ELECTRONIC PROPERTIES OF PSEUDO-ELLIPTIC QUANTUM RINGS: INFLUENCE OF IMPURITY POSITION AND ELECTRON SPIN

Doina BEJAN[1], Cristina STAN[2]*, and Alina PETRESCU-NIȚĂ[3]

We present a theoretical study on the influence of donor impurity position and Zeeman effect and Rashba and Dresselhaus spin-orbit couplings on the electronic properties of a GaAs/GaAlAs pseudo-elliptic quantum ring submitted to a magnetic field. The electronic spectra without/with spin were computed in the framework of the effective mass approximation for four representative positions of the impurity along the x-axis: ring center, inner and outer edges and ring middle. Our results reveal that the electronic spectrum of the ring with impurity placed at the ring middle differs greatly from the spectra obtained for the other positions of the impurity. This feature was correlated with the binding energy which is largest for this position of the impurity. The energy splitting produced by the electron spin through Zeeman effect and Rashba and Dresselhaus spin-orbit couplings increases at the magnetic field strengthening but is always lower than the Zeeman splitting.

Keywords: quantum ring, donor impurity, spin-orbit interaction, Zeeman effect, binding energy, magnetic field.

1. Introduction

There is a growing interest in the study of electron spin effects in low-dimensional semiconductor structures because their atom-like properties, together with a high flexibility in size, shape and carriers density, make them very attractive to build new devices such as electron spin beam splitters [1], spin field effect transistors or magneto-resistive random-access memory [2, 3] based on spin dynamics.

The electron spin controls the design of energy shells but also the optical absorption or magnetic properties of semiconductor quantum nanostructures. One

[1] Assoc. Prof., Faculty of Physics, University of Bucharest, Bucharest, Romania, e-mail: doinitabejan@yahoo.com
[2]* Prof., Faculty of Applied Sciences, "Politehnica" University of Bucharest, Bucharest, Romania, e-mail: cristina.stan@upb.ro
[3] Assoc. Prof., Faculty of Applied Sciences, "Politehnica" University of Bucharest, Bucharest, Romania, e-mail: alina.petrescu@ upb.ro

way to manipulate the spin is via spin-orbit interaction since it translates the spatial motion of an electron into rotation of its spin. The origin of spin-orbit interaction (SOI) in semiconductor nanostructures is attributed to two distinct mechanisms: the Dresselhaus SOI coupling [4] which is due to bulk inversion asymmetry of the lattice and the Rashba SOI coupling [5], determined by structure inversion asymmetry along the growth direction. Both SOI result in the splitting of electron energy levels and in the mixing of the electron spin states.

The impurities influence the electronic properties of these structures, allowing a proper tailoring of the transition energy, and in turn modify both optical and magnetic properties [6-9].

The purpose of this paper is to analyse the influence of donor impurity position and of Zeeman effect, Rashba and Dresselhaus spin-orbit couplings on the electronic properties of a GaAs/GaAlAs pseudo-elliptic quantum ring (PEQR) submitted to a magnetic field. The quantum ring-type structure with a pseudo-elliptic shape, suggested by AFM images of InGaAs self-assembled rings [10], is modeled by an outer ellipsis and an inner circle.

The electronic spectra obtained in this paper will be used to deduce the magnetic properties of the ring in a following paper. The outline of the paper is as follows: In Section 2, the theoretical framework is briefly given. Numerical results presented in Section 3 are followed by the conclusions given in Section 4.

2. Theory

For the mathematical modeling, we consider a conduction band electron confined into a PEQR under the simultaneous action of the Coulomb attraction due to an ionized donor and a magnetic field perpendicular to the ring plane. In the framework of the effective mass approximation, the single-particle Hamiltonian is:

$$H_0 = \frac{\hbar^2 k^2}{2m^*} + V\left(\vec{r}_{\parallel}\right) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r\left|\vec{r}-\vec{r}_i\right|} \tag{1}$$

where $\vec{k} = -i\nabla + e\vec{A}/\hbar$ with $\vec{A} = B/2(-y, x, 0)$ the potential vector in the Coulomb gauge ($\nabla\vec{A} = 0$), m^* is the effective mass of the electron, e is the absolute value of the electron charge, $\vec{r} = (x, y, z)$ is the position vector of the electron, $\vec{r}_i = (x_i, y_i)$ is the position vector of the donor impurity in the ring plane, $\vec{r}_{\parallel} = (x, y)$ is its projection on the ring plane. $V\left(\vec{r}_{\parallel}\right)$ is the confinement potential, defined as:

$$V\left(\vec{r}_{||}\right)=\frac{\hbar^2}{2m^*}\frac{\lambda^2}{x^2+y^2}+\frac{m^*}{2}\left(\omega_{0x}^2x^2+\omega_{0y}^2y^2\right), \tag{2}$$

where λ is the dimensionless parameter measuring the strength of the inverse square potential (describing the forbidden hollow region inside the ring) and ω_{0x}, ω_{0y} are the confinement frequencies of the parabolic potential.

In our computation, we consider a constant height of the ring, smaller than the in-plane dimensions. Under such conditions, the electron has a fast-movement along the z-direction and a slow-movement in the *xy*-plane that ensures the adiabatic separation of motions. It also guarantees that is only one allowed quantum state along *z,* so that the motion in the *xy*-plane determines completely the electronic properties of our ring. Such a flat QR, with no (or very little) vertical variation of height, can be easily achieved by droplet molecular epitaxy technique [11]. Consequently, the in-plane motion in the absence of SOI is described by the Hamiltonian:

$$H_{0||}=-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\frac{ieB\hbar}{2m^*}\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)+\frac{e^2B^2}{8m^*}\left(x^2+y^2\right)+V\left(\vec{r}_{||}\right)$$
$$-\frac{e^2}{4\pi\varepsilon_0\varepsilon_r\sqrt{\left(x-x_i\right)^2+\left(y-y_i\right)^2+d_{cutoff}^2}}\ . \tag{3}$$

Here we introduced a cut off distance to regularize the Coulomb potential which is singular at the origin [12].

Including the spin through the Zeeman effect and spin-orbit interaction, we get:

$$H=H_{0||}I_2+\frac{1}{2}g\mu_B B\sigma_z+H_R+H_D\ . \tag{4}$$

In Eq. 4, I_2 stands for the 2x2 identity matrix, μ_B is the Bohr magneton, g represents the Landé factor for the bound electron, σ_i *(i=x, y, z)* are the *i* component of the Pauli matrices vector and H_R, H_D introduce the Rashba [4] and Dresselhaus [5] spin-orbit interactions with α and β intensities, respectively. For *x* and *y* axes oriented parallel to [100] and [010] crystal directions, respectively, the spin-orbit coupling terms along *z* axis are:

$$H_R=\alpha\left(\vec{\sigma}\times\vec{k}\right)_z=\alpha\left(\sigma_x k_y-\sigma_y k_x\right) \tag{5}$$

$$H_D=\beta\left(\sigma_x k_x-\sigma_y k_y\right). \tag{6}$$

The energies (denoted E_{0j} for the ring without spin and E_j for the ring with spin) were numerically computed using the finite element method [13].

3. Results and discussion

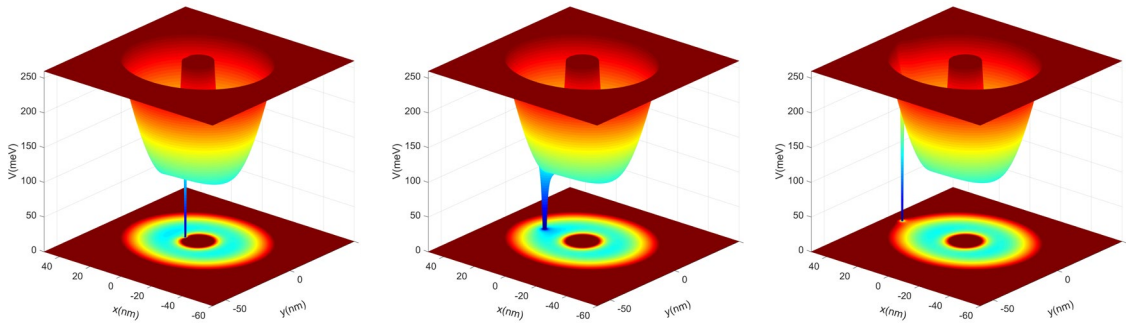
For easy comparison of the results, we use in this work the same parameters for the ring as in our previous papers, where we studied the influences of geometry, internal distortions and magnetic and electric fields on this particular QR [14-18]. The numerical values are: $m^* = 0.067 m_0$ (where m_0 is the mass of a free electron), ε_r=12.55, λ^2=30, ω_{0x}=28.42 THz, ω_{0y}=31.58 THz, V_0=260 meV (for GaAs/$Ga_{0.65}Al_{0.35}As$). The inner radius of the pseudo-elliptic ring $R_1 = \sqrt{\hbar^2\lambda^2/2m^*V_0} = 8.10\,\text{nm}$ corresponds to the value of $|\vec{r}_{||}|$ where the first term of Eq. 2 is equal to V_0 and the outer ellipse semiaxes $R_{x(y)} = \sqrt{2V_0 / m^* \omega_{0x(y)}^2}$ (R_x=41.10 nm and R_y=36.68 nm) are determined by the equality of the second term of the potential with V_0 [19].

Other parameters are: height h=2 nm [19], $N_0 = 5 \cdot 10^{22} m^{-3}$ [20], $d_{cuttoff}$=10^{-4} nm and temperature T=4 K. Considering a finite quantum well along the growth direction z, definite by V_0=260 meV and L_z=2 nm, the allowed energies for the electron, calculated using a discrete variable representation technique, are 184.65 meV, 264.63 meV, 270.83 meV, etc. Therefore, there is only one bounded state at E_{0z}=184.65 meV, and we can consider that all analyzed electron energies are relative to E_{0z}, the total energy of the electron being $E_{Tj} = E_{0z} + E_j$.

For the SOIs and Zeeman effect we have taken the most popular values from the literature for GaAs nanostructures [21,22]: α=5.4 meV·nm, β=10.8 meV·nm and g=-2.15.

The confining potentials of the pseudo-elliptic quantum ring in the presence of the impurity are represented in Fig. 1 for three positions of the donor impurity along the x direction: the edge of inner circle at x_i=R_1=8.1 nm, the middle distance

between the inner circle and outer ellipsis at $x_i=(R_1+R_x)/2=24.6$ nm (hereafter referred to as the ring middle) and finally, the edge of the outer ellipsis at $x_i=R_x=41.1$ nm.



a) b) c)

Fig. 1 The 3D potential profile of the pseudo-elliptic ring with an impurity at: a) $x_i=8.1$ nm, edge of inner circle; b) $x_i=24.6$ nm, the middle distance between the inner circle and outer ellipsis; c) $x_i=41.1$ nm, the edge of outer ellipsis. The infinite potential was cut with a horizontal plane at $V_0=260$ meV.

We computed the energy spectra as functions of the magnetic field for the ring with donor impurity in the three positions showed in Fig. 1 and also for the ring with impurity placed in the ring center ($x_i=0$).

Figure 2 shows the energy spectra of PEQR in the absence of Zeeman effect and spin-orbit interaction. All the spectra are obtained varying B from 0 to 10 T with a step size of 0.2 T.

The spectrum of the ring with on center impurity is quite comparable to that of the ring without impurity, analyzed in our previous papers [14,17], showing Aharonov-Bohm-like oscillations.

The influence of the impurity is stronger for a placement at the edge of inner circle at $x_i=8.1$ nm. The energies are lowered and the first four states are completely decoupled. Also, the oscillations of the first three states are washed out.

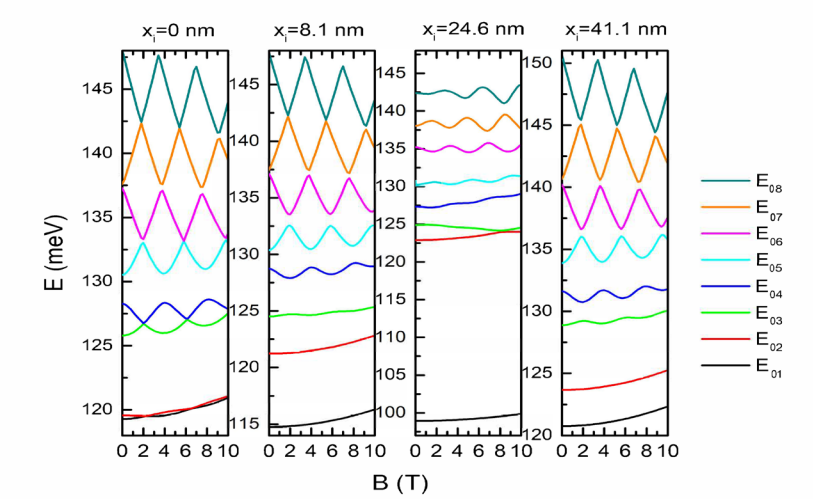


Fig. 2 The energies of the lowest states of the ring with an impurity at: x_i=0, the ring center; x_i=8.1 nm, edge of inner circle; x_i=24.6 nm, the middle distance between the inner circle and outer ellipsis; x_i=41.1 nm, the edge of outer ellipsis.

When the impurity is placed at the middle of the ring, we observe the strongest impact on the energy. All the represented levels are decoupled and the oscillations are suppressed for the first five levels. Also, the energy values are the lowest ones.

The impurity influence is again reduced for the position on the edge of the outer ellipsis. The energy spectrum looks like the spectrum of PEQR with impurity on the edge of inner circle but with higher energies.

The influence of the position impurity on the energy spectra may be better understood through its binding energy, illustrated in Fig. 3 as a function of the magnetic field.

The binding energy is defined as the energy difference between the electron energy in the ring without impurity (see [17], Fig. 1c) and the energy of the electron in the confined impurity. We can see that the binding energy is highest for the impurity placed at the middle of the ring than at the edges or the ring center. This feature is a consequence of the fact that the impurity experiences the lowest value of the potential in middle, since it is close to the potential's minimum. Also, the binding energy increases slightly with the magnetic field for the impurity placed in middle, but is almost constant when the impurity is placed at the ring edges or ring center, demonstrating that shallow donors are less influenced by the magnetic field.

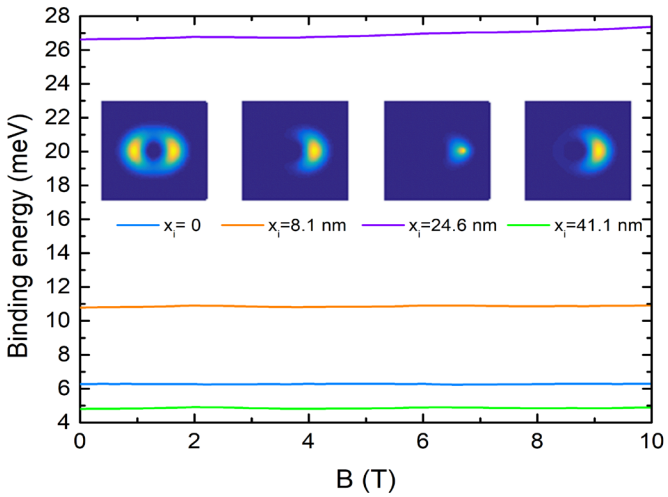


Fig. 3 The binding energy of the impurity as a function of the magnetic field. Inset: *xy*-projection of the WFs of the ground states of the ring with impurity in the four considered positions, at B=0.

In the inset of Fig. 3 there are presented the wave functions of the ground states (WFGSs) computed at B=0, for the four studied positions of the impurity in the ring.

It is easily observed a strong localization in the case of x_i=24.6 nm. Also, one can see that for the impurity in the ring center, the WFGS has two symmetric lobes while for the other impurity positions the WFGSs have only one maximum centered on the position impurity. It can be noticed too that the spread of the WFGSs maximum is correlated to the corresponding binding energy. For instance, for the impurity in the middle, the WFGS localization is augmented by the increased binding energy due to the rise in the experienced confinement.

Figure 4 represents the energy spectra of the PEQR with impurity in the presence of both Zeeman effect and spin-orbit interaction. As general observations, the energy levels are split into two levels, but the Aharonov-Bohm oscillations are preserved. To each level corresponds always a spin-up and a spin-down eigenfunction [14,21,22].

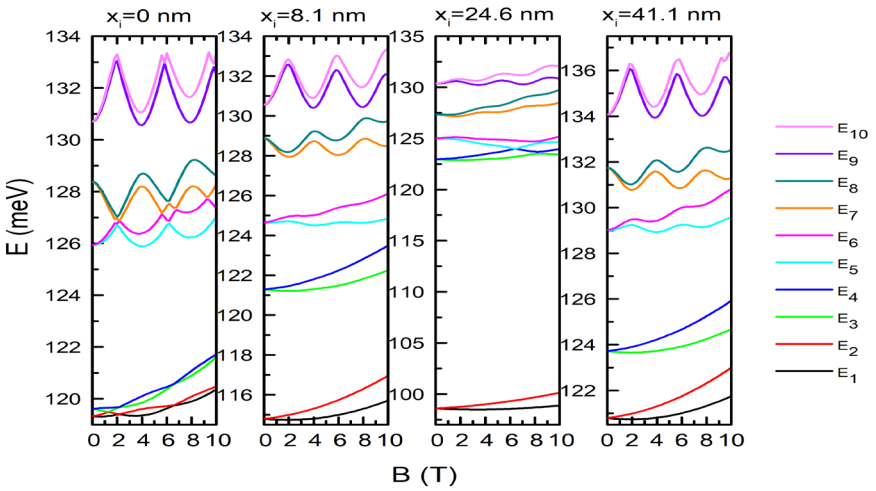


Fig. 4 The energies of the lowest states of the ring with Zeeman effect and spin orbit interaction for an impurity at: x_i=0, the ring center; x_i=8.1nm, edge of inner circle; x_i=24.6 nm, the middle distance between the inner circle and outer ellipsis; x_i=41.1 nm, the edge of outer ellipsis.

The energy spectrum of the PEQR with impurity at the edge of inner circle strongly resembles to the spectrum of the PEQR with impurity at the edge of outer ellipsis and has no anticrossings. Consequently, in both spectra, each level of the corresponding spectrum without spin is just split in two branches. On the contrary, the spectra of the PEQR with on center/middle impurity present anticrossings between states when the magnetic field is gradually increased.

Table 1

The total spin splitting ($\Delta E_{12}=E_2-E_1$) at strong magnetic fields

B (T)	20	30	40
impurity at 8.1 nm	2.37 meV	3.58 meV	4.73 meV
impurity at 24.6 nm	2.43 meV	3.65 meV	4.88 meV
impurity at 41.1 nm	2.36 meV	3.08 meV	3.68 meV

The SOIs shift down the entire spectrum approximately with a constant value $\left(\alpha^2+\beta^2\right)\frac{m^*}{\hbar^2}=0.129$ meV (exact value for this shift only at B=0). The energy splitting produced by SOI increases at the magnetic field strengthening but is always little lower than the one produced only by the Zeeman effect. For instance, at B=10 T, the Zeeman splitting is 1.245 meV, but the total split produced by Zeeman effect and SOI is 1.207 meV for the ring with impurity in the ring middle and 1.170 meV

for the ring with impurity at inner/outer edges. However, at greater values of the B, the total spin splitting augments achieving values of few meV, as can be seen in Table 1. The maximum splitting appears in the ring with impurity at the ring middle, followed closely by the splitting for the ring with impurity at the edge of the inner circle. From Fig. 3 and Table 1, we deduce that the total spin splitting can be correlated with the binding energy.

4. Conclusions

In this paper, we have studied the electronic properties of a GaAs/GaAlAs pseudo-elliptic quantum ring. The influence of the Zeeman effect and spin-orbit interaction have been addressed for four positions of the donor impurity.

The computed energy spectra present Aharonov-Bohm-like oscillations for the highest states, for all impurity positions, and more or less for the lowest states. The strongest influence on the energy spectrum is found for the impurity placement in the ring middle i.e. the middle distance between the inner circle and outer ellipsis. This characteristic was correlated with the binding energy which is largest for this position of the impurity, and is reflected by the minimum spread of the wave function of the ground state. We found that the electron spin preserves the Aharonov-Bohm oscillations but splits the energy levels and removes the spin degeneracy. The effect of the spin-orbit coupling is very low on these structures. It just reduces the Zeeman splitting without additional effects. However, the total spin-splitting increases with the magnetic field achieving values of few meV at very strong magnetic fields.

These results will be used in the following paper [23] to compute the magnetization and the magnetic susceptibility of the pseudo-elliptic quantum rings.

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