



One-electron quantum ring of non-uniform thickness in magnetic field



F. Rodríguez-Prada*, L.F. García, I.D. Mikhailov

Escuela de Física, Universidad Industrial de Santander, A. A. 678, Bucaramanga, Colombia

HIGHLIGHTS

- Model of a one-electron crater-like quantum ring with non-uniform thickness.
- Variations on the ring morphology change its optoelectronic and magnetic properties.
- A small non-uniformity of the crater thickness might suppress the electron rotation.
- The bigger the number of the valleys, the larger are tunnel currents.

ARTICLE INFO

Article history:

Received 8 July 2013

Received in revised form

29 September 2013

Accepted 9 October 2013

Available online 23 October 2013

Keywords:

Nanoring

Aharonov–Bohm oscillation

Crater like Quantum Ring

Non uniform thickness

ABSTRACT

We consider a model of a quantum ring in the form of a thin layer, whose thickness increases linearly between inner and outer radii. We show that in the structural adiabatic limit, when the quantum ring thickness is much smaller than its lateral dimension, the wave equation for the electron confined in such structure can be completely separated. We use analytical solutions found for this model as the base functions for analyzing the effect of the structural non-homogeneity on the electronic spectrum and the Aharonov–Bohm oscillations of the energy levels, in the framework of the exact diagonalization method we found that the pattern of the electron's possible pathways in its displacements generated by the external magnetic field, forms a quasi-one-dimensional region along a guideline marked by a set of highest points of the crater. Therefore, the Aharonov–Bohm oscillations of the energy levels in a crater-shaped quantum dot without non-uniformities are similar to those in 1D quantum ring independently on the crater width. We show that a slight non-uniformity produced by a single valley and single mountain suppresses the oscillations of several lower levels due to the localization of the corresponding rotational states close to the mountain. Nevertheless, when the non-uniformity becomes substantial due to the presence of multiple valleys and mountains, the rotational electron motion and the Aharonov–Bohm oscillations generated by the external magnetic field are restored, owing to the electron tunneling through mountains. We consider that our model of crater-shaped structure would be applicable in the analysis of a variety of more complicated problems related to systems of few carriers confined in nanostructures with ring-like geometry, as a starting point in the framework of the diagonalization method.

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1. Introduction

One of the simplest, and most completely treated recently, fields of application of the effective mass approximation for semiconductor structures is the theory of quantum dots (QDs) with one or two carriers confined inside them. For one-particle QDs with spherical or axial symmetry, the calculations of the energy spectrum can be performed exactly [1]. Besides, two-particle problems for such structures are still relatively simple enough, so that various exact [2] or approximation [3] methods

have been used recently in numerous works to carry out calculations to a high degree of accuracy for two-electron QDs or electron–hole pair confined in quantum dots [4]. QDs hence could furnish an excellent way of testing the validity of the quantum theory of solids. The development of new semiconductor growth techniques have made possible the fabrication of the self-assembled quantum rings (QRs) [5], which in the presence of the external magnetic field manifest a topologically determined quantum-interference phenomenon, known as the Aharonov–Bohm (AB) effect [6,7]. Such effect consists in oscillation of the ground and the excited states energies in the increasing magnetic field applied along the ring axis. But, it is also well-known that the diminishing of the size of the QR's central hole or the presence of any non-uniformity in a quasi-1D QR leads to a partial or total

* Corresponding author. Tel.: +57 7 6344000x2746; fax: +57 7 6332477.
E-mail address: inlogin@gmail.com (F. Rodríguez-Prada).

quenching of the AB oscillation of the energy levels [8,9]. The crucial question arises therefore, whether the manufactured rings, mainly non-uniform volcano-shaped could manifest the AB oscillations, peculiar to an ideally circular ring. As shown in Ref. [10], even though the fabricated quantum dots have in their shape a strong non-uniformity, they still exhibit in the presence of the magnetic field in their spectrum interference, patterns typical for the quantum behavior of electrons in a 1D circular structure. A similar analysis for two-particle QDs is much more complicated. It is known that two-electron problem can be solved exactly only for 1D QRs, or for QDs with parabolic confinement [1–3]. One can use the exact solutions for two-electron QD with parabolic confinement as basis functions for solving a correspondent problem for non-uniform QDs in the framework of the diagonalization method [10]. However, this set of a basis functions is not proper to QDs structures with a central hole. In the present work we propose other set of functions that are exact solutions of the wave equation for a one-particle crater-like QD whose thickness increases linearly between the inner and outer radii with different slopes in different radial directions. We believe that our model could give an explanation of a weak sensibility of the peculiar electronic properties of the rings to the presence of multiple structural defects and the variation of the ring's width.

2. Theory

Recently developed new technique called “droplet homoepitaxy” enables one to fabricate new QR morphologies that may find use in optoelectronic applications [11]. It was shown that the non-uniform stripes in the radial directions are formed due to the presence of the anisotropic strain in the rings fabricated by means of this method [11]. Surface of such heterostructure seems as a crater divided in various regions between radially directed valleys. Therefore we consider below a model of a crater-like non-isotropic QD in the form of a thin layer, in which the dependency of the thickness d on the distance ρ from the axis and polar angle φ is given by the relation:

$$d(\rho, \varphi) = h_0 \rho \vartheta(\rho - \rho_a) \vartheta(\rho_b - \rho) / \sqrt{\rho_b^2 + \sigma^2 \rho^2 f^2(\varphi)}; \quad f(\varphi) = \sin k\varphi \quad (1)$$

here $\vartheta(x) = 0$ for $x < 0$ and $\vartheta(x) = 1$ for $x > 0$ represent the Heaviside step-function, ρ_a and ρ_b are the inner and outer radii of the crater, respectively, σ is the non-uniformity's scale parameter, and $f(\varphi)$ is a fitting function which is selected for modeling an actual volcano-shaped non-uniform structure. As $\sigma = 0$, this relation describes an axially symmetric crater, whose thickness is increased linearly in the radial direction from a minimum value at the central hole frontier up to top value h_0 at the exterior frontier. On the contrary, as $\sigma \rightarrow \infty$ relation (1) describes a non-uniform ring with rectangular cross-sections in all radial directions. In this work we consider a particular case given by the set of three functions $f(\varphi) = \sin k\varphi$ with $k = 1/2, 2, 4$. The schematic images of corresponding morphologies are shown in Fig. 1.

Below, we assume a simple 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. In our calculations we use the effective Bohr radius $a_0^* = \hbar^2 \epsilon / m^* e^2$, the effective Rydberg $Ry^* = e^2 / 2\epsilon a_0^*$ and $\gamma = e\hbar B / 2m^* c Ry^*$ as units of length, energy and the dimensionless magnetic field strength, respectively, m^* being the electron effective mass and ϵ the dielectric constant.

The thicknesses of actual quantum dots manufactured up to now are much smaller than their lateral dimensions. Due to such feature of the QD's morphology one can take advantage of the adiabatic approximation in which the fast movement in the transversal direction of the electron and in its plane slow displacements can be considered in turn [2]. In the framework of this approximation, one should first analyze the fast electron motion in the z direction at different electron's in-plane positions with polar coordinates (ρ, φ) , that are treated as parameters (*cf.* electron motion for fixed nuclear position in molecular problems). Once the correspondent ground state energies $E_z(\rho, \varphi)$ at each in-plane points are found (in our case $E_z(\rho, \varphi) = \pi^2 / d^2(\rho, \varphi)$) then the renormalized 2D Hamiltonian describing the effective-mass approximation of the in-plane electron slow motion in the presence of the magnetic field in QD whose profile is given by Eq. (1) can be written as

$$H(\sigma) = -\frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{1}{\rho^2} \left[\frac{\partial^2}{\partial \varphi^2} - \frac{\pi^2 \rho_b^2}{h_0^2} \right] + i\gamma \frac{\partial}{\partial \varphi} + \frac{\gamma^2 \rho^2}{4} + \frac{\pi^2}{h_0^2} \sigma^2 f^2(\varphi); \quad \rho_a < \rho < \rho_b \quad (2)$$

For uniform crater ($\sigma = 0$) eigenfunctions of the Hamiltonian (2) depending on two quantum numbers, radial n and angular m can be found exactly in a form of the linear combination of Hypergeometric confluent functions:

$$\Psi_{n,m}(\rho, \varphi) = C e^{im\varphi} \rho^v e^{-\gamma \rho^2/4} [M(a, c; \gamma \rho^2/2) + \lambda U(a, c; \gamma \rho^2/2)]; \\ m = 0, \pm 1, \pm 2, \dots$$

$$a = (1/2)[v + 1 - (E_{n,m} - \gamma m)/\gamma]; \quad c = v + 1; \quad v = \sqrt{m^2 + \pi^2 \rho_b^2 / h_0^2} \\ \lambda = -M(a, c; \gamma \rho_b^2/2) / U(a, c; \gamma \rho_b^2/2), \quad (3)$$

here $E_{n,m}$ is the electron energy which is found as a solution with number n of the transcendental equation that arises from the boundary conditions $\Psi_{n,m}(\rho_a, \varphi) = \Psi_{n,m}(\rho_b, \varphi) = 0$:

$$M(a, c; \gamma \rho_a^2/2) U(a, c; \gamma \rho_b^2/2) - M(a, c; \gamma \rho_b^2/2) U(a, c; \gamma \rho_a^2/2) = 0 \quad (4)$$

Once Eq. (4) is solved, and the energies $E_{n,m}$ and the wave functions $\Psi_{n,m}(\rho, \varphi)$ are found then one can calculate the matrix elements

$$\langle nm | H(\sigma) | n' m' \rangle = E_{nm} \delta_{n,n'} \delta_{m,m'} + \left\langle m \left| \frac{\pi^2}{h_0^2} \sigma^2 f^2(\varphi) \right| m' \right\rangle \delta_{n,n'} \quad (5)$$

For the function $f(\varphi) = \sin k\varphi$, chosen for our calculations, the matrix elements (5) can be found explicitly:

$$\langle nm | H(\sigma) | n' m' \rangle = \left[E_{nm} \delta_{m,m'} + \frac{\pi^2}{4h_0^2} \sigma^2 (2\delta_{m,m'} - \delta_{m,m'+2k} + \delta_{m,m'-2k}) \right] \delta_{n,n'} \quad (6)$$

Thus a simple algorithm can be applied in order to find the energies of the one-electron non-uniform crater-like QR in the framework of the exact diagonalization method, that is reduced to

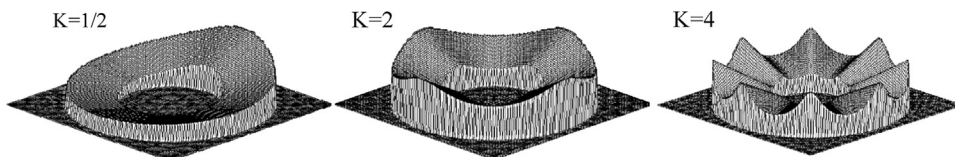


Fig. 1. 3D images of three different models of non-uniform quantum rings.

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