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I. S. Hnidko, V. I. Gutsul, I. P. Koziarskyi, O. M. Makhanets, "Influence of electric field on electronic optical quantum transitions in a quantum dot - quantum ring semiconductor nanostructure," Proc. SPIE 12126, Fifteenth International Conference on Correlation Optics, 121260Y (20 December 2021); doi: 10.1117/12.2615553

SPIE.

Event: Fifteenth International Conference on Correlation Optics, 2021, Chernivtsi, Ukraine

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Influence of electric field on electronic optical quantum transitions in a quantum dot - quantum ring semiconductor nanostructure

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ABSTRACT

In the model of effective masses and rectangular potentials, the influence of a homogeneous electric field on the energy spectrum, electron wave functions, and oscillator strengths of intraband quantum transitions in a semiconductor ($GaAs/Al_xGa_{1-}xAs$) quantum dot-quantum ring nanostructure is theoretically investigated. In the presence of an electric field, the stationary Schrödinger equations for quasiparticles are not analytically solved. For their approximate solution, the unknown wave functions are sought in the form of an expansion over a complete set of cylindrically symmetric wave functions, and the electron energy is found from the solution of the corresponding secular equation.

It is shown that the electric field significantly affects the localization of the electron in the multilayer nanostructure. In this case, both the electron energy and the strength of the oscillators of intraband quantum transitions depend non-monotonically on the magnitude of the electric field strength.

Keywords: quantum dot, quantum ring, electron, energy spectrum, oscillator strength, electric field

1. INTRODUCTION

Improving the experimental possibilities of growing semiconductor nanostructures has allowed scientists to create ordered arrays of concentric simple and double quantum rings and to study the luminescence spectra in them[1-3].

The unique properties of quasiparticles in such nanostructures make it possible to use them in devices of modern nanoelectronics: photodetectors[4], semiconductor lasers[5], elementary qubits of quantum computers[6].

Theoretical models for calculating the spectra of basic quasiparticles (electrons, phonons, excitons,…) in such structures and their interactions between themselves and external electric and magnetic fields are also being intensively developed and improved.

Thus, the authors[7, 8] investigated the dependence of the electron energy spectrum in a simple cylindrical semiconductor quantum ring on the uniform electric field strength perpendicular to the axial axis of the ring. They showed that, depending on the ratio between the inner and outer radii of the rings, at certain strengths, these dependences can be complex and non-monotonic.

In[9-12], the authors investigated the dependence of the spectral parameters of the electron on the induction of a uniform magnetic field and the electric field strength in double quantum rings based on $GaAs/Al_xGa_{1-x}As$ semiconductors. In particular, they showed that the electron in the ground state can be localized either in the inner or in the outer ring, depending on the value of the magnetic field induction, the electric field strength and the thickness of the nanorings. It is also established that the electron energies and the forces of the oscillators of intraband quantum transitions depend non-monotonically on the magnitude of the electric field strength F and the induction of the magnetic field B. In particular, anticrossings of energy levels are observed in the dependences of energies on F or B (Aaoronov-Bohm effect), and maxima and minima are clearly expressed in the dependences of oscillator forces. The reason for this behavior is a change in the localization of the electron in the space of two nano rings in different quantum states with a change in the electric field strength or magnetic field induction.

Exciton and polaron effects in nano rings were studied in[13, 14]. The calculations performed by the authors showed that it is possible to purposefully control the location of the electron in the system of double nanoring using electric and magnetic fields.

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Fifteenth International Conference on Correlation Optics, edited by Oleg V. Angelsky, Proc. of SPIE Vol. 12126, 121260Y
© 2021 SPIE · 0277-786X · doi: 10.1117/12.2615553

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In this paper, the influence of a homogeneous electric field on the energy spectrum and wave functions of an electron, as well as on the oscillator strengths of intraband quantum transitions in a quantum dot - quantum ring semiconductor nanostructure, will be theoretically investigated.

2. THEORY OF ENERGY SPECTRUM, WAVE FUNCTIONS AND OSCILLATOR STRENGTHS OF INTRABAND QUANTUM TRANSITIONS OF ELECTRON IN A QUANTUM DOT - QUANTUM RING SEMICONDUCTOR NANOSTRUCTURE

The 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), is investigated in this work. The cross-section by the plane $z = 0$ and the potential energy profile of such a nanostructure is shown in Fig. 1. The electric field strength vector $\vec{F}$ is directed along the *Ox* axis.

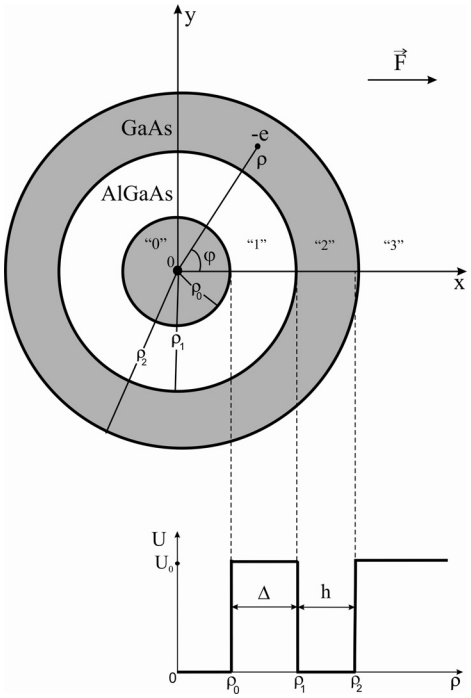

Fig. 1. Cross-section of nanostructure (height $L = 5$ nm) by plane $z = 0$ and potential energy profile.

All subsequent calculations will be performed in the model of effective masses and rectangular potentials in a cylindrical coordinate system (ρ, φ, *z*) with the *Oz* axis directed along the axial axis of the nanostructure.

Therefore, the effective electron masses are considered to be known in all areas of the nanostructure

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

In order to find the energy spectrum and wave functions of an electron, it is necessary to solve the stationary Schrödinger equation

$$\hat{H}\Psi(\rho,\varphi,z) = E\,\Psi(\rho,\varphi,z), \tag{2}$$

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with the Hamiltonian

$$\widehat{H}=\frac{1}{2\mu(\vec{r})}\left[-\hbar^2\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right)\right]-\frac{\hbar^2}{2\mu(\vec{r})}\frac{\partial^2}{\partial z^2}+U(\vec{r})-|e|F\rho\cos\varphi\,, \tag{3}$$

where e is the electron charge, F is the electric field strength, $U(\vec{r})$ is the dimensional quantization potential.

Since the electric field does not affect the energy spectrum of the electron during its movement in the axial direction, and the electron itself is mainly located in the region of quantum wells of the nanostructure and almost does not penetrate into the region of barriers, the corresponding energy $U(\vec{r})$ should be given as

$$U(\vec{r})=U(z)+U(\rho)\,,\ U(z)=\begin{cases}U_0, & |z|>L/2,\\ 0, & |z|\le L/2,\end{cases}\quad U(\rho)=\begin{cases}U_0, & \rho_0\le\rho\le\rho_1, \quad \rho>\rho_2,\\ 0, & 0<\rho<\rho_0, \quad \rho_1<\rho\le\rho_2.\end{cases}, \tag{4}$$

Then the variable z in the Schrödinger equation (2) with the Hamiltonian (3) can be separated, and the wave function can be given as

$$\Psi(\vec{r})=\Phi(\rho,\varphi)\,f(z)\,, \tag{5}$$

The Schrödinger equation for the z-th component of the wave function is solved exactly[15]

$$f(z)=\begin{cases}\begin{cases}A^{(+)}\cos(k_0 z)\\ A^{(-)}\sin(k_0 z)\end{cases}, & 0\le z\le L/2\\ B\exp(-k_1 z), & z>L/2\end{cases}, \tag{6}$$

The unknown coefficients ($A^{(\pm)}$, B) in (6) and the dispersion equations are found from the conditions of continuity of the wave function $f(z)$ and the probability density flux at the boundary $z = L/2$ together with the normalization condition

$$\frac{k_0}{\mu_0}tg(k_0\frac{L}{2})=\frac{k_1}{\mu_1}\,,\ \frac{k_0}{\mu_0}ctg(k_0\frac{L}{2})=-\frac{k_1}{\mu_1}\,,\ k_0=\sqrt{2\mu_0 E_{n_z}/\hbar^2}\,,\ k_1=\sqrt{2\mu_1(U_0-E_{n_z})/\hbar^2}\,. \tag{7}$$

The energy spectrum of an electron during its axial motion (E_{n_z}) is found from equations (7). The quantum number n_z numbers the solutions of these equations.

If there is no electric field, then the corresponding radial-angular Schrödinger equation with Hamiltonian (3) is also solved analytically exactly

$$\Phi^{\,0}_{n_\rho m}(\rho,\varphi)=\frac{1}{\sqrt{2\pi}}R_{n_\rho m}(\rho)\,e^{im\varphi}\,, \tag{8}$$

here n_ρ and m are the radial and magnetic quantum numbers. The radial wave functions have the form

$$R_{n_\rho m n_z}(\rho,\varphi)=\begin{cases}A_m^{(0)}J_m(\chi_0\rho), & 0\le\rho\le\rho_0,\\ A_m^{(1)}I_m(\chi_1\rho)+B_m^{(1)}K_m(\chi_1\rho), & \rho_0<\rho\le\rho_1,\\ A_m^{(2)}J_m(\chi_0\rho)+B_m^{(1)}N_m(\chi_0\rho), & \rho_1<\rho\le\rho_2,\\ B_m^{(3)}K_m(\chi_1\rho), & \rho>\rho_2,\end{cases}, \tag{9}$$

where J_m, N_m are the cylindrical Bessel functions of the first and second kind, I_m, K_m are the cylindrical modified Bessel

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functions of the first and second kind, $\chi_0 = \sqrt{2\mu_0 (U_0 - E^0_{n_\rho m})/\hbar^2}$, $\chi_1 = \sqrt{2\mu_1 E^0_{n_\rho m}/\hbar^2}$.

All unknown coefficients in (9), as well as the electron energy spectrum ($E^0_{n_\rho m}$), are found from the conditions of continuity of radial wave functions and the corresponding fluxes of probability densities at all heterointerfaces of the nanostructure

$$\begin{cases} R^{(i)}_{n_\rho m n_z}(\rho_i) = R^{(i+1)}_{n_\rho m n_z}(\rho_i) \\ \dfrac{1}{\mu_i}\dfrac{\partial R^{(i)}_{n_\rho m n_z}(\rho)}{\partial \rho}\Big|_{\rho=\rho_i} = \dfrac{1}{\mu_{i+1}}\dfrac{\partial R^{(i+1)}_{n_\rho m n_z}(\rho)}{\partial \rho}\Big|_{\rho=\rho_i} \end{cases} \quad (i = 0,1,2), \tag{10}$$

and rationing conditions $\int_0^\infty \left| R_{n_\rho m n_z}(\rho) \right|^2 \rho d\rho = 1$. The quantum number n_ρ numbers the solutions of the corresponding dispersion equations for a fixed m.

If an external electric field with strength F is applied to the nanostructure, then the corresponding Schrödinger equation with Hamiltonian (3) cannot be solved analytically exactly. To find the energy spectrum of an electron at F ≠ 0, we present unknown wave functions in the form of an expansion over a complete orthonormal set of wave functions (9)

$$\Phi_n(\rho,\varphi) = \frac{1}{\sqrt{2\pi}} \sum_{n_\rho} \sum_m c^n_{n_\rho m} R_{n_\rho m}(\rho) e^{im\varphi} . \tag{11}$$

Substituting expansion (11) into the Schrödinger equation with Hamiltonian (3), multiplying by $\Phi^*_n(\rho,\varphi)$ and integrating over ρ and φ, we obtain the secular equation:

$$\left| H_{n_\rho m, n'_\rho m'} - E_n \delta_{n_\rho, n'_\rho} \delta_{m,m'} \right| = 0 , \tag{12}$$

with matrix elements

$$H_{n_\rho m, n'_\rho m'} = E_{n_\rho m} \delta_{n_\rho, n'_\rho} \delta_{m,m'} + \left(\delta_{m',m+1} + \delta_{m',m-1} \right) \frac{eF}{2} \int_0^\infty R_{n_\rho m}(\rho) R_{n'_\rho m'}(\rho) \rho^2 \, d\rho , \tag{13}$$

Note that, as can be seen from (11) and (12), the new states of the electron in its transverse motion are now characterized by only one quantum number n.

Finding the eigenvalues and eigenvectors of the matrix (12), the energy spectrum E_n and the wave functions $\Phi_n(\rho,\varphi)$ of the electron in its transverse motion are obtained.

Therefore, both the full wave functions of the electron $\psi_{n n_z}(\vec{r})$ (5) and its energy $E_{n n_z} = E_n + E_{n_z}$ are now known.

The obtained energies and wave functions of the electron also make it possible to estimate the oscillator strengths of intraband optical quantum transitions by the formula[16]

$$f^{n'n'_z}_{n n_z} \sim (E_{n'n'_z} - E_{n n_z}) \left| M^{n'n'_z}_{n n_z} \right|^2 , \tag{14}$$

where

$$M^{n'n'_z}_{n n_z} = \iiint \psi^*_{n'n'_z}(\rho,\varphi,z) \sqrt{\mu(\rho)} \; e\rho^2 \cos(\varphi) \psi_{n n_z}(\rho,\varphi,z) \, d\rho \, d\varphi \, dz \tag{15}$$

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is the transition dipole moment.

3. ANALYSIS AND DISCUSSION OF RESULTS

The dependence of the electron spectrum and oscillator forces of intraband quantum transitions on the magnitude of the electric field strength (F) was studied on the example of double GaAs/$Al_xGa_{1-x}As$ nano rings with the following physical parameters μ_0 = 0.063 m_0, μ_1 = 0.096 m_0, U_0 = 297 meV (m_0 is the electron mass in vacuum); lattice constant of the GaAs medium a_{GaAs} = 5.65 Å. Since all subsequent calculations of the spectral parameters of the electron were performed for the quantum number n_z = 1, it is further omitted for convenience.

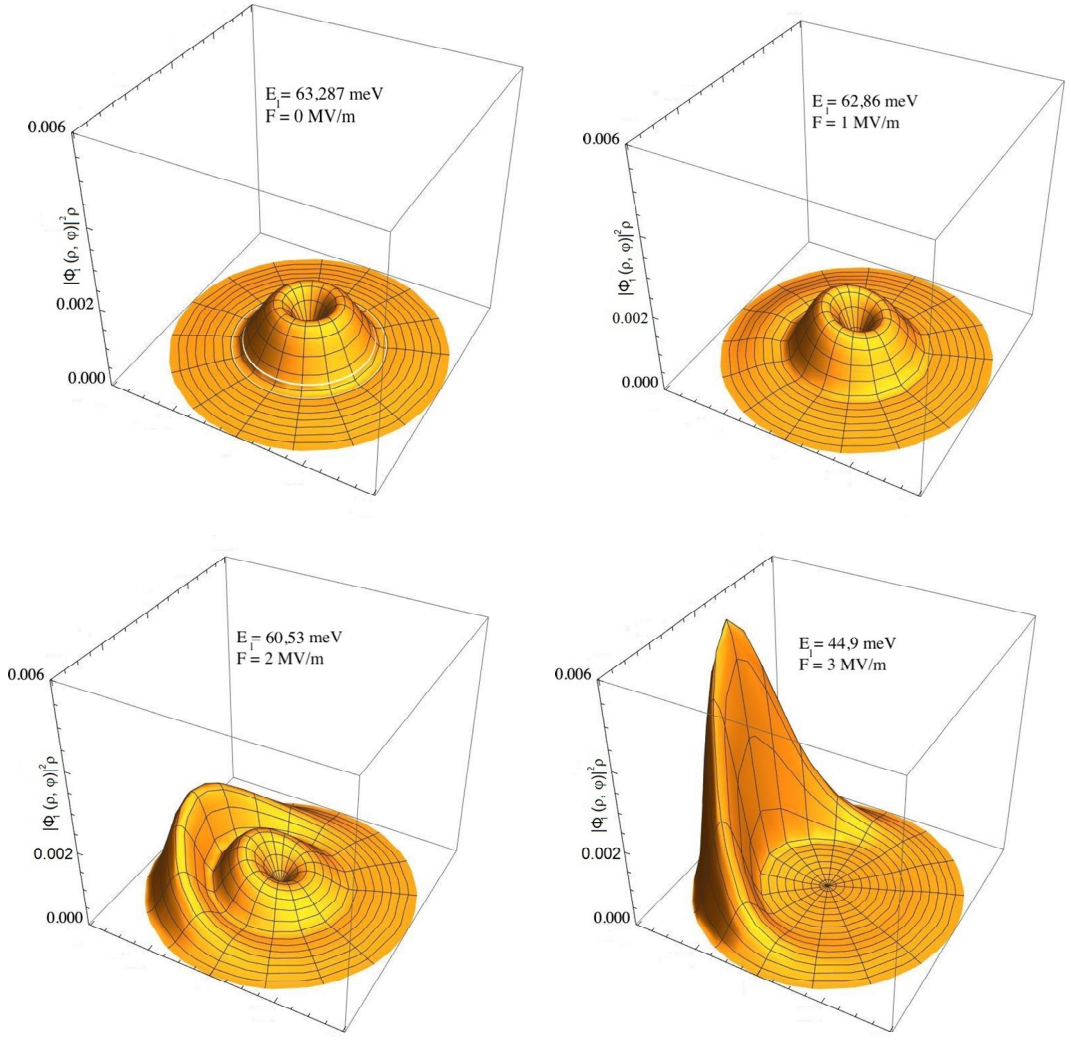

Fig. 2. Probability density of an electron in a nanosystem in the ground state $|\Phi_1(\rho,\varphi)|^2\,\rho$ at $L = 5$ nm, $\rho_0 = 18\,a_{GaAs}$, $\Delta = 3\,a_{GaS}$, $h = 17\,a_{GaS}$ and at different values of electric field strength F =0; 1; 2; 3,5 MV/m.

Fig. 2 shows the probability density of an electron in a nanosystem in the ground state $|\Phi_1(\rho,\varphi)|^2\,\rho$ at $L = 5$ nm, $\rho_0 = 18\,a_{GaAs}$, $\Delta = 3\,a_{GaS}$, $h = 17\,a_{GaS}$ and at different values of electric field strength F =0; 1; 2; 3,5 MV/m. The dimensions of the nanostructure are selected so that the electron in the absence of an electric field is localized in a

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quantum dot of radius ρ_0. The figure shows that the angular distribution of the probability density is uniform in this case. An increase in F affects the change in the localization of the electron in the nanostructure. With an increase in the electric field strength, an electron in the ground state tunnels from a quantum dot to a quantum nanoring so that at F = 3.5 MV/m it is completely localized in a nanoring of thickness h. As can be seen from the figure, in this case, its angular probability distribution becomes sharply nonuniform with a sharp maximum near the outer boundary of the nanoring.

Fig. 3 a, b shows the dependences of the electron energies E_n on the magnitude of the electric field strength (F) at $L = 5$ nm, $h = 17\, a_{GaS}$, $\rho_0 = 0$, $\Delta = 21\, a_{GaS}$ (Fig. 3, a) and $\rho_0 = 18\, a_{GaAs}$, $\Delta = 3\, a_{GaS}$ (Fig. 3, b). That is, Fig. 3a corresponds to a simpler nanostructure, which contains only one nanoring (there is no quantum dot) with a thickness of h = $17a_{GaS}$ and an inner radius of ρ_1 = $21a_{GaS}$, and Fig. 3b corresponds to a nanostructure with a quantum dot and a nanoring of the same geometric dimensions. On the left in both figures there are quantum numbers n_ρ, m, which characterize the corresponding energy levels in the absence of a field.

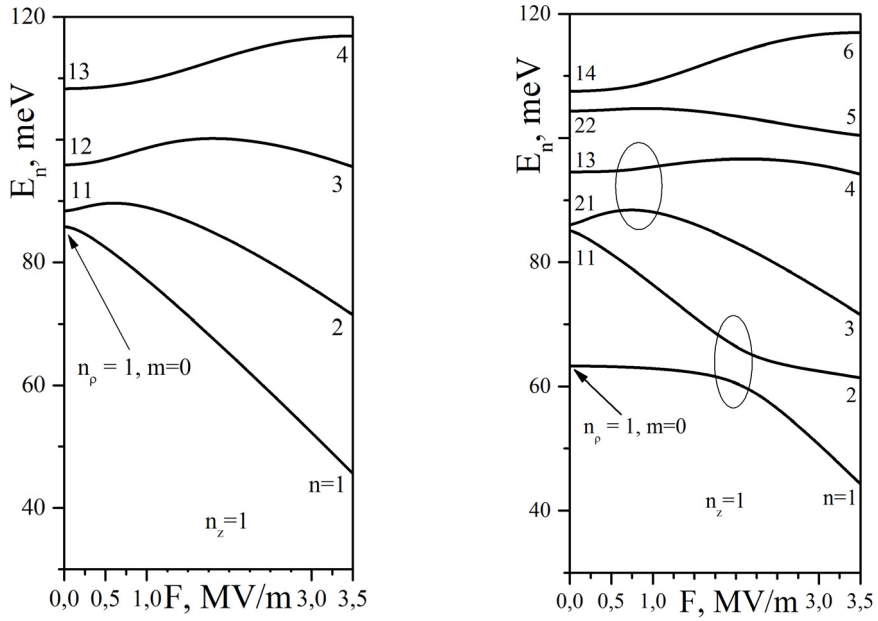

Fig. 3. Dependences of the electron energies E_n on the magnitude of the electric field strength (F) at $L = 5$ nm, $h = 17\, a_{GaS}$, $\rho_0 = 0$, $\Delta = 21\, a_{GaS}$ (a) and $\rho_0 = 18\, a_{GaAs}$, $\Delta = 3\, a_{GaS}$ (b).

Fig. 3a, b shows that in both cases the ground state energy (n = 1) only decreases with increasing F. However, this is no longer the case for excited states. Thus, in the case of a simple nanostructure (Fig. 3a), the energy of states with n = 2,3,4 first increases, and only then decreases. The same applies to nanostructures with a quantum dot and a nanoring, where the energy of states with n = 3,4,5,6 increases. In the general case, the increase or decrease of electron energies with increasing F is due to the nature of the angular distribution of the probability density of the quasiparticle in the nanostructure relative to the direction of the electric field strength (Fig. 2 for the ground state).

Note that in the case of a quantum dot - quantum ring nanostructure (Fig. 3b) the potential barrier that separates them has a finite height and width. Therefore, an electron can tunnel from one quantum well to another under the action of an electric field. This leads to the appearance of anticrossing energy levels (for example, (1) and (2) at $F \sim 2$ MV/m, (3) and (4) at $F \sim 1$ MV/m in Fig. 3b). The cause of anticrossing is a change in the localization of the electron between the quantum dot and the outer ring in adjacent quantum states with increasing electric field strength. In this case, the probabilities of the electron being in states 1 and 2 (3 and 4) either in the quantum dot or in the quantum ring are equalized for such strength values. Note that this effect is not observed in a simple nanoring with one potential well (Fig. 3a).

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Note that quite similar series of levels in the quantum number n appear at n_z = 2, 3, ..., however, they will simply be located in the higher-energy regions of the spectrum.

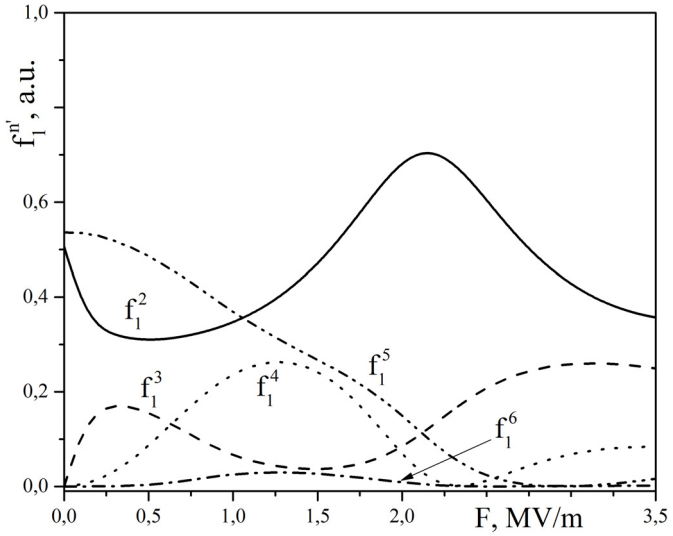

Fig. 4. Dependences of the oscillator forces of intraband quantum transitions $f_1^{n'}$ on the magnitude of the electric field strength (F) at L =5 nm, $h = 17a_{GaS}$, $\rho_0 = 18a_{GaAs}$, $\Delta = 3a_{GaS}$.

The possibility of localization of an electron (located in different states) in the region of a quantum dot or nanoring leads to a complex and non-monotonic dependence of the oscillator strengths of intraband quantum transitions ($f_1^{n'}$) on F with pronounced maxima and minima (Fig. 4). It turns out that such a non-monotonic behavior of $f_1^{n'}$ is mainly due to the overlap of the electron wave functions in the corresponding quantum states. Thus, the maximum on the curve f_1^2 at $F \approx 2.3$ MV/m corresponds to the case when the electron in states (1) and (2) is localized mainly in the nanoring. In this case, the overlap of the corresponding wave functions in (15) is significant, and the oscillator strength is maximum. The oscillator strength acquires its minimum value at F ≈ 0.5 MV/m. At this value of the electric field strength, the electron in the ground state is localized mainly in the quantum dot, and in the first excited state in the nanoring. The wave functions in the corresponding states overlap weakly and the oscillator strength of the corresponding transition is small. Similarly, the non-monotonic behavior of the oscillator strengths of quantum transitions between other states can be explained by a change in the localization of an electron in the space of a tunnel-connected quantum dot and nanoring under the action of an electric field.

Note also that for the oscillator strengths, as can be seen from Fig. 4, the rule of Thomas-Reich-Kuhn sums are fulfilled $\sum_{n'} f_1^{n'} = const$.

4. CONCLUSIONS

The dependence of the electron energy spectrum and the oscillator forces of intraband quantum transitions on the value of the electric field strength (F) in the quantum dot - quantum ring nanostructure based on GaAs/$Al_xGa_{1-x}As$ semiconductors was studied in the model of effective masses and rectangular potentials.

It is shown that the electric field significantly changes the distribution of the probability density of finding a quasiparticle in a nanosystem. Thus, if in the ground state in the absence of a field the electron is in a quantum dot, then with increasing electric field strength the quasiparticle tunnels into the nanoring. In this case, angular probability distribution becomes sharply nonuniform with a sharp maximum near the outer boundary of the nanoring.

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The electron energies and the oscillator strengths of the intraband quantum transitions non-monotonically depend on the magnitude of the electric field strength. In particular, in the energy dependences on *F*, anticrossings of energy levels are observed, and in the dependences of the oscillator forces on *F*, maxima and minima are clearly expressed. The reason for this behavior is the change in the localization of the electron in the space of the nanostructure in different quantum states with a change in the electric field strength.

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