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Specific features of the electronic states and interband absorption coefficient in a cylindrical nanotube of finite thickness with a vertical potential of confinement

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ABSTRACT

In this paper the features of one-electron states in a circular cylindrical sector are investigated. The finite thickness of the cylinder and the spatial expansion of the barrier, which runs along the cylinder generatrix, are taken into account. In the framework of the proposed model the distribution of electrons in the quantum states, as well as features of interband absorption of electromagnetic radiation, is theoretically investigated.

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1. Introduction: statement of the problem

Recently a considerable interest is observed in study of the physical properties of two-dimensional electron gas on the curved surface of a semiconductor. Theoretical studies discussed models like quantum cylinder [1–3], quantum sphere [4–6] and nanotubes of different geometries (see e.g. Refs. [7–9]). Also, experiments have been conducted on faceted surfaces of GaAs/GaAlAs structures containing two-dimensional electron gas [10,11]. It is worth highlighting the success of relatively recent technology which allows separating a thin layer of stressed GaAs/GaAlAs, GaAs/$In_xGa_{1-x}As$ heterojunction along with two-dimensional electron gas, using special techniques (lift-off), and to bent at any angle up to π order (see e.g. Refs. [12,13]). Currently the spectrum of curved two-dimensional electron gas, its plasma modes, magnetotransport (see Refs. [2,14,15] and references therein), and the optical properties (see e.g. Ref. [9]) are theoretically studied in sufficient details.

However, in existing theoretical studies of the physical properties of cylindrical nanolayers the following limitations of the problem statement can be observed. First, usually it is assumed that the charge carriers are localized on the surface of nanolayers (see e.g. Refs. [1,2,7–10]); thus the finite thickness of the sample is neglected. While describing a wide range of phenomena, this approach is mostly justified, but as a result the unique properties of a quantum cylinder are lost (i.e. the properties combining the characteristic physical features of both a quantum wire and quantum film [16]).

Second, the additional potential resulting from the growth of nanostructure is usually modeled either by straight δ-barrier (passing along the cylinder) [14], or an extended spiral δ-barrier [7–9], which means that they neglect the actually existing spatial expansion of the potential barrier. Note that in paper [14] the ballistic transport in a sector of a circular cylinder is studied but under a condition when the finiteness of barrier's size has small influence on electronic states. In this paper we propose a more realistic model of a circular tube sector. This model allows us to take into account both the finiteness of the cylinder's thickness and the spatial expansion of the barrier.

The model under study is a composition of materials $B/A/B$ in a form of a circular cylindrical layer with height L, inner and outer radii R_1 and R_2 respectively and with thickness of the layer $d=R_2-R_1$ (A is the circular cylindrical nanolayer and B is the surrounding environment). The additional barrier that limits the azimuthal motion of the electrons is directed along the cylinder's generatrix and has an angular width of $2\varphi_0$ (Fig. 1).

We will assume that the band characteristics of the constituent elements of the $B/A/B$ composition are such that the limiting

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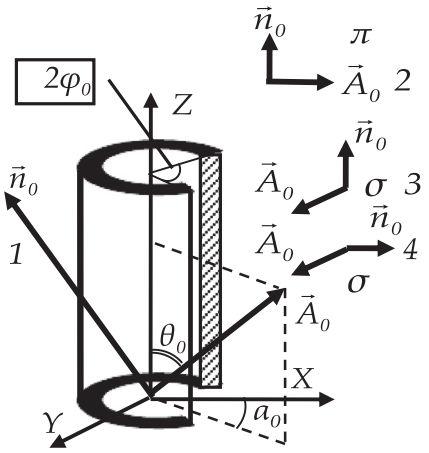

Fig. 1. The shape of nanostructure and orientation of the vectors $\vec{A}_0$ and n_0 for different cases of incidence of light wave (see Section 4).

potentials along radial and azimuthal directions can be approximated by an infinitely deep potential well with sufficient accuracy

$$V(\rho,\varphi)=\begin{cases}0, & R_1<\rho<R_2, \quad \varphi_0<\varphi<2\pi-\varphi_0\\ \infty & \rho\le R_1,\rho\ge R_2, \quad \varphi_0\ge\varphi\ge 2\pi-\varphi_0\end{cases} \tag{1}$$

Within the proposed model, the spectrum of an electron, the distribution of electrons in the quantum states as well as the specific features of intra-band absorption of electromagnetic radiation was theoretically studied.

2. The specific features of the electronic states of the nanosystem

We will present the enveloping wave function of the electrons with the potential of interaction (1) as

$$\Psi_{\text{tot}}(\rho,\varphi,z)=\Psi(\rho)\Phi(\varphi)\sqrt{\frac{1}{L}}\exp(ikz) \tag{2}$$

Bearing in mind the boundary conditions

$$\Psi(R_1)=\Psi(R_2)=0 \quad \text{and} \quad \Phi(\varphi_0)=\Phi(2\pi-\varphi_0)=0.$$

After solving the Schrodinger equation we obtain the following expressions for $\Psi(\rho)$ and $\Phi(\varphi)$:

$$\Psi(\rho)=C_\rho\left(J_\nu\left(\frac{\rho\sqrt{\eta}}{d}\right)N_\nu\left(\frac{R_1\sqrt{\eta}}{d}\right)-J_\nu\left(\frac{R_1\sqrt{\eta}}{d}\right)N_\nu\left(\frac{\rho\sqrt{\eta}}{d}\right)\right) \tag{3}$$

$$\Phi(\varphi)=\frac{1}{\sqrt{\pi-\varphi_0}}\cdot\begin{cases}\sin\frac{\pi m(\pi-\varphi)}{2(\pi-\varphi_0)}, & m=\pm 2,\pm 4,\ldots\\ \cos\frac{\pi m(\pi-\varphi)}{2(\pi-\varphi_0)}, & m=\pm 1,\pm 3,\ldots\end{cases} \tag{4}$$

Accordingly for the energy spectrum we will obtain

$$E=\frac{\hbar^2}{2m^*d^2}\eta(n,\nu)+\frac{\hbar^2k_z^2}{2m^*} \tag{5}$$

In formulas (3)–(5) the following notations are used. $J_\nu(\eta x)$ and $N_\nu(\eta x)$ are Bessel's and Neumann's functions of νth order, respectively, where $\nu=\frac{\pi m}{2(\pi-\varphi_0)}$.

For the η parameter which determines the energy of the transverse motion, a transcendental equation is obtained

$$J_\nu\left(\frac{R_2\sqrt{\eta}}{d}\right)N_\nu\left(\frac{R_1\sqrt{\eta}}{d}\right)-J_\nu\left(\frac{R_1\sqrt{\eta}}{d}\right)N_\nu\left(\frac{R_2\sqrt{\eta}}{d}\right)=0, \tag{6}$$

where n is the number of the root of Eq. (6).

Note that the states of azimuthal motion are symmetrically relative to the X axis (the equidistant points from the edges of the barrier are physically equivalent) so that the azimuthal wave function (4) has certain parity relative to $\varphi\to 2\pi-\varphi$ conversion. In relation to the specified conversion the wave functions with quantum numbers $m=2,4,\ldots$ are odd, and the states with quantum numbers $m=1,3,\ldots$ are even. In general, for arbitrary relations between geometric quantities R_1, R_2 and φ_0, the normalization factor C_ρ of the radial wave function, and the parameter η can be determined only by numerical methods.

Let us consider a particular case of practical interest. Suppose that for sufficiently thin nanotubes, when nanotube's thickness is much smaller than its radius, the following relation is true:

$$\beta=\frac{(4\nu^2-1)d}{8R_1\sqrt{\eta}}\ll 1 \tag{7}$$

Then, using Hankel's asymptotic expansions for Bessel and Neumann functions, we obtain the following equation for the wave function (e.g. [17]):

$$\Psi_{n,m,k}(\rho,\varphi,z)=\sqrt{\frac{2}{dL(\pi-\varphi_0)}}\frac{\sin\frac{\pi n}{d}(\rho-R_1)}{\sqrt{\rho}}\exp(ikz)\cdot\begin{cases}\sin\frac{\pi m(\pi-\varphi)}{2(\pi-\varphi_0)}, & m=\pm 2,\pm 4,\ldots\\ \cos\frac{\pi m(\pi-\varphi)}{2(\pi-\varphi_0)}, & m=\pm 1,\pm 3,\ldots\end{cases} \tag{8}$$

Aiming to solve the transcendental equation (6) we will use a less strict assumption

$$\frac{(4\nu^2-1)d^2}{8R_1R_2\sqrt{\eta}}\ll 1 \tag{9}$$

Then, from Eq. (6), for the energy spectrum of electrons we will have

$$E=\varepsilon_1 n^2+\varepsilon_2\left(m^2-\left(\frac{\pi-\varphi_0}{\pi}\right)^2\right)+\frac{\hbar^2k_z^2}{2m^*} \tag{10}$$

where $\varepsilon_1=\hbar^2\pi^2/2m^*d^2$ and $\varepsilon_2=\hbar^2\pi^2/2m^*l_0^2$ are the energy quanta of radial and azimuthal movements respectively, $l_0=2(\pi-\varphi_0)R$ is the length of the arc of the region of electrons' allowed motion, $R_0=\sqrt{R_1R_2}$ is the effective radius of the particle localization in the radial direction and $n=1,2,\ldots$ is the radial quantum number.

From expressions (9) and (10) it follows that the energy of the electron's azimuthal motion is much smaller than the energy of its radial motion; hence the energy spectrum of the nanosystem consists of separate series. Each series consists of a basic degree of spatial quantization with certain quantum number n (radial quantization) above which the energy levels with the quantum numbers $m=1,2,\ldots$ are located (azimuthal quantization).

At the end of the section we will discuss the applicability of the infinitely deep potential well model and provide numerical estimates. Obviously, the choice of the infinitely deep well model is justified if the forbidden bands of contacting materials overlap, and the magnitude of the energy band discontinuities V_e is more than the energy of the particles' size quantization in the layer.

Double heterojunctions $Ga_{1-x}Al_xAs/GaAs$, ($x=0.42$, $V_e=0.36$ eV) and $Ga_xIn_{1-x}As/Al_yIn_{1-y}As$ ($x=0.47$, $y=0.48$, $V_e=0.52$ eV) [18] satisfy these conditions with sufficient accuracy. In particular, if considering that many physical properties of the sample (filling degree of levels, dependence of frequency on the absorption coefficient) are determined by the relative difference of energy between the first two levels $\Delta\varepsilon_{12}/\varepsilon_1$, then estimates show that for the first heterojunction $Ga_{1-x}Al_xAs/GaAs$ we get $\Delta\varepsilon_{12}/\varepsilon_1\approx 2.823$ for $d=80$ Å and $\Delta\varepsilon_{12}/\varepsilon_1\approx 2.903$ for $d=100$ Å. For comparison, recall that for the infinitely deep well model $\Delta\varepsilon_{12}/\varepsilon_1=3$ and does not depend on the thickness of the well.

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