OPTICAL OSCILLATOR STRENGTHS FOR THE ELECTRON QUANTUM TRANSITIONS IN ELLIPTIC NANOTUBES⋆

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The electron energy spectrum and the wave functions in semiconductor elliptic nanotube constructed on the base of GaAs crystal are calculated within the effective mass approximation. The dependences of optical oscillator strengths for the quantum intersubband transitions in dipole approximation on the focus distance are obtained and analyzed. There are established the selection rules and polarization effects for intersubband optical transitions for electrons in elliptic nanotube are predicted.

Key words: elliptic semiconductor nanotube, optical oscillator strengths, electron energy spectrum.

1. INTRODUCTION

The development of modern semiconductor electronics and transition to the nanoelectronics are tightly bound to the utilization of semiconductor nanomaterials and nanotechnologies. It is believed that their use in nanoelectronics would allow to create nanostructure microprocessors, terabit memory schemes and increase the passing ability of connection channels. The development of nanoelectronics anticipates the phenomena of size quantization of charge carriers energy spectra in new semiconductor devices. Recently, the great interest of the researches has been attracted by one dimensional semiconductor nanostructures, studied both theoretically and experimentally. The modern technologies allow growing semiconductor quantum wire and nanotubes with different shape of transversal cross.

The theoretical investigations are mainly performed for the cylindrical quantum wires for which there are already obtained the exact solutions of Schrodinger equation within Bessel functions. The semiconductor quantum wires and nanotubes with complicated shape of transversal cross, recently successfully grown by different methods [1, 2] are theoretically studied not enough. The theory of quasiparticle spectra in elliptic quantum wires (EQW) is established in ref. [3–5].

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It the paper it is performed the investigation of electron energy spectra and wave functions and are calculated the oscillator strengths of its quantum transitions in elliptic semiconductor nanotubes (ESN).

2. HAMILTONIAN OF THE SYSTEM AND SOLUTIONS OF SCHRODINGER EQUATION

It is studied the elliptic semiconductor nanotube GaAs, confined by inner and outer cylinder with semi axes a_1, b_1 and a_2, b_2, respectively, embedded into the dielectric matrix or vacuum. The coordinate system is chosen in such a way that Oz axis is directed along the tube, Ox and Oy – along semi axes a and b, respectively. An electron is freely moving in the direction along nanotube with the energy $E_z = \hbar^2 k_z^2 / 2\mu$, where μ – its effective mass. The energy, caused by transversal movement of quasiparticle is obtained as a solution of Schrodinger equation

$$-\frac{\hbar^2}{2\mu}\Delta\Psi(x, y) + U(x, y)\Psi(x, y) = E\Psi(x, y), \tag{1}$$

where $U(x, y)$ – rectangular potential of size quantization.

Eq. (1) in the elliptic coordinate system (ξ, η, z), using the relationships

$$\left.\begin{array}{lll} x = f \cosh\xi \cos\eta, & 0 \le \xi < \infty \\ y = f \sinh\xi \sin\eta, & 0 \le \eta < 2\pi \\ z = z, & -\infty < z < +\infty \end{array}\right\}, \tag{2}$$

is rewritten as

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

where $f = \sqrt{a_1^2 - b_1^2} = \sqrt{a_2^2 - b_2^2}$ – focus distance of inner and outer ellipse and $k = \sqrt{2\mu E}/\hbar$. When the nanotube walls are impenetrable for the electron, the variables in the wave function can be separated, ref. [4]

$$\Psi_{nm}(\xi, \eta) = R_{nm}(\xi)\theta_m(\eta). \tag{4}$$

The radial $R_{nm}(\xi)$ and angular $\theta_m(\eta)$ parts of wave function satisfy Mathieu equations

$$\partial^2\theta_m(\eta)/\partial\eta^2 + (c - 2q_{nm}\cos 2\eta)\theta_m(\eta) = 0\,, \tag{5}$$

$$\partial^2 R_{nm}(\xi)/\partial\xi^2 - (c - 2q_{nm}\cosh 2\xi)R_{nm}(\xi) = 0 \tag{6}$$

where $q_{nm} = f^2 k_{nm}^2 / 4$, c – the separating constant.

The detail analysis of angular and radial Mathieu equations and their general solutions have been performed in refs. [3, 4]. The solutions of eq. (5), satisfying the periodical conditions, are even $ce_m(q,\eta)$ and odd $se_m(q,\eta)$ Mathieu functions of the first kind. The solutions of radial eq. (6) is linear combination of even and odd modified Mathieu functions of the first and second kind:

$$R_{nm}(q_{nm},\xi)=\begin{cases} A_m^e Je_m(q_{nm},\xi)+B_m^e Ne_m(q_{nm},\xi) \ , & even \quad states, \\ A_m^o Jo_m(q_{nm},\xi)+B_m^o No_m(q_{nm},\xi) \ , & odd \quad states. \end{cases} \tag{7}$$

The relationships between A_m^e, A_m^o, B_m^e, B_m^o coefficients and electron energy spectrum are defined by the boundary conditions:

$$\left.\begin{matrix} A_m^e Je_m(q,\xi_1)+B_m^e Ne_m(q,\xi_1)=0 \\ A_m^e Je_m(q,\xi_2)+B_m^e Ne_m(q,\xi_2)=0 \end{matrix}\right\}, \quad \left.\begin{matrix} A_m^o Jo_m(q,\xi_1)+B_m^o No_m(q,\xi_1)=0 \\ A_m^o Jo_m(q,\xi_2)+B_m^o No_m(q,\xi_2)=0 \end{matrix}\right\}, \tag{8}$$

where $\xi_1=\operatorname{arctanh}(b_1/a_1)$, $\xi_2=\operatorname{arctanh}(b_2/a_2)$.

The systems of eqs. (8) respectively A_m^e, A_m^o, B_m^e, B_m^o coefficients have the non zero solutions only at the magnitudes $q_{nm}^{e(o)}$, satisfying corresponding dispersion equations

$$Je_m(q,\xi_1)Ne_m(q,\xi_2)-Ne_m(q,\xi_1)Je_m(q,\xi_2)=0, \tag{9}$$

$$Jo_m(q,\xi_1)No_m(q,\xi_2)-No_m(q,\xi_1)Jo_m(q,\xi_2)=0. \tag{10}$$

The magnitudes $q_{nm}^{e(o)}=f^2\dfrac{\mu}{2\hbar^2}E_{nm}^{e(o)}$, satisfying dispersion eqs. (9, 10) determine the infinite set of quasiparticle discrete energy levels $E_{nm}^{e(o)}$, where $n = 1, 2 \ldots$ – main quantum number denoting number of the root of the respective equation.

The oscillator strengths fixing the probabilities of optical quantum transitions are given by the expressions

$$F_{nl}^{n'l'}=\frac{2\mu}{e^2\hbar^2}(E_{n'm'}-E_{nm})\left\langle nm\left|d_e\right|n'm'\right\rangle^2, \tag{11}$$

where E_{nm} and $E_{n'm'}$ – the energies of the first and last states, d_e – operator of dipole moment projection at the polarization direction.

3. RESULTS OF CALCULATIONS AND THEIR DISCUSSION

The computer calculations of the electron energies were performed for the elliptic nanotube GaAs with impenetrable walls at k = 0. The effective masses of

electron and lattice constant of bulk semiconductors GaAs are: $\mu = 0.067m_0$ (m_0 – the mass of free electron) and $a_{GaAs} = 5.62$ Å, respectively.

In Fig. 1 there are shown the energy dependences of even E^e_{nm} (solid curves) and odd E^o_{nm} (dash curves) electron states on the magnitude of inner ellipse big semi axis (a_1) at $f = 4{,}5\ a_{GaAs}$ and $\Delta a = a_2 - a_1 = 5\ a_{GaAs}$. In case $a_1 \to f$, $b_1 \to 0$, the inner ellipse degenerates into the segment with a_1 length. Its increasing at the constant magnitude of focus distance brings to the rapid degeneration of elliptic nanotube into the circle one, what is proved by the relationships a_1/b_1, written at the top axis of the figure. As a result, the energies of even and odd states, obtained from eqs. (9, 10), become closer to each other and approach the values of the energies in cylindrical nanotube. The further increasing of a_1 causes the degeneration of the energies over the quantum number m and it is obtained the electron energy spectrum in plane semiconductor layer with thickness Δa.

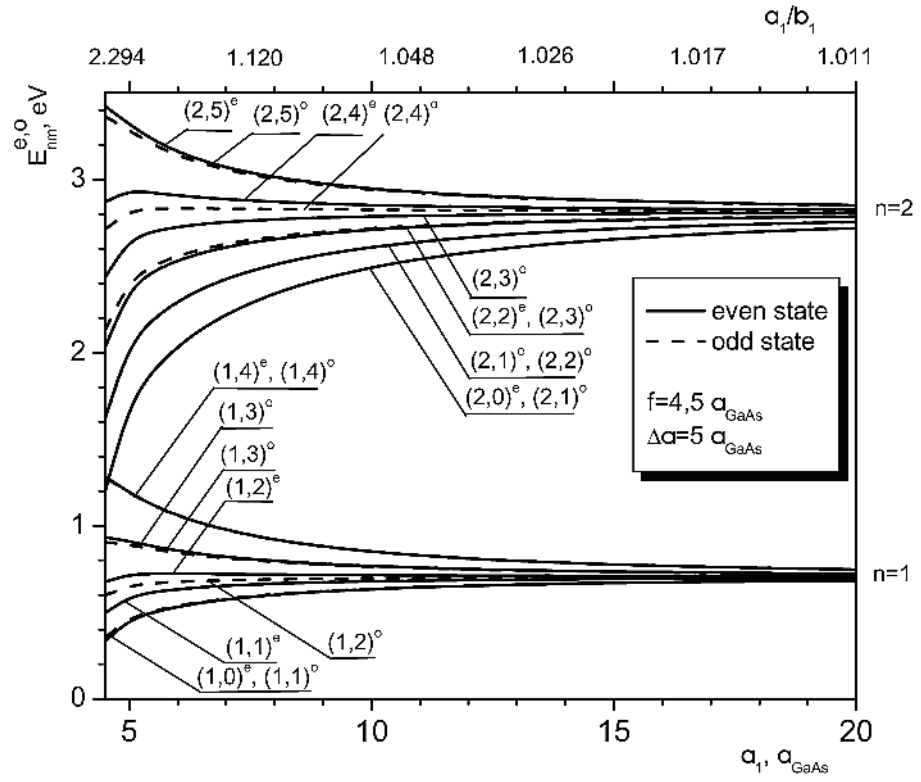

Fig. 1 – Dependence of electron energy spectrum in elliptic nanotube on a_1 magnitude at the constant thickness $\Delta a = 5\ a_{GaAs}$.

At the Fig. 1 one can see that at the small magnitudes of magnetic quantum number the energies of even states $(n, m)^e$ are close to the energies odd states $(n, m + 1)^o$. For the big m it is observed the rapprochement of energies of $(n, m)^e$ and $(n, m)^o$ states.

Such behavior of the spectrum can be explained analyzing Fig. 2, where it is shown the dependence of electron energy in nanotube on the magnitude of the focus distance (the magnitude $f = 4.5\ a_{\mathrm{GaAs}}$, at which the graphics presented at Fig. 1 are calculated, is shown by dash-dotted vertical line). From Fig. 2 it is clear that at $f = 0$ (ellipse degenerates into the circle) the energies of even and odd states coincide. The increasing of focus distance at the constant a_1 and Δa values causes the shift of all energy levels into the region of smaller energies due to the size quantization effect and the increasing of Δb magnitude. Herein, the energy levels are splitting and the energies of the odd states are decreasing faster, approaching the neigbour even states with the smaller (by one) magnitude of quantum number m. At the increasing of latter the magnitude of the energy levels splitting becomes smaller. In limit case ($f = a_1$) the inner ellipse degenerates into a segment and elliptic nanotube becomes similar to the elliptic quantum wire with $a_2 = a_1 + \Delta a$ and $b_2 = (a_2^2 - f^2)^{1/2}$ semi axes. Its energy spectra is formed in the following way: the ground energy level is obtained from the coinciding

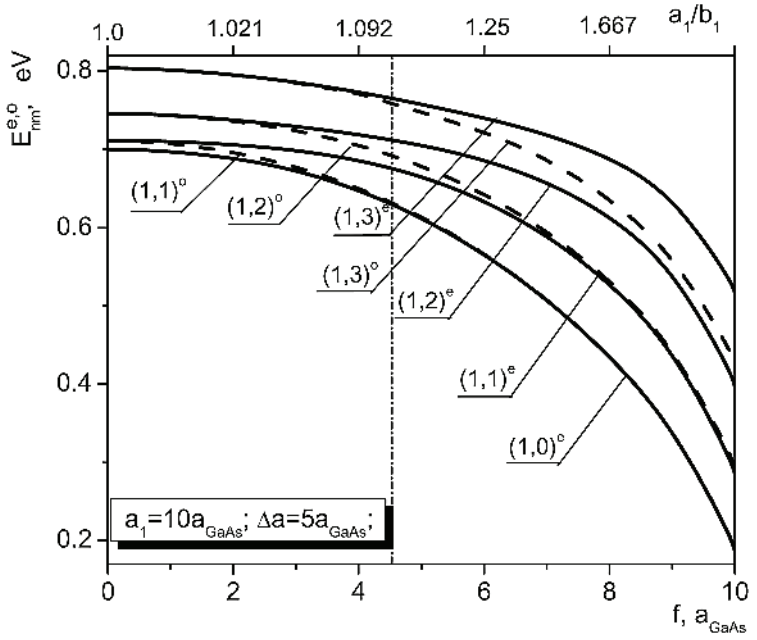

Fig. 2 – Dependence of electron energy spectrum in GaAs nanotube on the magnitude of focus distance (f) at a_1 =10 a_{GaAs}. Solid curves – even states, dash – odd states.

levels $(1, 0)^e$ and $(1, 1)^o$. The energy levels of quantum wire even states $(n, m)^e$ are obtained from the corresponding energy levels of elliptic nanotube and the energies of odd states $(n, m)^o$ from the states $(n, m+1)^o$ of elliptic nanotube. Such energy spectrum does not coincide to the energy spectrum of elliptic quantum wire with a_2 and b_2 semi axes, calculated according to the theory developed in refs. [3–5].

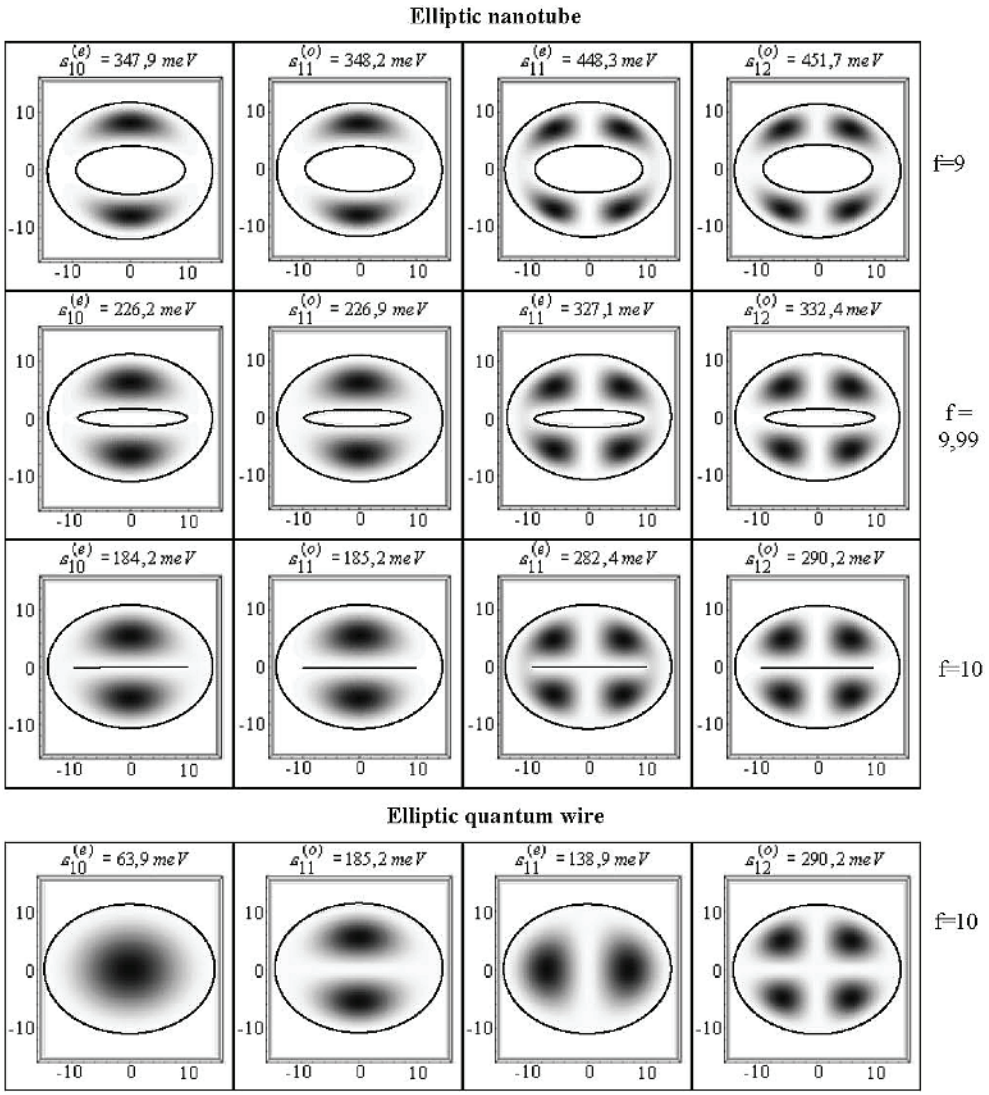

Fig. 3 – Distribution of probability density of electron location in the states $(1, 0)^e$, $(1, 1)^o$, $(1, 1)^e$ and $(1, 2)^o$ in ESN at $a_1 = 10\ a_{GaAs}$, $\Delta a = 5\ a_{GaAs}$ and different focus distances $f = 9\ a_{GaAs}$, $9.99\ a_{GaAs}$, $10\ a_{GaAs}$ and EQW at $a = 15\ a_{GaAs}$ and $f = 10\ a_{GaAs}$.

The difference in electron energy spectra in degenerated elliptic nanotubes and elliptic quantum wire can be explained studying the distribution of probability density of electron location in these nanosystems, presented in Fig. 3.

Fig. 3 proves that the energies of the odd states of degenerated nanotube are totally equal to the energies of the respective states in the elliptic wire. For the even states of nanotube the presence of degenerated inner ellipse, in all points of which the wave function is equal to zero, brings to the essential increasing of quasiparticle energy.

Analysis of $\langle nm|d_e|n'm'\rangle$ matrix element magnitude, defining the oscillator strength, opens the ability to determine the selection rules for the allowed intersubband transitions in dipole approximation. The calculations show that the matrix element is not equal to zero only for the transitions with $\Delta m = \pm 1$. The same selection rules exist also for the cylindrical quantum wires and nanotubes.

Dependence of oscillator strength of several allowed quantum transitions on the magnitude of focus distance is presented in Fig. 4.

Fig. 4 proves that the transitions between quantum states with different pairing are *y*-polarized and the transitions between the states with equal pairing – *x*-polarized. The oscillator strength of *y*-polarized light is decreasing and oscillator strength of *x*-polarized light is increasing for the bigger focus distance of nanotube. Since, the intensity of light, emitted in the direction of small ellipse semi axis at the big magnitudes of focus distance is more than the intensity of

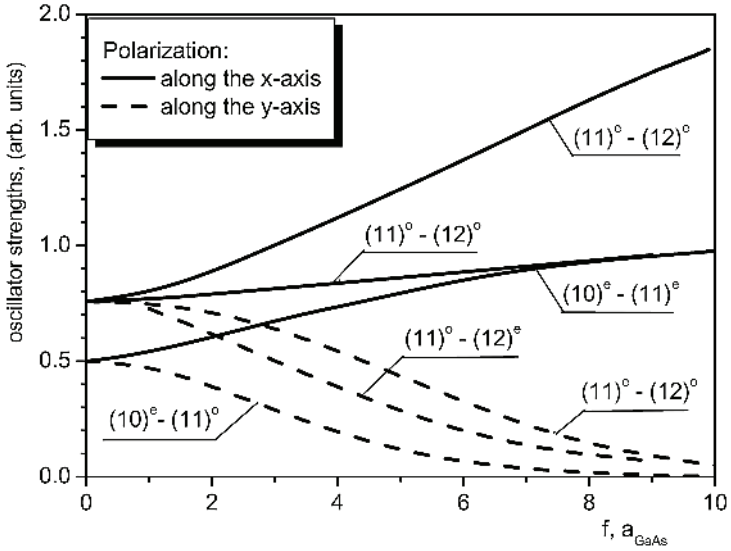

Fig. 4 – Dependence of oscillator strength of intersubband quantum transitions on the nanotube focus distance.

light emitted along the big semi axis. Such polarization peculiarities of nanotubes can find the practical utilization for the modern optoelectronic devices.

From the Fig. 4 one can also see that at $f = 0$, when the elliptic nanotube degenerates into the cylindrical one, the intensity of x- and y-polarized light emitting coincide, as it must be for the system, isotropic in radial direction.

4. CONCLUSION

The peculiarities of energy spectra and distribution of probability density of the location of quasiparticle in nanoheterosystem are investigated. It is established that in ESN the degeneration of energy spectrum is taken off. In limit cases the obtained energy spectra for ESN are the same as the known spectra of quasiparticles in cylindrical nanotubes and elliptic quantum wires.

It is shown that the magnitude of the splitting of energy levels of even and odd states and also the oscillator strengths of intersubband transitions depend on the ellipticity of nanotube. Such properties of nanotubes can be used in optical devices of one axis pressure and the other optoelectronics instruments of modern nanotechnologies.

It is established that the light, emitted due to the quantum transition between the states with different pairing, is linearly polarized along the small ellipse axis and due to the transitions between the states with equal pairing – along the big ellipse semi axis. This property can be utilized in light emitting devices.

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