Magnetoexciton in type-II semiconductor nanocone

M Herrera-Torres, J Sierra-Ortega, L F Garcia, and I D Mikhailov
1 Grupo de Investigación en Teoría de la Materia Condensada, Universidad del Magdalena, Santa Marta, Colombia
2 Grupo de Física Computacional en Materia Condensada, Universidad Industrial de Santander, Bucaramanga, Colombia

E-mail: jsierraortega@gmail.com

Abstract. We study spectral properties of heavy-hole exciton captured by a type-II InP/GaAs nanocone in the effective mass approximation. Assuming that the effective mass of the hole is essentially larger than of the electron, we solve the two-particle Schrödinger equation by using the adiabatic approximation and the Fourier series expansion method. We analyze the alteration of the averaged spatial separation of the electron and the hole, the period of the Aharonov–Bohm oscillations of the energy levels and the magnetic momenta as functions of the external magnetic field, applied along the symmetry axis. Our theoretical analysis reveals a possibility for controlling the electric polarization in type-II semiconductor structure with captured exciton, by means of the applying of an external magnetic field.

1. Introduction
Lately, there has been a great deal attention to study of type II semiconductor nanostructures, which offer an additional possibility for an increase of the electron-hole spatial separation facilitating on this way the control of the spectral, and the electric and magnetic properties of these structures by capturing an exciton. Separate localization of the carriers in type-II axially symmetrical heterostructures in the presence of the external magnetic field, can facilitate the observation of the stable Aharonov-Bohm(AB) effects manifested in the appearance of the persistent currents, oscillations of the exciton ground state energy and the magnetic moment, and crossovers of the energy levels [1-6]. Nanowires with type-II nanocone structures like Si/Ge, CdTe/CdZn/TeZnO and InGaAs/InGaAsP have been synthesized recently for solar cell applications [7-9], in which the electron is confined inside the cone while the hole, attained to the electron, is located at the surrounding matrix close to the conical lateral junction. The AB effect in such structure has interesting peculiarities, related to an additional degree of freedom acquired by the hole along the lateral cone’s junction [10,11]. The centrifugal force pushes the hole toward the cone’s bottom, while the diamagnetic force drives it to the top. As the magnetic field is increased the diamagnetic force becomes prevailing and the hole begins to climb from the bottom to the top. Such redistribution of the hole’s probability density under external magnetic field produces an electric polarization of the structure along the symmetry axis.

Below, we analyze a similar problem for magnetoexciton, in which the electron is trapped inside the type II nanocone, and the hole bounded to the electron is located outside of the cone.

2. Theoretical model
We consider a conically shaped InP nanostructure embedded in GaAs matrix, where the electron is retained inside the nanocone, while the hole, bounded to the electron, is mainly located within a thin
shell-region, encompassing the conical antidot. A vertical cross-section along the symmetry axis of this nanostructure is schematically represented in Figure 1. The geometrical parameters of the structure are given by the height \( H \), the bottom \( R_b \) and the top \( R_t \) radii for the conical core. In our model, the external homogeneous magnetic field \( B \) is parallel to the \( Z \)-axis and the Equation (1) for the lateral frontier surface in cylindrical coordinates has the following form:

\[
\rho(z) = R_b - z \tan \alpha; \quad \tan \alpha = (R_b - R_t)/H
\]  

(1)

In our calculations we use \( m^e_0 \) = 0.45\( m_0 \) and \( m^\ast_e \) = 0.08\( m_0 \) as the effective mass of the hole and electron in the GaAs and InP materials respectively and the dielectric constant \( \varepsilon \) = 12. As the effective mass of the hole is larger than the electron one, we take advantage of the adiabatic approximation [12,13] to represent the exciton wave function for the low-lying states in cylindrical coordinates as the Equation (2):

\[
\Psi_{l_h}(z_e, z_h, \theta_h) = \psi_e(z_e)e^{il_h \theta_h} \varphi_h(z_h); \quad l_h = 0, \pm 1, \pm 2, \ldots
\]  

(2)

Here and the following \( l_h \) is the angular momentum of the hole, \( \psi_e(z_e) \) describes the fast electron motion inside de cone and \( \varphi_h(z_h) \) defines the slow hole motion around the cone’s lateral border. We use the effective Bohr radius \( a^\ast_0 = 4\pi\varepsilon_0\hbar^2/\mu^e \), the effective Rydberg \( R^\ast_y = e^2/8\pi\varepsilon_0\varepsilon a^\ast_0 \) and parameter \( \gamma = eB/2\mu^e R^\ast_y \) as units of the distance, the energy and the magnetic field strength respectively. being \( \mu^\ast = m^e_0 m^h_0/(m^e_0 + m^h_0) \) the reduced mass and \( \mu^e = m^e_0/\mu^\ast \); \( \mu_h = m^h_0/\mu^\ast \). In framework of the two-step adiabatic approximation, we first find the ground state energy \( E_e(z_h) \) of the fast electron motion along the cone’s lateral border, by solving the Equation (3):

\[
-\psi_e''(z_e)/\mu_e + V_e(z_e, z_h)\psi_e(z_e) = E_e(z_h)\psi_e(z_e); \quad \psi_e(0) = \psi_e(H) = 0
\]  

(3)

where the electron potential energy \( V_e(z_e, z_h) \) is a sum of the infinite-barrier confinement energy inside the cone and the Coulomb attraction to the hole, whose axial coordinate \( z_h \) is considered as a fixed parameter. The energy \( E_e(z_h) \), we then use as adiabatic potential to find the energies of the exciton \( E_X(l_h) \) as eigenvalues of the problem for a slow rotation of the hole around the cone with angular momentum \( l_h \) (Equation (4)),

\[
-\psi_e''(z_h)/\mu_h + [V_h(z_h, l_h) + E_e(z_h)]\varphi(z_h) = E_X(l_h)\varphi(z_h); \quad \varphi(0) = \varphi(H) = 0; \quad l_h = 0, \pm 1, \pm 2, \ldots
\]  

(4)

\[\text{Figure 1. InP/GaAs nanocone structure.}\]
Here, \( V_h(z_h, l_h) = (l_h/z_h \tan \alpha - \gamma z_h \tan \alpha/2)^2 \). The energies and eigenfunctions of Equation (3) and Equation (4), which satisfy the boundary conditions, can be found by using the Fourier series expansion method, representing wave functions as the Equation (5):

\[
\psi_e(z_e) = \sum_{n_e=1}^{\infty} C_n \sin \left( \frac{n_e \pi z_e}{H} \right); \quad \varphi(z_h) = \sum_{n_h=1}^{\infty} B_n \sin \left( \frac{m_h z_h}{H} \right);
\]

Substitution of the Equation (5) at Equation (3) and Equation (4) provides the following system of secular equations for unknown coefficients of the Fourier expansions:

\[
\frac{\pi^2 n^2}{\mu_e H^2} C_n + \sum_{n'=1}^{\infty} \bar{V}_e(n, n') C_n' = E_e(z_h) C_n; \quad \frac{\pi^2 n^2}{\mu_h H^2} B_n + \sum_{n'=1}^{\infty} \bar{V}_h(n, n') B_n' = E_h(z_h) B_n
\]

\[
H. \bar{V}_p(n, n') = [l_p(n - n') - l_p(n + n')]; \quad p = e, h;
\]

\[
I_e(\bar{n}) = \int_0^H V_e(z) \cos \left( \frac{\pi n z}{H} \right) dz; \quad I_h(\bar{n}) = \int_0^H [V_h(z) + E_e(z)] \cos \left( \frac{m \pi z}{H} \right) dz
\]

3. Results

The adiabatic potential, found as the lowest eigenvalue of the first problem (3) defines the most probable z-position of the hole bound to the electron and the average electron-hole separation in the zero-magnetic field case. In Figure 2, it is shown the adiabatic potentials calculated for nanocones with different aperture angles. When the aperture angle is zero (case of the wire), the potential minimum position is at the middle of the cone height. As the aperture angle increases, the position of the minimum is displaced toward the cone’s bottom.

![Figure 2. Adiabatic potential.](image)

In Figure 3 we present results for some lower exciton energies corresponding to the radial quantum numbers \( n_h = 1 \) (solid lines) and \( n_h = 2 \) (dash lines) as functions of the magnetic field. From Figure 3(c), we can see that when the aperture angle is small, the AB oscillations are similar to those in a nanotube [9], with an almost periodic variation of the ground state energy and with the almost horizontal straight envelope dotted line. The period of the AB oscillations \( \Delta \gamma \) is the same as for 1D quantum ring \( \Delta \gamma = 2/R^2 \), with \( R = 40 \text{nm} \), i.e. for the cone’s radius at the middle of its height. Comparing the similar curves in Figure 3(a) and Figure 3(b) one can see that the increase of the cone’s aperture angle produces a successive growth of the slope of the straight envelope dot line. The period and the amplitude of the oscillation of the ground state energy successively drops with the increase of the external magnetic field. We associate this AB oscillations period reduction with a process of climbing of the hole horizontal circular paths with different angular momenta around the cone lateral junction under increasing...
magnetic field, from the bottom of the cone toward its top. A detailed discussion of the nature of the AB effect for cone-shaped nanostructures has been previously given in reference [10].

![Figure 3](image-url)

**Figure 3.** Exciton energies with different hole’s angular momentum and two different radial quantum numbers, as functions of the external magnetic field in type II nanocones with three different top radii.

The climbing of the hole circular paths in the presence of the external magnetic field supports the increase of the electron-hole separation resulting in the formation of a permanent electric dipole moment. The evolution of the dependencies of the electron-hole separation along the symmetry axis on the applied magnetic field with the reduction of the aperture angle is shown in Figure 4, which we calculate as: 

\[
\langle |z_{eh}| \rangle = \int_0^H |\varphi_{l_h}(z_h)|^2 d_z h \int_0^H (z_h - z_o) |\psi_h(z_o)|^2 d_z h; \quad l_h = 0, \pm 1, \pm 2, \ldots
\]

In all cases, one can see a monotone growth of the electron-hole separation up to its threshold value, resulting in formation of a giant permanent electric dipole moment when the magnetic field increasing becomes superior to a critical value. This is a manifestation of a possible magnetoelectricity in conical nanostructures with trapped excitons, which allow us to induce and control the electric dipole of the structure by means of variation of the external magnetic field. As the aperture angle is small as in Figure 4(a), the threshold value of the separation is low.

![Figure 4](image-url)

**Figure 4.** Electron-hole separations along the Z-axis in cones with four different aperture angles, as functions of the magnetic field for states with five lower angular momentum.
The threshold value of the carrier’s separation grows successively with increase of the aperture angle while the critical value of the magnetic field depends very weakly on the aperture angle. We associate such behavior of the electric dipole moment to the interplay between the magnetic confinement and the electron-hole attraction.

The magnetic confinement compresses the hole’s circular tracks toward the symmetry axis and push them upwards along the cone’s border, while the electron-hole attraction holds the hole close to the cone’s bottom. As the aperture angle is small, the contribution of the electron-hole attraction and the electron confinement to the total energy is prevailing and the threshold value for the induced dipole moment is relatively low. With an increase of the aperture angle, the role of the diamagnetic magnetic confinement becomes dominant, the hole climbs upwards along the cone’s border, while the electron remains close the cone’s bottom because of the structural confinement is stronger than the electron-hole attraction. Curves intersections of the energy dependencies on the magnetic field in Figure 3 are associated to an abrupt alteration of the magnetic momenta of the corresponding states, which are proportional to the first derivative of the corresponding energies with respect to the dimensionless external magnetic field. For example, the magnetic moment at zero temperature for the state with number $k$ can be found numerically by using the relation $M_k = \mu_B dE_k(\gamma)/d\gamma$, being $\mu_B$ the Bohr magneton. In Figure 5, we display the energies dependencies of the exciton ground states energy on the magnetic field. In insets are shown their first derivatives corresponding to magnetic moment. It is seen that the separations between minima points and the amplitude of the ground state energy oscillation are consistently reduced, as the aperture angle grows, transforming in an almost linear dependence.

![Figure 5](image_url)

**Figure 5.** Energies of exciton as functions of the external magnetic field in a type II nancone with three different aperture angles. In inset are shown similar dependencies for magnetic moment.

4. **Conclusions**

In summary, we show that the probability of the spatial distributions of the hole, encompassing lateral cone’s border outside type-II nanocone, depends mainly on the interplay between the Coulomb attraction to the electron, which hold it close to the bottom, and the diamagnetic force, which pushes it upward. When the magnetic field rises, the peaks of the hole distributions corresponding to different angular momentum begin to climb successively one by one from base toward the top, pushed up by the diamagnetic force, in the order of the ascending angular momentum. Besides, we show that such redistribution of the hole probability density produces a substantial decrease of the amplitude and the period of the AB oscillations of the ground state energy as function of the magnetic field. Thus, our theoretical analysis reveals a new possibility for controlling the electric dipole moment of the type-II semiconductor nancones by means the applying of the magnetic field.

**Acknowledgements**

This work was financed by the Universidad del Magdalena through Vicerrectoría de Investigación and the Universidad Industrial de Santander (UIS) through Vicerrectoría de Investigación y Extensión, DIEF de Ciencias (Cod. 1350).
References

[1] Chaplik A 2002 JETP Lett, 75(6) 292
[2] Kalameitsev A, Kovalev V, Govorov A, and Kotthaus J 1998 JETP Lett. 68(8) 669
[3] Janssens K, Patroens B and Peeters F 2001 Phys. Rev. B 64 155324
[4] Govorov A, Ulloa S, Karrai K and Warburton R 2002 Phys. Rev. B 66 081309(R)
[5] Xia Y, Yang P, Sun Y, Wu Y, Mayers B, Gates B, Yin Y, Klim F and Yan H 2003 Advanced Materials 15 353
[6] Alivisatos A 1996 Science 271 933
[7] Wang K, Chen J, Zhou W, Zhang Y, Yan Y and Pern J 2008 Advanced Materials 20 3248
[8] Lin H M, Chen Y L, Yang J, Liu Y C, Yin K M, Kai J J, Chen F R, Chen L C, Chen Y F and Chen C C 2003 Nano Lett. 3 537
[9] Medvid A, Dmytruk I, Onufrijevs P and Pundyk I 2007 Physica Status Solidi (c) 4 3066
[10] Garcia L F, Mikhailov I, and Sierra-Ortega J 2016 Journal of Nanomaterials 2016 ID496174
[11] Garcia L F, Gutiérrez W and Mikhailov I 2017 Journal of Nanomaterials 2017 ID 5658796
[12] Janssens K, Peeters F and Schweigert 2001 J. Appl. Phys. Rev. B 63 205311
[13] Porras L and Mikhailov I 2013 Physica E: Low-dimensional Systems and Nanostructures 53 41