Investigation of Quantum Waveguides (Solution of Helmholtz's Equation at any Arbitrary Cross sectional Area)

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Abstract

Introduction: Nowadays extraordinary properties of nano world and economical problems are the reasons for directing techniques toward micro implements, electronic circuits dimensions have been reduced to 10 to 100 nano meters. Moreover microstructures in cells with nano meter dimensions have been investigated by biologists, there are structures in electronic and biology which are very similar to the billiards and the electromagnetic waveguides but their dimensions are in nano meter range, therefore they were called quantum waveguides and billiards.

Aim: In this research billiards and quantum waveguides at any arbitrary cross sectional area have been investigated.

Method: A considerable effort was devoted in solving Helmholtz's equation with two dimensional cross sectional areas. Linear combinations of plane waves or Heller methods for several types of connective and no connective billiards with regular and irregular shapes have been used. Then eigenvalues and eigenvectors were calculated. At the final part by applying a simple method billiard type (chaotic or quiet) in a quantum scale has been realized.

Results and Discussions: In this paper two types of circular and stadium billiards have been studied and by using Heller's method and applying the numerical solution, energy levels together with the function forms have been attained.

Conclusions: This paper shows that Heller's method despite its quickness and simplicity is a very accurate method for finding eigenvalues and eigenvectors. Although in high eigenvalues the calculation is weighted, nevertheless this method is an acceptable computational method for the investigation of quantum nanobilliards such as quantum points.

***Keywords*:** Billiard, Quantum waveguide, Helmholtz's equation, Heller methods

Introduction

Nowadays extraordinary properties of nano world and economical problems are the reasons for directing techniques toward micro implements, electronic circuits dimensions have been reduced to 10 to 100 nano meters. [1] Moreover microstructures in cells with nano

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meter dimensions have been investigated by biologists, there are structures in electronic and biology which are very similar to the billiards and the electromagnetic waveguides but their dimensions are in nano meter range, therefore they were called quantum waveguides and billiards.

A region in space with a defined and closed boundary is called a billiard. This space can be assumed multidimensional but in this study two dimensional billiards in plane space have been investigated. Actually with a physical view these structures are live quantum waveguides and quantum mechanics can be used for their recognitions.

About one hundred years ago Edwin Abott imagined a world with only two dimensions and now his imagination has come through. In fact the two dimensional quantum waveguide and the two dimensional world are the same. The problem of finding the levels for the quantum billiards with desired shapes can be solved by the numerical method not the analytical one. Quantum billiards are very important, nowadays the accuracy of producing electronic instruments is in atomic scale and they are called nano devices. Therefore billiards are suitable models for forecasting and analysing the behaviour of these devices. Imagine a cylindrical waveguide with an arbitrary cross sectional area, to simplify suppose that the cross sectional area does not change along the cylinder. Postulate the rim is full conductive and the existent electromagnetic field is time dependent . Also it is assumed that the above waveguide is filled with a substance with dielectric coefficient of ε and magnetic permeability coefficient of μ. It can be demonstrated that in a such waveguide with constant cross sectional area after establishing marginal circumstances Maxwell's equations would be transformed to Helmholtz's equations. It means

$$(\nabla_t^2 + \gamma^2)\psi = 0 \quad , \quad \gamma^2 = \mu\varepsilon\frac{\omega^2}{c^2} - k^2 \tag{1}$$

Where ω is the wave frequency and k is the wave number. If in the billiards as two dimensional structures the interior potential assumed zero and the billiard walls imagined being hard, Helmholtz's equation is the movement equation and the particles behaviour depends on boundaries shape. According to their boundaries shapes, the billiards can be divided into two groups of regular and irregular ones. In Irregular billiards, the particle behaviour is chaotic in classical limit. In that case it is not possible to find an analytical solution for the particle movement equation. Therefore the numerical methods can be used to obtain energy spectrum.

The purpose of this paper was to present a technique on the basis of a computational method and it has been demonstrated that contrary to its simplicity this technique has superior potency in finding eigenstates and eigenvalues of quantum nanobilliards. In the following part, theory of Heller's method has been presented and at the result and discussion section, by using this method eigenvalues and eigenvectors for two circular and stadium billiards have been obtained. Meanwhile by comparing these results with the analytical ones, various features of billiards for instance their chaotic behaviour has been studied.

Material and Method

As it was mentioned earlier at the introduction, since Schrödinger's equation in a potential well with hard walls would be converted to Helmholtz's equation, for a billiard with an arbitrary shape energy levels can be obtained only by numerical method. The energy spectrum for a particle which is trapped in a billiard can be attained by solving a time independent Schrödinger's equation with proper boundary conditions. The most ordinary case is when the interior potential of a billiard (domain D) is zero and the particle can move freely

and also the potential on the boundary (Γ) is suddenly changing to infinity. In this situation the billiard boundary is called hard boundary. Therefore with this assumption Schrödinger's equation would be

$$(\nabla^2 + k^2)\psi(r) = 0, \qquad r \in D \tag{2}$$

Hard boundary is the reason for Dirichlet boundary conditions:

$$\psi(r)\big|_{r\in\Gamma} = 0 \tag{3}$$

Where, k is the wave number and is equal to $\sqrt{\frac{2ME}{\hbar}}$, M is the mass, E is the accumulated energy and $\hbar$ is equal to Planck's constant divided by 2π.

As it can be seen problem of obtaining energy levels is leading to solving Helmholtz's equation with Dirichlet boundary conditions. When the billiard shape is regular such as circle or square, equation (2) can be separated according to the variables and then can be converted into one dimensional potential well problem which was already solved by analytical method and afterward energy level can be obtained. Generally a function for a particle in the surroundings can be written as a linear sum of a series of basis functions.

$$\psi(r) = \sum_{n=1}^{N} C_n \phi_n \tag{4}$$

If $N\rightarrow\infty$ then $\Psi(r)$ can be calculated with a very high accuracy but it is obvious that computer can do calculation to limited values of N not to infinity. Therefore to be able to obtain accurate $\Psi(r)$ by a limited N, the selected basis function should converge enough. Selected basis functions can be divided into two major groups: E dependent and E independent.

The E independent basis preserves the linearity of the eigenvalues problem, giving a matrix eigenvalues equations which returns many solutions (E_μ, X_μ) at once. With these basis functions if N for the eigenstate is required the dimension of matrix should be greater than or equal to N and this is a major restriction.

The second group can be used if green function (for example eigenstates of H in domain D with different boundary conditions) is known analytically. By using the green function and the points on the boundary Γ, the dimensionality of the problem can be reduced from d to 1- d. Dimension reduction during computations is causing the base numbers for N lessening from $O\left(\frac{V}{\lambda_B^d}\right)$ to $O\left(\frac{A}{\lambda_B^{d-1}}\right)$.

Where, V is the volume of domain D, A is the surface area of region Γ *and* λ_B is the quantum wavelength of particle at the energy of interest.

Boundary Integral Method (BIM) and Plane Wave Decomposition Method (PWDM) are two examples of the second group. Here both methods have been explained in brief. [2] There are four steps which are similar in both methods BIM and PWDM but different in details.

- Selection of basis functions
- Definition of Matrix A
- Method of creating Ψ
- Description of quantum values of S for obtaining energy levels

Plane Wave Decomposition Method (PWDM) was presented by E.J. Heller in 1984. [3] This method is less complicated in comparison to the other methods and moreover is very

powerful in obtaining energy levels of billiards with arbitrary shape. This method is consisted of four following steps.

- Selection of basis functions:

In this method linear sum of plane waves can be used for formation of maximum wave. It means

$$\psi(r) = \sum_{j=1}^{N} C_j Cos\left(k_{xj} y + k_{yj} + \phi_j\right) \quad (5)$$

Where, $k_{xj} = k\ cos\ \theta_j$, $k_{yj} = k\ sin\ \theta_j$, $E = k^2$, N is the number of plain waves for formation of wave functions and ϕ_j is a random phases drawn from the interval [0 , 2π].

If the points on the boundary were distributed uniformly then $\theta_j = 2j\pi/N$ can be used to specify direction angles of wave vectors k. Because the basis functions are the solutions for Schrödinger's equation in domain D therefore appointing boundary conditions are only remaining. The random phases role in basis wave functions are to spread the origin of the plane waves all over the billiard region, and at the same time this results in reducing CPU time by almost a factor of 10.

- Definition of Matrix *A:*

To build matrix A for each arbitrary k, the point which belongs to the boundary surface (Γ) would be taken equal to zero and then at an arbitrary point inside domain D wave function would be given the value of 1. These points are called primary nodes. The forming condition of the matrix is $M \geq N$. These equations are establishing an inhomogeneous set of equations. It means

$$A\ .C\ =\ b \quad (6)$$

A is a matrix with the dimension of M x N and

$$A_{ij}^{(k)} = Cos\left(k_{xj} x_i + k_{yj} y_i + \phi_j\right) \quad (7)$$

Where, C is the coefficients in equation (5) and also it is a vector with the dimension of N. b is a vector which all of its members are zero except one.

Method of creating Ψ

Here it is assumed that $M=N$ and matrix A is a squared matrix. This matrix often posses multitude singularity, therefore to solve equation (6) Singular Value Decomposition method (SVD) should be applied. [4]

Description of quantum values of *S* for obtaining energy levels

After creating an expression for $\Psi(r)$, wave function could be calculated for some points on the boundary except the primary nodes. These points are called secondary nodes. The consequent wave function at the secondary nodes can be used for computation of tension S for this value of k. Tension is the sum of the squares of the wave functions at all the secondary nodes:

$$S(k) = \sum_i \left|\psi(r_i)\right|^2 \quad (8)$$

If k is the eigenvalue of energy then $S(k)$ should be equal to zero. Actually tension has a positive value; therefore problem of finding eigenvalues would be changed to obtaining minimum local tension in an energy interval. Then by using k which was the result of the minimum tensions, values of C_i can be calculated again and afterwards the wave function of eigenstate of the system can be attained. Note that the resulting wave function at this step has

not been normalized and before investigating its properties or its usage the wave function should be normalized directly.

Besides above methods, there are many other methods for the numerical solution of Helmholtz's equation, for example Kaufman's method which uses a limited potential at the billiard wall for transaction from a zero potential zone inside of the billiard to its hard wall. [5] Robnik developed a recording method to convert the irregular billiards to a regular shape. [6] The scaling method was another way which was invented by Vergini and Saraceno in 1995 and it was a combination of Heller's method and the scaling method which was published by Barnet in 2001.[7,8] These methods have been used for the extraction of energy spectrum of the billiards with arbitrary shapes and any of them have their own strength and weakness.

Result and Discussion

A computerized program in Fortran language has been written to solve Helmholtz's equation by the numerical method and the results for ideal shapes have been reported. In this part two types of circular and stadium billiards have been studied and by using Heller's method and applying the numerical solution, energy levels together with the function forms have been attained. Because the circular shape can also be solved by numerical method, this solution could be a reason to prove the validity of this method and the computerized program. The solution of Helmholtz's equation in a circular billiard is a separation method. If Helmholtz's equation was written in the polar system, after solving the problem it can be seen that the radial equation is identical to Bessel's equation and the answer to the angular equation is $e^{-in\theta}$. If the surface area of the billiard would be equal to π, the eigenvalues of energy (k_{nm}) are the roots of Bessel's equation and therefore eigenvalues of energy for the circular billiards can be calculated. Some of the corresponding wave numbers and eigenvalues of energy can be seen in Table 1.

Table 1- For a circle with a radius of 1, the eigenvalues of energy (k_{nm}) are the roots of Bessel function. In this table, some of the corresponding wave numbers and eigenvalues of energy can be seen.

n	1	2	3	4
k_{n0}	2.405	5.520	8.654	11.797
k_{n1}	3.832	7.016	10.173	
k_{n2}	5.136	8.417	11.620	

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In the numerical solution, the following equation is the selected wave function:

$$\psi(r) = \sum_{j=1}^{N} A_j Cos\left(k_{xj} y + k_{yj} + \phi\right) + B_j Cos\left(k_{xj} y + k_{yj} + \phi\right) \qquad (9)$$

Where, $k_{xj} = k \cos\theta_j$, $k_{yj} = k \sin\theta_j$ and $E = k^2$.

About 700 points on the boundary have been chosen and the quantities of the secondary nodes are four times of the primary nodes. Following each calculation and finding the function by using the primary nodes for these points, the tension function can be attained. These results have been shown on Figure 1.Once more the accuracy and the beauty of this method can be proved by comparing minimum points in this diagram with the results in Table 1. The remaining minimum points are related to the solutions with the greater *n* or some types of Bessel's functions greater than 3. The results of solving the problem by the numerical method, the eigenvectors for several eigenvalues, have been plotted in Figure 2.

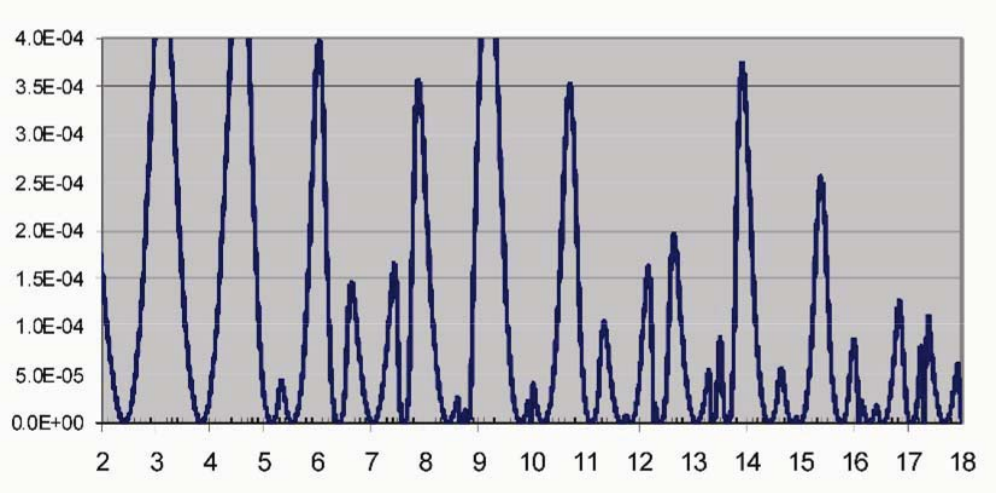

Fig 1- Diagram of tension function (according to k) for the circular billiards.

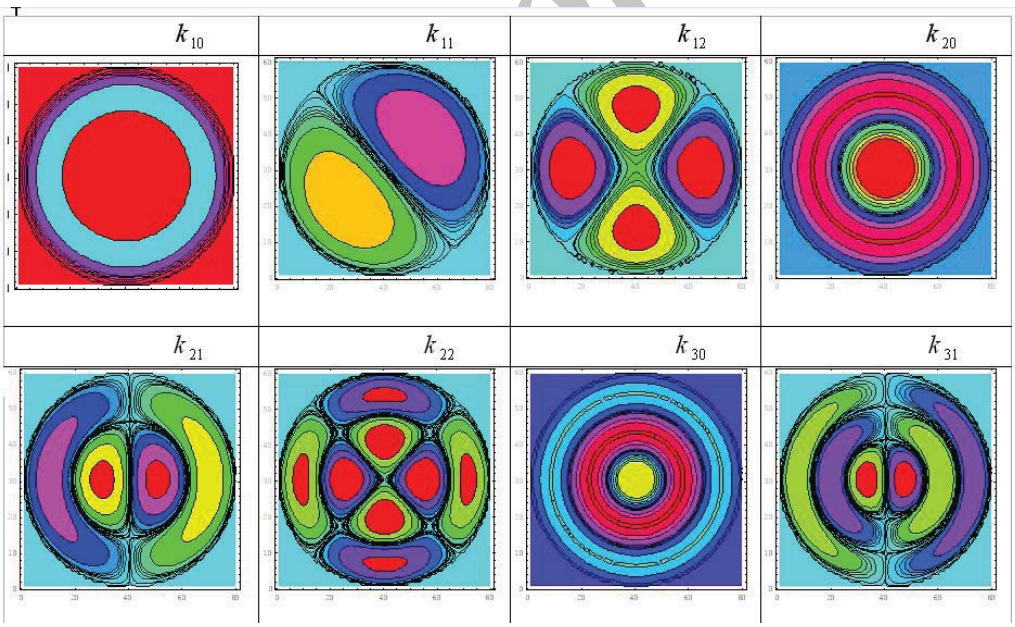

Fig 2-The results of solving the circular billiards problem by numerical method, for several eigenvalues have been plotted.

One of the remarkable results of the figures of Bessel's functions group (in identical Bessel's functions only the values of n are different) is that the figures have shapes which belong to the same group and this endorsing the results. Therefore it can be said that the shape belongs to:

Bessel's group type > 3	when $k = 6.4$
Bessel's group type 2	when $k = 15.2$
Bessel's group type 1	when $k = 16.64$

Another point is the number of peaks which can be obtained by *2mn* formula except for Bessel's group type 1, for this type it is equal to *n*. Therefore

shape of $k = 16.64$	Bessel's group type 1	10 extremum	$n = 5$
shape of $k = 15.2$	Bessel's group type 2	16 extremum	$n = 4$

Considering the above results and proving the quality of the solution method and the written program now is the time to investigate more complicated wave shapes which cannot be solved by the analytical method. Imagine a stadium billiard consisting of two semicircles which are connected by two parallel lines. Stadium boundaries have singularity in places where semicircles are linked to lines. Except radius *R* and the length of joint line *a*, stadium can be expressed according to such parameters like η and the surface area of the billiard *A*, here η is equal to *a/R*. This stadium has two axis of symmetry, vertical and horizontal axis. Therefore it includes minimum of four types of the symmetry, odd-odd, odd-even, even-even and even-odd. Here again Fourier expansion has been assumed as the function and the results would be obtained. At the selected stadium which is used for finding eigenvalues and eigenvectors $\eta = a/R = 0.5$ and surface area is equal to $0.25(\pi+1)$.

The number of primary nodes and *N* value have been presumed 66 and 3 respectively and the quantity of the secondary nodes have been taken four times of the primary ones. The results of the calculations at the secondary nodes, tension, have been plotted in Figure 3. Wide range of *k* values is the reason for dividing the diagram into two diagrams with two different values. Minimal points are clear and they are allowable values of *k* for the billiard with stadium shape. In Table 2 minimum values or indeed eigenvalues have been listed according to the orders which they are situated on the diagram.

Table 2- Minimum values or indeed eigenvalues have been listed according to the orders which they are situated on the diagram of Fi.3.

No.	k	No.	k	No.	k
1	3.91	14	13.16	27	18.4
2	5.56	15	13.31	28	18.14
3	6.815	16	13.92	29	18.6
4	7.445	17	14.28	30	18.66
5	8.12	18	14.973	31	19.18
6	9.36	19	15.06	32	19.675
7	9.765	20	15.34	33	16.917
8	9.845	21	15.96	34	19.9555
9	11	22	16.195	35	20.26
10	11.275	23	16.655	36	20.37
11	11.5	24	16.807	37	20.475
12	12.55	25	16.94	38	21.2
13	12.88	26	17.05		

For determination of the symmetry type, knowing the function shape (eigenvector) and k values is essential. In Figure 4, for this stadium, the stylish function configurations for different values of k have been plotted and besides k values the symmetry types have been specified.

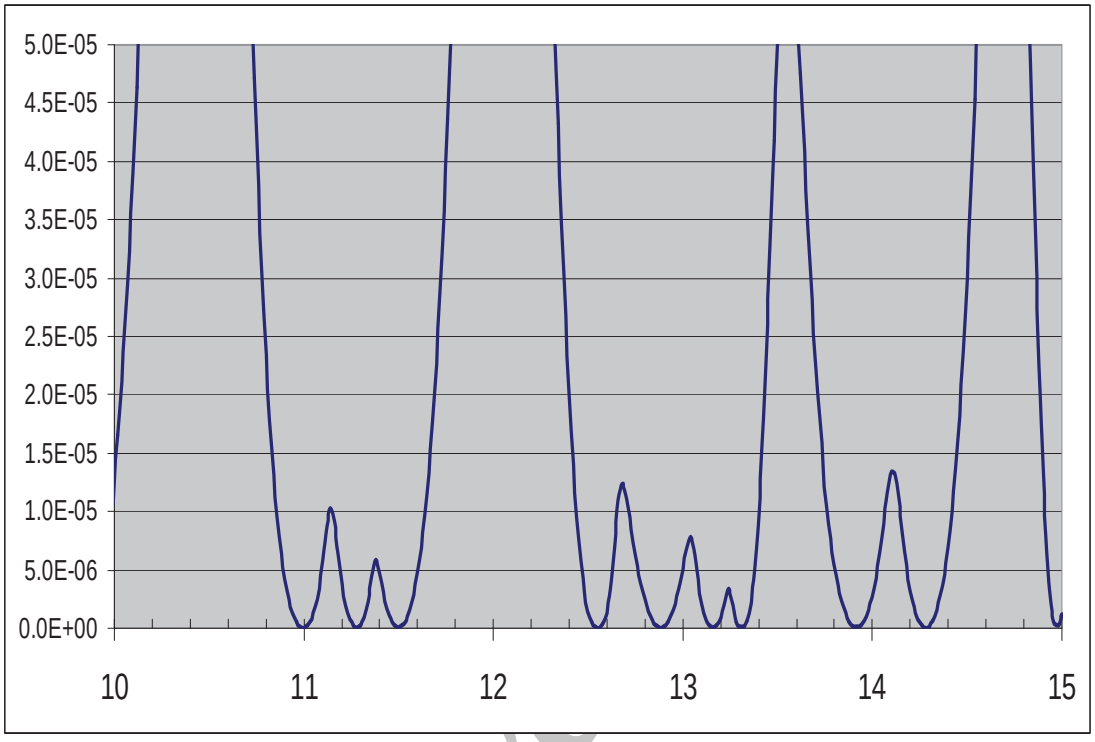

Fig 3- Diagram of tension function (according to k) for the billiard with stadium shape.

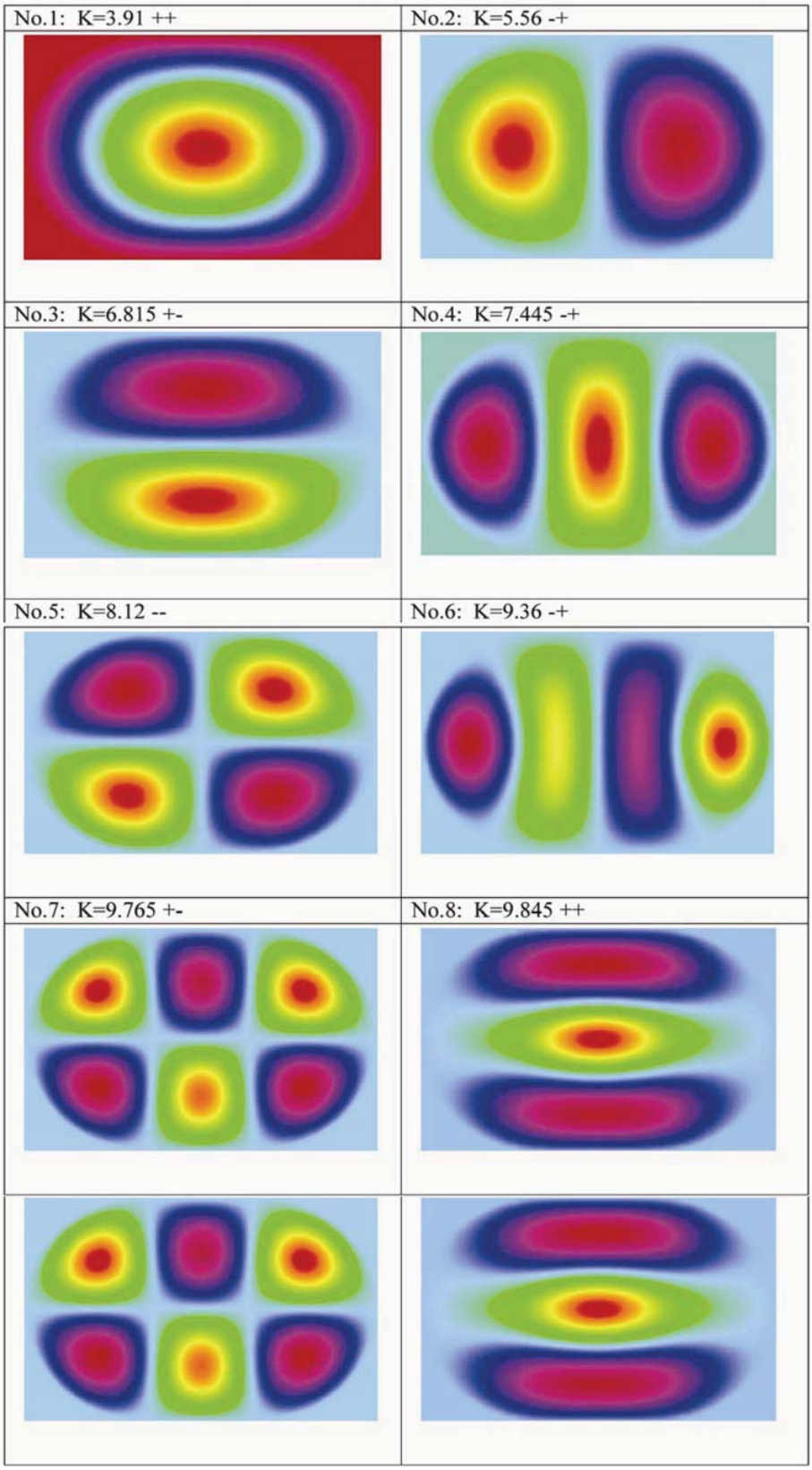

Fig. 4- Several calculated eigenvectors for the billiard with stadium shape.

The orders of symmetries according to their k values have been shown in Table 3.

Table 3- The orders of symmetries according to their k values have been shown.

Symmetry kind	--	-+	+-	++
K number (number of extremums)	5 (4)	2 (2)	3 (2)	1 (1)
K number (number of extremums)	11 (8)	4 (3)	7 (6)	8 (3)
K number (number of extremums)	16 (8)	6 (4)	13 (10)	10 (6)

The values inside of the parenthesis are number of extremums of the functions. As it is clear the first excited state of the symmetry is after the first states of the other symmetries, which shows this type of symmetry has high energy. This is happening in the other excited states of symmetry. The reason that the first excited state symmetry (2)+- is before the first excited state symmetry (3)-+ could be because of the dragging of the shape toward the horizontal direction rather than the vertical state. Therefore the slope of the graph in the horizontal direction for changing the sign is less and it imposes lower energy. For this reason, two states of excited symmetry with extremum number of 8 with 5 numbers difference, one would place in position 11 and the other one in position 16. The values of wave function on the billiard boundary and its behaviour on the border of the stadium billiard and also beauty of its symmetry inside of the stadium, all show sufficient accuracy of this method.

One important question which is discussed after obtaining energy spectrum of different quantum billiards, would be how chaotic appears in the quantum system? In the classical mechanic field the particle movement in some billiards such as the stadium billiard is chaotic, but is the quantum stadium also chaotic? And if it is chaotic, how it is recognizable? There are some different ways for the recognition of being chaotic in the quantum systems such as

- The behaviour of roots curve of the wave function
- The statistic distribution of separation of the billiard levels

Here the first method has been studied in summary. Investigation of roots curve of the wave function is one of the criteria in recognition of a chaotic billiard. If the billiard is in the XY plane and the values of wave function according to one eigenenrgy for the points inside of the billiard to be plotted, roots curve of wave function could be obtained by attaining the intersection points of wave function in the XY plane.

Roots curve of the chaotic billiards and the quiet billiards could be separated by two characters. First, in roots curve of the chaotic billiard there is not any symmetry and it is completely random and the second character is inexistency of any intersection points on the curve in roots curve of the chaotic billiard. It means in the regular billiards, roots curves cross each other but not in the chaotic billiards. Of course it is important to note that there are some regular billiards which their roots curves also do not cross each other, but it is certain that if there is any intersection point that billiard is not chaotic and Helmholtz's equation in a coordinate system can be solved by the separation method. Regarding two billiards which in the fourth part their energy spectrum were obtained, roots curve of the wave function can be seen by the specific colour of roots interval in the plotted figures of the functions. This indicates that the circular billiard is regular and the stadium billiard is chaotic.

Conclusions

In this research nanobilliards and quantum waveguides with any arbitrary cross sectional areas were investigated. Then the numerical solution methods in solving Helmholtz's equation with two dimensional cross sectional areas were introduced and here

after by linear combination of plane waves or Heller's methods, the numerical solution of Helmholtz's equation in some types of connective billiards with circular and stadium shapes were studied. Eigenvalues and eigenvectors of these billiards were calculated and afterwards by considering the number of extremum and the connection between the order of eigenvalues and eigenvectors, the quality of eigenvectors were perused. Then by applying a simple method the billiard type (chaotic or quiet) in the quantum scale was obtained. The results show that Heller's method despite its quickness and simplicity is a very accurate method for finding eigenvalues and eigenvectors. Although in high eigenvalues the calculation is weighted, nevertheless this method is an acceptable computational method for the investigation of quantum nanobilliards such as quantum points.

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