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ON THE HEXAGONAL QUANTUM BILLIARD

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Abstract. In the paper a planar classical quantum billiard in the hexagonal type areas with the hard wall conditions is considered. The process is described by the Helmholtz Equation in the hexagon and hexagonal rug with the homogeneous boundary conditions. By means of the conformal mapping method the problem is reduced to the elliptic partial differential equation in the rectangle with the homogeneous boundary condition. It is assumed that one parameter of mapping is sufficiently small. In this case the equation is simplified and analyzed. The asymptotic solutions are obtained. The spectrum and the corresponding eigenfunctions are found near the boundary of the hexagon. The wave functions are found in terms of the Bessel's functions. The results are applied for the estimation of the energy levels of electrons in graphene.

Keywords and phrases: Quantum chaos, Helmholtz Equation, Bessel's functions, graphene.

AMS subject classification (2010): 39A14, 35M11, 35Q40, 32H04.

Introduction

Quantum Billiard is a dynamical system, which describes a motion of a free particle inside a closed domain D with a piece-wise smooth boundary S [2, 3, 7-11, 13-17, 19-22]. In this case the Schrödinger Equation for a free particle assumes the form of the Helmholtz Equation and the spectrum of the Helmholtz Equation reflects the energy levels of the particle.

In the paper the following equation with the homogeneous boundary condition, when D is the hexagon, is considered

$$\Delta u(x,y) + \frac{2m}{h^2} E u(x,y) = 0 \qquad u|_S = 0, \tag{1*}$$

where S is a boundary of D, u is the wave function of the particle, $\lambda^2 = \dfrac{2m}{h^2}E$ is the constant to be determined, E is the energy of the particle, m is mass, h is Planck's constant.

In some cases it is more convenient to replace the condition $u|_S = 0$ by the condition [2, 14, 17,19, 20, 22]

$$\iint\limits_D |u|^2 dxdy = 1.$$

The hexagonal type areas are very important, as the atoms of Carbon and its allotropes are arranged in the hexagonal type structures [4, 7, 17, 19, 20] and has a lot of applications in microeletronics. For example, graphene is a one-atom thick sheet of carbon atoms which form a hexagonal structure ([4], see "One atom thick billiard" https//sites.google.com/a/ucr.edu/physics-lau/) and electrons in such structures behave like quantum billiard balls [4, 7, 17, 21].

The problem is investigated by means of the conformal mapping and partial differential equation. The Helmholtz Equation (1*) is transformed to the equation of the elliptic type. One parameter of the mapping is chosen sufficiently small, the initial equation is simplified and replaced by the approximate elliptic equation.The wave function and eigenvalues of this equation are found.

Statement of the problem

Let D be the hexagon of the plane $z_0 = x_0+iy_0$, with the vertexes $a_1, a_2, a_3, a_4, a_5, a_6$ ($a_1 = 0$, $Re\, a_4 = 0$), and with the axis of symmetry a_1a_4 (Fig.1). In this area we consider the following problem

Problem 1. To find a real function $u(x_0, y_0)$ in D having second order derivatives, satisfying the equation

$$\Delta u(x_0, y_0) + \lambda^2 u(x_0, y_0) = 0 \tag{1}$$

and the boundary condition

$$u|_S = 0, \tag{2}$$

where λ is the constant to be determined, S is the boundary of D.

By means of the conformal mapping we reduce Problem 1 to the elliptic partial differential equation in the rectangle.

At first we map the area D at the upper half-plane of the complex plane $z = x+iy$, by the Schwartz-Christoffel formula [1, 6, 15, 17] with the following correspondence of points

$$a_1 \leftrightarrow 0, a_2 \leftrightarrow a, a_3 \leftrightarrow b, a_4 \leftrightarrow \infty, a_5 \leftrightarrow -a, a_6 \leftrightarrow -b; a, b > 0;$$

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

where C is the definite constant, which is determined from the formula

$$a_3 - a_2 = C \int_a^b t^{-1/3}(t^2 - a^2)^{-1/3}(t^2 - b^2)^{-1/3}dt.$$

Let $z = f(w)$ be the conformal mapping of the rectangle $D_0\{-a_0/2 \le u \le a_0/2;\ 0 \le \nu \le b_0\}$ with the boundary S_0 of the plane $w(w = \xi + i\eta)$, on the upper half-plane of z. This mapping will be given by [1, 6, 15, 17]

$$z = sn\left(\frac{w}{C_0}\right), \tag{4}$$

or

$$w = C_0 \int_0^z (1 - t^2)^{-1/2}(1 - k^2t^2)^{-1/2}dt,$$

with the following correspondence of points

$$0 \leftrightarrow 0, a \leftrightarrow a_0/2, b \leftrightarrow a_0/2 + ib_0, \infty \leftrightarrow ib_0, -a \leftrightarrow -a_0/2 + ib_0, -b \leftrightarrow -a_0/2;\; a_0, b_0 > 0$$

(Fig. 2), where sn is the Jakobi "sinus" with the modulus k, having the periods $2a_0$ and $2b_0, C_0$ is the definite constant which is defined from the tables [15, 18], a_0 will be chosen accordingly in the following.

By the mappings (3), (4) Problem 1 could be reduced to the following problem

Problem 2. To find a real function $u_0(\xi, \eta)$ in D_0 having second order derivatives, satisfying the following equation

$$\Delta u_0(\xi, \eta) + \lambda^2 |f'(w)|^2 u_0(\xi, \eta) = 0, \qquad (5)$$

with the boundary condition

$$u_0|_{S_0} = 0,$$

where $u_0(\xi, \eta) = u(f(w))$, and λ is the constant to be determined.

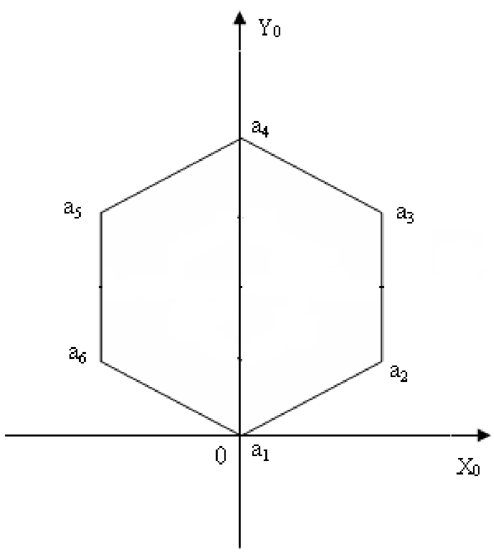

Fig. 1. The hexagonal area

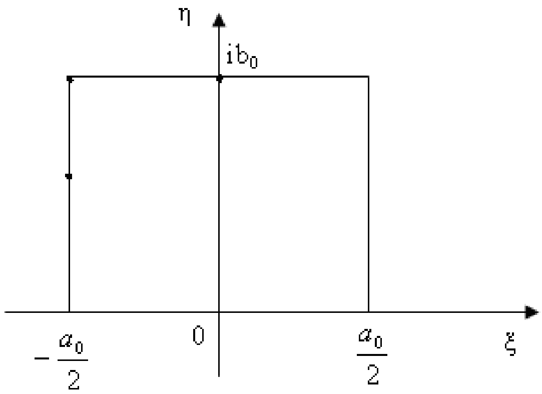

Fig. 2. The image of the hexagon by the mapping $z = f(w)$

Solution of Problem 2

It is obvious that

$$|f'_w(w)|^2 = |f'_z(w)|^2 \cdot |z'_w(w)|^2. \tag{6}$$

If we suppose $a = 1,\ b = 1/k$, from (3), (4), (6) after simple transformations we obtain

$$f'_w(w)^2 = C_1^2 \left(\frac{cn\dfrac{w}{C_0} dn\dfrac{w}{C_0}}{sn\dfrac{w}{C_0}} \right)^{2/3}. \tag{7}$$

where $C_1 = k^{2/3}\frac{C}{C_0}$ and sn, cn, dn are the Jacobi functions [1, 5, 6, 15].

As three parameters of the conformal mapping can be chosen arbitrarily, we can assume that $q = e^{-\pi\chi}$, $(\chi = \frac{2b_0}{a_0})$, is sufficiently small and we can use formulas [5, 6, 15]

$$\begin{aligned} sn(w/C_0) &\approx \sin\gamma(1 + 4q\cos^2\gamma),\\ cn(w/C_0) &\approx \cos\gamma(1 - 4q\sin^2\gamma),\\ dn(w/C_0) &\approx (1 - 8q\sin^2\gamma), \end{aligned} \tag{8}$$

where $\gamma = \frac{\pi w}{a_0 C_0}$. Without loss of generality we can also suppose $q \approx 0$ [1, 5, 6, 15], then the formulas (8) could be simplified and one obtains, (a_0 will be chosen in the following way)

$$\begin{aligned} sn(w/C_0) &\approx \sin\gamma,\\ cn(w/C_0) &\approx \cos\gamma,\\ dn(w/C_0) &\approx 1,\\ k \approx 0,0213,\ b_0 &= \frac{5a_0}{3},\ C_0 \approx \frac{a_0}{3}. \end{aligned} \tag{9}$$

Putting (9) into (7) we can write the approximate formula

$$|f'_w(w)|^2 \approx |C_1|^2 \left(\frac{1+V}{1-V}\right)^{2/3}, \tag{10}$$

where

$$V = \frac{\cos(2\pi\xi/a_0c_0)}{\cosh(2\pi\eta/a_0c_0)},$$

By using (10) Equation (5) may be rewritten as

$$\Delta u_0(\xi,\eta) + \lambda^2|C_1|^2 \left(\frac{1+V}{1-V}\right)^{2/3} u_0(\xi,\eta) = 0. \tag{11}$$

Hence, we obtain the degenerated elliptic equation.

Now, let us choose a_0 in such a way, that $\left(\frac{6\pi\xi}{a_0^2}\right)^4$ and $\left(\frac{6\pi\eta}{a_0^2}\right)^4$ are negligible. Taking into account (9) and

$$\cos\left(\frac{2\pi\xi}{a_0c_0}\right)^2 \approx 1-\frac{1}{2}\left(\frac{6\pi\xi}{a_0^2}\right)^2, \quad cosh\left(\frac{2\pi\eta}{a_0c_0}\right)^2 \approx 1+\frac{1}{2}\left(\frac{6\pi\eta}{a_0^2}\right)^2,$$

from (11) we obtain

$$\frac{\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}}{\left(1+9\frac{\pi^2}{a_0^4}\eta^2-9\frac{\pi^2}{a_0^4}\xi^2\right)^{2/3}}\Delta u_0(\xi,\eta)+\lambda^2|C_1|^2u_0(\xi,\eta)=0. \tag{12}$$

By using the approximate formula

$$\left(1+9\frac{\pi^2}{a_0^4}\eta^2-9\frac{\pi^2}{a_0^4}\xi^2\right)^{-2/3} \approx \left(1-\left(6\frac{\pi^2}{a_0^4}\eta^2-6\frac{\pi^2}{a_0^4}\xi^2\right)+\frac{5}{9}\left(9\frac{\pi^2}{a_0^4}\eta^2-9\frac{\pi^2}{a_0^4}\xi^2\right)^2\right)$$

and neglecting the terms

$$6\frac{\pi^2}{a_0^4}\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2),\ \ 45\left(\frac{\pi^2}{a_0^4}\right)^2\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)^2,$$

from (12) one obtains the approximate equation

$$\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}\Delta u_0(\xi,\eta)+\lambda^2|C_1|^2u_0(\xi,\eta)=0 \tag{13}$$

In our case we have the following estimations

$$\left(\frac{6\pi\xi}{a_0^2}\right)^4 \le \left(\frac{3\pi}{a_0}\right)^4, \ \left(\frac{6\pi\eta}{a_0^2}\right)^4 \le \left(\frac{10\pi}{a_0}\right)^4,$$

$$\Big|6\frac{\pi^2}{a_0^4}\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)Big| \le 150\left(\frac{109}{108}\right)^{2/3}\left(\frac{\pi}{a_0}\right)^{10/3}, \tag{14}$$

$$45\left(\frac{\pi^2}{a_0^4}\right)^2\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)^2 \le 5^5\left(\frac{109}{108}\right)^{2/3}\left(\frac{\pi}{a_0}\right)^{16/3},$$

$$\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3} \le 109^{2/3}\left(\frac{\pi}{2a_0}\right)^{4/3}.$$

For example, if $a_0=10^3$, then by (14)

$$\left(\frac{6\pi\xi}{a_0^2}\right)^4 \le 7.9\times 10^{-9}, \ \left(\frac{6\pi\eta}{a_0^2}\right)^4 \le 9.7\times 10^{-7},$$

$$\left|6\frac{\pi^2}{a_0^4}\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)\right| \le 6.8\times 10^{-7},$$

$$45\left(\frac{\pi^2}{a_0^4}\right)^2\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)^2 \le 1.4\times 10^{-10},$$

$$\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3} \le 4.2\times 10^{-3}.$$

If $a_0 = 10^4$,then by (14)

$$\left(\frac{6\pi\xi}{a_0^2}\right)^4 \le 7.9\times 10^{-13},\quad \left(\frac{6\pi\xi}{a_0^2}\right)^4 \le 9.7\times 10^{-11},$$

$$\left|6\frac{\pi^2}{a_0^4}\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)\right| \le 3.2\times 10^{-10},$$

$$45\left(\frac{\pi^2}{a_0^4}\right)^2\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)^2 \le 6.5\times 10^{-16},$$

$$\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3} \le 2\times 10^{-4},$$

If $a_0 = 10^5$, then

$$\left(\frac{6\pi\xi}{a_0^2}\right)^4 \le 7.9\times 10^{-17},\quad \left(\frac{6\pi\xi}{a_0^2}\right)^4 \le 9.7\times 10^{-15},$$

$$\left|6\frac{\pi^2}{a_0^4}\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)\right| \le 1.5\times 10^{-13},$$

$$45\left(\frac{\pi^2}{a_0^4}\right)^2\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3}(\eta^2-\xi^2)^2 \le 3\times 10^{-21},$$

$$\left(\frac{9\pi^2}{a_0^4}\right)^{2/3}(\eta^2+\xi^2)^{2/3} \le 9\times 10^{-6}.$$

In the polar coordinates $\xi = r\cos\varphi, \eta = r\sin\varphi$ equation (13) becomes

$$\Delta u_0(r,\varphi) + \frac{1}{r}\frac{\partial u}{\partial r} + \lambda^2|C_1|^2\left(\frac{a_0^4}{9\pi^2}\right)^{2/3} r^{-4/3}u_0(r,\varphi) = 0. \tag{15}$$

By the separation of variables $u_0 = u_1(r)u_2(\varphi)$ from (15) we obtain

$$\frac{u_1''}{u_1} + \frac{1}{r}\frac{u_1'}{u_1} + \lambda_0^2 r^{-4/3} = \beta, \tag{16}$$

$$u_2'' + \beta u_2 = 0,$$

where $\beta \ge 0$ is some constant and

$$\lambda_0^2 = \lambda^2 |C_1|^2 \left(\frac{a_0^4}{9\pi^2}\right)^{2/3}.$$

Suppose $,\varphi \le \varepsilon_0$, $\varepsilon_0^4 \approx 0$, then for $\beta = 0$, $u_2 = A\varphi$ where A is some constant, which will be calculated from the condition

$$\int_0^{\varepsilon_0} \int_0^{a_0/2} r\,|u|^2\, d\varphi dr = 1. \quad (17)$$

We can rewrite the first equation of (16) in the form

$$u_1'' + \frac{1}{r} u_1' + \lambda_0^2 r^{-4/3} = 0. \quad (18)$$

By the notation $r^{1/3} = t$, equation (18) becomes

$$u_1'' + t^{-1} u_1' + 9\lambda_0^2 u_1 = 0.$$

The solution of this equation is $u_1(t) = I_0(3\lambda_0 t)$ and hence the solution of (18) will be [5, 15]

$$u_1(r) = I_0(3\lambda_0 r^{1/3}), \quad (19)$$

where I_0 is Bessel's function.

Consequently, we can calculate the spectrum of the equation (18)by the boundary condition $I_0(3\lambda_0(\frac{a_0}{2})^{1/3}) = 0$.

By using Maple and formulas (9) one obtains

$$\Big|\int_a^{k^{-1}} t^{-1/3}(t^2 - a^2)^{-1/3}(t^2 - b^2)^{-1/3} dt\Big| = 0.342848,$$

$$|C| = |a_3 - a_2|/0.342848, \quad |C_1| = k^{2/3}\frac{|C|}{C_0} \approx 2^{2/3}10^{-1/3}\frac{|a_3 - a_2|}{a_0}, \quad (20)$$

$$\lambda_n^2 = \frac{\lambda_0^2}{|C_1|}\left(\frac{3\pi}{a_0^2}\right)^{4/3} = (10\pi^2)^{2/3}\frac{c_n^2}{6^{2/3}}\frac{a_0^{-4/3}}{|a_3 - a_2|^2}, \quad n = 1, 2, 3, \ldots$$

where c_n are zeros of Bessel's function I_0[15]

$$c_n \approx \frac{3\pi}{4} + n\pi,$$

$$c_1 \approx 2.4, \; c_2 \approx 5.5, \;\; c_3 \approx 8.7, \;\; c_4 \approx 11.7, \;\; c_5 \approx 14.9, \ldots$$

The constant A will be calculated from the formula (17)

$$\int_0^{\varepsilon_0} \int_0^{a_0/2} r\,|u|^2\, d\varphi dr = A^2\, \varepsilon_0^3/3 \int_0^{a_0/2} r|I_0^2(3\lambda_0 r^{1/3})|^2 dr = 1.$$

Note 1. As we have symmetry, then in the area$D_{b_0-\varepsilon_0} = \{-a_0/2 \le \xi \le a_0/2,$ $b_0 - \varepsilon_0 \le \eta \le b_0\}$the solutions of the Problem 2 will be the similar to the solutions of equation (18).

Now, let us consider (11) in the area D_ε near the line $\xi = 0$ with the conditions

$$\left(\frac{6\pi\xi}{a_0^2}\right)^2 \approx 0, \qquad \iint_{D_\varepsilon} |u|^2 d\xi d\eta = 1, \tag{21}$$

where $D_\varepsilon = \{-\varepsilon \le \xi \le \varepsilon; \quad 0 \le \eta \le b_0\}$, ε is sufficiently small. For example, if $\varepsilon = 10^{-4},\ a_0 = 10^{-3}$, then $\left(\frac{6\pi\xi}{a_0^2}\right)^2 \le 4.10^{-18}$.

By the conditions (21), (11) takes the form

$$th^{4/3}\left(\frac{3\pi\eta}{a_0^2}\right)\Delta u_0(\xi,\eta) + \lambda^2|C_1|^2 u_0(\xi,\eta) = 0. \tag{22}$$

In (22) we can suppose $th^2\left(\frac{3\pi\eta}{a_0^2}\right) \approx \left(\frac{3\pi\eta}{a_0^2}\right)^2$, then the equation (22) may be rewritten as

$$\Delta u_0(\xi,\eta) + \lambda^2|C_1|^2\left(\frac{a_0^2}{3\pi}\right)^{4/3}\eta^{-4/3}u_0(\xi,\eta) = 0. \tag{23}$$

By the separation of variables $u_0(\xi,\eta) = u_1(\xi)u_2(\eta)$ from (23) we obtain

$$\Delta u_1(\xi) + \beta u_1(\xi) = 0, \ \ \beta \ge 0, \tag{24}$$

$$\Delta u_2(\eta) + (\lambda_0^2\eta^{-4/3} - \beta)u_2(\eta) = 0, \tag{25}$$

where

$$\lambda_0^2 = \lambda^2|C_1|^2\left(\frac{a_0^2}{3\pi}\right)^{4/3}. \tag{26}$$

Here we suppose $\beta = 0$, hence (24) gives $u_1 = B(a_0/2 - \xi)$ (B is constant, which will be determined from condition (21)). The solution of (25) will be represented in terms of Bessel's function $I_{3/2}$ [5,15]

$$u_1(\eta) = \sqrt{\eta}I_{3/2}(3\lambda_0\eta^{1/3}), \tag{27}$$

where

$$I_{3/2}(3\lambda_0\eta^{1/3}) = \sqrt{\frac{2}{\pi}}(3\lambda_0)^{-3/2}\eta^{-1/2}\sin(3\lambda_0\eta^{1/3}) - \sqrt{\frac{2}{\pi}}(3\lambda_0)^{-1/2}\eta^{-1/6}\cos(3\lambda_0\eta^{1/3}). \tag{28}$$

(27)and (28) gives

$$u_1(\eta) = \sqrt{\frac{2}{\pi}}(3\lambda_0)^{-3/2}\left[\sin(3\lambda_0\eta^{1/3}) - 3\lambda_0\eta^{1/3}\cos(3\lambda_0\eta^{1/3})\right]$$

The eigenvalues of Problem 2 will be found from the boundary condition

$$\sin(3\lambda_0(b_0)^{1/3}) - 3\lambda_0(b_0)^{1/3}\cos(3\lambda_0(b_0)^{1/3}) = 0,$$

where $b_0 = \frac{5a_0}{3}$.

Consequently, $3\lambda_0(\frac{5a_0}{3})^{1/3}$ will be zeros of Bessel's function $I_{_{3/2}}(3\lambda_0\eta^{1/3})$ and the spectrum of (25)could be determined by using Maple and formulas (20), (26),

$$3\lambda_0(\frac{5a_0}{3})^{1/3} = d_n,$$

$$\lambda_n^2 = \frac{\lambda_0^2}{|C_1|}\left(\frac{3\pi}{a_0^2}\right)^{4/3} = (10\pi^2)^{2/3}\frac{d_n^2}{20^{2/3}}\frac{a_0^{-4/3}}{|a_3-a_2|^2}, \quad n = 1,2,3,\ldots \tag{29}$$

where d_n are zeros of Bessel's function $I_{_{3/2}}$[15]

$$d_n \approx \frac{3\pi}{2} + n\pi$$

$$d_1 \approx 4.4934, \;\; d_2 \approx 7.7252, \;\; d_3 \approx 10.9041, \;\; d_4 \approx 14.0662, \;\; d_5 \approx 17.2208\ldots$$

The constant B will be calculated from the formula (21)

$$\iint\limits_{D_\varepsilon} |u|^2 d\xi d\eta = B^2\frac{a_0^2\varepsilon}{2}\int\limits_0^{b_0} \eta\left[I_{3/2}(3\lambda_0\eta^{1/3})\right]^2 d\eta = 1. \tag{30}$$

Note 2. The functions I_0 and $I_{3/2}$ have the following asymptotics [5,15]

$$I_\nu(3\lambda_0 r^{1/3}) \approx \sqrt{\frac{2}{3\pi\lambda_0 r^{1/3}}}\cos\left(3\lambda_0 r^{1/3} - \nu\frac{\pi}{2} - \frac{\pi}{4}\right), \;\; \nu = 0, 3/2.$$

According to (13), (15), (19), (20), (23),(27),(29) we conclude.

Conclusion

1. Near the boundary $\eta = 0$ and $\eta = b_0$ the solutions of the Problem 2 are given by

$$u_{n_1}(\xi,\eta) = A_{n_1}\mathrm{arctg}\frac{\eta}{\xi}I_0(3\lambda_0(\eta^2+\xi^2)^{1/3}), \tag{31}$$

where

$$\begin{aligned} \lambda_0^2 &= \lambda_{n_1}^2|C_1|^2\left(\frac{a_0^4}{9\pi^2}\right)^{2/3}, \quad |C_1| \approx 2^{2/3}10^{-1/3}\frac{|a_3-a_2|}{a_0}, \\ \lambda_{n_1}^2 &= (10\pi^2)^{4/3}\frac{c_{n_1}^2}{6^{2/3}}\frac{a_0^{-4/3}}{|a_3-a_2|^2}, \quad n_1 = 1,2,3,\ldots, \end{aligned} \tag{32}$$

λ_{n_1} is the spectrum of Problem 1 and c_{n_1} are zeros of Bessel's function I_0, A_{n_1} are the definite constants

$$A_{n_1}^2 = (3/\varepsilon_0^3)\left(\int\limits_0^{a_0/2} rI_0^2(3\lambda_0 r^{1/3})dr\right)^{-1}. \tag{33}$$

2. Near the line $\xi = 0$ the solutions of Problem 2 will be given by

$$u_{n_2}(\xi,\eta) = B_{n_2(}a_0/2\xi)\sqrt{\eta}I_{3/2}(3\lambda_0\eta^{1/3}), \tag{34}$$

where

$$\lambda_0^2 = \lambda_{n_1}^2|C_1|^2\left(\frac{a_0^4}{9\pi^2}\right)^{2/3}, \quad |C_1| \approx 2^{2/3}10^{-1/3}\frac{|a_3-a_2|}{a_0},$$
$$\lambda_{n_2}^2 = (10\pi^2)^{4/3}\frac{d_{n_2}^2}{20^{2/3}}\frac{a_0^{-4/3}}{|a_3-a_2|^2}, \quad n_2 = 1,2,3,\dots, \tag{35}$$

where λ_{n_2} is the spectrum of Problem 1, d_{n_2}, $n_2 = 1,2,3,\dots$, are zeros of Bassel's function $I_{3/2}$,B_{n_2} are the definite constants

$$B_{n_2}^2 = \left(\frac{2}{a_0^2\varepsilon}\right)\left(\int_0^{b_0}\eta\left[I_{3/2}(3\lambda_0\eta^{1/3})\right]^2 d\eta\right)^{-1}. \tag{36}$$

The energy of the particle will be calculated from the formulas [2,14,16]

$$E_{n_1} = \lambda_{n_1}^2\frac{h^2}{2m} = \frac{4.5\times10^2}{3}(10\pi^2)^{4/3}\frac{c_{n_1}^2}{6^{2/3}}\frac{a_0^{-4/3}}{|a_3-a_2|^2}\times10^{-20}, \quad n_1 = 1,2,3,\dots,$$
$$E_{n_2} = \lambda_{n_2}^2\frac{h^2}{2m} = \frac{4.5\times10^2}{3}(10\pi^2)^{4/3}\frac{d_{n_2}^2}{20^{2/3}}\frac{a_0^{-4/3}}{|a_3-a_2|^2}\times10^{-20}, \quad n_2 = 1,2,3,\dots, \tag{37}$$

Below, on Table 1 the numerical results are given for $|a_3 - a_2| = 10^{-10}$ by using Maple

$a_0 = 10^4$	ε	λ_0^2		$\lvert E\rvert$(eV)
$c_1 = 2.4$	10^{-3}	0.046745	$A \approx \sqrt{6}\times10^{-1}$	0.553961
$d_1 = 4.49$	10^{-6}	0.073319	$B \approx 2\times10^{-8}$	0.8688876

Table 1.

Note 1. As $f(w)$ is a holomorphic function, we can continue it through the sides a_2a_3 and a_6a_5. Hence, we obtain the quantum billiard in the hexagonal rug (Fig.3). Consequently, for this problem equation (5) will be valid. So, the solutions will be the same as for the hexagon and given by formulas (31),(32), (33),(34),(35),(36), (37). The boundary conditions will depend on the number of cells in the rug.

Also, we can continue $f(w)$ through the sides a_3a_4,a_4a_5 and a_6a_1, a_1a_2. So we obtain billiard in the hexagonal flower (Fig. 4), where energy levels of particles will be calculated by formula (37).

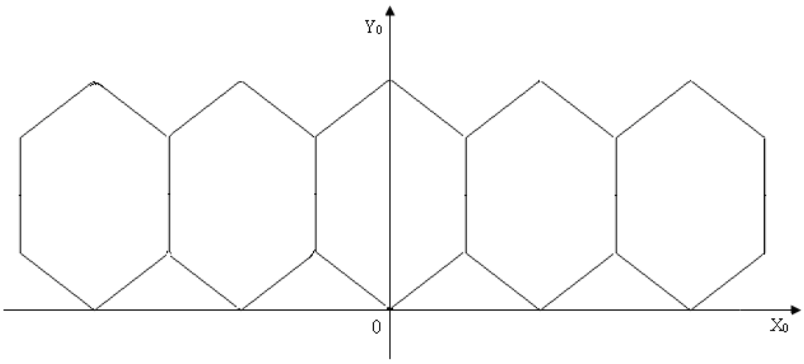

Fig. 3. The hexagonal rug

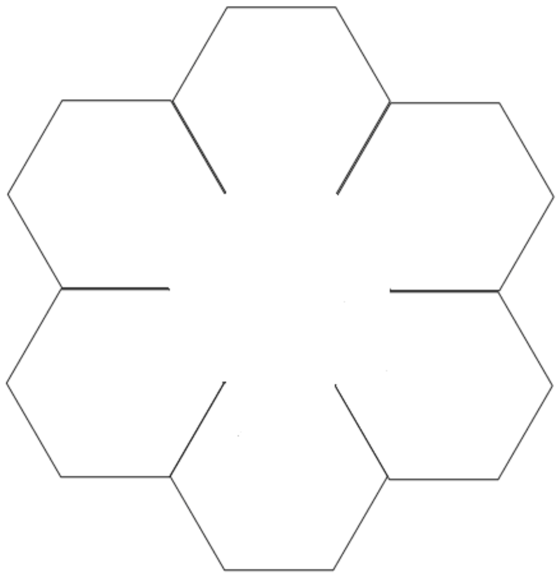

Fig. 4. Hexagonal flower

Note 2. Let us consider a half of the hexagon $D' = a_1a_2a_3a_4$ (Fig.1). For this area we can consider the following problem

Problem 3. To find a real function $u(x_0, y_0)$ in D' having second order derivatives, satisfying the equation

$$\Delta u(x_0, y_0) + \lambda^2 u(x_0, y_0) = 0,$$

and the boundary conditions

$$u\big|_{a_1a_4} = 0, \quad u\big|_{a_2a_3} = 0,$$

where λ is the constant to be determined.

The function $f(w)$ map the area D' at the rectangle D'_0 with the vertexes $(0,0)$, $(a_0/2, 0)$, $(a_0/2, b_0), (0, b_0)$. We can continue $f(w)$ through the sides a_1a_2 and a_3a_4 (step by step)and obtain the mapping of the hexagon with the hexagonal hall at the rectangle $D'_0 = \{0 \leq \xi \leq a_0/2; 0 \leq \eta \leq 6b_0\}$ (Fig. 5). So we can consider the billiard in the hexagon with the hexagonal hall. In this cases equation (11) will be valid. for the area $D'_\varepsilon = \{0 \leq \xi \leq a_0/2; 0 \leq \eta \leq \varepsilon\}$the equation (11) may be rewritten as

$$\Delta u_0(\xi, \eta) + \lambda^2 |C_1|^2 \left(\frac{a_0^2}{3\pi}\right)^{4/3} \xi^{-4/3} u_0(\xi, \eta) = 0,$$

This equation can be solved in analogy with (23) with the boundary condition

$$I_{3/2}(3\lambda_0(a_0/2)^{1/3}) = 0.$$

Near the line $\eta = 0$ we obtain the following solutions

$$u_{n_2}(\xi, \eta) = B_{n_2}\sqrt{\xi} I_{3/2}(3\lambda_0 \xi^{1/3}), \quad n_2 = 1, 2, 3, \ldots,$$

where λ_0 and B_{n_2} are given by (35) and (36).

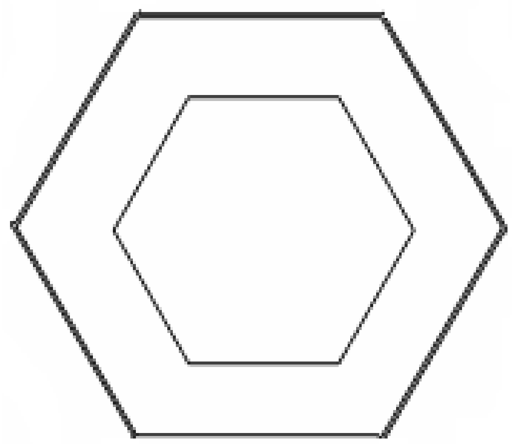

Fig. 5. Hexagon with the hexagonal hall

Note 3. By using the solutions of Problem 2 it is easy to obtain the solutions of the same problem for the particle trapped in 3D potential box of the hexagonal configuration $D \times \{0 \leq \zeta \leq c_0\}$. This problem can be solved in analogy with Problem 2 and the solutions will be given by

$$U = \sqrt{\frac{2}{c_0}} u_n(\xi, \eta) sin \frac{\pi n_1}{c_0}, \quad n, n_1 = 1, 2, 3, \ldots,$$

where $u_n(\xi, \eta)$ are given by (31),(32) or (34),(35) and corresponding energy eigenvalues are given by

$$E_n = \lambda_n^2 \frac{h^2}{2m} \frac{n_1^2}{c_0^2}, \quad n, n_1 = 1, 2, 3, \ldots$$

Note 4. Problem 1 could also be applied for the description of the growth of the single crystal of hexagonal configuration [12].

Discussion. The complete system of solutions of Problem 2 will be found if equation (11) or the equation

$$u_1'' + t^{-1} u_1' + 9(\lambda_0^2 - \beta t^4) u_1 = 0.$$

is solved globally.

Example. Now we consider the electron transport in graphene and find energy levels of the electron. “As an emergent electronic material and model system for condensed-matter physics, graphene and its electrical transport properties have become a subject of intense focus. By performing low-temperature transport spectroscopy on single-layer and bilayer graphene, we observe ballistic propagation and quantum interference of multiply reflected waves of charges from normal electrodes and multiple Andreev reflections from superconducting electrodes, thereby realizing quantum billiards in which scattering only occurs at the boundaries.”(“Phase-Coherent Transport in Graphene Quantum Billiards” (Science, Vol. 317, Issue 5844, Pages 1530-1533, 2007).

Graphen is a one-atom thick sheet of carbon atoms arranged in hexagonal rings in which scattering occurs at the boundaries. Hence, we can apply our results (Fig.3). The width of the side of the hexagonal cell is about 0.14×10^{-10} [17, 21].As we have billiard in the hexagonal rug, we can use formulas (31), (32), (33). Here we suppose, that the rug has 7 cells and by using Maple we have obtained the following result (Table 2)

a_0	d	ε	λ_0^2	A	$\|E\|$(eV)
10^4	2.4	10^{-6}	0.046745	$\sqrt{2} \times 10^{-6}$	0.553961

Table 2.

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