Optical singularities in doped quantum-well wires

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We present the calculation of emission and absorption spectra of single quantum-well wires doped with electrons. By solving an effective Bethe-Salpeter equation we show the inadequacy of an on-site electron-hole interaction for describing the optical singularities appearing at the band bottom and at the Fermi edge. With the use of a statically screened Coulomb interaction we study the necessity of hole localization in order to get significant singularities. The effect of wire width, carrier density, and temperature is analyzed in the cases of having electrons in one or two subbands. The existing experimental evidence in multiwires is discussed in light of our results.

I. INTRODUCTION

Low-dimensional systems are practically produced by modulation-doped semiconductor heterojunctions. They are ideal for studying many-body properties of an electron gas because the interaction of the carriers with scattering centers is very weak as confirmed by the high mobilities of the samples.[1] Looking for such many-body effects, the optical properties of quantum wells (QW) have been extensively studied.[2] In particular, the possibility of finding singularities in emission and absorption spectra of these quasi-two-dimensional (2D) systems has received much attention.[2–17] In three dimensions strong localization of the hole is essential for having important many-body effects,[18–21] but in QW the reduction of the dimensionality favors exciton and Fermi-edge singularities (FES) with respect to bulk systems. Then, hole localization is not so crucial, although still necessary, so that singularities are experimentally observed.[3–11] An even better candidate is a quantum-well wire (QWW) where singularities associated with the quasi-one-dimensionality should be even stronger. Different fabrication techniques have recently made feasible such systems allowing the experimental search of singularities[11,22–24] and provoking an increasing theoretical interest.[11,25–27] Experiments made in spatially indirect multiwires[11] clearly show FES provided that the QWW are narrow enough. Such features have not been observed so clearly in direct wires[24] and multiwires[22] probably because they were too wide. As far as the theoretical analysis is concerned, there are calculations with an on-site potential for the electron-hole coupling either within a ladder approximation[25] or making an exact calculation in a finite system.[11,27] The main difficulty in such descriptions is the choice of the on-site potential as we will discuss in detail in this paper. A screened Coulomb interaction has been also considered[26] in the case of quasi-one-dimensional electrons confined in a parabolic potential in one direction while they are free to move in the other one and assuming strong localization of the holes.

The aim of this paper is to investigate the importance on the optical singularities in QWW of a reliable interaction between electrons and holes as well as the necessity or not of the hole localization. We consider a single wire with parabolic potentials with the same center both for the holes and the electrons at variance with some experimental situations where the two type of particles are in different spatial regions.[11,23] The holes are described in the simplest diagonal approach where the coupling between heavy and light subbands is only included by adequately varying the effective masses. By considering the actual eigenfunctions of these potentials as well as the Coulomb interaction screened by a statically consistent response function, which includes electron-electron interaction by means of fluctuation effects,[28] we compute the absorption and emission spectra of a quasi-one-dimensional (1D) electron gas within a ladder approximation for the correlation function. This approximation includes the most singular terms in the correlation function.[18–20] We devote our attention to two different cases where the Fermi level is either in the first or second 1D subband. Then, different selection rules for the light polarization appear due to the symmetry of the electronic wave functions.

The paper is organized as follows. Section II is devoted to the description of the model used for computing absorption and emission spectra. In Sec. III some results are presented to discuss the inadequacy of an on-site interaction in the description of FES. Once we have shown the necessity of using a more realistic Coulomb interaction, we analyze in Sec. IV the effect of the hole effective mass on the possibility of obtaining both band-edge and Fermi-edge optical singularities in quasi-1D systems with different widths of the wire. After having shown that localization of the hole is essential for obtaining strong singularities, we analyze them in Sec. V as a function of temperature, density of carriers, and other physical parameters. A discussion of experiments in light of our results and some conclusions are given in Sec. VI.

II. DESCRIPTION OF THE MODEL

We are interested in describing the optical properties of a single n-doped wire in which the electron and

hole states coexist in the same spatial region. Typical widths of actual wires are of the order of a few hundred angstroms, so the states are labeled by a quantum wave number k along the wire direction and a subband index n that for the cases of interest (densities of 10^5–10^6 cm^{-1}) is typically 0 or 1. Therefore we will consider at most a couple of bands for electrons while the holes are described in a diagonal approach so that only the heavy-hole subband is included. Both the emission and absorption spectra are computed from the linear optical susceptibility $\chi(\omega)$ that it is related to the electron-hole Green's function $G_{n_v,n_c;n'_v,n'_c}(k,k',\omega)$ by

$$\chi(\omega) = -\sum_{n_v,n_c;n'_v,n'_c;k,k'} \langle n_v,k|\epsilon\cdot\mathbf{p}|n_c,k\rangle \times\langle n'_c,k'|\epsilon\cdot\mathbf{p}|n'_v,k'\rangle \times G_{n_v,n_c;n'_v,n'_c}(k,k',\omega), \quad (1)$$

where $|n_v,k\rangle$ and $|n_c,k'\rangle$ are valence and conduction states, respectively, labeled by their subband index n and wave vector k, ϵ is the light polarization, and $\mathbf{p}$ is the momentum operator. The absorption intensity is directly given by the imaginary part of the susceptibility $\chi(\omega)$ while the luminescence spectrum is proportional to $g(\omega)\mathrm{Im}[\chi(\omega)]$, where $g(\omega) = \{\exp[(\omega-\mu_e-\mu_h)/(k_BT)]-1\}^{-1}$ is the Bose distribution function and μ_e and μ_h are the electron and hole chemical potentials, respectively.[20,21] The matrix elements of $\epsilon\cdot\mathbf{p}$ will be discussed below for the particular set of eigenstates that we are going to use. The key quantity in Eq. (1) is the Green's function that can be obtained from the noninteracting electron-hole Green's function $G^0_{n_v,n_c}(k,-k,\omega)$ by means of a perturbative expansion in terms of a static electron-hole interaction potential $V_{n_v,n_c;n'_v,n'_c}(k-k')$.[20] Before discussing in detail the ingredients G^0 and V, let us pay some attention to the perturbative procedure itself. The expansion is enormously simplified when the interaction is approximated by an on-site potential so that its Fourier transform is independent of k and k'. The main simplification comes from the fact that, when the appropriate hole spectral function is considered, the ladder diagrams are the most singular and the inclusion of all the crossed diagrams can be avoided.[18–21] Then, in this ladder approximation, the Green's function is given by a Bethe-Salpeter equation

$$G_{n_v,n_c;n'_v,n'_c}(k,k',\omega) = G^0_{n_v,n_c}(k,-k,\omega)\delta_{n_v,n'_v}\delta_{n_c,n'_c}\delta(k+k') + \frac{1}{L}\sum_{n''_v,n''_c,k''} G^0_{n_v,n_c}(k,-k,\omega)V_{n_v,n_c;n''_v,n''_c}(k-k'')G_{n''_v,n''_c;n'_v,n'_c}(k'',k',\omega), \quad (2)$$

L being the wire length. In spite of the fact that an on-site interaction involves some problems, to be discussed below, and an actual screened Coulomb interaction is required, we will keep the ladder approximation in the analysis of the optical spectra of doped QWW. The ladder equation (2) is rather easy to work with by discretizing the k space. If a mesh is defined between two cut-off values $\pm k_c$ with k_c sufficiently larger than the Fermi wave vector, the Green's function $G_{n_v,n_c;n'_v,n'_c}(k,k',\omega)$ is obtained from the inversion of a matrix $[1-G^0V]$ in the discrete indices k,k'. The results shown in this paper have been obtained from matrices with sizes of the order of 500. Let us now discuss the ingredients G^0 and V involved in the ladder equation (2) starting with the interaction because it is useful in the discussion of the noninteracting electron-hole Green's function.

A. Electron-hole interaction

As mentioned above when discussing the ladder equation (2), the easiest way to proceed is to use an on-site potential $V_{0,n_c;0,n'_c}(k) = U_{0,n_c;0,n'_c}$ independent of the electron and hole wave vectors. Then, the ladder equation can be easily solved. For instance, in the simple case of just one conduction band, the relation between the two Green's functions integrated in k space takes the simple form

$$G_{0,0;0,0}(\omega) = \frac{G^0_{0,0}(\omega)}{1-U_{0,0;0,0}G^0_{0,0}(\omega)}. \quad (3)$$

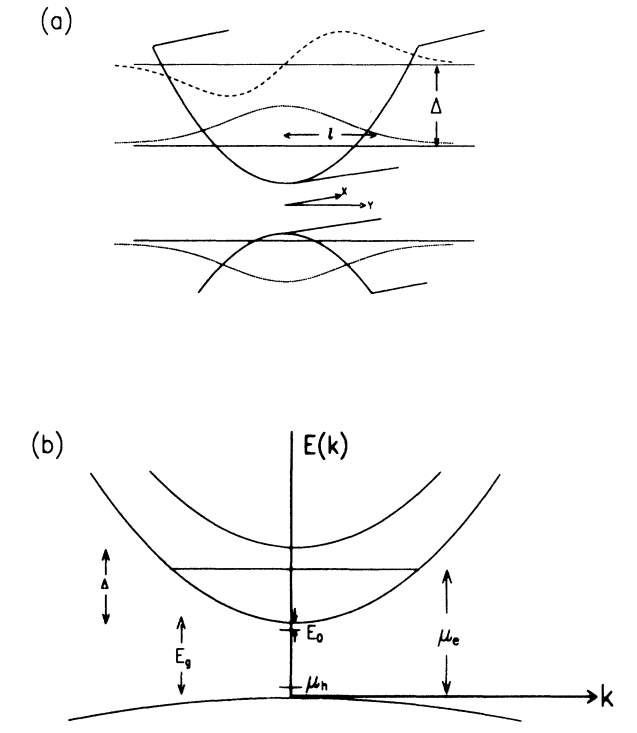

FIG. 1. Potential profile, wave functions (a) and band structure (b) of our model for the quantum-well wire. The magnitudes of interest are schematically shown.

This simple model could make sense because considering the hole as a scattering center for electrons, the optical spectra would be essentially controlled just by the phase shifts at the bottom of the conduction band and at the Fermi energy, i.e., only two parameters which could be associated with $U_{0,n_c;0,n_c'}$. However, the difficulty is the determination of such a parameter, which in turn determines very critically all the optical properties. In particular, as we will show in Sec. III, a small change (a few percent) in the coupling (U) quenches the FES. Therefore, a more adequate description is to consider the actual screened Coulomb interaction between an electron and a hole. For such a task one needs the quasiparticle wave functions. Firstly, we will consider that electrons and holes are completely confined in the xy plane. Then, the carriers are free to move along the x direction (the wire direction) while they are confined by parabolic potentials in the y direction as schematically shown in Fig. 1. We take the two parabolas in such a way that the ratio of separations Δ between the two first levels is just given by the inverse ratio between effective masses, i.e., $\Delta_e/\Delta_h = m_h^*/m_e^*$, as it would occur for infinite well potentials. Then the wave function of each of those carriers is of the form

$$\psi_{n,k}(x,y,z) = \sqrt{\frac{\delta(z)}{TL}}\frac{e^{ikx}}{\sqrt{L}}\sqrt{\frac{1}{2^n n!\sqrt{\pi}l}}e^{-y^2/2l^2}H_n\left(\frac{y}{l}\right), \tag{4}$$

where H_n is the Hermite polynomial corresponding to the nth subband, and both electrons and holes have the same characteristic length $l = \sqrt{\hbar/m_e^*\Delta_e}$ (hitherto we will use Δ for the characteristic frequency of the harmonic potential confining electrons). From the wave functions of electrons and holes, it is straightforward to get the unscreened Coulomb interaction between them.[28] As mentioned above, we are going to restrict ourselves to one heavy-hole subband and two electron subbands so that the necessary components of the unscreened electron-hole interaction that we need are

$$V^0_{0,0;0,0}(k) = -\frac{e^2}{\varepsilon_s}e^{l^2k^2/4}K_0(l^2k^2/4), \tag{5}$$

$$V^0_{0,1;0,1}(k) = -\frac{e^2}{\varepsilon_s}e^{l^2k^2/4}\left[K_0(l^2k^2/4) + \frac{l^2k^2}{4}[K_0(l^2k^2/4) - K_1(l^2k^2/4)]\right], \tag{6}$$

$$V^0_{0,0;0,1}(k) = 0, \tag{7}$$

K_0 and K_1 being modified Bessel functions of the second kind and ε_s the effective dielectric constant of the system fitted to give the adequate exciton binding energy $E_0(\simeq 6$ meV) of the kind of QW we are interested in. It must be pointed out that if one would consider the hole wave function completely localized [i.e., $\delta(x)\delta(y)$], the factors $\frac{1}{4}$ in the interactions V^0 should be replaced by $\frac{1}{8}$.[26]

Once we have the unscreened potential, we need to screen it in order to get the adequate electron-hole interaction. Two ingredients are required for the screening: the electron-electron interaction and the electron polarizability obtained from such interaction at zero temperature. Provided that l is the same for electrons and holes, the electron-electron interaction has the same shape that the electron-hole interaction has with just a change sign. On top of the matrix elements given in Eqs. (5)–(7), we also need the elements $V^0_{0,0;1,1}$ and $V^0_{1,1;1,1}$. The former is not necessary because it is only required in the screening of an interaction which is zero due to the symmetry of the potentials we have choosen. As far as the other one is concerned, it takes the form

$$V^0_{1,1;1,1}(k) = \frac{e^2}{\varepsilon_s}e^{l^2k^2/4}\left[\left(1 + \frac{l^2k^2}{2} + \frac{l^4k^4}{4}\right)K_0(l^2k^2/4) - \left(\frac{l^2k^2}{4} + \frac{l^4k^4}{16}\right)K_1(l^2k^2/4)\right], \tag{8}$$

where we have already written the sign corresponding to electron-electron interaction. The only lacking ingredient is the electron polarizability. In order to include some electron-electron effects in the polarizability, we take the form obtained from a generalized quantum Langevin approach which includes fluctuation effects by means of a diffusion constant.[28] Due to the symmetry of the potentials we only need the intrasubband matrix elements of the electron polarizability given by

$$\chi_{n,n}(k,\omega) = -\frac{m_e^*}{\pi k}\ln\frac{(lk_{Fn} + lk/2)^2 + a^2l^2k^2 - (\omega/lk\Delta)^2 - 2ia\omega/\Delta}{(lk_{Fn} - lk/2)^2 + a^2l^2k^2 - (\omega/lk\Delta)^2 - 2ia\omega/\Delta}, \tag{9}$$

where k_{Fn} is the Fermi wave vector of the nth subband and a is an adimensional parameter related to the diffusion constant.[28] Then, with all those ingredients, the statically screened electron-hole interaction is given by

$$V_{0,n;0,n'}(k) = \sum_{n'',n'''}[\varepsilon^{-1}(k,0)]_{n,n';n'',n'''}V^0_{0,n'';0,n'''}(k), \tag{10}$$

where the dielectric function is given by

$$[\varepsilon(k,\omega)]_{n,n';n'',n'''} = \delta_{n,n''}\delta_{n',n'''} - \chi_{n,n'}(k,\omega)V^0_{n,n';n'',n'''}(k). \quad (11)$$

B. Noninteracting electron-hole Green's function

The pair Green's function of noninteracting electron-hole pairs G^0 requires some attention because it contains two physical effects that are very important in the optical spectra: the temperature and lifetime of the individual quasiparticles electron and hole. Then, taking into account that the system is n-doped and at low temperatures so that only holes at the upper subband are considered, i.e., $n_v = 0$, the expression is

$$G^0_{0,n_c}(k,-k,\omega) = \int \frac{d\omega_{n_c}}{2\pi} \int \frac{d\omega_h}{2\pi} A_{n_c}(k,\omega_{n_c}) A_h(-k,\omega_h) \times \frac{1 - f_e(\omega_{n_c}) - f_h(\omega_h)}{\omega - \omega_{n_c} - \omega_h + i\delta}, \quad (12)$$

where $\delta = 0^+$ and f_e and f_h are the Fermi distribution functions of the quasiparticles. Lifetime effects are included in the spectral functions of the electron A_{n_c} and the hole A_h. Such effects are not important for the electron case because its lifetime implies a broadening much smaller than the electron chemical potential, so that

$$A_{n_c}(k,\omega) = 2\pi\delta[\omega - E_{n_c}(k)], \quad (13)$$

$E_{n_c}(k) = E_g + \hbar^2k^2/(2m_e^*) + n\hbar\Delta$ being the electron dispersion relation of the nth band with E_g the energy gap and m_e^* the electron effective mass. However, the case of the hole is more complicated. The ground-state wave functions of the conduction-electron system, with and without the valence-hole potential, are orthogonal so that just pair excitations of the conduction-electron gas break the symmetry giving the possibility of observing optical transitions; this is the well-known orthogonality catastrophe.[20] Such pair excitations are the essential dynamical effects responsible for a hole spectral function different from a δ function, so that we do not include other effects like plasmon excitation, Auger processes, and electron-phonon interaction which produce satellites, Lorentzian, and Gaussian shapes of the hole spectral function, respectively. It must be stressed that this is the approach consistent with the ladder approximation made above for the correlation function.[20] In the simplest approach, the contribution of the electron-hole pairs in the first conduction subband to the spectral function for the valence-band hole is obtained from a response function $R(\omega)$ within the static screening picture given by[15,20]

$$R(\omega) = \frac{1}{2\pi^2}\int dk \left[\frac{V^0_{0,0;0,0}}{|\varepsilon(k,0)|}\right]^2 [-\mathrm{Im}\chi_{0,0}(k,\omega)]. \quad (14)$$

From the expressions of Sec. II A it is straightforward to obtain, after some algebra, $R(\omega) \to g\omega$ as the asymtotic limit for $l \to 0$ and $\omega \to 0$, where

$$g = \frac{2}{\pi^2}\frac{1}{1 + \{\ln[1 + 1/(a^2)]/\pi\}^2}. \quad (15)$$

g does not vary very much with the value of a which is taken to be 0.1 along this paper. Equation (15) brings to a hole spectral function[20]

$$A_h(-k,\omega) = \frac{2\sin(\pi g)\Gamma(1-g)}{\mu_e}\frac{e^{-|\Omega|}}{|\Omega|^{(1-g)}}\theta[\pm\Omega], \quad (16)$$

where $\Omega = [\omega - E_h(k)]/\mu_e$, $E_h(k) = -\hbar^2k^2/(2m_h^*)$ being the hole dispersion relation with m_h^* the hole effective mass. The Heaviside step function $\theta[\pm(\Omega)]$ in Eq. (16) is a consequence of the sudden creation or annihilation of a hole at the valence band in the absorption and emission processes, respectively. This abrupt spectral function of the hole produces some computational unstabilities when solving Eq. (2). Therefore, the numerical calculations require us to introduce some imaginary parts in the frequency and to pay some attention to the associated fitting and convergence problems.

III. ON-SITE VERSUS COULOMB INTERACTION

Let us start by discussing the emission and absorption spectra for a system in the quantum limit in which the electron chemical potential is well below the bottom of the second conduction subband. In this case only electrons at the first subband are playing an important role so that the matrix elements of $\epsilon \cdot \mathbf{p}$, which are independent of the wave vector, have no effect on the spectra. This is different in the case of higher bands as will be discussed below.

An on-site interaction has been used[25,27] in the study of optical singularities in QWW because its inherent simplicity due to the lack of dependence of the coupling on the wave vector k. In the scheme we use, the problem reduces to solve Eq. (3) which is rather simple because $U_{0,0;0,0}$ is constant.[25] The origin of the FES is very easy to understand graphically as shown in Fig. 2. For those values of ω where $\mathrm{Re}G^0_{0,0}(\omega) = 1/U_{0,0;0,0}$ there are two peaks in the optical spectra with a width given by $\mathrm{Im}G^0_{0,0}(\omega)$. When such a width is large, these two peaks collapse in one. Then, the existence and strengh of the FES are extremely dependent on the value of $U_{0,0;0,0}$. So, it is possible to obtain any result by choosing the value of U, as shown in Fig. 3. Here, absorption and emission spectra for typical values of the effective masses, electron density, and temperature are presented for three different values of U. One could argue that a way of determining the adequate value for the on-site interaction should be to make some kind of average of the actual Coulomb interaction. A good possibility is to perform such an average to get the right value of some magnitude determined by the interaction as, for instance, the parameter g appearing in the hole spectral function. For the Coulomb interaction g is given by Eq. (15) while for the on-site interaction it

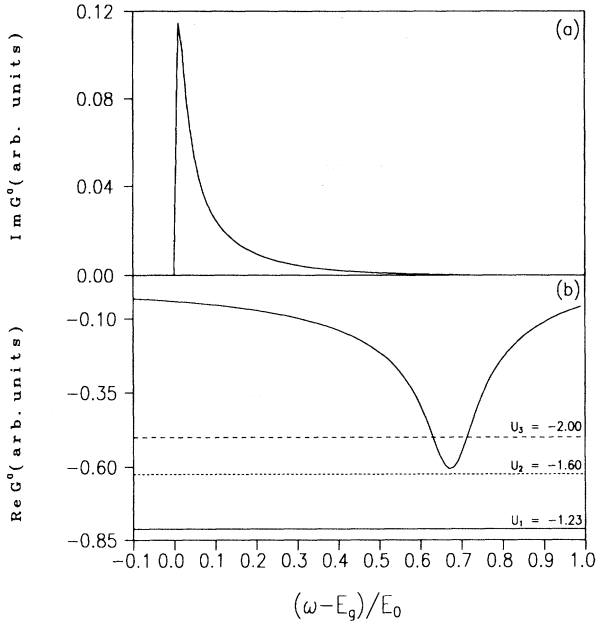

FIG. 2. Noninteracting electron-hole-pair Green's function for electrons in the first subband of a wire with a ratio of effective masses $m_h^*/m_e^* = 8$, $\mu_e = E_g + 0.6E_0$. The straight lines at values of $1/U$ are included as an indication of the possible solutions of the Bethe-Salpeter equation (see text).

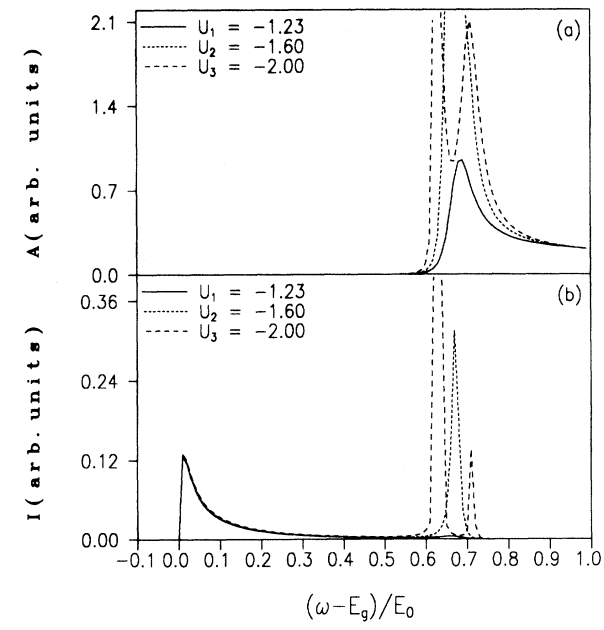

FIG. 3. Absorption (a) and emission (b) spectra of a wire at $T = 0.02E_0/k_B$ with electron chemical potential $\mu_e = E_g + 0.6E_0$ for different values of the on-site potential U between electrons and holes.

is straightforward to repeat the calculation, getting

$$g_0 = \frac{m_e U_{0,0;0,0}^2}{4\pi^2 \mu_e}. \tag{17}$$

By imposing $g = g_0$ one gets the desired average for the on-site interaction $U_{0,0;0,0}$. The trouble is that such an interaction would depend on the electron density. In the cases of Figs. 2 and 3 the value obtained with this procedure should be 1.23, the one labeled as U_1 that gives a tiny FES. With some other procedure of averaging perhaps it should be possible to get a more satisfactory result, but the uncertainty due to the value of the interaction would remain. Therefore we discard such a simple model interaction and work with the adequate Coulomb interaction described in Sec. II.

IV. EFFECT OF THE HOLE LOCALIZATION

Once we have shown that it is necessary to use the screened Coulomb interaction, we address ourselves in this section to the physically important question of the requirement of hole localization for having edge singularities. Such a localization is responsible for the singularities observed in the x-ray spectra of metals.[18–20] In two- and three-dimensional systems with mobile holes, there are no singularities due to peak broadenings produced by indirect transitions from the top of the valence band to the Fermi level accompained by low-energy excitations of the Fermi sea to ensure momentum conservation. In 1D systems this broadening mechanism is not efficient because allowed low-energy excitations are only with either 0 or $2k_F$ momentum. Therefore, quasi-1D systems are a good candidate for presenting singularities even for cases with mobile holes.[27] So, we are going to apply our model with a screened Coulomb interaction to analyze the possibility of having singularities with mobile holes.

In order to work in the range of experimental wire widths, we start with a parabolic wire with a width $2\sqrt{2}l$ of the order of 400 Å. The adequate magnitude to represent the wire is the level separation Δ that is equal to 1 (in units of E_0 as everywhere for energies in this paper and taking the electron effective mass of GaAs). Typical electron densities correspond to Fermi energies of the order of 0.6 which is the value we start with. Since, for the moment, we want a system without any extrinsic holes we take $\mu_h = 1$ (i.e., well within the gap). A low temperature where singularities can be expected is $T = 0.02$ (in units of E_0/k_B). In order to describe a mobile hole we can take for its effective mass a value of 8 (in units of the electron effective mass) at most. The absorption and emission spectra obtained with those parameters is shown in Fig. 4. The continuous lines correspond to the results obtained from $G(\omega)$ while the dashed lines are obtained with the use of $G_0(\omega)$ so that the difference is the many-body effect produced by the screened electron-hole interaction. The FES are more clear in absorption (the small oscillations in the figure are due to the integrals in k made with an accuracy which maintains a reasonable amount of computing time) while in emission it is rather weak. However, if one just looks at the complete

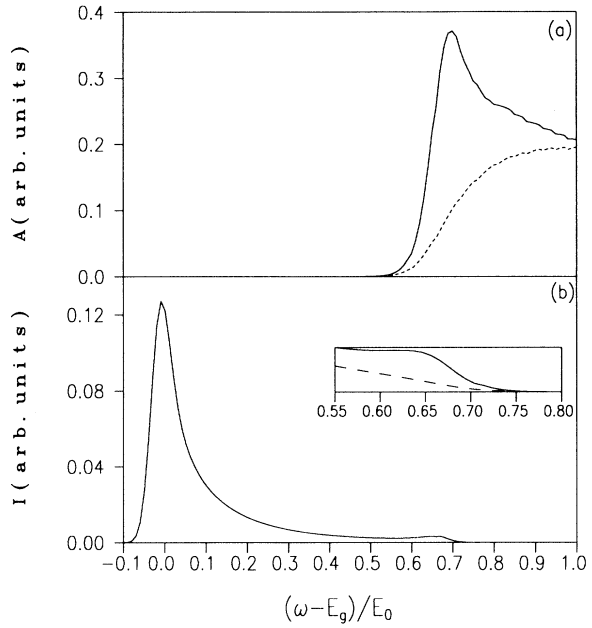

FIG. 4. Absorption (a) and emission (b) spectra of a wire at $T = 0.02E_0/k_B$ with electron chemical potential $\mu_e = E_g + 0.6E_0$, $\Delta = E_0$, and $m_h^* = 8m_e^*$ for both screened Coulomb interacting (continuous lines) and noninteracting (dashed lines) electron-hole pairs. In the case of emission the difference is only apparent close to the Fermi level as is shown in the inset.

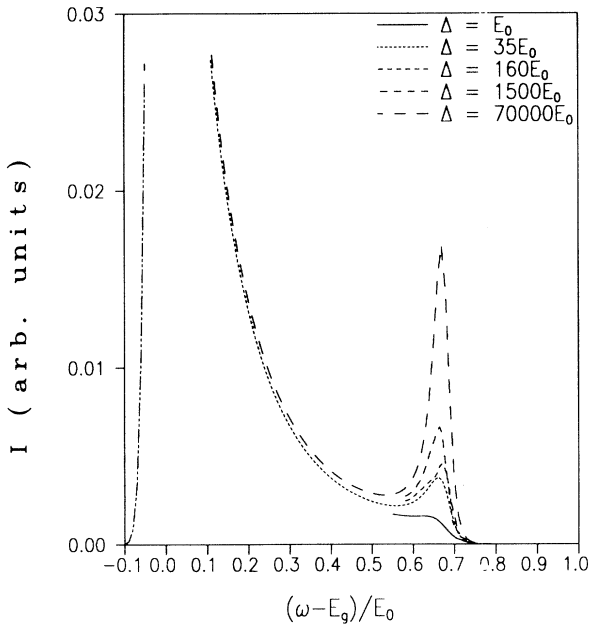

FIG. 5. Emission spectra of wires with different widths (i.e., different band separations Δ) at $T = 0.02E_0/k_B$ with electron chemical potential $\mu_e = E_g + 0.6E_0$ and $m_h^* = 8m_e^*$. The interaction between electrons and holes is a screened Coulomb one.

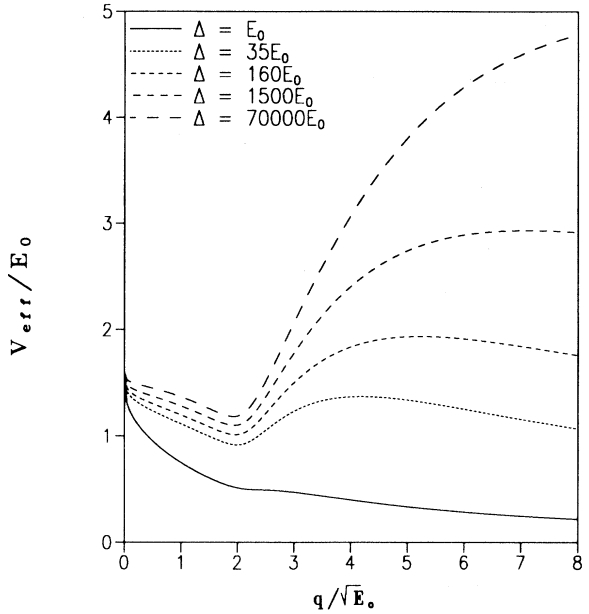

FIG. 6. Electron-hole screened Coulomb interaction for wires of different widths represented by the band separation Δ.

result (continuous lines) and tries to detect singularities by comparing with background values, the existence of FES is not so evident. A possibility to get stronger singularities is to reinforce the bare Coulomb attraction effect by decreasing the width of the wire, i.e., by having a more one-dimensional system. This is shown in

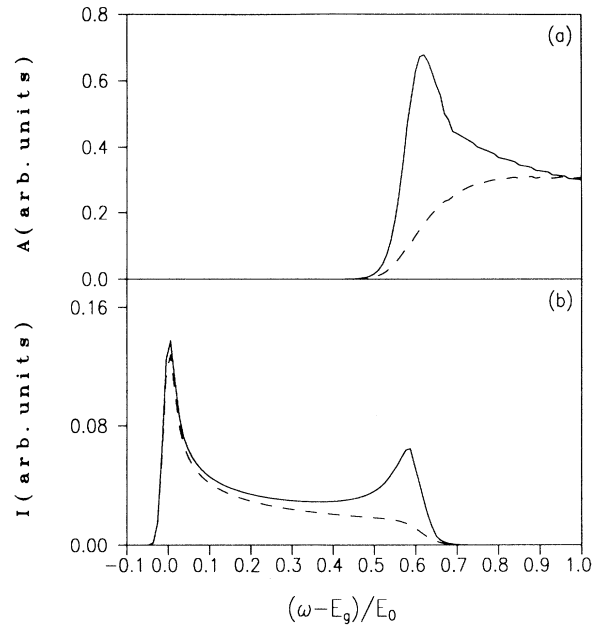

FIG. 7. Absorption (a) and emission (b) spectra of a wire at $T = 0.02E_0/k_B$ with electron chemical potential $\mu_e = E_g + 0.6E_0$, $\Delta = E_0$, and $m_h^* = 1000m_e^*$ for both screened Coulomb interacting (continuous lines) and noninteracting (dashed lines) electron-hole pairs.

Fig. 5 where the emission spectrum is shown for different values of Δ. FES neatly exist for values of Δ larger than 35 which means widths of the wire below 65 Å are clearly far narrower than the presently available wires. The singularity seems to saturate, and does not increase strongly for extremely narrow wires. This is understood by looking in Fig. 6 to the screened electron-hole interaction $V_{0,0;0,0}(k)$ for different values of Δ. The potential does not depend crucially on Δ in the region of $k \leq 2k_F$, which is the one of interest for computing the optical susceptibility $\chi(\omega)$. Since FES seem to be observed in wider multiwires,[11] a much more plausible explanation is to consider a localized hole. In our picture the simplest way of taking into account the localization is to increase the effective mass. The mass can be considered as infinite when $\hbar^2 k_F^2/(2m_h^*) \ll k_B T$. Therefore we present in Fig. 7 the absorption and emission spectra for $m_h^* = 1000$ and $\Delta = 1$. Now the singularities are very clear not only when comparing with the noninteracting case but also by themselves comparing peaks with backgrounds. This tends to suggest that the experimentally observed FES are connected with localized holes. Therefore, hereafter we are going to discuss the effect of different magnitudes for the case of a very large hole effective mass. Figure 8 shows that in this case of infinite hole mass the FES of the emission spectrum is stronger than the bottom band singularity for widths of the wire of 100 Å or smaller.

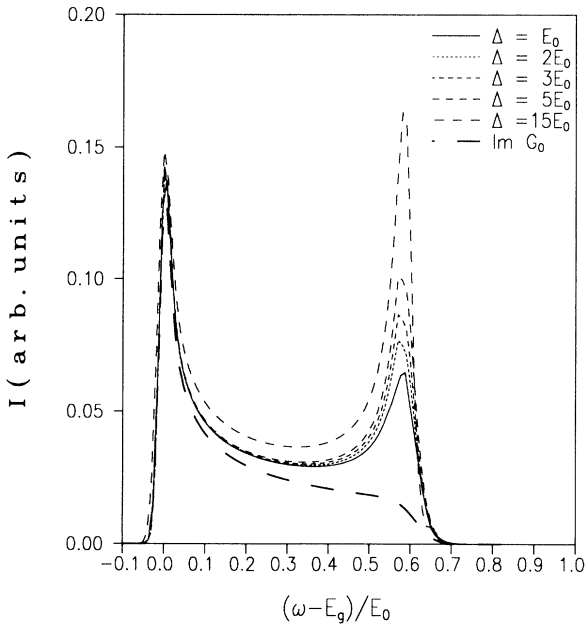

FIG. 8. Emission spectra of wires with different widths (i.e., different band separations Δ) at $T = 0.02E_0/k_B$ with electron chemical potential $\mu_e = E_g + 0.6E_0$ and $m_h^* = 1000m_e^*$. The interaction between electrons and holes is a screened Coulomb one. The lowest dashed line showing no peak corresponds to noninteracting electron-hole pairs.

V. EFFECT OF THE CARRIERS DISTRIBUTION

In this section we are going to study how singularities are affected by the distribution of electrons and holes, i.e., the effect of T and μ_e. As discussed above, all the results correspond to $m_h^* = 1000$ and $\Delta = 1$, implying a width of the wire around 400 Å. In order to simplify the discussion, we will start with a system where just one electron band is occupied at low temperature, i.e., $\mu_e < E_g + \Delta$. Although the difference between these two magnitudes would be small, the fact that we have a symmetric potential precludes the possibility of having a mixing between the first and the second electron subband produced by the Green's function as can happen in other systems.[25] For different polarizations one can have transitions from the top of the valence band to the even- or odd-parity electron bands, but they never interfere each other. Therefore, for the moment, we just consider the polarization which gives transitions to the first electron band.

A. Effect of the electron density

In the expressions of Sec. II it is not clear how the FES are affected by the variation of μ_e. In order to study this effect we compute just the emission spectrum where, as mentioned above, the singularity is easier to analyze by comparing with the background. We take a case with low temperature ($T = 0.02$) and no extrinsic holes ($\mu_h = 1$). Figure 9 shows the results for different

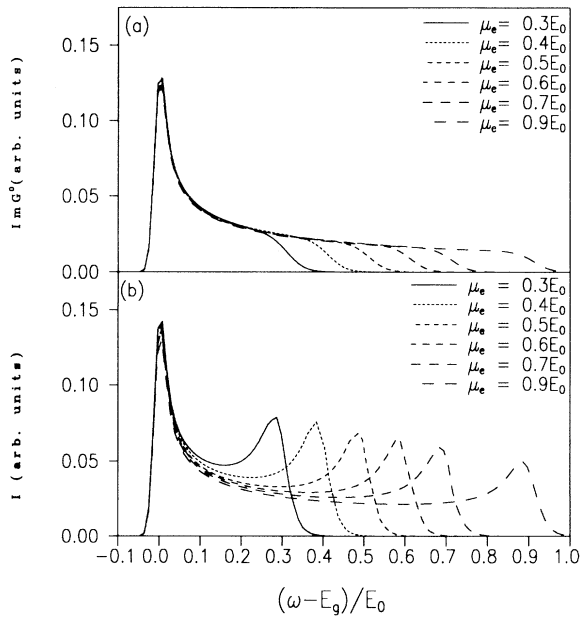

FIG. 9. Emission spectra of a wire with different electron chemical potentials μ_e at $T = 0.02E_0/k_B$ with $\Delta = E_0$ and $m_h^* = 1000m_e^*$. The two parts correspond to noninteracting (a) and interacting (screened Coulomb coupling) electron-hole pairs, respectively.

values of the electron chemical potential. For higher temperatures everything is smoother as will be discussed in the next section. The FES are not extremely dependent on the chemical potential although they slowly tend to disappear for high densities. When μ_e increases, the discontinuity at the Fermi level of G^0 slightly decreases, as shown in Fig. 9(b), due to the shape of 1D densities of states. This effect is compensated by an increase of the interaction in the region of wave vectors between 0 and $2k_F$, as shown in Fig. 10, where such an interaction is given for different electron densities.

B. Effect of the temperature

In order to see the effect of the temperature we concentrate again in the spectra of a wire with $\Delta = 1$ and $m_h = 1000$. We take $\mu_e = E_g + 0.6E_0$ which is an intermediate value among the ones above considered. Figure 11 shows the emission spectrum for different temperatures in the range between 0.02 and 0.10 (i.e., between 1.4 and 7 K). We have used a chemical potential for the holes $\mu_h = 0.01$ so that the total number of holes (and consequently the scale of the spectrum) does not change appreciably in the range of temperatures of interest as it occurs usually in the experiments.[11] The main result to be drawn is the disappearance of the FES for a temperature rather smaller than μ_e. In fact, such a disappearance does not depend significantly on μ_e. In Fig. 12 we show the absorption spectra for the same three temperatures of Fig. 11. Once again the FES are quenched for temperatures significantly smaller than μ_e. This result will be important below when discussing the experimental situation and the possible effect coming from a second electron subband.

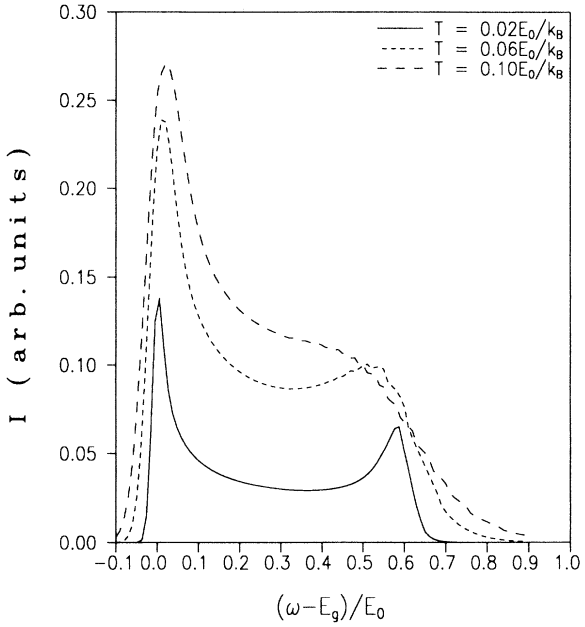

FIG. 11. Temperature variation of the emission spectrum of a wire with $\mu_e = E_g + 0.6E_0$, $\Delta = E_0$, and $m_h^* = 1000m_e^*$.

C. Second subband

Hitherto we have just discussed a case in which only one electron subband is occupied. A rather interesting case is that in which the electron Fermi level lies in the second subband. Then, in principle, the possibility exists of two singularities coming from the bottoms of the first and second subband and a double FES produced by the

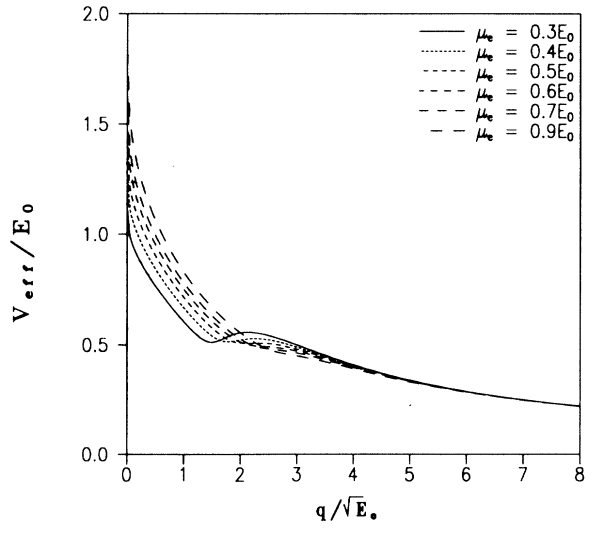

FIG. 10. Screened Coulomb interaction for different occupations of a wire with $\Delta = E_0$, $T = 0.02E_0/k_B$, and $m_h^* = 1000m_e^*$.

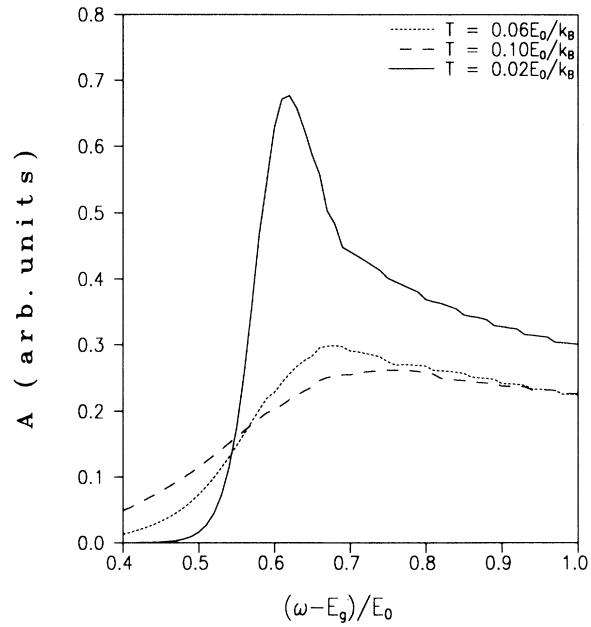

FIG. 12. Temperature variation of the absorption spectrum of a wire with $\mu_e = \mathcal{E}_g + 0.6E_0$, $\Delta = E_0$, and $m_h^* = 1000m_e^*$.

contributions of the Fermi levels at the two subbands. In order to analyze these possibilities, it becomes quite important to take care of the matrix elements of $\epsilon \cdot \mathbf{p}$ in Eq. (1), which are different for the two electron subbands so that the relative intensity of the different transitions can be known. After some algebra it is straightforward to obtain

$$\langle n_v = 0, k|\epsilon \cdot \mathbf{p}|n_c = 0, k\rangle = P_a \mathbf{u_x} + (P_a - P_b)\mathbf{u_y} \quad (18)$$

and

$$\langle n_v = 0, k|\epsilon \cdot \mathbf{p}|n_c = 1, k\rangle = ikl\sqrt{2\sqrt{2}}P_b \mathbf{u_y}, \quad (19)$$

where

$$P_a = \int d\mathbf{r} \frac{e^{-(y/l)^2}}{l\sqrt{\pi}} u_s \partial_x u_{p_x} \quad (20)$$

and

$$P_b = \int d\mathbf{r} \frac{e^{-(y/l)^2}}{l\sqrt{\pi}} \frac{y}{l^2} u_s u_{p_x}, \quad (21)$$

u_s and u_{p_x} being s and p atomic orbitals. From Eqs. (18) and (19) it is easy to see that the matrix element for the first electron subband is greater than or equal to the one of the second subband divided by $kl(2\sqrt{2})^{1/2}$. Since those u functions are difficult to manage, we take the most advantageous case for the second subband in which $P_a = P_b$ so that the only difference between the two matrix elements is just $ikl(2\sqrt{2})^{1/2}$. Then the singularity of the bottom of the second subband typical of any 1D system is going to be quenched by the factor k but the FES can still have some contribution of the second subband. We think that this ansatz overestimates the effect of the second subband which, anyway, is smaller than that of the first subband, as is shown in Fig. 13 for the emission spectra of the two bands separately. There it is clearly seen that, with increasing temperature, the effect of the first subband remains dominant, although less singular, around the Fermi level. Moreover, the quenching of that singularity is not directly related to the electron chemical potential as sometimes suggested.[11] We do not present results for the absorption because they are similar but less illustrative since there is no effect coming from the factor k appearing in emission. A possibility for the separating the effects of the first and second subbands should be to take advantage of the polarization rules contained in Eqs. (18) and (19).

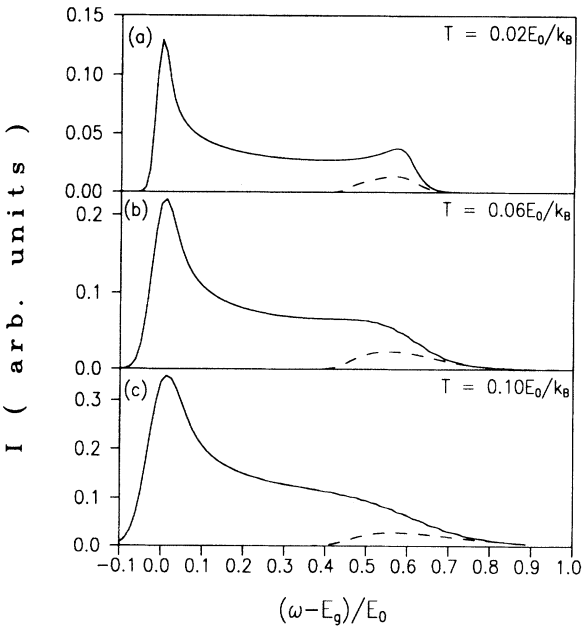

FIG. 13. Emission spectrum of a wire with $m_h^* = 1000m_e^*$, $\mu_e = E_g + 0.6E_0$, and $\Delta = 0.45E_0$, i.e., with electrons in the two first subbands for three different temperatures. Continuous lines give the contribution coming from the first subband while dashed lines give the contribution coming from the second subband.

VI. COMPARISON WITH THE EXPERIMENTS

Our results are for a single wire with electrons and holes in the same spatial region. Therefore they cannot be directly compared with experiments for multiwires for electrons and holes at different positions.[11] However, we think that some very general results should be applicable to any system made with wires. The first one is that although formally optical singularities exist for hole effective masses typical of perfect wires, in practice just with infinite m_h^* one gets clearly appreciable optical singularities. The only way of getting singularities with small hole masses should be to have wires much narrower than the ones presently available. Therefore, we think that the already observed[11] singularities are most probably connected with holes localized either by impurities or by some disordered variation of the wire width. An experimental fact rather difficult to understand is that the singularity of the band bottom is not observed in the emission experiments. Calleja *et al.*[11] suggest that this is probably once again connected with some variations in the wire width which would alter the energy position of such a feature in a random way with respect to the FES, which are the reference because they are always at the same energy. We find that singularities coming from the bottom of the bands are significantly more intense than the FES. Since width fluctuations only reduce the intensity of these peaks in, at most, a factor of 2 (Ref. 29), the lack of those peaks does not seem to be completely understood. We think that this disappearance should be typical of systems with electrons and holes spatially separated; therefore we have some work in progress along this line. A final comment is required for the case in which there are electrons in two conduction subbands. In this case our results are less directly comparable to the experiments[11] because the symmetry and selection rules are different, but we think that our result indicat-

ing that the FES are related to states in the first subband more than to those in the second one is still applicable to the presently available systems. As we have already mentioned we intend to work theoretically with the other system but it should also be interesting to have experiments in a case similar to ours because its high symmetry would give new and interesting possibilities along the lines of our theoretical results.

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