On the Energy Levels of Electrons in 2D Carbon Nanostructures

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***Abstract*—The quantum properties of materials essentially depend on their molecular structure. In the paper the mathematical model of quantum properties of 2D carbon nanostructures is studied from the nonrelativistic viewpoint. The energy levels of electrons in such structures are connected with the spectral problem for the stationary Schrödinger equation in the areas of hexagonal configuration. By means of the conformal mapping method the Schrödinger equation is reduced to the degenerated elliptic equation in the rectangle with the appropriate boundary conditions. This equation is solved analytically. The eigenvalues and eigenfunctions are obtained in new variables and consequently, the possible energy levels of electrons in 2D carbon nanostructures are derived numerically.**

Besides, the quantum billiard problem for some closed areas inscribed in the hexagon is solved.

***Index Terms*—Carbon, quantum billiard, Schrödinger equation**

I. Introduction

NANOSTRUCTURES and their unique quantum properties are widely used in electronic devices. Quantum effect is the essential part of those devices. Nanostructures properties are significantly different from their similar materials at macro scale [5],[6],[10],[13],[14]. The phenomena of quantum confinement and resonance tun-neling becomes significant, when the dimensions of the ma-terials are less than 10nm. Here we will focus on 2D carbon nanostructures (Fig.1 , Fig.2, Fig,3).

2D carbon nanostructure represents hexagonal honeycomb structure. The carbon atoms in those nanostructures are arrange in the hexagonal rings and electrons confined in such structures behave like quantum billiard balls [5],[10], [12],[13], [14] . Carbon is the sixth element (group 14), with a ground state electron configuration $1s^2 2s^2 2p^2$, four outer electrons are valence electrons [13],[14]. Graphene - 2D sheet of carbon is the strongest material ever tested and was studied in 2004 by Andre Gein and Konstantin Novoselov [5], [13],[14]. The side of the elementary cell (hexagon) in the carbon nanostructure is about $0.14nm$.

Here we consider the quantum billiard problem in one cell of this structure- hexagon or in the hexagonal rug (Fig.1 , Fig.2, Fig,3). The atoms are represented as the points at the vertices of the hexagon. We study this problem from the non-relativistic point of view, i.e. in the hexagonal area we consider the Schrödinger equation for the wave-function of the electron with the appropriate boundary conditions [1], [6], [9], [10], [11], [12] (quantum billiard problem).In this paper by means of the conformal mapping method the equation is reduced to the elliptic equation with the appropriate boundary conditions [7], [8]. As three parameters of the mapping can be chosen arbitrarily the equation is simplified and is solved analytically. The eigenvalues and eigenfunctions are obtained and energy levels of electrons are estimated.

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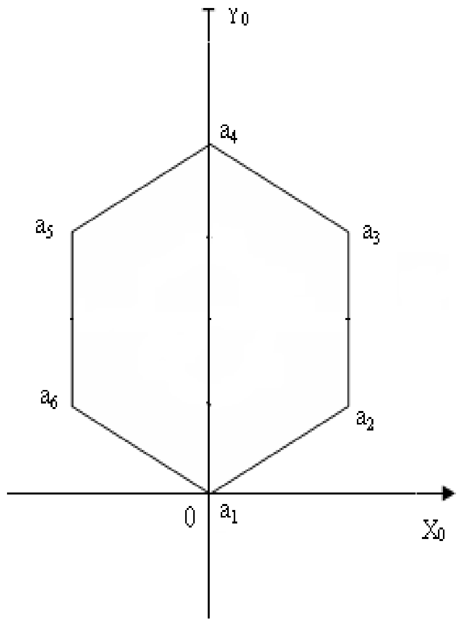

Fig.1. The hexagonal area The atoms are presented as points at the vertexes.

II. Statement of the Problem

From the non-relativistic viewpoint the wave function of the electrons satisfies the Schrödinger Equation in some area with the appropriate condition at the boundary.

Let D be a bounded connected area in z-plane, ($z = x + iy$) (Fig.1, Fig.2 or Fig.3). In this area we consider the following problem (quantum billiard problem) [1],[6],[9],[10],[11],[12].

Problem 1.

To find a real function $\psi(x, y)$ in D having second order derivatives , satisfying the equation

$$\Delta\psi(x, y) + \lambda_0{}^2\psi(x, y) = 0, \qquad (1)$$

and the conditions

$$\psi\big|_S = 0, \qquad \iint_D |\psi|^2 dxdy = 1, \qquad (2)$$

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where S is a boundary of D or the closed curve inscribed in D, ψ is the wave function of the particle, λ_0 is the constant to be determined,

$$\lambda_0{}^2 = \frac{8\pi^2 m}{h^2} E, \qquad (3)$$

E is the energy of the particle, m is mass of the electron and h is Planck's constant

$$\mathrm{m} \approx 9.1\times 10^{-31}\,\mathrm{kg};\ \mathrm{h} \approx 4.1\times 10^{-15}\, eV\cdot \mathrm{sec}\,.$$

The function $|\psi|^2$ is the probability of the location of the "electron cloud" in the region D.

Additionally we demand, $|\psi| \neq 0$ in D.

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

$$E_n = -\frac{m}{(2\varepsilon_0)^2 h^2} e^4 \frac{1}{n^2},\ n = 1,2,3,... \qquad (4)$$

where e is the electron charge, ε_0 is the vacuum permittivity,

$$\mathrm{e}^2 = v_1 \frac{mh}{2\pi},\ \mathrm{v}_1 \approx 2.3\times 10^6\, m/\mathrm{sec},$$

v_1 is the velocity of the electron, n is a quantum number. By the formula (4) he obtained the different quantum states of the electron in the Hydrogen atom. For example the ground state of the electron in the hydrogen atom is

$$E_0 = \frac{h^2}{8\pi^2 m r_1^2} \approx -13.6.eV,\ \mathrm{r}_1 \approx 5\times 10^{-11} m.$$

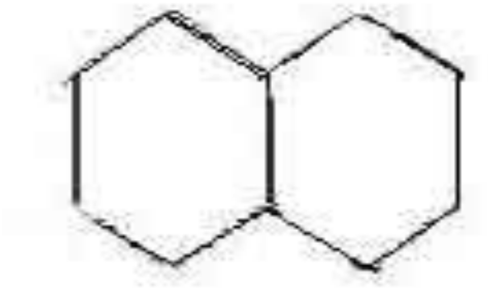

Fig.2. The hexagonal rug with two hexagonal cells.

III. SOLUTION OF PROBLEM 1 BY MEANS OF THE CONFORMAL MAPPING METHOD

We will consider three cases:

1. D is the hexagon (Fig. 1),
2. D is the composition of two hexagons (Fig. 2),
3. D is the composition of three hexagons (Fig. 3).

1. Let D be the hexagon of z-plane , $z = x + iy$, with the vertices $a_1 = 0, a_2, a_3, a_4 (\operatorname{Re} a_4 = 0), a_5, a_6$ and with the axis of symmetry $a_1 a_4$ (Fig.1). We consider Problem 1 in this case.

We will solve this problem by means of the conformal mapping method. As three parameters of the mapping could be chosen arbitrarily Problem 1 will be simplified [3],[4],[7],[8].

Let us consider conformal mapping $f(w)$ of the rectangle $D_0\{-a_0/2 \le \xi \le a_0/2; 0 \le \eta \le b_0\}$ of $w = \xi + i\eta$ plane on the area D, with the following correspondence of points (Fig. 4)

$$a_1 \leftrightarrow 0,\ a_2 \leftrightarrow a_0/2,\ a_3 \leftrightarrow a_0/2 + ib_0,\ a_4 \leftrightarrow ib_0,$$
$$a_5 \leftrightarrow -a_0/2 + ib_0,\ a_6 \leftrightarrow -a_0/2;\ a_0, b_0 > 0$$

The function $f(w)$ is given by the formula [3],[4]

$$z = f(w) = C\int_0^{z_0} t^{-1/3}\left(t^2 - a^2\right)^{-1/3}\left(t^2 - b^2\right)^{-1/3} dt,$$

$$z_0 = sn\left(\frac{w}{C_0}\right),$$

$$w = C_0 \int_0^{z_0} \left(1 - t^2\right)^{-1/2}\left(1 - k^2 t^2\right)^{-1/2} dt, \qquad (5)$$

where

$$|C| = \frac{|a_3 - a_2|}{k_0},$$

$$C_0 \approx \frac{a_0}{\pi},\ k_0 = \int_a^b t^{-1/3}\left(t^2 - a^2\right)^{-1/3}\left(t^2 - b^2\right)^{-1/3} dt, \qquad (6)$$

sn is the Jacobi "sinus" with the modulus k [3],[4], $a = 1; b = 1/k$.

By the mapping (5) Problem 1 will be reduced to the following problem

Problem 2.

To find a real function $\psi_0(\xi,\eta)$ in D_0 having second order derivatives, satisfying the following equation

$$\Delta\psi_0(\xi,\eta) + \lambda_0{}^2 \left|f'(w)\right|^2 \psi_0(\xi,\eta) = 0, \qquad (7)$$

and the boundary conditions

$$\psi|_{S_0} = 0,\ \iint_{D_0} |\psi_0|^2 \left|f'(w)\right|^2 d\xi d\eta = 1,\ |\psi| \neq 0,$$

where $\psi_0(\xi,\eta) = u(f(w))$, and λ is the constant to be determined, S_0 is the closed line inscribed in D_0.

It is obvious, that

$$|f_w{}'(w)|^2 = \left|f_{z_0}{}'(w)\right|^2 . |z_0{}'(w)|^2 . \qquad (8)$$

If we suppose $a = 1, b = 1/k$, from (5), (6), (8) after simple transformations one obtains

$$|f_w{}'(w)|^2 = C_1^2 \left(\frac{sn\frac{w}{C_0}}{cn\frac{w}{C_0} dn\frac{w}{C_0}}\right)^{2/3}, \qquad (9)$$

where $C_1 = k^{2/3} C / C_0$; sn, cn, dn are the Jacobi functions [3], [4].

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As three parameters of the conformal mapping can be chosen arbitrarily, we can assume, that $q = e^{-\pi\chi}$, ($\chi = \dfrac{2b_0}{a_0}$), is sufficiently small and use the formulas [3], 4]

$$sn(w/C_0) \approx \sin\gamma,$$
$$cn(w/C_0) \approx \cos\gamma, \; dn(w/C_0) \approx 1, \qquad (10)$$

$$\gamma = \frac{\pi w}{a_0 C_0}, \; b_0 = \frac{5}{3}a_0, C_0 \approx \frac{a_0}{\pi}, k \approx 0.0213.$$

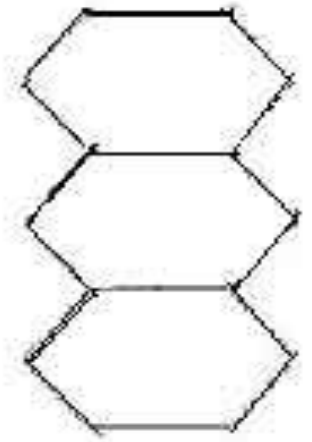

Fig.3. The hexagonal rug with three hexagonal cells.

Taking into account (10) in (6) and (9) and by using "Maple" we obtain

$$|f_w'(w)|^2 \approx C_1^2 \left(\frac{\cosh(2\pi\eta/a_0C_0) + \cos(2\pi\xi/a_0C_0)}{\cosh(2\pi\eta/a_0C_0) - \cos(2\pi\xi/a_0C_0)} \right)^{2/3},$$

$$\int_a^{1/k} t^{-1/3}\left(t^2 - a^2\right)^{-1/3}\left(t^2 - b^2\right)^{-1/3} dt \approx 0.342848, \qquad (11)$$
$$|C| = |a_3 - a_2| / 0.342848.$$

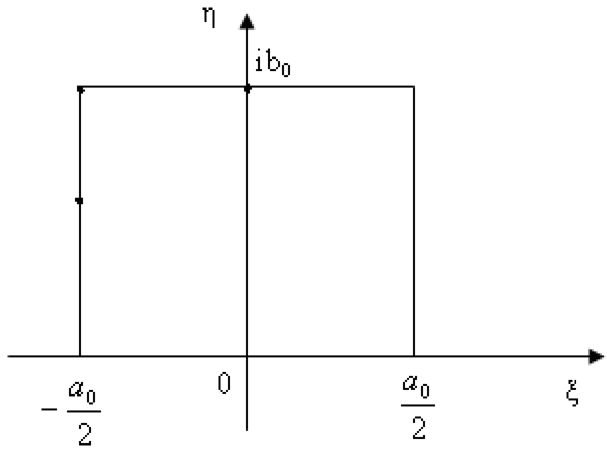

Fig.4.Rectangle

$$D_0\{-a_0/2 \le x_0 \le a_0/2; 0 \le y_0 \le b_0\}.$$

In new variables

$$\xi_0 = 2\pi\xi / a_0C_0, \eta_0 = 2\pi\eta / a_0C_0 \qquad (12)$$

by using (11) the equation (7) could be rewritten as

$$a_1^2 \Delta\psi_0(\xi_0,\eta_0) + \lambda_0{}^2 C_1^2 \left(\frac{\cosh(\eta_0) + \cos(\xi_0)}{\cosh(\eta_0) - \cos(\xi_0)} \right)^{2/3} \psi_0(\xi_0,\eta_0) = 0, \qquad (13)$$

where $a_1 = 2\pi^2 / a_0^2$.

Let us choose the parameter a_0 of the mapping in such a way that the quantity a_0^{-6} is negligible, then we can use well-known formulas

$$\cos(\xi_0) \approx 1 - \xi_0^2/2 + \xi_0^4/24,$$
$$\cosh(\eta_0) \approx 1 + \eta_0^2/2 + \eta_0^4/24 \quad . \qquad (14)$$

Putting (14) into (13) one obtains

$$a_1^2 \Delta\psi_0(\xi_0,\eta_0) + \lambda_0{}^2 C_1^2 \times \left(\frac{4 + \eta_0^2 - \xi_0^2 + \frac{1}{12}\left(\left(\eta_0^2 + \xi_0^2\right)^2 - 2\eta_0^2\xi_0^2\right)}{\eta_0^2 + \xi_0^2 + \frac{1}{12}\left(\eta_0^2 - \xi_0^2\right)\left(\eta_0^2 + \xi_0^2\right)} \right)^{2/3} \times \qquad (15)$$

$$\psi_0(\xi_0,\eta_0) = 0.$$

In the cylindrical coordinate system $\xi_0 = r\cos\varphi, \quad \eta_0 = r\sin\varphi$ (15) becomes

$$a_1^2 . r^{4/3}\left(\frac{\partial^2\psi_0}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2\psi_0}{\partial\varphi^2} + \frac{1}{r}\frac{\partial\psi_0}{\partial r}\right) + \lambda^2 \times \quad (16)$$

$$\left(\frac{4 - r^2\cos 2\varphi + \frac{r^4}{24}\left(\cos^2 2\varphi + 1\right)}{1 - \frac{1}{12}r^2\cos 2\varphi}\right)^{2/3} \psi_0(r,\varphi) = 0$$

where $\lambda^2 = \lambda_0{}^2 C_1^2$.

As $r^2 = \left(\xi_0^2 + \eta_0^2\right) \le 2\pi^4 / a_0^2$ and r^6 is negligible , taking into account the formula

$$(1 + r^2)^\alpha \approx 1 + \alpha r^2 + \frac{\alpha(\alpha-1)}{2!}r^4 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}r^6, \quad (17)$$

the equation (16) can be rewritten as

$$a_1^2 . r^{4/3}\left(r^2\frac{\partial^2\psi_0}{\partial r^2} + \frac{\partial^2\psi_0}{\partial\varphi^2} + r\frac{\partial\psi_0}{\partial r}\right) + \lambda_0{}^2 C_1^2 r^2 2^{4/3}\left(1 - \frac{r^2}{9}\cos 2\varphi\right)\psi_0(r,\varphi) = 0. \quad (18)$$

We now admit that $\lambda_0{}^2 C_1^2 r^4$ is negligible and finally the equation (18) takes the form

$$a_1^2\left(r^2\frac{\partial^2\psi_0}{\partial r^2} + \frac{\partial^2\psi_0}{\partial\varphi^2} + r\frac{\partial\psi_0}{\partial r}\right) + 2^{4/3}\lambda_0{}^2 C_1^2 r^{2/3}\psi_0(r,\varphi) = 0, \quad (19)$$

with the boundary condition

$$\psi\big|_{S_0} = 0, \quad (20)$$

where S_0 is the boundary of the area D_0^*: $\xi_0^2 + \eta_0^2 = \left(2\pi\xi / a_0 C_0\right)^2 + \left(2\pi\eta / a_0 C_0\right)^2 \le 2\pi^4 / a_0^2$, $\xi_0 \ge 0, \quad \eta_0 \ge 0.$

By the separation of the variables $\psi_0(r,\varphi) = u_1(r)u_2(\varphi)$ from the equation (20) one obtains

$$u_2''(\varphi) + \beta u_2(\varphi) = 0, \quad (21)$$

$$r^2 u_1''(r) + r u_1'(r) + \left(\frac{2^{4/3}}{a_1^2}\lambda_0^2 r^{2/3} - \beta\right)u_1(r) = 0. \quad (22)$$

The solutions of (21) satisfying the condition $u_2(0) = u_2(\pi) = 0$ are given by [15]

$$u_2(\varphi) = C^* \sin\sqrt{\beta}\,\varphi; \quad \beta = n^2; n = 1,2,\ldots \quad (23)$$

where C^* is a certain constant.

Now, let us consider the equation (22). By introducing a new variable $r_0 = r^{1/3}$ the equation (22) takes the form

$$r_0^2 u_1''(r) + r_0 u_1' + 9\left(\frac{2^{4/3}}{a_1^2}\lambda_0^2 r_0^2 - \beta\right)u_1 = 0. \quad (24)$$

We seek for the non-negative solutions of (22). The solutions of the equation (24) are given in terms of Bessel's functions [3], [4]

$$u_1(r_0) = I_{3\sqrt{\beta}}\left(3\lambda_1 r_0\right), \quad \lambda_1^2 = \frac{2^{4/3}}{a_1^2}\lambda_0{}^2 C_1^2 . \quad (25)$$

Taking into account (23) and (25) we obtain the solutions of the equation (19)

$$\psi_{0n}(r,\varphi) = C^* \sin n\varphi\, I_{3n}\left(3\lambda_1 r^{1/3}\right); n = 1,2,\ldots \quad (26)$$

The functions $\psi_{0n}(r,\varphi), n = 1,2,\ldots$ are the eigenfunctions of the equation (19) and corresponding eigenvalues will be calculated from the condition (20)

$$3\lambda_{1n}\left(2^{1/2}\pi^2 / a_0\right)^{1/3} = \frac{3\times 2^{5/6}}{a_1}\lambda_{on} C_1\left(\pi^2 / a_0\right)^{1/3} = \alpha_{0(3n)}, n = 1,2,\ldots \quad (27)$$

where $\alpha_{0(3n)}, n = 1,2,\ldots$ are zeroes of Bessel's functions I_{3n},

$$C_1 = \left(\pi k^{2/3} / k_0\right)\frac{|a_3 - a_2|}{a_0} \approx \sqrt[3]{0.4}\,\frac{|a_3 - a_2|}{a_0}. \quad (28)$$

As we have the additional condition $|\psi| \ne 0$ in D_0^*, only the case of $n = 1$ is acceptable .

Hence, the wave function of the problem 1 in terms of $\xi_0 = r\cos\varphi, \quad \eta_0 = r\sin\varphi$ will be given by

$$\psi_{01}(r,\varphi) = C^* \sin\varphi\, I_3\left(3\lambda_1 r^{1/3}\right)$$

and from (3), (27) and (28) we can calculate λ_{01} and corresponding energy level

$$E_1 = \lambda_{01}{}^2\frac{h^2}{8\pi^2 m} . \quad (29)$$

According to (27) and (28) one obtains

$$\frac{3\times 2^{5/6}}{a_1}\lambda_{o1} C_1\left(\pi^2 / a_0\right)^{1/3} \approx \lambda_{o1} a_0^{2/3}\frac{|a_3 - a_2|}{2} = \alpha_{0(3)}. \quad (30)$$

For the carbon structure $|a_3 - a_2| \approx 0.14\times 10^{-9} m$ [10], [13], [14] and by (29) and (30) we have

$$E_1 = \lambda_{01}{}^2\frac{h^2}{8\pi^2 m} \approx 14.4\times a_0^{-4/3}\alpha_{0(3)}^2, \quad (31)$$

$\alpha_{0(3)}$ is the first zero of Bessel's function I_3, $\alpha_{0(3)} \approx 6.4$ [4].

For $a_0 = 10$ the formula (31) gives $|E_1| \approx 29.5 eV$.

2. Now, let us suppose that the area D consists of two hexagons (Fig. 2). We can continue the function

$f(w)$ given by the formula (5) through the segment $[-a_0/2,0]$ and then then obtain the conformal mapping of the rectangle $D_0^2\{-a_0/2 \le \xi \le a_0/2; -b_0 \le \eta \le b_0\}$ cut along the segment $[0, a_0/2]$ on the area D. In this case as previously we reduce the equation (1) to the equation (19) with the boundary conditions $\psi|_{S_0} = 0$

where S_0 is the boundary of the area D_0^*: $\xi_0^2 + \eta_0^2 = (2\pi\xi/a_0C_0)^2 + (2\pi\eta/a_0C_0)^2 \le 2\pi^4/a_0^2$.
In this case the eigenfunction of the Problem 2 will be

$$\psi_0(r,\varphi) = C^*\varphi\, I_0\left(3\lambda_1 r^{1/3}\right)$$

and the eigenvalues will be calculated from the formula

$$3\lambda_{1n}\left(2^{1/2}\pi^2/a_0\right)^{1/3} = \frac{3\times 2^{5/6}}{a_1}\lambda_{on}C_1\left(\pi^2/a_0\right)^{1/3}$$

$$= \alpha_{0(n)},\ n = 1,2,...$$

where , $\alpha_{0(n)}$ are zeroes of the Bessel function I_0. By the additional condition $|\psi| \ne 0$ in D_0^* we consider only case of $n = 1$ and taken into account $\alpha_{0(0)} \approx 2.4$ one obtains

$$E_1 = \lambda_{01}^{\ 2}\frac{h^2}{8\pi^2 m} \approx 14.4\times a_0^{-4/3}\alpha_{0(0)}^2 \approx 83{,}5\times a_0^{-4/3}.$$

For $a_0 = 10$ we have $|E_1| \approx 8eV$.

3. Finally, we consider D as the composition of three hexagons (Fig.3). We continue the function $f(w)$ through the sides $[-a_0/2, ib_0]$ and $[a_0/2, ib_0]$ and obtain the conformal mapping of the rectangle $D_0^3\{-a_0/2 - a_0 \le \xi \le a_0/2 + a_0; 0 \le \eta \le b_0\}$ on the area D.

In this case the equation (1) will be reduced to the equation (19) with the boundary condition $\psi|_{S_0} = 0,$

where S_0 is the boundary of the area D_0^*: $\xi_0^2 + \eta_0^2 = (2\pi\xi/a_0C_0)^2 + (2\pi\eta/a_0C_0)^2 \le 18\pi^4/a_0^2$, $\xi_0 \ge 0, \quad \eta_0 \ge 0.$

Analogously to the first section of the paper the eigenfunctions of the problem 2 will be

$$\psi_{01}(r,\varphi) = C^*\sin\varphi\, I_3\left(3\lambda_1 r^{1/3}\right)$$

and corresponding eigenvalue satisfies the condition

$$3\lambda_{11}\left(2^{1/2}3\pi^2/a_0\right)^{1/3} =$$

$$\frac{3\times 2^{5/6}}{a_1}\lambda_{o1}C_1\left(3\pi^2/a_0\right)^{1/3} = \alpha_{0(3)}.$$

In this case we obtain the following energy level

$$E_1 = \lambda_{01}^{\ 2}\frac{h^2}{8\pi^2 m} \approx 7.2\times a_0^{-4/3}\alpha_{0(3)}^2,$$

For $a_0 = 10$ -- $|E_1| \approx 14.4eV$.

IV. SOLUTION OF PROBLEM 1 FOR SOME CLOSED AREAS INSCRIBED IN THE HEXAGON

Let us state the problem 1 in terms of polar coordinates $x = r\cos\varphi, \quad y = r\sin\varphi$

Problem 3.

To find a real function $\psi(r,\varphi)$ in $D_0 \subset D$ having second order derivatives , satisfying the equation

$$\frac{\partial^2\psi}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{1}{r}\frac{\partial\psi}{\partial r} + \lambda_0^2\psi(r,\varphi) = 0,$$

and the conditions

$$\psi|_S = 0, \quad |\psi| \ne 0,\ in\ D_0,\ \iint_D |\psi|^2 dxdy = 1,$$

where S is a boundary of the area D_0 inscribed in D, ψ is the wave function of the particle, λ_0 is the constant to be determined $\lambda_0^{\ 2} = 8\pi^2 mE/h^2$.

We will consider 4 cases :

1. D_0 is the circle with the radius $r = a\sqrt{3}/2$ inscribed in D.
2. D_0 is the spherical sector bonded with the lines $\varphi = \pi/d \quad ; \varphi = \pi - \pi/d;\ 2 < d < 6,\ d \ne 4$ and $r^2 = d_0^2$; (Fig.5)
3. D_0 is the spherical sector bonded with the lines $\varphi = \pi/4 \quad ; \varphi = \pi - \pi/4$ and $r^2 = 3a^2/2$; (Fig.6)
4. D_0 is the spherical sector bonded with the lines $\varphi = \pi/6 \quad ; \varphi = \pi/2$ and $r^2 = |a_3 - a_2|^2 = a^2$;

where d is the real number, a is the length of the side of the hexagon, $d_0 = a\dfrac{\sqrt{3}}{2\cos\pi/d}$.

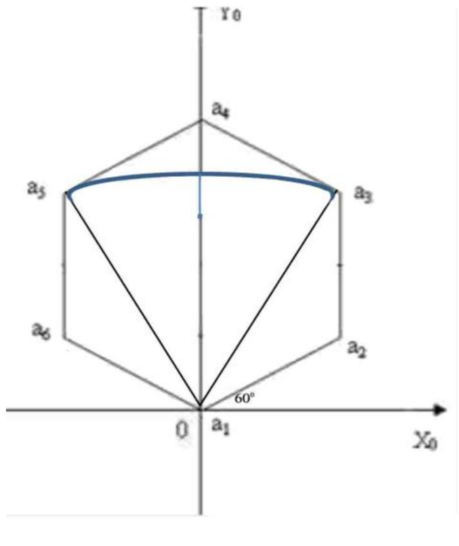

Fig.5.The sector inscribed into the hexagon.

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V. SOLUTION OF PROBLEM 3

By the separation of the variables ,as in previous section, we obtain that the eigenfunctions and eigenvalue of the problem 3 are :

1. $\psi(r,\varphi)=C_1^* I_0(\lambda_0 r)$, $\lambda_0 = 2\alpha_o/\sqrt{3}a$, where C_1^* is a certain constant, I_0 is the Bessel function, $\alpha_o \approx 2.4$. Corresponding energy level will be $|E_0| \approx 20.7eV$.

2. $\psi_d(r,\varphi)=C_1^* I_d(\lambda_0 r)\sin d\varphi, \lambda_d = \alpha_d / d_0$, (32)

$$\psi_{d/2}(r,\varphi)=C_2^* I_{d/2}(\lambda_0 r)\cos(\frac{\varphi d}{2}), \lambda_{d/2} d_0 = \alpha_{d/2}/d_0,$$

where $I_{d/2}$ and I_d are the Bessel functions, C_1^* and C_2^* are certain constants, $\alpha_{d/2}$, α_d are first zeroes of the Bessel functions $I_{d/2}$ and I_d correspondingly.

Corresponding energy levels will be given by

$$|E_d| = h^2 d_0^2 / 8\pi^2 \alpha_d^2 \quad , \quad |E_{d/2}| = h^2 d_0^2 / 8\pi^2 \alpha_{d/2}^2.$$

Example. Below we consider the case of $d = 3$ (Fig.5). By the formulas (32) the corresponding eigenfunctions and eigenvalues will be

$$\psi_3(r,\varphi)=C_1^* I_3(\lambda_0 r)\sin 3\varphi, \lambda_3 = \alpha_3 / d_0$$

$$\psi_{3/2}(r,\varphi)=C_2^* I_{3/2}(\lambda_0 r)\cos(3\varphi/2), \lambda_{3/2} = \alpha_{3/2}/d_0;$$

where $d_0 = \sqrt{3}a$, $\alpha_3 \approx 6.4$, $\alpha_{3/2} \approx 4.5$.

Consequently, the possible energy levels are

$|E_d| \approx 48eV$ and $|E_{d/2}| \approx 24eV$.

3. In case of Fig.6 the eigenfunctions and eigenvalues of the problem 3 are $\psi_2(r,\varphi)=C_2^* I_2(\lambda_0 r)\cos(2\varphi)$; $\lambda_2 = \alpha_2\sqrt{2}/a\sqrt{3}$; $\alpha_2 \approx 5.1$; and the corresponding energy level will be $|E_2| \approx 62.4eV$.

4. In the forth case the eigenfunctions and eigenvalues of the problem 3 are $\psi_3(r,\varphi)=C_1^* I_3(\lambda_0 r)\sin(3\varphi)$; $\lambda_3 = \alpha_3 / a$ and the energy level-$|E_3| \approx 147.6eV$.

REMARK. In the hexagonal rug the movement of the electron in the rectangle with the sides $la\sqrt{3}; a$, where l is the number of elementary cells (hexagons), is also possible. In this case the energy levels will be calculated from the well known formula [1] ,[6],[9],[10]

$$E_{n_1,n_2} = \frac{h^2}{8m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{3l^2a^2}\right), \ n_1, n_2 = 1,2,... \quad (33)$$

For example, in case of 20 samples ($l = 20$) the energy levels for $n_1 = n_2 = 1$, are $|E_{1,1}| \approx 32.4eV$; and

for $n_1 = 1, n_2 = 10$, -- $|E_{1,10}| \approx 32.7eV$.

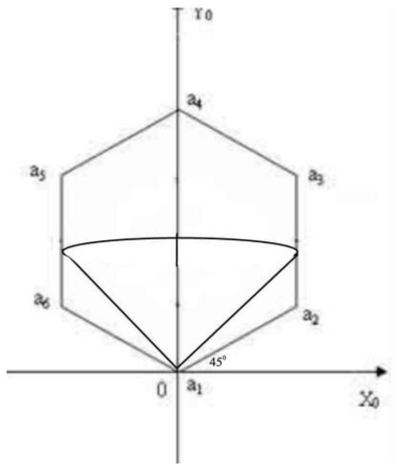

Fig.6.The sector inscribed into the hexagon.

VI. CONCLUSION

In the carbon nanostructures the possible energy levels of the electrons are:

1.In one cell (hexagon)

$|E_0| \approx 20.7eV$, $|E_1| \approx 29.5eV$,$|E_{3/2}| \approx 24eV$, $|E_2| \approx 62.4eV$,$|E_3| \approx 48eV$,$|E_4| \approx 147.6eV$.

2.In the rug with two cells $|E_0| \approx 32.4eV$, $|E_1| \approx 8eV$.

3.In the rug with 3 cells $|E_0| \approx 32.4eV$, $|E_1| \approx 14.4eV$.

4.In the rug with several cells are given by the formula (33).

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