

Effect of variation of the central-hole depth and the axial anisotropy on the AB oscillations in a wide nanoring

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Abstract. The effect of the external magnetic field on the spectral properties of one-electron non-uniform quantum ring with radially directed hills is analysed. The corresponding one-particle wave equation is separable in the adiabatic limit, when the layer thickness is essentially smaller than its lateral dimension. Our calculations show that the presence of a single axially directed hill as well as a rise of the central hole thickness produce a quenching of the Aharonov-Bohm (AB) oscillations of the lower energy levels and of the magnetic momentum. However, as the number of radially directed hills is increased, the system exhibits again oscillations, resulted from an enhancement of tunnelling circular currents.

1. Introduction

The development of new semiconductor growth techniques has made possible the fabrication of the self-assembled quantum rings (QRs) which in the presence of the magnetic field exhibit an interesting quantum-interference phenomenon, denominated AB effect [1]. Theoretical analysis of this phenomenon reveals its delicate nature related to a destructive interference induced by a possibility to appearance of multiple different spatially separated paths in QR under a diminishing of the central-hole dimension or any non-uniformity that breaks the axial symmetry [2,7]. This destructive interference disappears if the ring is sufficiently narrow, and uniform. However, further numerical analysis of more realistic 3D model of non-uniform crater-like QRs shows that, although the real QR shape differs strongly from an idealized circular-symmetric narrow ring structure, AB-type oscillations in the magnetization survive [8,10].

A 3D exactly solvable model of the crater-like one-electron QR, proposed recently in reference [11,12] provides an explanation of the stability of the AB oscillations with respect to structural non-uniformities. In the presence of the magnetic field applied along the symmetry axis, more probable electron paths in this model are clustered close to the crater's rim being similar to those in quasi-one-dimensional quantum rings independently on the crater width. However, any slight non-uniformity produced by a single radially directed valley or single hill suppresses the oscillations of several lower levels due to the localization of the corresponding rotational states. Nevertheless, when the non-uniformity becomes substantial due to the presence of multiple valleys and hills, the AB oscillations generated by the external magnetic field becomes again possible owing to the electron tunnelling through thin potential barriers.

It is possible to extend the model considered in reference [11,12] in order to analyse additionally the effect of the variation of the width and the depth of the central-hole on the AB oscillations. In this extended model, proposed in this paper, the crater's height between the central hole and the outer border

grows linearly with different slopes at different radial directions in the case of non-uniform structure, while the corresponding slopes in the central-hole at all radial directions are zero. By varying the depth and the radius of the central hole in this model, one can analyse a successive change of the spectral and magnetic properties during a transformation of the nanostructure morphology, from disk-like to ring-like.

2. Theoretical model

It is considered a model of a crater-like non-uniform QD as a thin layer whose thickness d depends on polar coordinates (ρ, φ) as:

$$d(\rho, \varphi) = [h_a \vartheta(\rho_a - \rho) + h_b \rho / \rho_b \vartheta(\rho - \rho_a)] \vartheta(\rho_b - \rho) / \sqrt{1 + \sigma(\rho / \rho_b)^2 f^2(\varphi)}; \quad h_a = h_b \rho_a / \rho_b; \quad (1)$$

Here $f(\varphi) = \sin p\varphi$, $p = 1/2, 1, 2, \dots$ and $\vartheta(x)$ is Heaviside step function, equal to zero, for $x < 0$ and to one, for $x > 0$; h_a is the layer thickness at the bottom of the crater and ρ_a is the radius of the central hole and h_b, ρ_b are corresponding values for height and radius of outer border of the isotropic crater. In the relation (1), the parameter σ and the function $f(\varphi)$ describe the degree and the type of the anisotropy of the crater, respectively. As $p = 1/2$, the structure has a single radially directed hill, as $p = 1$ two radially directed hills, separated by two valleys, as $p = 2$ four hills, etc. In Figure 1 can be observed examples of 3D images of corresponding models of layers with profiles given by the relations (1) for $\sigma = 1$ and $p = 1, 2$, or 4.

In order to simplify our numerical analysis in what follows, it is considered a model with the infinite-barrier confinement potential $V(\mathbf{r})$, which is supposed to be equal to zero inside the crater and to infinity otherwise. The external homogeneous magnetic field $\mathbf{B} = B \hat{z}$ is applied along the Z-axis. The effective Bohr radius $a_0^* = \hbar^2 / m^* e^2$, the effective Rydberg $R_y^* = e^2 / 2\epsilon a_0^*$ and $\gamma = e B / 2m^* c R_y^*$ as units of length, energy and the dimensionless magnetic field strength are used below, being m^* the electron effective mass and ϵ the dielectric constant.



Figure 1. 3D images of non-uniform quantum ring with morphology given by the relation (1).

As the thicknesses of actual self-assembled QDs manufactured up to now are much smaller than their lateral dimensions one can take advantage of the adiabatic approximation assuming a model with infinite-barrier confinement. In framework of this approximation, the fast movement of the electron along the Z-axis inside the layer is supposed to be independent on its in-plane slow displacements [13,15]. Therefore, the ground state energy for each the electron in-plane position given by polar coordinates (ρ, φ) , given by the well-known expression corresponding to infinite-barrier quantum well of width $d(\rho, \varphi)$, in dimensionless units is:

$$E_z(\rho, \varphi) = \pi^2 / d^2(\rho, \varphi) \quad (2)$$

Following the adiabatic approximation procedure, one can consider afterwards the in-plane electron motion as 2D problem with additional adiabatic potential given by this function. The renormalized 2D Hamiltonian describing in the effective-mass approximation the in-plane electron slow motion inside the layer with profile given by Equation (1) in the presence of the adiabatic potential (2) and the magnetic field applied along Z- axis has the following form:

$$H = -\Delta_{\rho,\varphi} - i\gamma \frac{\partial}{\partial \varphi} + \frac{\gamma^2 \rho^2}{4} + \frac{\pi^2}{h_a^2} \left(1 + \left(\frac{\rho}{\rho_a} \right)^2 \right) \vartheta(\rho_a - \rho) + \sigma \frac{\pi^2 f^2(\varphi)}{h_a^2} \left[\left(\frac{\rho}{\rho_a} \right)^2 \vartheta(\rho_a - \rho) + \vartheta(\rho - \rho_a) \right] \quad (3)$$

For the uniform crater ($\sigma = 0$) eigenfunctions of the Hamiltonian (3) depends on two quantum numbers, radial $n = 1, 2, 3, \dots$ and angular $m = \pm 1, \pm 2, \pm 3, \dots$ and they can be found exactly in a form of the linear combination of Hypergeometric confluent functions. The energies $E^{(0)}(n, m)$ and the wave functions $\phi_{n,m}(\rho)$ of the uniform crater, found by solving the transcendental equation, can be used further to calculate the matrix elements $\langle \phi_{n,m} | U | \phi_{n',m'} \rangle$ of the perturbation U induced by the non-uniformity and given by the relation (3). Resulting matrix elements of the Hamiltonian for non-uniform crater are:

$$\begin{aligned} \langle \phi_{n,m} | H | \phi_{n',m'} \rangle &= E^{(0)}(n, m) \delta_{n,n'} \delta_{m,m'} + \langle nm | \eta | n'm' \rangle (2\delta_{m,m'} - \delta_{m,m'+2p} - \delta_{m,m'-2p}) \\ \langle n | \eta | n' \rangle &= \frac{\pi^2 \sigma}{4h_a^2} \left[\int_0^{\rho_a} \phi_{n,m}(\rho) \phi_{n',m'}(\rho) \left(\frac{\rho}{\rho_a} \right)^2 \rho d\rho + \int_{\rho_a}^{\rho_b} \phi_{n,m}(\rho) \phi_{n',m'}(\rho) \rho d\rho \right] \end{aligned} \quad (4)$$

In what follows, the results of calculation of some lower energies $E_m(\gamma)$ corresponding to radial quantum number $n = 1$ and of the magnetic moment $p_m(\gamma)$ at zero temperature, as functions of the magnetic field γ , are presented. The magnetic moment $p_m(\gamma)$ at zero temperature, one can calculate according to the Hellmann-Feynman theorem, as follows:

$$p_m = -\mu_B \frac{\partial E_1}{\partial \gamma} \quad (5)$$

3. Results and discussion

The geometrical parameters used below are: a typical value for the InAs/GaAs material effective Bohr radius $a_0^* \approx 10nm$, the outer radius $\rho_b = 20nm$ and the height of crater at the rim $h_b = 4nm$, dimensions close to those of crater like QDs fabricated earlier by means of the droplet epitaxial technique [16,18]. The layer thickness at the bottom of the crater is considered as variable between $h_a = 1nm$ and $h_a = 3.5nm$.

In order to facilitate the interpretation of numerical results, it has been found the electron density distribution in a simple model with infinite-barrier confinement and in crater-like uniform InAs/GaAs structures with profile given by the relation (1) for $\sigma = 0$, by using the software of COMSOL MULTIPHYSICS (v.5.1) [19]. At first row of Figure 2, it is presented contour plots of the radial charge distribution in a plane through the axis of symmetry of uniform craters with central-hole thicknesses $h_a = 1, 2$, and $3.5nm$, calculated for infinite-barrier model, while at the second row are shown a similar result, obtained for the finite barrier model, using material parameters of InAs and GaAs.

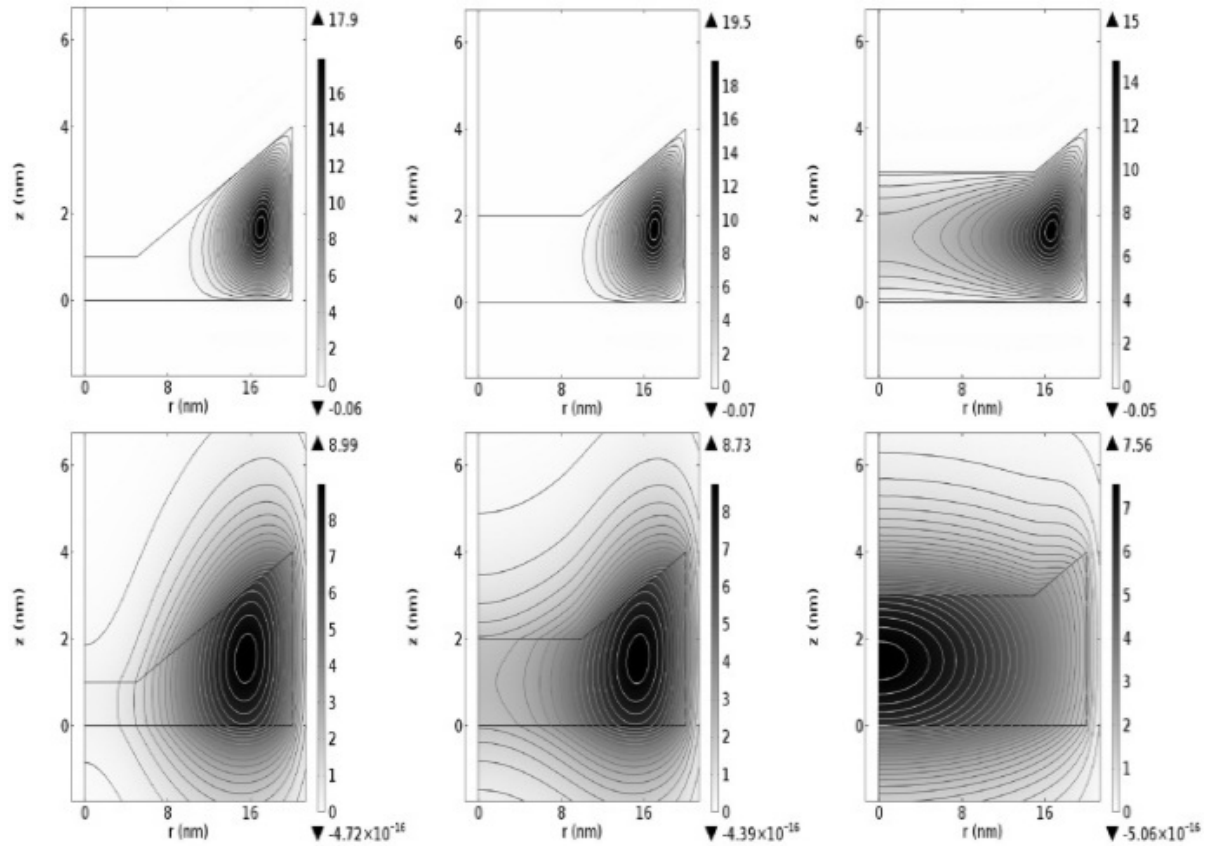


Figure 2. Contour plots of the density of the radial charge distribution in a plane through the axis of symmetry of uniform craters with three different central-hole depths in the ground state calculated for models with infinite (first row) and finite (second row) barrier heights.

For h_a less than 3.5nm, one can observe AB oscillations of energy levels, typical for a 1D ring-like structure, which generate multiple crossovers between the curves with different magnetic quantum numbers m . As it is well known, the period of AB oscillations, $\Delta\gamma$ in 1D QR of the radius R is equal in dimensionless units to $\Delta\gamma = 2/R^2$. According to this estimation, AB oscillations of energy levels at the first column of Figure 3 at the crater with the layer thickness in central hole region $h_a = 2\text{nm}$ are similar to one-dimensional QR of radius $R = 18.3\text{nm}$, those at the second column for $h_a = 3\text{nm}$ to a QR with radius $R = 17.3\text{nm}$, while at the third column for $h_a = 3.5\text{nm}$ AB oscillations are absent. It is largely consistent with results of calculation of the charge distribution presented in Figure 2, where one can see that for $h_a < 3.5\text{nm}$, 80-90% of the electric charge is localized inside a narrow region close to the outer border, while for $h_a \geq 3.5\text{nm}$ the electric charge leaks inside the central-hole region. It results in transformation of the ring-like charge distribution in the disk-like one. When initially h_a grows from 2nm to 3nm the maximum of the density is displaced slightly toward the border, the confinement is increased and the averaged value of the electron rotation radius is enlarged.

A rise of the energy band bottom and an increase of the period of the AB oscillation in Figure 3 is associated with such change of the charge distribution. For $h_a \geq 3.5\text{nm}$ the electron configuration becomes rather similar to one of the disc-like structure for which there are no the AB oscillation of the energy levels.

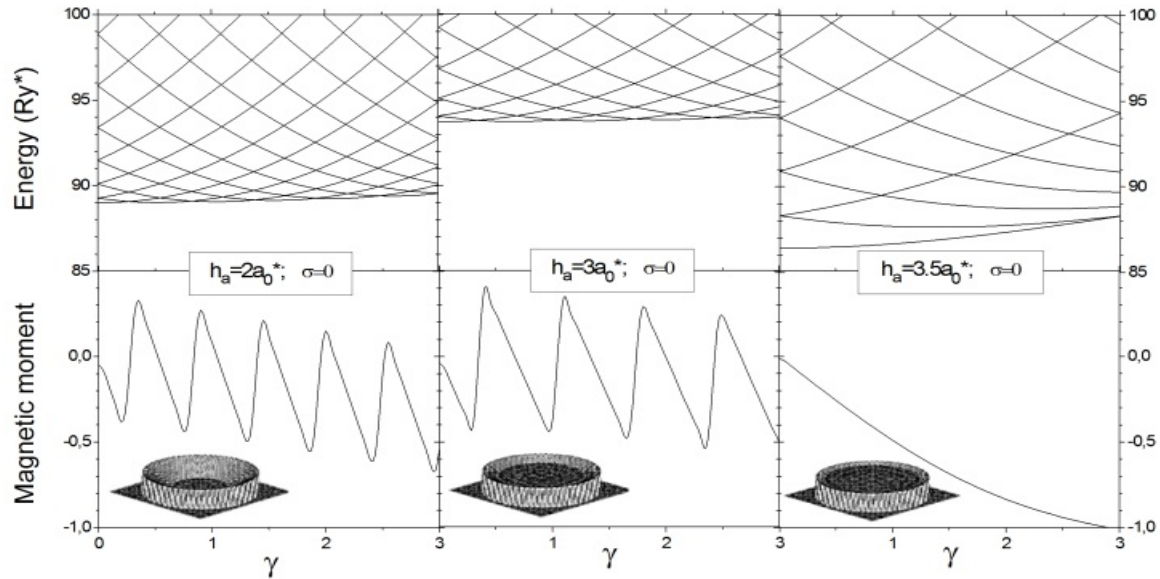


Figure 3. Lower energies (upper row) and induced magnetic momenta (lower row) in one-electron axially symmetrical crater-like QDs as functions of the external magnetic field for three different depths of the central-hole. Corresponding images are shown at the bottom of the Figure.

In Figure 4 similar curves are presented for wide axially non-uniform QRs, whose morphology is given by the layer thickness dependency specified by the relation (1) with parameters, inner and outer radii and thicknesses $h_a = 1nm$, $\rho_a = 5nm$ and $h_b = 4nm$, $\rho_b = 20nm$, respectively. In the first row is displayed the energies dependencies on the external magnetic field in the uniform crater ($\sigma = 0$) and in non-uniform structures with one, two and four radially directed hills, corresponding to parameters $p = 1/2$, $p = 1$, and $p = 2$, respectively, for $\sigma = 0.01$ in the relation (1). Similar dependencies for induced magnetic momenta are observed in the second row of Figure 4.

In Figure 4 is shown a similarity of the curves of the energies dependencies on the magnetic field for upper energy levels, which are due to rotational states. The electron density distribution in these states is practically insensible to the structural non-uniformity due to the fact, that the energy of the electron in these states are superior than the heights of barriers generated by the axial non-uniformity. On the contrary, the magnetic field dependencies of five lower levels and the magnetization in the single-hill structure ($p = 1/2$) in Figure 4 do not exhibit any oscillation, such as observed in the second column of Figure 4.

This effect is attributed to a localization of the lower rotational states, induced by single hill-type non-uniformity, and to relate to this localization insensibility to the external magnetic field.

It is seen also, that these lower energies in the third and fourth columns, for cases of non-uniform craters with two ($p = 1$), and four ($p = 2$) hills, are clustered inside separated bands with two and four levels in each one, respectively. The presence of a single radially directed hill in the crater produces an effective adiabatic potential with a wide barrier that impedes a cyclic displacement of the electron with a low energy along the rotational path. With a growth of the number of the hills, the potential barriers along circular paths between adjacent hills become narrower.

The bigger the number of the hills, the narrower are the barriers for circular paths and the larger is the tunnelling current generated by the external magnetic field. An increase of the tunnelling current provides a growth of the amplitude of the AB oscillations and a clustering of the vibrational levels in separated non-crossing bands, while inside each band one can see in Figure 4 multiple crossovers and reordering of the levels, typical for AB oscillations.

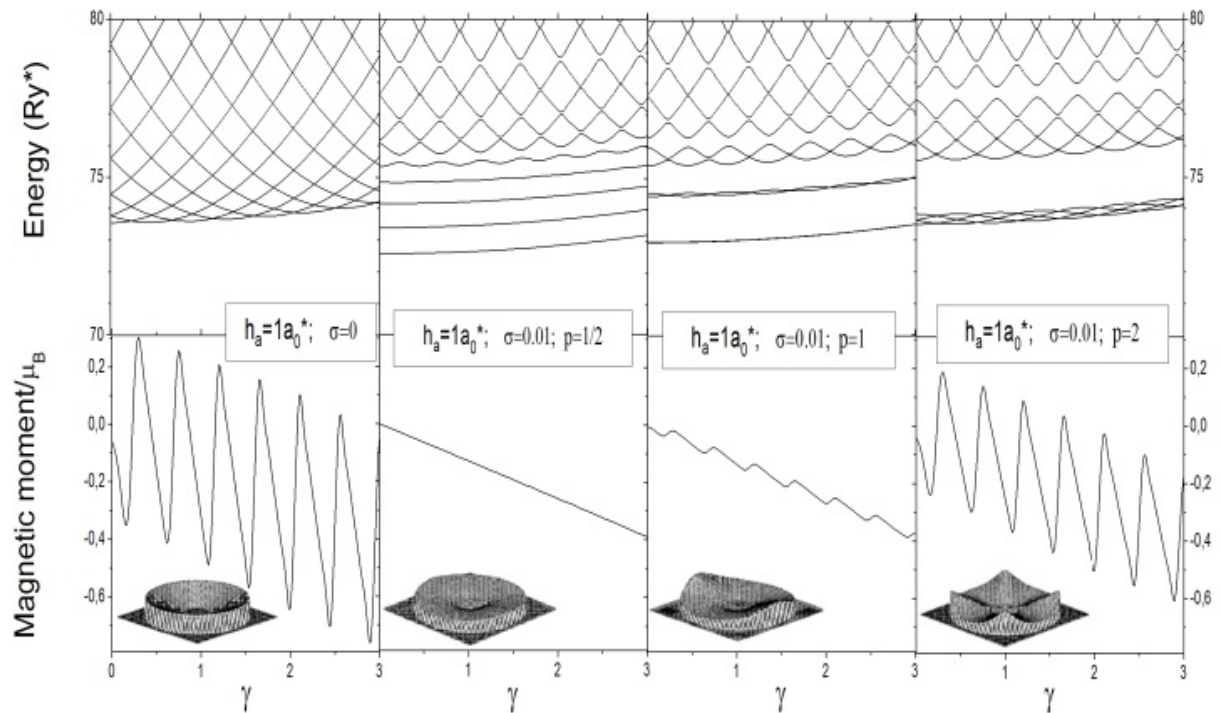


Figure 4. Lower energies (upper row) and induced magnetic momenta (lower row) in one-electron non-uniform crater-like QDs with different number of radially directed hills as functions of the external magnetic field. Corresponding images are shown at the bottom of the Figure.

The period of AB oscillations in the first column of Figure 4 for uniform crater-like wide QR with inner and outer radii 5nm and 20nm, respectively coincides with the corresponding value in 1D QR of the radius 20nm. It means that lines of the circular current induced by the magnetic field in uniform crater goes along the external border. It is interesting that AB oscillations in a non-uniform crater with multiple hills and valleys restored due to induced tunnelling current have the same period of oscillation as it one can observe at the last column of Figure 4. It means that lines of the circular tunnelling current induced by the magnetic field in non-uniform crater also goes along the outer border.

4. Conclusions

In this work is presented a theoretical analysis of the effect of the variation of the depth of the central hole in uniform and in non-uniform crater-like quantum dots on their energies and the induced magnetic momenta dependencies on the external magnetic field applied in the Z-axis direction. To this end is used a simple model of one-electron crater-like quantum dot with ideally circulate inner and outer radii but with non-uniform thickness due to the presence of radially directed hills. It is shown that in the adiabatic limit, when the thickness of the crater grows linearly in all radial directions keeping its value significantly smaller than the outer radius, the energies and wave functions of the electron can be found analytically.

The dependencies of the energies and induced magnetic momentum on the magnetic field in uniform craters reveal the presence of the AB oscillations typical for 1D quantum ring independently of the size of the central hole of the crater until the layer thickness of the central-hole region becomes almost equal to the thickness of the outer border. This result is attributed to a strong confinement that retains the electron in the crater-like structure inside a very narrow circulate region close to the exterior frontier, independently on width of the crater and the value of the external magnetic field, in contrast to the case of nanorings with rectangular cross-sections.

Similar analysis for crater-like non-uniform nanostructures with radially directed hills show that the barriers in the effective adiabatic potential in the regions of the valleys between adjacent hills along the circular paths, provides a localization of the electron in the vicinities of tops of the hills if the electron energy is smaller than barrier height. It has been shown that in the case of the crater-like structure with a single hill, a small non-uniformity of the crater thickness might suppress the electron rotation induced by the external magnetic field in various lower energy states, producing a quenching of the AB oscillations of the corresponding energy levels. The higher the non-uniformity, the bigger is the number of the separated levels whose energies does not depend on the external magnetic field. Its consider that these states (whose energies does not exhibit AB oscillations) as vibrations, localized close to the hill.

It was also found that an increase of the number of hills in a non-uniform crater produces the assembling of the localized states in independent sub-bands. The number of levels inside of each of them coincides with the number of hills in nanostructures, while the dependencies of the energies inside sub-bands on the magnetic field exhibit AB oscillations with crossovers between them, similar to those for extended states. The period of these oscillations, coincide with those for the extended states. These oscillations are attributed to the tunnelling currents generated by the external magnetic field. The bigger the number of the valleys, the larger are tunnelling currents, the wider are these bands, and the higher are the amplitudes of the corresponding AB oscillations. It has been shown that it is due the fact that the increase of the number of the valleys produces a reduction of the wide of the potential barriers between adjacent hills, making easier the tunnelling through narrower barriers along circular paths.

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