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Exciton Molecules in Quantum Wells: Influence of the Well Width Fluctuations*

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Abstract. The influence of the well width fluctuations on the dependence of the binding energy of excitonic complexes in quantum wells is studied by using the path-integral Monte-Carlo technique. The results are compared with available experimental data and a good agreement is found.

1 Introduction

Coulomb-bound few-particle systems in semiconductors are formed when interacting electrons (e) and holes (h) bind. In particular, an electron and hole bound together will form an exciton, while more electrons and holes will form the so-called exciton molecules, e.g., $2e(h) + h(e)$ form a trion and $2e + 2h$ form a biexciton. It is well known that in nanostructured semiconductors such as quantum wells (QWs), the binding energy of such excitonic complexes is substantially increased [1]. But the measured increase is larger than theoretically predicted. For the trion system this may be even a factor of two. It has been argued that the extra increase observed experimentally could be ascribed to the presence of quantum well width fluctuations which traps the Coulomb-bound few-particle system in the plane orthogonal to the quantum well growth axis [2, 3]. This interface

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defect would enhance the confinement of the excitonic complexes and as a consequence it would increase the binding energy of the system.

In this paper we make a quantitative investigation of the binding energy of the exciton, trion, and biexciton in a QW in the presence of an interface defect. In Sect. 2 we present the Hamiltonian of the problem and discuss the approach used to solve the system. In Sect. 3 we present our results and compare them to available experimental data.

2 Theoretical Tools

We consider a single $GaAs/Al_{0.3}Ga_{0.75}As$ quantum well structure. In the isotropic effective mass approximation the Hamiltonian for N_e electrons and N_h holes can be written as

$$H = \sum_{i=1}^{N_e,N_h} \left[-\frac{\hbar^2}{2m_i}\nabla^2 + V_{e(h)}(z_i) + V_{e(h)}^{\mathrm{loc}}(\mathbf{r}_i) \right] + \sum_{i<j=1}^{N_e,N_h} \frac{e_i\, e_j}{\epsilon|\mathbf{r}_i - \mathbf{r}_j|}, \qquad (1)$$

where m_i and e_i are the mass and charge of the i-th particle; ϵ is the dielectric constant, which we assume equal in the well and the barrier; $V_{e(h)}$ is the confinement potential due to the QW; $V_{e(h)}^{\mathrm{loc}}$ is the lateral (localization) confinement which is due to the fluctuations of the QW width. We take the quantum-well growth direction as the z-direction. We consider the following heights of the square-well potential: $V_e = 216\,\mathrm{meV}$ for electrons and $V_h = 163\,\mathrm{meV}$ for holes, and we use the following material parameters: $\epsilon = 12.58$, $m_e = 0.067\,m_0$, $m_h = 0.34\,m_0$, where m_0 is the mass of the free electron. The units for energy and length are $2R_y^* = e^2/(\epsilon\, a_B) = 11.58\,\mathrm{meV}$, $a_B = \hbar^2\epsilon/(m_e\, e^2) = 99.7\,\mathring{\mathrm{A}}$, respectively. To limit the number of parameters, we simulate the interface defects through a cylindrically symmetric potential with a lateral radius R and height $V_{e(h)}^{\mathrm{loc}}$. The potential height is determined by the zero-point energy and was obtained as the difference between the lowest energy levels of the electron (hole) in two QW's with the widths L and $L + \delta$, where δ is an integer number of monolayer (ML)-thicknesses, see Fig. 1. In the case when the quantum well height goes to infinity, the height of the potential will be $V_i^{\mathrm{loc}} = \hbar\pi^2/m_i L^2 - \hbar\pi^2/m_i(L+\delta)^2$. Because of the difference in mass between the electron and the hole, the height of the localization potential will also be different, see Fig. 2.

To solve the Hamiltonian we use the path-integral Monte-Carlo approach [4, 5]. The starting point is the N-particle density matrix of the exciton complex under study. As wavefunction of the density matrix in the z-direction we take for the

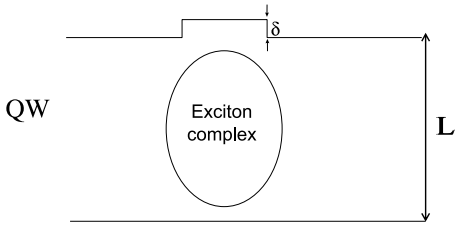

Fig. 1. Schematic view of a quantum well with well width fluctuation (interface defect)

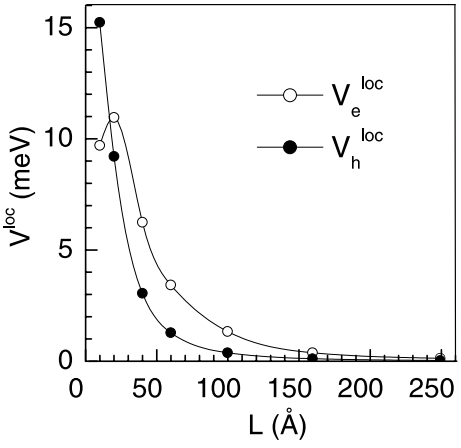

Fig. 2. The height of the localization potential $V_e(h)^{\mathrm{loc}}$ versus the well width

electron and the hole density matrices the ones of the non-interacting particle confined in the quantum well $\rho(Z_i, \beta)$. This allows us to introduce an effective two-dimensional (2D) in-plane interaction potential V_{eff}^{xy},

$$V_{\mathrm{eff}}^{xy} = \int dZ_e\, dZ_h \sum_{i<j} \frac{e_i\, e_j}{\epsilon|\mathbf{r}_i - \mathbf{r}_j|}\ \rho(Z_e, \beta)\rho(Z_h, \beta) \left[\int dZ_e\, dZ_h\ \rho(Z_e, \beta)\rho(Z_h, \beta) \right]^{-1}.$$

3 Results

In this section we investigate the influence of the interface defect (i.e., defect width and height) on the ground state of the exciton and excitonic complexes confined in a quantum well. In particular, we analyze the modification of the binding energies and of the average interparticle distances in the ground state of excitons (X), positive and negative trions ($X^{\pm}$), and biexcitons (X_2).

For an ideal QW, i.e., without interface defects, we define the binding energy of the exciton, charged exciton, and biexciton as

$$\begin{aligned} E_B(X) &= E_e + E_h - E(X), \\ E_B(X^{\pm}) &= E(X) + E_{h(e)} - E(X^{\pm}), \\ E_B(X_2) &= 2E(X) - E(X_2), \end{aligned} \tag{2}$$

where $E_{e(h)}$ is the energy of a single electron (hole) in the given quantum well with a free-particle mean kinetic (thermal) energy k_BT, and $E(A)$ is the total energy of the excitonic complex A. If an interface defect is present and a localization potential is included in our calculations, then the above definitions must be modified. All energies must be replaced by the corresponding energies of particles localized in the defect potential.

First we discuss the results for the binding energies of the ground state of various excitonic complexes as a function of the diameter (D) of the interface defect (see Fig. 3). We took a QW width of $L = 60\,\text{Å}$ and a defect of depth $\delta = 1\,\text{ML} = 2.8\,\text{Å}$, which leads to the following heights of the electron and hole localization potentials, $V_e^{\mathrm{loc}} = 3.43\,\text{meV}$ and $V_h^{\mathrm{loc}} = 1.28\,\text{meV}$, respectively. Notice that for all excitonic complexes the binding energy is increased by the presence of

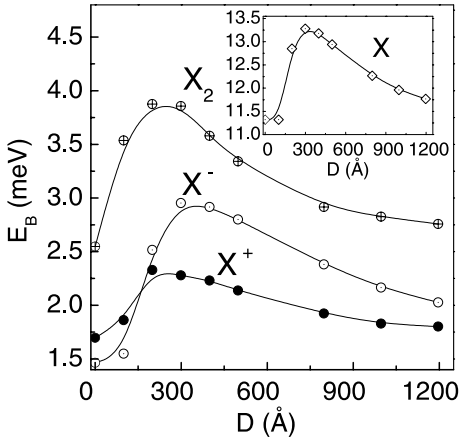

Fig. 3. The binding energy of the exciton, trion, and biexciton versus the diameter of the quantum well width fluctuation, in a quantum well of width 60 Å. The width of the fluctuation is 1 ML

a defect. In particular, it increases with the diameter D of the trapping potential up to some maximum after which it slowly decreases. For defect diameters exceeding $D \approx 800$ Å all binding energies tend towards saturation because, in the large defect limit, the system approaches an ideal QW, but 1 ML wider than the original one. Notice that the X^- is much more sensitive to the presence of the defect than the X_2 and the X^+. The X^- is in fact the lightest of the three complexes and therefore more mobile.

Secondly, in Fig. 4 we present a comparison between our theoretical results and the experimental data of refs. [6, 7] for the binding energy of the positive and negative trion as function of the quantum well width. Here the localization is assumed to have diameter $D = 300$ Å. Notice that if $L < D/2$ the presence of the

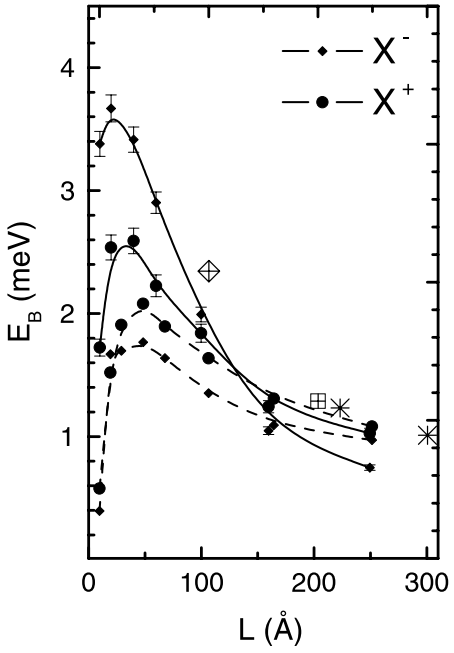

Fig. 4. Binding energies of positive and negative trions versus quantum well width. The results are for $GaAs/Al_{0.3}Ga_{0.7}As$ QWs. Symbols: experimental data for the X^- from refs. [6, 7], lines with small symbols: PIMC results with (solid curves) and without (dashed curves) localization

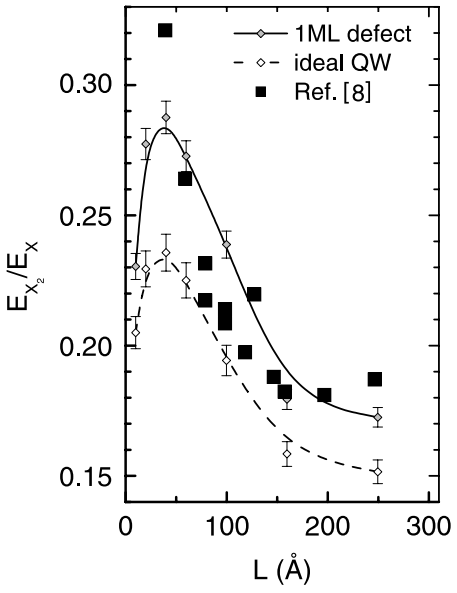

Fig. 5. The Fano factor for the negative trions versus quantum well width. The results are for GaAs/$Al_{0.3}Ga_{0.7}As$ QWs. Symbols: experimental data of ref. [8], lines with small symbols: PIMC results with (solid curves) and without (dashed curves) localization

localization defect increases the binding energy, in the case of the negative trion even doubles the binding energy for a well width of 50 Å. On the other hand, if $L > D/2$ the binding energy is lower than the energy of the system without localization. Notice how the experimental data reported for the negative trion at $L = 100$ Å is much closer to the value of the binding energy obtained when the confinement is included.

Third, in Fig. 5 we plot the so-called *Fano factor*, i.e., $E_B(X_2)/E_B(X)$ for the non-localized and the localized positive and negative trion and compare them with the experimental results from ref. [8]. The localization potential is considered as due to a 1 ML defect with diameter $D = 400$ Å. The theoretical result for an ideal QW, i.e., without localization, is shown by the dashed lines. For the well widths $L \geq 50$ Å, all theoretical and experimental results indicate a monotonic decrease of the Fano factor with increasing well widths. For the ideal quantum well the Fano factor starts from the value 0.15 for large L and reaches a maximum value of about 0.24 around $L = 50$ Å, where the QW confinement has the strongest localization effect on the electron (and hole) wave functions along the growth direction. With the localization included (solid line) our calculation shows a systematic increase of the Fano factor $E_B(X_2)/E_B(X)$. The experimental values for the Fano factor [8], solid squares in Fig. 4 by solid symbols, are mostly located between the two theoretical curves. In an intermediate range, i.e., around 70 Å $\leq L \leq 130$ Å, there is an indication that the experimental results correspond to non-localized excitonic complexes, whereas for widths larger than 150 Å and smaller than 60 Å, there is a better agreement if the assumption of predominantly localized complexes is made.

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