Effects of an electron gas on the negative trion in semiconductor quantum wells

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Abstract

We present here the results of calculations of the negative trion binding energy in the presence of an electron gas. The screening of the Coulomb interaction and the Pauli exclusion principle are considered. Our results show a rapid ionization of the negative trion due to the Pauli exclusion principle while the screening is mainly responsible for the weakening of the trion binding energy.

PACS 71.35.Lk, 78.66.Fd

Keywords: semiconductor quantum wells, two dimensional electron gas, optical properties

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I. INTRODUCTION

The optical properties of low-dimensional semiconductors are strongly influenced by Coulomb interactions. In the case of intrinsic quantum wells (QWs), the optically created electron-hole pair forms a bound state, the exciton, which dominates the optical transitions [1]. In the presence of an electron gas, in modulated-doped samples, the exciton is quenched and the optical properties are dominated by band-to-band transitions. Coulomb correlations may eventually manifest themselves in the optical response of the system. This many-body effect is characterized by an enhancement of the spectrum intensity known as the Fermi edge singularity [2]. The situation is quite different in the case of low-carrier densities. In this regime, the electron-hole pair may still hold a bound state. The exciton interacts with the electron gas (in the case of n-doped samples) eventually binding an extra electron forming a bound complex, the negative trion (X\(^{-}\)). This state is the ground state of the system while the exciton (X\(^{0}\)) is an excited state. In this picture, the second electron is only weakly bound since its binding energy originates from the interaction between the electron and a neutral exciton through its dipole. As a consequence, the spectrum lines associated with the X\(^{-}\) and the X\(^{0}\) are separated by an energy of the order of few meV. This makes the observation of the X\(^{-}\) a difficult task only recently achieved in high-quality samples. Since its first observation [3], the trion has been intensively studied, both experimentally [4] and theoretically [5]. One of the aspects that has not been considered yet is the influence of the excess of electrons in the trion properties. Here we address this issue by calculating the negative trion binding energy in the presence of an excess of electrons in semiconductor QWs. Our results show that while the screening of the Coulomb interaction decreases the binding energy, the phase-space filling effects originated from the Pauli exclusion principle rapidly ionize the trion complex.
II. MODEL

We consider the stability of the ground state of two electrons and one hole complex in a semiconductor QW in the presence of a degenerate population of electrons in the lowest QW conduction subband. The trion states can be labeled by their total spin, $S$, total angular momentum, $M$, and total wave-vector, $K_{CM}$. In the absence of external fields, only the $M = 0$ singlet ($S = 0$) is a bound state. We calculate the $K_{CM} = 0$ bound state variationally by expanding the trion wave-function in a symmetrized two-relative particles plane-wave basis for the in-plane coordinates. Along the growth direction (z-direction), the component of the wave-function is taken as being the QW conduction and valence ground states. The Pauli exclusion principle is taken into account by limiting the relative particle plane-waves to $k$ values above the Fermi wave-vector, $k_F$. The orbital part of the singlet wave-function $\Psi_{S,M,K_{CM}}$, for the ground state is written as:

$$\Psi_{0,0,0}(\rho_1, \rho_2) = \chi_0(z_{e1})\chi_0(z_{e2})\phi_0(z_h) \sum_{\lambda_1, \lambda_2} a_{\lambda_1\lambda_2} \left\{ S \sum_{\vec{k}_1, \vec{k}_2(k_1, k_2 < k_F)} \alpha(\vec{k}_1, \vec{k}_2; \lambda_1, \lambda_2) e^{i\vec{k}_1.\vec{\rho}_1} e^{i\vec{k}_2.\vec{\rho}_2} \right\}$$

(1)

where $\chi_0(z)$ and $\phi_0(z)$ are the conduction and valence QW ground states, the $\lambda_i$’s are numerical parameters chosen within physically meaningful values and $a_{\lambda_1\lambda_2}$’s are the linear variational parameters. The $\alpha(\vec{k}_1, \vec{k}_2; \lambda_1, \lambda_2)$ are chosen so that for $k_F = 0$ the wave-function is a symmetrized expansion in non-orthogonal two single-relative-particle gaussian functions parameterized by $\lambda_i$ is limited to the s-like relative states [6]. This is enough to obtain a good description of the trion binding energy. For a better quantitative result it is necessary, however, to include higher relative angular momenta.

The screening of the Coulomb interaction is considered within the Random-Phase Approximation (RPA) [7]. Within this approximation, the Coulomb interaction is in-plane Fourier transformed and the $q$-dependent Coulomb interaction is screened by the RPA static-dielectric constant, $\epsilon_{RPA}(q) = 1 + \frac{2}{qa_0} F(q) g(q)$, where $a_0$ is the three-dimensional Bohr radius, $F(q)$ is the usual QW form factor and $g(q) = 1 - \sqrt{1 - (\frac{2k_F}{q})^2} Y(q - 2k_F)$, where $Y(x)$ is the step function ($Y = 0$ if $x < 0$ and $Y = 1$ if $x > 0$). The trion ground-state
is calculated by diagonalizing the generalized eigenvalue problem obtained by projecting the
total two-electrons and one-hole Hamiltonian into the wave-function of Eq. 1. To obtain
the conditions for the stability of the trion we calculate the exciton plus a non-interacting
electron ground state within the same approximation.

III. RESULTS AND DISCUSSION

We considered a single 100 Å symmetrically n-modulated-doped GaAs-(Ga,Al)As QW.
Figure 1 shows (a) the exciton energy and (b) the trion energy relative to the non-interacting
particles total energy as a function of the electron density when only the screening is consid-
ered (dotted-line), when only the Pauli exclusion principle effect is considered (dashed-line)
and when both effects are included (full line). Here we subtracted the kinetic energy of the
relative particle with \( k_F \) wave-vector for the exciton and twice this value for the trion. This
garanties that the exciton and the trion states are not degenerate with available scattering
states and is a true bound state. We observe that the screening decreases the binding energy
already at very weak electron concentrations (\( n_e \)). However, even for large concentrations, it
remains a sizable although weak binding energy. On the other hand, the Pauli exclusion
principle is almost ineffective up to \( n_e \) of the order of \( 10^9 \) cm\(^{-2}\). For higher concentrations,
the binding energy is rapidly quenched at \( n_e=4 \times 10^{10} \) cm\(^{-2}\). The combined effects show
an exciton binding energy which decreases with \( n_e \) and is quenched for a concentration of
\( 10^{10} \) cm\(^{-2}\). The same behavior is observed for the trion energy, where it was extracted twice
the relative Fermi energy, following the same arguments as in the exciton case.

The stability of the \( X^- \) complex, however, must be established by comparing its total
energy with the next two-electrons one-hole state, that is, when the one electron and the hole
form the bound excitonic state and the extra electron is at the lowest available scattered
state, that is, at the Fermi energy. The trion binding energy is defined as the difference
between this two energies: \( E_{X^-}^b = E_{X^0} + e_F - E_{X^-} \). In Figure 2 we plot this value as a
function \( n_e \). When we consider only the screening effects, the trion binding energy remains
roughly the same up to values of $n_e$ of the order of $5 \times 10^{10}$ cm$^{-2}$, when it increases almost linearly with it. The decrease in the binding energy due to the screening is compensated by the energy of the extra electron up to concentrations of the order of $5 \times 10^{10}$ cm$^{-2}$, giving an almost constant trion binding energy. Once the screening effects is saturated, the energy increases with the Fermi energy almost linearly. The situation changes completely when we consider the Pauli exclusion principle. In this case, the trion binding energy quenches already at values of $n_e$ of the order of $5 \times 10^9$ cm$^{-2}$. When we consider both, the screening and the Pauli exclusion principle, the trion ionizes at concentrations of the order of $2 \times 10^9$ cm$^{-2}$. In actual samples, the nominal excess of electrons is above this value. However, the trion and the exciton emission lines remains stable and no quenching of the photoluminescence is observed. A more complex trion wave function gives higher values for the trion binding energy and one should expect the quenching to happen at higher concentrations. This will not, however, change the qualitative picture. One of the reasons to understand the trion stability is the effect of interface fluctuations. It may trap the trion, increasing the energy necessary to ionize it or, it may trap the electrons making them less effective in the quenching of the bound state. More experimental and theoretical work is necessary to elucidate this problem.

The authors are grateful to G. Bastard and B. Deveaud-Pledran for stimulating discussions. This work is supported by FAPESP (Brazil) and CNPq (Brazil).
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FIGURES

FIG. 1. (a) Exciton binding energy and (b) negative trion binding energy relative to the effective gap for a 100 Å QW as a function of $n_e$ when we include the effects of the screening (dash-dotted line), the Pauli exclusion principle (dashed-line) and when both effects are considered (full line).

FIG. 2. Trion binding energy as a function of the electron concentration for the same cases as in Figure 1.
