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APPLICATION OF THE SCHRODINGER EQUATION TO A PARTICLE IN A ONE-DIMENSIONAL POTENTIAL WELL

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ABSTRACT

It is impossible for students to master the basic ideas and conclusions of quantum mechanics without solving a certain set of problems. Problems play a significant role in the educational process, forming not only logical thinking, but also influencing the overall development of the students.

The article poses and solves problems about stationary one-dimensional problems in quantum mechanics.

Keywords: Trigonometric function, excited state, eigen wave function, Hamilton operator.

Introduction

There is great interest in solving and discussing mathematical problems of quantum mechanics in theoretical physics and other fields related to physics. Quantum mechanics is the most important achievement of the 20th century. It is one of the most important branches of physics focusing on nanoscale systems relevant to optics, chemistry, and electronics. Only quantum mechanics can describe the reality of orbitals and energy levels in atoms. In addition to the wave nature, quantum mechanics can shed light on the quantization of light and its corpuscular nature [1].

Literature

The equations of quantum mechanics are described in various concepts in the matrix mechanics of W.Heisenberg, the wave mechanics of E.Schrodinger, and the “vector” algebra of states of P. Dirak. E. Schrodinger proved the equivalence of wave and matrix mechanics and combined them under the general name of quantum mechanics. Although the above forms of quantum mechanics are described in specific ways and have different mathematical tools, they are focused on the study of the same micro-object, the final results are the same and can be transferred from one to another. Since wave mechanics is simpler and more obvious from the mathematical point of view, the basic concepts and laws of quantum mechanics are described based on the Schrodinger equation [2].

The Schrodinger equation was discovered based on experimental results to describe the wave and corpuscular particle motion in different potential fields. Therefore, they cannot be derived using the laws of classical physics, which ruled until quantum mechanics. Schrodinger's equations are given ready-made like Newton's second law [3]:

$$-\frac{\hbar}{i}\frac{d\Psi}{dt} = -\frac{\hbar^2}{2m}\nabla^2\Psi + U\Psi \qquad (1)$$

(1) is the complete Schrödinger equation. It allows one to study the motion of particles in time-dependent fields. Equation (1) can be expressed in a simpler form using the Hamilton operator:

$$\hat{H}\Psi = E\Psi \qquad (2)$$

The Schrodinger equation is a second order linear partial differential equation. Therefore, the Ψ function, which is a solution to the equation, must satisfy the following conditions:
1. It itself and its first-order derivative are continuous;
2. Unambiguous;
3. Finiteness (since the probability cannot be > 1),
4. Satisfies the boundary conditions arising from the requirements of the specific issue.

RESEARCH METHODOLOGY

The study used analysis and synthesis of scientific and scientific-methodological literature, pedagogical observations, and methods of pedagogical experience.

RESULTS

Using the functions ψ and Ψ, which are solutions to the Schrodinger equations, the probability of finding a particle in the region defined by these functions is found.
1. The particle is in a one-dimensional rectangular potential with side a. Determine the probability of finding a particle in the lowest energy state in the region $0 \le x \le l/3$ [4].
Solution:

$$U(x) = 0, \quad 0 \le x \le l$$
$$U(x) = \infty, \quad x < 0, x > l$$

$x = 0, x = l$ - coordinates of the pit walls (Fig.1, a).

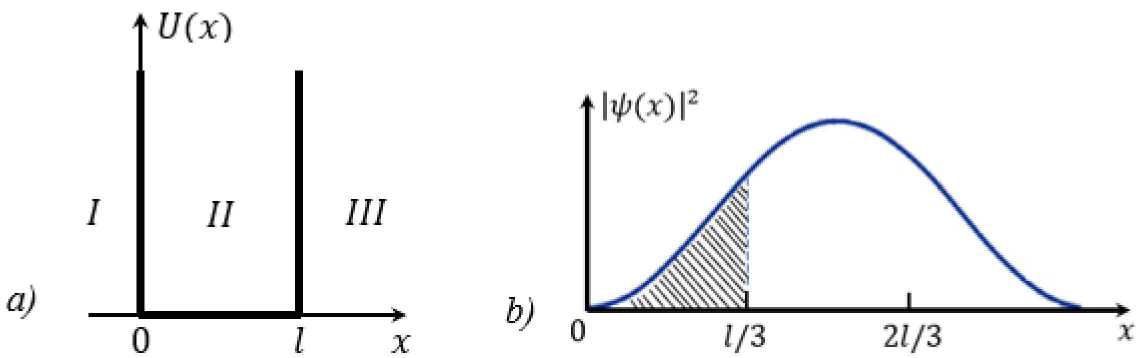

Fig.1.

Since its walls are absolutely impermeable, the particle cannot be in areas I and III, that is, the probability of finding a particle in these areas is zero, from which it is known that $\psi_1 = \psi_3 = 0$. For field II, we write the Shrodinger equation for:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

If we denote $k^2 = \frac{2mE}{\hbar^2}$, the above expression takes the form:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2mE}{\hbar^2}\psi = 0$$

We look for a solution to this differential equation in the form

$\psi(x) = A\,sin\,(kx + \alpha)$ (1)

From the condition of continuity of the wave function $\psi(0) = 0$. It follows that $\alpha = 0$. Since $\psi(l) = 0$
And equals

$$A\,si\,n\,kl = 0$$

So, the simplest trigonometric equation was obtained. To solve it
$kl = \pi n \quad (n = 1,2,3,\ldots)$. from this

$$k = \frac{\pi n}{l}$$

Then expression (1) will take the following form:

$$\psi_n(x) = A\,sin\frac{\pi n}{l}x$$

Let us determine the coefficient A from the conditions for normalizing the wave function:

$$\int_0^l |\psi(x)|^2 dx = 1$$

$$A^2 \int_0^a sin^2\frac{\pi n}{l}xdx = 1$$

$$\frac{A^2}{2}\int_0^l \left(1 - cos\frac{2\pi n}{l}x\right)dx = \frac{A^2}{2}l - \frac{A^2}{2}\sin\frac{2\pi nx}{l}\frac{l}{2\pi n}\Big|_0^l = \frac{A^2}{2}l = 1;$$

$$A = \sqrt{\frac{2}{l}}.$$

$\psi_n(x) = \sqrt{\frac{2}{l}}\sin\frac{\pi n}{l}x -$ is the normalized eigenfunction.

According to the conditions of the problem, the particle has the lowest energy, from which it is known that n=1. Wave function for this case

$$\psi_1(x) = \sqrt{\frac{2}{l}}\sin\frac{\pi}{l}x$$

Let us determine the probability of finding a particle in the region $0 \leq x \leq l/3$ [7]:

$$\omega = \int_0^{l/3} |\psi_1(x)|^2 dx = \frac{2}{l}\int_0^{l/3} \sin^2\frac{\pi n}{l} x dx =$$

$$= \frac{1}{l}\int_0^{l/3} \left(1 - \cos\frac{2\pi x}{l}\right) dx = \frac{1}{l}\cdot\frac{l}{3} - \frac{1}{l}\cdot\frac{l}{2\pi}\cdot \sin\frac{2\pi x}{l}\bigg|_0^{\frac{l}{3}} = 0{,}195$$

The value of the ω function is equal to the area of the shaded area in Fig.1b.

2. The particle is in a one-dimensional rectangular potential well with side l. Determine the coordinates of the point at which the probability of finding a particle is greatest, around points with coordinate x at the first and second energy levels [5].

Solution: The squared modulus of the wave function represents the probability density of particle detection:

$$\rho(x) = |\psi(x)|^2$$

According to the conditions of the problem, the particle is in a one-dimensional potential. Therefore, the particle density function

$$\psi(x) = \sqrt{\frac{2}{l}} \sin\frac{\pi n}{l} x$$

for n = 1

$$\rho_1(x) = |\psi_1(x)|^2 = \frac{2}{l}\sin^2\frac{\pi x}{l}$$

At the point where the trigonometric function reaches its maximum value, the particle detection probability density reaches its maximum value, which corresponds to the point $x = l/2$ [7] (Fig.2, a).

for n = 2

$$\rho_2(x) = |\psi_2(x)|^2 = \frac{2}{l}\sin^2\frac{2\pi x}{l}$$

in this case, from the solution of the trigonometric function, it is known that the points at which the probability density of particle detection reaches its maximum value are $x = l/4$ and $x = 3l/4$ (Fig.2, b).

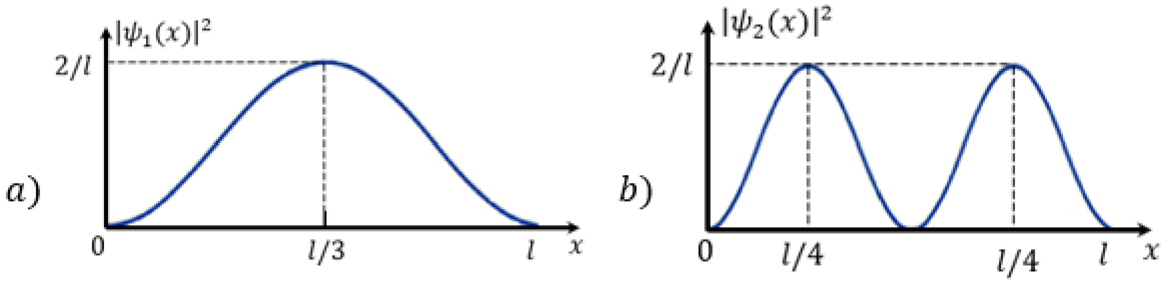

Fig.2. A plot of particle detection probability density versus its coordinate.
a) for n=1, b) n=2 cases.

One way to think of a particle is to think of $|\psi_2(x)|^2$ as a "cloud," where high density corresponds to high probability of detection (Fig 3).

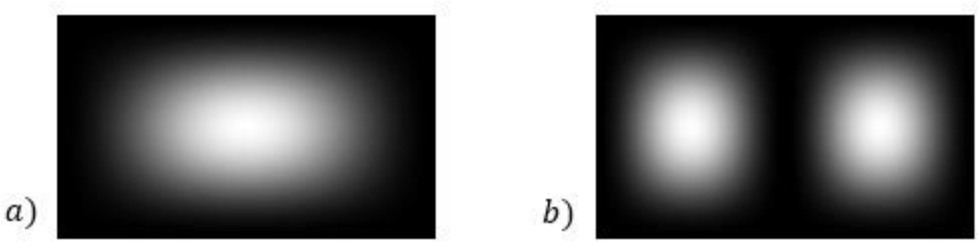

Fig.3. Electronic "cloud", for a) n=1, b) n=2 cases.

In Fig.3 it can be seen that with n = 1 the particle detection probability density reaches its maximum value at one point, and with n = 2 it reaches its maximum value at two points. This corresponds to the graph presented in fig.2 [8].

CONCLUSION

The Schrodinger equation is the fundamental equation of non-relativistic quantum mechanics. It can take different forms depending on the potential field in which the particle is located.

The article found the wave function by solving the Schrödinger equation. The wave function itself has no physical meaning, but the square of its modulus has a physical meaning and means the probability of detecting a particle in a given area.

Teaching students to solve problems involving one-dimensional potential wells provides a foundation for them to solve problems involving two-dimensional and three-dimensional potential wells.

The problems given as examples in the article will help strengthen students' theoretical knowledge on the topic "The Schrodinger Equation" in the science of quantum mechanics. From the solutions to the problems, it is clear that to solve this type of problem, students need to have basic knowledge, such as "Trigonometric function", "Derivative operation", "Finding the original function", "Graphing". complex functions" from a mathematics course.

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