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

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Motivation for research

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.

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. Calculations of the electron energy spectrum are performed by the method of expansion of the wave functions of the quasiparticle by a complete set of cylindrical wave functions obtained as an exact solution of the Schrödinger equation in the nanosystem in the absence of impurities.

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

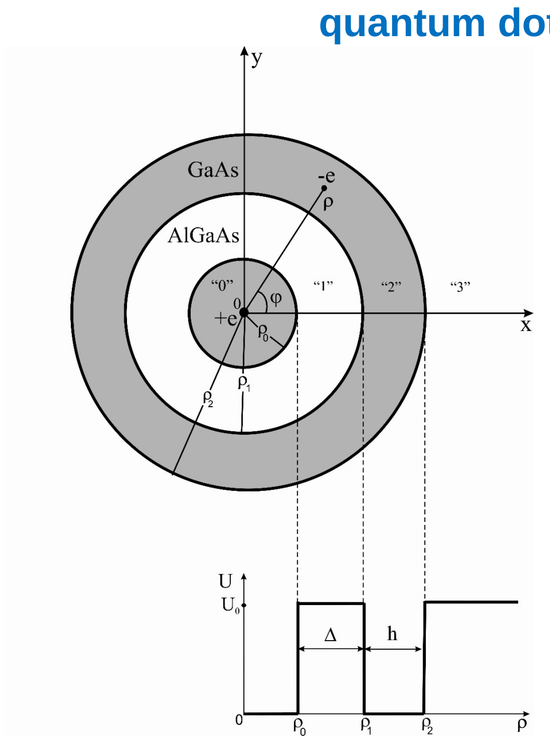

Fig.1. Cross section and energy scheme of the nanostructure

The paper investigates a nanostructure of height *L*, consisting of a cylindrical semiconductor 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 Fig. 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

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

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

$$\hat{H}=-\frac{\hbar^2}{2}\vec{\nabla}_{\rho,\varphi}\frac{1}{\mu(\rho)}\vec{\nabla}_{\rho,\varphi}+U(\rho)-\frac{\hbar^2}{2\mu(\rho)}\frac{\partial^2}{\partial z^2}+V(\rho,z) \qquad (2)$$

$U(\rho)$ - dimensional quantization potential.

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

$$\Psi^{(0)}_{n_\rho m n_z}(\vec{r})=\frac{1}{\sqrt{2\pi}}e^{im\varphi}R_{n_\rho m n_z}(\rho)\,f_{n_z}(z) \qquad (3)$$

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

$$R_{n_\rho m n_z}(\rho,\varphi)=\begin{cases}A^{(0)}_m J_m(k_0\rho), & 0\le\rho\le\rho_0\\ A^{(1)}_m I_m(k_1\rho)+B^{(1)}_m K_m(k_1\rho), & \rho_0<\rho\le\rho_1\\ A^{(2)}_m J_m(k_0\rho)+B^{(1)}_m N_m(k_0\rho), & \rho_1<\rho\le\rho_2\\ B^{(3)}_m K_m(k_1\rho), & \rho>\rho_1\end{cases} \qquad (5)$$

$m=0,\pm1,\pm2,..$- magnetic quantum number $n_\rho=1,2,3,...$ - radial quantum number

J_m, N_m - Bessel functions of integer order I_m, K_m - modified Bessel functions

All unknown coefficients in (5), as well as the electron energy spectrum, 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 and the normalization condition.

In order to solve the Schrödinger equation with the Hamiltonian (2) we write the unknown wave functions in the form of expansion of the complete set of wave functions (3)

$$\Psi_{nm}(\vec{r})=\frac{1}{\sqrt{2\pi}}e^{im\varphi}\sum_{n_\rho}\sum_{n_z}c^{nm}_{n_\rho n_z}R_{n_\rho m n_z}(\rho)\,f_{n_z}(z) \qquad (6)$$

Substituting the expansion (6) into the Schrödinger equation with the Hamiltonian (2), we obtain the secular equation

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

$$H^m_{n_\rho n_z,n'_\rho n'_z}=E_{n_\rho m n_z}\delta_{n_\rho,n'_\rho}\delta_{n_z,n'_z}- \qquad (7)$$

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

The problem of finding the energy spectrum and wave functions 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

$$F^{n'm'}_{nm}\sim(E_{n'm'}-E_{nm})\left|M^{n'm'}_{nm}\right|^2 \qquad M^{n'm'}_{nm}=\left\langle n'm'\left|\sqrt{\mu(\rho)}\;e\rho\cos(\varphi)\right|nm\right\rangle \qquad (8)$$

Analysis and discussion of results

The calculation and analysis of the electron spectrum properties and the oscillator strengths were performed by numerical methods on the example of a nanostructure based on GaAs/$Al_{0.4}Ga_{0.6}As$ semiconductors

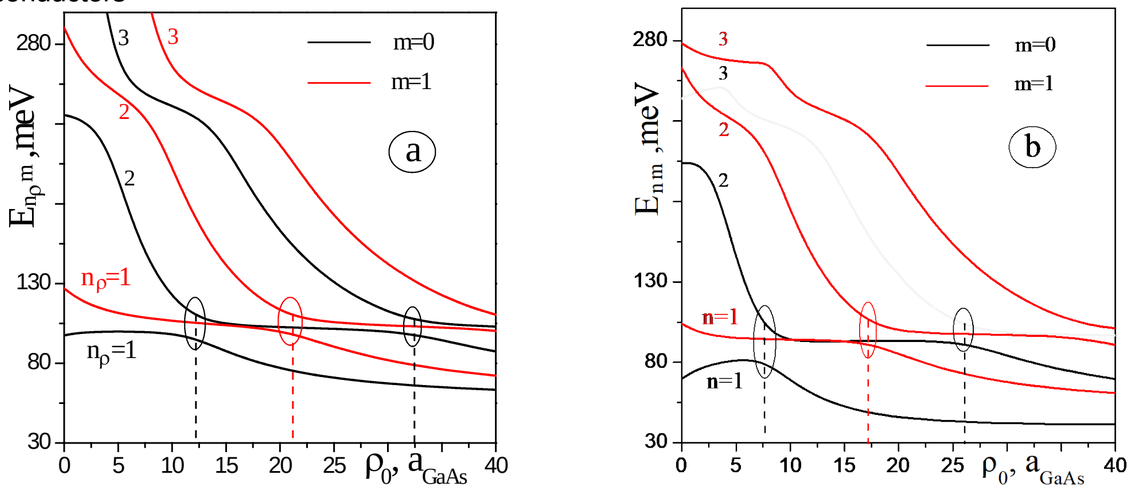

Fig. 2. Dependences on the radius (ρ_0) of the quantum dot of the electron energies in the nanostructure without an impurity (Fig. 2, a) and with an impurity (Fig. 2, b) at $\Delta=3a_{GaAs}$, $h=18a_{GaAs}$, $L=18a_{GaAs}$.

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 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. The attractive 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.

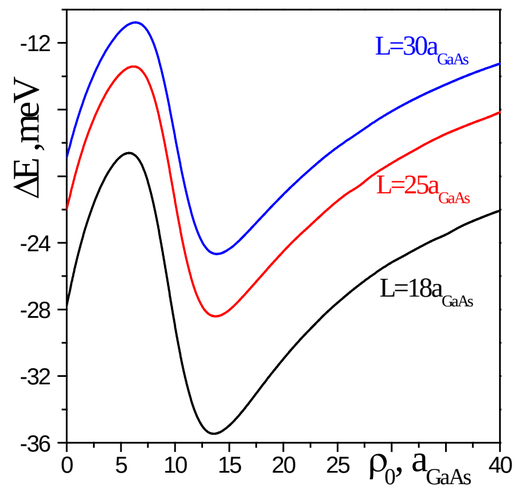

Fig. 3. Dependences on the radius of the quantum dot of the binding energy of the electron ground state at $\Delta=3a_{GaAs}$, $h=18a_{GaAs}$.

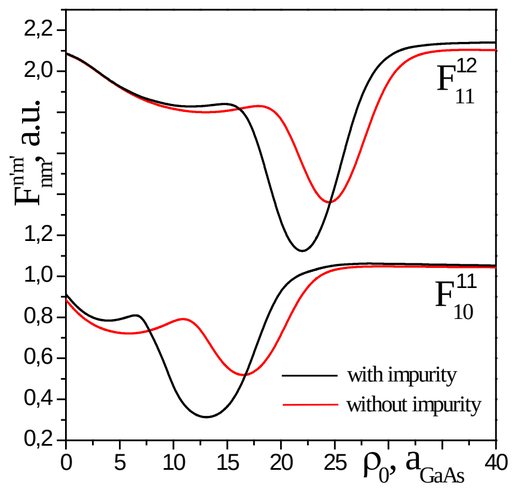

Fig. 4. Dependences on the radius of the quantum dot of the oscillator strengths of the intraband quantum transitions of the electron between states (10) -> (11) and (11) -> (12) at $h=18a_{GaAs}$, $\Delta=3a_{GaAs}$, $L=18a_{GaAs}$.

As can be seen from Fig. 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 value at $\rho_0\approx7a_{GaAs}$. 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, the electron begins to tunnel into the quantum dot region, the distance between it and the impurity decreases, and the binding energy increases. The binding energy acquires the maximum value at $\rho_0\approx14a_{GaAs}$. At this value of the radius, the electron is already completely localized in the region of the quantum dot.

Note that at $\rho_0\to\infty$, $L\to\infty$ the binding energy reaches saturation, and its value is ~ 8 meV, which corresponds to the value of the binding energy of the electron with the impurity in the massive GaAs crystal.

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

Note 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.

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.

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2. *M. Zervos* Electronic properties of core-shell nanowire resonant tunneling diodes // Nanoscale Research Letters. – 2014. – **9**. – P. 509.