

# Magneto-electric effect in non-uniform quantum nanotube

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**Abstract.** A model of non-uniform core-shell type nanostructure with a donor located at a bottleneck point of the core is considered. It is shown that such structure can have a giant polarizability, which, besides can be controlled by applying of the external magnetic field. Presented theoretical analysis reveals a new possibility for the coupling between the polarization and magnetization arising from the quantum-size effect in non-uniform semiconductor nanowires.

## 1. Introduction

Nanostructures with tubular architecture have exceptional physical properties of great interest for potential applications in electronic devices, solar cells, and sensing. The ring-like geometry of these structures offers an opportunity for controlling their spectral and electrical properties by applying of an external magnetic field. On the other hand, their reduced dimensionality along the axis retains electric carriers within a narrow conducting channel, making them very sensible to the external electric field. One could expect that the combination of these properties offer an additional possibility in device design related to control of the magnetization or polarization by an electric field or magnetic field. Different techniques of crystal growth have been used to fabricate narrow GaAs/AlAs and InAs/GaAs nanotubes (NTs) [1-3], which, as it has been demonstrated, exhibit in their photoluminescence spectrum the Aharonov-Bohm (AB) oscillations in the presence of the external magnetic field [4]. Earlier, it has been also reported on fabrication of non-vertically aligned GaN/GaP core/shell nanowires with variable cross section dimensions [5, 6].

The charge probability distribution along the symmetry axis of the excessive electron inside a NT with variable radius in the ground and excited states is nonhomogeneous, the narrower is the cross section the smaller is the probability for finding the electron close to this point. However, the distribution can be easily changed in the presence of the external and the electric field due to a high electric and magnetic polarizability of such structure. In this paper, it is presented a theoretical analysis of a possibility for designing a tubular architecture with a giant electric polarizability, which besides can be controlled by the external magnetic field.

## 2. Theoretical model

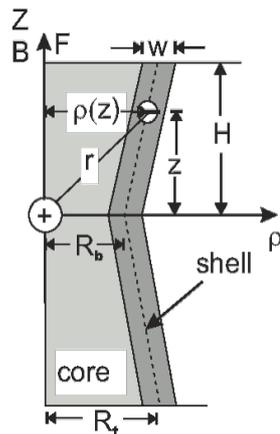
To this end, below it is considered a model of axially symmetric nanowire with the core/shell type heterojunction, and with a shape of the vertical cross-section along the symmetry axis, schematically represented in Figure 1. In this model, the shell region presents a tube-shaped quantum well with variable radius, capable to trap the excessive electron, released from the on-axis donor, located at the bottleneck point. The corresponding geometrical parameters of the structure are the height,  $H$  the centreline radius



$R_b$  at the bottleneck, the centreline radius  $R_t$  at extreme points of the tube, and the shell thickness  $W$ . The external fields, applied parallel to the  $Z$ -axis, are magnetic  $B$  and electric  $F$ . In this model, the shell region presents a tube-shaped quantum well with variable radius, capable to trap the excessive electron, released from the on-axis donor, located at the bottleneck point. The shell layer along the core's lateral frontier regarded below as an infinite-barrier antidot, presents a narrow cylindrical nanotube with the centreline radius depending on the coordinate  $z$  as follows:

$$R_c(z) = R_b + (R_t - R_b) \cdot |z/H|^n; \quad n = 1, 2 \quad (1)$$

The core/shell frontier presents a hard wall for the electron is located within the quasi-2D region defined in cylindrical coordinates as  $\{R_c(z) - w/2 < \rho < R_c(z) + w/2; 0 < \varphi < 2\pi; 0 < z < H\}$ , in which the electron circulates around the core, encompassing the cone's lateral surface. The electrostatic attraction and the external magnetic field  $B$  press the electron circular tracks toward the bottleneck point while the external electric field  $F$  and the structural confinement push them toward one of two extreme points of the structure. The competition between these two groups of forces can change drastically the electron-donor separation resulting in the inducing of a giant dipole momentum.



**Figure 1.** Vertical cross-section of the nanowire with core/shell type junction and with on-axis donor.

In our calculations there are used effective Bohr radius  $a_0^* = \sqrt{2\epsilon/m^*} e^2$  and the effective Rydberg,  $R_y^* = e^2/2\epsilon a_0^*$  as units of the length and energy, while the values  $\xi = eF a_0^*/R_y^*$ ;  $\gamma = e B/2m^* R_y^*$  as dimensionless parameters of electric field  $F$  and magnetic field  $B$ , respectively, being  $m^*$  the electron effective mass and  $\epsilon$  dielectric constant of the shell material parameters. By using the adiabatic approximation [7,8] and considering the ratio  $w/R_c(z)$  as a small parameter one can represent wave functions for low-lying energy levels as follows:  $\Psi_m(\rho, \varphi, z) = e^{im\varphi} \phi(\rho) f_m(z)$ ;  $m = 0, \pm 1, \pm 2, \dots$ . Here  $m$  is the  $Z$ -projection of the angular momentum,  $\phi(\rho)$  is the radial eigenfunction corresponding to the lowest energy in the circular 2D ring of the width  $w$  and the radius  $R_c(z)$ , while the axial part of the wave function  $f_m(z)$  in the limit  $w/\rho_c(z) \rightarrow 0$  is the solution of the one-dimensional boundary problem with the adiabatic potential  $V_{eff}(z)$ :

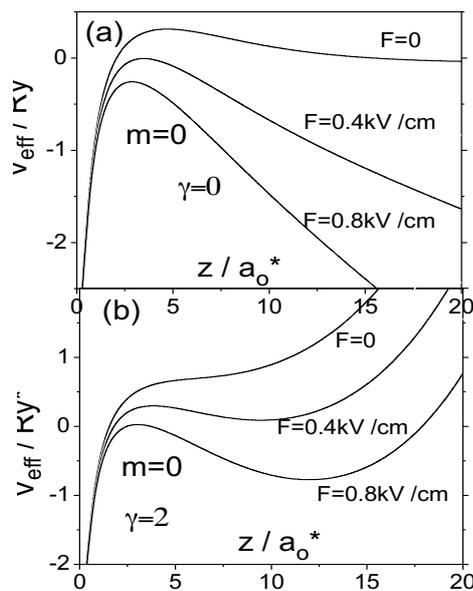
$$-f_m''(z) + V_{eff}(z) f_m(z) = E_m \cdot f_m(z); \quad -H < z < H; \quad f_m(\pm H) = 0 \quad (2a)$$

$$V_{eff}^{(m)}(z) = \xi \cdot z + (m^2 + 1/2) / R_c^2(z) + \gamma^2 \cdot R_c^2(z) / 4 - 2 / \sqrt{z^2 + R_c^2(z)} - \gamma \cdot m \quad (2b)$$

### 3. Results and discussion

Eigenvalues of Equation (2) are found by means of the numerical trigonometric sweep method [9,10]. Results, presented below are given for the structure with parameters,  $R_b = 1a_0^*$ ,  $R_t = 4a_0^*$  and  $H = 20a_0^*$ . The type of the tube's profile no homogeneity in our model (1) is given by the parameter  $n$ . Below, the profile is called as linear if  $n = 1$  and parabolic if  $n = 2$ . In presented below calculations dimensionless units typical for GaAs material  $a_0^* \approx 1nm$ ,  $Ry^* \approx 6meV$  are used.

Classical electron paths present circular horizontal tracks whose radii  $R_c(z)$  depend on the distance  $|z|$  from the bottleneck point, given by the minimum position  $z_{min}$  of the adiabatic potential (2b). The stationary point position  $z_{min}$  in accordance with Equation (2b) is defined by interplay between two groups of forces. One of them is induced by the external electric field and the centrifugal force, both pushing the electron toward one of two extremes, and other induced by the magnetic confinement and the Coulomb attraction to the donor that drive the electron toward the bottleneck point  $z = 0$ . Analyzing the displacement of  $z_{min}$  provided by external fields one can give a simple interpretation of the spectral, electric and magnetic properties of this structure. In Figure 2 it is presented the curves of the adiabatic potentials  $V_{eff}^{(0)}(z)$  for states with zero angular momentum ( $m = 0$ ), for two different magnetic fields  $\gamma = 0$  and  $\gamma = 2$ , and for three different values of the electric field. At the zero magnetic field case ( $\gamma = 0$ ) the potential curves presented in Figure 2(a) have two minima, one deep main minimum, close to the donor ( $z = 0$ ) and other, the shallow minimum located at the extreme of the NT ( $z = H$ ). As the electric field increasing surpasses the value  $F = 0.5kV/cm$ , the second minimum becomes more profound, while the electron in its ground state is jumped from the bottleneck point ( $z = 0$ ) up to the tube extreme ( $z = H$ ), generating in this way a giant dipole momentum.



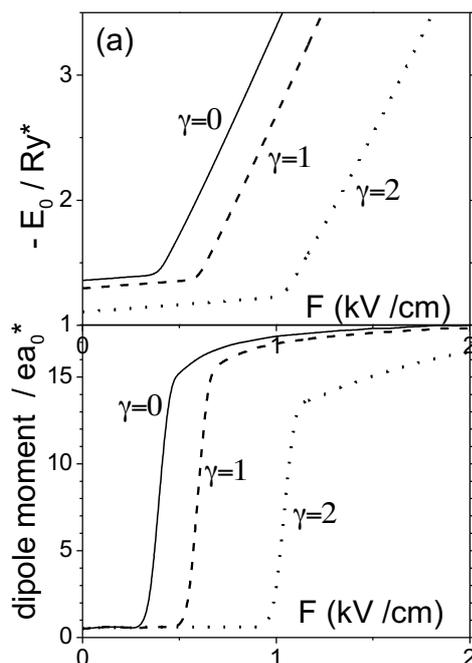
**Figure 2.** Adiabatic potential along symmetry axis of the nanotube with linear profile in the presence of external fields.

The shape of the potential curves is changed essentially in the presence of the magnetic field as it can be seen from Figure 2(b), where similar results for  $\gamma = 2$  are shown. If the electric field pushes the electron toward the tube's extremes, the diamagnetic confinement (the third term in Equation 2(b) drives it toward the bottleneck point and therefore under increasing external magnetic field the second minimum in the adiabatic potential in Figure 2(b) is successively displaced in the direction of the bottleneck point. Such modification of the adiabatic potential under external field affected also the charge distribution in the ground state of the structure. In Figure 3(a) are presented results of calculation of the electron ground state energy  $E_0$  as function of the electric field, found by solving eigenvalue problem (2). For small electric field the ground state energy is almost constant about  $1Ry^*$  due to the fact that the electron-donor separation remains unchanged until  $F$  increasing reaches a critical value. As  $F$  further increases, the electron-donor separation is changed abruptly and the energies begin to grow linearly with a sharply increased slopes. In Figure 3 the curves are presented for three different values of the external magnetic field applied at the same direction. The larger applied magnetic field, the greater is the critical value of the electric field at which the charge distribution and the slopes of curves are changed significantly.

In Figure 3(b) it is presented the electric moment  $d$  of the structure at zero temperature as function of the electric field calculated by means of the numerical derivation of the ground state energy  $E_0$  accordingly to the relation:

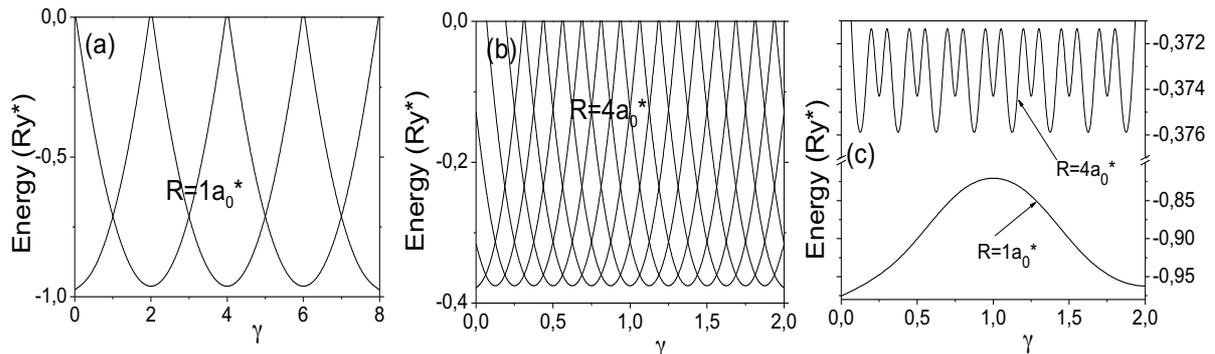
$$d = -ea_0^* \cdot \partial E_0 / \partial \xi \quad (3)$$

It is seen that the value of the dipole moment of the structure for small electric field corresponds to the electron-donor separation about  $1a_0^*$  and rises abruptly up to a value corresponding to a giant electron-donor separation close to  $20a_0^*$ , as the electric field exceeds its critical value. The value of the critical electric field can be changed by applying the magnetic field. As the magnetic field increased, the jump of the curves of the dipole moment dependency becomes smoother. The curves presented in Figure 3 point out a possibility of the existence of the magnetoelectric effect in nanostructures with tubular architecture.



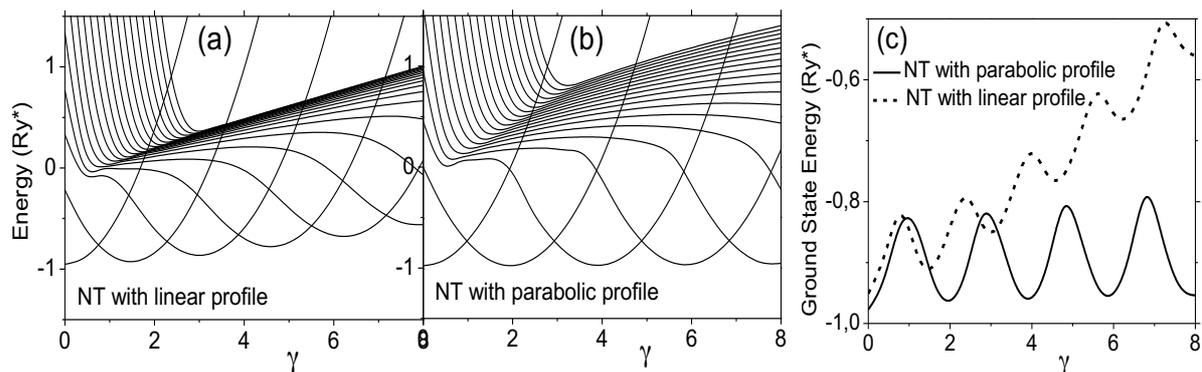
**Figure 3.** (a) Ground state energy and (b) Dipole moment as functions of the external electric field, given for three different values of external magnetic field.

Other manifestation of the quantum-size magnetoelectric effect in tubular nanostructures one could reveal by analyzing AB oscillations of the energy levels in the presence of the external magnetic field. AB oscillations of energy levels in homogeneous tubes are similar to those in one-dimensional quantum, where the period of the oscillation of the ground state energies  $\Delta\gamma$  depends on the radius  $R$  as  $\Delta\gamma = 2/R^2$ . One can observe in Figure 4 AB oscillations of the eigenvalues  $E_m$  of the Equation 2 for some lower levels  $m = 0, \pm 1, \pm 2$ , in uniform nanotubes with radii  $R = 1a_0^*$  and  $R = 4a_0^*$ , where periods of oscillations are equal to  $\Delta\gamma = 2$  and  $\Delta\gamma = 1/8$ , respectively.



**Figure 4.** Lower energies as functions of the external magnetic field in uniform nanotubes with radii: (a)  $R_c = 1a_0^*$  and (b)  $R_c = 4a_0^*$ . In (c) the comparison of the oscillations of the ground state energy in nanotubes with different radii are shown.

In order to demonstrate that the shape of the AB oscillation in tubes with non-uniform profiles are changed essentially, in Figure 5 are shown the lower eigenvalues of the problem (2) as functions of the external magnetic field for the zero-electric field case and for two type of profiles, linear ( $n = 1$ ) and parabolic ( $n = 2$ ) with parameters  $R_b = 1a_0^*$ ,  $R_t = 4a_0^*$  and  $H = 20a_0^*$ .

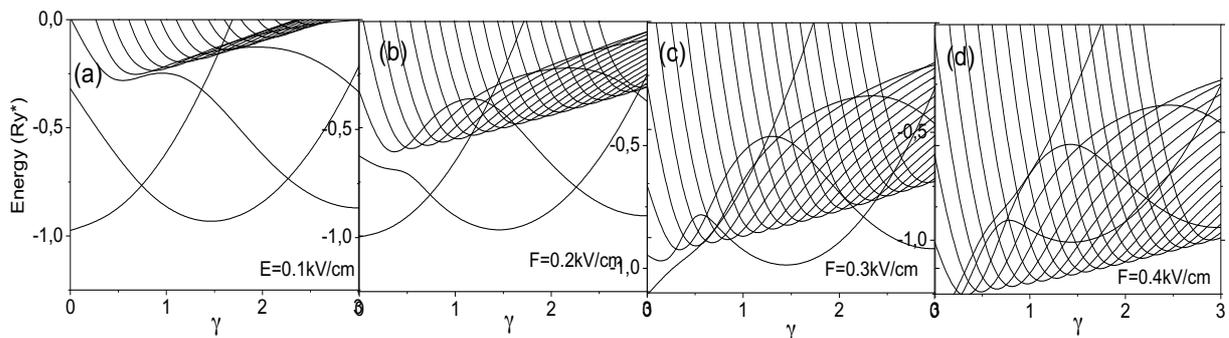


**Figure 5.** Lower energies as functions of the external magnetic field in non-uniform nanotubes with parameters  $R_b = 1a_0^*$ ,  $R_t = 4a_0^*$  and  $H = 20a_0^*$ , for (a) linear profile, (b) parabolic profile and (c) comparison of the oscillations of the ground state energy in tubes with different profiles.

It is seen that in both cases the period of oscillation of the lowest energy level is equal to  $\Delta\gamma = 2$ , coinciding with the corresponding value for the 1D quantum ring of the radius  $R_b = 1a^*$ . This result demonstrates that in the zero electric field case the electron is mainly localized close to the bottleneck point  $z = 0$ . In spite of a general similarity of the curves of the AB oscillations for both types of profiles one can see particular differences on their magnetic field dependencies. The comparison of the curves

for the excited states in Figures 5(a) and 5(b) reveals that unlike the linear profile for which all excited states in the high magnetic field becomes almost degenerated, the splitting between excited states in nanotubes with parabolic profile remains meaningful for all magnetic field values. There is also a significant difference in the magnetic field dependence of the ground state energies of these two types of non-uniform profiles, as it can be seen from Figure 5(c). One can observe a similarity of the oscillations of the ground state energy in Figure 4(a) for the uniform NT of radius  $R = 1a_0$  \* and for non-uniform NT with the parabolic profile in Figure 5(c), the periods and amplitudes of the NT oscillations in both cases are practically equals. Unlike, for non-uniform NT with linear profile the AB oscillation of the ground state energy level in Figure 5(c) exhibits a weakly reduced amplitude and increased period and a linear trend with slope different of zero. These differences are associated with a significantly larger separation, existing between the donor and electron in the excited states in the non-uniform structure with linear profile, in comparison with one in the parabolic profile structure.

One can expect that the curves of the AB oscillations should be very sensible to applying the external electric field, which by forcing the electron to move away the donor also makes to rise its rotation radius. In Figure 6, there are presented lower energies as functions of the external magnetic field in non-uniform NT with linear profile for four different values of the external electric field.



**Figure 6.** Successive transformation of curves of the Aharonov-Bohm oscillations under increasing electric field in non-uniform nanotube with linear profile.

It is seen that there is two group of the curves of the energies dependencies with different periods of the AB oscillations, equal approximately to  $\Delta\gamma = 2$  and  $\Delta\gamma = 1/8$ , respectively. The first group with the large period of the oscillation can be attributed to the states with small dipole momenta when the electron is located close to the bottleneck point  $z = 0$ , while the second group corresponds to states with large dipole momenta as the electron is located close to the end of the NT. One can observe in Figure 6 a successive convergence of these two groups of levels with increase of the electric field when the electric field is grown from zero to 0.3kV/cm. As the electric field further increases and exceeds a critical value, the period of the AB oscillations is dropped abruptly, from  $\Delta\gamma = 2$  to  $\Delta\gamma = 1/8$ . In this way, by applying the external electric field it is possible to change also magnetic properties of the structure.

#### 4. Conclusions

A simple model, in which on-axis donor is located at the bottleneck point of structure, is considered in order to analyze the effect of the electric and magnetic fields applied along the symmetry axis of non-uniform nanotubes on their spectral, electric and magnetic properties. It is revealed that such structure can exhibit a giant polarizability under external electric field, which besides can be controlled by applying additional magnetic field. The analysis of the Aharonov-Bohm oscillations under external electric field reveals their significant sensibility to applied external electric field that can change magnetic properties in this structure abruptly. Our theoretical analysis predicts a possibility of the existence of the magnetoelectric effect, arising from the quantum-size effect in non-uniform nanotubes.

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