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Fermi-edge singularities in the optical absorption and emission of doped indirect quantum wires

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Fermi-edge singularities in the optical spectra of doped indirect quantum wires are theoretically analyzed by using a screened Coulomb interaction. In the extreme quantum limit in which the Fermi level lies in the lowest electron subband, strong singularities appear when three requisites are fulfilled: (i) infinite hole mass, (ii) Fermi energy slightly smaller than the intersubband spacing for electrons, and (iii) a transverse separation of the order of 100 nm exists between the electron and the hole. In such a case the optical singularity associated with the bottom of the electron subband is negligible with respect to the one at the Fermi level. These results allow a clarifying discussion on the available experimental information.

Available experiments[1–5] on the optical properties of modulation-doped quantum wires have raised an interesting polemic about the possibility of observing Fermi-edge singularities (FES) in quasi-one-dimensional (1D) systems. Some optical absorption and emission measurements,[2] performed in the extreme quantum limit having carriers only in the first 1D subband, clearly show a strong peak at the Fermi energy. In contrast, some other experiments,[3–5] performed in rather similar conditions, do not seem to detect such FES in the optical spectra. One more puzzling feature of the luminescence experiments[2] is that the peak at the Fermi level is not accompanied in the spectra by another peak, lower in energy, connected with the singularity at the bottom of the 1D density of states. In other words, only in some cases is the FES observed with such a strong intensity that the bottom peak is negligible in comparison. No convincing explanation is obtained from the published theoretical models describing the optical properties of quantum wires.[6–10] Strictly 1D approaches[6,8,9] using model on site electron-hole interactions give always a singularity associated with the bottom the band and can also give a FES just by adequately choosing the coupling parameter. However, since there is no physical way of determining such a parameter, those models do not throw any light on the experimental controversy. More reliable calculations,[7,10] in which the actual screened Coulomb interaction between the carriers is used, clearly establish that the existence of the FES needs an infinite effective mass for the hole. In all the theoretical emission spectra, there is always a bottom singularity accompanying the FES in disagreement with the experiments. Theory also fails in understanding why some experiments do not detect singularities in spite of the similitude to the cases where those singularities are observed. The problem of the works[7,10] using screened Coulomb interaction is probably due to the fact that the calculations are made for electrons and holes coexisting in the space while the experiments are usually performed with indirect wires. In fact, these models have an important deficiency because they involve selection rules which prevent the coupling between spatially symmetric and antisymmetric wave functions.[10] This decouples even and odd subbands canceling any possible FES enhancement associated with the Fermi level in the lowest subband and very close to the bottom of the next subband.[6,11] In this paper we present a theoretical analysis that solves all these difficulties and completely clarifies the experimental situation.

In order to compute the absorption and emission spectra of a quantum wire, we follow the theoretical procedure that we developed in Ref. 10. All the optical properties are obtained 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 key quantity in Eq. (1) is the interacting Green's function. As discussed in Ref. 10, $G_{n_v,n_c;n'_v,n'_c}(k,k',\omega)$ can be obtained from the noninteracting electron-hole Green's function $G^0_{n_v,n_c}(k,-k,\omega)$ and from the static electron-hole interaction potential $V_{n_v,n_c;n'_v,n'_c}(k-k')$ by means of a Bethe-Salpeter equation provided that a spectral function for the hole is included to give the adequate power-law shape of the singularity. The Bethe-Salpeter equation

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

where L is the wire length, is solved by discretizing the k space. If a mesh is defined between two cutoff 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'. G^0 is the same in the case of a direct or an indirect wire, so that we use the same one as that in Ref. 10 including the hole spectral function. The physically essential difference appears in the electron-hole interaction. We consider that both electrons and holes are completely confined in the xy plane. The electrons are free to move as a plane wave along the x direction (the wire direction) while they are confined by parabolic potentials in the y direction having a wave function[10] proportional to $\exp(-y^2/2l^2)H_n(y/l)$, where H_n is the Hermite polinomial corresponding to the nth subband. Their characteristic width is $l=\sqrt{\hbar/m_e^*\Delta}$. For the holes we are interested in a wave function displaced a distance a in the y direction with respect to the electrons. Since the only requirement for having strong FES is to have infinite hole mass, we have two possibilities: (i) extended holes in the x direction with zero mobility due to random fluctuations of the potential in the y direction, and (ii) localized holes due to trapping in impurities or any other defect. In the case of direct wires these two possibilities do not give qualitative differences for the FES.[12] Therefore, we can work with any one of them, and choose the first one. We use for the hole a plane wave in the x direction and a localized part in the y direction given by $\exp[-(y-a)^2/2l^2]H_n[(y-a)/l]$. In this way the spatial width of the holes is the same as that of electrons as happens in the experiments.[1–5] From the wave functions of electrons and holes, it is straightforward to get the unscreened Coulomb interaction between them. We 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

$$V^0_{0,0;0,0}(k)=-\sqrt{2}e^2/(l\varepsilon_s\sqrt{\pi})e^{-a^2/2l^2}2\mathcal{I}(a,k),$$

$$V^0_{0,1;0,0}(k)=-\sqrt{2}e^2/(l\varepsilon_s\sqrt{\pi})e^{-a^2/2l^2}\sqrt{2}\left[(a/l)-l\frac{d}{da}\right]\times\mathcal{I}(a,k),$$

$$V^0_{0,1;0,1}(k)=-\sqrt{2}e^2/(l\varepsilon_s\sqrt{\pi})e^{-a^2/2l^2}\times\left[1+(a^2/l^2)-2a\frac{d}{da}+l^2\frac{d^2}{da^2}\right]\mathcal{I}(a,k),$$

where

$$\mathcal{I}(a,k)=\int_0^\infty dy\,e^{-y^2/2l^2}\cosh(ay/l^2)K_0(ky),$$

K_0 being a modified Bessel function of second kind and ε_s the effective dielectric constant of the system fitted to give an adequate exciton binding energy $E_0=6$ meV. The screening of the Coulomb interaction is only due to electrons so that it is exactly the same than for direct wires where we used a random-phase approximation.[10,13] The crucial difference with respect to direct wires is that here $V^0_{0,1;0,0}(k)$ is different from zero allowing the coupling between odd and even electronic bands which brings to a strong enhancement of the FES when the Fermi level lies just below the bottom of one of the bands, as we will see below.

Let us apply our model to some cases with typical parameters in order to understand the experiments. Experiments in which the FES have been detected[2] are performed with wires having a Fermi energy in the range 3.5–4.5 meV and an intersubband spacing Δ roughly 0.5 meV higher than E_F. Therefore, we work in the extreme quantum limit in which the Fermi level lies below the bottom of the second subband. We perform our calculations with $E_F=0.6E_0$ and Δ varying in the range between $0.64E_0$ and $0.8E_0$ in order to understand the importance of the separation between E_F and Δ. Also to cover the experimental range, we take the temperature $0.02E_0/k_B\simeq1.4$ K $\le T\le0.1E_0/k_B\simeq7$ K. The electron effective mass is that of GaAs while for the holes we take infinite mass in order to get a significant FES as discussed above. The last parameter of interest is the separation a of electron and holes. Experiments[2] with $a=100$ nm show FES while others[3] with $a=250$ nm do not. Therefore, we will cover the range $0\le a\le250$ nm. A very important point in our calculations is that the momentum matrix elements in Eq. (1) are taken as constant so that only effects of the electron-hole Green's function are responsible for the features in the spectra. Figure 1 shows the absorption (a) and emission (b) spectra for $T=0.02E_0/k_B$, $E_F=0.6E_0$, and $a=100$ nm for three different values of Δ. From the figure it is quite clear that the FES is associated with the difference between the Fermi level and the subband separation. When such a difference is of the order of 1 meV or greater the FES becomes inappreciable (the high-frequency peak is not a FES but a transition to the second subband). Due to the asymmetry of the potential, $G_{0,0;0,1}$ couples $G_{0,0;0,0}$ with $G_{0,1;0,1}$. The latter gives a very strong contribution to the total emission. In a direct wire the off-diagonal term is zero and no strong singularity appears even when the intersubband separation is slightly larger than the Fermi energy.

Once the importance of the proximity of E_F and Δ is established, let us analyze the importance of the electron-hole spatial separation as the key to understand differences between experiments. Figure 2 shows the emission spectra for several values of a for wires with $T=0.02E_0/k_B$, $E_F=0.6E_0$, and $\Delta=0.7E_0$. The absorption spectra are not shown because they do not give any insight on the physics behind the experimental features. Both for small and large values of a the FES is rather weak. Only in the range between 50 and 100 nm does the singularity become strong. Our results show a maximum of $V_{0,0;0,1}$ in that range while the two diagonal terms $V_{0,0;0,0}$ and $V_{0,1;0,1}$ decrease monotonically with increasing a. For $a\to0$ the symmetry tends to decouple the first and second electron subbands and the singularity weakens. For very large a the interaction between the electron and the hole is so small that the second term of Eq. (2) goes to zero and the Green's function tends to be G_0 which does not present singularities at all.[14] Our results are in agreement both with experiments[2] which present FES in wires having $a=100$

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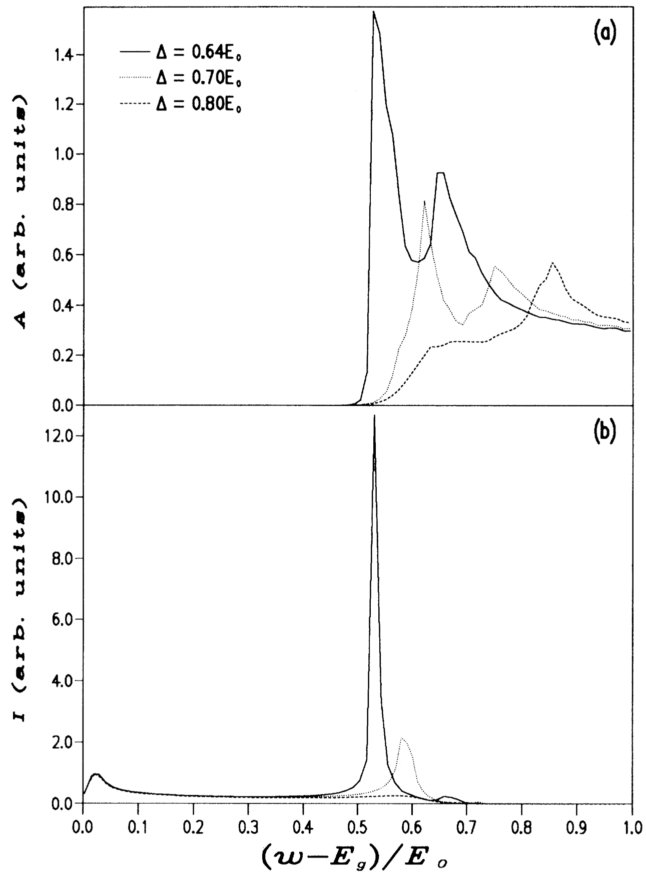

FIG. 1. Absorption (a) and emission (b) spectra of an indirect wire at $T = 0.02E_0/k_B$ with Fermi energy $E_F = 0.6E_0$ and electron-hole separation $a = 100$ nm for different values Δ. E_g is the single-particle band gap.

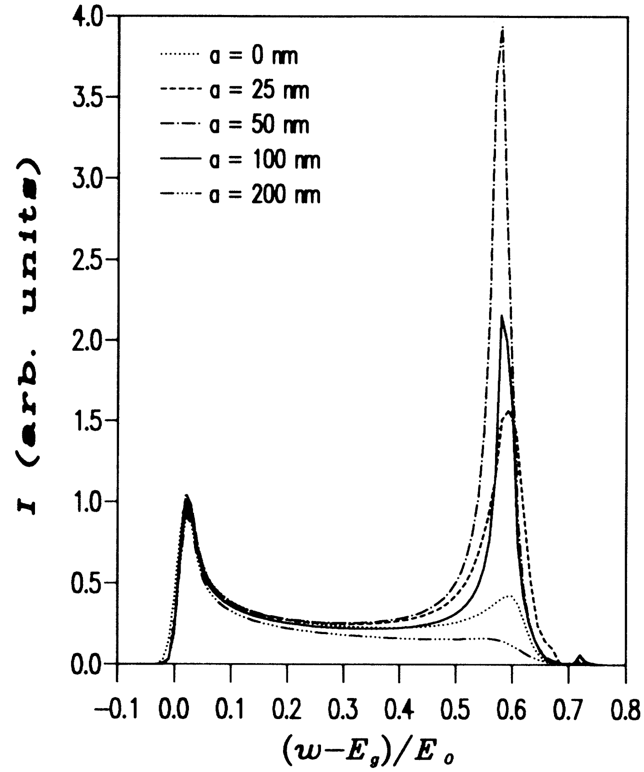

FIG. 2. Emission spectra of several wires with different electron-hole separations a at $T = 0.02E_0/k_B$, $E_F = 0.6E_0$, and subband separation $\Delta = 0.7E_0$.

nm and with those[3] which do not have singularity in wires having $a = 250$ nm. Moreover, the FES is so strong that the bottom singularity becomes negligible in the whole emission spectrum as experimentally observed.[2] Finally, another property comparable with the experiment is presented in Fig. 3. There, the emission spectrum for a wire with $E_F = 0.6E_0$, $\Delta = 0.7E_0$, and $a = 100$ nm is given for several temperatures. For a temperature of 7 K, much smaller than E_F, the FES has weakened so much that it is comparable to the bottom singularities of the first ($\omega - E_g \simeq 0$) and the second ($\omega - E_g \simeq 0.7E_0$) subband, i.e., something undetectable in the experiment. This again agrees with the experimental temperature dependence.

Finally, a very important point must be stressed. The calculation has been performed in a single indirect wire while the experiments are done with multiple wires. For a perfect array of wires, the symmetry should be restored so that the off-diagonal term of the Green's function should be zero again and the decoupling between first and second subband would tend to quench the FES. However, this is not the case in actual samples. The hole does not move along the x direction most probably due to fluctuations of the wire potential. The position x_i of such a localization is completely random for different wires i of

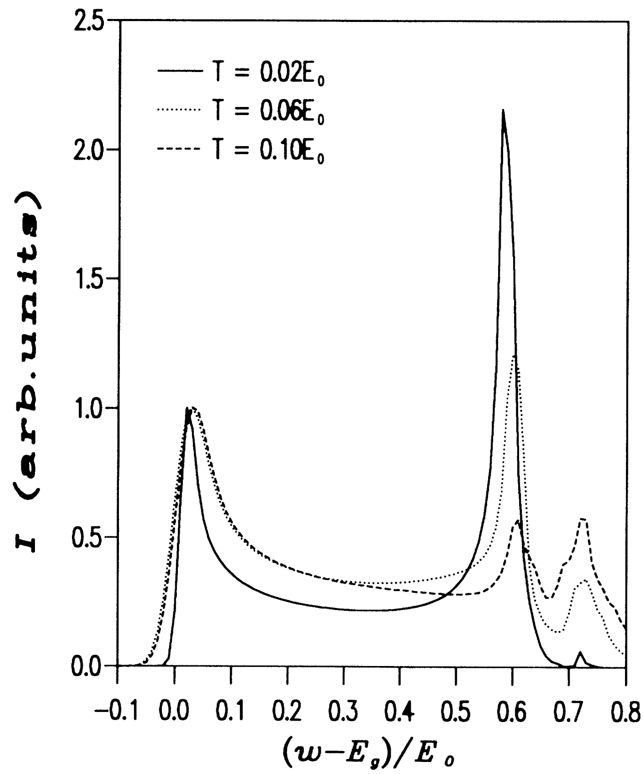

FIG. 3. Emission spectrum of an indirect wire with electron-hole separation $a = 100$ nm, $E_F = 0.6E_0$, and $\Delta = 0.7E_0$ for different temperatures.

the array and the system is not symmetric any more. We can modelize this effect in the following way: each electronic wave function in the wire i sees at its right a hole with a plane wave $\exp\{ik(x-x_i)\}$. The same electron sees at its left a hole having $\exp\{ik(x-x_{i-1})\}$. When averaging to the whole array, the phase $\exp\{ik(x_i-x_{i-1})\}$ cancels the contributions of one of the holes (for instance, the "left" hole) and the total result is just n times that of a single indirect wire simply having a "right" hole. In other words, the symmetry is not restored by the existence of a multiple array and all the results presented here for a single indirect wire are perfectly comparable with actual experiments.

In summary, we have studied the optical absorption and emission spectra of indirect wires in the extreme quantum limit in which the Fermi level lies in the lowest conduction subband. In order to observe FES, three requisites are needed: (i) infinite hole mass produced either by impurities or disorder along the wire, (ii) a Fermi energy slightly smaller than the intersubband spacing for electrons, and (iii) an intermediate spatial separation (of the order of 100 nm) between the electron and the hole.

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