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ON THE QUANTUM PROPERTIES OF 3D CARBON NANOSTRUCTURES

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Abstract. The mathematical model, connected with the quantum properties of 3D carbon nanostructures, is studied from the non-relativistic viewpoint. Stationary Schrödinger equation with the homogeneous boundary conditions is solved in the prism with the hexagonal cross-section. The analytic solutions are obtained and the energies of electrons are estimated.

Keywords and phrases: Carbon nanostructure, quantum billiard, Schrödinger equation.

AMS subject classification (2010): 39A14, 35M11, 81Q05, 81Q60.

1 Introduction. Carbon nanostructures have unique quantum properties and they are the significant part of nanodevices [4, 9, 11, 12]. Carbon is a most common element with oxygen, hydrogen, helium on the earth. Its atomic number is 6. Carbon has 4 electrons on the outer shell. Those electrons are available to form covalent bonds. Each carbon atom can form covalent bonds with 2, 3 or 4 other carbon atoms. Graphene, buckyballs, nanotubes are important carbon nanostructures. Electrons, confined in those structures, behave like quantum billiard balls. In 2013 the bilayer graphene-3D honeycomb of hexagonally arranged carbon was produced. We consider the mathematical model of quantum properties of this structure from the non-relativistic point of view and interpreted it as the quantum billiard problem i.e. we consider the stationary Schrödinger equation for the free particle in the bounded area D with the homogeneous boundary conditions [1, 5-8, 9, 10]. In our paper we consider one cell of this nanostructure- the area D is a prism with hexagonal cross section (D represents one cell of nanostructure with twelve carbon atoms at the vertices, from 1 to 6 electrons can move freely at those structure). We admit, that in the nanostructure electrons can have only certain energy levels. Our purpose is to find possible energy levels of electrons confined in D.

2 Statement of the problem. Let D be a prism with the hexagonal cross-section $D = D_0 \times \{0 \leq z \leq z_0\}$ in $xoyz$-space (Fig.1), where D_0 is the hexagon of the plane $w_0 = x + iy$, with the vertices $a_1, a_2, a_3, a_4, a_5, a_6$ ($a_1 = 0,\ Re\, a_4 = 0$), and with the axis of symmetry $a_1 a_4$ (Fig.2), z_0 is a certain constant. In the area D we consider the following spectral problem

Problem. To find a real function $u(x, y, z)$ in D having second order derivatives, satisfying the equation

$$\Delta u(x, y, z) + \lambda^2 u(x, y, z) = 0 \tag{1}$$

and the conditions

$$u|_S = 0,\ \iint\limits_D |u|^2 dxdydz = 1,\ u \neq 0\, in\, D, \tag{2}$$

where S is the boundary of D, λ is the constant to be determined $\lambda^2 = 8\pi^2 mE/h^2$, E is the energy of the electron, $m \approx 9.1 \times 10^{-31}\, kg$ is mass, $h \approx 4.1 \times 10^{-15}\, eV.sec$ is Planck's constant.

Remark 1. In 1913 Niels Bohr has calculated the energy levels of electron in the Hydrogen atom by the formula [2]

$$E = -\frac{e^4\, 2\pi^2 m}{h^2\, n^2},\; e^2 = \frac{h^2}{4\pi^2 m\, r_1^2},\; r_1 = 5 \times 10^{-11} m,\; n = 1, 2, 3 \cdots,$$

where e is the electron charge. For $n = 1$, $E = -e^4\, 2\pi^2 m/h^2 \approx -13.6\, eV$.

3 Solution of the problem. By the separation of the variables $u(x, y, z) = u_1(z)u_2(x, y)$ equation (1) split into two equations

$$u_1'' + \beta u_1 = 0,\; u_1(0) = u_1(z_0) = 0, \tag{3}$$

and

$$u_2'' + (\lambda^2 - \beta)u_2 = 0,\; u|_{S_0} = 0, \tag{4}$$

where $\beta \geq 0$ is some constant,S_0 is the boundary of D_0.

The solutions of equation (3) are well-known and are given by

$$u_1(z) = C^* \sin \sqrt{\beta} z,\;\; \beta = \pi^2 n^2/z_0^2,\;\; n = 1, 2, \cdots \tag{5}$$

where C^* is a certain constant.

The solution of equation (4) satisfying the conditions (2) was obtained by the author in the previous works by means of the conformal mapping method [5, 6, 7] and is given by

$$u_2(x(\xi), y(\eta)) = C^* \sin \varphi I_3(3\lambda_1 r^{1/3}), \tag{6}$$

where $\xi = Re\, w; \eta = Im\, w; \varphi = \operatorname{arctg} \eta/\xi;$

$$r^2 = \left(\frac{2\pi\xi}{a_0 C_0}\right)^2 + \left(\frac{2\pi\eta}{a_0 C_0}\right)^2; \lambda_1^2 = \frac{2^{4/3}(\lambda^2 - \beta)C_1^2}{a_1^2}; \tag{7}$$

$$\begin{gathered} w = C_0 \int_0^{w_1} (1 - t^2)^{-1/2}(1 - k^2 t^2)^{-1/2} dt; w_0 = C \int_0^{w_1} t^{-1/3}(t^2 - a^2)^{-1/3}(t^2 - b^2)^{-1/3} dt, \\ w_1 = sn\, w/C_0; |C| = |a_3 - a_2|/k_0; C_0 \approx a_0/\pi; |C_1| = k^{2/3}|C|/C_0; a_1 = 2\pi^2/a_0^2; \end{gathered} \tag{8}$$

sn is the Jakobi "sinus" with the modulus k,I_3 is the Bessel function [3],

$$k \approx 0,0213; k_0 \approx 0,342848; a = 1; b = 1/k; a_0 = 10; a_3 - a_2 \approx 0.14 \times 10^{-9} m.$$

Consequently, according to (5) and (6) the wave function of the Problem will be given by the formula

$$u(z, x(\xi), y(\eta)) = C^* \sin(\pi z/z_0) \sin \varphi I_3(3\lambda_1 r^{1/3}),$$

where r, φ, λ_1 are given by formulas (7), (8).

Energy levels of the electron will be calculated by the formula

$$E = \lambda_0^2 h^2/8\pi^2 m; \lambda_0^2 = \lambda_1 a_1^2/2^{4/3}C_1^2 + \beta; \lambda_1 \approx \alpha_{0(3)}/3;$$

where $\alpha_{0(3)} \approx 6.4$ is zero of the Bessel function I_3 [3]. Taking into the account $h^2/8\pi^2 m \approx 3.4 \times 10^{-20}$ for $z_0 = 10^{-9}m$ we obtain $|E| \approx 28.3\, eV$.

In case of $\lambda_0^2 = \beta$ the solution of the Problem is a harmonic function given by the formula $u = Im\, w_2$, where $w_2 = f^{-1}(w_0)$,

$$w_0 = f(w_2) = C_1 \int_0^{w_2} (t^2 - b_2^2)^{-1/3}(t^2 - b_3^2)^{-1/2} dt + a_4/2,$$

C_1, $b_2\, b_3$ are definite constants and the corresponding energy level is $|E| \approx 0.32\, eV$.

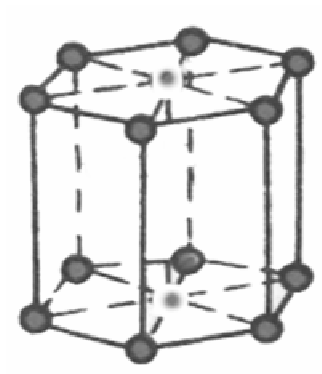
Remark 2. The following scenario is also possible: the movement of the electron inside the prism having as the cross-section the spherical sector $\pi/6 \le \varphi_0 \le 5\pi/6$, $r_0^2 = |a_3 - a_2|^2, x = r_0 \cos\varphi_0$, $y = r_0 \sin\varphi_0$ (the part of the initial prism D) (Fig.2). According to the previous results of the author [7] the eigenfunction of the Problem will be given by

$$u(z, x, y) = C^* \sin(\pi z/z_0) \sin 3\varphi_0 I_3(\lambda_0 r_0); \lambda_0 = \alpha_{0(3)}/|a_3 - a_2|;$$

where C^* is the definite constant. The corresponding energy level for $z_0 = 10^{-9}m$ is

$$|E| = (\lambda_0^2 + \beta)h^2/8\pi^2 m = ((\alpha_{0(3)}/|a_3 - a_2|)^2 + \beta)h^2/8\pi^2 m \approx 139.7\, eV.$$

The mechanical properties of nanostructures was studied in [13]



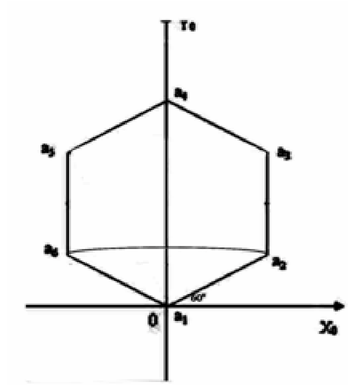


Figure 1: Hexagonal prism. Figure 2: Hexagon in *xoy* plane.

4 Conclusions. The possible energy levels of electrons at the carbon nanostructures represented by the hexagonal prism are $|E| \approx 28.3\, eV$, $|E| \approx 0.32\, eV$,$|E| \approx 139.7\, eV$.

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