MAGNETIC 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 the Zeeman effect, Rashba and Dresselhaus spin-orbit couplings and donor impurity position on the magnetic properties of a GaAs/GaAlAs pseudo-elliptic quantum ring. We found that the effects of the impurity on the magnetization are strongest when the impurity is placed at the ring middle. The average total energy, the magnetization and the magnetic susceptibility were computed using both Boltzmann and Fermi-Dirac statistics. If the electron spin is not included, both distributions lead to linear variations of the magnetization versus the magnetic field. The ring is diamagnetic having a susceptibility that increases slightly with the magnetic field. When electron spin is considered, the susceptibility decreases slowly with the field for the Fermi-Dirac distribution but shows a larger decrement with the magnetic field if Boltzmann distribution is used. In this latter case, the ring with impurity in the middle is paramagnetic at weak fields and diamagnetic for higher values of magnetic fields.

Keywords*:* quantum ring, donor impurity, spin-orbit interaction, Zeeman effect, magnetization, susceptibility.

1. Introduction

In the last years, there is a growing interest in the use of the electron spin in addition to its charge for information processing. Achieving a control on the spin manipulation has an important role in spintronics [1,2] and is a promising tool in the development of new, faster, and more powerful devices [3-5].

A lot of papers focused on the theoretical study of the magnetization and magnetic susceptibility of low-dimensional semiconductor nanostructures such as

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

quantum wells (QW) [6,7], quantum dots (QD) [8-16], quantum well wires (QWW) [17,18] and quantum rings (QRs) [19-24] taking into account one or more electrons in the presence or in the absence of the Zeeman effect and/or spin-orbit interaction. The effects of impurity, size, geometry, temperature, pressure, external fields and noise on the magnetic properties were also studied and their specific influence was evidenced [6-29].

In many papers [6,7,11-12,17,18], the susceptibility of the donor impurity was calculated as the second order derivative of the diamagnetic part of the electron energy in magnetic field, neglecting completely the spin effects. In other papers, the susceptibility was deduced from the magnetization that was calculated as the derivative of the energy of the fundamental state [21] or of a given state [14,16] including in this later case the Zeeman effect. Other methods to compute the magnetization have used: i) the derivative of the total energy of the quantum system taken as a sum over the energy levels [19,20]; ii) the derivative of the mean total energy of the system calculated using the canonical ensemble formula [10,13,14,23,24]; iii) the derivative of the average energy of a system connected to a reservoir and having a fixed chemical potential [8,9].

The effect of spin-orbit interaction on the magnetization and susceptibility was included only in few of the cited works [8,9,13,15,24].

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 magnetic properties of a GaAs/GaAlAs pseudo-elliptic quantum ring (PEQR). The average total energy and the magnetic properties were computed using comparatively the Boltzmann and Fermi-Dirac statistics. We demonstrate that the impurity position, as well as the electron spin, influences the magnetic properties and that some differences appear between the magnetic properties calculated with different statistics.

2. Theory

The energies for the ring without/with spin were numerically computed using the finite element method [30] for four positions of the impurity positions of the donor impurity along the x direction: ring center x_i=0, 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, in the theoretical framework described in our previous paper [31].

The Fermi level E_F at a given temperature is determined from the charge neutrality condition:

$$N_0 = \sum_{j=1}^{N_{max}} \rho_j \tag{1}$$

where N_0 is the total electron density in GaAs (that can be controlled through doping), N_{max} is the total number of energy levels lower than the barrier V_0 (the barrier potential for electrons in GaAs surrounded by a $Ga_{1-x}Al_xAs$ material) and ρ_j is the density of the electrons at thermal equilibrium in the subband E_j [8, 32,33]:

$$\rho_j = N_0 f_{FD}(E_j) = N_0\left[1 + exp\left(\frac{E_j - E_F}{k_B T}\right)\right]^{-1}. \tag{2}$$

Here, f_{FD} is the Fermi-Dirac distribution function, T is the absolute temperature and k_B is the Boltzmann constant.

In the literature, the average energy of quantum nanostructures is calculated using either the Fermi-Dirac statistic, specific to a system connected to a reservoir and having a fixed chemical potential [8,9]:

$$\langle E_T \rangle_{FD} = \frac{\sum_{j=1}^{N_{max}} \rho_j E_j}{\sum_{j=1}^{N_{max}} \rho_j} = \frac{\sum_{j=1}^{N_{max}} N_0 E_j f_{FD}(E_j)}{\sum_{j=1}^{N_{max}} N_0 f_{FD}(E_j)} = \frac{\sum_{j=1}^{N_{max}} E_j f_{FD}(E_j)}{\sum_{j=1}^{N_{max}} f_{FD}(E_j)}. \tag{3}$$

or using the formula of the mean values for the canonical ensemble [10,13,15,23,24]:

$$\langle E_T \rangle = \frac{\sum_{j=1}^{N_{max}} E_j \, exp\left(-\frac{Ej}{k_B T}\right)}{\sum_{j=1}^{N_{max}} exp\left(-\frac{Ej}{k_B T}\right)} \tag{4}$$

Eq. 4 can be also derived assuming a Boltzmann distribution on the energy levels of the quantum nanostructure [34]. In this case, the density of the electrons at thermal equilibrium on the E_j level is:

$$\rho_{Bj} = N_0 \frac{exp\left(-\frac{Ej}{k_B T}\right)}{\sum_{j=1}^{N_{max}} exp\left(-\frac{Ej}{k_B T}\right)} \tag{5}$$

It is obvious that ρ_{Bj} satisfies also Eq. 1 and that $\langle E_T \rangle_B = \frac{\sum_{j=1}^{N_{max}} \rho_{Bj} E_j}{\sum_{j=1}^{N_{max}} \rho_{Bj}}$ leads to Eq. 4. In the following we shall call the average energy given by Eq. 4 as the Boltzmann average energy $\langle E_T \rangle_B$.

The magnetic properties of the quantum ring are described by the magnetization and the magnetic susceptibility that are computed as:

$$M = -\frac{\partial \langle E_T \rangle}{\partial B} \tag{6}$$

and

$$\chi = \frac{\partial M}{\partial B} = -\frac{\partial^2 \langle E_T \rangle}{\partial B^2}. \tag{7}$$

For the computation of the average energy and magnetic properties of the ring we comparatively consider the both statistics. At this point, we want to emphasize that, from Eq. 2 and Eq. 1, one obtains

$$N_0 = \sum_{j=1}^{N_{max}} N_0 f_{FD}\left(E_j\right) \rightarrow 1 = \sum_{j=1}^{N_{max}} f_{FD}\left(E_j\right) \tag{8}$$

which is the same equation that was used in [8,9] for one electron per ring or QD. Therefore, N_0 does not play any role in determining the nanostructure Fermi level or its average energy and consequently it will not influence the magnetic properties of the ring.

Moreover, the Boltzmann statistics is valid only for distinguishable particle and must be replaced by Fermi-Dirac or Bose-Einstein statistics when the particles are indistinguishable. So, for electrons, we must use Fermi-Dirac statistic, especially because our ring contains around $2 \cdot 10^5$ atoms. Even that, when the average number of particles per quantum state is small [34], the Boltzmann and Fermi-Dirac formulas for the average total energy coincide, we will demonstrate in this work that the different statistical approaches may lead to some differences in the magnetic properties when the electron spin is considered.

3. Results and discussion

We use in this work the same numerical values for the parameters of the ring as in our previous paper [31].

We computed the Fermi level for B varying from 0 to 10 T with a step size of 0.2 T (using the data represented in Figs. 2 and 4 in [31]). In Fig. 1 it is represented the dependence of the Fermi energy on the magnetic field for the two analyzed cases: PEQR without spin (Fig. 1, full lines) and PEQR with SOI and Zeeman effect (Fig. 1, dashed lines).

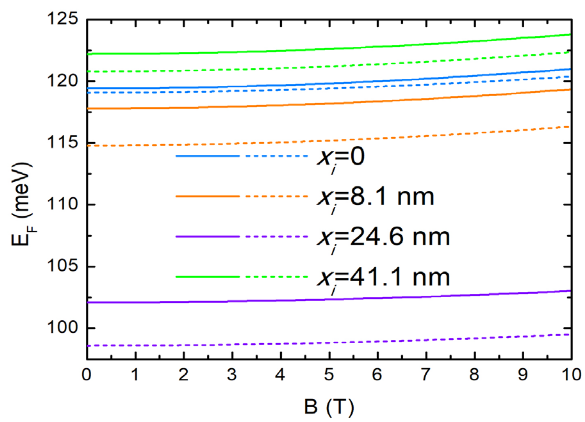

Fig. 1 The Fermi level of the pseudo-elliptic ring versus the magnetic field for different positions of the impurity without spin (full line) and with Zeeman and SOI (dashed line).

For the PEQR without spin, the Fermi level is always placed between the E_{01} (ground state) and E_{02} (first excited state) even for the impurity located in the ring center, where these two levels are very close. When spin-orbit interaction (SOI) and Zeeman effect are included, the levels splitting leads to lower values for the Fermi level. It goes below E_1 for small B values for the PEQR with on center impurity or an impurity placed at the outer ellipsis edge. However, the Fermi levels in Fig. 1 have a similar dependence with magnetic fields, for all impurity positions. This is a direct consequence of the fact that the inclusion of electron spin just splits the levels without altering their oscillations (see I).

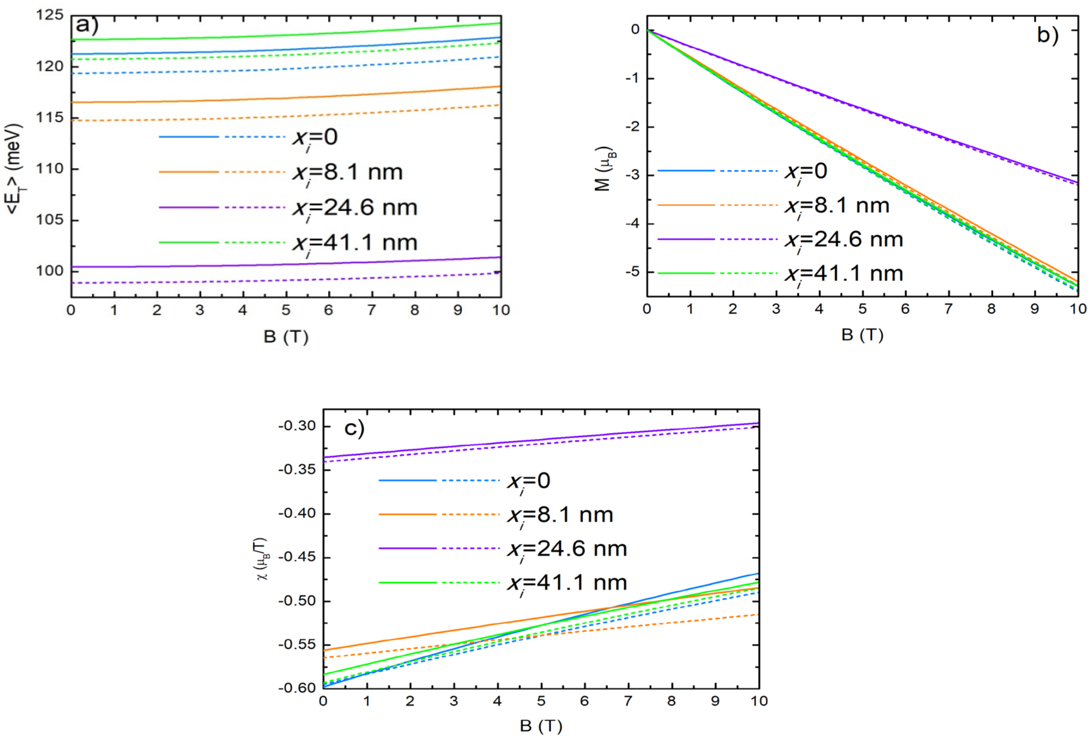

Fig. 2 a) The mean total energy of the pseudo-elliptic ring without spin b) magnetization and c) the susceptibility versus the magnetic field for different positions of the impurity. In all graphs, are represented with full line the results obtained with Fermi-Dirac distribution and with dashed line the results obtained with Boltzmann distribution.

The average total energy, calculated using the Fermi-Dirac distribution (Eq. 3) and the Boltzmann distribution (Eq. 4), is presented in Fig. 2a for the PEQR without spin. It can be seen that the values obtained with the Fermi-Dirac distribution are slightly higher. For both distributions, $\langle E_T \rangle$ was fitted with the function:

$$\langle E_T \rangle = \langle E_T \rangle_0 + \frac{\beta B^2}{1 + \alpha B} \tag{9}$$

where $\langle E_T \rangle_0$ represents the value at B=0. This function was proposed first for excitons in a quantum disk [35] but extended for hydrogenic impurity in a domeshape quantum dot [36] because this impurity behaves like an exciton with infinite hole effective mass. For all $\langle E_T \rangle$ we obtained a very good match. The values of α are very low (see Table 1), showing that actually $\langle E_T \rangle \cong \beta B^2$. For this reason, the magnetization as function of B has a linear variation, as can be seen in Fig. 2b. The magnetization is zero at B=0 and goes to negative values at the augment of the magnetic field. The susceptibility increases very slowly with the magnetic field but remains negative at the magnetic field strengthening having slightly different values for the two statistics. Such an increment of the susceptibility was obtained also for the diamagnetic susceptibility of a donor in a quantum well [6]. Consequently, the ring with impurity is diamagnetic at all field values if spin effects are not included.

It can be observed that the absolute values of the magnetization and susceptibility are lowest for the impurity placed in the ring middle where the impurity experiences the highest binding energy.

When electron spin is included, the dependence $\langle E_T \rangle = f(B)$ can still be well fitted with Eq. 9 for the Fermi-Dirac distribution. For the Boltzmann distribution, the average total energy can be fitted by Eq. 9 but also, equally, by a polynomial of third order without linear term

$$\langle E_T \rangle = \langle E_T \rangle_0 + aB^2 + cB^3 \tag{10}$$

except for the PEQR with impurity placed in the ring middle. In this case, the curve resulting from Boltzmann distribution can be well fitted only by Eq. 10, which determines a quadratic dependence in magnetization, as seen in Fig. 3b. Such dependence evidences that, in this case, the Boltzmann distribution might be inappropriate, because experimentally, only a quadratic dependence was found for $In_{0.55}Al_{0.45}As$ self-assembled quantum dots at low values of the magnetic field followed by a linear dependence at high values [35,37].

The inset of Fig. 3a presents a zooming around 100 meV where $\langle E_T \rangle_B$ was vertically translated to superpose over $\langle E_T \rangle_{FD}$ at B=0 to demonstrate that, in this particular case, the two statistics predict different dependences for the total energy versus magnetic field.

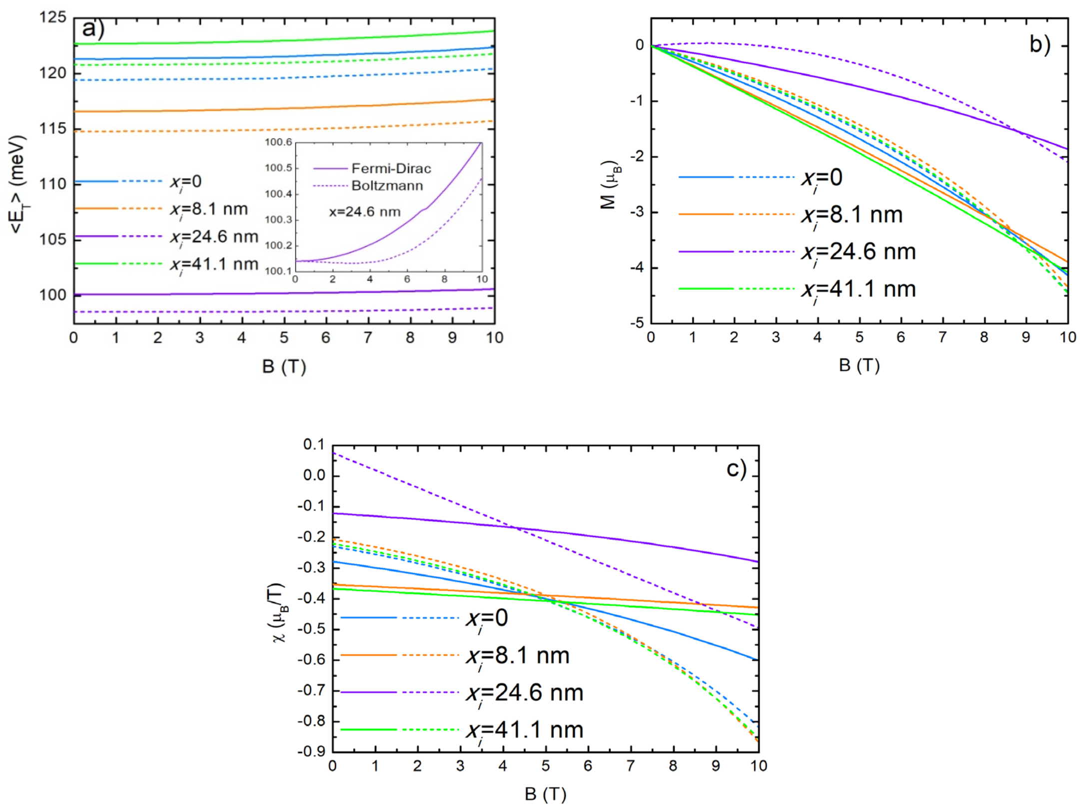

Fig. 3 a) The mean total energy of the pseudo-elliptic ring with spin, b) magnetization and c) the susceptibility versus the magnetic field for different positions of the impurity. In all graphs, are represented with full line the results obtained with Fermi-Dirac distribution and with dashed line the results obtained with Boltzmann distribution.

The magnetization takes now different values for the two distributions and for the different positions of the impurity. Due to the low values of α (see Table 1), the magnetization has almost a linear variation with B for the Fermi-Dirac distribution as in the absence of the electron spin. For the Boltzmann distribution, the magnetization shows a quadratic distribution for all impurity position even if $\left\langle E_T \right\rangle_B$ was calculated with Eq. 10 for the impurity in the ring middle and with Eq. 9 for the other impurity positions.

The values of susceptibility are negative and decrease slowly with B for the Fermi-Dirac distribution. Therefore, for this statistical approach, the electron spin has little influence on the diamagnetic behavior of the ring with impurity. It just lowers its magnetization and susceptibility (in absolute value) and leads to a decrement of the susceptibility instead an increment at the field strengthening as obtained in the spin absence.

Table 1

Theoretical values of α and β obtained for Fermi-Dirac distribution

impurity position	α_{FD}(meV/T) without spin	β_{FD}(meV/T^2) without spin	α_{FD}(meV/T) with spin	β_{FD}(meV/T^2) with spin
x_i=0	0.00852	0.0173	-0.0226	0.0087
x_i=8.1	0.00471	0.01609	-0.0062	0.01023
x_i=24.6	0.00422	0.0097	-0.02431	0.00351
x_i=41.1	0.00687	0.01689	-0.00672	0.01063

When Boltzmann distribution is considered (see Fig. 3c, dashed lines), the susceptibility has a larger decrement with B for all impurity positions. For the PEQR with impurity at x_i=24.6 nm, the system is in the paramagnetic phase at weak fields (χ>0) and, at the critical value B=1.327 T, it crosses into the diamagnetic phase (χ<0).

4. Conclusions

In this paper, we have studied the magnetic 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.

We computed the average total energy, the magnetization and the magnetic susceptibility using both Fermi-Dirac and Boltzmann statistics. If the spin is not considered, both distributions lead to a similar linear variation of the magnetization with magnetic field, that determines a diamagnetic behavior of the nanostructure, with a negative susceptibility that increases slowly with the magnetic field. The absolute values of the magnetization and susceptibility are lowest for the impurity placed in the ring middle where the impurity experiences the highest binding energy.

When spin-orbit interaction and Zeeman effect are added in the computation, differences in magnetization appear for the two distributions used, because the Fermi-Dirac distribution leads again to a negative value of the susceptibility decreasing slightly with the field, while the Boltzmann distribution leads to a decrement of the susceptibility with a larger variation at the magnetic field strengthening. The ring with an impurity at the ring middle is paramagnetic at weak fields and becomes diamagnetic starting from a critical intensity of the magnetic field.

Our work evidences the role played by the impurity position and electron spin in the evaluation of the magnetic properties of the rings, but also of the distribution used in computation. As the values of the susceptibility and magnetization are within the range detectable with current experimental techniques, experimental measurements could show if the susceptibility increases or decreases slightly or has an important lowering with the magnetic field, confirming in this way our results.

REFERENCES

[1] *S. Maekawa, S. O. Valenzuela, E. Saitoh, and T. Kimura* (eds.), *Spin Current*, Oxford University Press, Oxford, 2012.

[2] *J. Xia, W. Ge, and K. Chang*, *Semiconductor Spintronics*, World Scientific, Singapore, 2012.

[3] *L. Zhang, P. Brusheim, H.Q. Xu,* "Multimode electron transport through quantum waveguides with spin-orbit interaction modulation: Applications of the scattering matrix formalism", Phys. Rev. B **72** (2005) 045347.

[4] *Madhav K. Singh, Pradeep K. Jha, Aranya B. Bhattacherjee*, *"Spin and tunneling dynamics in an asymmetrical double quantum dot with spin-orbit coupling: Selective spin transport device"*, J. Appl. Phys. **122** (2017) 114301.

[5] *P. Földi, O. Kálmán, M. G. Benedict, and F. M. Peeters*, "Quantum rings as electron spin beam splitters", Phys. Rev. B **73** (2006) 155325.

[6] *E. Kilicarslan, S. Sakiroğlu, M. Köksal, H. Sari, I. Sökmen*, " The effects of the magnetic field and dielectric screening on the diamagnetic susceptibility of a donor in a quantum well with anisotropic effective mass", Physica E **42** (2010) 1531.

[7] *E. Kasapoğlu, F. Ungan, H. Sari, I. Sökmen*, "The diamagnetic susceptibilities of donors in quantum wells with anisotropic effective mass", Superlattices Microstruct. **46** (2009) 817.

[8] *O. Voskoboynikov, O. Bauga, C. P. Lee, O. Tretyak*, "Magnetic properties of parabolic quantum dots in the presence of the spin-orbit interaction", J. Appl. Phys. **94** (2003) 5891.

[9] *J. Lee, H. N. Spector, W. C. Chou, C. S. Chu*, " Rashba spin splitting in parabolic quantum dots", J. Appl. Phys. **99** (2006) 113708.

[10] *B. Boyacioglu, A. Chatterjee*, "Dia-and paramagnetism and total susceptibility of GaAs quantum dots with Gaussian confinement", Physica E **44** (2012) 1826.

[11] *B. Vaseghi, T. Sajadi*, "Simultaneous effects of pressure and temperature on the binding energy and diamagnetic susceptibility of a laser dressed donor in a spherical quantum dot", Physica B **407** (2012) 2790.

[12] *A. Bera, S. Saha, J. Ganguly, M. Ghosh*, "Exploring diamagnetic susceptibility of impurity doped quantum dots in presence of Gaussian white noise", J. Phys. Chem. Solids **98** (2016) 190.

[13] *D. S. Kumar, S. Mukhopadhyay, A. Chatterjee*," Effect of Rashba interaction and Coulomb correlation on the ground state energy of a GaAs quantum dot with parabolic confinement", J. Magn. Magn. Mater. **418** (2016) 169-174.

[14] *A. Boda*, "Magnetic moment and susceptibility of an impurity in a parabolic quantum dot", J. Magn. Magn. Mater. **483** (2019) 83.

[15] *J. D. Castaño-Yepes, D. A. Amor-Quiroza, C.F. Ramirez-Gutierrez, Edgar A. Gómez,* "Impact of a topological defect and Rashba spin-orbit interaction on the thermo-magnetic and optical properties of a 2D semiconductor quantum dot with Gaussian confinement", Physica E **109** (2019) 59.

[16] *K. L. Jahan, B. Boyacioglu, A. Chatterjee*, "Effect of confinement potential shape on the electronic, thermodynamic, magnetic and transport properties of a GaAs quantum dot at finite temperature ", Sci. Rep. **9** (2019) 15824
[17] *R. Khordad*," Diamagnetic susceptibility of hydrogenic donor impurity in a V-groove GaAs/Ga1- x Al x As quantum wire", Eur. Phys. J. B **78** (2010) 399.
[18] *E. C. Niculescu, A. Radu*, "Laser-induced diamagnetic anisotropy of coaxial nanowires", Curr. Appl. Phys.**10** (2010) 1354.
[19] *W. C. Tan, J.C. Inkson*, "Magnetization, persistent currents, and their relation in quantum rings and dots", Phys. Rev. B **60** (1999) 5626.
[20] *O. Voskoboynikov, Y. Li, H. M. Lu, C. F. Shih, C. P. Lee*, "Energy states and magnetization in nanoscale quantum rings"Phys. Rev. B **66** (2002) 155306.
[21] *V. M. Fomin, V. N. Gladilin, S. N. Klimin, J. T. Devreese, N. A. J. M. Kleemans , P. M. Koenraad*, "Theory of electron energy spectrum and Aharonov-Bohm effect in self-assembled Inx Ga1-x As quantum rings in GaAs" Phys. Rev. B **77** (2008) 205326.
[22] *V. A. Margulis, V. A. Mironov*, "Magnetic moment of an one-dimensional ring with spin-orbit interaction", Physica E **43** (2011) 905.
[23] *M. K. Elsaid, A. Shaer, E. Hjaz, M. H. Yahya*, "mpurity effects on the magnetization and magnetic susceptibility of an electron.", Chin. J. Phys. **64** (2020) 9.
[24] *Hong-Yi Chen, P. Pietiläinen and T. Chakraborty*, "Some unique magnetic properties of nanoscale quantum rings subjected to a Rashba spin-orbit interaction", Phys. Rev. B **78** (2008) 073407.
[25] *E. Niculescu, G. Tiriba, A. Spandonid*e, "Optical absorption in pyramid-shaped quantum dots under applied electric and magnetic fields", U.P.B. Sci. Bull., Series A, **77** (2015) 229.
[26] *D. Bejan, C. Stan*, "Influence of spin–orbit interaction, Zeeman effect and light polarisation on the electronic and optical properties of pseudo-elliptic quantum rings under magnetic field", Philos. Mag. **100** (2020) 749.
[27] *D. Bejan, C. Stan*, "Electron spin and donor impurity effects on the absorption spectra of pseudo-elliptic quantum rings under magnetic field", Philos. Mag. **101** (2021) 1871.
[28] *D. Bejan, C. Stan*, "Aharonov-Bohm oscillations in pseudo-elliptic quantum rings: influence of geometry, eccentricity and electric field", Eur. Phys. J. Plus **134** (2019) 127.
[29] *D. Bejan*, "Donor impurity-related nonlinear optical rectification in a two-dimensional quantum ring under magnetic field", Phys. Lett. A **381** (2017) 3307.
[30] *R. D. Cook, D. S. Malkus, M. E. Plesha*, "Concepts and Applications of Finite Element Analysis", 3rd edition, John Wiley & Sons, New York, 1989.
[31] *D. Bejan, C. Stan, A. Petrescu-Niță*, "Electronic properties of pseudo-elliptic quantum rings: influence of impurity position and electron spin", U.P.B. Sci. Bull., Series A, **83** (2021) 253.
[32] *C.M. Duque, Ruben E. Acosta, A.L. Morales, M.E. Mora-Ramos, R.L. Restrepo, J.H. Ojeda, E. Kasapoglu, C.A. Duque*, "Optical coefficients in a semiconductor quantum ring: Electric field and donor impurity effects", Opt. Mat. **60** (2016) 148.
[33] *D. Ahn and S. L. Chuang*, "Calculation of Linear and Nonlinear. Intersubband Optical Absorptions in a Quantum well with an Applied Electric Field", IEEE J. Quantum Electron. **23** (1987) 2196.
[34] *A. N. Matveev*, *Molecular Physics*, Mir Publishers, Moscow, 1985.
[35] *K. L. Janssens, F.M. Peeters, V. A. Schweigert,* "Magnetic-field dependence of the exciton energy in a quantum disk", Phys. Rev. B **63** (2001) 205311.

[36] *E.C. Niculescu, C. Stan, M. Cristea, C. Trusca*, "Magnetic-field dependence of the impurity states in a dome-shaped quantum dot", Chem. Phys. 493 (2017) 32.

[37] *P. D. Wang, J. L. Merz, S. Fafard, R. Leon, D. Leonard, G. Medeiros-Ribeiro, M. Oestreich, P. M. Petroff, K. Uchida, N. Miura, H. Akiyama, and H. Sakaki*, "Magnetoluminescence studies of InyAs1−yAs self-assembled quantum dots in AlxGa1−xAs matrices", Phys. Rev. B **53** (1996) 16 458.