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Microparticles in One-Dimensional, Two-Dimensional and Three-Dimensional Rectangular Potential Holes

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Abstract. Behavior of microparticle in potential hole has been studied. One-dimensional, two-dimensional and three-dimensional potential holes with infinitive deepness (with infinitively high walls) and flat bottom were observed. The stationary case was discussed. The wave function, describing the particle state, probabilities of the particle being in the given hole and its energy, depending on dimensional sizes were determined. For each case the dependencies of the wave function and its squared modulus were presented on one, two and three coordinates, respectively.

Keywords: microparticle, potential hole with infinitively high walls, wave function, stationary case, energy

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1. Introduction

From the beginning of 20th century, the physical theory, describing the movement rules of a microparticle, gives the connections between measured values in microscopic experiments and particle characteristic magnitudes; this theory is called quantum mechanics. Quantum-mechanic regularities control the rules of micro-world physics [1, 2].

For solvation of movement problem in classical physics Newton's second rule is written. To solve it means to find the resolution of the main equation in dynamics, i.e., to determine the position of a particle at the random moment of time. So

$$m\frac{d^2\vec{r}}{dt^2} = \vec{F}(\vec{r}, \frac{d\vec{r}}{dt}, t).$$

If the resultant force is known, the movement rule is determined $\vec{r}(t)$ by solvation of heterogeneous linear differential equation of the second order. The main equation of dynamics assumes that both coordinate and velocity (impulse) were determined simultaneously. The classical particle moves by the certain trajectory.

In microworld physics to describe the movement, the idea of wave function is inserted [3-5]. Generally, it is a complex function and does not have any physical meaning. Instead of this, the squared modulus of the wave function has a physical meaning [3]. The squared modulus of the wave function in the given point of space and at the given moment of time is a density of probability of particle revelation. Let's appoint the wave function, which describes a micro-particle, as $\psi(\vec{r}, t)$. In the volume unit dV, in the vicinity of radius-vector $\vec{r}$ at the t moment of time the probability of particle finding is determined as $|\psi(\vec{r}, t)|^2 dV$ or $|\psi(\vec{r}, t)|^2 = \frac{dW}{dV}$. Function $\psi(\vec{r}, t)$ depends on $\vec{r}$- and t, it is continuously and normalized to unit – $\int |\psi(\vec{r}, t)|^2 dV = 1$.

The main equation of quantum mechanics is Schrödinger equation, which is impossible to take out. It can be justified, but not taken out [6-8]. Based on the understanding of wave package and using the rules of operator arithmetic, let's write the main equation, the solution of which will be the wave function

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + U\psi\ . \qquad (1)$$

The last equation is the main rule of non-relativistic quantum mechanics and is called Schrödinger equation. The given operator ∇^2 in Descartes coordinate system has the following form

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\,.$$

If the potential energy $U(\vec{r},t)$ is known, it means that the probability density of particle finding is known as well.

In general case the potential energy of particle interaction $U(\vec{r},t)$ depends on both coordinates and time.

The presented work is aimed at studying the stationary movement. In this case the interaction potential energy does not depend on time $U(\vec{r})$. It means that the wave function may be presented as a product of two derivatives – $\psi(\vec{r},t) = \psi_r(\vec{r})\cdot\psi_t(t)$. One of these functions depends only on radius, another – only time. Replacing the wave function in Schrödinger equation (1), we will receive

$$i\hbar\frac{\partial\psi_t(t)}{\partial t}\psi_r(\vec{r}) = \psi_t(t) - \frac{\hbar^2}{2m}\nabla^2\psi_r(\vec{r}) + U(\vec{r})\psi_r(\vec{r}))\ .$$

The last expression dividing into $\psi_r(\vec{r})\cdot\psi_t(t)$, we will receive

$$\frac{1}{\psi_t(t)}i\hbar\frac{\partial\psi_t(t)}{\partial t} = \frac{1}{\psi_r(\vec{r})}(-\frac{\hbar^2}{2m}\nabla^2\psi_r(\vec{r}) + U(\vec{r})\psi_r(\vec{r}))\ .$$

Left part of the last equation does not contain coordinates and can be dependent only on time. The right part does not contain time and can be dependent only on coordinates. The obtained equation should describe each moment of time and each point of space. It means that both the right and left sides depend on neither time, nor coordinates. In other words, it is a constant value. This constant value is appointed through E. Thus, the last equation may be written by the following way

$$\frac{1}{\psi_t(t)}i\hbar\frac{\partial\psi_t(t)}{\partial t} = E, \qquad (2)$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_r(\vec{r}) + U(\vec{r})\psi_r(\vec{r}) = E\psi_r.$$

Integrating equation (2), we will receive $\psi_t = Ae^{-\frac{i}{\hbar}Et}$. It is obvious from the aforementioned that the physical meaning is peculiar not for the wave function, but for the square of its module

$$|\psi(\vec{r},t)|^2 = |\psi_r(\vec{r})|^2\cdot|\psi_t(t)|^2 = |\psi_r(\vec{r})|^2\cdot|A|^2\ . \qquad (3)$$

It is obvious from here, that the time dependence of the wave function does not play any role. It means that the stationary movement will be described by an equation, where only the coordinate part of the wave function $\psi_r(\vec{r})$ will contribute. In this case Schrödinger equation will have the following shape (4)

$$\nabla^2\psi_r(\vec{r}) + \frac{2m}{\hbar^2}\left(E - U(\vec{r})\right)\psi_r(\vec{r}) = 0\ . \qquad (4)$$

Equation (4) is known as stationary Schrödinger equation [9, 10].

2. Theoretical Approach: Movement of quantum particle in one-dimensional, two-dimensional and three-dimensional rectangular potential hole

One-dimensional rectangular potential hole. Let's observe infinitively deep (with infinitively high walls), one-dimensional potential hole with flat bottom. Analytically such hole can be presented by the following mode:

$$U(x) = \begin{cases} \infty, x < 0 \\ 0, 0 < x < a \,.. \\ \infty, x > a \end{cases} \quad (5)$$

The start point of energy calculation was chosen in a such way that the hole bottom corresponds to the energy value $E = 0$.

Let's choose the coordinate's axis start point in left marginal part of the hole. Presumably, the hole length is a (Fig. 1).

According to the equation (5) the particle cannot be in the right and left intervals in Fig. 1. It can be only in the middle interval $0 < x < a$

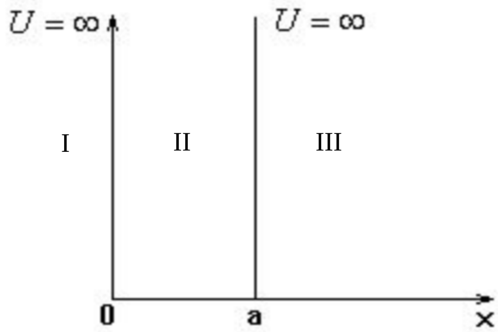

Fig. 1. Particle in one-dimensional potential hole.

Taking into account the equation (5) and the fact that $U = U(x)$ and there is no time dependence, stationary Schrödinger equation can be written as

$$\nabla^2 \psi_r(\vec{r}) + \frac{2m}{\hbar^2}(E - U(x))\psi_r(\vec{r}) = 0.$$

As far as the one-dimensional case is discussed, so $\psi_r = \psi_r(x)$, and $\nabla^2 = \frac{\partial^2}{\partial x^2}$. The last equation will accept the following shape

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left(E - U(x)\right)\psi(x) = 0.$$

In those points of space, where $U(x) = \infty$, the wave function is equal to zero, i.e., in these intervals the particle cannot be found. These intervals correspond to parts I and III, shown in Fig. 1. Therefore, it is necessary to solve the problem in the second interval, where this particle can be.

In the interval $0 < x < a$ Schrödinger equation, will accept the following shape

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}E\psi(x) = 0\,. \quad (6)$$

Let's search the solvation of the equation (6) with this form $\psi(x) = Asin(kx + \varphi_0)$, where we will do the following appointment $k = \frac{\sqrt{2mE}}{\hbar}$. The constant A, parameter k and initial phase φ_0 will be determined by the wave function normalization and marginal conditions respectively. Thus,

$$\psi(x = 0) = 0, it\ is\ followed\ that\ \varphi_0 = 0,$$

$$\psi(x = a) = 0, it\ is\ followed\ that\ \sin(ka) = 0, i.e.\ ka = \pi n, where\ n = 1, 2, 3, \ldots$$

On the other hand, replacing the value of k, we will receive $\frac{\sqrt{2mE}}{\hbar} a = \pi n$, from where we will receive for the wave function and energy

$$E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2 , \quad (7)$$

$$\psi_n(x) = Asin\left(\frac{\pi n}{a} x\right) . \quad (8)$$

From the normalization condition of the wave function, it is known that $\int_0^a |\psi_n(x)|^2 dx = 1$. Replacing the equation (8) we will receive

$$\int_0^a A^2 sin^2\left(\frac{\pi n}{a} x\right) dx = 1.$$

To calculate the last integral, let's do the replacement of variable: $\frac{\pi n}{a} x \equiv z$. In this case we will receive

$$A^2 \frac{a}{\pi n} \int_0^{\pi n} sin^2 z\, dz = 1.$$

Calculating this integral we will determine A

$$A = \sqrt{\frac{2}{a}} \quad (9).$$

Therefore, from the formulae (7)-(9) we will obtain that in infinitively deep rectangular potential hole the wave function, describing the particle state and energy have the following shapes

$$\psi_n(x) = \sqrt{\frac{2}{a}} sin\left(\frac{\pi n}{a} x\right), and\ E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2, where\ n = 1, 2, 3, \ldots \quad (10)$$

The parameter n is called quantum number.

Two-dimensional rectangular potential hole. Now let's consider the case, when the particle is in two-dimensional rectangular hole with infinitively high walls. Coordinates of a particle x, y change in interval $0 < x < a, 0 < y < b$, where values a and b are the sizes of the potential hole. The shape of two-dimensional potential hole is presented in Fig. 2.

In this case the potential hole analytically can be presented in the following form

$$U(x,y) = \begin{cases} \infty, if \begin{cases} x < 0 \\ y < 0 \end{cases} \\ 0, if \begin{cases} 0 < x < a \\ 0 < y < b \end{cases} \\ \infty, if \begin{cases} x > a \\ y > b \end{cases} \end{cases} \quad (11)$$

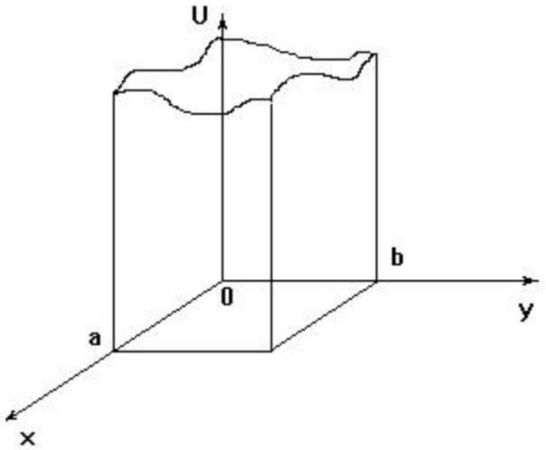

Fig. 2. Particle in two-dimensional potential hole.

The particle can be only in interval $0 < x < a, 0 < y < b$, where stationary Schrödinger equation will accept the following shape

$$\frac{d^2\psi(x,y)}{dx^2} + \frac{d^2\psi(x,y)}{dy^2} + \frac{2m}{\hbar^2} E\psi(x,y) = 0 \quad (12)$$

Like one-dimensional case the solution of the equation (11) is searched in the following way – the values of constants $\psi_n(x,y) = Asin(k_1 x + \varphi_{01}) \cdot sin(k_2 y + \varphi_{02})$: k_1, k_2, φ_{01}, φ_{02} are determined from border conditions of two-dimensional wave function $\psi_n(x,y)$. Those are

$$\psi_n(0,y) = 0 \implies sin\varphi_{01} = 0 \implies \varphi_{01} = 0$$
$$\psi_n(x,0) = 0 \implies sin\varphi_{02} = 0 \implies \varphi_{02} = 0$$
$$\psi_n(a,y) = 0 \implies sink_1 a = 0 \implies k_1 a = \pi n_1$$
$$\psi_n(x,b) = 0 \implies sink_2 b = 0 \implies k_2 b = \pi n_2$$

Thus, the two-dimensional wave function will turn into

$$\psi_n(x,y) = Asin\left(\frac{\pi n_1}{a} x\right) \cdot sin\left(\frac{\pi n_2}{b} y\right), \quad (13)$$

Where quantum numbers are $n_1, n_2 = 1, 2, 3, ...$ The value of constant A is determined by normalization of the wave function

$$\int_0^a \int_0^b |\psi_n(x,y)|^2 \, dydx = 1 \implies \int_0^a \int_0^b sin^2\left(\frac{\pi n_1}{a} x\right) \cdot sin^2\left(\frac{\pi n_2}{b} y\right) A^2 \, dy \, dx = 1.$$

Calculating the mentioned double integral, the following value for constant A, will be received

$$A = \sqrt{\frac{4}{ab}} \; . \quad (14)$$

If to replace the wave function by the shape (13) in Schrödinger equation (12), the following equation will be received for the energy:

$$\frac{2m}{\hbar^2}E = (\frac{\pi n_1}{a})^2 + (\frac{\pi n_2}{b})^2,$$
$$E_{n_1,n_2} = \frac{\pi^2\hbar^2}{2m}(\frac{{n_1}^2}{a^2} + \frac{{n_2}^2}{b^2}) \ . \quad (15)$$

Taking into account the equations (13)-(15), the wave function, describing the particle in two-dimensional potential hole, and its energy will obtain the following forms

$$\psi_n(x,y) = \sqrt{\frac{4}{ab}} sin\left(\frac{\pi n_1}{a}x\right) \cdot sin\left(\frac{\pi n_2}{b}y\right), and\ E_{n_1,n_2} = \frac{\pi^2\hbar^2}{2m}\left(\frac{{n_1}^2}{a^2} + \frac{{n_2}^2}{b^2}\right), where\ n_1, n_2 = 1, 2, 3, .. \quad (16)$$

Three-dimensional rectangular potential hole. Let's discuss the case, when the particle is in three-dimensional rectangular potential hole with infinitively high walls. Coordinates of a particle x, y, z change in interval $0 < x < a, 0 < y < b, 0 < z < c$, where the values of a, b and c are the sizes of the potential hole. The shape of three-dimensional potential hole is presented in Fig. 3.

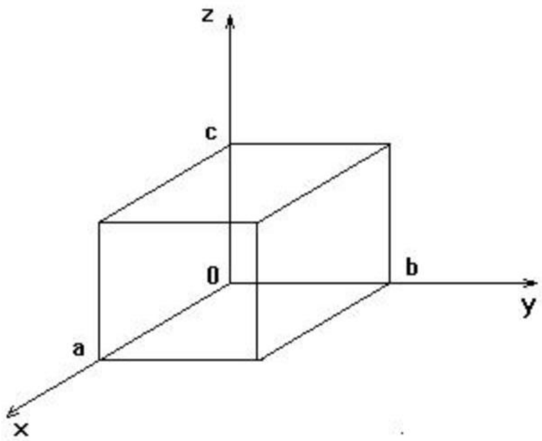

Fig. 3. Particle in three-dimensional potential hole.

In this case the potential hole analytically may be presented in the following form

$$U(x,y,z) = \begin{cases} \infty, if \begin{cases} x < 0 \\ y < 0 \\ z < 0 \end{cases} \\ 0, if \begin{cases} 0 < x < a \\ 0 < y < b \\ 0 < z < c \end{cases} . \\ \infty, if \begin{cases} x > a \\ y > b \\ z > c \end{cases} \end{cases} \quad (17)$$

The particle can be only in the interval $0 < x < a, 0 < y < b, 0 < z < c$, where stationary Schrödinger equation can accept the following shape

$$\frac{d^2\psi(x,y,z)}{dx^2} + \frac{d^2\psi(x,y,z)}{dy^2} + \frac{d^2\psi(x,y,z)}{dz^2} + \frac{2m}{\hbar^2}E\psi(x,y,z) = 0 \ . \quad (18)$$

Like one-dimensional and two-dimensional cases, the solution of the equation (18) is searched in the following way – $\psi_n(x, y, z) = Asin(k_1x + \varphi_{01}) \cdot sin(k_2y + \varphi_{02}) \cdot \sin(k_3x + \varphi_{03})$. The values of the constants k_1, k_2, k_3 φ_{01}, φ_{02}, φ_{03} are determined from the border conditions of three-dimensional wave function. Those are

$$\psi_n(0, y, z) = 0 \Rightarrow sin\varphi_{01} = 0 \Rightarrow \varphi_{01} = 0$$
$$\psi_n(x, 0, z) = 0 \Rightarrow sin\varphi_{02} = 0 \Rightarrow \varphi_{02} = 0$$
$$\psi_n(x, y, 0) = 0 \Rightarrow sin\varphi_{03} = 0 \Rightarrow \varphi_{03} = 0$$
$$\psi_n(a, y, z) = 0 \Rightarrow sink_1a = 0 \Rightarrow k_1a = \pi n_1$$
$$\psi_n(x, b, z) = 0 \Rightarrow sink_2b = 0 \Rightarrow k_2b = \pi n_2$$
$$\psi_n(x, y, c) = 0 \Rightarrow sink_3c = 0 \Rightarrow k_3c = \pi n_3$$

Thus, the three-dimensional wave function will turn into

$$\psi_n(x, y, z) = Asin(\frac{\pi n_1}{a}x) \cdot sin(\frac{\pi n_2}{b}y) \cdot sin(\frac{\pi n_3}{c}z) , \tag{19}$$

Where three quantum numbers are $n_1, n_2, n_3 = 1, 2, 3, ...$ The value of the constant of A in the equation (18) is determined by the normalization of the wave function

$$\int_0^a\int_0^b\int_0^c A^2 sin^2\left(\frac{\pi n_1}{a}x\right) \cdot sin^2\left(\frac{\pi n_2}{b}y\right) sin^2\left(\frac{\pi n_3}{c}z\right) dzdydx = 1.$$

Calculating the mentioned triple integral, the value of A constant will be equal to

$$A = \sqrt{\frac{8}{abc}} \tag{20}$$

If to replace the wave function (19) in Schrödinger equation (18), the following equation for the energy will be obtained

$$\frac{2m}{\hbar^2}E = (\frac{\pi n_1}{a})^2 + (\frac{\pi n_2}{b})^2 + (\frac{\pi n_3}{c})^2,$$
$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2m}\left(\frac{{n_1}^2}{a^2} + \frac{{n_2}^2}{b^2} + \frac{{n_3}^2}{c^2}\right) . \tag{21}$$

Taking into account the equations (19)-(21) the wave function, describing the particle in three-dimensional potential hole, and its energy will have the shapes

$$\psi_n(x, y, z) = \sqrt{\frac{8}{abc}} sin\left(\frac{\pi n_1}{a}x\right) \cdot sin\left(\frac{\pi n_2}{b}y\right) \cdot sin\left(\frac{\pi n_3}{c}z\right), and$$
$$E_{n_1,n_2,n_3} = \frac{\pi^2\hbar^2}{2m}\left(\frac{{n_1}^2}{a^2} + \frac{{n_2}^2}{b^2} + \frac{{n_3}^2}{c^2}\right), where\ n_1, n_2, n_3 = 1, 2, 3, ... \tag{22}$$

Density of the probability of the particle to be in one-dimensional, two-dimensional and three-dimensional rectangular potential hole with infinitively high walls is determined by the formula

$$dW = |\psi(\vec{r})|^2 dV , \tag{23}$$

where the value of $|\psi(\vec{r})|^2$ can be determined through the formulae (10), (16) and (22) respectively.

Via MATLAB program software it has been written a program, throughout which the dependencies of the squared moduli of the wave functions in both discussed cases on coordinates are constructed for the different values n_1, and n_1, n_2 respectively (Fig. 4 and Fig. 5).

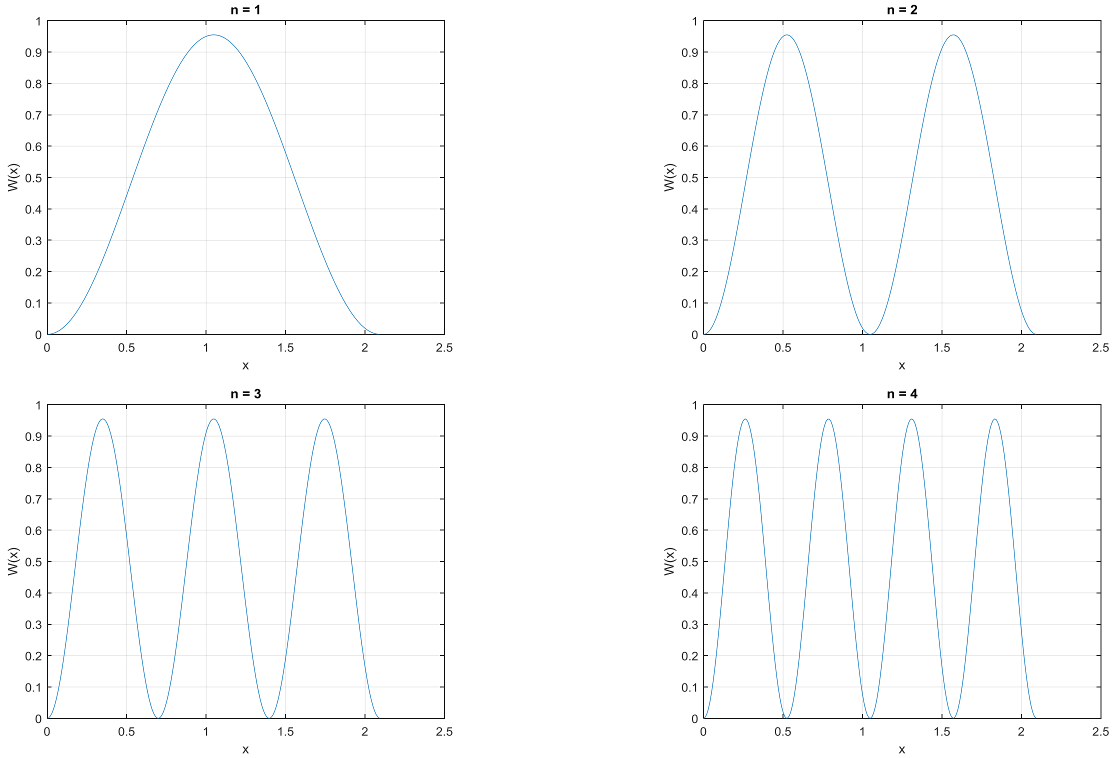

Fig. 4. The distribution of the probability of the particle to be in one-dimensional, rectangular potential hole with infinitively high walls for $n = 1,2,3,4$. Hole length was equal to $a = 2\pi/3$.

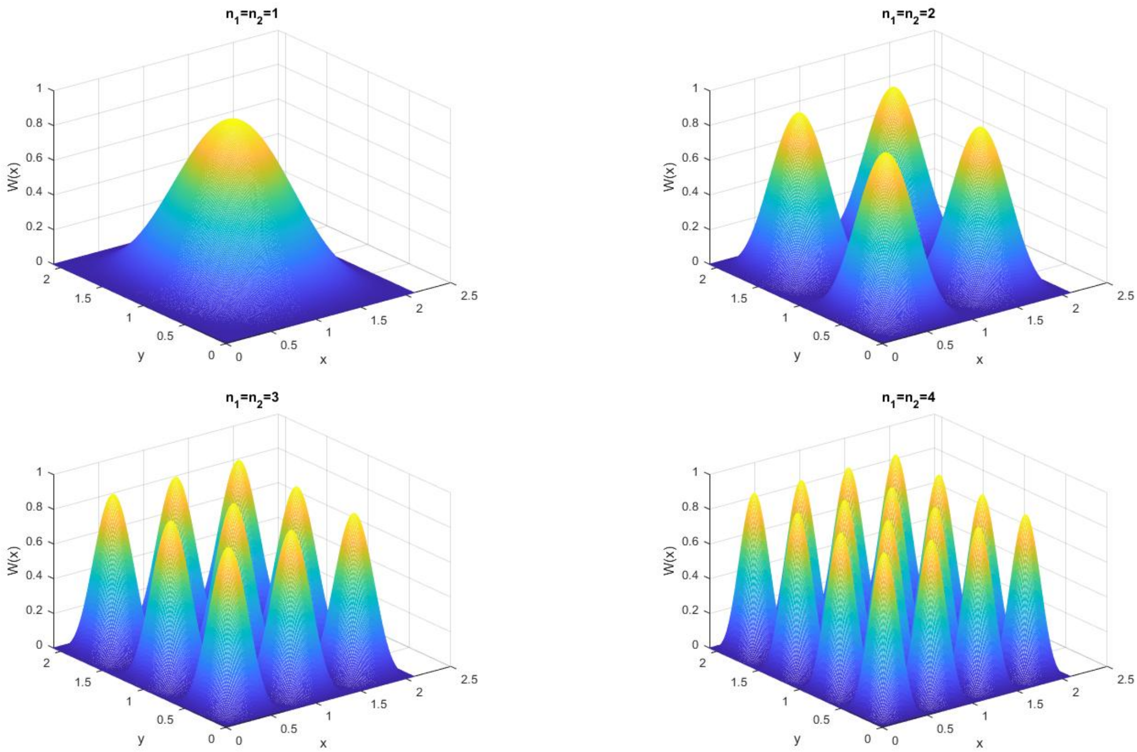

Fig. 5. The distribution of the probability of the particle to be in two-dimensional, rectangular potential hole with infinitively high walls for $n_1 = n_2 = 1, 2, 3, 4$. Hole sizes are equal to $a = b = \frac{2\pi}{3}$.

These dependencies on coordinates for one-dimensional and two-dimensional cases were constructed digitally (Figs. 4 and 5). It is obvious from the presented curves that the higher is the energy value, the smaller is the probability of the particle to be in this hole. The mentioned intervals on the Figures correspond to internodal spaces.

3. Conclusions

In the presented work solving stationary Schrödinger equation analytically, the wave function, describing the particle state in rectangular potential hole with infinitively high walls, has been calculated. The calculations were made for three cases: when the potential hole was one-dimensional, two-dimensional and three-dimensional. The equations were solved in Descartes coordinate system. Particle energy formula was obtained for three different cases. The results show that the energies accept discrete values and these values depend on dimensional sizes and squared values of quantum numbers $\{n_1\}$, $\{n_1, n_2\}$ and $\{n_1, n_2, n_3\}$ respectively. The squared modulus of the wave function for each case was obtained analytically. In other words, the probability distributions of the particle being at any point inside potential hole were determined. The code was written numerically throughout MatLab standard package, and using this code the dependencies of the squared modulus of the wave function on coordinates were constructed for both one-dimensional and two-dimensional cases. It is obvious from the presented figures that along with quantum number enhancement (energy value rises), the number of nodes increases. Permeable intervals for particle being were broken up to sub-intervals, in which the probability of particle revelation decreases (in nodes it is practically equal to zero). In frames of potential hole, the increase of nodes of the wave function leads to enhancement of the particle energy.

Authors Contributions

Hasmik Shahinyan formulated the problem and its way of solvation as well as she composed and edited the text of manuscript. The author N.J. Grigoryan developed calculation, and L.S. Ghazaryan, participated in the writing of the text.

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