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Stability of Charged Exciton States in Quantum Wires*

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Abstract. We show that the order of energies of negative (X^-) and positive (X^+) trions in quantum wires is determined by the relative electron and hole lateral confinements. For equal electron and hole confinement, X^+ has a larger binding energy, but a small imbalance towards a stronger hole localization changes the order of the X^- and X^+ recombination lines in the photoluminescence spectrum.

1 Introduction

We study the exciton trions formed when an electron or a hole is bound to a neutral exciton (X). The binding energies of the complexes in nanostructures, i.e., in quantum wells [1–4] and quantum wires [5–7] are measured in photoluminescence (PL) spectroscopy as shifts between the spectral lines of the complexes with respect to the exciton energy line. Due to the larger effective mass of the hole, in bulk [8] as well as in strictly two-dimensional confinement [2] the binding energy of positive trions (X^+) is larger than the negative trion (X^-) binding energy. However, in quantum wells the observed [4] X^- and X^+ binding energies are nearly equal, which is explained [3, 4] by a stronger hole quantum-well localization enhancing the hole-hole interaction. In quantum dots the localization-related hole-hole interaction enhancement leads to the interchange of the order of the X^- and X^+ recombination lines in the (PL) spectrum already for quantum dot diameters as large as 24 donor Bohr radii [10].

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The present work is motivated by a recent experimental study [7] on trions in V-groove GaAs/AlGaAs quantum wires. The X^- was found to be distinctly more stable than X^+ (binding energies of X^- and X^+ were determined as -4.2 and -2.9 meV, respectively). In a previous theoretical study [5] of trions in quantum wires X^+ was found to be more stable than X^-, which was obtained in the case of equal hole and electron confinement. A crossing of X^- and X^+ PL lines as function of the wire width has previously been obtained in a quantum Monte-Carlo study [6] of a quantum wire with a square well confinement potential. Here, we demonstrate that the observed [7] order of X^- and X^+ energy lines is due to the enhanced hole localization.

2 Theory

We apply the single band model for the electron and the hole and consider a harmonic oscillator confinement potential in the directions perpendicular ("lateral") to the wire with $l_{e(h)}$ the oscillator length for the electron (hole) [9]. We assume that the lateral confinement is strong, so that only the lowest subband for the electron and hole is occupied. This assumption allows for a reduction of the Schrödinger equation to an effective two-dimensional form, which can be solved numerically with an exact inclusion of the interparticle correlations along the wire [9]. We adopt the donor units, i.e., donor Bohr radius $a_d = 4\pi\epsilon_0\epsilon\hbar^2/m_e e^2$ for the unit of length and twice the donor Rydberg $2R_d = \hbar^2/m_e a_d^2$ as the unit of energy, where m_e is the band electron effective mass and ϵ is the dielectric constant. The effective negative trion Hamiltonian after separation of the centre-of-mass motion written with respect to the dissociated system is

$$H_-^{\mathrm{rel}} = -\frac{1}{2\mu}\left(\frac{\partial^2}{\partial z_{eh1}^2} + \frac{\partial^2}{\partial z_{eh2}^2}\right) - \frac{1}{\sigma}\frac{\partial^2}{\partial z_{eh1}\partial z_{eh2}} + V^{\mathrm{ef}}(l_e; z_{eh1} - z_{eh2}) - V^{\mathrm{ef}}(l_{eh}; z_{eh1}) - V^{\mathrm{ef}}(l_{eh}; z_{eh2}), \tag{1}$$

with the reduced mass of an electron-hole pair $\mu = \sigma/(1+\sigma)$, $\sigma = m_h/m_e$, and the coordinates of the relative electron-hole positions $z_{eh1} = z_h - z_{e1}$ and $z_{eh2} = z_h - z_{e2}$ along the wire. In Eq. (1) $l_{eh} = \sqrt{(l_e^2 + l_h^2)/2}$ and V^{ef} is the effective one-dimensional interaction potential [5]

$$V^{\mathrm{ef}}(l; z) = (\pi/2)^{1/2}\,\mathrm{erfc}(|z|/\sqrt{2}l)\exp(z^2/2l^2)/l, \tag{2}$$

finite at the origin ($V^{\mathrm{ef}}(l;0) = 1/l$) and approaching the $1/z$ asymptotic at large z. The Hamiltonian for X^+ has the form (1) but with $1/\sigma$ standing in front of the mixed derivative replaced by 1 [9].

3 Results

We consider a quantum wire made of GaAs ($m_h = 0.45m_0$, $m_e = 0.067m_0$, $2R_d = 11.9$ meV, $a_d = 9.8$ nm). Fig. 1 shows the wave function of (a) X^-, (b) X^+ trions for equal hole and electron oscillator lengths of the lateral confinement. The interaction potentials in the trion Hamiltonians have a minimum along the $z_{eh1} = 0$ and $z_{eh2} = 0$ axis corresponding to an electron and a hole in the same position and a

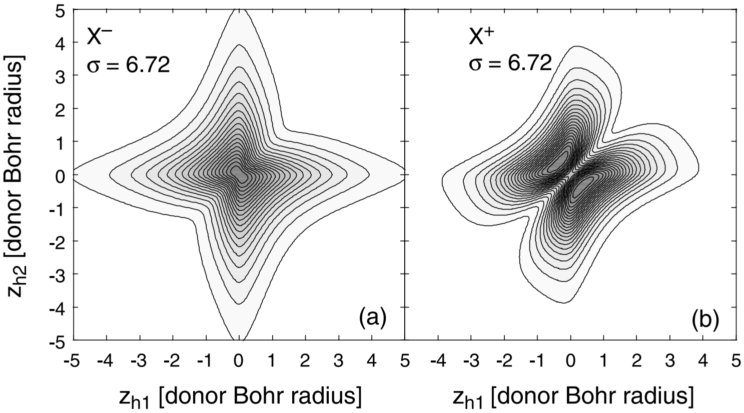

Fig. 1. Contour plots of the wave function for (**a**) X^- and (**b**) X^+ trions for $l_e = l_h = L = 0.2$ with a mass ratio $\sigma = 6.72$ corresponding to GaAs

maximum along the diagonal $z_{eh1} = z_{eh2}$ corresponding to both electrons (for X^-) or both holes (for X^+) at the same position. Fig. 1 shows that the electrons in X^- with light effective masses tunnel easily through the diagonal barrier due to the inter-electron repulsion. On the other hand the diagonal barrier is effectively much larger for the heavy-mass holes which leads to the appearance of the characteristic maxima separated by the minimum elongated along the diagonal [see Fig. 1b].

The X^+ and X^- binding energies are plotted in Fig. 2. Both trions are equally stable for $l_h = 0.92 l_e - 0.38$ nm (see the black line in Fig. 2). For l_h larger (smaller) than $0.92 l_e - 0.38$ nm X^+ is more (less) stable than X^-. The fit of the calculated X^- and X^+ binding energies to the experimental data [7] is obtained at the crossing of the thick gray dotted lines, i.e., for $l_e = 2.95$ nm and $l_h = 1.3$ nm. The obtained fit corresponds to realistic values which give a general idea on the particle localization in the wire (the measurements [7] were performed on a V-groove GaAs/AlGaAs

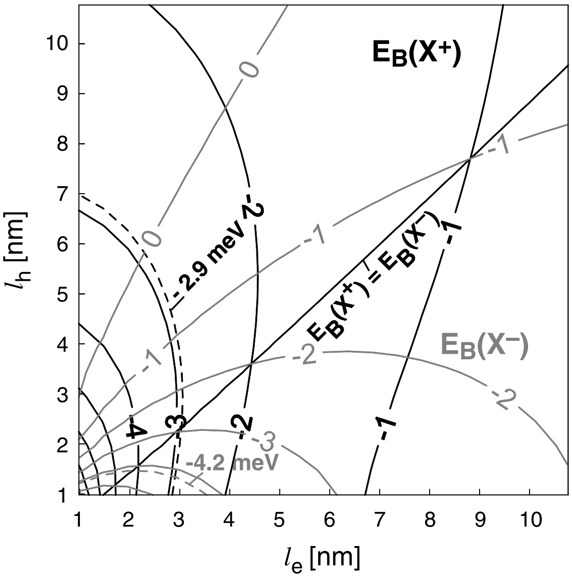

Fig. 2. Contour plot of the binding energies for positive (dark grey lines) and negative (light grey lines) trions (in meV) as function of the electron and hole confinement lengths for GaAs material parameters. Below (above) the black line X^- (X^+) trion is more stable. The dashed lines correspond to experimental [7] data, $E_B(X^-) = 4.2$ meV and $E_B(X^+) = 2.9$ meV

quantum wire with a thickness of the GaAs crescent of 3 nm at the centre). Obviously, a more realistic model is required to extract details of the confinement from the experimental data.

4 Conclusions

We found that the order of the X^- and X^+ PL lines is interchanged when the lateral confinement of the hole is stronger than the one for the electron due to the modification of the effective interactions in the trion complexes. The present results provide an explanation for the recently experimentally observed larger stability of the negative trion in quantum wires [7]. The magnetic field oriented parallel to the axis of the wire will tend to equalize the electron and hole localization enhancing stronger the X^+ binding energy, which can result in a crossing of the X^+ and X^- lines [9].

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