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Impurity effect on the spectral parameters of an electron in a quantum dot–quantum ring semiconductor nanostructure

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ABSTRACT

In the model of effective masses and rectangular potentials, the effect of a hydrogen-like donor impurity on the energy spectrum, electron wave functions and oscillator strengths of intraband quantum transitions in a quantum dot–quantum ring semiconductor nanostructure ($GaAs/Al_xGa_{1-x}As$) is studied theoretically. The stationary Schrödinger equation for an electron interacting with an impurity cannot be solved analytically exactly. For its approximate solution, the unknown wave functions are sought in the form of an expansion over a complete set of cylindrically symmetric wave functions in the nanostructure without impurity, and the electron energy is found by solving the corresponding secular equation. The dependences of the energy spectrum, the binding energy of the electron with the impurity and the oscillator strengths of the quantum intraband transitions on the geometric parameters of the nanostructure are analyzed.

KEYWORDS

Semiconductor nanostructure; quantum dot; quantum ring; donor impurity; electron energy; oscillator strengths

1. Introduction

Multilayer semiconductor nanostructures have been studied both theoretically and experimentally for quite a long time. The unique properties of quasiparticles in such systems make it possible to use them as basic elements in devices of modern nanoelectronics: tunnel nanodiodes, nanolasers, nanodetectors [1, 2].

A special place among various types of multilayer nanostructures is occupied by semiconductor quantum rings. As a rule, they have a cylindrical symmetry, as well as quantum wires, however, in contrast to them, their height is finite and amounts to a few nanometers. So, the movement of charge carriers in such nanosystems is limited in all three dimensions. Therefore, in this aspect, they are similar to cylindrical quantum dots. Modern experimental possibilities make it possible to obtain nanoheterostructures with cylindrical quantum nanorings [3–6] and to study the spectra of quasiparticles in them.

As for the theoretical models for calculating the spectra of main quasiparticles (electrons, phonons, excitons …) in such structures and their interaction between themselves and external fields, they are also intensively developing and improving [7–13].

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Obviously, the presence of impurities in nanostructures with quantum dots and rings will significantly change their physical properties, which, in turn, will affect the physical characteristics of nanodevices that will be created on their basis.

The study of the binding energy of an electron with an impurity in nanostructures with cylindrical symmetry faces mathematical difficulties, which are related to the fact that it is necessary to match the nonspherical symmetry of the nanosystem with the spherical symmetry of the Coulomb potential energy of interaction between the electron and the impurity. Therefore, in the vast majority of studies on the electron spectrum renormalized by the impurity, the variational Ritz method is used [14–18]. This method is quite accurate and simple to describe only the ground state of the electron. The choice of the trial variational function for excited states is ambiguous and cumbersome [16]. Much more informative is the effective potential energy method, which was previously used for the theoretical study of the exciton spectrum in simple and multilayer semiconductor nanotubes [19]. However, this method also gives slightly underestimated values of the binding energy of the electron with the impurity as the size of the nanostructure increases.

In this work, the effect of the donor impurity on the energy spectrum and strength of the oscillators of intraband quantum transitions of an electron in the quantum dot--quantum ring nanostructure based on GaAs/$Al_xGa_{1-x}As$ semiconductors is investigated in the model of effective masses and rectangular potentials. The corresponding Schrödinger equation for an electron interacting with an impurity is solved by expanding the unknown wave function over a complete set of cylindrically symmetric wave functions, and the electron energy is found by solving the corresponding secular equation. The proposed method makes it possible to physically substantiate and adequately study the spectral parameters of the electron in a wide range of geometric parameters of the nanostructure.

2. Theory of the energy spectrum and wave functions of an electron interacting with an impurity in a quantum dot–quantum ring semiconductor nanostructure

The paper investigates a nanostructure of height L, consisting of a cylindrical semiconductor quantum dot (quantum well, GaAs medium), which through a finite potential barrier ($Al_xGa_{1-x}As$ medium) is tunnel-connected to a coaxial cylindrical nanoring (quantum well, GaAs medium). The cross section and energy diagram of such a nanostructure is shown in Figure 1. The donor impurity is located on the axial axis of the nanostructure at the origin. It creates an attractive Coulomb potential for the electron

$$V(\rho, z) = -\frac{e^2}{\varepsilon(\rho)\sqrt{\rho^2 + z^2}} \tag{1}$$

For reasons of symmetry, all subsequent calculations should be performed in a cylindrical coordinate system (ρ, φ, z) with the Oz axis along the axial axis of the nanostructure.

The effective masses, dielectric constants and potential energies of the electron are considered to be known in all areas of multilayer nanostructure.

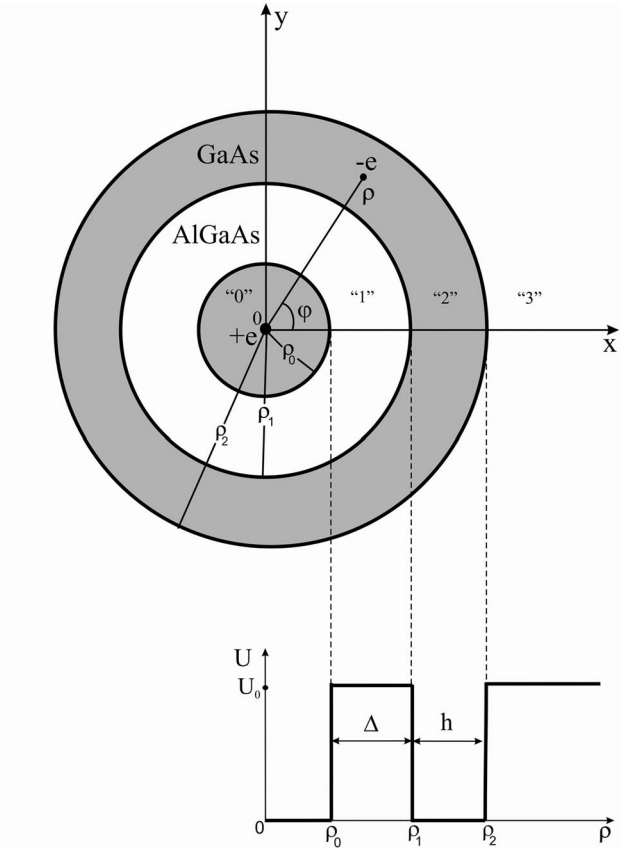

Figure 1. Cross section and energy scheme of the nanostructure.

$$\varepsilon(\rho) = \begin{cases} \varepsilon_0 \\ \varepsilon_1 \end{cases}, \ \mu(\rho) = \begin{cases} \mu_0 \\ \mu_1 \end{cases}, \ \mathrm{U}(\rho) = \begin{cases} 0, & 0 \le \rho \le \rho_0, \quad \rho_1 \le \rho \le \rho_2, \\ \mathrm{U}_0, & \rho_0 < \rho < \rho_1, \ \rho > \rho_2. \end{cases} \tag{2}$$

It is assumed that the limiting potential along the Oz axis is such that at $|z| > \frac{\mathrm{L}}{2}$ $U(z) = \infty$. Also note that in the case of the studied nanostructure based on GaAs/$\mathrm{Al_xGa_{1-x}As}$ semiconductors, the dielectric constants of the contacting media are very close. Therefore, the system can always be considered a continuum with a constant average dielectric constant $\bar{\varepsilon} = (\varepsilon_0 + \varepsilon_1)/2$.

In order to investigate the effect of an impurity on the energy spectrum and wave functions of an electron, it is necessary to solve the stationary Schrödinger equation with the Hamiltonian

$$\widehat{H} = -\frac{\hbar^2}{2} \overrightarrow{\nabla}_{\rho,\varphi} \frac{1}{\mu(\rho)} \overrightarrow{\nabla}_{\rho,\varphi} + U(\rho) - \frac{\hbar^2}{2\mu(\rho)} \frac{\partial^2}{\partial z^2} + V(\rho, z). \tag{3}$$

In the absence of impurities, the corresponding stationary Schrödinger equation is solved analytically exactly, and the wave functions are obtained in the form

$$\Psi^{(0)}_{n_\rho m n_z}(\vec{r}) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} R_{n_\rho m n_z}(\rho) f_{n_z}(z), \tag{4}$$

where

$$f_{n_z}(z) = \sqrt{\frac{2}{L}} \begin{cases} \cos\left(\frac{\pi n_z}{L} z\right), & n_z = 1, 3, 5, \ldots \\ \sin\left(\frac{\pi n_z}{L} z\right), & n_z = 2, 4, 6, \ldots \end{cases}, \tag{5}$$

$$R_{n_\rho m n_z}(\rho, \varphi) = \begin{cases} A_m^{(0)} J_m(k_0 \rho), & 0 \le \rho \le \rho_0 \\ A_m^{(1)} I_m(k_1 \rho) + B_m^{(1)} K_m(k_1 \rho), & \rho_0 < \rho \le \rho_1 \\ A_m^{(2)} J_m(k_0 \rho) + B_m^{(1)} N_m(k_0 \rho), & \rho_1 < \rho \le \rho_2 \\ B_m^{(3)} K_m(k_1 \rho), & \rho > \rho_1 \end{cases} \tag{6}$$

Here $m = 0, \pm 1, \pm 2, ..$– magnetic quantum number, $n_\rho = 1, 2, 3, \ldots$ – radial quantum number, J_m, N_m– Bessel functions of integer order; I_m, K_m– modified Bessel functions, $k_0 = \sqrt{2\mu_0 E/\hbar^2 - \pi^2 n_z^2/L^2}$, $k_1 = \sqrt{2\mu_1(U_0 - E)/\hbar^2 + \pi^2 n_z^2/L^2}$.

All unknown coefficients in (6), as well as the electron energy spectrum ($E_{n_\rho m n_z}$) are found from the conditions of continuity of the radial wave functions and the corresponding fluxes of the probability densities at all heterointerfaces of the nanostructure

$$\begin{cases} R^{(i)}_{n_\rho m n_z}(\rho_i) = R^{(i+1)}_{n_\rho m n_z}(\rho_i) \\ \frac{1}{\mu_i} \frac{\partial R^{(i)}_{n_\rho m n_z}(\rho)}{\partial \rho} \Big|_{\rho=\rho_i} = \frac{1}{\mu_{i+1}} \frac{\partial R^{(i+1)}_{n_\rho m n_z}(\rho)}{\partial \rho} \Big|_{\rho=\rho_i} \ (i = 0, 1, 2) \end{cases} \tag{7}$$

and the normalization condition $\int_0^\infty \left| R_{n_\rho m n_z}(\rho) \right|^2 \rho d\rho = 1$.

In order to solve the Schrödinger equation with the Hamiltonian (3) we write the unknown wave functions in the form of expansion of the complete set of wave functions (4)

$$\Psi_{n m}(\vec{r}) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \sum_{n_\rho} \sum_{n_z} c^{n m}_{n_\rho n_z} R_{n_\rho m n_z}(\rho) f_{n_z}(z) \,. \tag{8}$$

Substituting the expansion (8) into the Schrödinger equation with the Hamiltonian (3), we obtain the secular equation

$$\left| H^m_{n_\rho n_z,\, n'_\rho n'_z} - E_{n m}\, \delta_{n_\rho, n'_\rho} \delta_{n_z, n'_z} \right| = 0, \tag{9}$$

where the matrix elements $H_{n_\rho n_z,\, n'_\rho n'_z}$ have the form

$$H^m_{n_\rho n_z,\, n'_\rho n'_z} = E_{n_\rho m n_z} \delta_{n_\rho, n'_\rho} \delta_{n_z, n'_z} - \\ - \frac{2}{L} e^2 \bar{\varepsilon} \int_{-L/2}^{L/2} dz \int_0^\infty \rho \, d\rho \, \frac{R_{n_\rho m n_z}(\rho)\, R_{n'_\rho m n'_z}(\rho) f_{n_z}(z) f_{n'_z}(z)}{\sqrt{\rho^2 + z^2}} \,. \tag{10}$$

Note that, as can be seen from (8) and (9), the new electron states are now characterized by only two quantum numbers n and m.

The problem of finding the energy spectrum $E_{n m}$ and wave functions $\Psi_{n m}(\vec{r})$ is now reduced to the calculation of eigenvalues and eigenvectors of the resulting matrix.

The found energy spectrum and wave functions also make it possible to estimate the oscillator strengths of intraband optical quantum electron transitions by a known formula [20]:

$$F_{n\,m}^{n'm'} \sim (E_{n'\,m'} - E_{n\,m}) \left| M_{n\,m}^{n'm'} \right|^2, \tag{11}$$

where

$$M_{n\,m}^{n'\mathrm{m}'} = \langle n'\mathrm{m}' \Big| \sqrt{\mu(\rho)}\; e\rho\cos(\varphi) | n\,m \rangle \tag{12}$$

- transition dipole moment.

Note that using the explicit form of wave functions (8) it is easy to establish selection rules according to which only those transitions between the electron energy levels is nonzero probable for which the difference in magnetic quantum numbers is ± 1 ($\Delta m = \pm 1$).

3. Analysis and discussion of results

The following study of the electronic spectrum and oscillator strengths of intraband optical quantum transitions and their dependence on the geometric parameters of the system was carried out for a nanostructure based on GaAs/$Al_{0.4}Ga_{0.6}As$ semiconductors with the following physical parameters: $\varepsilon_0 \approx \varepsilon_1 = 13$, $\mu_0 = 0,063m_0$, $\mu_1 = 0,096m_0$, $U_0 = 297\ meV$, (m_0 – electron mass in vacuum); the lattice constant of the GaAs medium $a_{GaAs} = 5,65\,A^o$.

Figure 2 shows the dependences on the radius (ρ_0) of the quantum dot of the electron energies in the nanostructure without an impurity (Figure 2a) and with an impurity (Figure 2b) at $\Delta = 3a_{GaAs}$, $h = 18a_{GaAs}$, $L = 18a_{GaAs}$.

Figure 2 shows that the electron energies nonmonotonically depend on the radius of the quantum dot. This non-monotonicity is manifested in the alternation of horizontal and descending sections, i.e. the so-called anticrossing of energy levels of the same symmetry is manifested. In this case, the horizontal sections correspond to the electronic

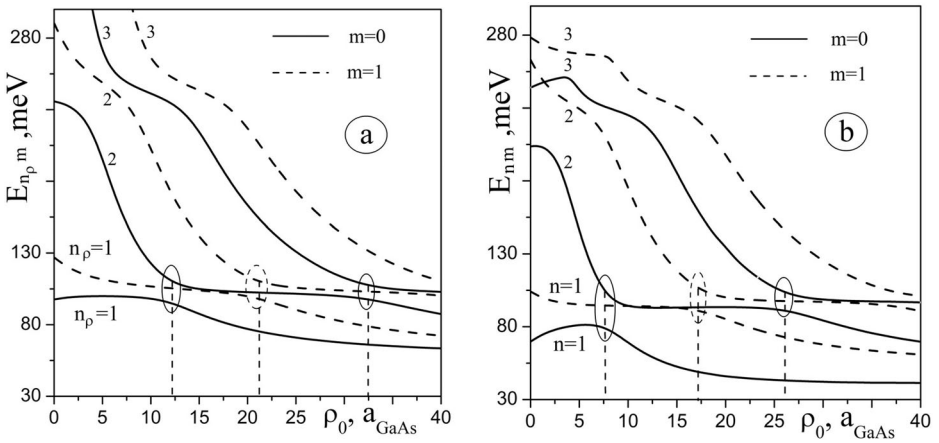

Figure 2. Dependences on the radius (ρ_0) of the quantum dot of the electron energies in the nanostructure without an impurity (a) and with an impurity (b) at $\Delta = 3a_{GaAs}$, $h = 18a_{GaAs}$, $L = 18a_{GaAs}$.

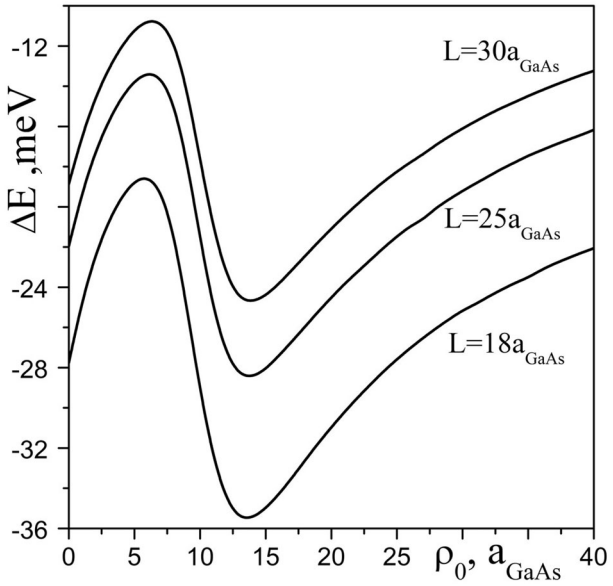

Figure 3. Dependences on the radius of the quantum dot (ρ_0) of the binding energy of the electron with the impurity at the ground state at $\Delta = 3a_{GaAs}$, $h = 18a_{GaAs}$ and at different values of the height of the nanostructure $L = 18a_{GaAs}$, $L = 25a_{GaAs}$, $L = 30a_{GaAs}$.

states in which the quasiparticle is located in the outer nano ring with an overwhelming probability. In those states that correspond to the descending sections, the electron is mainly localized in the quantum dot, and an increase in its radius leads to a decrease in the resonance energy.

A comparison of both figures shows that the presence of a donor impurity does not lead to significant qualitative changes in the behavior of the electronic spectrum. However, attractive Coulomb impurity potential (1) decreases the height of the potential barrier separating the quantum dot and the nanoring, and also significantly increases the depth of the inner potential well (medium "0"). Therefore, the energies of the electron in all states in the nanostructure with the impurity are shifted to the low-energy region of the spectrum, and the anticrossings are shifted to the region of smaller radii of the quantum dot.

Figure 3 shows the dependences on the radius of the quantum dot (ρ_0) of the binding energy of the electron with the impurity at the ground state at $\Delta = 3a_{GaAs}$, $h = 18a_{GaAs}$ and different values of the height of the nanostructure $L = 18a_{GaAs}$, $L = 25a_{GaAs}$, $L = 30a_{GaAs}$.

As can be seen from Figure 3, the binding energy of the electron with the impurity nonmonotonically depends on the radius of the quantum dot and reaches certain maximum and minimum values. The binding energy acquires its minimum modulo value at $\rho_0 \approx 7\, a_{GaAs}$. In this case, the electron with an overwhelming probability is localized in the outer nanoring, and the distance between it and the impurity is significant. With increasing radius ρ_0, the electron begins to tunnel into the quantum dot region, the distance between it and the impurity decreases, and the binding energy modulo increases. The binding energy acquires the maximum value at $\rho_0 \approx 14\, a_{GaAs}$. The electron is already completely localized in the region of the quantum dot at this value of the radius.

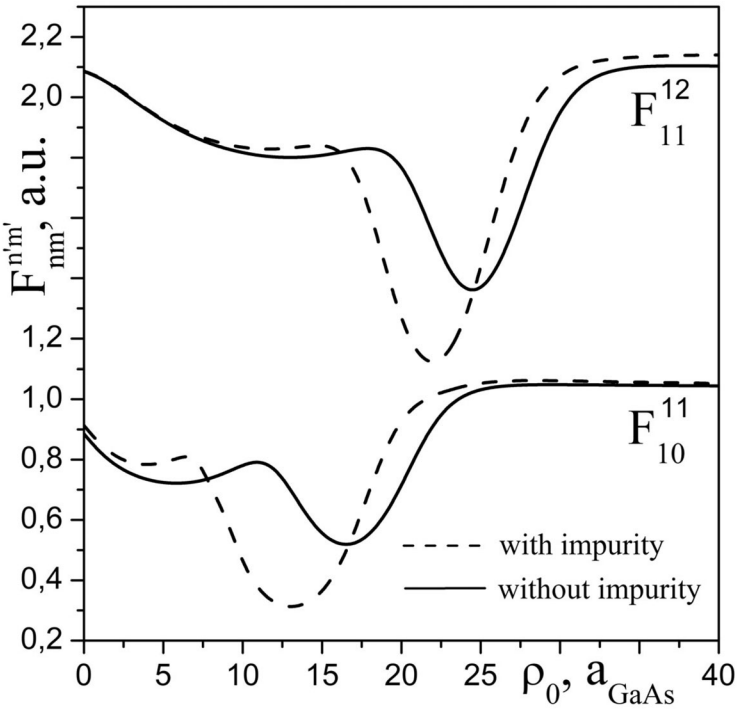

Figure 4. Dependences on the radius (ρ_0) of the quantum dot of the oscillator strengths of the intra-band quantum transitions of the electron between states ((10) → (11), (11) → (12)) at $\Delta = 3a_{GaAs}$, $h = 18a_{GaAs}$ and at different values of the height of the nanostructure $L = 18a_{GaAs}$.

The absolute value of the binding energy decreases with increasing height of the nanostructure (Figure 3). The binding energy reaches saturation, and its value is $\sim$ 8 meV at $\rho_0 \to \infty$, $L \to \infty$, which corresponds to the value of the binding energy of the electron with the impurity in the bulk GaAs crystal. This confirms the correctness and adequacy of the method used in the work.

Also note that since the absolute value of the binding energy decreases in the region of the radii of the quantum dot $0 \leq \rho_0 \leq 5\ a_{GaAs}$, the energy of the ground quantum state of the electron first increases slightly with increasing ρ_0, then reaches a maximum, and only then decreases (Figure 2b).

The dependences of the oscillator strengths on ρ_0 are also complex and nonmonotonic (Figure 4), since the electron, being in different states, can be localized either in the region of the quantum dot or in the outer nanoring. As can be seen from Figure 4, for both types of transitions ((10) → (11), (11) → (12)), a bright minimum is observed in these dependences. The presence of a minimum in this dependence is entirely due to the small overlap of the wave functions of the electron in the corresponding states. The overlap of the electron wave functions in the quantum states with $m = 0$ ($m = 1$) and $m = 1$ ($m = 2$) is significant in the region of small or large radii of the quantum dot, so the intensity of the transition is significant.

Note also that the presence of an impurity leads to a shift in the minimum value of the oscillator strength to the region of smaller radii of the quantum dot, and its value decreases even further.

4. Conclusions

In the model of effective masses and rectangular potential energies, one of the possible theoretical approaches to studying the spectral parameters of an electron in a semiconductor quantum dot–quantum ring nanostructure with a donor hydrogen-like impurity on the axial axis is proposed. The method makes it possible to physically substantiate and adequately investigate the spectral parameters of an electron in a wide range of geometric parameters of the nanostructure.

It is shown that both the binding energies of an electron with an impurity and the oscillator strengths of the intraband quantum transitions of an electron depend in a complex and non-monotonous manner on the quantum dot radius, reaching certain minimum and maximum values.

This feature of the behavior of the spectral parameters of the electron is entirely due to the complex nature of the distribution function of the probability density of finding an electron (which interacts with the impurity) in the space of the multilayer nanostructure.

The introduction of the impurity leads to a decrease in the electron energy, as well as to a shift of anticrossings and all maximum and minimum values of the oscillator strengths to the region of smaller radii of the quantum dot.

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