Abstract

We present a model to take into account the interface defects contribution on the binding energy of charged exciton in GaAs/Al$_{0.3}$Ga$_{0.7}$As quantum wells. The dependence of the binding energy gain and of the trion size on the quantum well width are variationally calculated. We show that the trion is more sensitive to interface defects than the exciton.

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I. INTRODUCTION

When low power is used to excite an intrinsic quantum well (QW), its photoluminescence spectrum is dominated by an exciton which is analogous to the H atom in semiconductor physics. This complex is formed by the Coulomb attraction between one electron and one hole. In the case of lightly modulation doped samples, the presence of extra carriers inside the QW gives rise to new bound states through the attraction of an extra electron (n-doped) or hole (p-doped) by the excitonic electrical dipole forming a charged complex, the trion, which may be negatively charged, $X^-$, or positively charged, $X^+$, respectively. Lampert [1] was the first author to propose the stability of such charged complexes in semiconductors. However, the first experimental observation was only possible in QWs and it was made by Kheng et al. [2]. The influence of carrier localization potentials on the trion experimental observations is an interesting and open question. Some experimental works show evidences of carrier localization [3] while other results indicate that the trion is composed by free carriers [4]. Moreover, the measured binding energies are consistently higher than the theoretical ones, indicating the possibility of trapped electrons. To shed some light on this question, we variationally calculated the binding energies of charged exciton in GaAs/Al$_{0.3}$Ga$_{0.7}$As QWs including the presence of structural defects represented by attractive gaussian potentials. This kind of defect is always present at the QW interface due to the interdiffusion of well and barrier materials during the QW growth process.
II. MODEL

We describe the QW, a GaAs layer between two Al$_{0.3}$Ga$_{0.7}$As layers, using the effective mass and envelope function frameworks. We start with the assumption that the QW confinement is strong enough and that the interface defects are weak enough to make reasonable the use of the noninteracting electron and hole ground states in ideal QWs as the z-part (growth direction) of the one particle trial wavefunction. The axial symmetry will be preserved by the defect potential. This leads us to describe the X$^-$ in-plane motion in terms of a center of mass ($\vec{R}$) and relative coordinates considering the following intuitive picture: the X$^-$ is composed by an exciton and a distant electron bound to its electrical dipole [5]. Consequently, the relative coordinates are given by one electron relative to the hole ($\vec{\rho}_1$) and the other one relative the center of mass (CM) of this particle ($\vec{\rho}_2$) in the X$^-$ case. We assume parabolic energy dispersions, so the equivalent X$^+$ coordinates are obtained through the interchange between electrons and holes.

The two electrons (holes in the case of X$^+$) indistinguishability leads us to use a Slater determinant as basis. We assume that the internal degrees of freedom are not strongly affected by the defect potential [6,7], in other words, its main effect is the localization of the CM, which is weakly coupled to the internal dynamics. In the absence of structural defects and external fields, only the singlet trion state with total angular momentum in the z direction equal to zero is a bound state. Therefore, we consider only this configuration for the orbital part of the charged exciton trial wavefunction:

$$\Psi_0 = N_{i,j,m} \chi_0(z_h) \chi_0(z_{e1}) \chi_0(z_{e2}) \phi_m^0(\vec{R}) \times \left[ \phi_1^0(\vec{\rho}_1) \phi_2^0(\vec{\rho}_2) + \phi_3^0(\vec{\rho}_3) \phi_4^0(\vec{\rho}_4) \right],$$  \hspace{1cm} (1)

where $N_{i,j,m}$ is the determinant normalization, $\chi_0(z)$ is the fundamental electron (e) or hole
(h) ideal QW state, $\phi_i^0(\vec{\rho})$ is a s-like one particle wavefunction (plane wave for the CM in ideal QWs). The coordinates $\vec{\rho}_3$ and $\vec{\rho}_4$ are obtained through the interchange between electrons 1 and 2 in the relative coordinates $(\vec{\rho}_1, \vec{\rho}_2)$.

We limit our basis to the fundamental QW states and s-like orbitals. Although it is known that they are not sufficient for a quantitative trion description [8], the present choice retains the main physical results of the defects influence on the trion states. We chose gaussian one particle wavefunctions to describe the in-plane motion because of their good trion description in the absence of defects [8]. This basis also helps due to the analytical results for the calculation of all the contributions on the trion Hamiltonian, including the defect ones.

The actual form of the interface defects is not known and it depends on the sample growth conditions. Because of this, we represent all the defects by a gaussian potential:

$$V_{def}(e, h) = V_{e,h}Y\left(\frac{L}{2} < z_{e,h} < \frac{L}{2} + \delta\right)\exp\left[-\left(\frac{\vec{\rho}_{e,h}}{D}\right)^2\right]$$

Here, we used electron (e) and hole (h) absolute coordinates, $V_{e,(h)}$ is the QW confining potentials for electrons (holes), $Y(z)$ is the step function ($Y(z)=1$ if $z>0$ and $Y(z)=0$ if $z<0$) and $L$ is the QW width. The defect parameters are $\delta$, the defect depth in the z direction, and $D$, the defect radius in the xy plane.

The charged exciton binding energy is defined as the difference between the energy of this charged complex and the energy of a trapped exciton ($X^0$) plus an in-plane free electron (hole), in the $X^- (X^+)$ case.
III. RESULTS AND DISCUSSIONS

Since we are considering a GaAs/Al$_{0.3}$Ga$_{0.7}$As QW, the effective parameters used are: $m_e=0.067m_0$, $m_{hz}=0.377m_0$, $m_{hxy}=0.112m_0$, $\varepsilon=13.2$ for the well and barrier materials. The conduction band off-set is 0.6.

Figure 1 shows the energy gain due to the interface defect presence as a function of QW width for $X^-$ (squares), $X^+$ (open circles) and excitons (triangles). The following defect parameters were considered: $D = 250$ Å and $\delta = 1$ GaAs monolayer. Our results show that the $X^-$ has the most significant energy gain. We present the results for the QW width range in which the internal degrees of freedom are weakly affected, i.e., the binding energy gain is less than 40%. The binding energy is the energy distance between each complex and the respective continuum. Figure 2 shows the percentage of binding energy that is gained due to the defect presence as a function of the QW width. We considered the same defect parameters as in Fig. 1. As one can see again, the $X^-$ is the most strongly affected complex by the defect, mainly in the narrow QW range. This happens because the carrier wavefunction probability inside the defect is greater for narrow QWs, particularly for electrons (inset of Fig. 2). Our results show that a single monolayer fluctuation is sufficient to produce a drastic effect on the trion binding energy.

Figure 3 shows the CM mean radius as a function of the QW width for the same complexes and defect parameters considered in Fig. 1. It also shows that the $X^-$ is more strongly localized by the defect than the exciton. This is in agreement with the experimental findings of Eytan et al. However, they attributed the origin of this strong localization of charged complexes to fluctuations in the electrical potential of remote ionized donors. Our results
show that even for strictly structural defects the $X^-$ is more affected than the exciton.

In conclusion, we presented a simple model to take into account the interface defects contribution on the trion binding energy. Our results show that the structural imperfections are more important in the case of narrow QWs and that the charged exciton are more strongly localized than the neutral one even in the case of strictly structural defects. This may explain why the theoretical results have, in general, better agreement with the experiments in the wide QW limit \[ \text{[5,8]} \]. Our results also show that the negative trion is more sensitive to the structural imperfections than the positive one.

IV. ACKNOWLEDGEMENTS

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FIGURES

FIG. 1. $X^-$ (squares), $X^+$ (open circles) and exciton (triangles) energy gain due to interface defects presence as a function of QW width. The defect parameters are: radius, $D = 250$ Å, and depth, $\delta = 1$ GaAs monolayer.

FIG. 2. $X^-$ (squares), $X^+$ (open circles) and exciton (triangles) relative energy gain as a function of QW width. Inset: probability of finding an electron (solid line) or a hole (dashed line) inside the region of the defect as a function of QW width for an ideal QW. The defect parameters are the same as in Fig. 1.

FIG. 3. CM mean radius as a function of QW width for $X^-$ (squares), $X^+$ (open circles) and exciton (triangles). The defect parameters are the same as in Fig. 1.
CM mean radius ($10^3 \text{Å}$)

Quantum well width (Å)

Dacal et al. - Figure 3