Vertically coupled non-uniform quantum rings with two separated electrons in threading magnetic field

J. H. Marín¹, F. A. Rodriguez-Prada², and I. D. Mikhailov²

¹Escuela de Física, Universidad Nacional de Colombia, Medellín, Colombia
A.A. 3840
²Escuela de Física, Universidad Industrial de Santander, Bucaramanga, Colombia A.A. 678

E-mail: jhmarca65@gmail.com; jhmarin@unal.edu.co

Abstract. We propose a simple method for calculating the energy spectrum of two separated electrons in vertically coupled narrow quantum rings with non-uniform cross-sections heights. We present numerical results for energies of some low-lying levels as a function of the magnetic flux for a particular case, in which one of two rings is uniform and other has a locally distorted height. The effect of the distortion on the Aharonov-Bohm oscillations is studied.

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 clearly manifested only in a narrow and homogeneous ring [3]. In 1D QRs the two-electron problem is separated exactly both for a single QR [4] and two vertically stacked QRs [5]. The QR’s properties are changed drastically if the ring is non-uniform. 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 [6] due to the electron localization near the defect. The samples of 3D rings, used in the experiment for observing the AB effect, have finite but very small and variable thicknesses with drastically different crystalline shapes [7]. The properties of a thin 3D ring is similar to those of a 2D ring, only if the 3D ring thickness is uniform, otherwise the potential energy corresponding to the electron in-plane motion is non-homogeneous. For example, the increase of the ring height from 4 nm up to 4.5 nm lowers the energy of the electron about 20%. This effect may be more interesting for the model of two-electron vertically stacked QRs when the strongly correlated electrons should be mainly located on the opposite sides of the rings. Therefore the localization of one of them should lead to the localization of the other one and to the quenching of the AB oscillations. In the present work, we analyze the model of two separated electrons, in two coaxial and vertically stacked thin QRs, schematically presented in figure 1, where the lower and upper rings have the same width and different centerline radii \( R_1 = R \) and \( R_2 = \alpha R \), respectively, being the separation between them \( d = \beta R \). The external magnetic field \( \mathbf{B} \) is applied along the z-axis. The lower ring is considered as homogeneous with fixed thickness \( h_1 \) (\( h_1 = h \)), while the thickness of the
upper ring is supposed to be dependent on the polar angle as \( h_2 = \hbar \sqrt{1 + \alpha^2 \theta_2^2}; (-\pi < \theta_2 < \pi) \). The smaller the parameter \( \sigma \), the smoother is the surface of the upper ring.

2. Theory

In the effective mass approximation the dimensionless two-electron Hamiltonian can be written as:

\[
H = \sum_{j=1,2} H_0(r_j) + \frac{2}{|r_1 - r_2|}; \quad H_0(r_j) = -\Delta_j + V_j(r_j) + \frac{\gamma^2 \rho_j^2}{4} - iv \frac{\partial}{\partial \theta_j}
\]

Here \( V_1(r_1) \) and \( V_2(r_2) \) are infinite-barrier confinement potential in the lower and in the upper rings, respectively, and the effective Bohr radius \( a_0^* = \hbar^2 \varepsilon / m^* c^2 \), the effective Rydberg \( R_j^* = e^2 / 2 \varepsilon a_0^* \) and \( \gamma = eB / 2m^* cR_j^* \) are taken as units of length, energy and the conventional dimensionless magnetic field strength, respectively. For the sake of the mathematical convenience, we consider below only quasi-1D rings with large radius–width and width-thickness aspect ratios, i.e. \( h_j << w << R_j \), for which the two-electron wave function can be separated by using adiabatic approximation (AA) [8] and represented in the form: \( \Psi(r_1, r_2) = \psi(\theta_1, \theta_2) f(U)(\rho_1, \rho_2, z_1, z_2) \). Here \( \psi(\theta_1, \theta_2) \) is the variational function that describes the slow electrons rotation around \( z \)-axis and \( f(U)(\rho_1, \rho_2, z_1, z_2) \) the one-particle ground state wave function which describes the transversal fast motion of two non-interacting electrons in planes through the \( z \) axis with polar angles \( \theta_1 \) and \( \theta_2 \), respectively. The condition \( h_j << w \) allows us to apply the AA in order to separate \( z_j \) and \( \rho_j \) coordinates and to find this function in an analytical form. Starting from the Schrödinger variational principle [9] we find the energies of the low-lying states by minimizing the functional:

\[
E[\Psi] = \left< \frac{\delta}{\delta \psi} \right| H \left| \frac{\delta}{\delta \psi} \right> / \left| \frac{\delta}{\delta \psi} \right| f(U) \left| \frac{\delta}{\delta \psi} \right> \rightarrow \text{min}
\]

Taking the functional derivative with respect to \( \psi \) one can obtain the wave equation for \( \psi(\theta_1, \theta_2) \) [8].

\[
\hat{H}_s \psi = \varepsilon \psi; \quad \hat{H}_{sl} = -\frac{1}{\alpha^2} \left( \frac{\partial^2}{\partial \theta_1^2} - i \alpha^2 \Phi \right)^2 + \frac{\pi^2 \alpha^2 R^2}{\hbar^2} \theta_1^2 + a \Phi^2
\]

Here \( \varepsilon \) is normalized energy, \( \Phi \) is the magnetic flux through interior of the lower ring expressed in term of the magnetic flux unit \( \Phi_0 = \hbar e / c \), i.e. \( \Phi = B \cdot \pi R^2 / \Phi_0 \) and the terms of order \( \hbar^2 / R^2 \) and superior are neglected. The equation (3) in the centre-of-mass \( \Theta = (\theta_1 + \alpha^2 \theta_2) / (1 + \alpha^2) \) and relative \( \theta = \theta_1 - \theta_2 \) coordinates can be rewritten as:

\[
\hat{H}_s \psi(\Theta, \Theta) = \varepsilon \psi(\Theta, \Theta); \quad \hat{H}_{sl} = \hat{H}_s + \hat{H}_\theta - \frac{\pi^2 \alpha^2 R^2}{\hbar^2 p} \Theta; \quad p = 1 + \alpha^2; -\pi < \Theta < \pi; \quad -2\pi < \Theta < 2\pi
\]

Here \( \Theta = \theta_1 - \theta_2 \) is the total angular momentum, \( \Theta = \theta_1 + \alpha^2 \theta_2 \) is the total angular momentum. The equation (4) in the centre-of-mass \( \Theta = \psi(\Theta, \Theta) \) and relative \( \hat{H}_\theta \) parts of the Hamiltonian, for different values of centre-of-mass, \( M = 0, \pm 1, \pm 2, \ldots \) and relative angular, \( m = 0, \pm 1, \pm 2, \ldots \) momenta. The corresponding matrix elements of Hamiltonian \( \hat{H}_s \) by using these basis functions can be calculated analytically. We checked the accuracy of our method by comparing our results with those of references [4, 8] for 1D uniform two-electron QRs with different radii. Discrepancies between our results and those from references [4,8]
for the first 20 low-lying energy states is less than 5% when our Fourier series converge.

3. Results

We have performed numerical calculations of two-electron normalized energies \( \varepsilon = E \cdot R^2 \) as a function of the magnetic flux and for different geometric parameters of the ring in order to analyze the effect of the ring dimension and the smoothness of the ring surface. First, we calculate the energies one-electron single QR with smooth distortion of the surface thickness. Results are shown in Fig. 2.

![Figure 2](image2.png)

**Figure 2.** Renormalized energies of the one-electron low-lying states as functions of the magnetic flux for a single ring with two different radii and smoothness of the with parameters \( h = 0.2 \)

It is seen that a very small increase of the surface non-homogeneity, given by the variation of the parameter \( \sigma \) from 0.001 to 0.004 has produced a quenching of the AB oscillations of the lower energy levels similarly to one, found previously in the references [6] for non-uniform 1D and 2D rings. The physical reason for the flattening of the energy levels is similar to one given in references [6] for 2D non-uniform rings. The higher regions of the circular ring are more favourable for the electrons, i.e., they correspond to a lower effective potential. Therefore, low energy electrons are confined near the point corresponding to \( \theta_2 = 0 \), wherein the height attains its maximum value. Since the ring is thin, small variations in the height produce large variations in the transversal energy, thus confining the electron.

![Figure 3](image3.png)

**Figure 3.** Effect of non-homogeneity on the two-electron energy levels for QRs with same (\( \alpha = 1 \)), and different (\( \alpha = 1.5 \)) radii. Other parameters of QRs are \( R = 20a_0 \), \( w = 1a_0 \), \( h = 0.2a_0 \), \( \beta = 0.1 \)

The energy levels of two electrons in vertically coupled QRs as a function of magnetic flux have been plotted in Fig. 3. We choose the radius of the lower ring \( R = 20a_0 \) and the separation between rings very small (\( \beta = 0.1 \)) in order to compare our results with those from reference [4], where it has been shown that in two-electron 1D QR such dependencies are given by a set of curves with oscillations and multiples crossovers similar to those of an image of the fingerprints. As magnetic fingerprints are changed with the increase of the radius, it has been concluded that the Coulomb interaction of two electrons in 1D QRs of quantum size effects and magnetic fingerprints. A similar analysis for 3D non-uniform two-electron structures is more complicated because it involves various additional factors, related to a wider variety of possible rings morphologies. The curves presented on the left side of Figure 3 (\( \alpha = 1, \sigma = 0 \)) for two identical, uniform, very thin and sufficiently narrow rings, located closely one to another, are practically coincide with those presented in Figure 6 of Reference [4] for two-electron 1D QR. As one of the two uniform rings has the radius 50% larger (\( \alpha = 1.5, \sigma = 0 \)), the picture of the magnetic fingerprints has more intersections of the energy level curves and it looks like...
a superposition of fingerprints of rings with radii $20a_0$ and $30a_0$. One can see that the number of the energy levels, with quenched AB oscillations, increases with a rate, which is almost independent of the radii ratio, when the non-homogeneity parameter grows from 0 to 0.002.

**Figure 4.** Renormalized energies as functions of radii vertically stacked rings in zero- (figures (a) and (b)) and in a strong magnetic field (γ = 3, $B = 20T$, figures (c) and (d)). Structure have the parameters $\alpha = 4$, $\beta = 0.1$, $h = 0.01$, $w = 0.1$.

Finally, in Figure 4 we show the dependencies of normalized energies ($\varepsilon = E \cdot R^2$) on the lower (uniform) ring radius $R$, in zero and strong magnetic fields ($\gamma = 3$) for the case as the radius of the lower ring is much smaller ($\alpha = 4$) than of the upper. For radii given in Figure 4, the contribution of the normalized potential energy, which depends on the radius linearly, in the normalized Hamiltonian is larger than the contribution of the normalized kinetic energy, which is independent of radius. Therefore, the dependence of all energies on the radius is almost linear. It is seen from Figure 4 that in zero magnetic field case the levels are arranged into bands of sublevels with the same slopes, while when one of the rings is non-uniform the lines have two different slopes, providing many crossovers.

External magnetic field adds diamagnetic term in normalized energy proportional to $R^4$. As the result the abrupt increase of the energies is observed for large radii as a strong magnetic field is applied.

**4. Conclusion**

We have calculated the energies of two-electron vertically stacked rings with different radii in a threading magnetic field, focusing our attention on the effects of the rings thickness non-uniformity. For the model with only one non-uniform ring, we have obtained new results. We show that in rings with different radii, the curves of the higher energies as functions of the magnetic flux, give a picture with higher number of crossovers than in the rings with equal radii, due to the presence of the Aharonov–Bohm oscillations with two different periods, while the oscillations of the lower energies are quenched similarly in both cases.

**Acknowledgments**

This work was financed by Universidad Nacional de Medellín (UN) through the DIME Cod. QUIPU 20101007748 and the Excellence Center of Novel Materials ECNM, under Contract No. 043-2005.

**References**

[1] Lorke A, Luken R J, Govorov A O, Kotthaus J P, Garcia J M and Petroff P M, 2000 *Phys. Rev. Lett.* **84** 2223; Reimann S M and Manninen M 2002 *Rev. Mod. Phys.* **74** 1283

[2] Römer R A and Raikh M E 2000 *Phys. Rev. B* **62** 7045; Govorov A O, Ulloa S E, Karrai K and Warburton R J, 2002 *Phys. Rev. B* **66** 081309(R)

[3] Wendler L, Fomin V M and Chaplik A V 1994 *Superlatt. and Microstructure* **16** 311; Wendler L, Fomin V M 1995 *Phys. Rev. B* **51** 17814; Wendler L, Fomin V M, Chaplik A V and Govorov A O 1996 *Phys. Rev. B* **54** 4794; Wendler L and Fomin V M 1995 *Phys. Rev. B* **51** 17814

[4] Zhu J-L, Dai Z and Hu X 2003 *Phys. Rev. B* **68** 045324

[5] Marin J H, Garcia F and Mikhailov I D 2006 *Braz. Jour. of Phys.* **36**(3B) 940

[6] Pershin Y V and Piermarocchi C 2005 *Phys. Rev. B* **72** 195340; Bruno-Alfonso A and Latgé A 2008 *Phys. Rev. B* **77** 205303

[7] Haft D, Schulhauser C, Govorov A O, Warburton R J, Karrai K, Garcia J M; Schoenfeldd W, Petroff P M 2002 *Physica E* **13** 165; Kuroda T, Mano T, Ochia T, Sanguinetti S, Sakoda K, Kido G and Koguchi N 2005 *Phys. Rev. B* **72** 205301

[8] Marin J H, Gutiérrez W and Mikhailov I D 2010 *J. Phys.: Conference Series* **210** 012145