Peculiarities of the Aharonov-Bohm Effect for Interacting Electrons in Thin Quantum Rings

Abstract—The electronic states of a InSb, InAs and GaN quantum ring with a few interacting electrons in an applied magnetic field via the spin-density functional theory have been studied. It has been shown that Aharonov-Bohm effect strongly depends on the number of interacting electrons. The results indicate that in the case of two interacting electrons in the InSb, InAs and GaN ring, the Aharonov-Bohm effect oscillations become aperiodic. Quantum rings of different materials have the different Aharonov-Bohm effect in the case of two interacting electrons. The Aharonov-Bohm effect in a InSb, InAs and GaN quantum ring can be controlled by varying the number of interacting electrons.

Keywords—Aharonov-Bohm Effect, Quantum Ring, electron-electron interaction

I. INTRODUCTION

In recent years, considerable attention is paid to the study of low-dimensional systems in semiconductor heterostructures. In such systems, there are interesting effects associated with dimensional quantization and electron motion limitation. Research of similar effects is important for the development of modern nanoelectronics and the possibility of building quantum rs and devices. One of the directions of such investigation is the study of correlated electron systems in a magnetic field [1]. The most notable example is the fractional quantum Hall effect [1] and several unique phenomena in various nanoscale systems, such as the quantum dots (QDs) [2–4] and quantum rings (QRs) [5, 6]. QDs and QRs can be considered as the artificial atoms, whose sizes and number of electrons can be controlled by the applied electric field.

In the case of multielectron QDs or QRs, the interaction effects between charges (Exchange, Coulomb and Spin-orbit interactions strength) should be taken into account. For the description of the spin-orbital interaction on the magnetization of quantum rings, the Rashby approximation was used [7,8]. In order to calculate the effect of EE interaction in quantum-sized structures, the Hartree method, Hartree-Fock approximation and Spin density functional theory are generally used [9–14]. The effect of spin-orbit interaction on energy spectra of electrons in a parabolic confinement in InSb QDs and QRs in magnetic field has been explored in [15–17].

In a nanoscale quantum ring structure, bounded electrons exhibit topological quantum coherence, which famous as Aharonov-Bohm effect (AB) [18]. The characteristics of the one electron energy spectrum for a ring-shaped geometry permeated by quantizedmagnetic flux correspond to the increasing orbital moment of with a period of one quantum, [18].

In present work we have studied the electronic states of a InSb, InAs and GaN quantum rings with a few interacting electrons in an applied magnetic field via the spin-density functional theory. We have also compared the AB effect in a InSb, InAs and GaN quantum rings.

II. THEORY

The properties of quantum rings were described by the simple model potential for an insulated two-dimensional ring located in the plane XY [19,20].

\[ V_c(r) = \frac{a_1}{r^2} + a_2 r^2 - V_0 \] (1)

where \( V_0 = 2 \sqrt{a_1 a_2} \).

The movement of the electrons along the Z axis is bounded by an infinitely deep potential well (fig. 1. C). In this model the ring radius and width can be selected independently.

Potential (1) has the following properties:

a) there exists a minimum \( V(r_0) = 0 \):

\[ r = r_0 = \left( \frac{a_1}{a_2} \right)^{\frac{1}{4}} \] (2)

which determines the average ring radius;

6) at \( r \approx r_0 \) the potential has a simple parabolic shape

\[ V_c(r) = \frac{1}{2} m^* \omega_0^2 (r - r_0)^2 \] (fig.2), where the parameter \( \omega_0 = \frac{8a_2}{m^*} \) characterizes the size of 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) a 1D ring, at \( r_0 = const \) and \( \omega_0 \to \infty \);

(b) a 2D straight wire, at \( \omega_0 = const \) and \( r_0 \to \infty \);
(c) a quantum dot, at \( a_1 = 0 \);  
(d) an isolated antidot, \( a_2 = 0 \).  

Provided that a uniform magnetic field \( B \) is applied along the Z axis to which the vector potential corresponds: 
\[
A = \left(-\frac{B_y}{2}, \frac{B_x}{2}, 0\right), \quad B = (0,0;B). 
\]

A. One-electron Hamiltonian

The one-electron Hamiltonian can be written in polar coordinates \([r, \phi]\) [15]:  
\[
H_1 = -\frac{\hbar^2}{2m} \left[ \frac{\partial}{\partial r} \left( \frac{1}{r} \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right] - \frac{i}{2} m^* \omega_c(B) \frac{\partial}{\partial \phi} + \frac{1}{8} m^* \omega_c^2(B) r^2 + V_c(r) + \frac{1}{2} \sigma_z \mu_B g B, 
\]  
where 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. The last term describes the interaction between the electron spin and the magnetic field, where \( \mu_B = e\hbar / 2m_0 \) - the Bohr magneton, \( g - g \) factor, \( m_0 \) - the mass of free electron, \( \omega_c(B) = eB \frac{m^*}{m} \) - cyclotronic frequency, and \( \sigma_z \) - Pauli matrix.

Calculations of energy spectra of energies and types of wave functions for the Hamiltonian (3) are carried out in [21].

B. Spin-density functional theory

In calculations of the energies and wave functions of electrons located in a certain bounded area, electrostatic and electromagnetic interactions between particles should be taken into account. The exact solution of the problem is very complicated, therefore, some simplifications must be applied. The theory of the functional density is the basis for the description of electrons in the limiting potential. This theory allows us to construct an equivalent one-particle representation of a complex multi-particle problem. To calculate the electron spectra with electron-electron and spin-orbital interaction, the Kohn – Sham equation for a two-dimensional quasiparabolic quantum ring is solved. Also, self-consistent calculations have been carried out [9,10]:

\[
H_1 + \frac{e^2}{\kappa} \int \frac{\mathbf{w}_r(r')}{|\mathbf{r} - \mathbf{r}'|} \mathbf{w}_r(r') d^2r' = \mathbf{\psi}_n^\sigma(r) \mathbf{H}_n^\sigma \mathbf{\psi}_n^\sigma(r), \tag{4} 
\]

\[
\mathbf{w}(r) = \sum_\sigma \mathbf{w}_n^\sigma = \sum_\sigma \sum_\mathbf{H}_n^\sigma \mathbf{\psi}_n^\sigma(r)^2, \tag{5} 
\]

where \( H_1 \) - Hamiltonian of an electron in a one-electron approximation (equation 3). Index \( \sigma \) defines spin of electron, \( \zeta(r) \) - the local spin polarization, \( \kappa \) - the relative permittivity, \( E_{xc} \) - the functional of the exchange-correlation energy, which is used in the approximation of local density [11]. Here, and further atomic units are used, the radius is taken in the effective radius of Bohr (\( \hbar^2 / \kappa \mu^2 \)) and energy is taken in the effective units of Hartree (\( \hbar^2 / \kappa \mu^2 \)).

\[
E_{xc} = \int \mathbf{w}(r) \mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) d^2r, \tag{6} 
\]

\[
\zeta(r) = \frac{\mathbf{w}^\sigma(r) - \mathbf{w}^\uparrow(r)}{\mathbf{w}(r)}, \tag{7} 
\]

where \( \mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) \) - exchange-correlation energy per one particle of homogeneous spin - polarized gas. In turn, \( \mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) \) is considered as the sum of exchange and correlation energies [11]:

\[
\mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) = \mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) + \mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)). \tag{8} 
\]

Taking into account the electron-electron interaction, only the exchange energy is used:

\[
\mathbf{e}_{xc}(\mathbf{w}(r), \zeta(r)) = -\frac{4}{3\pi r_B} \int \frac{\mathbf{w}(r) \mathbf{w}(r')}{|r - r'|} \left[ (1 + \zeta^2)^{3/2} + (1 - \zeta^2)^{3/2} \right] d^2r', \tag{9} 
\]

where \( r_B \) - Bohr radius.

The energy of the ground state of a quantum ring, which is filled with N electrons, can be expressed as:
The solution of equation (4) is carried out by a self-consistent field method, where the states of the other electrons are known for the determination of the electron energy. The resulting solution is consequently used to specify the states and potential of other interacting electrons. The method of self-consistent calculations of Broyden was used [22].

III. RESULTS OF CALCULATIONS

The calculations were carried out for the GaN, InAs and InSb quantum rings.

### TABLE I. PARAMETERS OF QUANTUM RINGS

<table>
<thead>
<tr>
<th>QRs</th>
<th>m/m_e</th>
<th>G</th>
<th>k</th>
<th>a_1 (eV nm)^2</th>
<th>a_2 (meV nm)^2</th>
</tr>
</thead>
<tbody>
<tr>
<td>InSb</td>
<td>0.0136 [23]</td>
<td>-50.6 [23]</td>
<td>17.9</td>
<td>1700</td>
<td>1.4</td>
</tr>
<tr>
<td>InAs</td>
<td>0.0239 [23]</td>
<td>-15 [23]</td>
<td>14.6</td>
<td>700</td>
<td>0.57</td>
</tr>
<tr>
<td>GaN</td>
<td>0.242 [24]</td>
<td>2.06 [24]</td>
<td>9.5</td>
<td>180</td>
<td>0.125</td>
</tr>
</tbody>
</table>

The parameters of the quantum rings (a_1 and a_2) are chosen so that the sizes of the rings from different materials have the same dimensions, when the quantum ring is filled by one electron. The average radius is r_0 ≈ 33.3 nm, the width ∆r ≈ 9.3 nm.

The low-lying energy electron level in quantum rings with one electron are presented in Fig. 3 as a function of the magnetic field B. In the quantum rings with only one electron the ground state changes periodically with the increase of magnetic field (Fig. 3). This is the direct illustration of the Aharonov–Bohm effect in a quantum rings. Quantum rings of different materials differ by their effective masses and G-factors, while the Aharonov–Bohm effect is preserved in all three systems.

For quantum rings with two electrons, the several substantial differences can be observed between the energy spectra of the InSb, InAs and GaN QRs.

Fig. 3 The low-lying energy levels versus the magnetic field in quantum ring with one electron for (a) InSb, (b) InAs, (c) GaN. The arrow indicates the value of the total orbital angular momentum in the ground states of the electrons.
From Fig. 4 it can be seen that with two electrons in the InSb quantum ring the sequence of the changing in the total orbital moment of the system with the increase of the external magnetic field is also changing. For small values of the magnetic field the ground state is a singlet with $L = 0$ and the total electron spin $S = 0$. 
With an increase of the magnetic field the ground state changes to a triplet with \( L = -1 \) and \( S = +1 \). With further increase of the magnetic field all the observed crossings of the ground state correspond to triplet-triplet transitions between the states with odd number of total angular momentum \((|L| = 0, 1, 3, 5...))

Taking into account only the Coulomb interaction between electrons in the quantum ring does not introduce significant changes in the spectrum. Only small changes in the values of the magnetic fields that cause a change in the ground state can be observed (Fig. 4a, 4b).

Consideration of the exchange interaction leads to the fact that the levels with electrons with the same direction of spin become energetically more favorable. These levels shift downwards in relation to the levels with the electrons with different orientation of spins.

It is shown that the singlet level \((L = 0, S = 0)\) has been moved upwards (Fig. 4.c.) and the intersection of the states with \((L = 0, S = 0)\) and \((L = -1, S = +1)\) occurs at lower magnetic field values \(B \approx 0.08\)T (instead of \(B \approx 0.35\)T (Fig 4.a,b)).

A similar picture is observed for an InAs quantum ring, without taking into account electron-electron interaction (Fig. 5a). Total angular momentum changes by the same dependence as in InSb. \((|L| = 0, 1, 3, 5...))\). The Coulomb interaction (Figure 5b) leads to a change in this sequence. \((|L| = 0, 1, 2, 3, 5...))\). In magnetic fields from \(B_1 \approx 0.9\), to \(B_2 \approx 1.3\) the ground state becomes \((L = -2, S = 0)\). Both electrons have a projection of the orbital moment on the Z axis by -1 and spins are oriented in different directions. We observe the Aharonov–Bohm effect up to the values of the fields \(B = 2.3\)T \((| L | = 0, 1, 2, 3)\). Then again this effect becomes irregular.

Taking into account the exchange interaction of Fig. 5.c leads to a shift in the energy levels of electrons with different spin directions upwards. The sequence of the change of orbital moment becomes \((|L| = 1, 3, 5...))\).

It is important that, for the InSb quantum ring (Fig. 4c), with the exchange interaction for the low values of the magnetic field leads to the fact that the ground state remains with \(L = 0\). For the InAs quantum rings (Fig. 5c), this energy level shifts upwards and the state becomes the main state with \(L = -1\).

The total angular momentum for the GaN quantum ring (Fig. 6a, 6b) varies according to the same law as in InAs, taking into account the Coulomb interaction (Fig. 5b).

However, the magnetic fields where the ground state becomes \((L = -2, S = 0)\) have a small range in the vicinity from \(B = 1.170\) to \(B \approx 1.185\) (Fig. 6a), and \(B \approx 1.168\) to \(B \approx 1.174\) (Fig. 6b).

It should be emphasized that Coulomb and exchange interaction for GaN (Fig. 6c) as well as, InSb (Fig. 4c) and InAs (Fig. 5c), leads to the fact that levels with the electrons with the same spin direction become more energy efficient. Accordingly, the levels with \((L = 0, S = 0)\) and \((L = -2, S = 0)\) are shifted upwards. The value of energy shifting is large for GaN quantum ring. The sequence of the change of the orbital moment becomes \((|L| = 1, 3, 5...))\).

Fig. 6. The low-lying energy levels versus the magnetic field for GaN quantum ring with 2 electrons. (a) Without taking into account electron-electron interaction, (b) taking into account the Coulomb interaction between electrons, (c) taking into account the Coulomb and exchange interaction.
To summarize, we have studied the electronic states of a InSb, InAs and GaN quantum rings with a few interacting electrons in an applied magnetic field via the spin-density functional theory. Different materials of quantum rings, with different effective masses and G-factors, were considered. It has been found that the Zeeman interaction, Coulomb interaction and exchange interaction are major characteristics of the InSb, InAs and GaN QRs and exert a profound influence on the electron states. In particular, we investigated that Aharonov-Bohm effect strongly depends on the number of interacting electrons. Our results indicate that in the case of two interacting electrons in the InSb, InAs and GaN rings, the Aharonov-Bohm effect oscillations become periodic. Quantum rings of different materials have the different Aharonov-Bohm effect in the case of two interacting electrons. The Aharonov-Bohm effect (and thereby the persistent current) in a InSb, InAs and GaN quantum rings can be controlled by varying the number of interacting electrons.

REFERENCES


