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Electron energy spectrum and wave functions in complicated elliptic quantum wires

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Within the effective mass approximation the electron spectra in single and complicated elliptic quantum wire constructed on the base of $Al_xGa_{1-x}As$ crystals are researched. The exact energy spectrum of electron in elliptic quantum wire is obtained for the case of infinite potential barriers at the media interfaces at the different ratios between ellipse semi widths. The approximated electron energy spectrum in elliptic semiconductor quantum wire GaAs covered by the $Al_xGa_{1-x}As$ shell embedded into the dielectric medium is calculated. It is shown that in such system the splitting of energy spectrum is caused by the ellipticity of both media interfaces. The dependences of electron energy spectrum on the sizes and geometrical shape of the quantum wire cross-section are obtained. There one can see the anti crossing effect of the energy levels with the same symmetry.

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1. Introduction

The physics of semiconductors during the last decades has been transformed into the physics of low dimensional systems due to the modern technological achievements. There are a lot of experimental methods of the semiconductor nanosystems creation now (single and complicated quantum dots and wires with different geometrical shape). The modern methods of nanostructures creation allow to obtain the radial complicated nanowires. The core-shell nanowires enable passivation of interface states thereby improving the overall performance of the resultant semiconductor devices. The investigations of quantum wires covered by the external shell are of great interest because the experimental results [1] prove that the intensity of their photoluminescence increases by 20 times comparing to the single quantum wires. Moreover, core-multishell nanowires formed by sequential modulation of composition along the radial direction have the distinct ability to incorporate multifunction into an individual nanowire. In order to utilize the complicated quantum wires as light emitted devices it is necessary to study the influence of the shape and sizes of the quantum wire cross-section at the electron and hole energy spectra. The first attempts of such investigations were performed in [2] for the elliptic quantum wires with finite and infinite potential walls. In ref. [3] it was shown that for the elliptic nanowires with finite potential barrier one can obtain only the approximated solutions of Schrödinger equation.

The quasiparticle energy spectrum in core-shell elliptic quantum wires were not studied yet. But such investigations would be useful for interpretation of electron energy spectra in radial strained complicated nanowires.

2. Hamiltonian of the system. Solutions of Schrödinger equation

2.1 Single elliptic nanowire

The elliptic quantum wire (EQW) GaAs (“0”) embedded into the semiconductor or dielectric matrix (“1”) is under study. The coordinate system is chosen in such a way that Oz axis is directed along the wire axis. Electron potential energy and effective mass in Cartesian coordinates have the form

$$\mu(x,y)=\begin{cases}\mu_0, & x^2/a^2+y^2/b^2\le 1,\\ \mu_1, & x^2/a^2+y^2/b^2>1,\end{cases}$$
$$U(x,y)=\begin{cases}0, & x^2/a^2+y^2/b^2\le 1,\\ V, & x^2/a^2+y^2/b^2>1,\end{cases} \tag{1}$$

where a and b – ellipse semi axes.

Electron can perform a free movement in the direction along the quantum wire. Thanks to the tunnel effect the wave function of quasiparticle can penetrate into the medium “1” and part of energy caused by the longitudinal movement of electron would be $E_z=\hbar^2k_z^2/2\mu^*$, where μ^*-averaged effective mass, equal to μ_0 in the case of infinite potential barrier. The energy caused by the transversal movement of quasiparticle is found from the Schrodinger equation

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

Setting (1) into (2) there are obtained the following equations for every medium

$$\Delta\Psi^{(i)}(x,y)+k_i^2\Psi^{(i)}(x,y)=0\,,\quad (i=0,1), \tag{3}$$

where $k_i^2=\dfrac{2\mu_i}{\hbar^2}(E-V_i)$, $V_0=0$.

Taking into account the elliptic symmetry, eq.(3) is convenient to be solved in elliptic coordinates (ξ,η,z) bound to the Cartesian by the relationships

$$\left.\begin{aligned} x&=f\cosh\xi\cos\eta, && 0\le\xi<\infty\\ y&=f\sinh\xi\sin\eta, && 0\le\eta<2\pi\\ z&=z, && -\infty<z<+\infty \end{aligned}\right\}, \tag{4}$$

where $f=\sqrt{a^2-b^2}$ – focus distance, ξ – plays the role of radial coordinate and η – angular one. The radial coordinate (ξ) is defined by the ratio between ellipse semi widths ($\tanh\xi=b/a$). By changing in eq. (3) the Cartesian coordinates with the elliptic ones, one gets:

$$\left[\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}+\frac{f^2k_i^2}{2}(\cosh 2\xi-\cos 2\eta)\right]\Psi^{(i)}(\xi,\eta)=0 \qquad (i=0,1). \tag{5}$$

In ref. [3] it is shown that the variables in eq. (5) are not separated in general case because it is impossible to ensure the continuity of wave function at the elliptic interface between the media. Therefore, the wave function $\Psi^{(i)}(\xi,\eta)$ in *i*th medium can be written as

$$\Psi^{(i)}(\xi,\eta)=\sum_m C_m R_m^{(i)}(\xi)\theta_m^{(i)}(\eta), \tag{6}$$

where $R_m^{(i)}(\xi)$ - radial and $\theta_m^{(i)}(\eta)$ - angular part satisfying Mathieu equations

$$\partial^2\theta_m^{(i)}(\eta)/\partial\eta^2+(c-2q_i\cos 2\eta)\theta_m^{(i)}(\eta)=0, \tag{7}$$

$$\partial^2R_m^{(i)}(\xi)/\partial\xi^2-(c-2q_i\cosh 2\xi)R_m^{(i)}(\xi)=0, \tag{8}$$

here $q_i=f^2k_i^2/4$, c – separating constant.

The wave function allows to separate the variables only in the case of impenetrable walls at the interface of quantum wire. The quantum states of quasiparticle are characterized by the definite value of quantum number *m*

$$\Psi_m(\xi,\eta)=R_m(\xi)\theta_m(\eta). \tag{9}$$

The detail analysis of radial and angular Mathieu equations and their general solutions are presented in refs. [4, 5]. The equations (7) and (8) are the characteristic equations for the Mathieu functions. The solutions of eq. (7) are Mathieu functions of first and second kind. The periodical conditions can be satisfied only by even $ce_m(q,\eta)$ and odd $se_m(q,\eta)$ Mathieu function of first kind, since, the angular part of wave function is to be taken as

$$\theta_m(q,\eta)=\begin{cases} ce_m(q,\eta),\\ se_m(q,\eta).\end{cases} \tag{10}$$

The solution of radial equation (8) is the linear combination of even *(e)* and odd *(o)* modified Mathieu functions of first and second kind

$$R_m^e(q,\xi)=\begin{cases} A_m^eJe_m(q,\xi)+B_m^eNe_m(q,\xi)\,, & q>0\\ A_m^eIe_m(q,\xi)+B_m^eKe_m(q,\xi), & q<0\end{cases} \tag{11a}$$

$$R_m^o(q,\xi)=\begin{cases} A_m^oJo_m(q,\xi)+B_m^oNo_m(q,\xi), & q>0\\ A_m^oIo_m(q,\xi)+B_m^oKo_m(q,\xi), & q<0\end{cases} \tag{11b}$$

where $A_m^e, A_m^o, B_m^e, B_m^o$ – the coefficients determined by fitting and normalizing conditions.
Modified Mathieu functions, present in the radial wave function, have the complicated dependence on the separating constant (*c),* defined from the periodical condition for the angular part of the wave function (10) and are the same as the respective Bessel functions in the limit case when the elliptic coordinates tend to the cylindrical [12].

The energy spectrum of quasiparticle is obtained within the fitting conditions for the wave function. In case of impenetrable walls for the elliptic quantum wire, the even and odd wave functions at the surface of elliptic cylinder ($\xi=\xi_0$) are equal to zero. There radial parts would contain only the functions $Je_m(q,\xi)$ and $Jo_m(q,\xi)$ (coefficients $B_m^e=B_m^o=0$) in analogy to the cylindrical functions. Thus, the energies of even and odd states in EQW are characterized by the fixed magnitude of quantum number *m* and are defined by the equations

$$\mathrm{Je_m}(\mathrm{q},\xi)\big|_{\xi=\xi_0}=0,\quad \mathrm{m}=0,1,2,\ldots;\quad \mathrm{Jo_m}(\mathrm{q},\xi)\big|_{\xi=\xi_0}= \\ =0,\quad \mathrm{m}=1,2,\ldots \tag{12}$$

The values $q_{nm}^{e(o)}=f^2\,E_{nm}^{e(o)}\,\mu_0\big/2\hbar^2$, satisfying eqs.(12), determine the infinite number of quasiparticle discrete energy levels $E_{nm}^{e(o)}$, where *n*=1, 2 3,... – quantum number fixed by the order of the root of respective eq. (12).

2.2 Complicated elliptic quantum wire

The elliptic quantum thread (“0”) covered by elliptic shell (“1”) and embedded into the dielectric matrix (“2”) is under study. Electron potential energy and effective mass in Cartesian coordinates are the following

$$\mu(x,y)=\begin{cases}\mu_0, & x^2/a_0^2+y^2/b_0^2\le 1,\\ \mu_1, & x^2/a_0^2+y^2/b_0^2>1\ \cap\ x^2/a_1^2+y^2/b_1^2\le 1\\ \mu_2, & x^2/a_1^2+y^2/b_1^2>1\end{cases} \tag{13}$$

$$U(x,y)=\begin{cases} V_0, & x^2/a_0^2+y^2/b_0^2\le 1, \\ V_1, & x^2/a_0^2+y^2/b_0^2>1 \cap x^2/a_1^2+y^2/b_1^2\le 1 \\ V_2, & x^2/a_1^2+y^2/b_1^2>1 \end{cases} \qquad (14)$$

where a_0 , b_0 and a_1 , b_1 – the semi widths of inner and outer ellipse, respectively.

The radial wave functions for every part of nanosystem are given by (12). Assuming that the external dielectric medium forms the infinite potential barrier for the electron ($V_2=\infty$), the wave function at $\xi=\xi_1$ is equal to zero. At the media interface $\xi=\xi_0$ there is the finite skip of potential energy, since, using the conditions of wave function and density of probability current continuity for the even and odd states

$$\frac{1}{\mu_0}\frac{\partial R_m^{e(0)}(q_0,\xi)/\partial\xi}{R_m^{e(0)}(q_0,\xi)}\bigg|_{\xi=\xi_0}=\frac{1}{\mu_1}\frac{\partial R_m^{e(1)}(q_1,\xi)/\partial\xi}{R_m^{e(1)}(q_1,\xi)}\bigg|_{\xi=\xi_0} \qquad (15)$$

$$\frac{1}{\mu_0}\frac{\partial R_m^{o(0)}(q_0,\xi)/\partial\xi}{R_m^{o(0)}(q_0,\xi)}\bigg|_{\xi=\xi_0}=\frac{1}{\mu_1}\frac{\partial R_m^{o(1)}(q_1,\xi)/\partial\xi}{R_m^{o(1)}(q_1,\xi)}\bigg|_{\xi=\xi_0} \qquad (16)$$

it is obtained the dispersion equation for the electron energy spectrum for the case $V_1>V_0$.

$$\begin{cases} \dfrac{J'_m(q_0,\xi_0)}{\mu_0\ J_m(q_0,\xi_0)}-\dfrac{J'_m(q_1,\xi_0)N_m(q_1,\xi_1)-N'_m(q_1,\xi_0)J_m(q_1,\xi_1)}{\mu_1[J_m(q_1,\xi_0)N_m(q_1,\xi_1)-N_m(q_1,\xi_0)J_m(q_1,\xi_1)]}=0, \quad q_1\ge 0; \\ \dfrac{J'_m(q_0,\xi_0)}{\mu_0\ J_m(q_0,\xi_0)}-\dfrac{I'_m(q_1,\xi_0)K_m(q_1,\xi_1)-K'_m(q_1,\xi_0)I_m(q_1,\xi_1)}{\mu_1[I_m(q_1,\xi_0)K_m(q_1,\xi_1)-K_m(q_1,\xi_0)I_m(q_1,\xi_1)]}=0, \quad q_1<0; \end{cases} \qquad (17)$$

where

$$q_i=f^2k_i^2/4, \quad k_i^2=\frac{2\mu_i}{\hbar^2}(E-V_i), \qquad (18)$$

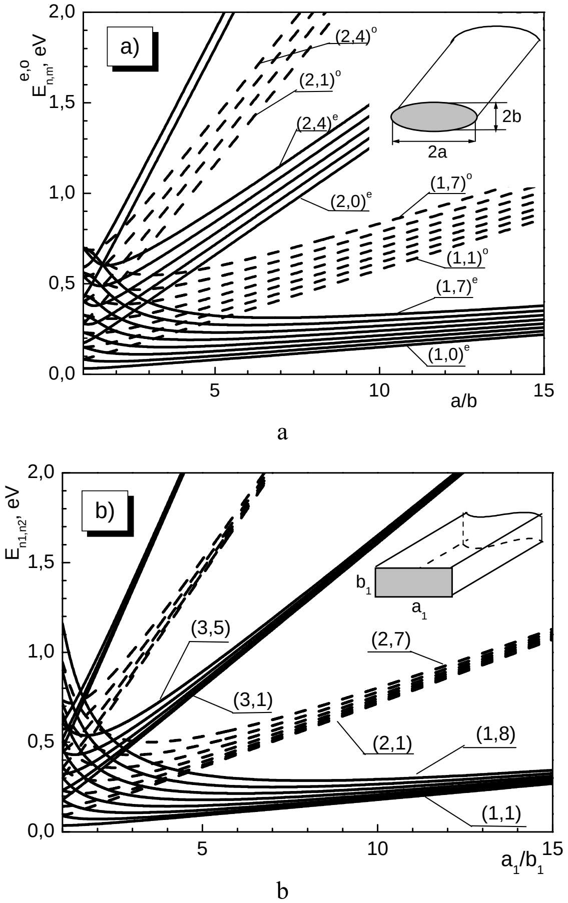
and functions $J_m(q,\xi)$, $N_m(q,\xi)$, $I_m(q,\xi)$, $K_m(q,\xi)$ are even or odd Mathieu functions for the defining of even and odd energies of electron ($E_{nm}^{e(o)}$), n=1, 2, 3 ... – quantum number fixing the order of the corresponding root of dispersion equation.

Such solutions are possible only for the complicated elliptic quantum wires with interfaces between ellipses which have the equal focus distances because it is demanded by the elliptic coordinate system (4).

3. Results and discussion

The computer calculations were performed using the following parameters of semiconductor crystals: x=0.12, $\mu_0=0.067m_0$, $\mu_1=(0.067+0.083\mathrm{x})\mathrm{m}_0\approx 0.77\mathrm{m}_0$, – the effective masses of electron in the inner thread and in the outer shell of quantum wire, respectively (m_0 – mass of pure electron), $\mathrm{V}=0.57(1.55\mathrm{x}+0.37\mathrm{x}^2)=0.109\,\mathrm{eV}$ – height of potential barrier for the electron at the media interface (“0” and “1”), $\mathrm{a}_{\mathrm{GaAs}}$=5,65 Å – lattice constant of bulk crystal GaAs.

In Fig. 2a there are presented the results obtained for the energies of electron transversal movement in EQW GaAs with impenetrable walls ($k_z=0$) depending on the ratio between ellipse semi widths ($\mathrm{a}_0/\mathrm{b}_0$) at its constant square (radius of the circle equal to the ellipse $R_0=\sqrt{a_0b_0}=10\,\text{íì}$). Even states are shown by solid curves and odd one – dashed. In fig.2b the electron energy spectrum in quantum wire with rectangular cross-section (of the same square as the elliptic one) is depicted for comparison.



a

b

Fig. 1. Dependence of electron energy spectrum in elliptic (a) and in rectangular (b) quantum wires GaAs with the same square of cross-section on the ratio a/b.

Fig. 1a proves that even and odd states create the sets of the levels, herein the energies of even states are located lower than the respective energies of odd states. The lowest energy belongs to the state $(1,0)^e$ staying non degenerated at a_0/b_0=1.

The qualitatively similar spectrum is observed in the quantum wire with rectangular cross-section (Fig. 1b). The increasing of cross-section square and a/b ratio causes arising of quasi continuum energy bands both in the EQW and in the rectangular one. In the limit case, when the ellipse is degenerated into the circle (a_0/b_0=1) and rectangular — into the square, the energies of even and odd states are coinciding.

In Fig. 2 the electron energies of even and odd states with $k_z = 0$, *m*=1 are presented for the complicated elliptic quantum wire GaAs/Al$_x$Ga$_{1-x}$As as functions of the magnitude of semi width a_0 of the inner thread (GaAs) of quantum wire at the constant thickness of the shell (Al$_x$Ga$_{1-x}$As) in the direction of OX axis ($\Delta a = 20a_{\mathrm{GaAs}}$) and constant focus distance ($f=15a_{\mathrm{GaAs}}$) of both confining elliptic cylinders (solid curves). The analogous dependences for the similar complicated cylindrical quantum wire (CQW) with the circle cross-section (dash curves) are shown for the comparison. Herein, the radii r_0 and r_1 for CQW were determined by the condition of equality of cross –section square of the inner thread and shell for the elliptic and cylindrical quantum wire: $r_0 = \sqrt{a_0 b_0}$, $r_1 = \sqrt{a_1 b_1}$.

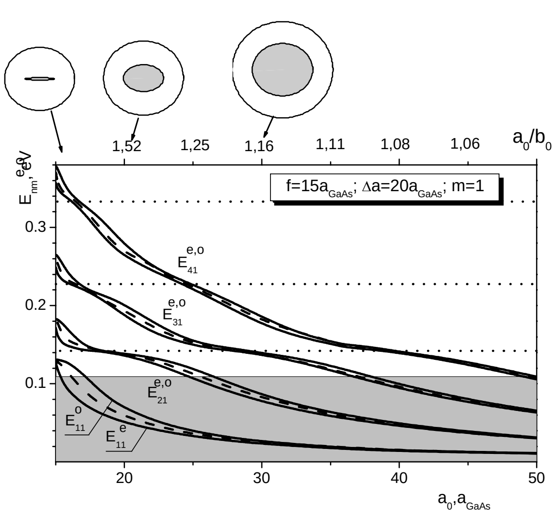


Fig. 2. Dependences of even (E^e_{nm}) and odd (E^o_{nm}) energy states of electron in EQW at m=1 (solid curves) and energies (E_{nm}) in the respective CQW (dash curves) on a_0.

From Fig. 2 it is clear that the energies of electron even states in EQW are always smaller and odd – bigger than the corresponding energies in CQW. Such splitting is big for the lower energy levels and decreases for the states with bigger main quantum number. It is explained by the fact that the ratio a_0/b_0 is always bigger than a_1/b_1 (because the focus distance of both ellipses is equal). Since the skip of potential energy at the inner interface is V=109 meV, then the electron in the states with bigger energy "feels" this interface less. At the increasing of a_0 the magnitude of the EQW elliptic cross-sections approach the circle (it is obvious from a_0/b_0 magnitudes shown at the up horizontal axis of the figure and pictures of the quantum wire cross-sections), the energies of even and odd electron states are coinciding and tending to the respective values in CQW. Toned region in Fig. 2 correspond to the energies lower the potential barrier. Here, the energy spectrum is monotonously decreasing. As for the energies higher the potential barrier, one can see the anti crossing effect because the nanosystem under research consists of two potential wells, every of which has the own system of energy levels. When the size of EQW inner thread increases, the energy levels which belong to the respective potential well tend to its bottom. Herein they are to cross the levels which belong to the well created by the shell (horizontal dot lines). Such crossings are forbidden for the states with the same quantum number (*m*) in the case when quantum wells ("0" and "1") create the sole system for the electron. As a result, the dependence of electron energy spectrum on a_0 magnitude in the region higher the potential barrier has non monotonous character. In the regions of energy levels anti crossings the quasiparticle changes its location in nanosystem.

In Fig. 3 there are shown the energy dependences of even E^e_{1m} (solid curves) and odd E^o_{1m} (dash curves) electron states on the thickness (Δa) of the elliptic shell (Al$_x$Ga$_{1-x}$As) at $a_0=10a_{\mathrm{GaAs}}$ and $f=5a_{\mathrm{GaAs}}$.

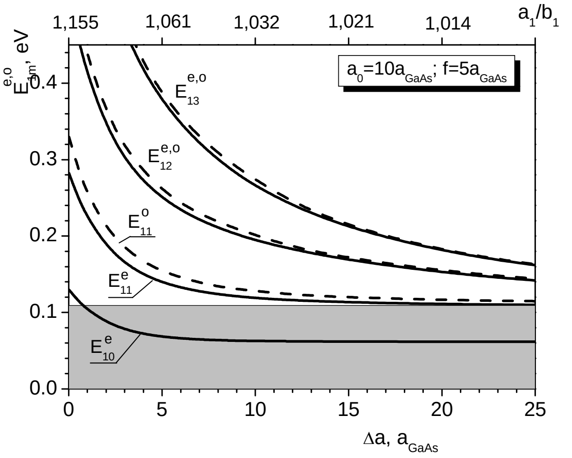


Fig. 3. Energy dependences of even (solid curves) and odd (dash curves) of electron states in complicated EQW at n=1 on thickness of elliptic shell.

Figure proves that these energies are monotonously decreasing. In the limit case (Δa=0) it is obtained the EQW with impenetrable potential wells. When the thickness of shell (Δa) increases, the size quantization becomes weaker and potential energy of electron in the shell is finite, since, the electron in the lowest energy state is bound by the potential well of the central part of the wire. At Δa>8 a$_{\mathrm{GaAs}}$ the energy dependence of the ground electron state on the thickness of the shell is saturating. The latter corresponds to the energy of electron in elliptic wire, embedded into the massive media Al$_x$Ga$_{1-x}$As. The energies of the excited electron states becoming closer to each other, tend to the bottom of the potential well created by the elliptic shell. The magnitude of the splitting of even and odd energy states becomes smaller with the increasing of the shell thickness because the ellipticity of the outer interface is decreasing (magnitude of the ratio between semi axes (a_1/b_1) is shown at the upper axis of the graphics.

5.Conclusions

In the elliptic coordinate system at the base of Mathieu functions in the framework of the effective mass approximation the energy spectrum of electron is calculated in quantum wire GaAs with impenetrable walls for the quasiparticle. The electron energy spectrum consists of the series of energy levels corresponding to the even and odd electron states and is qualitatively similar to the energy spectrum of quasiparticle in rectangular quantum wire. There are obtained the exact solutions of Schrödinger equation which can be used for the investigation of interaction of quasiparticles in quantum wires with elliptic cross-section.

The results of investigation of electron energy spectrum in complicated EQW consisting of elliptic semiconductor thread GaAs, covered by the shell $Al_xGa_{1-x}As$ prove that the splitting between the energies of even and odd states depends on the ellipticity of both media interfaces. Herein, even the small deformation of cylindrical quantum wire essentially influences at the electron energy spectrum. The anti-crossing effect of energy levels is observed for the states with equal symmetry in the region of energies higher than the potential barrier.

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