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Two-electron volcano-shaped quantum dot

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ABSTRACT

We propose a simple model of non-uniform volcano-shaped quantum dot that reflects the confinement details of the morphology of really fabricated GaAs/InAs nanorings and whose profile geometry, on the one hand, is described by means of simple analytical functions and, on the other hand, allows us to find exact one-particle wave functions. By using them as a basis function we calculate two-electron lower energies as functions of the external magnetic field applied along the growth axis. We show that the ring morphology and electron–electron interaction have great influence on the energy spectrum structure of nanoring and the Aharonov–Bohm oscillations.

1. Introduction

The self-assembled quantum rings (QRs) are the subject of extensive theoretical and experimental studies [1] due to their particular topology, which leads to the Aharonov–Bohm (AB) effect consisting in the appearance of the persistent currents and the energy oscillations in an increasing magnetic field, applied along the ring axis [2]. This effect is manifested clearly only in a narrow and homogeneous ring [3]. In 1D QRs the two-electron problem is separated exactly for both a single QR [4] and two vertically stacked QRs [5]. However, the analysis of a similar effect in wide QR is realized in the framework of the model with parabolic confinement by using the exact diagonalization method demonstrating a possibility to observe also the AB effect in two-electron wide QR [6]. On the other hand, the QRs properties in non-uniform rings should be quite different. It has been shown recently that any smooth and tiny variations in the 2D ring width or curvature may produce quenching of the AB oscillations of the lower energy levels [7] due to the electron localization near the defect. One could expect a similar transformation of the energy spectrum of two-electron QRs due to the presence of any type of the non-uniformities.

In order to ascertain it we below consider a model of a crater-like non-isotropic QD in the form of a thin layer, in which the dependency of the thickness on the distance from the axis and polar angle is given by relation:

$$h(\rho,\varphi)=h_0\rho/\sqrt{R^2+\sigma^2\rho^2 f_p(\varphi)}\,\vartheta(\rho_b-\rho)+h_0R/\sqrt{R^2+\sigma^2R^2 f_p(\varphi)}\,\vartheta(\rho-\rho_b) \quad (1)$$

Here $\vartheta(x)$ represents the Heaviside step-function, h_0 and R are the height and radius of the crater rim, 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 zero at the axis up to a maximum value at the crater rim and afterwards it is descended smoothly.

Below we consider a particular case of non-uniform volcano-shaped nanostructure whose profile is given by relation (1) with $f(\varphi)=\sin 2\varphi$ and $p=4$. The schematic images of corresponding morphologies given by relation (1) for the cases of a uniform crater ($\sigma=0$) are shown in Fig. 1(a, b) and a non-uniform crater ($\sigma\neq 0$) in Fig. 1(c).

There are two reasons to adopt the volcano profile in a form (1). One of them consists in the fact that the one-particle Hamiltonian in this case for thin layer becomes separable and the corresponding wave functions may be found analytically as we demonstrate below. On the other hand, as it can be found recently QRs fabricated by means of new technique called "droplet homoepitaxy" [8] exhibit the non-uniform stripes in the radial directions that are formed due to the presence of the anisotropic strain. The surface of such heterostructure seems as a crater divided into various regions between radially directed valleys similar to the one shown in Fig. 1(c). Below, we assume a simple model with the infinite-barrier confinement potential $V(r)$, which is supposed to be equal to zero inside the crater and $(0<z<h(\rho,\varphi))$ to infinity otherwise. The external homogeneous magnetic field B is applied along the Z axis. In our calculations we use the effective Bohr radius $a_0^*=\hbar^2\varepsilon/m^*e^2$, the effective Rydberg $R_y^*=e^2/2\varepsilon a_0^*$ and $\gamma=e\hbar B/2\,m^*cR_y^*$ as units of length, energy and the dimensionless magnetic field.

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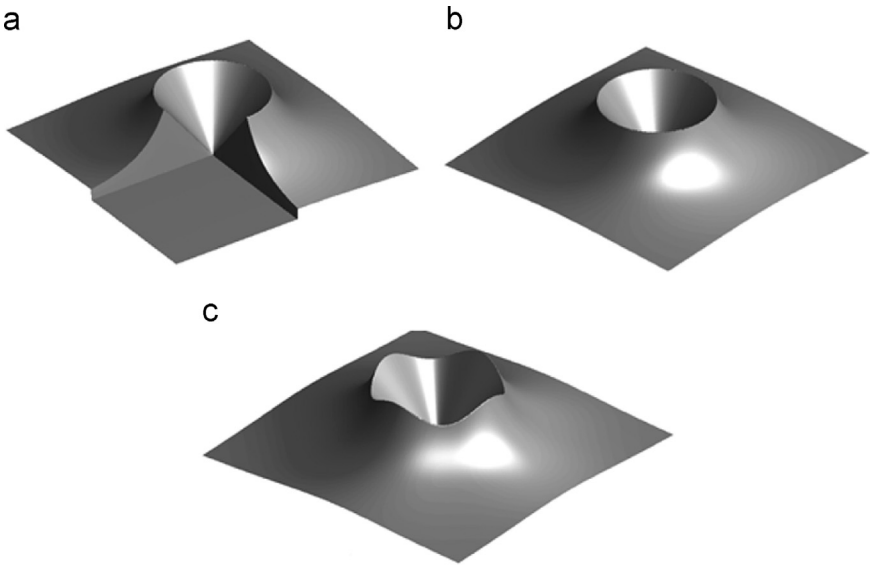

Fig. 1. Images of uniform (*a*, *b*) and non-uniform (*c*) QDs with profiles given by relation (1).

2. Theory

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 its in-plane slow displacements can be considered in turn [9]. In the framework of this approximation, one first should analyze the fast electron motion in the z direction at different electron's in-plane positions with polar coordinates (ρ,φ), which 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 $E_z(\rho,\varphi)=\pi^2/h^2(\rho,\varphi)$ then the renormalized 2D Hamiltonian describing in the effective-mass approximation the in-plane electron slow motion in the presence of the magnetic field in QD with profile given by Eq. (1) can be written as

$$H=H_0(\vec{\rho}_1)+H_0(\vec{\rho}_2)+V$$

$$V=\frac{\pi^2}{h_0^2}\sigma^2[f^p(\varphi_1)+f^p(\varphi_2)]+\frac{2}{|\vec{\rho}_1-\vec{\rho}_2|}$$

$$H_0(\rho)=-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}-\frac{1}{\rho^2}\left[\frac{\partial^2}{\partial\varphi^2}-\frac{\pi^2R^2}{h_0^2}\vartheta(R-\rho)\right]+i\gamma\frac{\partial}{\partial\varphi}+\frac{\rho^2}{4}\left[\gamma^2+\frac{4\pi^2}{h_0^2R^2}\vartheta(\rho-R)\right] \quad (2)$$

Eigenfunctions of the Hamiltonian (2) depending on two quantum numbers, radial n and angular m may be found exactly in a form of the linear combination of Hypergeometric confluent functions:

$$\phi_{n,m}(\rho,\varphi)=Ce^{im\varphi}\rho^{\nu}e^{-\gamma\rho^2/4}\left[M\left(a_1,c_1;\frac{\gamma_1\rho^2}{2}\right)J(R-\rho)+\lambda U\left(a_2,c_2;\frac{\gamma_2\rho^2}{2}\right)J(R-\rho)\right]$$

$$a_i=1/2\left[\nu_i+1-\frac{(E_{n,m}-\gamma_i m)}{\gamma_i}\right];\quad i=1,2$$

$$\lambda=\frac{M(a_1,c_1;\gamma_1R^2/2)}{U(a_1,c_1;\gamma_2R^2/2)};\quad m=0,\pm1,\pm2,\ldots$$

$$\nu_1=\sqrt{m^2+\pi^2/h_0^2R^2};\quad \nu_2=m;$$

$$\gamma_1=\sqrt{\gamma^2+4\pi^2/h_0^2R^2};\quad c_i=\nu_i+1 \quad (3)$$

The electron energies then are solution with number n of the transcendental equation:

$$M'(a_1,c_1;g_1r^2/4)U(a_2,c_2;g_2r^2/4)-M(a_1,c_1;g_1r^2/4)U'(a_2,c_2;g_2r^2/4)=0 \quad (4)$$

Eq. (4) is solved, $E_{n,m}$ and $\phi_{n,m}(r,j)$ are found that the energy spectrum of one- and two-electron volcano-shaped QD may be analyzed by using the diagonalization method considering the last term two-particle Hamiltonian as a perturbation. To this end we use two sets of the basis functions, one corresponding to the spin-singlet states ($S=0$) and the spin-triplet states ($S=1$).

$$\Psi^{(0)}_{j_1j_2}=k_{j_1j_2}[\Phi_{j_1}(\rho_1,\varphi_1)\Phi_{j_2}(\rho_2,\varphi_2)+\Phi_{j_2}(\rho_1,\varphi_1)\Phi_{j_1}(\rho_2,\varphi_2)] \quad (5)$$

$$\Psi^{(1)}_{j_1j_2}=1/\sqrt{2}[\Phi_{j_1}(\rho_1,\varphi_1)\Phi_{j_2}(\rho_2,\varphi_2)-\Phi_{j_2}(\rho_1,\varphi_1)\Phi_{j_1}(\rho_2,\varphi_2)] \quad (6)$$

Here $k_{j_1j_2}=1/\sqrt{2}$ if $j_1\neq j_2$ and $k_{j_1j_2}=1/2$ otherwise. The index $j_i(n_i,m_i);i=1,2$ labels the in-plane wave functions (3) with the radial n_i and m_i angular quantum numbers. We diagonalize the Hamiltonian (2) representing the wave function of two interacting electrons as a linear combination of the basis functions (5) and (6) as follows [6]:

$$\Psi^{(S)}=\sum_{j_1=1}^{j_{max}}\sum_{j_2=2}^{j_1-S}C_{j_1j_2}\Psi^{(S)}_{j_1j_2};\quad S=0.1 \quad (7)$$

The set of eigenfunctions allows us to calculate the energies of lower states with an acceptable accuracy by extending the matrix dimension step by step; until satisfactory convergence is achieved.

3. Results

In order to analyze the effect of the periodical non-uniformity on the electron spectral properties of one- and two-electron volcano-shaped QDs we have performed numerical calculations for low-lying energy levels as functions of the external magnetic field. In our numerical work, we assumed for the effective Bohr radius and the effective Rydberg the values $a_0^*\approx 10$ nm and