Exciton in type-II quantum dot

J Sierra-Ortega¹, R A Escorcia¹, and I D Mikhailov²
¹ Universidad del Magdalena, A. A. 731, Santa Marta, Colombia
² Universidad Industrial de Santander, A. A. 678, Bucaramanga, Colombia

E-mail: jsierraortega@gmail.com

Abstract We study the quantum-size effect and the influence of the external magnetic field on the exciton ground state energy in the type–II InP quantum disk, lens and pyramid deposited on a wetting layer and embedded in a GaInP matrix. We show that the charge distribution over and below quantum dot and wetting layer induced by trapped exciton strongly depends on the quantum dot morphology and the strength of the magnetic field.

1. Introduction
The study of the behaviour of Wannier excitons in both type-I and type-II self-assembled quantum dots (QDs) has attracted considerable attention in recent years. In type-I structures, such as InAs/GaAs or InAlAs/AlGaAs, both carriers, which forms exciton, are located inside the quantum dots, while in type-II structures such as InP/GaInP or GaSb/GaAs inside the dots can be located only electron or only hole. Separate localization of the carriers in type-II axially symmetrical heterostructures can lead to interesting effects such as persistent currents, oscillations of the exciton ground state energy, and crossovers of the energy levels [1]. At the same time, analysis realized recently shows that the modification of the density distribution in two-dimensional structures with broken symmetry produces a partial or total quenching of these effects for low-lying energy levels [2]. On the other hand, according to the results obtained previously for type-I QDs in form of the disk [3], lens, and pyramid [4] the three-dimensional density distribution of carriers in QDs is modified due to an appreciable tunnelling of carriers toward the matrix through the upper and lower QD’s junctions. As the electron is lighter than the hole it’s tunnelling toward the matrix is stronger than one of the electron. Therefore in the regions above and below the type-I QD with trapped exciton the negative charge exceeds the positive one, while in the central region of the QD the charge distribution is inverted. In this work we present results of similar calculations of the charge distributions, provided by the trapped exciton around and inside type-II QDs with different morphologies.

2. Theoretical model
We consider a model of axially symmetrical quantum-well structure in the form of thin InP layer whose thickness \(d\) depends on the distance \(\rho\) from the axis as:

\[
d(\rho) = d_b + d_0 \left[1 - \left(\frac{\rho}{R_0}\right)^2\right]^{1/n} \theta(R_0 - \rho)
\]

(1)

Here \(\theta(x) = 0\) for \(x < 0\) and \(\theta(x) = 1\) for \(x > 0\), \(d_b\) is the wetting layer (WL) thickness, \(R_0\) and \(d_0\) are

¹ Corresponding author: Tel.: +575 4308684; fax: +575 4213011. (J. Sierra-Ortega)
the QD base radius and maximum height over the WL, respectively. The structure is embedded in
GaInP matrix. The QD morphology according to relation (1) is controlled by means of the integer
shape-generating parameter \( n \) which is equal to 1, 2 or tends to infinity for conical pyramid-like, lens-
like and disk-like geometrical shapes, respectively. For sake of the mathematical convenience and,
besides, in accordance with the experiment, we assume, that the height-to-base radius aspect ratio in
all cases is small, i.e. \((d_{0} + d_{b}) / R_{0} \ll 1\). In our model type-II quantum dot the position vectors \( r_{i} \)
of the electron sited mainly inside the layer and of the hole sited mainly outside the layer (figure 1) are
given in cylindrical coordinates by the components \((\rho_{i}, \vartheta_{i}, z_{i})\). Here and in what follows indices
\( i = e, h \) correspond to the electron and the hole with the masses \( m_{e}, m_{h} \), respectively.

**Figure 1** The model of the exciton in II-type quantum dot

Below we use as the unit of length the exciton effective Bohr radius \( a_{0}^{*} = \hbar^{2} / e \mu e^{2} \), as the unit of
energy the effective Rydberg \( \text{Ry}^{*} = e^{2} / 2 \varepsilon a_{0}^{*} \), and \( \gamma = e \hbar B / 2 \mu c \text{Ry}^{*} \) as the unit of the strength of the
magnetic field \( B \) applied along the symmetry axis, being \( \mu = m_{e} m_{h} / (m_{e} + m_{h}) \) the reduced mass, \( e \)
the electron charge, and \( \varepsilon \) the dielectric constant. In the effective-mass approximation the dimensionless
Hamiltonian of the exciton corresponding to its ground state can be written as:

\[
\hat{H} = - \sum_{i = e, h} \left[ \hbar \left( \frac{1}{\rho_{i}} \frac{\partial}{\partial \rho_{i}} \rho_{i} \frac{\partial}{\partial \rho_{i}} + \frac{\partial^{2}}{\partial z_{i}^{2}} + \frac{\gamma^{2} \rho_{i}^{2}}{4} \right) + V_{i} (\rho_{i}, z_{i}) \right] - 2 / r_{eh} \tag{2}
\]

Here \( V_{e} (\rho_{e}, z_{e}) = 0 \) and \( V_{h} (\rho_{h}, z_{h}) = V_{ho} > 0 \) if \( 0 < z_{e} < d (\rho_{e}), i = e, h \), otherwise \( V_{e} (\rho_{e}, z_{e}) = V_{eo} > 0 \)
and \( V_{h} (\rho_{h}, z_{h}) = 0 \). \( \eta_{e} = \mu / m_{e}, \eta_{h} = \mu / m_{h} \), and \( r_{eh} \) is the electron-hole separation. In our model the
hole is retained close to the QD only due to the attraction to the electron trapped inside the layer and
therefore the typical scale for the distance between them is the effective Bohr radius. This value can
be assured by the presence of the factor \( \exp (-r_{eh}) \) in the ground state wave function. It is the reason
why we choose the trial function for the trapped exciton as follows:

\[
\Psi (r_{e}, r_{h}) = \chi (r_{eh}) f_{e} (\rho_{e}, z_{e}) \Phi (\rho_{h}), \quad \chi (r_{eh}) = \exp (-r_{eh}) \tag{3}
\]

Here an unknown envelope function \( \Phi (\rho_{h}) \) describes a modification of the Slater orbital due to the
presence of the repulsive \( V_{h} (\rho_{h}, z_{h}) \) and attractive, \( \gamma^{2} \rho_{h}^{2} / 4 \) potentials in the Hamiltonian (2) and
\( f_{e} (\rho_{e}, z_{e}) \) is the electron ground state wave function in QD, the exact solution of the equation:

\[
\left[ - \eta_{e} \Delta_{e} + V_{e} (\rho_{e}, z_{e}) + \frac{\gamma^{2} \rho_{e}^{2}}{4} \right] f_{e} (\rho_{e}, z_{e}) = E_{e} f_{e} (\rho_{e}, z_{e}) \tag{4}
\]

Taking into consideration that the structures under consideration have a small the height-to-base radius
aspect ratio we found the solution of the equation (4) corresponding to the lowest energy \( E_{e} \) by using
the procedure corresponding to the adiabatic approximation, described in reference [4]. The exciton
energy of the ground state \( E_{X} \) is found by minimizing the ratio:

\[
E_{X} = \left\langle \chi (r_{eh}) f_{e} (\rho_{e}, z_{e}) \Phi (\rho_{h}) \right| \hat{H} \left| \chi (r_{eh}) f_{e} (\rho_{e}, z_{e}) \Phi (\rho_{h}) \right\rangle / \left\langle \chi^{2} (r_{eh}) f_{e}^{2} (\rho_{e}, z_{e}) \Phi^{2} (\rho_{h}) \right\rangle \tag{5}
\]

Taking the functional derivative with respect to \( \Phi \) gives a wave equation of the form:

\[
- \frac{\eta_{h}}{J (\rho)} \frac{d}{d \rho} J (\rho) \frac{d \Phi (\rho)}{d \rho} + \tilde{V} (\rho) \Phi (\rho) = - E_{h} \Phi (\rho); \quad E_{h} = E_{e} - E_{X} , \tag{6}
\]
where $E_b$ is the exciton binding energy, $J(\rho)$ and $\tilde{V}(\rho)$ are the Jacobian and the effective potential energy as functions of the distance from the hole position to the axis, respectively, defined as:

$$J(\rho) = \left( \chi^2 f^2 e \delta(\rho_h - \rho) \right); \quad \tilde{V}(\rho) = -1 + \eta \chi^2 \rho^2 / 4 + \left\{ V_h(\rho_h, z_h) \chi^2 f^2 \delta(\rho_h - \rho) \right\}$$

(7)

The presence in these expressions of delta-function, $\delta(\rho_h - \rho)$, allows us to simplify essentially the calculation of the correspondent dependencies. By using the substitution $\Phi(\rho) = u(\rho) \sqrt{\rho / J(\rho)}$ the equation (6) is reduced to a form typical for two-dimensional central force problem

$$-\frac{\eta}{\rho} \frac{d}{d\rho} \rho \frac{du(\rho)}{d\rho} + V_{\text{eff}}(\rho) u(\rho) = E \Phi(\rho); \quad V_{\text{eff}}(\rho) = E + \tilde{V} + 0.5 \left( w' - 0.5 w^2 \right); \quad w(\rho) = J'(\rho) / J(\rho)$$

(8)

Here $V_{\text{eff}}$ is the effective potential which controls the in-plane motion of the hole around the QD. The potential curves $V_{\text{eff}}$ in the disk, the lens and the conical pyramid with the base radius 8nm, the thickness of the WL 2nm and the greatest QD height over the WL 3nm for the zero-magnetic field case are presented in Fig. 2. It is seen that the effective potentials strongly depends on the QDs morphology.

Figure 2 Effective potential curves for the in-plane motion of the hole in QDs with different profiles

3. Results and discussion

We solve one-dimensional wave equations (8) by using the trigonometric sweep method described in Ref. [3]. In our calculations we took the parameters: $m_e = 0.077 m_0, m_h = 0.6 m_0, V_e = 250 meV, V_h = -50 meV$, and $\varepsilon = 12.61$, which are typical for InP/GaInP system [5]. In order to understand the effect of the QD morphology on the exciton ground state energy we first calculated the density of the charge distribution inside and around the QD with trapped exciton, defined as the difference between the electron and the hole density distributions... It is clear that the change of the InP layer morphology should provide a variation of the averaged separation between the electron and the hole. For example, if in the disk-shaped QD the electron can be displaced inside the QD along the layer relatively easy, following to the motion of the hole, in the case of the conically-shaped QD the electron is mainly localized close to the axis. Therefore the mean distance between the electron and the hole in a conically-shaped QD is larger and the binding energy is inferior than those in the disk. In Fig. 3 we present contour plots, which correspond to the level lines of the charge density distributions along a cross section in the middle of the InP/GaInP quantum disk, lens and conical pyramid with trapped exciton. The left- and right-side parts of the figure correspond to the models of QDs without and with WL, respectively. It is seen that in contrast to the distribution obtained previously for the type-I QD in reference [4], the density of the radial charge distribution inside QDs is generally negative while outside QDs it is positive. Also, one can see that the region of the positive charge over and below QDs is extended toward axis while the morphology of the QD is changed from disk-shaped to conical-
shaped. The existence of the WL leads to a lowering of the effective barrier height for the in-plane electron motion reinforcing significantly its tunnelling in the lateral direction, resulting in a stronger charging of the peripheral regions in the lateral direction that can be seen in right-side plots of Fig. 3.

**Figure 3** Contour plots of the radial charge distribution density induced by captured exciton in a plane through the axis of symmetry of the InP/GaInP quantum disk, lens and conical pyramid with the base radii 10nm and the heights 4nm, and with 0 (left-side) and 2nm (right-side) thickness of the WL.

Comparing contour plots in Fig. 3 with those from reference [4] for type-I QDs one can observe that the charging of the central y peripheral regions in the type-II QDs is essentially stronger than one in the type-I QDs. It is due to the fact that the regions of the carriers’ localization in the type-I QDs are essentially overlapped while in the type-II QDs they are strongly separated.

**Figure 4** Exciton binding (a) and total (b) energies versus radii $R_0$ in QDs with different profiles.
In Fig. 4 we display the exciton binding and total energies dependencies on the base radii of the disk, the lens and the conical pyramid with height 4nm over WL, whose thickness is 2nm. It is interesting to note that for small QD radii ($R_0 < 15\text{nm}$) the largest binding energy has the exciton in the conical pyramid followed by the lens and disk, whereas for large QD radii this order is inverted. It is due to the fact that the motion of electron is mainly restricted in QD close to axis and that the largest confinement is provided in the conical pyramid followed by the lens, and the disk. Therefore, as the QD radius is greater than the effective Bohr radius (about 15nm), the largest separation between the hole and the electron is in the conical pyramid. The order is reversed for $R_0 < 15\text{nm}$ . One can see in Fig. 4(b) that the total energy dependencies in QDs with different shapes are rather similar being the energy in the conical pyramid for all base radii higher than those in the lens and in the lens higher than in the disk. In Fig. 5 we display the exciton binding energies dependences on the magnetic field strength for QDs with different shapes. It is seen that in all cases the exciton binding energy increases and that this increase is larger in the pyramid and the lens. The magnetic field affects mainly the density distribution of the hole, displacing its peak toward heterostructure axis, decreasing in this way the electron-hole separation and increasing the binding energy. Such modification of the distribution under magnetic field is less pronounced in disk-shaped QD.

![Figure 5](image_url)  
**Figure 5** Exciton binding energy as a function of the magnetic field in QDs with different profiles

4. Conclusions
In order to study the effect of the morphology on the charge distribution in type-II quantum dots with trapped exciton we propose a simple trial function for calculating the charge distribution and the ground state energy of the exciton in flat disk-shaped, lens-shaped, and cone-shaped InP/GaInP quantum dots with different base radii, heights and wetting layer thicknesses. We present novel contour plots of the radial charge distribution density induced by captured exciton in InP/GaInP quantum dots with different morphology. It is found a strong influence of the morphology on the charge distribution inside, over and below QD with trapped exciton and on the exciton energy dependencies on the QD radius and the magnetic field strength.

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