Optical absorption in core-shell quantum antidot with donor impurity under applied magnetic field

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***Abstract*— The influence of the magnetic field and off-central donor impurity on the energy spectrum and wave functions of an electron in the inverted core-shell QD are calculated. On this basis, the dependence of the binding energy and the absorption coefficient of electromagnetic waves by multilayer QD with an impurity on the magnetic field induction are investigated within the approximation of the effective mass and the rectangular potential profile of the nanosystem by the matrix method using the exact electron wave functions in nanosystem without perturbations.**

The linear, third-order nonlinear and total optical absorption coefficients (OACs) are calculated taking into account all possible intraband quantum transitions. The combined effect of donor position, magnetic field and core size on binding energies and optical absorption coefficients is observed. The results show that these effects cause significant changes on donor binding energy and optical absorption coefficient

Keywords—absorption coefficient, core-shell QD, donor inpurity, intraband transitions

I. INTRODUCTION

Recently, nanostructures have attracted much attention of scientists due to modern technology of their growth and wide range of their applications in electronic and optoelectronic devices. Today it has become possible to create multilayers spherical quantum dots (MSQD), which are called core-shell, core-shell-shell and others. Based on them, biosensors, fluorescent labels, light emitting devices, solar cells are already being created, and elements for the latest computer technology are being developed [1-4].

Depending on the potential barrier height of the external medium, MSQD can be opened and closed. The electron and hole quasi-stationary spectrum in an open spherical nanostructure was theoretically studied in [5].

Closed multilayers spherical nanostructures are characterized by a discrete electronic spectrum similar to the atomic spectrum. MSQDs, consisting of core and several layers of semiconductor materials with different band gaps, have the additional possibilities for the fabrication of optoelectronic devices. They have the complicated profile of electron and hole potential energy, with several potential wells and barriers. The absorption (radiation) energies depend on the size nanostructure potential wells. The MSQD with two or more potential wells are used for independent control of its absorption (radiation) spectrum. Change in the localization of quasiparticles in MSQD with several potential wells is accompanied by a significant change of its optical properties [6-7].

One of the most famous MSQD is so-called inverted core-shell QD, which consists of a core and shell (the core has a wider bandgap than the shell, see fig.1). Such nanosystems can have a large radius but strong confinement due to the large core and small thickness of the shell. The larger the radius of the system, the more sensitive it is to the magnetic field, and this can be used in magneto-optical devices.

To create electronic and optoelectronic devices based on such nanostructures it is necessary to study the influence of external fields and size of MSQD on the energy spectrum and distribution of the electron probability. On this basis, one can calculate the dependence of the absorption coefficient on the photon energy.

The presence of impurities can significantly change the performance of quantum devices and their optical properties. By changing the size of the MSQD layers and the positions of the impurities, one can adjust the energy of the quantized transitions, and thus obtain the necessary optical properties of the devices.

It is known that the application of an electric or magnetic field can provide information about nanosystems. Such external fields can also be used to control the properties of QD for application in various devices. The study of the external magnetic field influence on the oscillator forces of quantum transitions is necessary for a better understanding of the QD electronic and optical properties.

The exact analytical solutions of the Schrödinger equation are possible only if the spherical symmetry is preserved. Such solutions exist even in the quantum antidot with a central impurity [8-9]. The presence of off-central impurity or external fields violates the spherical symmetry, so the authors use approximate methods. The calculation of the binding energy of an electron with a shallow impurity ion, the oscillatory force of quantum transitions and the absorption coefficient under influence of the external magnetic or electric fields is performed by most authors in the approximation of the effective mass using variational [10-12] or matrix [13-24] methods.

The absorption coefficient is determined not only by transitions from the ground state but also between the electron excited states. The authors [19] investigated the magnetic field effect on optical transitions spherical QD GaAs and showed that partial contributions in OAC from quantum transitions between excited states are greater than from ground state. Thus, the quantum transitions between electron excited states play an important role in optical properties of nanosystems, which are placed in strong external fields.

In the present paper, we have calculated magnetic field dependence of electron energy spectra, binding energy electron with impurity and absorption coefficient from

intersubband quantum transitions electron in inverted core-shell QD with and without impurity.

II. THEORETICAL FRAMEWORK

The semiconductor MSQD $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ consisting of core $Al_{0.3}Ga_{0.7}As$ with the radius r_0, shell-well GaAs with the width $\Delta = r_1 - r_0$ and outer shell $Al_{0.3}Ga_{0.7}As$ is under research. The geometric scheme, the dimensions, and the scheme of the confinement potential are shown in Fig. 1.

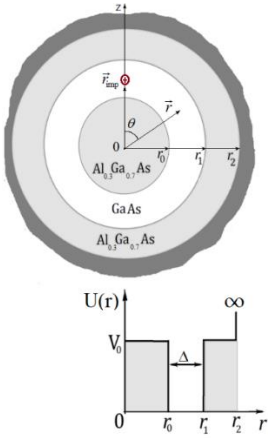

Fig. 1. Nanosystem geometric and potential scheme.

In order to investigate the magnetic field effect on the electron energy spectrum and wave functions in the nanosystem with impurity it is necessary to solve the Schrodinger equation

$$H\,\Psi_{jm}(\vec{r}) = E_{jm}\Psi_{jm}(\vec{r}) \tag{1}$$

with the Hamiltonian

$$H = -\vec{\nabla}\frac{1}{\mu^*(r)}\vec{\nabla} + \frac{\eta L_z}{\hbar\mu^*(r)} + \frac{\eta^2 r^2 sin^2\theta}{4\mu^*(r)} - \frac{Ze^2}{\varepsilon|\vec{r}-\vec{r}_{imp}|} + U(r), \tag{2}$$

where

$$U(r) = \begin{cases} V_0, & 0 < r \le r_0, r_1 < r \le r_2 \\ 0, & r_0 < r \le r_1 \\ \infty, & r > r_2 \end{cases}, \tag{3}$$

$$\mu(r) = \begin{cases} m_0, & 0 < r \le r_0, r_1 < r \le r_2, \\ m_1, & r_0 < r \le r_1 \end{cases} \tag{4}$$

$\eta = e\hbar B/(2m_e c\,Ry)$, $Ry = \hbar^2/(2m_e a_B^2)$ - Rydberg constant.

In order to solve the equation (1), the wave functions are expanded over the complete set of exact functions obtained without the magnetic field and impurity

$$\psi_{jm}(\vec{r}) = \sum_n \sum_l c_{nl}^{jm}\Phi_{nlm}(\vec{r}), \tag{5}$$

$$\phi_{nlm}(r) = R_{nl}(r)Y_{lm}(\theta,\varphi), \tag{6}$$

The analytical expression of the radial part is determined by Bessel functions

$$R_{n\ell}(r) = \begin{cases} A_{n\ell}^{(0)} i_\ell(k_{n\ell}^{(0)} r), & E_{nl} < V_1 \\ A_{n\ell}^{(0)} j_\ell(k_{n\ell}^{(0)} r), & E_{nl} \ge V_1 \\ A_{n\ell}^{(1)} j_\ell(k_{n\ell}^{(1)} r) + B_{n\ell}^{(1)} n_\ell(k_{n\ell}^{(1)} r) & \\ A_{n\ell}^{(2)} i_\ell(k_{n\ell}^{(2)} r) + B_{n\ell}^{(2)} \kappa_\ell(k_{n\ell}^{(2)} r), E_{nl} < V_2 & \\ A_{n\ell}^{(2)} j_\ell(k_{n\ell}^{(2)} r) + B_{n\ell}^{(2)} n_\ell(k_{n\ell}^{(2)} r), E_{nl} \ge V_2 & \end{cases}, \tag{7}$$

The unknown coefficients and electron energies E_{nl} are found using Ben Daniel-Duke boundary conditions on all interfaces

$$\left.\begin{aligned} & R_{n\ell}^{(i)}(r_i) = R_{n\ell}^{(i+1)}(r_i) \\ & \frac{1}{m_i}\frac{dR_{n\ell}^{e,h(i)}(r)}{dr}\bigg|_{r=r_i} = \frac{1}{m_{i+1}}\frac{dR_{n\ell}^{e,h(i+1)}(r)}{dr}\bigg|_{r=r_i} \end{aligned}\right\}, \quad i = 0,1 \tag{8}$$

To determine the coefficients c_{nl}^{jm} and energy spectrum $E_{\rm jm}$ we obtain the secular equation

$$\left|H_{n\ell,n'\ell} - E_{jm}\delta_{n,n'}\delta_{\ell,\ell'}\right| = 0 \tag{9}$$

$$H_{n'l',nl} = E_{nl}^0\delta_{n',n}\delta_{l',l} + eF\left(\alpha_{l,m}\delta_{l',l+1} + \beta_{l,m}\delta_{l',l-1}\right)U_{n'l',nl} + F_{n'l',nl}\,, \tag{10}$$

$$\alpha_{l,m} = \sqrt{\frac{l^2-(m+1)^2}{(2l+3)(2l+1)}}\,,\ \beta_{l,m} = \sqrt{\frac{l^2-m^2}{4l^2-1}}\,,\ U_{n'l',nl} = \int_0^{r_2} r^3 R_{n'l'}^*(r)R_{nl}(r)dr$$

$$F_{n'l',nl} = \iiint_V \Phi_{n'l'm}^*(\vec{r})\frac{2Z}{|\vec{r}-\vec{r}_{imp}|}\Phi_{nlm}(\vec{r})dV\,. \tag{11}$$

Using the obtained energies and wave functions of an electron, the binding energies of an impurity can be calculated:

$$E_b^{1s-f} = E_f^{Z=0} - E_{1s}^{Z=1} \tag{12}$$

For a spherical nanosystem, linear $\alpha^{(1)}(\omega)$, third-order nonlinear $\alpha^{(3)}(I,\omega)$ and total absorption coefficients are defined as follows, respectively

$$\alpha^{(1)}(\omega) = \omega\sqrt{\frac{\mu}{\varepsilon_R}}\frac{\sigma_v\hbar\Gamma_{fi}|M_{fi}|^2}{(E_{fi}-\hbar\omega)^2+(\hbar\Gamma_{fi})^2} \tag{13}$$

$$\alpha^{(3)}(I,\omega) = -\omega\sqrt{\frac{\mu}{\varepsilon_R}}\left(\frac{I}{2\varepsilon_0 n_r c}\right)\frac{\sigma_v\hbar\Gamma_{fi}|M_{fi}|^2}{\left[\left(E_{fi}-\hbar\omega\right)^2+\left(\hbar\Gamma_{fi}\right)^2\right]^2}\times$$

$$\times\left\{4|M_{fi}|^2 - \frac{(M_{ff}-M_{ii})^2\left[3E_{fi}^2-4E_{fi}^2\hbar\omega+\hbar^2\left(\omega^2-\Gamma_{fi}^2\right)\right]}{E_{fi}{}^2+(\hbar\Gamma_{fi})^2}\right\}, \tag{14}$$

$$\alpha(I,\omega) = \alpha^{(1)}(I,\omega) + \alpha^{(3)}(I,\omega) \tag{15}$$

The dipole transition matrix element is given by

$$M_{fi} = \left\langle\psi_i\left|er\cos\theta\right|\psi_f\right\rangle. \tag{16}$$

III. RESULTS AND DISCUSSION

The computer calculations have been performed for $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ nanostructure with the following physical parameters: x=0.3, m_0=0.067+0.083x,

m_1=0.067, V_0=0.6(1155 x+370 x^2) = 227.9 meV, ε=11,5 is the averaged dielectric constant. For comparison, nanostructures of two sizes have been considered: 1) r_0=5 nm, r_1=15 nm (Δ=10 nm), r_2=20 nm; 2) r_0=15 nm, r_1=25 nm (Δ=10 nm), r_2=30 nm.

In a spherical nanostructure without impurity and external fields, energy spectrum and wave function of an electron $E^0_{n\ell}$ are characterized by the radial (n) and orbital (l) quantum numbers. A potential well with a depth V_1=227.9 meV and a width Δ = 10 nm contains 11 energy levels (up to l = 6) at r_0=5 nm and 21 levels (up to l = 11) at r_0=15 nm. This quantity of terms in the expansion (6) is not sufficient to ensure high accuracy of calculation of the electron energies and wave functions in the presence of a non-central impurity [21-22]. Therefore, electron discrete states the energy higher than V_0 are also included in the orthonormal basis. There are enough of them for arbitrary accuracy, because the potential barrier at r=r_2 is infinite.

Dependencies of electron energies (at m=0) on magnetic field intensity B in the structure without impurity (dashed lines) and with donor impurity r_{imp}=(r_0+r_1)/2 (solid lines) are presented in Fig. 2. These energies are no longer characterized by a certain value of the orbital quantum number, because electron states are a combination of states with different values of l, but they are marked as 1s, 1p, 1d, 1f (at Z = 1) and $1s^0$, $1p^0$, $1d^0$, $1f^0$ (for Z = 0) in Fig.2 for convenience.

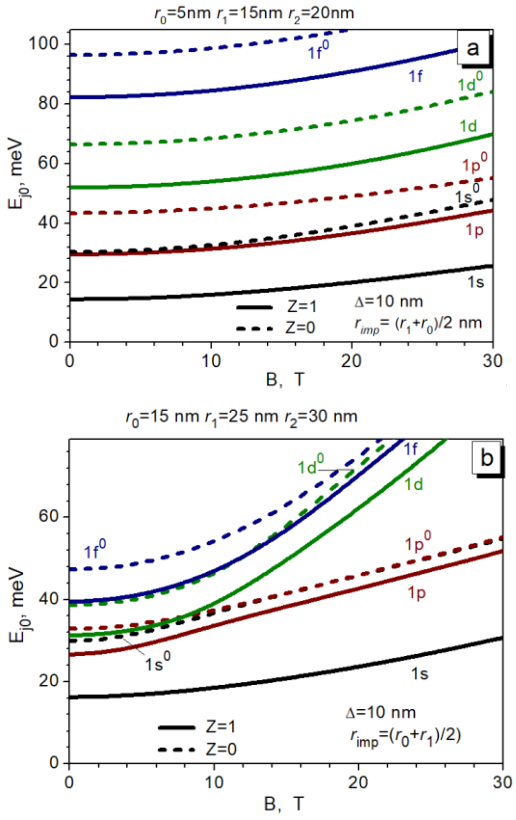

Fig. 2. Dependence of the electron energy spectra on the applied magnetic field in the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ multilayer spherical quantum dots with r_0 =5 nm, r_1 =15 nm and r_2 =20 nm (a) and r_0 =15 nm, r_1 =25 nm and r_2 =30 nm (b). The solid lines are for Z=1, whereas the dashed lines are for Z=0. In both panels the impurity is located at $r_{imp} = (r_0 + r_1)/2$.

Figure 2 shows that the magnetic field effect on the electron energy spectrum is small for the nanostructure with a small core (r_0 = 5 nm), and for nanostructure with a big core (r_0 = 15 nm) anticrossings of energy levels (1p, 1d) at B = 8 T and (1d, 1f) at B = 20 T are observed.

The energy levels $1s^0$ and $1p^0$ come together under magnetic field influence, and the electron density distribution becomes similar in these states. The same happens with the $1d^0$ and $1f^0$ energy levels. This effect has been described for the QD CdSe/ZnS [13] in details.

Figure 3 indicates the dependencies of transition energies on the magnetic field induction. Off-central donor impurity causes the increase of the 1p-1s and decrease of 1d-1p transition energies.

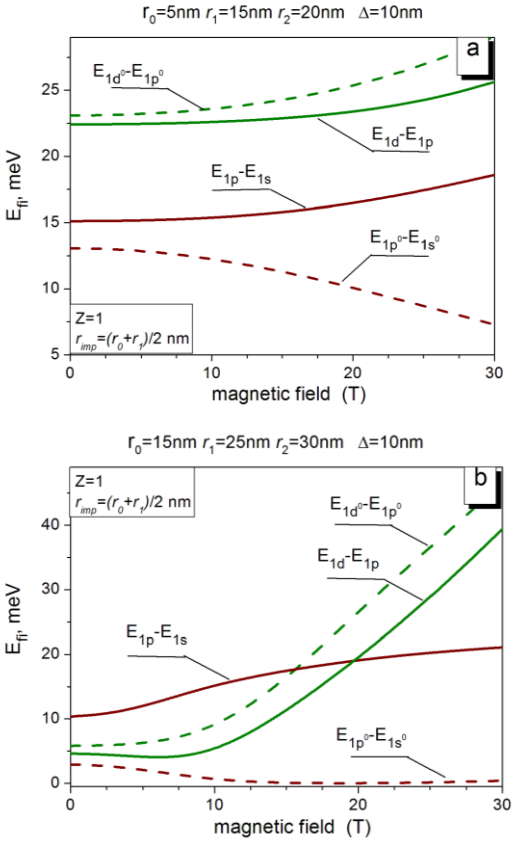

Fig. 3. Dependencies of transition energies on the applied magnetic field in MSQD with r_0 =5 nm, r_1 =15 nm and r_2 =20 nm (a) and r_0 =15 nm, r_1 =25 nm and r_2 =30 nm (b). Solid lines – MSQD with impurity (Z=1), dashed lines without impurity (Z=0).

Figure 4 indicates the linear, third-order nonlinear and total OACs in the MSQD with r_0=5nm (a) r_0=15nm (b) without impurity (Z=0) as function of the incident photon energy. Two peaks are formed by quantum transitions 1s-1p and 1p-1d correspondently. The energy distance between peaks is bigger at bigger magnetic field induction. The third-order nonlinear OAC is much smaller than linear OAC at r_0=5nm (Fig.4a). The value of nonlinear OAC increases with the growth of the core radius and the magnetic field induction. Therefore, at some region of photon energies, the total OAC becomes negative (Fig.4b). In this case, contribution of the quantum transition 1s-1p is much greater than 1p-1d.

The same dependencies have been obtained at the presence central donor impurity. Thus, central impurity does not change the AOC.

The third-order nonlinear OAC is significantly reduced in the case of off-central impurity ($r_{imp} = (r_0 + r_1)/2$.), especially under influence of a magnetic field (Fig.5). Besides this, two peaks of OAC converge into one.

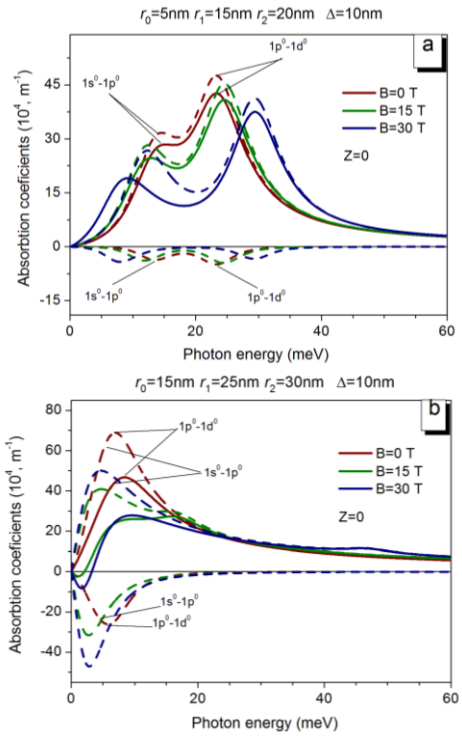

Fig. 4. Dependence of absorption coefficient on the applied magnetic field in the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ multilayer spherical quantum dots with r_0 =5 nm (a) and r_0 =15 nm (b) when Z=0.

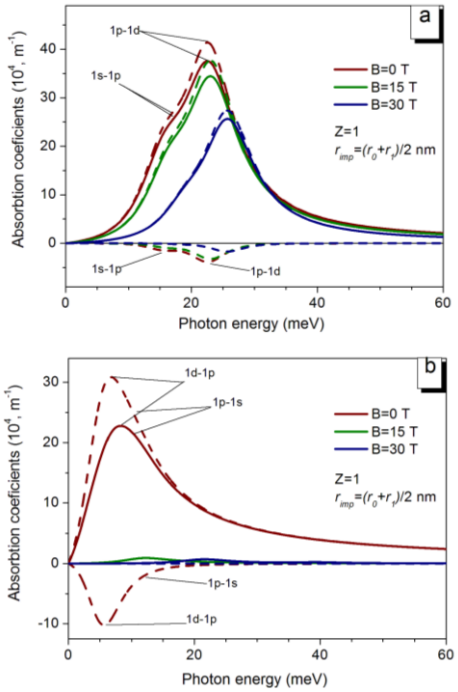

Fig. 5. Dependence of absorption coefficient on the applied magnetic field in the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ multilayer spherical quantum dots with r_0 =5 nm (a) and r_0 =15 nm (b) when Z=1 and $r_{imp} = (r_0 + r_1)/2$.

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