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Excitonic enhancement of the Fermi-edge singularity in the optical spectra of doped semiconductors

Joachim F. Mueller
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08855

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Low-temperature optical-absorption and -emission spectra are calculated for *n*-type doped semiconductors in which the Fermi level is nearly degenerate with the exciton of a higher conduction band. It is shown that in such a system the Fermi-edge singularity can be strongly enhanced by the hybridization with the excitonic resonance. In fact, due to this enhancement the Fermi-edge singularity, which is usually only observed in absorption, also becomes visible in the emission spectrum, in accordance with recent experimental findings.

I. INTRODUCTION

The optical spectra of (*n*-type) modulation-doped heterostructures are known to be strongly influenced by many-body electron hole correlations.[1] In particular, for a sufficiently narrow hole band, multiple scattering of electrons and holes gives rise to the appearance of a Fermi-edge singularity in the low-temperature absorption spectrum.[2,3] However, because of momentum conservation, this Fermi surface effect is usually not seen in the luminescence spectrum, since emission mainly involves holes near $k=0$.[4,5]

Recently, Chen *et al.*[6] reported an unusual enhancement of emission intensity near the Fermi edge. They found that this enhancement stems from the atomic exciton of a higher conduction subband, which in their sample is almost degenerate with the Fermi level. However, the strong decrease of this emission line with increasing temperature showed that it is not purely excitonic, but involves the Fermi-edge resonance of the degenerate two-dimensional electron gas. In fact, it is the involvement of the Fermi sea that enabled Chen *et al.* to subsequently use this emission line as an optical probe for the quantum Hall effect.

In this paper the influence of an excitonic resonance originating from a higher conduction band on the optical spectra of an *n*-type doped semiconductor is examined theoretically. The simplest model that describes such a system consists of three bands (see Fig. 1): a valence band v, a partially filled lower conduction band c_1, and an empty upper conduction band c_2. Within this model it turns out that the observed enhancement in luminescence intensity at the Fermi energy can be attributed to the hybridization between the v-c_1 Fermi-edge resonance and the v-c_2 excitonic resonance. A c_1 electron may scatter virtually into band c_2, where, together with a hole in the valence band, it forms a virtual v-c_2 exciton. This effect strongly enhances the optical matrix element and leads to the appearance of the sharp v-c_2 excitonic resonance in the v-c_1 luminescence line, even in the absence of a real c_2 population. Essential for the occurrence of this effect is the presence of a pronounced Fermi-edge singularity in the underlying v-c_1 optical transition. As a consequence, the theoretical spectra display a strong temperature dependence. When the thermal energy k_BT becomes comparable to the Fermi energy, the Fermi-edge resonance becomes smeared out and thus also the enhancement of the luminescence intensity at the Fermi edge decreases, in accordance with the experimental findings.

In Sec. II of this paper the luminescence spectrum and the corresponding absorption spectrum are derived within the three-band model. In Sec. III numerical results are discussed.

II. THREE-BAND-MODEL CALCULATION OF THE OPTICAL SPECTRA

In this section, the absorption coefficient and the luminescence spectrum of the three-band model sketched in Fig. 1 are derived. As usual, the optical spectra are determined by the linear optical susceptibility $\chi(\omega)$, the resonant part of which is related to the electron-hole–pair Green's function $G^{e\text{-}h}$ by[7]

$$\chi(\omega)=-\sum_{j,j',k,k'}\mu^*_{j,k}\mu_{j',k'}G^{e\text{-}h}_{j,j',k,k'}(\omega)\ , \tag{1}$$

where $\mu_{j,k}=\langle c_j,k|ez|v,k\rangle$, $j=1,2$ is the optical dipole matrix element, and $G^{e\text{-}h}_{j,j',k,k'}(\omega)$ is the Fourier transform of the retarded pair-correlation function,

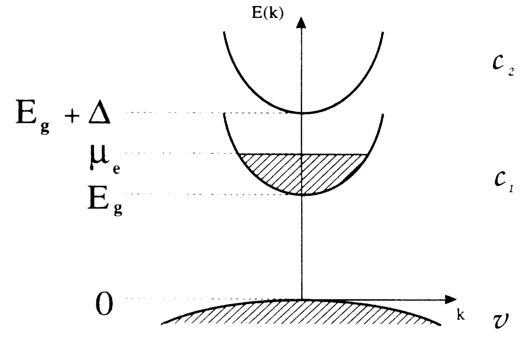


FIG. 1. Sketch of the three-band model discussed in the text.

$$G^{e\text{-}h}_{j,j',k,k'}(t-t') = -i\Theta(t-t')\langle [b_{-k}(t)a_{j,k}(t), a^{\dagger}_{j',k'}(t')b^{\dagger}_{-k'}(t')]\rangle \tag{2}$$

(with $\hbar=1$). Here, $a^{\dagger}_{j,k}$ and $b^{\dagger}_{k}$ denote creation operators for electrons and holes, respectively, k is the wave vector, $\Theta(\tau)$ is the Heaviside step function, and spin indices are suppressed. The dipole matrix element $\mu_{2,k}$ is assumed finite, as expected in asymmetric quantum-well structures.

An approximate solution for the pair Green's function $G^{e\text{-}h}$ can be obtained by summing the coupled ladder diagrams in the two channels v-c_1 and v-c_2. This yields the set of integral equations

$$G^{e\text{-}h}_{j,j',k,k'}(\omega) = G^{e\text{-}h,0}_{j,j',k,k'}(\omega) - \sum_{j'',k'',j''',k'''} G^{e\text{-}h,0}_{j,j'',k,k''}(\omega)V_{j'',j'''}(k''-k''')G^{e\text{-}h}_{j''',j',k''',k'}(\omega) , \tag{3}$$

where $G^{e\text{-}h,0}$ is the pair Green's function of noninteracting electron-hole pairs. In Eq. (3), $V_{i,j}=\langle c_i;v|V|c_j;v\rangle$ is the Coulomb matrix element for electron-hole scattering. For simplicity, other Coulomb matrix elements, such as $\langle c_i;c_j|V|c_{i'};c_{j'}\rangle$, are neglected in this calculation. The corresponding scattering processes cause exchange and correlation shifts of the single-particle energies and lead to the screening of the electron-hole interaction. Therefore, the single-particle energies in this calculation are renormalized energies, and V is an effective potential.

In general, Eq. (3) has to be solved numerically,[8] but for a qualitative discussion it is sufficient to proceed with the simplifying assumption that the interaction potential V is short ranged and thus wave vector independent:

$$V_{j,j'}(q) \rightarrow V_{j,j'} . \tag{4}$$

Also, for simplicity, the optical matrix elements are assumed k independent:

$$\mu_{j,k} \rightarrow \mu_j . \tag{5}$$

The optical susceptibility $\chi(\omega)$ can then be written as

$$\chi(\omega) = -\sum_{j,j'} \mu^*_j \mu_{j'} Q_{j,j'}(\omega) \tag{6}$$

with

$$Q_{j,j'}(\omega) = \sum_{k,k'} G^{e\text{-}h}_{j,j',k,k'}(\omega) . \tag{7}$$

With the help of Eq. (3), the contracted pair Green's functions $Q_{j,j'}$, Eq. (7), can be seen to satisfy the set of equations

$$\begin{aligned} Q_{1,1} &= Q^0_1 - Q^0_1 V_{1,1} Q_{1,1} - Q^0_1 V_{1,2} Q_{2,1} , \\ Q_{1,2} &= -Q^0_1 V_{1,1} Q_{1,2} - Q^0_1 V_{1,2} Q_{2,2} , \\ Q_{2,1} &= -Q^0_2 V_{2,1} Q_{1,1} - Q^0_2 V_{2,2} Q_{2,1} , \\ Q_{2,2} &= Q^0_2 - Q^0_2 V_{2,1} Q_{1,2} - Q^0_2 V_{2,2} Q_{2,2} , \end{aligned} \tag{8}$$

with Q^0_j being the contracted pair Green's function for noninteracting particles. At this point it is convenient to introduce the pair Green's function Q_j of a hole and a c_j electron in the absence of the coupling $V_{1,2}$:

$$Q_j = \frac{Q^0_j}{1+V_{j,j}Q^0_j} . \tag{9}$$

In terms of these functions one obtains for the optical susceptibility, Eq. (6),

$$\chi(\omega) = -\frac{|\mu_1|^2 Q_1 - (\mu^*_1\mu_2 V_{1,2} + \mu^*_2\mu_1 V_{2,1})Q_1 Q_2 + |\mu_2|^2 Q_2}{1-|V_{1,2}|^2 Q_1 Q_2} . \tag{10}$$

Both the absorption and the emission spectrum are proportional to the imaginary part $\chi''(\omega)$ of the optical susceptibility (10), which is given by

$$\chi''(\omega) = -\frac{Q''_1(|\mu_1 - \mu_2 V_{1,2} Q'_2|^2 + |\mu_2 V_{1,2} Q''_2|^2) + (1\leftrightarrow 2)}{[1-|V_{1,2}|^2(Q'_1Q'_2 - Q''_1Q''_2)]^2 + [|V_{1,2}|^2(Q'_1Q''_2 + Q''_1Q'_2)]^2} , \tag{11}$$

where Q'_j and Q''_j denote the real and the imaginary part of Q_j, respectively. Equation (11) reveals the factors by which the bare absorption coefficients for the optical transitions v-c_j, which are proportional to $\chi''_j(\omega) = -|\mu_j|^2 Q''_j(\omega)$, become enhanced due to the coupling $V_{1,2}$.

Knowing the absorption spectrum proportional to $\chi''(\omega)$, one can obtain the luminescence spectrum $I(\omega)$ by using the detailed balance relation

$$I(\omega) \propto g(\omega)\chi''(\omega) , \tag{12}$$

which holds under quasiequilibrium conditions.[7] In (12), $g(\omega)=\{\exp[(\omega-\mu_e-\mu_h)/T]-1\}^{-1}$ is the Bose distribution function (with $k_B=1$), and μ_e and μ_h are the chemical potentials of the electrons and holes, respectively. The same relation (12) also holds between the bare luminescence spectrum $I_j(\omega)$ and the bare absorption spectrum proportional to $\chi''_j(\omega)$. From Eq. (11) one thus obtains for the luminescence spectrum

$$I(\omega) = \frac{I_1(|1-\mu_2 V_{1,2} Q'_2/\mu_1|^2 + |\mu_2 V_{1,2} Q''_2/\mu_1|^2) + (1\leftrightarrow 2)}{[1-|V_{1,2}|^2(Q'_1Q'_2 - Q''_1Q''_2)]^2 + [|V_{1,2}|^2(Q'_1Q''_2 + Q''_1Q'_2)]^2} . \tag{13}$$

If the conduction band c_2 is unpopulated, then the term proportional to $I_2(\omega)$ in Eq. (13) vanishes and one is left with the bare c_1 luminescence spectrum $I_1(\omega)$, which, however, becomes enhanced by the virtual Coulomb transitions of electrons from the Fermi surface into the v-c_2 excitonic state.

III. NUMERICAL RESULTS

For the noninteracting pair Green's function Q_j^0 one has

$$Q_j^0(\omega)=\sum_k \int \frac{d\omega_j}{2\pi} \int \frac{d\omega_h}{2\pi} A_{j,k}(\omega_j)A_{h,-k}(\omega_h)\frac{1-f_e(\omega_j)-f_h(\omega_h)}{\omega+i\delta-\omega_j-\omega_h} \tag{14}$$

with $\delta=0^+$. In Eq. (14), $f_\alpha(\omega)=\{\exp[(\omega-\mu_\alpha)/T]+1\}^{-1}$, $\alpha=e,h$ is the Fermi distribution function, and $A_{j,k}$ and $A_{h,k}$ are the spectral functions for electrons and holes, respectively. For the electron spectral functions the quasiparticle approximation

$$A_{j,k}(\omega)=2\pi\delta(\omega-e_{j,k}) \tag{15}$$

with single-particle energies $e_{j,k}$ is used. Lifetime effects are incorporated by using a Gaussian broadening within the hole spectral function,

$$A_{h,k}(\omega)=2\pi\sqrt{\alpha/\pi}\exp\{-\alpha[(\omega-e_{h,k})/\gamma]^2\}/\gamma \tag{16}$$

with $\alpha=\ln 2$, broadening [half width at half maximum (HWHM)] γ, and single-particle energy $e_{h,k}$. Since the concentration of photogenerated holes can be assumed to be small, the distribution function f_h in Eq. (14) is neglected in the calculation of the absorption spectrum from Eq. (11), and in the calculation of the luminescence spectrum, Eq. (13), the hole population is kept only to leading order in f_h. The latter can be achieved by using the identity

$$g(\omega)[1-f_{j,k}-f_h(\omega-e_{j,k})]=f_{j,k}f_h(\omega-e_{j,k}) \tag{17}$$

with $f_{j,k}=f_e(e_{j,k})$. With Eq. (17) one finds for the functions $I_j(\omega)$ in Eq. (13)

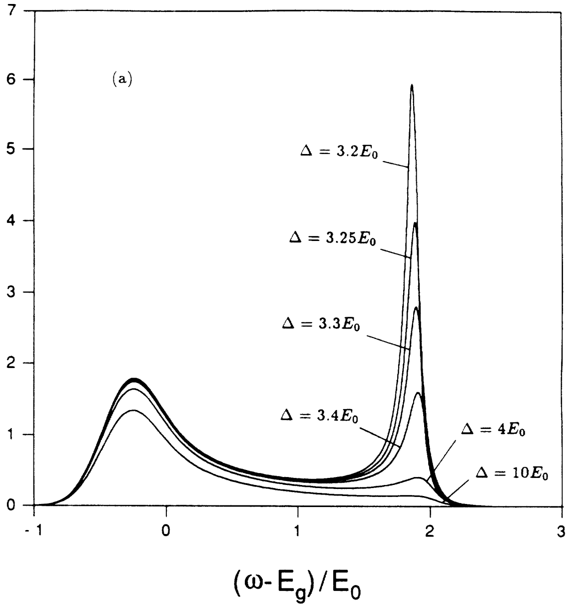
$$I_j(\omega)=\frac{I_j^0(\omega)}{|1+V_{j,j}Q_j^0(\omega)|^2}\ , \tag{18}$$

where

$$I_j^0(\omega)\propto|\mu_j|^2\sum_k A_{h,-k}(\omega-e_{j,k})f_{j,k}f_h(\omega-e_{j,k}) \tag{19}$$

is the luminescence spectrum of noninteracting electron-hole pairs. The hole distribution function is now only kept in expression (19) and can be neglected otherwise in Eq. (13).

For simplicity, the numerical evaluation of Eqs. (11) and (13) was carried out in one space dimension. The parameters used in the calculation were $\mu_1=\mu_2$, $V_{1,1}=V_{2,2}=5V_{1,2}>0$, effective masses $m_v/m_{c_1}=m_v/m_{c_2}=-8$, valence band v broadening (HWHM) $\gamma=0.23E_0$, $\mu_e(T=0)=E_g+2E_0$, and $\mu_h(T=0.1E_0)=-E_0$, where E_g is the band gap and E_0 is the exciton binding energy.



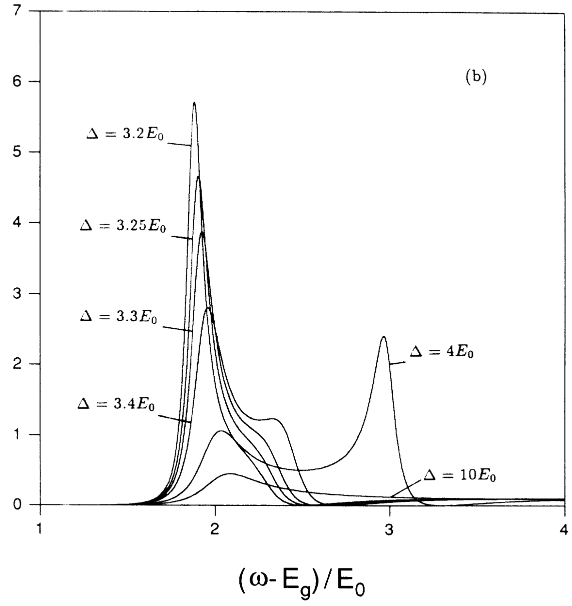


FIG. 2. (a) Emission and (b) absorption spectra in arbitrary units for various conduction-band splittings Δ and fixed temperature $T=0.1E_0$.

Figure 2(a) shows the resulting emission spectra for various conduction-band splittings Δ (Δ as defined in Fig.

1) and fixed temperature $T=0.1E_0$. At this low temperature the second conduction band is nearly unpopulated for all values of Δ considered here. Therefore, in the noninteracting case $V_{1,2}=0$, no luminescence involving the second conduction band would occur. For large conduction-band splitting, $\Delta=10E_0$, the unoccupied conduction band c_2 plays no role in luminescence, and one recovers the characteristic two-band emission spectrum with a peak near the band edge which, due to the valence-band broadening, appears somewhat below $\omega=E_g$, and a steplike high-energy edge near $\omega=E_g+(1-m_{c_1}/m_v)(\mu_e-E_g)\simeq\mu_e$. The latter feature is a remnant of the v-c_1 Fermi-edge singularity. In the corresponding absorption spectrum, Fig. 2(b), one finds a resonance at this energy, but in emission the effect is quite small, because only a few holes are available near $k=k_F$. However, when Δ is lowered towards $\mu_e-E_g+E_0$, the emission intensity at the Fermi edge increases dramatically. As in the data of Chen *et al.*, the enhanced emission at the Fermi edge exceeds by far that near $\omega=E_g$. The physical origin of this effect lies in the increasingly resonant transitions of electrons from the Fermi edge into the virtual v-c_2 exciton state, which in turn lead to the enhancement of the v-c_1 singularity in the spectrum.

In the corresponding absorption spectra shown in Fig. 2(b), the hybridization between the v-c_1 Fermi-edge resonance and the v-c_2 excitonic resonance with decreasing splitting Δ can be seen. For $\Delta=4E_0$ both lines are still resolved and the v-c_2 exciton line appears as a Fano resonance in the v-c_1 scattering continuum.[9] Since the coupling constant $V_{1,2}$ was assumed real and positive in this calculation, the Fano parameter q (Ref. 10) is negative, resulting in destructive interference on the high-energy side of the spectrum. However, on the low-energy side of the exciton line constructive interference with the Fermi-edge resonance occurs and leads to a very large peak as the two resonances merge.

Figure 3(a) shows the temperature dependence of the luminescence spectrum for $\Delta=3.2E_0$. Since there is nearly no real c_2 population, the whole temperature variation in this regime stems from the v-c_1 Fermi-edge resonance. A temperature increase makes more holes available at high energies. This results in a slight increase of the luminescence intensity at the Fermi energy as the temperature is increased from $T=0.1E_0$ [see Fig. 2(a)] to $T=0.12E_0$. However, in agreement with the data of Chen *et al.*, the enhancement at the Fermi edge disappears when the temperature is further increased, reflecting the deleterious effects of Fermi surface smearing on the v-c_1 singularity.

This decrease in oscillator strength at the Fermi energy with increasing temperature is also seen in the corresponding absorption spectra in Fig. 3(b), until at higher temperature ($T=0.7E_0$) the ordinary v-c_2 excitonic resonance recovers and regains its oscillator strength. This line at frequency $\omega=E_g+\Delta-E_0$ can also be seen in the corresponding luminescence spectrum in Fig. 3(a), because, due to the higher temperature, the emission spectrum now extends to higher frequencies. Also, due to the relatively high temperature, even the v-c_1 exciton begins to recover, shifting spectral weight towards the below gap region. The latter feature however is not realistic, since at high temperatures bound electron-hole pairs become ionized by phonons, an effect which was not taken into account in this calculation.

In conclusion, a simple theoretical model has been developed, which is in good qualitative agreement with the recent unexpected experimental findings. It was shown that the hybridization between the Fermi-edge

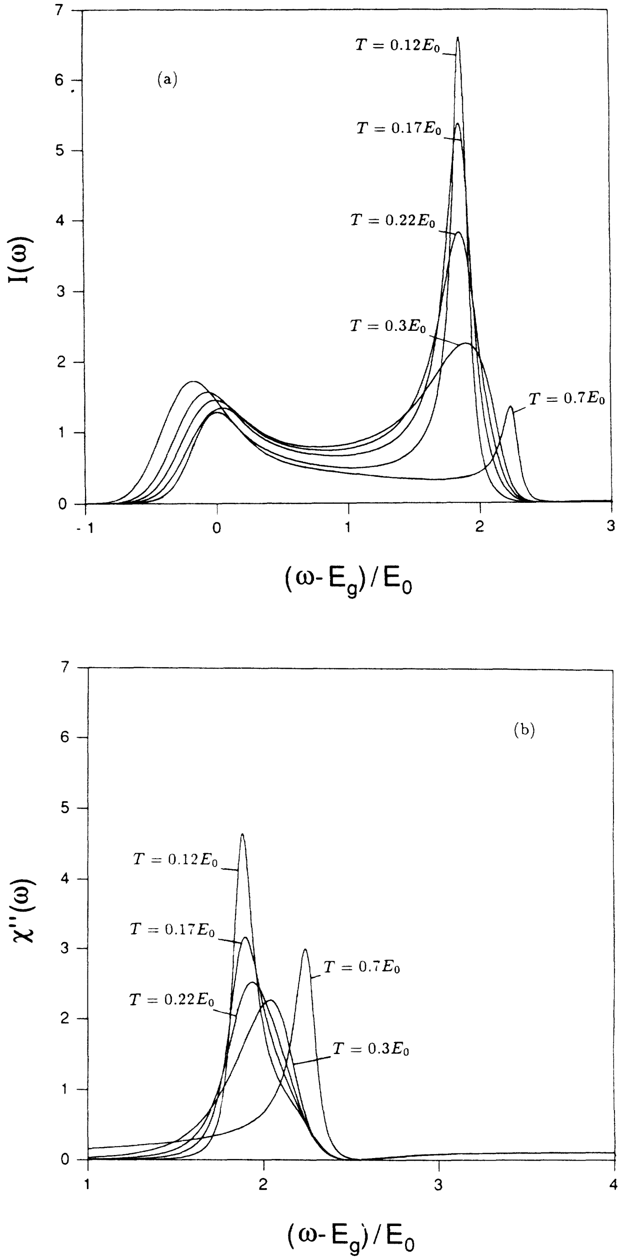


FIG. 3. (a) Emission and (b) absorption spectra in arbitrary units for various temperatures T and fixed conduction-band splitting $\Delta=3.2E_0$.

singularity of a degenerate electron gas and the excitonic resonance of a higher conduction band can make the Fermi-edge resonance, which is usually only seen in absorption, also observable in luminescence. In the future, we hope to investigate the remarkable magnetic field dependence of the effect in two dimensions.

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