Binding energy of charged excitons bound to interface defects of semiconductor quantum wells

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(Received 9 October 2001; published 8 March 2002)

We present a model that takes into account the interface-defects contribution to the binding energy of charged excitons (trions). We use Gaussian defect potentials and one-particle Gaussian basis set. All the Hamiltonian defect terms are analytically calculated for the *s*-like trial wave functions. The dependence of the binding energy and of the trion size on the quantum-well width and on the defect size are investigated using a variational method for GaAs/$Al_{0.3}Ga_{0.7}As$ quantum wells. We show that even in the case of strictly structural defects the trion is more strongly affected than the exciton.

DOI: 10.1103/PhysRevB.65.115325 PACS number(s): 68.35.Dv, 73.20.Mf, 73.21.Fg

I. INTRODUCTION

The stability of charged excitons (trions) was firstly proposed by Lampert.[1] A charged exciton is a complex formed when there is an excess of charge in a semiconductor and an extra electron or hole is bound by the electrical dipole of a neutral exciton. In the first case we have a negative complex (X^-) and in the second case we have a positive one (X^+). These complexes are analogous to the ions H^- and H_2^+ in atomic physics. The advantage of working with semiconductor materials is that the screening of electrical interactions gives rise to the possibility of obtaining, with magnetic fields accessible in laboratories, cyclotron energies of the same order of the Coulomb ones while, in the H^- and H_2^+ cases, this is only possible in astrophysical systems. The first trion binding-energy calculation[2] showed that its value is not large enough to be experimentally detected in semiconductor bulk materials. However, this value is one order of magnitude larger in semiconductor quantum wells.[3] This is a consequence of the carriers confinement inside the quantum well (QW) due to the energy-gap difference between the barrier and well materials. The first experimental observation of a trion spectrum was made by Kheng *et al.*[4] in a II-VI type QW. In this case the trion binding energy is more than twice the value for III-V systems.[5]

There has been an intense discussion in the literature about the influence of charge localization potentials on the trion experimental observations. Most of the theoretical results[6–9] show weaker binding energies than that experimentally observed.[10–13] This suggests that the trion may be trapped by some kind of QW interface defect. Eytan *et al.*[14] presented experimental evidences of X^- localization due to electrostatic potential fluctuations generated by the ionized donors at the barrier material. Dzyubenko and Sivachenko[15] showed that the optical activity of the X^- triplet state can only be possible due to a QW symmetry breaking. On the other hand, results from time-resolved photoluminescence indicate that the trion optical emission is dominated by free charged excitons.[16]

To shed some light on this problem, we present a simple model to include the interface-defects contribution in the trion Hamiltonian. This kind of defect is always present at the QW interface due to the mixture of well and barrier materials during the QW growth process. The protrusion of a material with lower gap in the region with a greater one gives rise to structural defects that are attractive for both electrons and holes in type-I QW's.

II. MODEL

We consider a semiconductor QW, more exactly a GaAs layer grown between two $Al_{0.3}Ga_{0.7}As$ layers. The carriers are confined in the GaAs layer. The effective-mass and envelope-function frameworks are used to describe the semiconductor materials and the QW, respectively. We neglect the band bending and the effect of the excess of carriers due to the doping. The QW width is in the z direction (growth direction). The valence and conduction subbands are approximated by parabolic dispersions that is more severe an approximation in the case of X^+ than in the case of X^-.

We start with the assumption that the QW confinement is strong enough to make a z and (x,y) separable wave function in the basis-set reasonable. We use the noninteracting electron and hole fundamental solutions for ideal QW's as the z part of the one-particle trial wave functions.

The axial symmetry will be preserved by the defect potential. This leads us to use polar coordinates to describe the X^- in-plane motion in terms of center of mass (CM) and relative coordinates following the classical picture of the X^-: an exciton and a distant electron bound to its electrical dipole.[8] Furthermore, the chosen coordinates have the additional advantage of eliminating from the in-plane trion Hamiltonian the terms that are proportional to the product of relative coordinate linear momenta. We define

$$\vec{R}=\frac{m_e(\vec{\rho}_{e1}+\vec{\rho}_{e2})+m_{hxy}\vec{\rho}_h}{M},$$

$$\vec{\rho}_1=\vec{\rho}_{e1}-\vec{\rho}_h, \qquad (1)$$

$$\vec{\rho}_2=\vec{\rho}_{e2}-\frac{m_e\vec{\rho}_{e1}+m_{hxy}\vec{\rho}_h}{m}.$$

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Here the electron mass is isotropic. On the other hand, the hole dispersion is strongly nonparabolic in QW's, but, as a first approximation, the off-diagonal terms of the Luttinger Hamiltonian can be neglected. In this case, the hole mass is anisotropic and shows a lighter in-plane value. Using this approximation, the X^+ in-plane coordinates are easily obtained from the previous ones through the electron and hole labels interchange. The negative trion CM mass is given by $M = m_{hxy} + 2m_e$ and $m = m_e + m_{hxy}$. We use the same mass values for the well and the barrier materials.

Due to the presence of the defect, the CM is not a free particle. We label the trion state through the following good quantum numbers: the total angular momentum in the z direction (including the CM contribution), and the total spin of the two electrons (X^-) or two holes (X^+), S $(S = S_1 + S_2)$, which allows us to separate the solutions in singlet and triplet states.

The two electrons (holes in the case of X^+) indistinguishability leads us to use a Slater determinant basis. We assume that the internal degrees of freedom are not strongly affected by the defect potential.[17,18] Consequently, the main effect of the interface roughness is the localization of the CM that is weakly coupled to the relative coordinates. This CM localization will stabilize the trion. 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.[10] Therefore, we consider only this configuration and the orbital part of the charged-exciton trial wave function is written as

$$\Psi_0 = N_{i,j,m} \chi_0(z_h) \chi_0(z_{e1}) \chi_0(z_{e2}) \phi_m^0(\vec{R}) \times [\phi_i^0(\vec{\rho}_1)\phi_j^0(\vec{\rho}_2) + \phi_i^0(\vec{\rho}_3)\phi_j^0(\vec{\rho}_4)], \quad (2)$$

where $N_{i,j,m}$ is the determinant normalization, $\chi_0(z)$ is the fundamental electron (e) or hole (h) ideal QW state, and $\phi_i^0(\vec{\rho})$ are s-like one-particle wave functions [Eq. (4)]. When an ideal QW is considered, the CM function $[\phi(\vec{R})]$ is a plane wave. The coordinates $\vec{\rho}_3$ and $\vec{\rho}_4$ are obtained through the interchange between electrons 1 and 2 in Eq. (1). They are related to $\vec{\rho}_1$ and $\vec{\rho}_2$ through

$$\vec{\rho}_3 = \frac{m_e}{m}\vec{\rho}_1 + \vec{\rho}_2, \qquad \vec{\rho}_4 = \left[1 - \left(\frac{m_e}{m}\right)^2\right]\vec{\rho}_1 - \frac{m_e}{m}\vec{\rho}_2. \quad (3)$$

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,[19] the present choice retains the main physical results of the defects influence on the trion states.

Using gaussian functions, it is possible to calculate analytically all the defect-potential contributions. Therefore, we chose this kind of variational wave function to represent the in-plane one-particle state

$$\phi_j^0(\vec{\rho}) = \frac{1}{\sqrt{2\pi}} \frac{2}{\lambda_j} \exp\left[-\frac{\rho^2}{\lambda_j^2}\right], \quad (4)$$

where λ_j is the variational parameter.

Analogously to the charged-exciton case, the trial wave function for the neutral complex, the exciton, is given by

$$\psi_0 = N_{i,j} \chi_0(z_h) \chi_0(z_e) \phi_i^0(\vec{R}_{ex}) \phi_j^0(\vec{\rho}), \quad (5)$$

where

$$\vec{R}_{ex} = \frac{m_e \vec{\rho}_e + + m_{hxy} \vec{\rho}_h}{m}, \qquad \vec{\rho} = \vec{\rho}_e - \vec{\rho}_h. \quad (6)$$

Next, we analyze the contribution of the different terms of the Hamiltonians.

A. Exciton Hamiltonian

The actual shape of the interface defects is not accurately known and it depends on the sample growth conditions. Because of this and for simplicity, we simulate the interface defects through a potential that displays a cylindrical symmetry with a Gaussian shape and lateral radius D. Using the relative coordinate for the in-plane motion, the exciton Hamiltonian is written as

$$H_{ex} = H(z_e) + H(z_h) + T_{xy} + V_c + V_{def}(e) + V_{def}(h), \quad (7)$$

where

$$H(z_{e,h}) = -\frac{\hbar^2}{2m_{e,hz}} \frac{\partial^2}{\partial z_{e,h}^2} + V_{we,wh} Y\left(\frac{L}{2} - |z_{e,h}|\right), \quad (8)$$

$$T_{xy} = -\frac{\hbar^2}{2m}\left[\frac{1}{R_{ex}}\frac{\partial}{\partial R_{ex}}\left(R_{ex}\frac{\partial}{\partial R_{ex}}\right) + \frac{1}{R_{ex}^2}\frac{\partial^2}{\partial \theta_{Rex}^2}\right] - \frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial \rho}\left(\rho\frac{\partial}{\partial \rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial \theta^2}\right], \quad (9)$$

$$V_c = -\frac{e^2}{\varepsilon\sqrt{(z_e - z_h)^2 + \rho^2}}, \quad (10)$$

$$V_{def}(e) = V_{we} Y\left(\frac{L}{2} < z_e < \frac{L}{2} + \delta\right) \exp\left[-\left(\frac{\vec{R}_{ex} + \frac{m_{hxy}}{m}\vec{\rho}}{D}\right)^2\right], \quad (11)$$

$$V_{def}(h) = V_{wh} Y\left(\frac{L}{2} < z_h < \frac{L}{2} + \delta\right) \exp\left[-\left(\frac{\vec{R}_{ex} - \frac{m_e}{m}\vec{\rho}}{D}\right)^2\right]. \quad (12)$$

Here the QW potential height for electrons (e) and holes (h) is given by $V_{we,wh}$, $Y(z)$ is the step function $[Y(z) = 1$ if $z > 0$ and $Y(z) = 0$ if $z < 0]$, L is the QW width, μ is the

exciton in-plane reduced mass, and ε is the GaAs dielectric constant. Since V_{we} and V_{wh} are the QW confining potentials for electrons and holes, respectively, we are assuming attractive defects for electrons and holes. The defect parameters are δ, the defect depth in the z direction, and D, the defect radius in the xy plane.

It is known from optical experiments that the trions have a small binding energy. Hence, the carriers localization on the defect should be weak. Therefore, we use $\delta=1$ ML $=2.83$ Å for GaAs and $D\sim 300$ Å.[18] These parameters ensure that the exciton or trion internal degrees of freedom are not strongly affected by the defect. On a more quantitative basis, our assumption states that the gain in the exciton binding energy due to the defect presence remains small compared to the distance between the $1S$ and $2S$ exciton levels in an ideal QW.[17,18]

B. Charged-exciton Hamiltonian

Analogously to the exciton case, using the relative coordinates for the in-plane motion [Eq. (1)], the X^- Hamiltonian is given by

$$H_{cex}=H(z_{e1})+H(z_{e2})+H(z_h)+T_{xy}+V_c+V_{def}(e1)+V_{def}(e2)+V_{def}(h), \tag{13}$$

where

$$T_{xy}=-\frac{\hbar^2}{2M}\left[\frac{1}{R}\frac{\partial}{\partial R}\left(R\frac{\partial}{\partial R}\right)+\frac{1}{R^2}\frac{\partial^2}{\partial\theta_R^2}\right]-\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho_1}\frac{\partial}{\partial\rho_1}\left(\rho_1\frac{\partial}{\partial\rho_1}\right)+\frac{1}{\rho_1^2}\frac{\partial^2}{\partial\theta_1^2}\right]-\frac{\hbar^2 M}{2m_e m}\left[\frac{1}{\rho_2}\frac{\partial}{\partial\rho_2}\left(\rho_2\frac{\partial}{\partial\rho_2}\right)+\frac{1}{\rho_2^2}\frac{\partial^2}{\partial\theta_2^2}\right], \tag{14}$$

$$V_c=-\frac{e^2}{\varepsilon\sqrt{(z_{e1}-z_h)^2+\rho_1^2}}-\frac{e^2}{\varepsilon\sqrt{(z_{e2}-z_h)^2+|\vec{\rho}_2+\frac{m_e}{m}\vec{\rho}_1|^2}}+\frac{e^2}{\varepsilon\sqrt{(z_{e1}-z_{e2})^2+\left|\frac{m_{hxy}}{m}\vec{\rho}_1-\vec{\rho}_2\right|^2}} \tag{15}$$

and the other terms follow the definition of Eq. (7). The X^+ parabolic Hamiltonian is immediately obtained through the interchange of electron and hole labels.

We would like to point out that an electron or hole is weakly bound to the interface defects we are considering here. Comparing with the exciton case, their binding energies are negligible. Therefore, the charged-exciton binding energy E_b is defined as the difference between the energy of this trapped charged complex and the energy of a trapped exciton

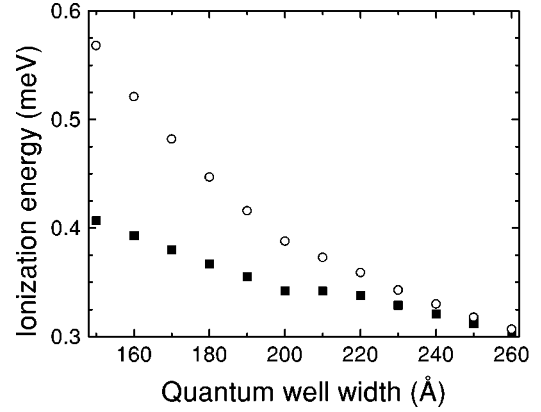

FIG. 1. X^- binding energy as a function of a GaAs QW width in the absence (squares) and presence (open circles) of interface defects. The defect parameters are: $D=300$ Å, $\delta=1$ GaAs monolayer.

(X^0) plus an in-plane *free* electron (hole), in the X^- (X^+) case. Taking the ground-state energy of these carriers as zero, one can write

$$E_b(X^-/X^+)=E(X^-/X^+)-E(X^0). \tag{16}$$

It is important to realize that the charged-exciton binding energy is a difference between two values obtained through variational calculations. This means that the calculated trion binding energy is not necessarily an upper limit of the actual value.

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- (valence-) band offset is 224.5 meV (149.6 meV).

Figure 1 shows the X^- binding energy as a function of the QW width in the cases of absence (squares) and presence (circles) of interface defects. Figure 2 shows the same calculations for the X^+. One can see that the defect potential is more important for narrow QW's. This is a consequence of

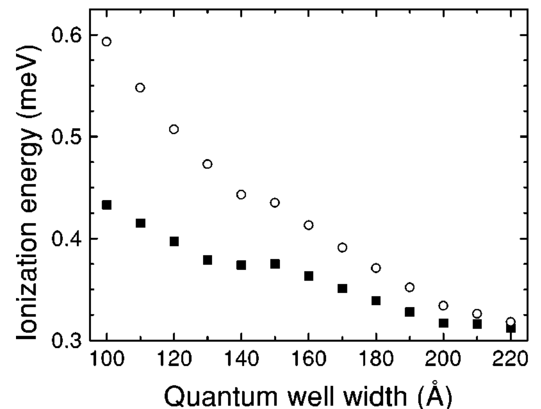

FIG. 2. The same as Fig. 1, but for the X^+

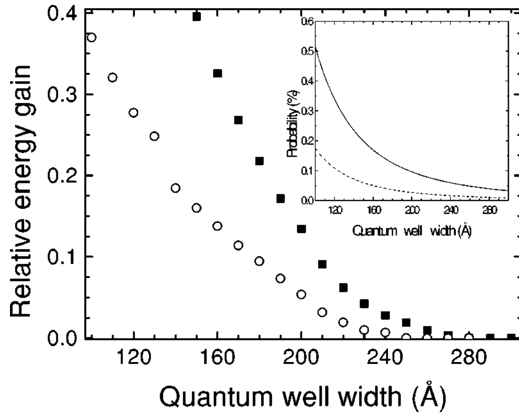

FIG. 3. X^- (squares) and X^+ (open circles) relative energy gain as a function of QW width. Inset: probability of finding an electron (solid line) or a hole (dashed line) inside the defect as a function of QW width. The defect parameters are $D=300$ Å, $\delta=1$ GaAs monolayer.

the greater amplitude of the carrier wave function inside the defect when narrow QW's are considered (inset of Fig. 3). Our results show that the defects play an important role and drastically affect the trion binding energy even in the case of a single monolayer fluctuation. They may also explain why the theoretical results have better experimental agreement in the wide QW limit.[8,19] Figures 1, 2, and 3 display only the results obtained in a QW width range where the trion internal degrees of freedom are not strongly affected by the defects. The criterion used was to show the points with less than 40% of energy gain due to the defect-potential presence. In the wide QW limit the trion CM is almost unbound and the binding energy tends to be that one in the ideal interface case.

It is important to realize that the X^- is more strongly affected by the defect than the X^+. This happens because the amplitude of the carrier wave function inside the defect is greater for electrons than for holes (inset of Fig. 3), basically because the electron is lighter than the hole. This feature is shown in Fig. 3, where we compare the X^- (squares) and the

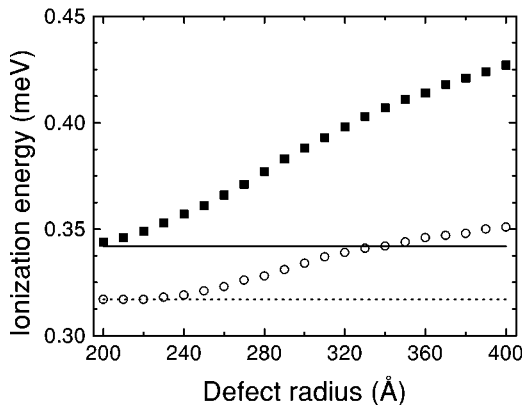

FIG. 4. X^- (squares) and X^+ (open circles) binding energies as a function of the defect radius. The horizontal lines are the X^- (solid) and the X^+ (dotted) binding energies in the absence of defects. The QW width is 200 Å and $\delta=1$ GaAs monolayer.

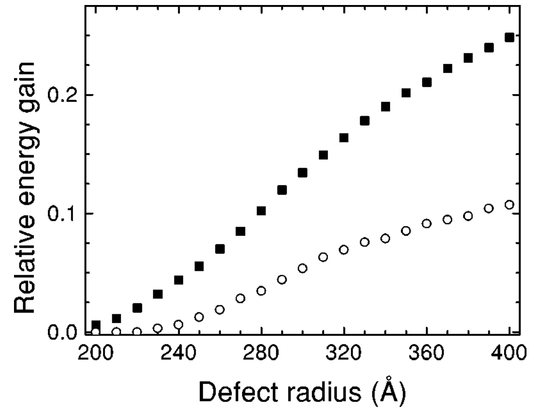

FIG. 5. X^- (squares) and X^+ (open circles) relative energy gain as a function of the defect radius. The QW width is 200 Å and $\delta=1$ GaAs monolayer.

X^+ (circles) relative energy gains, i.e., the binding-energy difference between the cases with and without defect divided by the binding energy without defect.

Figures 4 and 5 show the defect-radius influence on the trion binding energy. The QW width is 200 Å and the defect depth is one GaAs monolayer. For defect radii greater than ≈ 400 Å we expect a binding-energy saturation because, in the large defect-radius limit, the system tends to be equivalent to an ideal QW but 1 ML wider. Let us stress that the X^- (squares) and the X^+ (circles) binding energies get farther and farther with increasing defect radius. This is again a consequence of the greater electron sensitivity to the defect.

Figure 6 shows the CM mean radius of exciton (triangles), X^- (squares), and X^+ (circles) as a function of the QW width. Figure 7 shows the CM mean radii but as a function of the defect radius. One can see that the X^- is much more affected by the interface defects than the exciton, in other words, the X^- CM is more strongly localized by structural imperfections. This is in agreement with Eytan *et al.*[14] 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.

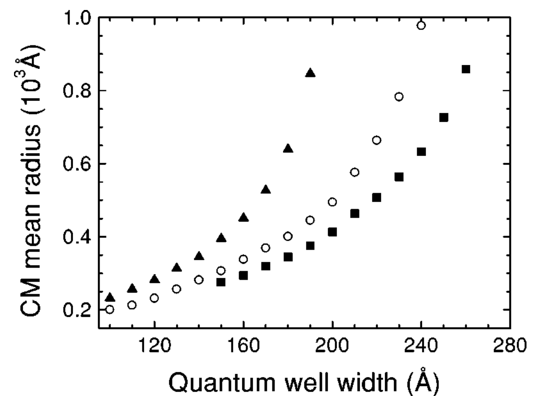

FIG. 6. CM mean radius as a function of QW width for the exciton (up triangles), X^- (squares) and X^+ (open circles). The defect parameters are: $D=300$ Å, $\delta=1$ GaAs monolayer.

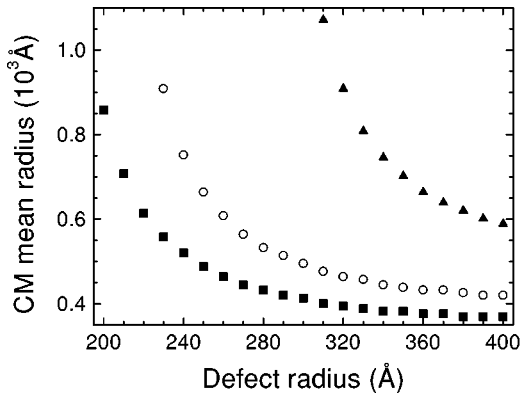

FIG. 7. CM mean radius as a function of the defect radius for the exciton (up triangles), X^- (squares) and X^+ (open circles). The QW width is 200 Å and $\delta = 1$ GaAs monolayer.

In the limits of wide QW's and small defect radii, when the defect is less important, the CM's are weakly localized. This can be seen through the tendency to very large CM radii in Figs. 6 and 7. The X^- points in Fig. 6 are interrupted in the narrow QW region where our approximations are less adequate.

IV. CONCLUSION

We have presented a simple model of the effect of the interface defects on the trion binding energy. The defects were represented by a Gaussian potential. Our results show that the structural imperfections are more important in the case of narrow QW's and that the charged excitons are more strongly localized than the neutral one, even in the case of strictly structural defects. This explains why the theoretical results have, in general, a better agreement with experiments in the wide QW limit. Our results also show that the negative trion is more sensitive to the structural imperfections than the positive one.

ACKNOWLEDGMENTS

This work was supported by FAPESP (Brazil), CNPq (Brazil), and by NEDO (Japan) and EEC Project No. [IST-1999-11311(SQID)].

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