

# Controlled Coulomb effects in core-shell quantum rings

Anna Sitek<sup>\*,‡</sup>, Miguel Urbaneja Torres<sup>\*</sup>, Kristinn Torfason<sup>\*</sup>, Vidar Gudmundsson<sup>¶</sup>,  
and Andrei Manolescu<sup>\*</sup>

<sup>\*</sup>*School of Science and Engineering, Reykjavik University, Menntavegur 1, IS-101 Reykjavik, Iceland*

<sup>‡</sup>*Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology, 50-370 Wrocław, Poland*

<sup>¶</sup>*Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland*  
*e-mail: annams@ru.is*

## ABSTRACT

We analyse theoretically the possibilities of contactless control of in-gap states formed by a pair of electrons confined in a triangular quantum ring. The in-gap states are corner-localized states associated with two electrons occupying the same corner area, and thus shifted to much higher energies than other corner states, but still they are below the energies of corner-side-localized states. We show how the energies, degeneracy and splittings between consecutive levels change with the orientation of an external electric field relatively to the polygonal cross section. We also show how absorption changes in the presence of external electric and magnetic fields.

**Keywords:** polygonal quantum rings, core-shell structures.

## 1. INTRODUCTION

Core-shell semiconductor nanowires represent a novel expanding field of research largely as a result of their rich electronic properties, related both to transport and optics, and constitute a great technological promise as building blocks of electronic nanodevices. Such nanowires consist of an embedded core covered by different materials and are typically grown vertically by the bottom-up methods. Due to the crystallographic structure, the wires exhibit polygonal cross sections, most often hexagonal although other shapes, like circular, square or triangular, are also feasible. The possibility to combine vertically two different materials allows for control of band alignment, and thus structures in which electrons are accumulated only in the shells may be achieved. Moreover, the polygonal nanotubes of finite thickness can be created by etching the core parts.

Core-shell nanowires short enough to confine the electrons along the growth direction, i.e. shorter than their wavelength, can be considered as quantum rings. Such structures are of particular interest due to the possibility of controlling the number of carriers in the system and its fluctuations [1, 2], and offer the possibility to study artificial atoms and their features as they exhibit shell structures similar to those of real atoms.

In this paper we focus on the manipulation possibilities of the in-gap states [3] created by a pair of electrons confined in a triangular ring. We show that an external electric field splits these states and moves them to different parts of the energy interval forbidden for non-interacting particles. It also considerably changes particle localization which depends on the field orientation relatively to the polygonal cross section. We explain why in the presence of the electric field parallel to one of the sides two optical transitions to energetically separated in-gap states take place, and why they are blocked when the ring is immersed in external (static) magnetic field.

## 2. THE MODEL

We study a system of two Coulomb interacting electrons confined in a triangular quantum ring. The sample is exposed to an external magnetic field  $B$  perpendicular to the ring's plane  $(x,y)$ , i.e., associated with a vector potential  $\mathbf{A} = B[-y, x, 0]/2$ . The sample is also subjected to an external electric field which can be rotated with respect to the cross section. We assume that it forms an angle  $\phi$  with the  $x$  axis,  $\mathbf{E} = E[\cos(\phi), \sin(\phi), 0]$ . The single-particle Hamiltonian is then

$$H = \frac{(-i\hbar\nabla + e\mathbf{A})^2}{2m_{\text{eff}}} - g_{\text{eff}}\mu_B\sigma_z B - e\mathbf{E}\cdot\mathbf{r}, \quad (1)$$

where  $m_{\text{eff}}$  is the electron effective mass,  $g_{\text{eff}}$  is the effective g-factor,  $e$  the electron charge,  $\sigma_z$  stands for the  $z$  Pauli matrix and  $\mathbf{r}$  defines the position.

To calculate single-particle eigenvalues ( $E_a$ ) and eigenstates ( $|\psi_a\rangle$ ) we use a discretization method based on a polar grid [4]. We construct a circular sample on which we superimpose polygonal constraints and redefine the grid such that it consists only of the sites situated between the boundaries. We solve the eigenvalue problem numerically and further use the results to construct the many-body Hamiltonian,

$$\hat{H} = \sum_a E_a a_a^\dagger a_a + \frac{1}{2} \sum_{abcd} V_{abcd} a_a^\dagger a_b^\dagger a_d a_c,$$

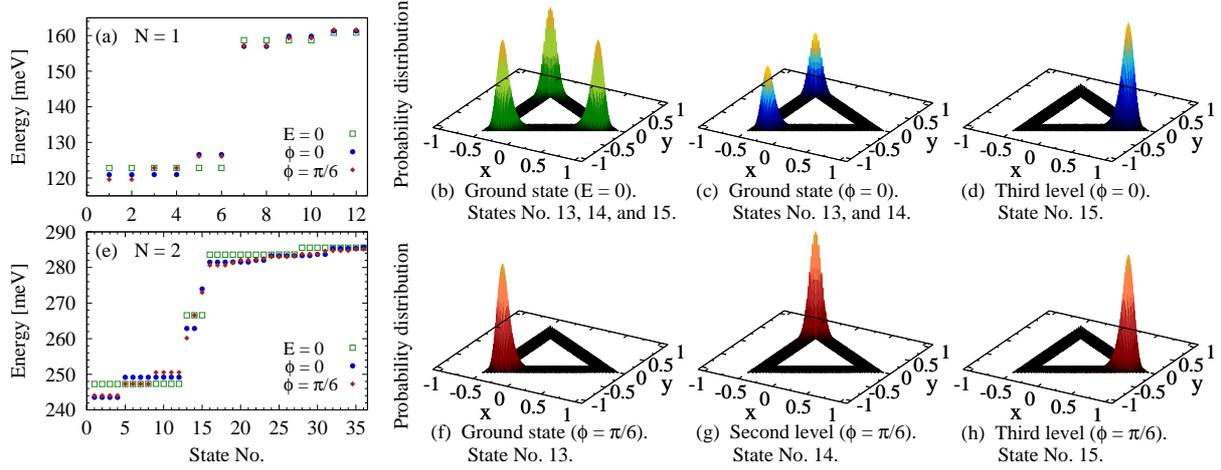


Figure 1: *Single-particle (a) and many-body (e) energy levels of electrons confined in a triangular quantum ring in the absence of external fields (green squares) and in the presence of an electric field of amplitude  $E = 0.11$  mV/nm parallel to the  $x$  axis (blue circles) and one of the sides (red diamonds). The number of particles ( $N$ ) is shown in each figure. (b-d) and (f-h) probability distributions associated with some of the levels shown in Figs. (a) and (e). The upper label refers to single-particle quantities while the lower labels to many-body ones.*

where  $a_a^\dagger$  and  $a_a$  create and annihilate, respectively, an electron in the state  $|\psi_a\rangle$  and  $V_{abcd}$  are the Coulomb integrals.

We study the absorption of clockwise polarized electromagnetic field by the pair of electrons occupying the triangular ring. The corresponding absorption coefficients are calculated in dipole and low temperature approximations according to the formula [5]

$$\alpha(\hbar\omega) = \mathcal{A} \hbar\omega \sum_f |\langle f | \boldsymbol{\varepsilon} \cdot \mathbf{d} | i \rangle|^2 \delta[\hbar\omega - (\mathcal{E}_f - \mathcal{E}_i)],$$

where  $\mathcal{A}$  is a constant amplitude,  $\omega$  the frequency of the electromagnetic field,  $\boldsymbol{\varepsilon}$  the unit polarization vector,  $\mathbf{d}$  is the electric dipole moment, and  $\mathcal{E}_{i,f}$  are the energies of the initial ( $|i\rangle$ ) and final ( $|f\rangle$ ) many-body states.

In the numerical calculations we use InAs material parameters which are:  $m_{\text{eff}} = 0.023$ ,  $g_{\text{eff}} = -14.9$ , and the relative permittivity  $\epsilon = 15$ . The studied sample is an equilateral triangular ring of height and side thickness equal to 75 and 10 nm, respectively.

### 3. RESULTS

Polygonal quantum rings have unique physical properties which depend on the number of corners and details of the sample symmetry. In particular, if there is a single electron confined in a symmetric (equilateral) sample, then its energy level degeneracy is determined solely by the number of vertices while the splittings between the levels depend on the aspect ratio between the side thickness and the radius of the external circumcircle. The ground state of an electron confined in a triangular ring is twofold (spin) degenerate and is followed by a sequence of alternating pairs of four- and twofold degenerate levels. The latter ones are degenerated due to spin, the fourfold degeneracy originates from spin and finite orbital momentum [Fig. 1(a) green squares]. Low-energy electrons occupy areas between internal and external boundaries and for sufficiently thin rings are completely depleted from sides [Fig. 1(b)]. These levels are energetically separated from higher (side-localized) states by a considerable energy gap which decreases with increasing the aspect ratio. Contrary to square and hexagonal rings, for the triangular case this gap never diminishes to values comparable to splittings in the corner domain [6, 7].

The degeneracy due to orbital momentum is lifted when the sample is exposed to an electric field parallel to the ring's plane. Irrespective of the field orientation, all the levels are spin degenerate. Beyond creating an energy splitting within each group of fourfold degenerate states, the field may also increase the splittings present in its absence. This stretching of the energy interval of every set of six states is particularly strong for the corner-localized domain [Fig. 1(a)]. The field strongly rearranges electron localization. If it acts along the  $x$  axis then the two lowest levels are quasi-degenerate and, due to the field direction, are shifted to lower energies while the addition to the third level (states No. 5 and 6) is positive and slightly larger [Fig. 1(a) blue circles]. The two close by levels are associated with the same probability distributions which form two maxima at the ends of the side perpendicular to the electric field [Fig. 1(c)]. Electrons excited to the third level occupy only the corner area with

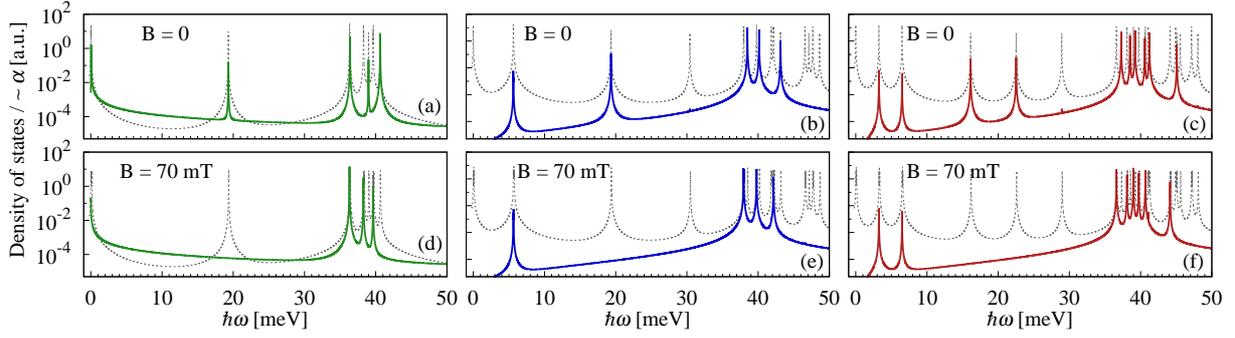


Figure 2: *Density of states (grey dotted) and absorption coefficients associated with the excitation of a ground state of a pair of Coulomb interacting electrons confined in a triangular quantum ring: in the absence of external fields (a), exposed to a static electric field of amplitude  $E = 0.11$  mV/nm parallel to the  $x$  axis (b), and to one of the sides (c). (d-f) exposed to external electric fields as in (a-c) and magnetic field of 70 mT.*

the highest value of the  $x$  coordinate [Fig. 1(d)]. Both probability distributions are symmetric with respect to the  $x$  axis, i.e., orientation of the electric field.

If the external field is parallel to one of the sides then the six lowest states are arranged into three well separated levels [Fig. 1(a) red diamonds]. In this domain the energy shifts are: positive and negative of the same magnitude for the corners located at the ends of the side parallel to the field, and negligibly small for the opposite corner. The contribution to the second level does not vanish totally due to the finite areas between internal and external boundaries. The corresponding probability distributions form maxima around single corners which are determined by the direction and orientation of the external field with respect to the polygon [Figs. 1(f)- 1(h)].

Energy levels of two Coulomb interacting electrons confined in a triangular quantum ring are arranged in groups of quasi-degenerate levels. The fifteen lowest states are built of only corner-localized single-particle states, and thus are associated with probability distributions of this type [Fig. 1(b)]. The ground state and the eleven consecutive states refer to particles distributed between two different corners. Due to the largest possible spatial separation, the contribution from Coulomb interaction to these states is the smallest. The opposite occurs for the smallest distance between particles, i.e., when the two electrons occupy the same corner area, which is possible for particles in a spin singlet state. The three states of this kind (states No. 13, 14, and 15) are shifted to much higher energies than other corner states. Since the spin of all three states is determined, their degeneracy is only of the orbital origin and resembles the arrangement of the lowest single-particle states with respect to spin. The higher states contain contributions from corner- and side-localized single-particle states, and thus are associated with mixed corner-side-localized probability distributions. These states are separated from the lower group of corner states by an energy interval which is of the order of the gap separating corner- from side-localized single-particle states and is 'broken' only by the three in-gap states [Fig. 1(a) green squares] [3].

The external electric field induces large splittings within quasi-degenerate groups of two-electron states. Like in the case of single-particle states, the most pronounced effects occur for corner-localized states, in particular for the in-gap states. If the field is parallel to the  $x$  axis, then the twelve lowest states are split into two groups separated by 5.6 meV, shifted to higher and lower energies with respect to the states in the absence of the field. The energy interval of in-gap states is also stretched. The two lowest states are nearly degenerate while the energy of the third one is 11 meV higher [Fig. 1(a) blue circles]. As the energy levels, the corresponding probability distributions also resemble single-particle ones. This means that the two lowest in-gap states contain only contributions from the single-particle ground state and the two states forming the second level, while the third level is built of the fifth and sixth single-particle states [Fig. 1(c) and 1(d)].

An electric field parallel to one of the sides rearranges the twelve lowest states into three fourfold degenerate levels equally separated from each other by 3.3 meV. In this case the energy of one of the in-gap states is decreased by 6.4 meV while the energy of another one is increased by the same amount with respect to the energies achieved in the absence of the field, the energy of the third one is negligibly affected. A pair of electrons in one of these states occupies one particular corner, i.e., each of the in-gap states is built of only two spin degenerate single-particle states [Figs. 1(f) - 1(h)].

In this paper we do not take into account spin-orbit interaction, and thus the analysed optical transitions conserve spin. Circularly polarized electromagnetic field impinging on a sample containing a pair of Coulomb interacting electrons may excite the system to one of the nearby corner states, to one of the in-gap states and to three states associated with mixed corner-side-localized probability distributions [Fig. 2(a)] [3]. The number of optically induced transitions does not change when the sample is exposed to an external electric field parallel to the  $x$  axis.

The ground state and the optically accessible in-gap state are associated with the same probability distributions [Fig. 1(c)]. Due to the identical contributions from the electric field, the energy shifts of both these states are the same which results in conserved energy required to excite the system to the in-gap state. The field creates a splitting in the lowest group of corner states. This increases the separation between the ground state and the lowest optically excited state, and thus the excitation of this state requires higher energy than in the absence of the field [Fig. 2(b)]. The number of optical transitions increases when the external electric field is parallel to one of the sides. Such a field mixes the degenerate or quasi-degenerate optically active states (excited by a clockwise and counterclockwise polarized electromagnetic field), and rearranges them into pairs of well separated states which may be excited from the ground state irrespective of the polarization type. In particular, it splits the lower in-gap states and breaks the previously forbidden gap with relatively distant states [Fig. 2(c)].

If the quantum ring is immersed in an external (static) magnetic field perpendicular to its plane, then all transitions to the in-gap states are blocked for relatively weak fields. All the in-gap states are well separated spin singlets which do not mix with other states for wide ranges of electric and magnetic fields. The opposite occurs within the group of twelve lower corner states. The ground state is either degenerate or separated from the second level by a very small energy interval. Due to the Zeeman splitting the degeneracy of all the levels is lifted. Moreover, for relatively weak fields the states originating from different levels may interchange. As a result the spin of the ground state changes, and thus the transition to the in-gap states is blocked [Figs. 2(d) - 2(f)].

#### 4. CONCLUSIONS

We analysed energy levels and the corresponding electron localization of a single electron and a pair of Coulomb interacting particles confined in a triangular quantum ring in the presence of an external electric field. We showed that the field lifts the degeneracies due to orbital momentum but conserves the twofold spin degeneracy of single-particle levels. Moreover, the field strongly redistributes particles within the ring. Depending on its orientation with respect to the cross section, the particles may be depleted from some regions of the sample.

The energy spectrum of a pair of Coulomb interacting electrons is even more affected by the field. The degenerate and quasi-degenerate levels are split into well separated groups of states. In particular, the in-gap states, i.e., pairs of electrons in a spin singlet state occupying the same corner area, are stretched, and thus associated with energies belonging to a wide range of energies forbidden for non-interacting particles. Irrespective of the external electric field, the in-gap states degeneracy and the corresponding probability distributions reproduce those of single-particle corner states with respect to spin. The absorption of the many-body system depends on the orientation of the electric field. The excitation of the in-gap states is unaffected if the field is perpendicular to one of the sides, but the field parallel to one side allows for optical transitions to two distant in-gap states. The excitation of the highest two-particle corner-localized states is blocked in the presence of a weak magnetic field perpendicular to the ring's plane.

#### ACKNOWLEDGEMENTS

This work was financed by the Icelandic Research Fund.

#### REFERENCES

- [1] A. Ballester, J. Planelles, and A. Bertoni, *Multi-particle states of semiconductor hexagonal rings: Artificial benzene*, J. Appl. Phys. **112**, 104317 (2012).
- [2] A. Ballester, C. Segarra, A. Bertoni, and J. Planelles, *Suppression of the aharonov-bohm effect in hexagonal quantum rings*, EPL **104**, 67004 (2013).
- [3] A. Sitek, M. Ţolea, M. Niță, L. Serra, V. Gudmundsson, and Andrei Manolescu, *In-gap corner states in core-shell polygonal quantum rings*, Sci. Rep. **7**, 40197 (2017).
- [4] C. Daday, A. Manolescu, D. C. Marinescu, and V. Gudmundsson, *Electronic charge and spin density distribution in a quantum ring with spin-orbit and coulomb interactions*, Phys. Rev. B **84**, 115311 (2011).
- [5] S. L. Chuang, *Physics of Optoelectronic Devices* (John Wiley and Sons, Inc., New York, 1995).
- [6] A. Sitek, L. Serra, V. Gudmundsson, and A. Manolescu, *Electron localization and optical absorption of polygonal quantum rings*, Phys. Rev. B **91**, 235429 (2015).
- [7] A. Sitek, G. Thorgilsson, V. Gudmundsson, and A. Manolescu, *Multi-domain electromagnetic absorption of triangular quantum rings*, Nanotechnology **27**, 225202 (2016).