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The exciton spectrum of the cylindrical quantum dot - quantum ring semiconductor nanostructure in an electric field

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In the model of effective masses and rectangular potentials for an electron and a hole, the influence of a uniform electric field on the energy spectrum and wave functions of the exciton and the oscillator strengths of interband quantum transitions in the semiconductor ($GaAs/Al_xGa_{1-x}As$) quantum dot-quantum ring nanostructure is theoretically investigated. The stationary Schrödinger equations for noninteracting quasiparticles in the presence of an electric field cannot be solved analytically. For their approximate solution, the unknown wave functions are sought in the form of an expansion over the complete set of cylindrically symmetric wave functions, and the electron energy is found by solving the corresponding secular equation. The exciton binding energy is found using perturbation theory.

The dependences of the energy spectra, the wave functions of an electron, hole, and exciton, and the intensity of interband optical quantum transitions on the magnitude of the electric field strength are analyzed.

Keywords: Quantum Dot, Nanoring, Exciton, Energy spectrum, Intensity, Electric field.

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Introduction

Currently, the experimental possibilities of creating various semiconductor nanostructures allow scientists to grow entire ordered arrays of concentric simple and double quantum rings with axial symmetry and to study the luminescence spectra in them [1-3].

The unique properties of quasiparticles (electrons, holes, excitons, ...) in such nanostructures, which are manifested during their interaction with each other and external electric and magnetic fields, make it possible to use them in modern nanoelectronics devices: semiconductor lasers [4], photodetectors [5], elementary qubits quantum computers [6].

Theoretical models for calculating spectra, wave functions of basic quasiparticles and intensities of intraband and interband optical quantum transitions in such structures are also intensively developed and improved.

In papers [7, 8], the authors investigated the dependence of the energy spectrum of an electron in a simple cylindrical semiconductor quantum ring on the intensity of a uniform electric field directed perpendicular to the axial axis of the ring. They showed that these dependencies are different for a certain range of changes in the electric field strength and are determined by the ratio between the inner and outer radii of the rings. In particular, anticrossing of energy levels can be observed in the corresponding dependencies.

In papers [9-12], the authors theoretically investigated the influence of electric and magnetic fields on the energy spectrum, wave functions and intensities of intraband quantum electron transitions in double quantum nanorings based on $GaAs/Al_xGa_{1-x}As$ semiconductors. The stationary Schrödinger equation for a quasiparticle in the presence of a magnetic field is solved analytically exactly, and the wave function is obtained as a superposition of confluent hypergeometric functions and generalized Laguerre polynomials. In the case of an electric field, this equation cannot be solved exactly. Therefore, the spectrum of an electron interacting with an electric field was found by the method of expanding the unknown wave function of the electron by the complete orthonormal set of wave functions of a quasiparticle in a nanosystem without a field and solving the resulting secular equation.

The authors showed that the electron in all states can be localized either in the inner or outer ring depending on the value of the magnetic induction (*B*), the strength of the electric (*F*) fields, and the ratio between the thicknesses of the nanorings. In this case, energy level anticrossings are observed in the corresponding dependences of the energy levels on *F* or *B*, and the maxima and minima of the intensities of the corresponding transitions are clearly pronounced in the dependence of the oscillator strengths. The authors found that the reason for this behavior is a change in the localization of an electron in the space of two nanorings in different quantum states with a change in the electric field strength or magnetic field induction.

Exciton and polaron effects in nanorings were studied in papers [13, 14]. The calculations performed by the authors showed that it is possible to purposefully control the location of an electron in a system of double nanorings using electric and magnetic fields. The energy of the ground state of the polaron decreases nonlinearly with increasing electric field strength, and, in general, the application of electric and magnetic fields leads to strengthening of the electron-phonon interaction.

In this work, we will theoretically investigate the influence of a uniform electric field on the energy spectrum and wave functions of the exciton (taking into account the energy of the electron-hole interaction), as well as on the intensity of interband quantum transitions in the quantum dot-quantum ring semiconductor nanostructure.

I. Theory of the energy spectrum and wave functions of an exciton in a quantum dot - quantum ring semiconductor nanostructure.

The paper presents studies of a nanostructure consisting of a cylindrical semiconductor quantum dot (quantum well, GaAs medium), which is tunnel-connected to a coaxial cylindrical nanoring (quantum well, GaAs medium) through a finite potential barrier ($Al_xGa_{1-x}As$ medium). The height of the nanostructure is *L*. The cross section by the plane z = 0 and the scheme of the potential energies of an electron and a hole of such a nanostructure in the absence of an electric field are shown in Fig. 1. The electric field intensity vector *F* is directed along the *Ox* axis.

For reasons of symmetry, all further calculations will be performed in a cylindrical coordinate system with the *Oz* axis along the axial axis of the nanostructure.

Since the lattice constants and the permittivities of the semiconductor elements of the nanostructure differ little from each other, we will use the model of effective masses and rectangular potentials to calculate the spectra and wave functions of an electron and a hole. We will consider them to be known in all areas of the investigated nanostructure:

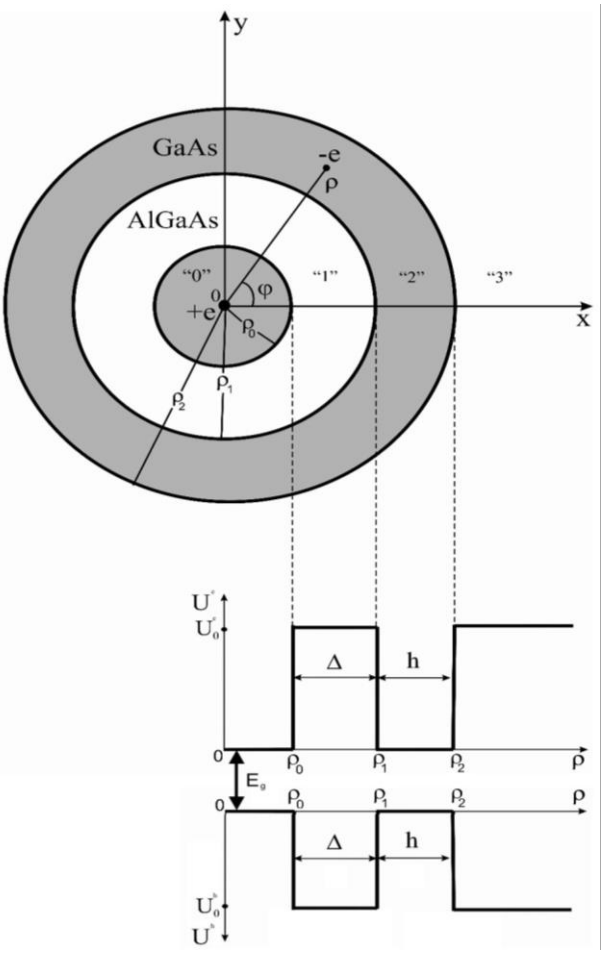


Fig. 1. Geometric and energy schemes of the nanostructure.

$$\mu^{(e,h)}(\vec{r}) = \begin{cases} \mu_0^{(e,h)}, & |z| \le L/2 \ \ and \ \ 0 \le \rho \le \rho_0, \ \rho_1 \le \rho \le \rho_2 \\ \mu_1^{(e,h)}, & |z| > L/2 \ \ or \ \ |z| \le L/2 \quad and \ \ \rho_0 < \rho \le \rho_1, \ \rho > \rho_2 \end{cases}, \tag{1}$$

$$U^{(e,h)}(\rho) = \begin{cases} U_0^{(e,h)}, & \rho_0 \le \rho \le \rho_1, \ \rho > \rho_2, \\ 0, & 0 < \rho < \rho_0, \ \ \rho_1 < \rho \le \rho_2 . \end{cases} \tag{2}$$

We will also assume that the exit of quasiparticles into the $|z| \le L/2$ region is impossible, since the electric field does not affect the energy spectrum of the electron and hole (and therefore the exciton) when both quasiparticles move along the *Oz* axis.

$$U^{(e,h)}(z) = \begin{cases} \infty, & |z| > L/2, \\ 0, & |z| \le L/2. \end{cases} \tag{3}$$

In order to find the energy spectrum and wave functions of the exciton in such a nanostructure, it is necessary to solve the stationary Schrödinger equation

$$\widehat{H}_{ex}(\vec{r}_e, \vec{r}_h)\Psi_{ex}(\vec{r}_e, \vec{r}_h) = E_{ex}\Psi_{ex}(\vec{r}_e, \vec{r}_h) \tag{4}$$

with the Hamiltonian

$$\widehat{H}_{ex}(\vec{r}_e, \vec{r}_h) = E_g + \widehat{H}_e(\vec{r}_e) + \widehat{H}_h(\vec{r}_h) + U(|\vec{r}_e - \vec{r}_h|). \tag{5}$$

Here, E_g is the band gap width of the nanosystem quantum well material;

$$\widehat{H}_i(\vec{r}_i) = \frac{1}{2\mu^{(i)}(\rho_i)}\left[-\hbar^2\left(\frac{\partial^2}{\partial\rho_i^2} + \frac{1}{\rho_i}\frac{\partial}{\partial\rho_i} + \frac{1}{\rho_i^2}\frac{\partial^2}{\partial\varphi_i^2}\right)\right] - \frac{\hbar^2}{2\mu^{(i)}(\rho_i)}\frac{\partial^2}{\partial z_i^2} + U^{(i)}(\vec{r}_i) \mp |e|F\rho_i\cos\varphi_i, \quad (i = e,h) \tag{6}$$

- the Hamiltonians of an electron and a hole in an electric field that do not interact with each other;

$$U(|\vec{r}_e - \vec{r}_h|) = -\frac{e^2}{\varepsilon(\vec{r}_e, \vec{r}_h)|\vec{r}_e - \vec{r}_h|} \tag{7}$$

- the potential energy of the interaction between an electron and a hole in a medium with permittivity $\varepsilon(\vec{r}_e, \vec{r}_h)$.

The Schrödinger equation (4) with the Hamiltonian (5) cannot be solved exactly. We will seek its approximate solution in the following way. Considering that the energy of interaction between an electron and a hole is two orders of magnitude less than the energy of their size quantization, we first find the last ones. At the same time, we will take into account the effect of the electric field, and then we will find the binding energy of both quasiparticles using the perturbation theory.

So, further we will solve the stationary Schrödinger equations for an electron and a hole that do not interact with each other

$$\widehat{H}_i\Psi_i(\rho_i, \varphi_i, z_i) = E_i\Psi_i(\rho_i, \varphi_i, z_i), \ \ (i = e,h) \tag{8}$$

The method of solving equations (8) will be given on the example of an electron, omitting the index *i*.

It can be seen from the form of the Hamiltonian (6) that the variable *z* in the corresponding Schrödinger equations (8) is separated, and it is advisable to look for the electron wave function in the form [13]

$$\Psi(\vec{r}) = F(\rho, \varphi)f_{n_z}(z) \tag{9}$$

Here

$$f_{n_z}(z) = \begin{cases} \cos\left(\frac{\pi n_z}{L}z\right), & n_z = 1,3,5,\ldots \\ \sin\left(\frac{\pi n_z}{L}z\right), & n_z = 2,4,6,\ldots \end{cases} \tag{10}$$

In the absence of an electric field, equation (8) also has exact solutions

$$F^0_{n_\rho m}(\rho, \varphi) = \frac{1}{\sqrt{2\pi}}R_{n_\rho m}(\rho)e^{im\varphi} \tag{11}$$

with radial functions

$$R^i_{n_\rho m}(\rho) = A^{(i)}_{n_\rho m}\, j^{(i)}_m(\chi\rho) + B^{(i)}_{n_\rho m}\, n^{(i)}_m(\chi\rho), \quad (i = 0,1,2,3) \tag{12}$$

$$j^{(i)}_m(\chi\rho) = \begin{cases} I_m(\chi_0\rho), & i = 1,3 \\ J_m(\chi_1\rho), & i = 0,2 \end{cases} \tag{13}$$

$$n^{(i)}_m(\chi\rho) = \begin{cases} K_m(\chi_0\rho), & i = 1,3 \\ N_m(\chi_1\rho), & i = 0,2 \end{cases} \tag{14}$$

Here n_ρ and m are radial and magnetic quantum numbers; J_m, N_m are cylindrical Bessel functions of the first and second kind; I_m, K_m are cylindrical modified Bessel functions of the first and second kind;

$$\chi_0 = \sqrt{2\mu_0\left(U_0 - E^0_{n_\rho m}\right)/\hbar^2 + \pi^2 n_z^2/L};$$

$$\chi_1 = \sqrt{2\mu_1 E^0_{n_\rho m}/\hbar^2 - \pi^2 n_z^2/L};$$

$$B^{(0)}_{n_\rho m} = 0,\ A^{(3)}_{n_\rho m} = 0$$

All the unknown coefficients $A^{(i)}_{n_\rho m}$, $B^{(i)}_{n_\rho m}$ in the wave functions and electron energies $E^0_{n_\rho m}$ are found from the conditions of continuity of the radial functions (12)–(14) and the probability density fluxes at the heteroboundaries of the nanostructure and the normalization condition.

Note that the wave functions (11) together with (10) form a complete orthonormal set.

Then, in order to find the energy spectrum and wave functions of an electron in a nanostructure at $F \neq 0$, we will represent these functions in the form of an expansion of the complete set of wave functions (11)

$$F_n(\rho,\varphi) = \frac{1}{\sqrt{2\pi}}\sum_{n_\rho}\sum_m c^n_{n_\rho m} R_{n_\rho m}(\rho) e^{im\varphi}. \qquad (15)$$

Substituting the expansion (15) into the Schrödinger equation with Hamiltonian (6), it is easy to obtain the secular equation

$$\left| H_{n_\rho m, n_\rho' m'} - E_{nn_z}\delta_{n_\rho, n_\rho'}\delta_{m,m'} \right| = 0 \qquad (16)$$

with matrix elements

$$H_{n_\rho m, n_\rho' m'} = E_{n_\rho m}\delta_{n_\rho, n_\rho'}\delta_{m,m'} + \left(\delta_{m',m+1} + \delta_{m',m-1}\right)\frac{eF}{2}\int_0^\infty R_{n_\rho m}(\rho)\, R_{n_\rho' m'}(\rho)\rho^2 d\rho\ . \qquad (17)$$

Now, in order to find the energy spectrum of a quasiparticle and its wave functions, it is necessary to find the eigenvalues and eigenvectors of the obtained matrix.

Since the summation is based on the indices n_ρ and m in (15), the new quantum states of the electron (hole) interacting with the electric field are now characterized by only one quantum number n.

So now we know both the complete wave functions of the electron $\Psi^e_{n^e n_z^e}(\vec{r})$ (9) and its energy $E^e_{n^e n_z^e}$. The wave functions ($\Psi^h_{n^h n_z^h}(\vec{r})$) and the hole energy ($E^h_{n^h n_z^h}$) are obtained in exactly the same way.

Then the exciton energy in the studied nanostructure is obtained in the form

$$E^{n^e n_z^e}_{n^h n_z^h} = E_g + E^e_{n^e n_z^e} + E^h_{n^h n_z^h} + \Delta E^{n^e n_z^e}_{n^h n_z^h} \qquad (18)$$

Here, $\Delta E^{n^e n_z^e}_{n^h n_z^h}$ is the exciton binding energy, which, due to its smallness, can be found according to the perturbation theory

$$\Delta E^{n^e n_z^e}_{n^h n_z^h} = -\frac{e^2}{\bar{\varepsilon}}\int d^3\vec{r}_e \int d^3\vec{r}_h \frac{\left|\Psi^e_{n^e n_z^e}(\vec{r})\Psi^h_{n^h n_z^h}(\vec{r})\right|^2}{\varepsilon(\vec{r}_e,\vec{r}_h)|\vec{r}_e - \vec{r}_h|} \qquad (19)$$

The obtained energies and wave functions of the electron and hole also make it possible to detect the intensity of interband optical quantum transitions using the well-known formula [15]

$$I^{n^e n_z^e}_{n^h n_z^h} \cong \left|\int \Psi^e_{n^e n_z^e}(\rho,\varphi,z)\Psi^h_{n^h n_z^h}(\rho,\varphi,z)\rho\, d\rho d\varphi dz\right|^2 \qquad (20)$$

The calculation and analysis of the exciton spectrum and the intensities of interband quantum transitions was performed by numerical methods for a nanostructure based on $GaAs/Al_{0.4}Ga_{0.6}As$ semiconductors.

II. Analysis and discussion of results.

The dependence of the electron, hole and exciton spectrum and the intensities of interband optical quantum transitions on the electric field strength (F) was studied using the example of a $GaAs/Al_{0.4}Ga_{0.6}As$ nanostructure with the following physical parameters: E_g = 1424 meV, $\varepsilon_0 \approx \varepsilon_1 = 13$, μ^e_0=0.096 m_0, μ^e_1=0.063 m_0, U^e_0=297 meV, μ^h_0=0.61 m_0, μ^h_1=0.51 m_0 U^h_0=224 meV (m_0 is the electron mass in vacuum); lattice constant of the medium $GaAs \cdot \alpha_{GaAs}$ =5.65 A^0.

Figures 2a, b, c, d shows the dependences of the energies of the electron (Fig. 2a, b) and hole (Fig. 2c, d) on the magnitude of the electric field strength (F) at L = 5 nm, $h = 17\alpha_{GaAs}$, $\rho_0 = 0$, $\Delta = 21\alpha_{GaS}$ (Fig. 2a, c) and $\rho_0 = 18\alpha_{GaAs}$, $\Delta = 3\alpha_{GaS}$ (Fig. 2b, d).

That is, Figures 2a,c correspond to a simpler nanostructure that contains only one nanoring (no quantum dot) with thickness $h = 17\alpha_{GaS}$ and inner radius $\rho_1 = 21\alpha_{GaS}$, and Figures 2b,d correspond to a nanostructure with a quantum dot and a nanoring of the same geometric dimensions. On the left of all the figures, the quantum numbers n_ρ, m are given, which characterize the corresponding energy levels in the absence of a field.

Figures 2a, c show that for both quasiparticles, in the absence of a quantum dot in the nanostructure, levels generated by the quantum number n_ρ = 1 and different values of the magnetic quantum number m are formed on the quantum well energy scale. In the presence of a quantum dot, "new" levels with different values of quantum numbers n_ρ appear in the energy spectra of both quasiparticles at F = 0 (Fig. 2b, d). The energy of the ground state of both the electron and the hole only decreases with increasing electric field strength F. However, the energy of excited states can increase with increasing F and only then decrease. In the general case, the increase or decrease of electron or hole energies with

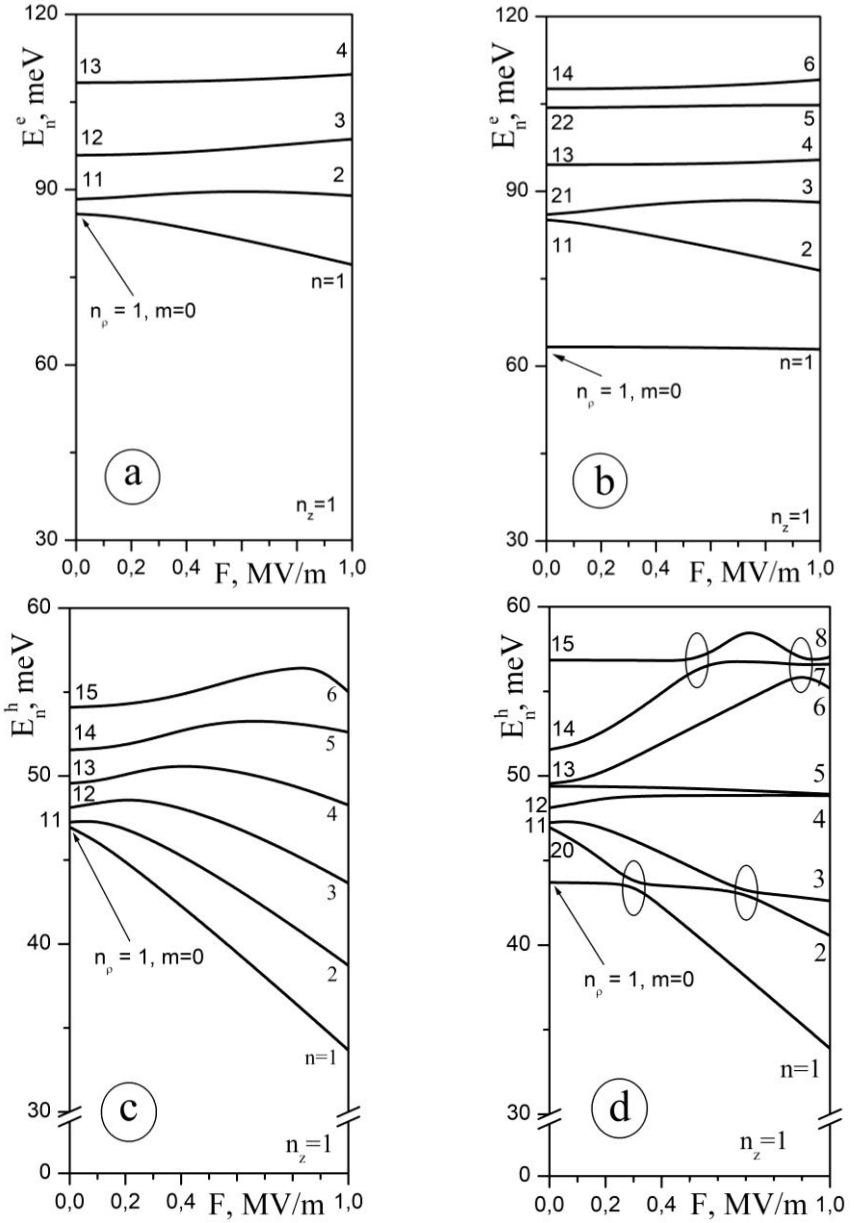


Рис.2. Dependences of the energies of the electron (Fig. 2a, b) and hole (Fig. 2c, d) on the magnitude of the electric field strength (F) at L=5 nm, $h = 17\alpha_{GaAs}$, $\rho_0 = 0$, $\Delta = 21\alpha_{GaS}$ ((Fig. 2a, c) and $\rho_0 = 18\alpha_{GaAs}$, $\Delta = 3\alpha_{GaS}$ (Fig. 2 b, d).

increasing F is due to the region of the nanostructure in which the quasiparticle is localized in the corresponding states and the nature of the angular distribution of the probability density with respect to the direction of the electric field strength.

As can be seen from Figures 2a, b, the electron energy weakly depends on the magnitude of the electric field strength. Since the effective mass of the hole is almost an order of magnitude greater than the mass of the electron, the density of its energy levels in the quantum well energy scale is significant, their dependence on F is sharply nonmonotonic with pronounced level anticrossings (Fig. 2d). The cause of anticrossings is the change in the localization of the quasiparticle between the quantum dot and the outer ring in the corresponding quantum states with an increase in the electric field strength [12]. Anticrossings occur where levels of different symmetry at $F = 0$ should have crossed. At this value of the strength at the anticrossing point, the probabilities of both quasiparticles being in the region of the quantum dot and the nanoring are the same and equal to 0.5.

Figures 3a, b shows the dependences of several lowest exciton levels (Fig. 3a) and the corresponding intensities of interband optical quantum transitions (Fig. 3b) on the magnitude of the electric field strength (F) at L = 5 nm, $h = 17\alpha_{GaS}$, $\rho_0 = 18\alpha_{GaAs}$, $\Delta = 3\alpha_{GaS}$.

Figure 3a shows that the dependence of the exciton levels on F nonmonotonically decreases with the manifestations of exciton anticrossing. The exciton binding energy calculated by formula (19) turns out to be two orders of magnitude smaller than the sum of the size-quantized energies of an electron and a hole. Therefore, the behavior of exciton levels with a change in strength F is completely determined by the peculiarities of the behavior of the electron and hole energies and their common contribution to (18).

It can be seen from Figure 3b that in the range of electric field strength change from 0 to 1 MV/m, only two transitions have significant intensity: I_1^1 from $F = 0$ to $F \approx 0.4$ MV/m and I_2^1 from $F \approx 0.2$ to $F \approx 0.7$ MV/m. The intensity of other transitions is low. The transition intensity I_1^1 is maximum at $F = 0$, and with increasing F it only decreases and is practically equal to zero at $F \approx 0.4$ MV/m. This behavior of the intensity can be explained by the following considerations.

Consider the evolution of the density of the

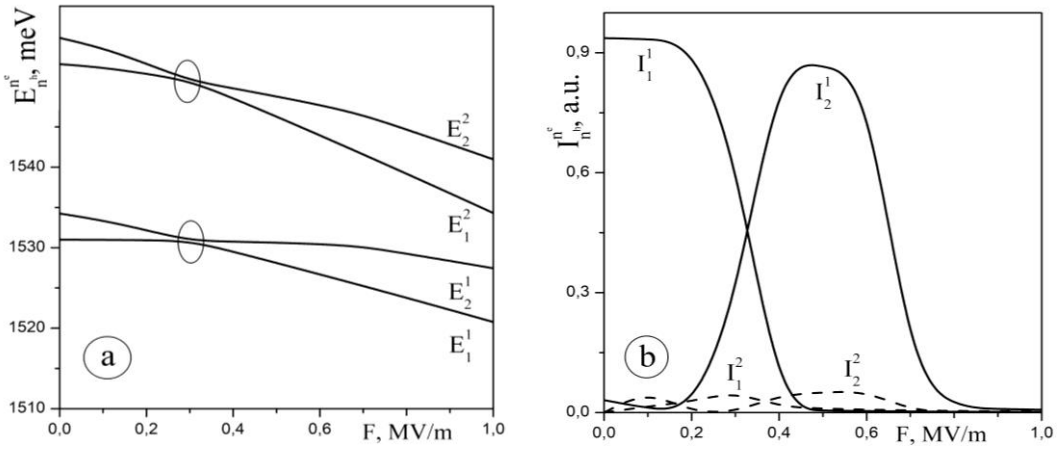
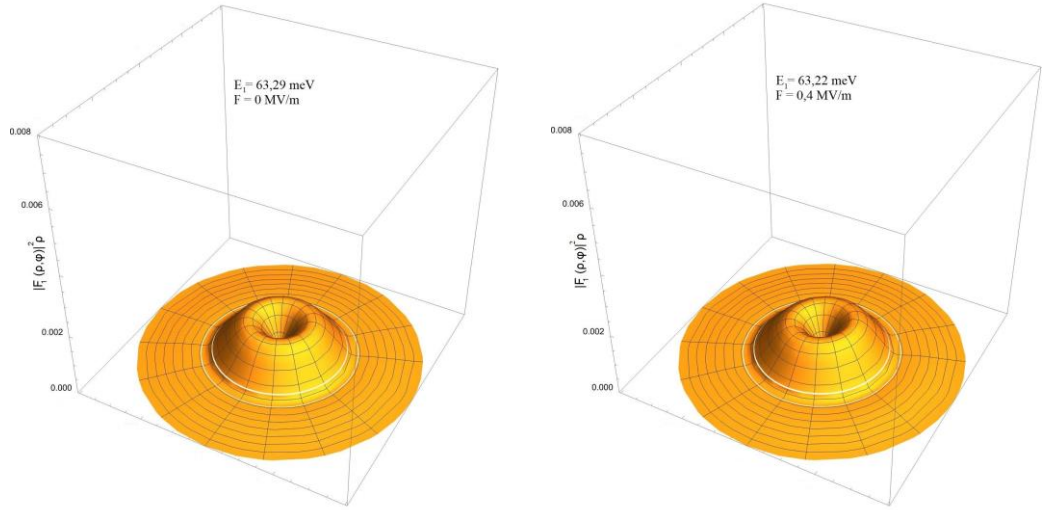


Fig. 3. Dependences of the exciton energies (Fig. 3a) and the intensities of interband optical quantum transitions (Fig. 3b) on the magnitude of the electric field strength (F) at L = 5 nm, $h = 17\alpha_{GaS}$, $\rho_0 = 18\alpha_{GaAs}$, $\Delta = 3\alpha_{GaS}$.

electron



hole

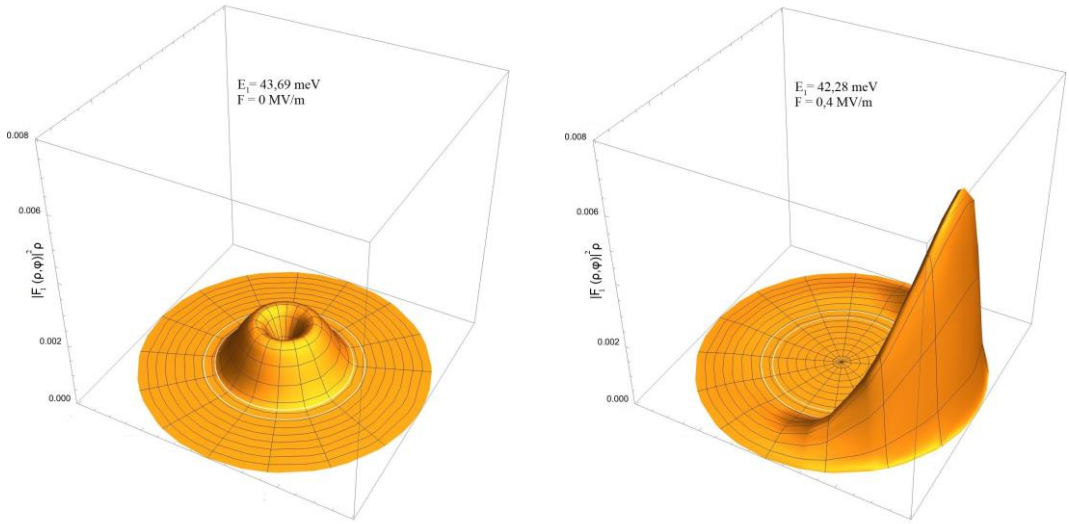


Fig. 4. The evolution of the probability density of finding an electron and a hole in the ground states in a nanostructure with a change in the electric field strength at L = 5 nm, $h = 17\alpha_{GaS}$, $\rho_0 = 18\alpha_{GaAs}$, $\Delta = 3\alpha_{GaS}$.

probability of finding an electron and a hole in the ground states in a nanostructure with an increase in the electric field strength (Fig. 4). As can be seen from Figure 4, at $F = 0$, the electron and hole in the ground state are localized in the quantum dot. In this case, the overlaps of the corresponding wave functions in (20), and hence the intensity of the transition, are significant. As the electric field strength increases, the hole begins to tunnel into the outer nanoring. At the same time, the overlap of the wave functions of both quasiparticles and, consequently, the intensity of the corresponding transition decreases. At $F \approx 0.4$ MV/m, the hole is completely localized in the outer ring, and the electron is in the quantum dot. The wave functions in the corresponding states overlap weakly and the intensity of such a transition turns out to be small.

The evolution of intensities with a change in electric field strength for other quantum states of an electron and a hole can be explained quite similarly.

Main results and conclusions

In the approximation of effective masses and rectangular potentials, the dependence of the energy spectrum of an electron, a hole, an exciton, and the intensities of interband quantum transitions on the magnitude of the electric field strength (F) in the quantum dot-quantum ring nanostructure was investigated. The basis of the nanostructure are $GaAs$ and $Al_{0.4}Ga_{0.6}As$ semiconductors.

It has been established that the location of quasiparticles in the nanostructure can be purposefully controlled by changing the magnitude of the electric field strength F. It is shown that when F changes in the range from 0 to 0.4 MV/m, the electron still does not change its localization, but the hole already tunnels through the finite potential barrier into the outer nanoring.

The hole and exciton energies and the intensity of interband quantum transitions as F varies from 0 to 1 MV/m depend nonmonotonically on the electric field strength. In particular, energy level anticrossings are observed in the dependences of the hole and exciton energies on F, and maxima are clearly pronounced in the dependences of the intensities of interband quantum transitions. The reason for this behavior is a change in the localization of the hole in the space of the nanostructure in different quantum states with a change in the electric field strength.

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Спектр екситона в циліндричній напівпровідниковій наноструктурі квантова точка – квантове кільце в електричному полі

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У моделі ефективних мас та прямокутних потенціалів для електрона і дірки теоретично досліджено вплив однорідного електричного поля на енергетичний спектр та хвильові функції екситона та сили осциляторів міжзонних квантових переходів у напівпровідниковій ($GaAs/Al_xGa_{1-x}As$) наноструктурі квантова точка – квантове кільце. Стаціонарні рівняння Шредінгера для невзаємодіючих квазічастинок за наявності електричного поля аналітично не розв'язуються. Для їх наближеного розв'язку невідомі хвильові функції шукаються у вигляді розкладу за повним набором циліндрично - симетричних хвильових функцій, а енергія електрона знаходиться із розв'язування відповідного секулярного рівняння. Енергія зв'язку екситона знаходиться з використанням теорії збурень.

Проаналізовано залежності енергетичних спектрів, хвильових функцій електрона, дірки й екситона та інтенсивностей міжзонних оптичних квантових переходів від величини напруженості електричного поля

Ключові слова: квантова точка, нанокільце, екситон, енергетичний спектр, інтенсивність, електричне поле.