Theory of electric field effect on the optical properties of elliptical quantum wire

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In the approximation of the effective mass, the electric field effect on the optical properties of the elliptical quantum wire (EQW) was investigated. In an elliptic coordinate system, exact solutions of the Schrödinger equation for an electron in an EQW with hard walls are obtained. The energy spectrum of a quasiparticle consists of energies of even and odd states, whose wave functions are expressed through even and odd Mathieu functions of the first kind. Using these solutions, an orthonormal basis was constructed. The influence of the electric field perpendicular to the quantum wire and parallel to the ellipse's major axis on the energies and forces of the oscillators of quantum electron transitions was calculated using the matrix method. It is shown that the ellipticity of the quantum wire leads to the removal of the degeneracy of the energy spectrum of quasiparticles, since the energies of even and odd electronic states depend differently on the ratio of the EQW semi-axes. The electron's ground state is the even state, which is nondegenerate because there is no corresponding odd state. The electric field has a greater effect on energy states with a lower value of the magnetic quantum number. As the electric field strength increases, the energies of even and odd states shift to the region of lower energies. The distribution of the electron density of the ground state shifts the most in the direction opposite to the direction of the electric field. This leads to a decrease in the strength of the oscillators of quantum transitions with an increase in the intensity of the electric field.

Keywords: elliptic quantum wire; energy spectrum; electric field; quantum transition; oscillators strength; matrix method.

Introduction

Semiconductor quantum nanostructures, including quantum wells, quantum wires, and quantum dots (QDs), demonstrate distinctive electronic and optical properties, making them subjects of extensive theoretical and experimental research by numerous scientists.

Remarkable technological advancements for growing semiconductor nanostructures have made it possible to obtain quantum dots and quantum wires of various shapes and sizes. Changing the size and shape of nanostructures leads to changes in their optical properties due to changes in the energy spectrum and wave functions of quasiparticles. In addition, external electric and magnetic fields affect the energy spectrum of quasiparticles. For the possibility of using nanostructures in real devices, many authors perform theoretical studies of the influence of shape, size, and external fields on the energies and oscillator strength of quantum transitions, which form the optical properties of nanostructures. Currently, in addition to the simplest spherical and cylindrical nanosystems, ellipsoidal [1-6], pyramidal [7-8], and lens-shaped quantum dots [9], elliptical rings [10-11], and elliptical quantum wires [12-17] are intensively studied. For this studies, various methods to solve the Schrödinger equation for an electron in nanostructures of various shapes are used. For spherical and cylindrical nanostructures, analytical solutions of this equation can be obtained, which are expressed in terms of Bessel functions. For QDs with the shape of an oblate ellipsoid, Kazarian and others obtained exact solutions of the equation in oblate spheroidal coordinates [1]. Boychuk et al. obtained the energy spectrum of an electron in an ellipsoidal QD using prolate spheroidal coordinates [2]. Sadeghi et al. investigated the effect of light polarization on the optical properties of GaAs/AlGaAs ellipsoidal quantum dots using the method of coordinate transformations. As a result of solving the Schrödinger equation, it is obtained in the form of Hermite polynomials [3]. The energy spectrum of electrons in elliptical quantum wires and elliptical nanotubes is obtained from exact solutions of the Schrödinger equation in elliptical coordinates [4-6]. Such solutions are obtained based on ordinary and modified Mathieu functions of the first and second kinds. Studies have shown that the energy spectrum of an electron in an elliptical quantum wire consists of energies of even and odd states, whose wave functions are expressed in terms of even and odd Mathieu functions, respectively.

The exact solutions of the Schrödinger equation are important because, based on them, it is possible to build an orthonormal basis for calculating the influence of external fields on the optical properties of elliptic-shaped quantum wires. The method of diagonalization based on the basis, which takes into account the boundary conditions that must be satisfied by the solutions of the problem, has advantages over other research methods. This method was used to study the effect of electric and magnetic fields on the optical properties of multilayer quantum dots [18-19]. It is shown that the results obtained by diagonalization method coincide with the results of the numerical solution of the Schrödinger equation obtained by the finite element method. For high accuracy, it is enough to take into account a small (5-10) number of terms in the expansion of the wave function. As a result, not only the solutions of the Schrödinger equation were obtained, but also the values of the partial contributions of the basis functions (the wave functions of the states of the unperturbed problem) to the formation of new wave functions. In this work, the influence of the electric field on the energy spectrum and wave functions of the electron at different ratios of the semi-axes of the ellipse is investigated using the diagonalization method based on the orthonormal basis, which takes into account the boundary conditions for the elliptic quantum wire.

Theoretical framework

The elliptic quantum wire (EQW) GaAs embedded into impenetrable for electron matrix is under study. The coordinate system is chosen in such a way that Oz axis is directed along the wire axis. The confinement potential in Cartesian coordinates have the form

$$U(x,y)=\begin{cases}0, & x^2/a^2+y^2/b^2\le 1,\\ \infty, & x^2/a^2+y^2/b^2>1,\end{cases} \qquad (1)$$

Where a ta b are the semi-axes of the ellipse. The electric field applied perpendicular to wire axis and along to Ox axis. An electron can perform a free movement in the direction along the quantum wire with energy $E_z = \hbar^2 k_z^2/2\mu^*$, where k_z – quasiparticle longitudinal quasimomentum and μ^*– electron effective mass. The energy caused by the transversal movement of quasiparticle is found from the Schrodinger equation

$$-\frac{\hbar^2}{2\mu^*}\Delta\Psi(x,y) + (|e|\, F\, x + U(x,y))\Psi(x,y) = E\Psi(x,y), \qquad (2)$$

where F– electric field strength. Equation (2) does not have an exact solution, so we first consider the solutions of the Schrödinger equation in the absence of an electric field. In elliptical coordinates at $F = 0$, the Schrödinger equation (2) will have the form

$$\left[\frac{\partial^2}{\partial\xi^2} + \frac{\partial^2}{\partial\eta^2} + \frac{f^2 k_i^2}{2}(\cosh 2\,\xi - \cos 2\,\eta)\right]\Phi(\xi,\eta) = 0, \qquad (3)$$

where (ξ, η, z) are elliptic coordinates related to Cartesian coordinates by the following relations

$$\begin{cases} x = f\cosh\xi\cos\eta\,, & 0 \le \xi < \infty \\ y = f\sinh\xi\sin\eta\,, & 0 \le \eta < 2\pi\ , \\ z = z, & -\infty < z < +\infty \end{cases} \qquad (4)$$

where $f = \sqrt{a^2 - b^2}$ is the focal length, ξ – radial coordinate, and η – angular coordinate. The wave function $\Phi(\xi,\eta)$ in elliptical coordinates allows separation of variables $\Phi(\xi,\eta) = R(\xi)\theta(\eta)$. The quantum states of a quasiparticle are characterized by a certain value of the quantum number m, since the radial $R(\xi)$ and angular $\theta(\eta)$ parts of the wave function satisfy the characteristic equations of the Mathieu function

$$\partial^2\theta_m(\eta)/\partial\eta^2 + (c - 2q\cos 2\,\eta)\theta_m(\eta) = 0 \qquad (5)$$

$$\partial^2 R_m(\xi)/\partial\xi^2 - (c - 2q\cosh 2\,\xi)R_m(\xi) = 0, \qquad (6)$$

where $q = f^2k^2/4$ and c – separation constant, which is found from the periodicity conditions of the angular part of the wave function. Since periodicity conditions can be satisfied only by Mathieu functions of the first kind (even – $ce_m(q,\eta)$, odd – $se_m(q,\eta)$), the angular part of the wave function will have the form

$$\theta_m(q,\eta) = \begin{cases} ce_m(q,\eta), \\ se_m(q,\eta). \end{cases} \quad (7)$$

The solutions of the radial equation (6) that satisfy the condition of convergence at $\xi \to 0$ are even – $Je_m(q,\xi)$ and odd – $Jo_m(q,\xi)$ modified Mathieu functions of the first kind. Therefore, the energies of the even E^e_{nm} and odd E^o_{nm} electron states with a certain value of the quantum number m are determined from the equations

$$\left.\begin{array}{l} Je_m(q,\xi)|_{\xi=\xi_0} = 0, \quad m = 0,1,2,\ldots \\ Jo_m(q,\xi)|_{\xi=\xi_0} = 0, \quad m = 1,2,\ldots \end{array}\right\}. \quad (8)$$

The values $q = q^{e(o)}_{nm} = f^2 \frac{\mu}{2\hbar^2} E^{e(o)}_{nm}$ that satisfy equation (8) determine the energy spectrum of the quasiparticle $E^{e(o)}_{nm}$, where $n = 1, 2, \ldots$ is the main quantum number, which is equal to the ordinal number of the corresponding equation root, and the quantum number m is determined by the order of the corresponding Mathieu functions. At the same time, as follows from (8), for $m = 0$ there is only an even state of a quasiparticle. On the basis of the orthogonal basis of the functions $\Phi^{e,o}_{nm}(\xi,\eta) = R^{e,o}_{nm}(\xi)\theta^{e,o}_m(\eta)$, which take into account the boundary conditions of the problem, we can find the solutions of equation (2). In the case of an electric field directed along the x–axis, the new wave functions $\Psi(\xi,\eta)$ preserve the parity/oddity property, so their expansion contains corresponding functions

$$\Psi^{e,o}_{n'j}(\xi,\eta) = \sum_{n,m} c^{n'j}_{nm} R^{e,o}_{nm}(\xi)\theta^{e,o}_m(\eta)\,. \quad (9)$$

The unknown coefficients $c_{nm}^{n\prime j}$ and the new energy spectrum $\tilde{E}_{n'j}^{e,o}$ can be found by the method of diagonalization of the corresponding secular equation.

Using the wave functions (9), it is possible to calculate the dipole moment and oscillator strength of the quantum intersubband transition at linear x- and y-polarization of the electromagnetic wave

$$F^{x}{}_{nj-n\prime j\prime} = \frac{2m}{\hbar^2}(E_{n'j'} - E_{nj}) < nj|x|n'j' >^2 \quad (10)$$

$$F^{y}{}_{nj-n\prime j\prime} = \frac{2m}{\hbar^2}(E_{n'j'} - E_{nj}) < nj|y|n'j' >^2. \quad (11)$$

Due to the properties of Mathieu functions, the oscillator strength of quantum transitions $F^{x}{}_{nj-n\prime j\prime}$ between even and odd electron states is zero, and for $F^{y}{}_{nj-n\prime j\prime}$ only mixed transitions (even-odd or odd-even) have a non-zero oscillator strength.

Analysis and discussion of results

cross-section

Numerical calculations were performed for an elliptic GaAs quantum wire of equal area with a cylindrical wire of radius $r_0 = 10$ nm, effective electron mass $\mu^* = 0.067\, m_e$, where m_e is the mass of a free electron. The electron density distribution in several lowest even and odd states in an elliptical quantum wire with the ratio of semi-axes $a/b = 2$ is shown in Figure 1 ($m = 0{,}1{,}2{,}3$ for even states and $m = 1{,}2{,}3{,}4$ for odd states). As can be seen from the figure, the distribution of the electron density is symmetrical with respect to the axes of the ellipse. Moreover, for all odd states, the electron density on the OX axis is zero, and for even states it is nonzero. The number of maxima along the Ox axis for odd states is equal to the quantum number m, and for even states it is equal to $(m + 1)$. The number of maxima along the Oy axis for even states is equal to $2n - 1$, and for odd states – $2n$.

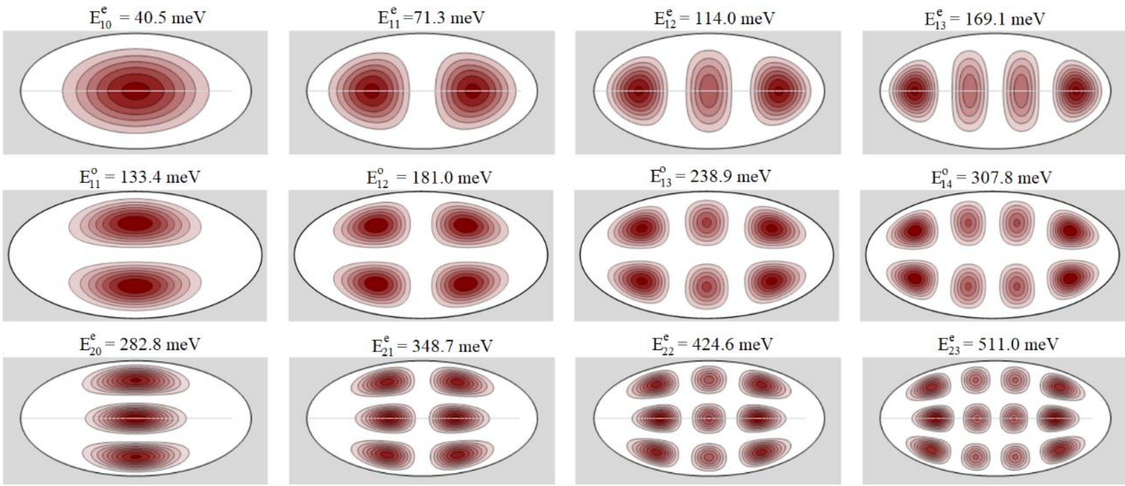

Figure 1. Distribution of the electron density in the even (1st and 3rd rows, $m = 0, 1, 2, 3$) and odd (2nd row, $m = 1, \ldots, 4$) states in the elliptical quantum wire $a/b = 2$.

Figure 2 shows the dependence of the energies of even and odd states of an electron in an elliptical quantum wire with ratio a/b=2. For the circle case ($a/b \to 1$), the energies of the even and odd states coincide, and as the a/b ratio increases, the energies of the even states have less energy than the odd states, and this energy difference increases with the increase of the a/b ratio.

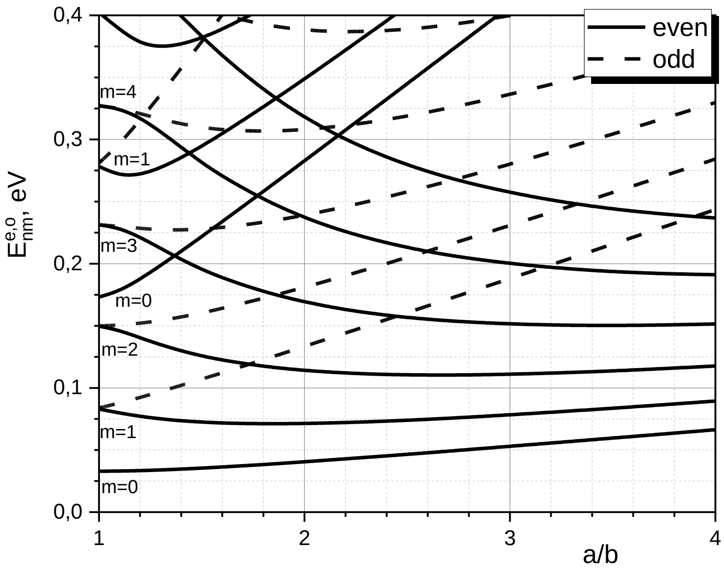

Figure 2. Dependence of the energy spectrum of an electron in an elliptical GaAs quantum wire on the ratio a/b.

Figure 3 shows the evolution of the electron density distribution under the electric field effect. The electron, as expected, moves in the direction opposite to the direction of the electric field. Moreover, this displacement is smaller for excited states. The contribution of various terms in the equation (10) can be estimated by the coefficients $c_{nm}^{n\prime j}$, the values of which for several lowest states at F=50 kV/cm and a/b=2 are given in Table 1 for even states and in Table 2 for odd states. It can be seen from the tables that the main contribution to the schedule is made by only a few states closest in energy. When the electric field becomes stronger, the number of terms that make a significant contribution increases.

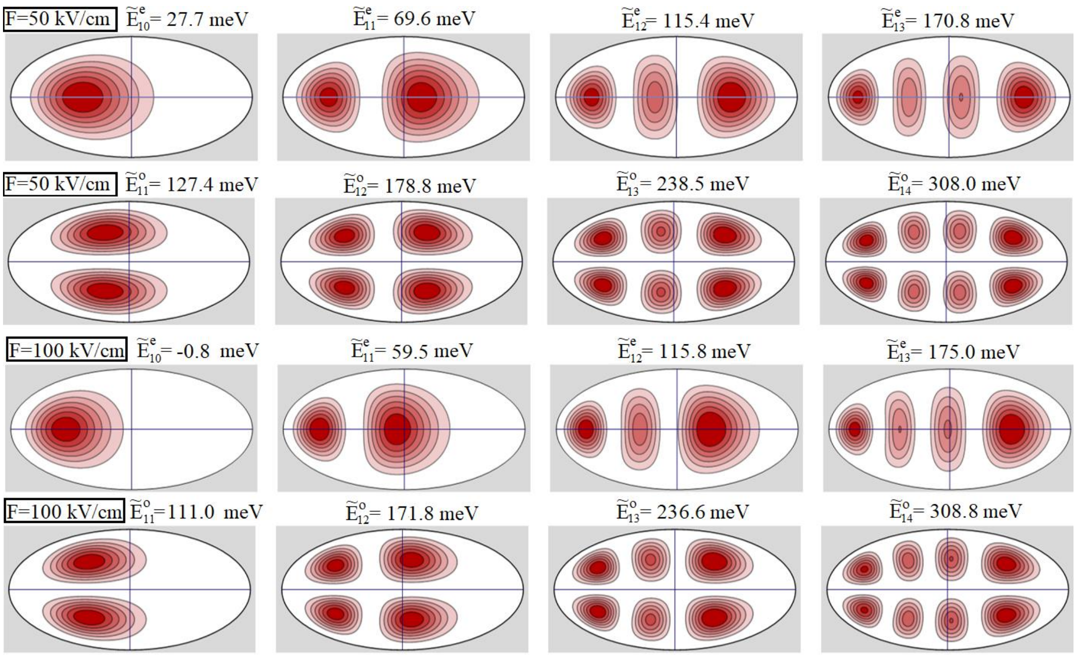

Figure 3. Distribution of electron density in even and odd states in an EQW at $F = 50$ and 100 kV/cm (a/b=2).

Table 1. Values of the coefficients $\left(c_{nm}^{1j}\right)^2$ for the expansion $\psi_{1j}^{e}(\vec{r})$ at j=0,1,2,3 (F=50 kV/cm, $r_0 = 10$ нм, $a/b = 2$).

r_0=10 нм, a/b=2		$\vert n,m >$	$\vert 1,0 >$	$\vert 1,1 >$	$\vert 1,2 >$	$\vert 1,3 >$	$\vert 1,4 >$	$\vert 1,5 >$	$\vert 1,6 >$
j	$\tilde{E}_{1j}^{e}$, меВ	E_{nm}^{e}, меВ	40.5	71.3	114.0	169.1	236.9	317.6	411.2
0	27.72	$(c_{nl}^{10})^2$	**0.7153**	0.2569	0.0260	0.0016	0.0001	10^{-6}	10^{-6}
1	69.6	$(c_{nm}^{1})^2$	0.2661	**0.4862**	0.2292	0.0175	0.0009	0.00005	10^{-6}
2	115.4	$(c_{nm}^{12})^2$	0.0179	0.2443	**0.5483**	0.1798	0.0090	0.0005	10^{-5}
3	170.8	$(c_{nm}^{13})^2$	0.0006	0.0120	0.1896	**0.6543**	0.1385	0.0047	0.0003

Table 2. Values of the coefficients $\left(c_{nm}^{1j}\right)^2$ for the expansion $\psi_{1j}^{o}(\vec{r})$ at *j*=1,2,3 (F=50 kV/cm, $r_0 = 10$ нм, $a/b = 2$).

r_0=10 нм, a/b=2		$\mid n,m >$	$\mid 1,1 >$	$\mid 1,2 >$	$\mid 1,3 >$	$\mid 1,4 >$	$\mid 1,5 >$	$\mid 1,6 >$	$\mid 1,7 >$
j	$\tilde{E}_{1j}^{o}$, меВ	E_{1m}^{o}, меВ	181.0	238.9	307.8	387.9	479.5	582.8	697.8
1	127.4	$(c_{nm}^{11})^2$	**0.8866**	0.1087	0.0045	0.0002	10^{-6}	10^{-7}	10^{-8}
2	178.8	$(c_{nm}^{12})^2$	0.1102	**0.7654**	0.1197	0.0044	0.0002	10^{-6}	10^{-7}
3	238.5	$(c_{nm}^{13})^2$	0.0031	0.1226	**0.7622**	0.1087	0.0033	0.0001	10^{-6}

Figure 4 shows the dependence of the energies of the even and odd states on the electric field strength. It can be seen from the figure that under the influence of the electric field, most of the states are shifted to the region of lower energies, but the ground state of the electron undergoes the largest shift. The magnitude of the excited state shift decreases with increasing quantum number j. When j>3, the electron energy depends little on the electric field, or even has a slight opposite shift to the region of higher energies.

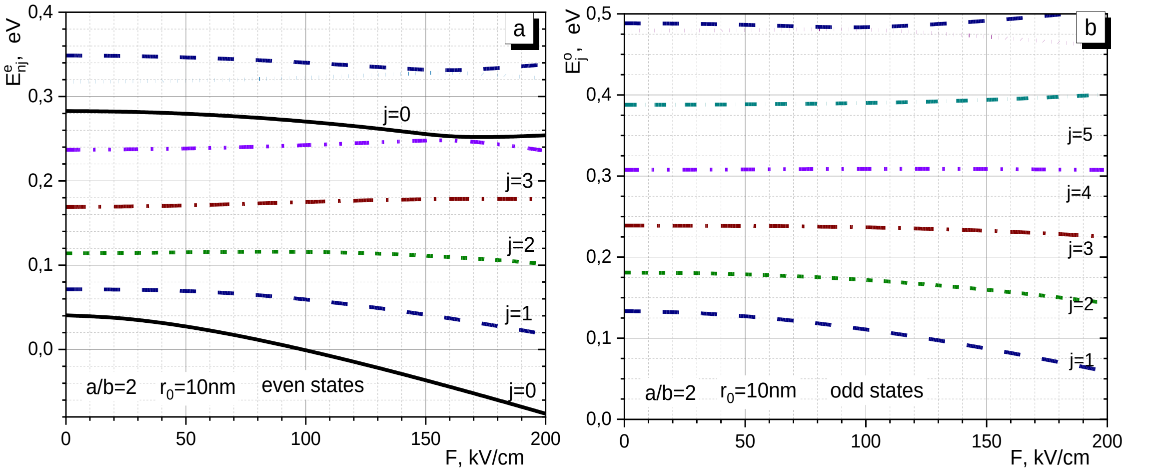

Figure 4. Dependence of the energy spectrum of an electron in an elliptical quantum wire on the electric field strength (energies of even states - **a**; energies of odd states - **b**).

Figure 5 shows the dependences of the energies and oscillator strength of the intersubband quantum transitions in an elliptical quantum wire under electric field effect. Calculations showed that transitions between quantum states with the same parity are possible only with x-polarization of an electromagnetic wave, and transitions between quantum states with different parity are possible only with y-polarization.

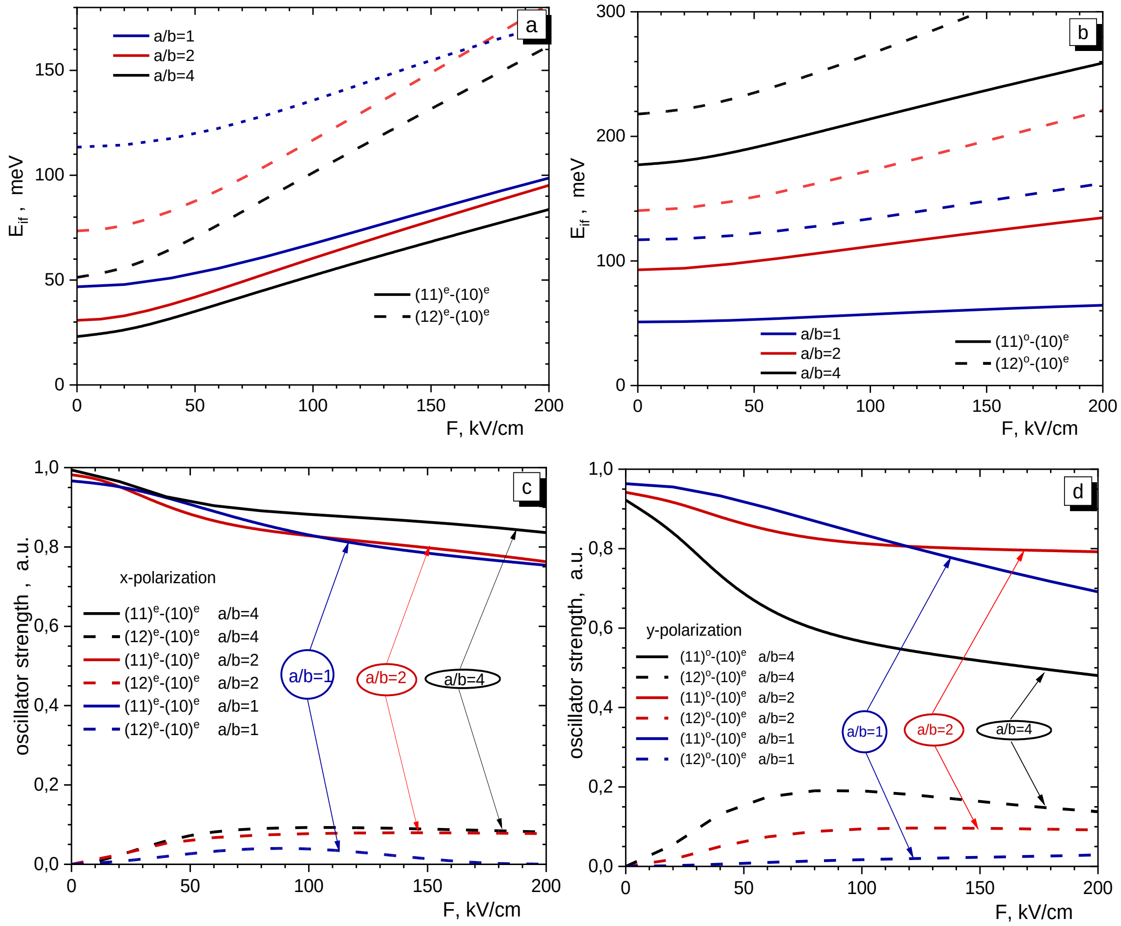

Figure 5. Dependencies of energies (a, b) and oscillator strength (b, c) of electron quantum transitions on the electric field strength between the electron ground state and even (a, c) and odd (b, d) excited states.

It can be seen from Figure 5 that for quantum transitions between the ground and excited states with $j = 1$ have the greatest oscillator strength. Moreover, at $F = 0$, only transitions with Δm=±1 are allowed by the selection rules. Under the influence of an electric field, the probability of transitions to the next excited states increases. At the same time, the Thomas-Kuhn sum rule is fulfilled: the sum of oscillator forces of all possible transitions from a given state is a constant value.

Conclusion

The influence of the electric field on the optical properties of elliptical quantum wire was theoretically investigated in the effective mass approximation. The wave functions and energy spectrum of electrons in an elliptical quantum wire under the influence of an electric field were obtained by the diagonalization method using the orthonormal basis of wave functions, which are exact solutions of the unperturbed Schrödinger equation.

The study reveals that an x-polarized electromagnetic wave induces quantum transitions from the ground state to even quantum states, while a y-polarized wave leads to transitions to odd states. Quantum transitions to the nearest excited state exhibit the highest probability, but with an increase in the electric field strength, the likelihood of transitions to other excited states also rises. The ellipticity of the quantum wire significantly impacts both the energies and the oscillator strength of quantum transitions.

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