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MAGNETIC PROPERTIES OF PARABOLIC GaSb AND InAs QUANTUM DOTS WITH SPIN-ORBIT AND ELECTRON-ELECTRON INTERACTION

A theoretical consideration of the influence of spin-orbit and electron-electron interactions on GaSb and InAs quantum dots occupied by a few electrons is presented in detail. The influence of spin-orbit and electron-electron interactions on the magnetic properties of quantum dots at low-temperature values is analyzed. The magnetic properties of quantum dots with a certain electron filling exhibit abrupt shifts in magnetization with changes in the applied magnetic field. The magnetization jump is a result of electron-electron or spin-orbit interactions.

Keywords: quantum dot, spin-orbit interaction, electron-electron interaction, magnetic properties, magnetization.

1. Introduction

Quantum dots (QDs) are unique structures with extraordinary electronic and optical properties. Quantum dots, as well as quantum rings, can be considered as artificial atoms. The creation of QDs is a particularly promising area in physics because of the possibility of using them as qubits in quantum computation [1, 2]. It is also an attractive material for fluorescence resonance energy transfer (FRET), a quantum-mechanical process that relies on the distance dependence of nonradiative energy transfer from an excited-state donor to the ground-state acceptor via long-range dipole-dipole interactions [3]. Semiconductor QDs are used in the development of optically active chemical sensors and biosensors [4], as well as in spintronics [1, 5, 6].

Devices based on electron spin have already demonstrated commercial relevance in information storage devices (spin valves in magnetic hard disk heads). Quantum rings and quantum dots can be used in devices related to spin transport. Spin–orbit (SO) interactions in low-dimensional quantum dot and quantum ring structures are now intensively investigated [7, 8].

Current theoretical research focuses on the consideration of spin dynamics of electrons in quantum dots and rings [6, 9], the magnetic properties of quantum-dimensional structures [5, 10, 11] and the magneto-optical properties of artificial atoms [7, 8, 12]. Recent experimental and theoretical studies have confirmed that SO splitting affects charge transfer and conductivity fluctuations at quantum dots subjected to a homogeneous magnetic field. It also affects infrared absorption by quantum dots.

Nanoscale semiconductor crystals or structures with quantum wells in which electron motion is confined by the applied electric potential can act as quantum dots. Such structures are often based on GaAs [13], whereas GaSb is used less frequently for such structures. GaSb is a III–V narrow band gap semiconductor with high hole mobility at room temperature. Therefore, it has significant technological potential in electronics and optoelectronics [14]. Based on GaSb, low-power, high-efficiency p-type field-effect transistors (FET) are being developed. Nanowires and quantum dots based on GaSb have also been the subject of intensive investigation [15–19]. Studies on the structure of the GaSb valence band reveal significant spin splitting of the main subzone caused by SO interaction. Therefore, GaSb is a suitable material for

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forming spin qubits, as well as traditional semiconductors such as GaAs [13].

The purpose of this work is to investigate the magnetic properties of GaSb QDs filled with 2–6 electrons. InAs QDs of the same size are also taken for comparison with GaSb ones. When analyzing this problem, the effects of electron-electron (EE) and SO interactions are taken into account. The temperature dependencies of the magnetizations of the QDs are also considered.

2. Method

2.1. One-electron Hamiltonian

Let us consider a QDs formed by an external electric field applied to 2D electron gas. The electron motion along the Z-axis is confined by an infinitely deep potential well [11].

Under the influence of a homogeneous magnetic field B, applied along the axis of symmetry of the quantum dot (z) the one-electron Hamiltonian in cylindrical coordinates $\{\rho, \phi\}$ is expressed as [19]:

$$H_1 = -\frac{\hbar^2}{2m(E)}\left[\frac{\partial}{\rho\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2}\right] - \\ - \frac{i}{2}m\omega_c(E,B)\frac{\partial}{\partial\rho} + \frac{1}{8}m(E)\omega_c^2(E,B)\rho^2 + \\ + V_c(\rho) + V_{so}^R(\rho,\phi) + \frac{1}{2}\sigma_z\mu_{\rm B}g(E)B, \quad (1)$$

where

$$V_c(\rho) = \frac{1}{2}m(E)\omega_0^2\rho^2, \quad (2)$$

V_c – effective parabolic longitudinal potential, $\hbar\omega_0$ is the characteristic energy, σ_z – z-component of the Pauli matrix, the effective mass of the electron is expressed in [20, 21] as:

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

where E is the electron energy in the conduction band, $m(0)$ – the effective mass of the electron at the bottom of the conduction band, E_g and Δ – band gap and spin–orbit splitting of the valence band, respectively

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

ω_c – cyclotron frequency of the electron,

$$g(E) = 2\left[1 - \frac{m_0}{m(E)}\frac{\Delta}{3(E+E_g)+2\Delta}\right], \quad (4)$$

it is an effective g-factor in a semiconductor [22], $\mu_{\rm B} = \frac{e\hbar}{2m_0}$ – the Bohr magneton. e – the charge of the electron, m_0 – the mass of free electron.

The potential of spin-orbit interaction introduced by Rashba was taken into account [20, 23–25]:

$$V_{so}^R(\rho,\phi) = \sigma_z\alpha\frac{\partial V_c(\rho)}{\partial\rho}\left(k_\phi + \frac{e}{2\hbar}B\rho\right), \quad (5)$$

where $k_\phi = -i(1/\rho)\partial/\partial\phi$, and α – the parameter of spin-orbit interaction introduced by Rashba [20]. The Hamiltonian energies can be obtained by self-consistent equation calculations (6), (3), (4) [19]:

$$E_{n,l,\sigma} = \hbar\Omega_\sigma(E_{n,l,\sigma},B)(2n+|l|+1) \times \\ \times l\frac{\hbar\omega_c(E_{n,l,\sigma},B)}{2} \times \\ \times\sigma\left[\frac{\mu_{\rm B}}{2}g(E_{n,l,\sigma})B + l\alpha m(E_{n,l,\sigma})\omega_0^2\right]. \quad (6)$$

Wave functions of electrons are:

$$\Psi_{n,l,\sigma}(\rho,\psi) = \frac{1}{\sqrt{2\pi}}\exp(il\phi)\sqrt{\frac{2}{l_B^2}} \times \\ \times\left[\frac{n!}{(n+|l|)!}\right]^{\frac{1}{2}}\exp\left(-\frac{\rho^2}{2l_B^2}\right)\left(\frac{\rho^2}{l_B^2}\right)^{\frac{|l|}{2}}L_n^{|l|}\left(\frac{\rho^2}{l_B^2}\right), \quad (7)$$

where

$$\Omega_\sigma^2 = \omega_0^2 + \frac{\omega_c^2(E,B)}{4} + \sigma\alpha\frac{m(E)\omega_0^2}{\hbar}\omega_c^2(E,B),$$

$l_B = \sqrt{\hbar/m\Omega_\sigma}$, $L_n^{|l|}$ – generalized Laguerre polynomial, n – the principal quantum number, l and $s = \pm 1$ – projection of the orbital and spin quantum numbers on the z-axis, respectively.

2.2. The Kohn–Sham equations theory of spin functional density

We use atomic units to take the radius in the effective Bohr units $\kappa\hbar^2/m^*e^2$ and energy in effective Hartree units $m^*e^4/\kappa^2\hbar^2$ (κ – relative permittivity).

We solve the Kohn–Sham equation for a two-dimensional parabolic quantum dot, and perform self-consistent calculations [26]:

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

$$\times \Psi^{\sigma}_{n,l}(\mathbf{r}) = \varepsilon^{\sigma}_{n,l}\Psi^{\sigma}_{n,l}(\mathbf{r}), \tag{8}$$

$$w(\mathbf{r}) = \sum_{\sigma} w^{\sigma}(\mathbf{r}) = \sum_{\sigma}\sum_{n,l} \left|\Psi^{\sigma}_{n,l}(\mathbf{r})\right|^2, \tag{9}$$

where index σ – determines the spin of electrons, $\zeta(\mathbf{r})$ – is local spin polarization, κ – relative permittivity, and E_{xc} – the functional of the exchange-correlation energy used in local-density approximation [27]

$$E_{xc} = \int w(\mathbf{r})\,\varepsilon_{xc}\left[w(\mathbf{r}), \quad \zeta(\mathbf{r})\right] d(\mathbf{r}), \tag{10}$$

$$\zeta(\mathbf{r}) = \frac{w^{\uparrow}(\mathbf{r}) - w^{\downarrow}(\mathbf{r})}{w(\mathbf{r})}, \tag{11}$$

where $\varepsilon_{xc}\left[w(\mathbf{r}), \zeta(\mathbf{r})\right]$ – exchange-correlation energy per particle of homogeneous spin-polarized gas. While $\varepsilon_{xc}\left[w(\mathbf{r}), \zeta(\mathbf{r})\right]$ is considered as the sum of exchange and correlation energies [27]:

$$\varepsilon_{xc}\left[w(\mathbf{r}), \zeta(\mathbf{r})\right] =$$

$$= \varepsilon_x\left[w(\mathbf{r}), \zeta(\mathbf{r})\right] + \varepsilon_c\left[w(\mathbf{r}), \zeta(\mathbf{r})\right]. \tag{12}$$

Regarding the electron-electron interaction, we will take into account only the exchange energy.

In the case of two-dimensional electron gas, the exchange interaction is expressed as:

$$\varepsilon\left[w, \zeta\right] = -\frac{4}{3r_{\mathrm{B}}}\sqrt{\frac{2w}{\pi}}\left[(1+\zeta)^{\frac{3}{2}} + (1-\zeta)^{\frac{3}{2}}\right], \tag{13}$$

where r_{B} – Bohr radius.

The basic energy state of a quantum dot filled with N electrons can be expressed as:

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

$$- \sum_{\sigma} w^{\sigma}(\mathbf{r})\,\frac{\delta E_{xc}(w,\zeta)}{\delta w^{\sigma}(\mathbf{r})}\,d\mathbf{r} + E_{xc}. \tag{14}$$

At zero temperature, the magnetization can be found in the form:

$$M = -\frac{\partial E_{\mathrm{tot}}}{\partial B}, \tag{15}$$

where E_{tot} – is a ground state of the electron system.

When considering the temperature dependencies of magnetization, we follow the thermodynamic model discussed in [28]. The temperature dependence of the magnetization takes the form:

$$M = -\frac{\sum_i \frac{\partial E_i}{\partial B}\exp\left(-\frac{E_i}{kt}\right)}{\sum_i \exp\left(-\frac{E_i}{kt}\right)}, \tag{16}$$

where partial derivatives are evaluated as operator expectation values for the interacting state i.

3. Results of Calculations

We have theoretically investigated the effects of spin–orbit and electron–electron interactions on the magnetization of quantum dots (magnetic moment) at low temperatures. These quantum dots were occupied by a few electrons.

For the InAs QDs dot, we choose $m(0) = 0.0239m_0$, $E_g = 0.42$ eV, $\Delta = 0.38$ eV, $\alpha = 1.1$ nm^2, $\kappa = 14.6$ [19, 29, 30]. Let us consider a quantum dot with the following parameters: $\hbar\omega_0 = 0.0318$ eV, average radius $r_0 = 14$ nm for the case of one electron in QD. For the GaSb QDs we choose $\alpha = 0.33$ nm^2, $\kappa = 15.69$ [30, 31]. We will analyze a quantum dot with the following parameters: $\hbar\omega_0 = 0.0185$ eV, average radius $r_0 = 14$ nm. The selected quantum dot size is consistent with the characteristic dimensions of similar nanostructures. At this scale, the effects of interest in our study are sufficiently pronounced to be reliably observed and analyzed.

The calculated magnetization of quantum dots with 2–6 electrons is shown in Figs. 1 and 2. For comparison, magnetization for the same number of electrons but without spin–orbit or electron–electron interaction is also presented in the same figures.

The magnetization dependence of InAs QDs filled with 2–6 electrons is shown in Fig. 1. As we can observe from Fig. 1, *a*, e in the case where the quantum dot is filled with two and six electrons, the effect of the spin–orbit interaction is practically negligible. For QDs containing six electrons, electron–electron interactions modify the slope of the magnetization as a function of the applied magnetic field.

QDs with two and six electrons behave as artificial atoms with closed outer electron shells. Consequently, the diamagnetic properties of InAs are observed in Fig. 1, *a*.

The InAs QDs filled with three electrons with spin–orbit and EE interaction are presented in Fig. 2, *b*. It

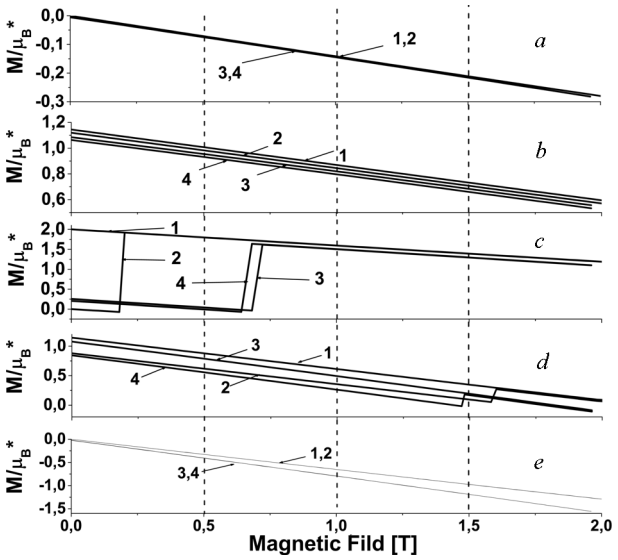

Fig. 1. Magnetization of an InAs quantum dot at zero temperature: for two electrons (*a*); for three electrons (*b*); for four electrons (*c*); for five electrons (*d*); for six electrons (*e*). Index *1* indicates calculations without SO and EE interactions, *2* – with SO and without EE interaction, *3* – without SO and with EE interaction, *4* – with SO and EE interactions

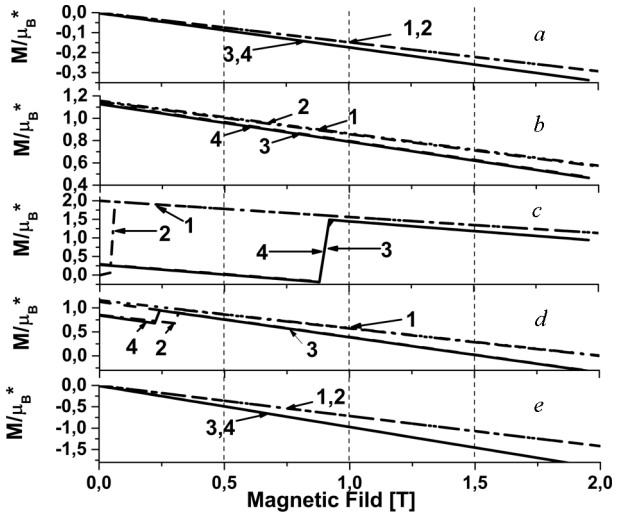

Fig. 2. Magnetization of GaSb quantum dot at zero temperature: for two electrons (*a*); for three electrons (*b*); for four electrons (*c*); for five electrons (*d*); for six electrons (*e*). Index *1* indicates calculations without SO and EE interactions, *2* – with SO and without EE interaction, *3* – without SO and with EE interaction, *4* – with SO and EE interactions

leads to a small shift of the dependence of the magnetization on the external magnetic field. A QDs with 3 electrons exhibits paramagnetic properties.

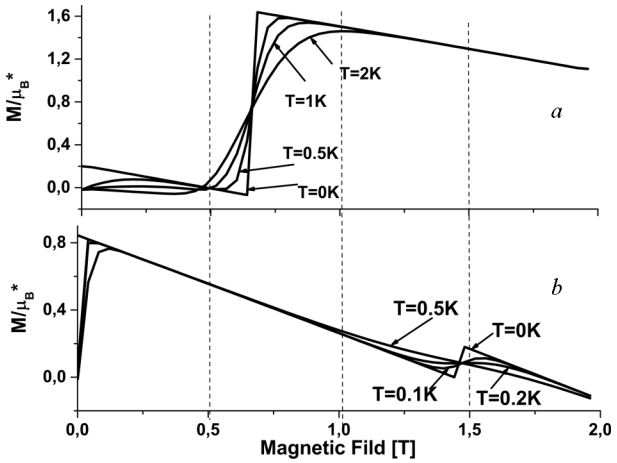

Fig. 3. Temperature dependencies of the magnetization of the InAs quantum dot on the external magnetic field, calculated with SO and EE interactions. for four electrons (*a*); for five electrons in QD (*b*)

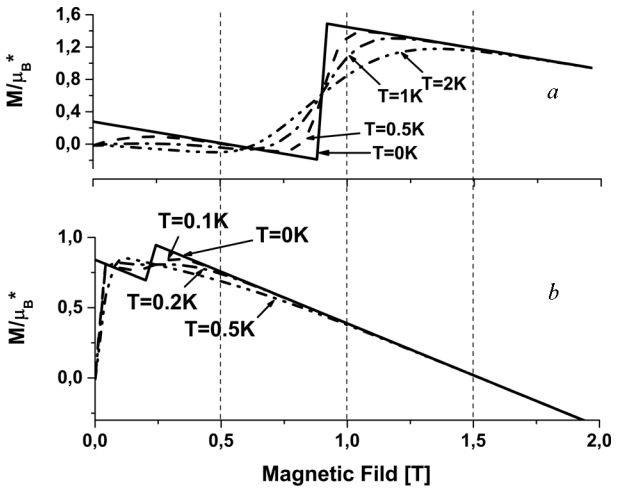

Fig. 4. Temperature dependencies of the magnetization of the GaSb QDs on the external magnetic field, taking into account both SO and EE interactions. For four electrons (*a*); for five electrons in QD (*b*)

As can be observed in Fig. 1, *c*, in the case of QDs is filled with four electrons without taking into account electron–electron interaction, taking into account the spin–orbit interaction leads to a magnetization jump (index 2). As can be observed in Fig. 1, *c*, in the case of four electrons being filled without spin–orbit interaction, the electron–electron interaction also leads to the appearance of a magnetization jump (index 3), but in the region of strong magnetic fields. Taking into account both electron–electron and spin–orbit in-

teractions (Fig. 1, *c*, index 4) leads to a shift of the magnetization jump toward lower magnetic fields.

As can be seen in Fig. 1, *d*, ($N = 5$) electron–electron interaction does not lead to a magnetization jump (index 3). Taking into account the spin–orbit interaction leads to the formation of corresponding magnetization jumps (index 2, 4).

This magnetization jump (Fig. 1, *d*) is important for regulating the magnetic properties of QDs (artificial atoms) by the applied external magnetic field. Changing the size of the QDs (modifying the confinement potential) leads to the shift of the magnetization jump to different values of the magnetic field.

Figure 2 shows the dependence of the magnetization of the GaSb QDs on the magnetic-field strength. In the case when the QDs are filled with 2 or 6 electrons (Fig. 2, *a, e*), the effect of spin–orbit interaction is negligible. EE interaction leads to a change in the slope of the magnetization on the magnetic field. In the case when the QDs are filled with 3 electrons (Fig. 2, *b*) the influence of spin–orbit interaction becomes more noticeable, but does not change the general tendency.

Let us compare Fig. 1, *c* with Fig. 2, *c*. Spin–orbit interaction leads to a shift in magnetization (index 2). In Fig. 2, *c*, the jump occurs at smaller magnetic-field values (this is due to the smaller strength of the spin–orbit interaction in GaSb). Taking into account the EE interaction (indices 3 and 4), the spin–orbit interaction also leads to the shift in the magnetic-field value at which the magnetization jump occurs. However, due to the relatively weak spin–orbit interaction, this change is small.

Magnetization jumps are observed in Fig. 2, *d*, ($N = 5$), as a consequence of spin–orbit interaction. In contrast to InAs QDs, for GaSb QDs certain jumps occur at much smaller magnetic-field values (Fig. 1, *d*). This is also a consequence of the lower strength of spin–orbit interaction for QDs with GaSb compared to InAs QD.

The most important result was obtained for the case of QDs filled with 4 and 5 electrons. The temperature dependencies of the magnetization of InAs and GaSb QDs are presented in Figs. 3 and 4, respectively, for different values of the applied magnetic field. As can be observed from Fig. 3, *a* and Fig. 4, *a*, due to the larger magnitude of the electron–electron interaction, the magnetization jump in GaSb QDs with 4 electrons (Fig. 4, *a*) occurs at larger values of magnetic fields, compared to InAs QDs (Fig. 3, *a*). As the temperature increases, the step-like behavior of the magnetization becomes less pronounced.

In the case of filling of the QDs with 5 electrons (Fig. 3, *b*, Fig. 4, *b*), the magnetization jumps occur only as a result of the SO interaction. For GaSb the strength of spin–orbit interaction is lower than for InAs. Therefore, we see that in GaSb QDs (Fig. 4, *b*), the magnetization jump occurs at smaller values of the applied magnetic field than for InAs QDs (Fig. 3, *b*). The magnitude of the magnetization jumps does not differ significantly. As can be seen from Fig. 3, *b* and Fig. 4, *b*, when the temperature is increased to $T = 0.10$ K, the magnetization jump is substantially smoothed, and at the temperature $T = 0.30$ K the jump disappears.

4. Conclusions

The magnetic properties of GaSb QDs and InAs QDs with a parabolic confinement potential have been considered in this article. The magnetic properties of quantum dots depend on the number of confined electrons and on the geometric parameters of the structures.

As a result of the spin-orbit interaction, energy-level splitting occurs at zero magnetic field in QDs. The splitting of energy levels leads to the energy-level crossings in the case of an applied magnetic field. This has a significant effect on the magnetic properties of quantum dots. A jump of magnetization also occurs in the case of QDs filled with 5 electrons. The magnitude of the shift depends on the magnetization induced by the applied magnetic field. The position of this jump depends on the magnitude of the spin-orbit interaction (InAs and GaSb have different values of SO interaction) and, to a large extent, on the size of the QDs.

Consideration of electron-electron interaction also leads to the splitting of energy levels. In the case of four electrons in QDs, the influence of spin-orbit and electron-electron interactions leads to similar magnetization dependencies. The magnetic field values at which the magnetization jump occurs are largely determined by the EE interaction (quantum dot size, material dielectric constant, effective electron mass).

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МАГНІТНІ ВЛАСТИВОСТІ
ПАРАБОЛІЧНИХ КВАНТОВИХ КІЛЕЦЬ
GaSb ТА InAs ЗІ СПІН-ОРБІТАЛЬНОЮ
ТА ЕЛЕКТРОН-ЕЛЕКТРОННОЮ ВЗАЄМОДІЄЮ

Детально представлено теоретичний розгляд впливу спін-орбітальної та електрон-електронної взаємодій на квантові точки GaSb і InAs, заповнені кількома електронами. Проаналізовано вплив спін-орбітальної та електрон-електронної взаємодій на магнітні властивості квантових точок за низьких температур. Магнітні властивості квантових точок з певним електронним заповненням виявляють різку зміну намагніченості зі зміною величини прикладеного магнітного поля. Стрибок намагніченості є результатом електрон-електронної або спін-орбітальної взаємодій.

Ключові слова: квантова точка, спін-орбітальна взаємодія, електрон-електронна взаємодія, магнітні властивості, намагніченість.