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MAGNETIC PROPERTIES OF QUANTUM RINGS IN THE PRESENCE OF SPIN-ORBIT AND ELECTRON-ELECTRON INTERACTIONS

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The separate and combined influences of the spin-orbit and electron-electron interactions on the electron magnetization in quantum rings have been studied theoretically on the basis of the spin-density-functional theory and the Kohn–Sham equation used for the calculation of electron states in two-dimensional parabolic quantum rings containing from two to six electrons. The magnetization of electrons in a quantum ring is calculated at zero temperature. The revealed abrupt changes in the ring magnetization are associated with the crossing of electron states that occurs if the spin-orbit and/or electron-electron interactions are taken into consideration.

K e y w o r d s: Kohn–Sham, qubit, Hartree–Fock, Broyden, Rashba, quantum dots, spin-orbit splitting.

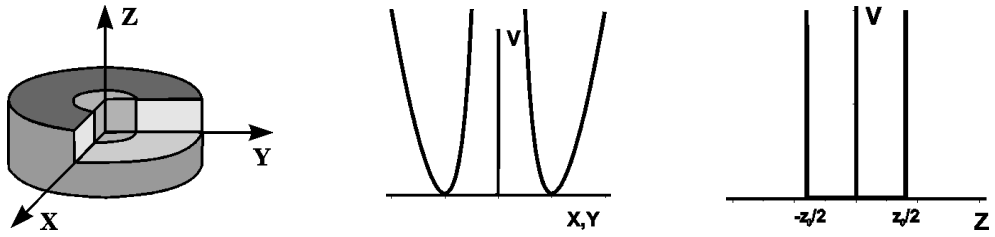
1. Introduction

Spintronics is a branch of electronics, in which the principle of device operation is based on the use of electron's spin degree of freedom. Some devices belonging to this group have already proved their importance even at the commercial level. In particular, spin-valve reading heads of hard disks can serve as an example of such an application. The review of this direction can be found in work [1].

This research is devoted to quantum rings (QRs). The study of those systems is challenging, because both QRs and quantum dots (QDs) can be regarded as artificial atoms. In contrast to ordinary atomic systems, QRs possess a variety of features including the possibility to manipulate their magnetic properties with the use of an external electric field [2, 3]. Quantum rings can be used as qubits in quantum computers. Therefore, their properties studied in this work should be taken into consideration when designing such devices.

The aim of this work is to analyze the influence of the spin-orbit interaction in weak magnetic fields on the magnetic properties of small semiconducting QRs. The magnetization of QRs in a quasiparabolic potential for electrons was calculated with regard for for the spin-orbit (SO) and electron-electron (EE) interactions. In the previous works, theoretical researches of the magnetic properties of QDs with regard for the SO [4] and EE [5] couplings were carried out. The magnetic properties of QRs taking the SO interaction into account were also calculated [6], but the EE coupling for QRs was not considered.

To describe the influence of spin-orbit interaction on QR magnetization, the Rashba approximation was applied [7, 8]. While calculating the influence of EE coupling in quantum-sized structures, the Hartree and Hartree–Fock approximations, as well as the theory of spin density functional are used [9–13]. In work [14], various approaches to the calculation of electron ground state energies in QDs were compared in detail (the cases of filling a QD with two to thirteen electrons were examined). In particular, it was shown that the calculation error for the energies of electron ground states obtained in the framework of the spin-density functional theory does not exceed 2.5%. Therefore, the mentioned theory is also applied in this



a *b* *c*

Fig. 1. Schematic images of a quantum ring and the corresponding potential profiles

work to describe the EE interaction in structures of the same class.

2. Method

To describe the properties of magnetic rings, a simple model potential for an insulated two-dimensional ring located in the plane XY was used [15,16] (see Fig. 1),

$$V_c(r) = \frac{a_1}{r^2} + a_2 r^2 - V_0, \tag{1}$$

where $V_0 = 2\sqrt{a_1 a_2}$. In this model, both the ring radius and width can be selected independently. In the previous works [15, 16], the energy spectrum and the magnetization at zero temperature were calculated, as well as the wave functions in a constant magnetic field applied perpendicularly to the ring plane. Neither the SO, nor the EE interaction was taken into consideration in those works.

Potential (1) has the following properties:

(a) there exists a minimum $V(r_0) = 0$ at

$$r = r_0 = \left(\frac{a_1}{a_2}\right)^{1/4}, \tag{2}$$

which determines the average ring radius;

(b) at $r \approx r_0$, the potential has a simple parabolic shape $V(r) \approx \frac{1}{2} m\omega_0^2 (r - r_0)^2$ (Fig. 2), where the parameter $\omega_0 = \sqrt{\frac{8a_2}{m}}$ characterizes the size of the potential well, and m is the effective electron mass.

Potential (1) can also be used to describe a number of other physical systems, in particular, a 1D ring (at $r_0 = \text{const}$ and $\omega_0 \to \infty$), a 2D straight wire (at $\omega_0 = \text{const}$ and $r_0 \to \infty$), a quantum dot (at $a_1 = 0$), an isolated antidot (at $a_2 = 0$), and others.

2.1. One-electron Hamiltonian

Provided that a uniform magnetic field **B** is applied along the QR symmetry axis (the z-axis), the one-

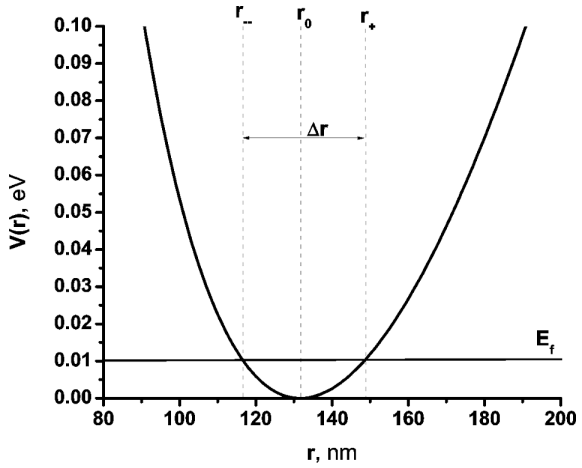


Fig. 2. Profile of the quantum-ring potential

electron Hamiltonian can be written down in the polar coordinates $\{r, \varphi\}$ [17] as follows:

$$H_1 = -\frac{\hbar^2}{2m(E)}\left[\frac{\partial}{r\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\right] - \frac{i}{2} m\omega_c(E,B) \times$$
$$\times \frac{\partial}{\partial \phi} + \frac{1}{8} m(E)\omega_c^2(E,B) r^2 + V_c(r) + V_{so}^{\mathrm{R}}(r,\phi) +$$
$$+ \frac{1}{2}\sigma_z \mu_{\mathrm{B}} g(E) B. \tag{3}$$

Here, the first term is responsible for the kinetic energy of the electron, the second and third terms describe the influence of a magnetic field on the electron motion, $V_c(r)$ is the confining potential, $V_{so}^{\mathrm{R}}(r,\phi)$ the energy of spin-orbit interaction, and the last term describes the interaction between the electron spin and the magnetic field. For the effective mass, we use the expression [8, 18]

$$\frac{1}{m(E)} = \frac{1}{m(0)} \frac{E_g(E_g + \Delta)}{(3E_g + 2\Delta)} \left[\frac{2}{E + E_g} + \frac{1}{E + E_g + \Delta}\right], \tag{4}$$

where E and $m(E)$ are the electron energy and mass, respectively, in the conduction band; $m(0)$ is the effective electron mass near the conduction band bottom; E_g the energy gap width; and Δ the spin-orbit splitting of the valence band. In formula (3), the quantity

$$\omega_c(E,B) = \frac{eB}{m(E)}$$

is the electron cyclotron frequency, and σ_z is the Pauli z-matrix. For the g-factor, we used the expression [19]

$$g(E) = 2\left[1 - \frac{m_0}{m(E)}\frac{\Delta}{3(E_g+E)+2\Delta}\right], \tag{5}$$

$\mu_{\rm B} = e\hbar/2m_0$ is the Bohr magneton, e the electron charge, and m_0 the free electron mass.

The operator of SO interaction energy, which was introduced by Rashba, is taken in the form [8, 20–22]

$$V_{so}^{\rm R}(r,\phi) = \sigma_z \alpha \frac{dV_c(r)}{dr}\left(k_\phi + \frac{e}{2\hbar}Br\right), \tag{6}$$

where $k_\phi = -i(1/r)\partial/\partial\phi$, and α is the parameter of the spin-orbit interaction introduced by Rashba [8].

The stationary Schrödinger equation with Hamiltonian (3) has no analytical solution, so it was solved numerically. The results of corresponding calculations and the electron wave function are presented in work [6].

2.2. Spin density functional theory

While calculating the energies and the wave functions of electrons confined in a certain region, electrostatic and electromagnetic interactions between particles have to be taken into account. The exact solution of this problem is extremely difficult, and a number of simplifications have to be applied. The density functional theory forms a basis for the description of electrons in a confining potential. This theory allows one to give an equivalent one-particle formulation for the complicated many-particle problem.

When calculating the electron spectra for a two-dimensional quasiparabolic quantum ring taking the EE and SO interactions into account simultaneously, the corresponding Kohn–Sham equation was solved self-consistently [9, 11],

$$\left[H_1 + \frac{e^2}{\kappa}\int \frac{w(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}dr' + \frac{\delta E_{xc}(w,\zeta)}{\delta w^\sigma(\mathbf{r})}\right]\psi_{n,l}^\sigma(\mathbf{r}) =$$

$$= \varepsilon_{n,l}^\sigma \psi_{n,l}^\sigma(\mathbf{r}), \tag{7}$$

$$w(\mathbf{r}) = \sum_\sigma w^\sigma(\mathbf{r}) = \sum_\sigma \sum_{n,l} \left|\psi_{n,l}^\sigma(\mathbf{r})\right|^2, \tag{8}$$

where H_1 is the electron Hamiltonian in the one-electron approximation (Eq. (3)). The superscript σ corresponds to the electron spin, $\zeta(\mathbf{r})$ is the local spin polarization, κ the dielectric constant, and E_{xc} the functional of exchange-correlation energy, which was used in the local density approximation [10]. Hereafter, the atomic units are used, the radius is reckoned in terms of the effective Bohr radius ($\kappa\hbar^2/m^*e^2$), and the energy is taken in effective Hartree units ($m^*e^4/\kappa^2\hbar^2$).

$$E_{xc} = \int w(\mathbf{r})\varepsilon_{xc}[w(\mathbf{r}),\zeta(\mathbf{r})]d\mathbf{r}, \tag{9}$$

$$\zeta(\mathbf{r}) = \frac{w^\uparrow(\mathbf{r}) - w^\downarrow(\mathbf{r})}{w(\mathbf{r})}, \tag{10}$$

where $\varepsilon_{xc}[w(\mathbf{r}),\zeta(\mathbf{r})]$ is the exchange-correlation energy per one particle in a uniform spin-polarized gas, which is considered to be a sum of the exchange and correlation energies [10],

$$\varepsilon_{xc}[w(\mathbf{r}),\zeta(\mathbf{r})] = \varepsilon_x[w(\mathbf{r}),\zeta(\mathbf{r})] + \varepsilon_c[w(\mathbf{r}),\zeta(\mathbf{r})]. \tag{11}$$

Below, while considering the electron-electron interaction, only the exchange energy component will be taken into consideration. In the case of two-dimensional electron gas, the exchange interaction looks like

$$\varepsilon_x[w,\zeta] = -\frac{4}{3r_{\rm B}}\sqrt{\frac{2w}{\pi}}\left[(1+\zeta)^{3/2} + (1-\zeta)^{3/2}\right], \tag{12}$$

where $r_{\rm B}$ is the Bohr radius. Then, the ground-state energy of a quantum ring with N electrons has the form

$$E_{\rm tot}(N) = \sum_{n,l,\sigma}\varepsilon_{n,l}^\sigma + \frac{e^2}{2\kappa}\int\frac{w(\mathbf{r})w(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d\mathbf{r}d\mathbf{r}' -$$

$$-\sum_\sigma\int w^\sigma(\mathbf{r})\frac{\delta E_{xc}(w,\zeta)}{\delta w^\sigma(\mathbf{r})}d\mathbf{r} + E_{xc}. \tag{13}$$

At zero temperature, the magnetization is determined as follows:

$$M = -\frac{\partial E_{\rm tot}}{\partial B}. \tag{14}$$

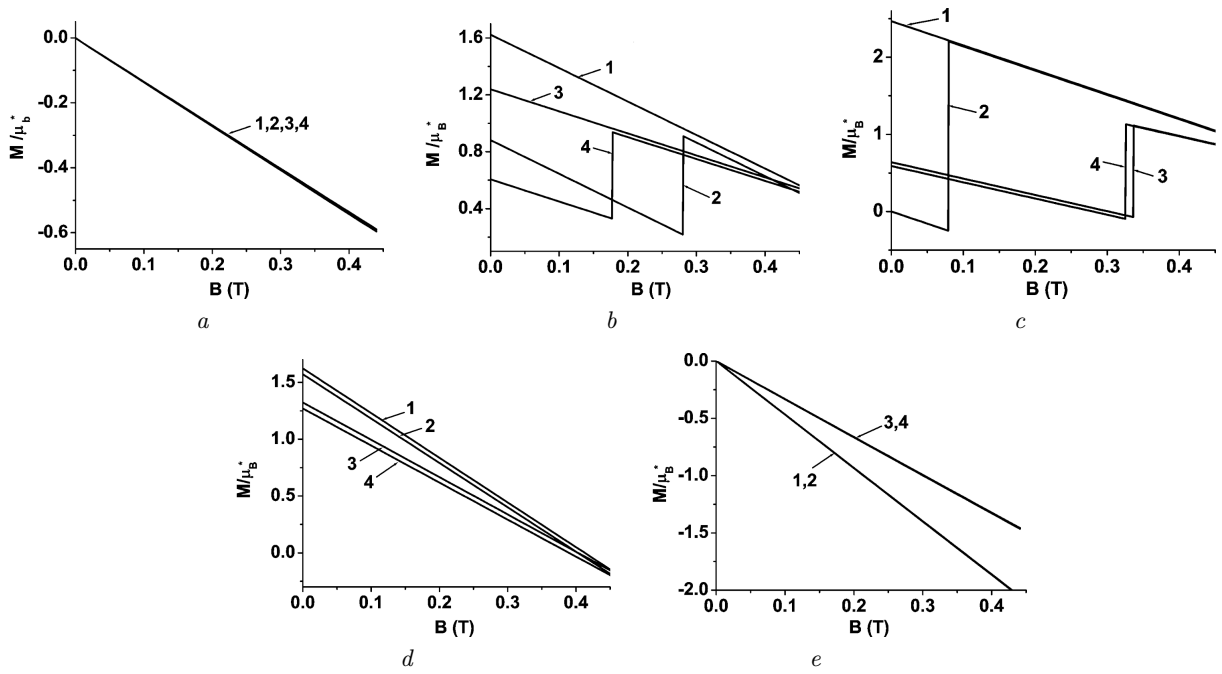


Fig. 3. Dependences of the magnetization in the InSb quantum ring filled with two to six electrons (panels *a* to *e*, respectively) on the magnetic applied field. The ring dimensions are $r_0 \approx 26$ nm and $\Delta r \approx 18$ nm. Calculations were carried out taking no SO and EE interactions into account (curves *1*), taking only SO interaction into account (curves *2*), taking only EE interaction into account (curves *3*), and taking both SO and EE interactions into account (curves *4*). $\mu_{\rm B}^* = e\hbar/2m(0)$

The solution of Eq. (7) was obtained in the framework of the self-consistent field approach. Namely, the energy of an electron was determined assuming that the states of other electrons were known. Then, the obtained solution was used to correct the states of other electrons and the potential created by them. While carrying out self-consistent calculations, the Broyden algorithm [23] was used.

3. Results of Calculations

The influence of spin-orbit and electron-electron interactions on the ring magnetization (ring's magnetic moment) at zero temperature and a small number of electrons in the quantum ring was studied theoretically. For an InSb quantum ring, the following parameters were selected [17, 18, 24]: $m(0) = 0.014m_0$, $E_g = 0.24$ eV, $\Delta = 0.81$ eV, and $\alpha = 5$ nm^2. Consider quantum rings with the following widths Δr and average radii r_0:

(a) $r_0 \approx 26$ nm, $\Delta r \approx 18$ nm ($a_1 = 31.5$ eV(nm)^2, $a_2 = 0.094$ meV/nm^2;

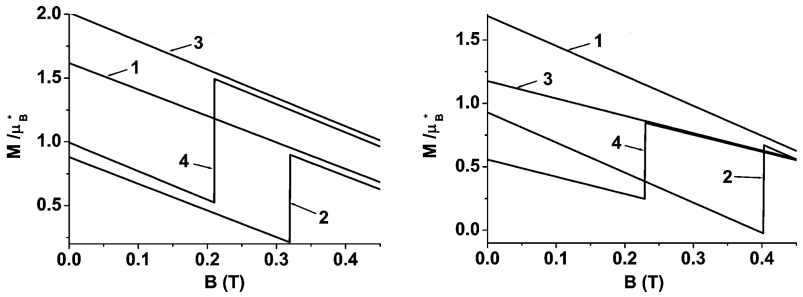
(b) $r_0 \approx 24$ nm, $\Delta r \approx 18$ nm ($a_1 = 67$ eV(nm)^2, $a_2 = 0.145$ meV/nm^2);

(c) $r_0 \approx 26$ nm, $\Delta r \approx 16$ nm ($a_1 = 43$ eV(nm)^2, $a_2 = 0.094$ meV/nm^2).

The parameters a_1 and a_2 (see Eq. (1)) were so selected to trace the influence of small changes in the average radius (item b) and the width (item c) of a QR on the magnetic properties of rings. The QR sizes selected for calculations correspond to the typical dimensions of structures that are grown up experimentally [25].

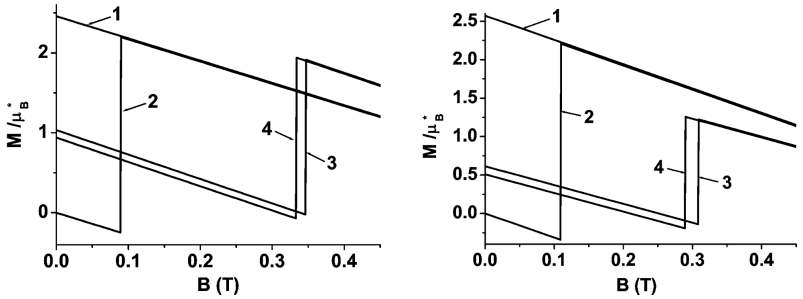
The calculated magnetizations of quantum rings with two to six electrons are illustrated in Figs. 3 to 5. For the sake of comparison, the magnetizations calculated for rings with the same number of electrons, but taking no account of spin-orbit or electron-electron interaction, are also depicted in the relevant figures.

First, consider the quantum ring (a) with the dimensions $r_0 \approx 26$ nm and $\Delta r \approx 18$ nm. From Figs. 3, *a*, *d*, and *e*, one can see that, in the case where the quantum ring is filled with two, five, or six electrons, the influence of the spin-orbit interaction is almost unnoticeable. The electron-electron interaction gives rise to a variation in the slope of the magnetization dependence on the magnetic field. If the QR



a *b*

Fig. 4. Dependences of the magnetization in an InSb quantum ring filled with three electrons on the magnetic applied field. The ring dimensions are $r_0 \approx 24$ nm and $\Delta r \approx 18$ nm (panel *a*) and $r_0 \approx 26$ nm and $\Delta r \approx 16$ nm (panel *a*). The curve notation is the same as in Fig. 3



a *b*

Fig. 5. The same as in Fig. 4, but for quantum rings filled with four electrons

is filled with two (Fig. 3, *a*) and six (Fig. 3, *e*) electrons, the quantum ring reveals diamagnetic properties. This behavior corresponds to the situation when the external electron shells are filled.

As one can see from Fig. 3, *c*, if the ring is filled with four electrons, the account of the electron-electron interaction brings about the emergence of a jump in the magnetization (curve *2*). If the ring is filled with four electrons, the account of the electron-electron interaction also results in the emergence of a jump in the magnetization, but at higher magnetic fields (curve *3*). With regard for both electron-electron and spin-orbit interactions (Fig. 3, *c*, curve *4*) shifts the magnetization jump toward lower fields. At the same time, the electron-electron interaction alone does not induce the emergence of a magnetization jump (Fig. 3, *d*, curve *3*). The latter arises when the spin-orbit interaction is also taken into account (curves *2* and *4*).

In Fig. 4, the dependences of the ring magnetization on the magnetic field are exhibited for QR (b) with the dimensions $r_0 \approx 24$ nm and $\Delta r \approx 18$ nm (Fig. 4, *a*) and QR (c) with the dimensions $r_0 \approx 26$ nm and $\Delta r \approx 16$ nm (Fig. 4, *b*), the both filled with 3 electrons. In Fig. 4,*a*, the number of electrons in the ring is the same as in Fig. 3, *b*, but the average ring radius is smaller. The ring with the dependences shown in Fig. 4, *b* has a smaller width in comparison with the ring corresponding to the dependences in Fig. 2, *b*. One can see that a decrease of either the average ring radius or the ring width results in the enhancement of the influence of both the spin-orbit and electron-electron interactions. The considered changes in the QR sizes shift the magnetization jump toward higher magnetic fields (Figs. 3, *b*; 4, *a*; and 4, *b*).

In Fig. 5, the dependences of the ring magnetization on the magnetic field are exhibited for QR (b) with the dimensions $r_0 \approx 24$ nm and $\Delta r \approx 18$ nm (Fig. 5, *a*) and QR (c) with the dimensions $r_0 \approx$ ≈ 26 nm and $\Delta r \approx 16$ nm (Fig. 4, *b*), the both being filled with 4 electrons. The figures also demonstrate that there is a shift in the positions of the magnetization jumps. Namely, the jumps become shifted

toward higher magnetic fields. The distance between magnetization jumps when both the SO and EE interactions are taken into account is larger than if only the EE interaction is considered (Figs. 3, *c*; 5, *a*; and 5, *b*; curves *3* and *4*).

4. Conclusions

Quantum rings with completely filled external electron shells – with two (Fig. 3, *a*) or six (Fig. 3, *e*) electrons in the QR – behave like diamagnetics. The account of both SO and EE interactions does not change the magnetic properties of QRs with filled external shells. If the external electron shell of a QR is not filled, there may emerge jumps in the dependence of the ring magnetization on the applied magnetic field (Figs. 3, *b*, 3, *c*, 4, and 5). Those jumps are the consequences of the SO and EE interactions.

The influence of the SO and EE interactions results in the splitting of energy levels in the zero magnetic field for the electrons in the quantum ring. The splitting brings about the possibility of the crossing between the energy levels if an external magnetic field is applied. This is the factor that is responsible for the emergence of jumps in the ring magnetization. If either or both of QR sizes – the average radius and the width – diminishes, the influence of the SO and EE interactions becomes stronger. Therefore, by changing the material or the geometry of QRs, it is possible to control their magnetic properties.

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МАГНІТНІ ВЛАСТИВОСТІ КВАНТОВИХ КІЛЕЦЬ ПРИ ВРАХУВАННІ СПІН-ОРБІТАЛЬНОЇ ТА ЕЛЕКТРОН-ЕЛЕКТРОННОЇ ВЗАЄМОДІЇ

Р е з ю м е

У роботі наведено теоретичний розгляд впливу спін-орбітальної (СО) та електрон-електронної (ЕЕ) взаємодій на електронну намагніченість квантових кілець (КК). У дослідженні використано теорію функціонала густини та рівняння Кона–Шема для розрахунку енергетичних рівнів електронів у дворозмірному квазіпараболічному квантовому кільці, заповненому 2–6-ма електронами. Намагніченість електронів у квантовому кільці розрахована при нульовій температурі. Різка зміна намагніченості пов'язана з перетином енергетичних рівнів електронів (ці перетини є наслідком врахування спін-орбітальної або електрон-електронної взаємодії).