Electric polarizability of type-II semiconductor nanocone induced by magnetoexciton

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Abstract. We present a theoretical analysis of the possibility of formation of a permanent electric dipole moment in the presence of the electric and magnetic fields, which are simultaneously applied along the symmetry axis of a CdS/ZnSe type II nanocone, induced by a trapped exciton. We show that the external magnetic field applied along the cone’s axis increases the electric dipole moment forcing the electron to climb along the cone’s border via the diamagnetic confinement, meanwhile the electric field may cause either growth or reduction of the electric dipole moment.

1. Introduction

Type-II semiconductor nanowires can more effectively enhance light absorption and increasing coupling efficiency in comparison with planar nanostructures [1-4]. In particular, type-II core-shell nanowire structure offers a novel mechanism of charge separation in their junctions in the radial direction, which can act similarly as a p-n junction, but without requirement of a doping. Nanowires with type-II core/shell heterojunctions like ZnO/ZnSe a GaN/GaP core/shell nanowires have been synthesized earlier for solar cell applications [5,6]. A special morphology of type-II nanowires allows us to control their spectral, electric and magnetic properties by applying the external electric and magnetic fields. As in these structures there is a single conducting channel, the separation of positive and negative charges and the polarizability of these structures are very sensitive to the applying of the external electric field along the symmetry axis. Besides, when the axially symmetrical type II nanowire has a conical geometry, an external magnetic field applied along the symmetry axis can change additionally the electric polarizability in such structures due to the Aharonov-Bohm (AB) effect [7,8]. The type-II core-shell CdS/ZnSe nanostructure has been synthesized and their properties have been studied earlier [9-12]. Below, we present a theoretical analysis of the electric polarizability of a magnetoexciton trapped in a type II semiconductor nanocone, in which the heavy hole is mainly retained inside the nanocone close to the symmetry axis, while the electron, bound to the hole encompasses the cone lateral border. Assuming that the effective mass of the hole is essentially larger than of the electron, we solve the corresponding two-particle Schrödinger equation in the adiabatic approximation [13,14]. Our calculation shows that the diamagnetic confinement, provided by the growing external magnetic field, applied along the symmetry axis, pushes the electron upwards increasing suddenly the electron-hole separation and the electric dipole momentum of the structure as the magnetic field surpass a threshold value. Similar behavior is detected for the dipole momentum dependence on the electric field. In
addition, the dipole momentum dependencies reveal a reciprocal relation between electric and magnetic fields; the magnetic field affects the polarizability induced by the electric field and vice versa. This proves a possible existence of the magnetoelectric effect, induced by the quantum confinement in quasi-one-dimensional nanostructures, such as wires, cones or rods.

2. Theoretical model
In order to study the energies and dipole momenta dependencies on the external electric and magnetic fields, we consider a model of a CdS nanocone embedded in a ZnSe matrix. A vertical cross-section along the symmetry axis of this nanostructure is schematically represented in Figure 1. The conduction and valence bands potential mismatches at junctions of this structure retain the hole inside the wire, while the electron, linked to the hole, encompasses the conical antidot within a thin shell-region. The geometrical parameters of the model are the aperture angle \( \alpha \), the cone’s height \( H \), the bottom \( R_b \) and the top \( R_t \) radii. The external homogeneous magnetic \( B \) and electrical \( F \) fields are applied parallel to the \( Z \)-axis.

It is consider a simplified tractable model, in which we suppose that the hole confined inside the cone is mainly situated close to the symmetry axis and its position is given by a single \( z \)-coordinates \( z_h \), while the electron with cylindrical coordinates \( \rho_e, \theta_e, z_e \) attained to the hole, is displaced within the narrow region along the surface of the cone’s lateral border, where coordinates \( \rho_e, z_e \) are related as the follow Equation (1):

\[
\rho_e(z_e) = R_b - z_e \tan \alpha; \quad \tan \alpha = (R_b - R_t)/H
\]  

Figure 1. CdS/ZnSe nanocone structure.
In our calculations we use, the effective mass, \( m^*_e = 0.14m_0 \) for the electron in the ZnSe [6,7] and \( m^*_h = 0.81m_0 \) for the hole in the CdS [15], and the dielectric constant \( \varepsilon = 10 \) for both materials. In what follows we use dimensionless units: the effective Bohr radius \( a^*_0 = 4\pi\varepsilon_0\varepsilon_0^*a_0^2/\mu^*e^2 \), the effective Rydberg \( R^*_\gamma = e^2/8\pi\varepsilon_0\varepsilon_0^*a_0^2 \), the parameters \( \gamma = e^2h^2/2\mu^*R^*_\gamma \) and \( \beta = e^2a_0^2/R^*_\gamma \) as units of the distance, the energy and the magnetic and electric field strengths respectively, being \( \mu^* = m^*_e^2m^*_h/\left(m^*_e + m^*_h\right) \) the reduced mass and \( \mu^*_h = m^*_e^2/\mu^*; \mu^*_h = m^*_e^2/\mu^* \). Due to the axial symmetry of the structure, the angular momentum of the electron \( l_e \) is a good quantum number and the corresponding two-particle wave functions in our simplified model can be represented as the Equation (2):

\[
\psi_{l_e} = \left(z_e, \theta_e, z_h\right) = \ e^{i\hbar z_e^0} \Phi_{l_e}(z_e, z_h); \ l_e = 0, \pm 1, \pm 2, ...
\]  

(2)

Since the effective mass of the hole is essentially larger than one of the electrons we can take the advantage of the adiabatic approximation in order to represent approximately the exciton wave function for the low-lying states in cylindrical coordinates as in Equation (3):

\[
\Phi_{l_e}(z_e, z_h) = \psi_{l_e}(z_e, z_h) \varphi(z_h); \ l_e = 0, \pm 1, \pm 2, ...
\]  

(3)

Where the first factor describes the fast electron motion around the lateral cone’s border while the second factor defines the slow hole motion along the symmetry axis. In framework of the two-step adiabatic approximation, we first find the ground state energy of the fast electron motion, considering the hole’s coordinate \( z_h \) as parameter, and by solving the Equation (4):

\[
-\frac{1}{\mu_e} \frac{\partial^2\psi_{l_e}(z_e,z_h)}{\partial z_e^2} + V_e(z_e,z_h)\psi_{l_e}(z_e,z_h) = E_e(z_h,l_e)\psi_{l_e}(z_e,z_h); \ l_e = 0, \pm 1, \pm 2, ...
\]  

(4)

With the potential (Equation (5)),

\[
V_e(z_e,z_h) = \left(\frac{l_e}{\rho_e(z_e)} - \frac{\gamma \varphi(z_e)}{2}\right)^2 - \frac{2}{\left(\rho_e(z_e)^2+(z_e-z_h)^2\right)} - \beta F
\]  

(5)

The ground state energies \( E_e = (z_h,l_e) \) present here the adiabatic potentials for the slow motion of the hole described by the wave function \( \varphi(z_h) \), which is the solution of the Equation (6) (eigenvalue problem):

\[
-\frac{1}{\mu_h} \frac{\partial^2\varphi(z_h)}{\partial z_h^2} + V_h(z_h) + E_e(z_h,l_e)\varphi(z_h) = E_X(l_e)\varphi(z_h); \ V_h(z_h) = \frac{\pi^2}{\rho^2_e(z_h)} + \beta F
\]  

(6)

Here, \( E_X(l_e) \) is the exciton energy in the state with the electron angular momentum \( l_e \). The energies and eigenfunctions of Equation (4) and Equation (6), which satisfy the boundary conditions at extremes of the cone, we can find by using the Fourier series expansion method, representing wave functions as the Equation (7):

\[
\psi_{l_e}(z_e,z_h) = \sum_{n_e=1}^{\infty} C_n \sin \left(\frac{m_e z_e}{H}\right); \ \varphi(z_h) = \sum_{n_h=1}^{\infty} B_n \sin \left(\frac{\pi n_h z_h}{H}\right)
\]  

(7)

Substitution of the Equation (7) at Equation (4) and Equation (6) provides the following system of secular equations for unknown coefficients of the Fourier expansions:

\[
\left(\frac{\pi^2 n^2}{\mu_e H^2}\right)C_n + \sum_{n'=1}^{\infty} V_1(n,n')C_n' = E_e(z_h) \cdot C_n; \ \left(\frac{\pi^2 n^2}{\mu_h H^2}\right)B_n + \sum_{n''=-\infty}^{\infty} V_2(n,n'')B_n'' = E_e(z_h) \cdot B_n''
\]  

(8)
\[ V = 10 = d, I = 4 \]

3. Results

In order to analyze the effect of the electric and magnetic fields on the polarizability of the trapped exciton in type II conical nanocone, we have first performed numerical calculations for the exciton lowlying energy levels as functions of the external electric field. For our calculations, we choose the geometrical parameters, the bottom and the top radii \( R_b = 10 \text{ nm}, R_t = 9 \text{ nm} \) and the cone’s height \( H = 50 \text{ nm} \), respectively. In Figure 2, we display the exciton energies as functions of the external electric field obtained by solving the eigenvalue problems (8) for two different values of the external magnetic fields applied along the symmetry axis. Lowest energies of the exciton states in the adiabatic approximation depend on the electron angular momentum \( l_e \) and the hole’s axial quantum number \( n_h \), i.e. \( E_X = E_X(l_e, n_h) \). In the zero-magnetic-field, in Figure 2(a) the electron circular paths around cone’s lateral border, in all states with different angular momenta begin to climb under the increasing electric field, maintaining the sequence of the energy levels with different quantum numbers \( l_e \). The greater \( l_e \), the greater is the contribution of the centrifugal term in the total energy of the corresponding state. Therefore, all states with lower energies in Figure 2(a) have angular momenta \( l_e = 0 \) or \( l_e = 1 \).

An essential reordering of the energy levels happens in the presence of the magnetic field, as a result of AB effect. In Figure 2(b) it is observable the lowest energies with different angular momenta up to \( l_e = 6 \). Such reordering of the energy levels in conical-shaped nanostructure has been recently explained [7,8] by the interplay between forces induced by three terms in the Hamiltonian, centrifugal, paramagnetic and diamagnetic. In the presence of the magnetic field, the electron trajectory with different angular momenta form aligned tracks in a sequence of horizontal circular loops, climbing one by one under the increasing magnetic field in ascending order of the angular momentum, from the cone’s bottom to its top. Unlike the electron, the heavy hole, confined inside the cone, has a very weak response to external fields and it remains close to the bottom of the cone. Therefore, external electric and magnetic fields increase the separation between the electron and the hole providing the formation of a permanent electric dipole moment.

**Figure 2.** Exciton energies as functions of the electric field.

In Figure 3(a) and Figure 3(b) we display results of calculation of dipole momenta for different exciton states as functions of the electric field. The dependence of the dipole moment on the external electric field exhibits in all cases a drastic variation of the polarizability as the electric field surpasses a critical value. When the electric field is weak, the electron and the hole are located close to the bottom of the cone being held by electrostatic attraction, but if the electric field becomes larger than a critical
value, the electron jumps along the lateral border of the cone toward the cone’s top, while the heavy hole remains close to the bottom. The jump of the electron can be additionally facilitated by the applying of the external magnetic field, which by compressing the circular tracks also pushes the electron upwards.

In Figure 3(a) and Figure 3(b), we can observe how an increase of the magnetic field allows us to diminish the critical value of the electric field associated with the formation of the giant permanent electric dipole moment.

Thus, the applying of the magnetic field additionally increases the polarizability of the structure facilitating on this way the separation between the electron and the hole induced by the electric field. It is expected a reciprocal effect, in which the increasing magnetic field were able to induce by itself an abruptly growing electric dipole moment, forced by the jump upwards of the electron under the magnetic confinement, which in addition could be controlled by the applying of the electric field.

Results of calculation of the dipole moment for different exciton states as function of the magnetic field, are presented in Figure 3(c) and Figure 3(d) in the presence of the electric fields applied at two opposite directions. In both cases, it is observable the existence of the phase transition between states with the small and the giant dipole moments when the magnetic field surpasses a critical value. We consider that it is a manifestation of the abrupt magnetoelectric polarization, related to jumps of the electron's orbits, encompassing the lateral border of the cone with different angular momenta, induced by the growing magnetic field. It is seen that the position of the critical point depends strongly on the direction of the applied electric field and therefore the electric field can be used for shifting the critical value of the magnetic field that generate the phase transition in the structure, as well as the magnetic field can be used to shift the critical value of the electric field that generate a giant dipole.

![Figure 3](image-url)
4. Conclusions
We show the existence of abrupt changes in the curves of the dependencies of the electric dipole moment on external electric and magnetic fields accompanied by the formation of the giant permanent electric dipole moment for strong electric and magnetic fields. We associate this effect with the interplay between the centrifugal and the electrostatic attraction forces pushing the electron circular orbits toward the cone’s bottom, and the diamagnetic and electric forces induced by the external fields forcing them to climb toward the cone top. Our theoretical analysis reveals a possible existence of the magnetoelectricity in type II nanostructures induced by the quantum-size confinement of the carriers.

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