Symmetry dependent electron localization and optical absorption of polygonal quantum rings

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ABSTRACT

We compare energy spectra, electron localization and optical absorption of square and diamond quantum rings and analyze how sample geometry affects those features. We show that low energy levels of diamond rings form two groups delocalized between opposite corners which results in increased number of optical transitions. We also show that contacts applied to corner areas allow for continuous change between square- and diamond-like behavior of the same sample, irrespective of its shape.

Keywords: polygonal quantum rings, core-multi-shell structures, absorption.

1. INTRODUCTION

Polygonal quantum rings are very short hollow or core-multi-shell wires in which electrons are confined only in one of the shells. The most common are hexagonal structures, but dodecagonal [1], triangular [2, 3] and tetragonal [4] core-shell wires have already been achieved. The main feature which distinguishes polygonal from circular structures is a unique carrier localization, which in the case of quantum wires leads to a formation of one-dimensional channels [5, 6, 7, 8, 9, 10]. As in the case of bent quantum wires [11], in the corner areas of polygonal rings effective quantum wells are formed which attract low-energy electrons and localize them only in the vicinity of the vertices [12, 13]. If the rings are externally and internally restricted by regular polygons, then the localization probability associated with the lowest states is equally distributed between all corners, but this may be easily turned into localization in single corners if the system symmetry is broken. Moreover, the existence of corners changes the energy degeneracy, i.e. splits degeneracies related to angular momentum conservation. For sufficiently narrow rings the polygon separates energy levels for which the probability distribution is localized only in the corner areas from higher, mostly side-localized, eigenvalues. Electron distribution also affects absorption of electromagnetic waves. In the presence of an external magnetic field and circularly polarized light only two transitions, each coupled to a different polarization, from the ground state to the corner- or side-localized states above the energy gap occur for symmetric samples [13].

In this paper we focus on square and diamond shaped rings, we show how probability distribution changes when the system symmetry is reduced, and how it affects absorption of electromagnetic field. We compare two cases: In the first case the system geometry is variable; we show that for a diamond ring the energy levels are only spin degenerated and the corner-localized states form two energy groups. The lower one with probability distribution equally shared by the two sharper corners and the higher group associated with electrons bound symmetrically to the wider corners. We show that diamond samples allow for twice as many optical transition than the square rings in the presence of one polarization type. In the second case we apply potentials to the corner areas and show how they allow to switch between square- and diamond-like carrier localization and absorption for one or another ring shape.

2. THE MODEL



Figure 1: Sample model - diamond constraints, for with the ratio between the diagonals is 0.8, applied on polar grid. Blue points indicate areas where an on-site potential was applied. For visibility we reduced the number of site points.

The sample model used in our calculations is based on a discretization method on a polar grid with diamond constraints defining the ring shape. The Hilbert space is spanned by vectors $|kj\sigma\rangle$, where k and j refer to the radial and angular coordinates, respectively, associated only with sites within the polygonal shell, δr and $\delta \phi$ are

the corresponding intervals and σ denotes spin. The Hamiltonian matrix element in these coordinates is [14]

$$H_{kj\sigma,k'j'\sigma'} = T\delta_{\sigma,\sigma'} \left[\left(t_r + t_\phi + \frac{1}{2} t_{\rm B}^2 \left(\frac{r_k}{4R_{\rm ext}} \right)^2 + V \right) \delta_{k,k'} \delta_{j,j'} - \left(t_\phi + t_{\rm B} \frac{i}{4\delta\phi} \right) \delta_{k,k'} \delta_{j,j'+1} + t_r \delta_{k,k'+1} \delta_{j,j'} + \text{H.c.} \right] + \frac{1}{2} T t_{\rm B} \gamma \left(\sigma_z \right)_{\sigma,\sigma'} \delta_{k,k'} \delta_{j,j'},$$

$$(1)$$

where $T = \hbar^2/(2m^*R_{ext}^2)$ is an energy factor, m^* the effective mass of the semiconductor material, R_{ext} is the external radius of the polar grid, $t_r = (R_{ext}/\delta r)^2$, $t_{\phi} = [R_{ext}/(r_k\delta\phi)]^2$, $t_{\rm B} = \hbar eB/(m^*T)$ is the cyclotron energy in units of T, e is the electron charge and B a magnetic field perpendicular to the ring plane (which lifts energy degeneracies due to spin and angular momentum), σ_z stands for the *z*th Pauli matrix, $\gamma = g^*m^*/(2m_e)$ is the ratio between the Zeeman gap and the cyclotron energy with g^* being the electron g-factor, m_e the free electron mass, and V stands for an on-site potential.

The optical absorption coefficient is calculated in the dipole and zero temperature approximations according to Refs. [15, 16, 17] and equals

$$\alpha(\hbar\omega) = A\hbar\omega \sum_{\rm f} |\langle f|\boldsymbol{\varepsilon}\cdot\boldsymbol{d}|i\rangle|^2 \delta\left(\hbar\omega - (E_{\rm f} - E_{\rm i})\right),$$

where A is a constant, $\boldsymbol{\varepsilon} = (1, \pm i) / \sqrt{2}$ the circular polarization of the electromagnetic field, \boldsymbol{d} the dipole moment and $E_{i,f}$ the energies of the initial and final states $|i, f\rangle$, respectively. The delta function was approximated by a Lorentzian $(\Gamma/2) / \{[\hbar\omega - (E_f - E_i)]^2 + (\Gamma/2)^2\}$, where Γ is a phenomenological broadening. Since we neglect spin-orbit coupling, optical transitions do not allow for spin flip.

3. RESULTS

In all of the cases analyzed below the external radius of the disk-shaped grid, which is also the largest radius of the tetragons, is set equal to 25 nm and the side thicknesses are equal to 5 nm. The material parameters correspond to InAs, where $m^* = 0.023m_e$ and $g^* = -14.9$ and thus the energy unit T introduced in the Hamiltonian (1) is approximately 2.8 meV and the ratio $\gamma = -0.171$. The samples consist of over 6000 grid points.



Figure 2: Energy levels (a). Density of states (gray - dotted) and absorption coefficients in the presence of clockwise (red - dashed) and counterclockwise (green - solid) polarization for the diamond ring shown in Fig. 1 initially containing one electron in the ground state [(b) and (c)].



Figure 3: Probability densities corresponding to the first 12 levels shown in Fig. 2(a). Corner states of the lowest (a) and second (b) energy groups, then purely side localized states (c), and finally higher states where side and corner localization coexists (d). For proper comparison the probability density in (c) and (d) was scaled by a factor of three.

In a recent study we analyzed regular polygons [13]. In the present paper we discuss what happens when the symmetry of the polygon is changing. To do so we modify the square ring by decreasing one diagonal to 40 nm and obtain a diamond quantum ring as shown in Fig. 1. Several low energy levels of this sample are plotted in Fig. 2(a), where one can distinguish two groups of states which look like four-fold degenerated energy levels, but in fact they are composed of two close-by spin (two-fold) degenerated eigenvalues [inset to Fig. 2(a)]. The shape and depth of the effective wells formed in the vicinity of the vertices depend on corner angles and areas. Sharper corners have a larger area between the external and the internal boundaries of the polygon, which results in formation of deeper wells. Thus the lowest energy states, No. 1-4, are localized in the sharpest corners [3(a)], and the higher energy states, No. 5-8, are spread between the (shallower) wells existing in the wider corners [3(b)]. This results in formation of an energy gap of about 50 meV in the corner state domain. For a square polygon the two groups of four states merge into a single group of eight states with a dispersion of about 5 meV [13] (also shown below). For the higher levels of the energy spectrum the probability distributions are spread over the polygon sides. The distribution corresponding to the first energy level above the corner localized groups, states No. 9-10, is purely delocalized between the side areas [Fig. 3(c)] similarly to the side states of a square ring. The localization pattern of the higher states includes a small probability of finding the electron in corner areas, but here in the sharper corners for the second state above the corner-localized group, No. 11-12 [Fig. 3(d)] or in the wider corner areas for the next energy level (not shown). This means that electron distribution for a diamond ring differs considerably from the one of a square sample only in the low-energy domain.

The symmetry reduction and formation of two different wells affects absorption of electromagnetic field. To remove the spin degeneracy we consider the diamond sample immersed in a weak magnetic field of 0.53 T, perpendicular to its plane, which produces a spin splitting of 0.48 meV. We assume the sample initially contains an electron in the ground state. As seen in Fig. 2, light which is circularly polarized in the sample plane may excite the electron to two other corner states [Fig. 2(b)] as well as to side-localized states [Fig. 2(c)] and all four transitions occur in the presence of both clockwise and counterclockwise polarization types. In the analogous case of a square ring only two, complementary transitions occur for each type of polarization [13].



Figure 4: Probability distribution associated with the ground state of a diamond sample with an on-site potential equal to 372 meV(a), corresponding energy levels (b), and absorption spectrum for magnetic field equal to 0.53 T [(c) and (d)].

An external electric field allows to control electron distribution within a ring. If it is applied in the plane of the polygon it affects all of the corners and changes the geometry of the effective wells formed in their vicinity. This may easily break wave function symmetry, and thus open all spin allowed transitions, or partially restore symmetric electron localization in asymmetric samples [13]. Even more precise control may be achieved if point contacts are applied in the corner areas which enable to control the depth of each well separately.

To model this later situation we applied an on-site potential in the wider corner areas of diamond sample as indicated by the blue points in Fig. 1. Negative potential deepens the quantum wells and thus shifts the energy levels of the sample and delocalizes low-energy carriers between all of the corners. The ratio of probability maxima depends on the value of the external potential and may be continuously adjusted, i.e., probability distribution may become equally distributed between all four corners as in the case of an ideal square ring [Fig. 4(a)]. In this case the energy spectrum is nearly indistinguishable from the one of square sample [Fig. 4(b) and Ref. [13]], but even levels which seem to be four-fold degenerated consists of pairs of very close only spin degenerated eigenvalues. In the case shown in Fig. 4 this splitting is a results of a small mismatch of the potential and could be reduced even further. As long as all corners are populated, even if the localization peaks differ considerably from each other, the energy spectrum resembles more the one of a square sample [13] than of a diamond ring [Fig. 2(a)].

Interesting effects are observed in the absorption spectrum if all of the corners are nearly equally populated. As seen in Figs. 4(c) and 4(d), two transitions from the ground state to corner- and side-localized states occur, but in each domain one of the absorption coefficient's maximum is about 1000 times smaller from the other one. Thus, irrespective of the sample shape, only two relevant transitions associated with one polarization type take place, as

in the case of square rings [13].

4. CONCLUSIONS

We studied electron localization and optical absorption of a diamond quantum ring and compared it to the square sample. We showed that this geometry induces two groups of low-energy states localized either in the sharper or in the wider corners, respectively. The probability distributions associated with higher energy levels are mostly spread over all polygon sides and resemble those of square rings. Diamond rings allow for more optical transitions in the presence of one circular polarization type than square rings. We also showed that gates applied in corner areas enable to achieve a wide range of electron localization patterns and thus different energy and absorption spectra within one sample irrespective of its shape which opens wide range of control possibilities.

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REFERENCES

- [1] T. Rieger, D. Grutzmacher, and M. I. Lepsa, Misfit dislocation free InAs/GaSb core-shell nanowires grown by molecular beam epitaxy, Nanoscale 7, 356 (2015).
- [2] F. Qian, Y. Li, S. Gradečak, Deli Wang, C. J. Barrelet, and Ch. M. Lieber, Gallium nitride-based nanowire radial heterostructures for nanophotonics, Nano Letters 4, 1975 (2004).
- [3] F. Qian, S. Gradečak, Yat Li, Ch.-Y. Wen, and Ch. M. Lieber, Core/multishell nanowire heterostructures as multicolor, high-efficiency light-emitting diodes, Nano Letters 5, 2287 (2005).
- [4] K. L. Kavanagh, I. Saveliev, M. Blumin, G. Swadener, and H. E. Ruda, Faster radial strain relaxation in InAs–GaAs core–shell heterowires, J. Appl. Phys. 111, 044301 (2012).
- [5] J. Jadczak, P. Plochocka, A. Mitioglu, I. Breslavetz, M. Royo, A. Bertoni, G. Goldoni, T. Smolenski, P. Kossacki, A. Kretinin, H. Shtrikman, and D. K. Maude, Unintentional high-density p-type modulation doping of a GaAs/AlAs core–multishell nanowire, Nano Letters 14, 2807 (2014).
- [6] A. Bertoni, M. Royo, F. Mahawish, and G. Goldoni, Electron and hole gas in modulation-doped AaAs/Al_{1-x}Ga_xas radial heterojunctions, Phys. Rev. B **84**, 205323 (2011).
- [7] M. Royo, A. Bertoni, and G. Goldoni, Landau levels, edge states, and magnetoconductance in AaAs/AlGaAs core-shell nanowires, Phys. Rev. B 87, 115316 (2013).
- [8] M. Royo, A. Bertoni, and G. Goldoni, Symmetries in the collective excitations of an electron gas in core-shell nanowires, Phys. Rev. B 89, 155416 (2014).
- [9] M. Fickenscher, T. Shi, H. E. Jackson, L. M. Smith, J. M. Yarrison-Rice, Ch. Zheng, P. Miller, J. Etheridge, B. M. Wong, Q. Gao, S. Deshpande, H. H. Tan, and Ch. Jagadish, Optical, structural, and numerical investigations of GaAs/AlGaAs core–multishell nanowire quantum well tubes, Nano Letters 13, 1016 (2013).
- [10] T. Shi, H. E. Jackson, L. M. Smith, N. Jiang, Q. Gao, H. H. Tan, Ch. Jagadish, Ch. Zheng, and J. Etheridge, Emergence of localized states in narrow GaAs/AlGaAs nanowire quantum well tubes, Nano Letters 15, 1876 (2015).
- [11] D. W. L. Sprung, H. Wu, and J. Martorell, Understanding quantum wires with circular bends, 71, 515 (1992).
- [12] A. Ballester, J. Planelles, and A. Bertoni, Multi-particle states of semiconductor hexagonal rings: Artificial benzene, J. Appl. Phys. 112, 104317 (2012).
- [13] A. Sitek, L. Serra, V. Gudmundsson, and A. Manolescu, Electron localization and optical absorption of polygonal quantum rings, arXiv:1503.09186 (2015).
- [14] 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).

- [15] H. Haug and S. W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, World Scientific, Singapore, 5th edition (2009).
- [16] S. L. Chuang, *Physics of Optoelectronic Devices*, John Wiley and Sons, Inc., New York (1995).
- [17] H. Hu, J.-L. Zhu, and J.-J. Xiong, Energy levels and far-infrared spectroscopy for two electrons in a nanoscopic semiconductor ring, Phys. Rev. B 62, 16777 (2000).