the Lee–Low–Pines transformation with an explicit dependence on the relative coordinate r and

$$\phi(r) = \frac{1}{\sqrt{4\pi}}\left[\frac{(2\gamma)^3}{2}\right]^{1/2} \mathrm{e}^{-\gamma r} \tag{32}$$

is the exciton envelope 1s wavefunction with γ as a variational parameter. The plasmon distribution functions $f_q(r)$ are calculated from the minimum condition

$$\frac{\delta}{\delta f_q(r)}\langle\Phi|\tilde{H}|\Psi\rangle = 0 \tag{33}$$

which produces the Eulerian partial differential equation

$$\frac{\hbar^2}{2\mu}\nabla_r^2 f_q - \frac{\hbar^2}{2\mu}\frac{\nabla\phi^2\cdot\nabla f_q}{\phi^2} + \left[\hbar\omega(q) + \frac{\hbar^2 q^2}{2M}\right]f_q = C(q)\eta_q(r) \tag{34}$$

whose solution has been already widely discussed [13–16]. An excellent approximation to $f_q(r)$ is given by

$$f_q(r) = \frac{2\mu C(q)}{\hbar^2}\left(\frac{\mathrm{e}^{\mathrm{i}s_2\boldsymbol{q}\cdot\boldsymbol{r}}}{\xi^2/4 + s_2^2q^2} - \frac{\mathrm{e}^{\mathrm{i}s_1\boldsymbol{q}\cdot\boldsymbol{r}}}{\xi^2/4 + s_1^2q^2}\right) \tag{35}$$

where

$$\xi = \left[4\gamma^2 + \frac{8\mu}{\hbar^2}\left(\hbar\omega(q) + \frac{\hbar^2q^2}{2M}\right)\right]^{1/2}. \tag{36}$$

The ground state energy on the trial wavefunction (30) with $Q = 0$ is

$$E(\gamma) = \langle\phi|\frac{p^2}{2\mu} + V_{\mathrm{eff}}(r;\,\gamma)|\phi\rangle \tag{37}$$

where we have defined an effective potential

$$V_{\rm eff}(r,\gamma) = -\frac{e^2}{\epsilon_0 r} - \frac{\nu\mu}{\pi^2\hbar^2}\int_0^\infty q^2 C^2(q)\left[\frac{2\mu}{\hbar^2}2a_{\rm e}(q)a_{\rm h}(q)\hbar\omega(q)\frac{\sin(qr)}{qr}\right.$$
$$\left.\times\left(a_{\rm e}^2(q)+a_{\rm h}^2(q)\right)\gamma^2+\left(a_{\rm e}(q)+a_{\rm h}(q)\right)\left(1-2\frac{\sin(qr)}{qr}\right)\right]{\rm d}q \qquad (38)$$

which, when averaged on the envelope (32) gives rise to the exciton total energy

$$E(\gamma) = \frac{\hbar^2\gamma^2}{2\mu} - \frac{e^2\gamma}{\epsilon_0} - \frac{\nu\mu}{\pi^2\hbar^2}\int_0^\infty q^2 C^2(q)\left[\frac{2\mu}{\hbar^2}2a_{\rm e}(q)a_{\rm h}(q)\hbar\omega(q)\frac{(2\gamma)^4}{(4\gamma^2+q^2)^2}\right.$$
$$\left.\times\left(a_{\rm e}^2(q)+a_{\rm h}^2(q)\right)\gamma^2+\left(a_{\rm e}(q)+a_{\rm h}(q)\right)\left(1-2\frac{(2\gamma)^4}{(4\gamma^2+q^2)^2}\right)\right]{\rm d}q \qquad (39)$$

where

$$a_{\rm i}(q) = \left(\gamma^2+\frac{2\mu}{\hbar}\omega(q)+\frac{\mu}{m_{\rm i}}q^2\right)^{-1} \qquad {\rm i} = {\rm e},\ {\rm h}. \qquad (40)$$

It is worth discussing in some detail equation (38). The first term is just the direct electron–hole Coulomb potential. Inside the integral we can distinguish two types of term: those with an explicit dependence on r and those that are constant. In both cases there is an explicit dependence on the exciton envelope wavefunction (32) through the parameter γ. The terms not dependent on r can be defined as self-energy terms with an explicit dependence on γ. However, the pair self-energy $E_{\rm self}$ given in equation (14) can be obtained from either (38) or (39) setting $\gamma = 0$. Since the limit $\gamma = 0$ means that the electron–hole pair are at infinite relative distance, we can state

$$E_{\rm self} = E(\gamma)_{\gamma=0}. \qquad (41)$$

The fact that the self-energy is obtained within the same Hamiltonian and approximations as that of the exciton is an important feature of our approach which, as we shall see, facilitates comparison with experimental data. The calculation of the integral in equation (38) can be done analytically only under the same restrictions discussed in the case of the induced charge density of section 3. Thus, neglecting the kinetic terms $\hbar^2q^2/2m_{\rm i}$, taking equation (4) for the plasmon dispersion and setting $\gamma = 0$ we obtain equation (22) for the effective potential. It is interesting to note that equation (22) has resulted from (21) because of an exact cancellation of the direct Coulomb interaction. This is still true, but only for $\gamma = 0$, that is, when the particles are at great distance from each other. For $\gamma \neq 0$ equation (38) is unable to produce a Coulombic potential exactly cancelling the direct Coulomb interaction (first term of equation (38)). The consequence of this is that the effective potential of equation (38) has a screened Coulombic tail for $\gamma \neq 0$. More precisely, it is possible to show from (38) that, apart from constant terms,

$$V_{\rm eff}(r)_{r\to 0} \sim -\frac{e^2}{\epsilon_0 r} \qquad (42)$$

$$V_{\rm eff}(r)_{r\to\infty} \sim -\frac{e^2}{\epsilon_0 r}\left(1-\frac{\hbar\omega_{\rm p}}{\hbar^2\gamma^2/2\mu+\hbar\omega_{\rm p}}\right). \qquad (43)$$

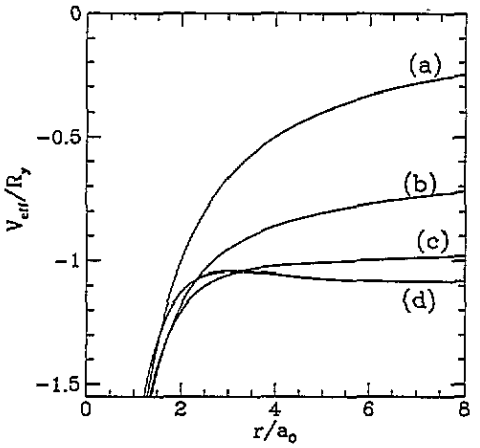

Figure 3. The effective potential as defined in equation (38) as a function of r for $n = 1.24 \times 10^{15}$ ($r_s = 5.0$) and for three different values of γ. (a) Coulomb potential, (b) $\gamma = 1.0$, (c) $\gamma = 0.5$, (d) $\gamma = 0.0$. Material parameters are those of GaAs.

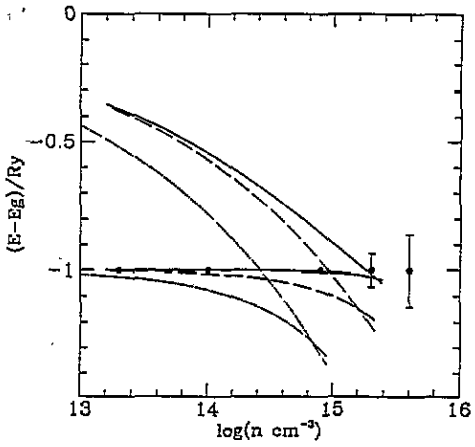

Figure 4. GaAs exciton energy and self-energy referred to the gap at $n = 0.0$. The dots are experimental points taken from [26]. The dot-dashed, the dashed and the full line corresponds to different approximations (see text).

Equation (43) shows the relative importance played by γ and $\hbar\omega_p$ in determining the screened Coulombic tail.

In figure 3 we present a plot of the effective potential numerically calculated from equation (38) with a free particle density of $n = 1.24 \times 10^{15}$ ($r_s = 5.0$) and for three different values of γ. Curve (a) is the bare direct Coulomb interaction whereas (b), (c) and (d) correspond to $\gamma = 1.0, 0.5, 0.0$ respectively. It is immediately seen that for $\gamma \neq 0$ there is a screened Coulombic tail.

5. Pauli blocking

As soon as an electron–hole gas is generated by optical pumping a Fermi sphere is formed and therefore the k-space available to the exciton for forming the ground state is reduced (Pauli blocking). In order to account for this effect we have changed the exciton envelope function in such a way to make it orthogonal to all plane waves inside the Fermi sphere. Taking for the Fourier transform of the envelope, the following expression

$$\phi(k) = \frac{(k^2 - k_F^2)^{1/4}}{k^{1/2}} g\left(\sqrt{k^2 - k_F^2}\right)\theta(k - k_F) \tag{44}$$

where k_F is the Fermi momentum, $\theta = 1$ when $k > k_F$ and is zero otherwise, and g is an arbitrary function of its argument, we have a normalization independent of k_F

$$\int_0^\infty k^2\phi^2(k)\,dk = \int_{k_F}^\infty k(k^2 - k_F^2)^{1/2} g^2\left(\sqrt{k^2 - k_F^2}\right) dk = \int_0^\infty u^2 g^2(u)\,du$$

and a kinetic energy (apart from $\hbar^2/2\mu$)

$$\int_0^\infty k^4\phi^2(k)\,dk = \int_{k_F}^\infty k^3(k^2 - k_F^2)^{1/2} g^2\left(\sqrt{k^2 - k_F^2}\right) dk = k_F^2 + \int_0^\infty u^4 g^2(u)\,du$$

which is the sum of the term one would get without orthogonalization and the kinetic energy k_F^2 of two particle sitting on the Fermi sphere. These two properties lead us to choose for $g(k)$ the Fourier transform of the envelope (32) $1/(\gamma^2+k^2)^2$ and write

$$\phi(r) = \frac{4\gamma^{5/2}}{\pi^{3/2}} \int_{k_F}^{\infty} \frac{k^{1/2}(k^2-k_F^2)^{1/4}}{(k^2-k_F^2+\gamma^2)^2} \frac{\sin(kr)}{r}\,\mathrm{d}k. \tag{45}$$

It is immediately apparent that this envelope reduces to (32) for $k_F = 0$. It is also interesting to study the asymptotic behaviour of $\phi(r)$

$$\phi(r)_{r\to\infty} = \frac{0.7743 k_F^{3/4}}{\gamma^{3/2}} \frac{\cos(\pi/8 + k_F r)}{r^{9/4}} \tag{46}$$

which on one side shows a delocalization of the exciton envelope depending on k_F and on the other the possibility of still defining the exciton average radius $\langle\phi|r|\phi\rangle$.

It should be mentioned that by changing the exciton envelope from (32) to (45), a new Eulerian differential equation for $f_q(r)$ from (33) is obtained so that both the approximation (35) and consequently the effective potential (38) should assume a different form. The calculation of an effective potential fully consistent with the envelope (45) is technically involved so that, at this stage, we have done the following approximation. The Eulerian partial differential equation (34) determining $f_q(r)$ has the term

$$\frac{\hbar^2}{2\mu} \frac{\nabla\phi^2(r)}{\phi^2(r)} \nabla f_q(r) \tag{47}$$

which is responsible for the coupling between the exciton envelope ϕ and the plasmon field. With the envelope (32) we have

$$\frac{\nabla\phi^2(r)}{\phi^2(r)} = -2\gamma \tag{48}$$

which allows an exact solution [13, 14] for $f_q(r)$ from which (35) is derived. With $\phi(r)$ defined in (45), we can approximate (48) with

$$\langle\phi|\frac{\nabla\phi^2(r)}{\phi^2(r)}|\phi\rangle = 4\pi \int_0^{\infty} r^2 \frac{\mathrm{d}\phi^2}{\mathrm{d}r}\,\mathrm{d}r = -8\pi \int_0^{\infty} r\phi^2\,\mathrm{d}r \tag{49}$$

and therefore define an effective variational parameter

$$\bar{\gamma} = 4\pi \int_0^{\infty} r\phi^2\,\mathrm{d}r \tag{50}$$

which substitutes γ in equation (35) and it is such that $\bar{\gamma} = \gamma$ when $k_F = 0$. With this sort of mean field approximation we are confident that most of the underlying physics has been captured. We shall see that this conclusion is supported by the excellent agreement with experimental data.

6. Numerical results

In this section we present a number of results obtained from the numerical minimization of equation (39) with respect to the parameter γ using differ levels of approximation. We shall also look at some quantities like the average exciton radius, absorption coefficient in an optical transition, average number of plasmon dressing the electron–hole pair, which are all useful for the characterization of the exciton. Although our theory is applicable to any semi-conductor, all the calculations refer to GaAs at $T = 0$ K with the plasmon dispersion given by equation (3) with the Lindhard static dielectric function (5). With these choices for the plasmon dispersion there are not adjustable parameters.

In figure 4 we show results of the minimization of equation (39) compared with experimental data of Fehrenbach *et al* [25, 26]. In this figure we draw simultaneously the exciton total energy (which, for the chosen units, tends to -1 at low density) and the free particle self-energy. There are three sets of results we wish to comment about, considering that the crossings between curves of the same type (full, dashed, dot-dashed) define the densities at which the exciton breaks in a free pair. The dot-dashed line is obtained assuming that the electron–hole pair can emit and reabsorb plasmons without recoil, that is, neglecting $\hbar^2 q^2/2m_i$ in equation (39). As we have seen, this corresponds to a static approximation. It is immediately seen that this approximation gives an overestimation of both the screening and self-energy. It fails in reproducing the persistence of the exciton line. A remarkable improvement is obtained when recoil terms are included (dashed line). The overall trend is towards a reduction of the screening. Finally, a more than satisfactory agreement with the experiment is obtained when Pauli blocking is included (full line) along the lines discussed in the previous section. Here the variational parameter is still γ and the actual values entering the effective potential are given by equation (50).

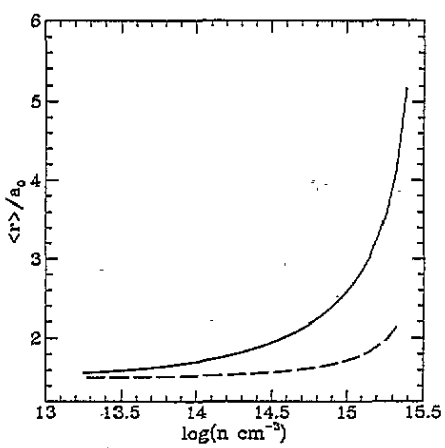

Figure 5. Exciton average radius as a function of density. The full line is calculated with the exciton envelope given in equation (45) whereas the dashed line from equation (32). Material parameters are those of GaAs.

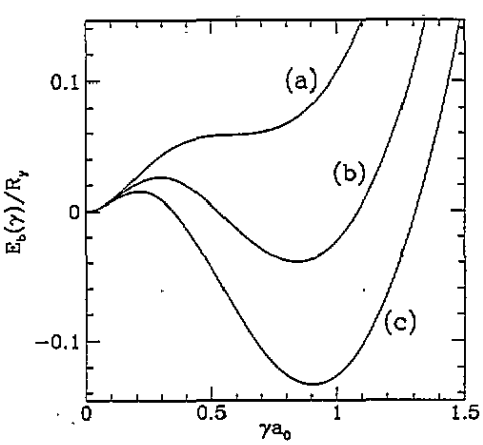

Figure 6. Exciton binding energy as a function of the variational parameter γ calculated with the envelope (32). The three curves correspond to the densities: (a), $n = 2.43 \times 10^{15}$ ($r_s = 4.0$); (b), $n = 1.24 \times 10^{15}$ ($r_s = 5.0$); (c), $n = 7.20 \times 10^{14}$ ($r_s = 6.0$). Material parameters are those of GaAs.

In figure 5 we present the average exciton radius $\langle r \rangle = \langle \phi | r | \phi \rangle$ as a function of the free particles' density. The values of γ used in this calculation are those that minimize the total

energy. The general trend is an increase of $\langle r \rangle$ with the density indicating that the effect of the screening is, as expected, to make the exciton larger. The orthogonalization of the exciton envelope to plane wave (full line) makes the exciton even larger, with $\langle r \rangle \sim 5$ Bohr radii near the transition from bound to unbound state.

In figure 6, the binding energy $E_b(\gamma) = E(\gamma) - E(0)$ is shown as a function of the variational parameter γ for three different densities. This figure shows the existence of either one or two minima according to whether or not the exciton forms in a bound state. For densities $n < 2.4 \times 10^{15}$ ($r_s > 4.0$), a bound state is formed so that the minimum at $\gamma \neq 0$ is lower than the one at $\gamma = 0$. Since $\gamma \to 0$ means a very large separation between the particles forming the exciton, in such a density range two free particles are unstable against the formation of a bound state. For $n > 2.4 \times 10^{15}$ ($r_s < 4.0$) the opposite occurs, that is, the exciton is unstable versus the formation of a free pair.

In figure 7 the values of $|\phi(0)|^2$ as a function of the free particle density are shown, again calculated with the values of γ which minimize the total energy at a given density. It is well known that this quantity is related to the exciton optical absorption and therefore its decreasing with the density of the screening particles is consistent with the experimental observation of a vanishing exciton line. There is not a great difference between the envelopes (32) and (45).

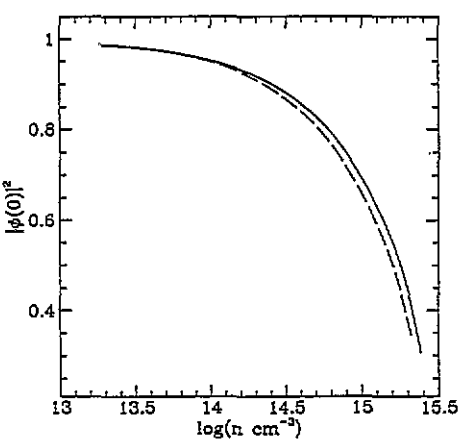

Figure 7. Modulus squared of $\phi(0)$ as a function of density normalized to the value at $n = 0.0$. The full line is calculated from the envelope (45) whereas the dashed line is from (32).

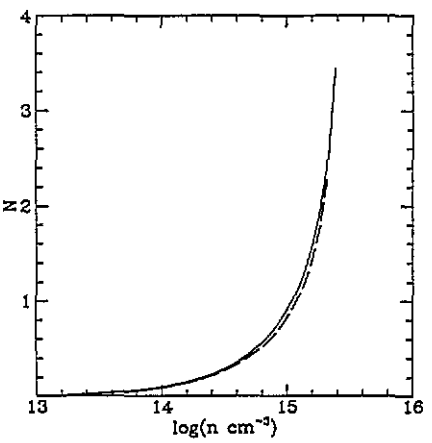

Figure 8. Average number of dressing plasmons as a function of density. The full line is calculated from the envelope (45) whereas the dashed line is from (32).

In figure 8 we show the average number of plasmons dressing the exciton as a function of density. As one would expect, N does increase with density, particularly near the ionization threshold, where $N \sim 3$. The fact that N is of the order of some units is consistent with our intermediate coupling [20] variational choice of equation (30).

In figure 9 the dilution parameter defined as $n\langle r \rangle^3$ is shown against the free particle densities. This parameter gives the average number of particles in the volume occupied by the exciton and defines the density range within which our single exciton theory is valid. It is in fact evident that if the dilution is bigger than one, then there would be a substantial overlap between different excitons and therefore the exciton–exciton interaction is no longer negligible. It is seen that there is a marked difference between the envelopes (32) and (45)

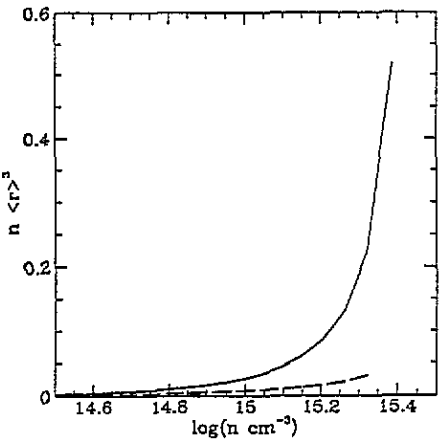

Figure 9. Dilution parameter as a function of density. The average radius is as in figure 9.

related to the delocalization of the exciton. However, $n\langle r\rangle^3$, in the density range of interest, is always less than 1, indicating that the exciton–exciton interaction is negligible.

7. Conclusion

In conclusion, we have shown that a theory describing the dynamical screening of an exciton embedded in a photogenerated electron–hole gas can be formulated in terms of electron (hole) plasmon interaction in a fashion similar to the electron–phonon interaction. We have underlined the importance of accounting for the recoils due to the emission and reabsorption of plasmons and the presence of a Fermi sphere which reduces the k-space available to the exciton wavefunction. A detailed study of the effective electron–hole interaction has shown that the screening depends on the average distance between the particles. This distance is proportional to γ^{-1} where γ is a variational parameter calculated, for each density, from the minimization of the exciton total energy. At low density the excitonic pair is separated by about one effective Bohr radius ($\gamma \to a_0^{-1}$), its kinetic energy is bigger than $\hbar\omega_p$, the electron–hole gas cannot follow the exciton and therefore the free electron–hole screening is not very effective. In contrast, at high densities the average exciton radius increases ($\gamma \to 0$), the kinetic energy is lower than $\hbar\omega_p$ and therefore the free charges have time to adjust themselves in such a way to make the screening more effecting. In the limit ($\gamma \to 0$) there is no Coulombic tail in the screened effective potential.

We have analytically shown that assuming the excitonic part very far apart ($\gamma \to 0$), neglecting the recoils and assuming a Thomas–Fermi dielectric function for the electron–hole gas, the effective interaction reduces to a Yukawa potential with a screening length given by the inverse of the Thomas–Fermi momentum. This is the bridge between our dynamical theory and previous Hamiltonian approach [7, 17].

A number of quantities such as the average number, N, of plasmon dressing, the exciton and the dilution parameter have been calculated to consistently support the approximations used. In particular, the behaviour of N with the free particle density justifies the use of an intermediate coupling scheme for the system ground state and the low (< 1) value of the dilution parameter is consistent with neglecting the exciton–exciton interactions.

Finally, the theory has been compared with experimental data relative to GaAs showing the ability of this approach of reproducing the persistence of the exciton line when the sample is under strong optical excitation and of giving at the same time the transition density from bound to unbound states.

Acknowledgment

This work has been partially supported by the EEC Human Capital and Mobility Program under the contract No ERBCHRXCT930124.

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