

Visualization of finite potential wells

M. Jeremić, M. Gocić, S. Trajković, and M. Milić

Abstract - The necessity to describe micro particles through probability is the most important feature of quantum theory. On the other hand, during their lectures, professors of physics face many problems related to students' understanding of quantum mechanics. They appear for any teaching style, book, school or the level of students' previous knowledge. In this article we will emphasize the need for physics teachers of quantum theory to visually illustrate some quantum theory phenomena in order to overcome understanding problems. Applications are developed in order to help students in improving and deepening the knowledge of this important subject.

An example of visualization for a rectangular potential barrier is described in this paper, for which it is necessary to calculate the probability of tunnelling, i.e. the probability that a particle can jump over the edge of the barrier if its energy is less than the potential barrier. This is one of the more complex forms of potential barriers that can have an analytical solution of the Schrödinger equation. Two versions of Computer applications were developed: PC and PocketPC application using Borland Delphi 7 and Visual Studio 2010.

Keywords - Potential wells, Schrödinger equation, Wave function.

I. INTRODUCTION

An old-fashioned tools and methods for presenting the quantum theory lectures cause many understanding problems to students that are attending them. Because of that teachers, professors and scientists have begun to investigate these problems [1], [2], [3], [4]. An interesting result is that most of the students' difficulties are universal [4], [5], and patterns of errors of quantum mechanics appear at all levels of lecturing.

In order to face this problem, we will first give a brief overview of the quantum theory basics. Due to its wavy nature, as well as the uncertainty relations that arise out of it, it is impossible to observe and analyse microparticles (quantum particles) in the classical sense. Namely, in the case of a classical particle, the equation of motion for a given particle can completely describe its position and impulse at a given time instant. Regardless of the fact that quantum particles do not allow this, there was a need to introduce a function, which would contain wavelike properties of a micro-particle; it would be a part of an equation that can be used for calculation of the

probability of finding a micro-particle, as well as its energy. The state of the system in quantum mechanics describes the wave functions $\Psi^a(x, y, z, t)$ that can be determined by solving the Schrödinger equation. However, it turned out that only the square of its module has physical meaning, and that is proportional to the probability of finding the particle W .

In general, the Schrödinger equation describes the change of the wave function over time, which depends on time and the coordinates (positions) of the particle $\Psi(r, t)$, which is shown in Eq. 1, while its form for the case of stationary state is given by Eq. 2 [6].

$$-\frac{\hbar^2}{2m}\Delta\Psi + U(x, y, z, t)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \quad (1)$$

It is well known from the basic of mathematics that the change of this function over time is determined by the partial derivative of the function with respect to time as the variable. Since Ψ is function of more variables therefore we need to use its partial derivatives

$$\Delta\Psi + \frac{2m}{\hbar^2}(E - U)\Psi = 0 \quad (2)$$

The equation will be solved for a few cases that may be of interest for further applications, and allow obtaining the solution in a closed form. The solution of the differential equation is a function that, when replaced into this equation, gives an identity. It should be emphasized that for the solution of a differential equation we assume any continuous function that has defined corresponding derivatives and which translates equation into an identity. The general expression for the normalization in this case is given by the following form:

$$\int |\Phi(x)|^2 dx = 1 \quad (3)$$

The integration is done along the areas where the particle can move. First, we will observe a particle with $V(x) = 0$.

There are several forms of wave functions that are used in practice, which contain trigonometric functions sinus and cosines. This function can represent a stationary wave that moves from left to right or vice versa. Their linear combination can also be a solution:

$$\Phi(x) = C \cdot \sin k \cdot x + D \cdot \cos k \cdot x \quad (4)$$

The choice of constants depends on the boundary conditions, that is, the conditions that the wave function should fulfil for the physical reasons. Depending on the direction of motion, some of the constants can have a zero value, while the free particle can have an arbitrary value of

M. Jeremić, M. Gocić, and S. Trajković are with the Faculty of Civil Engineering and Architecture, University of Niš, Aleksandra Medvedeva 14, Niš, miljan.jeremic@gmail.com, milan.gocic@gaf.ni.ac.rs, slavisa@gaf.ni.ac.rs.

M. Milić is with the Faculty of Electronic Engineering, University of Niš, Aleksandra Medvedeva 14, Niš, miljana.milic@elfak.ni.ac.rs.

positive energy.

The normalization problem can arise if the summation is done over the entire space, and consequently an infinite value can be expected. After this, we can observe a particle in a well with an infinite potential [7]. The extreme case of the well is shown in the following Figure:

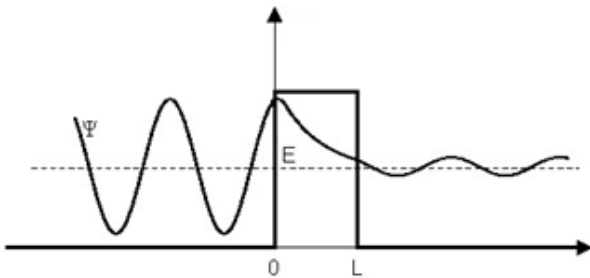


Fig. 1. Particle in a potential well

This well describes the situation when a particle cannot leave a certain space. Then, the probability of finding a particle outside the well, as well as at its borders is zero, and therefore, the wave function must also be zero [8]. Then, the wave number of a particle in an infinitely deep potential well can only have few exact values that correspond to the energy levels. The wave function can now be normalized. The calculation of these functions is illustrated in Figure 2.:

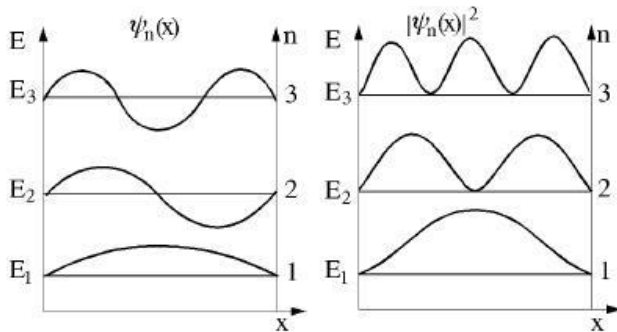


Fig. 2. Wave function

If we analyse the case of a finite potential barrier, there are two situations. In the first situation, the energy of the particle is greater than the energy of the barrier $E > V_0$. More interesting case is when the energy of the particle is smaller than the energy of the barrier. There is a finite, non-zero probability for the particle to appear in the well in Fig. 1, and it decreases with the distance from the boundary of that area.

This situation explains the tunnelling effect. On the left and right side of the barrier, the particles behave freely. As the probability is inversely proportional to the width of the barrier, it is clear that all this makes sense only if the barriers are narrow.

II. METHODS AND TOOLS

Borland Delphi 7 and Visual Studio 2010, were used as the environment for the application development [9].

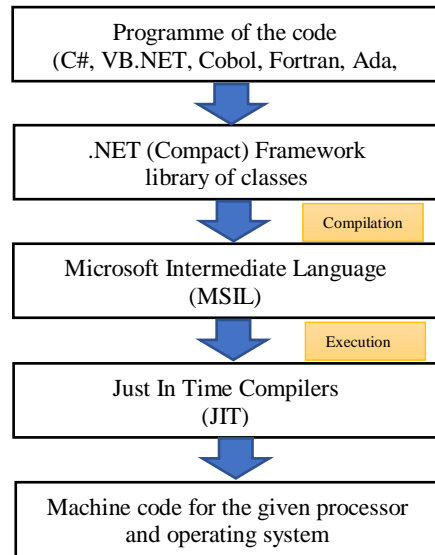


Fig. 3. Architecture of .NET application

Programming in Visual Studio is done with the support of .NET Framework. If, for example, both .NET application and .NET JIT compiler for Mac OS, are available, application developed for Windows OS would also work correctly for Mac OS. The architecture of the .NET application is shown in Fig. 5 [10]. For mobile versions of Windows OP, there are some "shorter" versions of .NET Framework, called .NET Compact Framework. It can be used for the development of PocketPC version of the application.

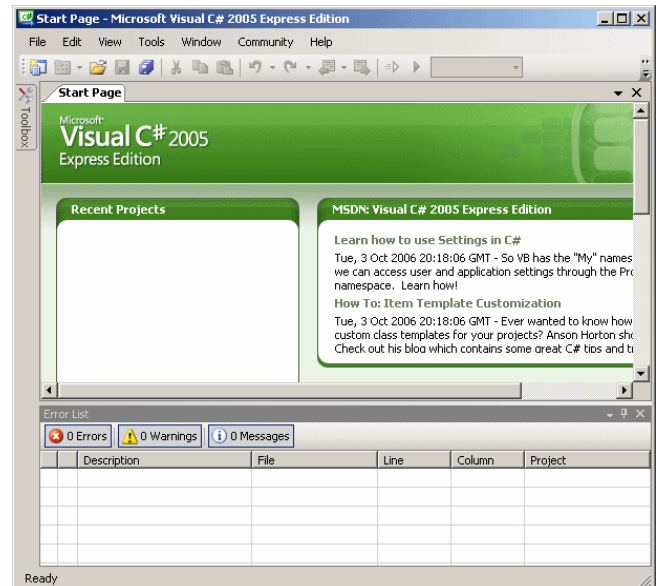


Fig. 4. Project in Visual Studio

Working in Visual Studio (for classical applications development) implies placing the objects/controls in the form/window and defining their visual characteristics and

properties during the program execution. After that, program coding, application testing and debugging need to be done.

Development of the program consisted of two parts: programming the PC application and programming the PocketPC application, using .NET Framework-a and .NET Compact Framework, respectively. Development of a PocketPC application version is illustrated in Fig. 2 [9], [11].

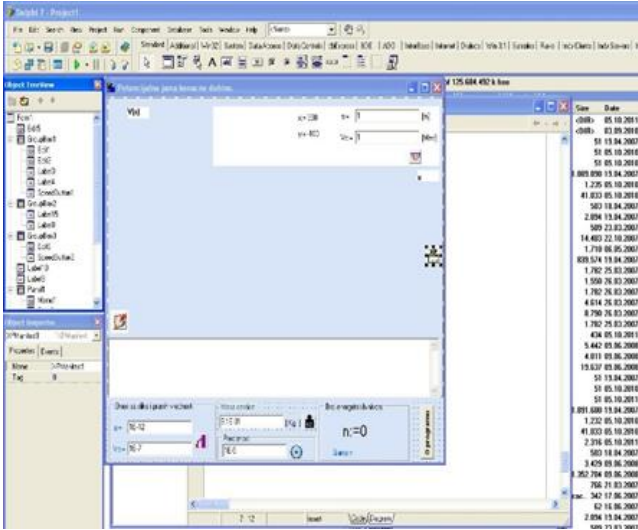


Fig. 5. Project in Delphi

For the PocketPC application it was enough to use textual INI basis for data storing due to fast and easy access. The alternative to these bases were Access and SQL bases, but their advanced functions for data manipulations were far too complex for this application. Every INI „base“ consist of Sections, while they consist of Keys that can store a certain value.

In order to verify the PocketPC application, both emulator and a real device were used. Microsoft ActiveSync was used to establish the communication with a device. This is also required during the execution of the program due to the requirements for a calendar and the synchronization between the files on the PocketPC with those on the computer. During the execution of the program, it stores a certain file in the PocketPC memory, which represents a sort of database placed in My Documents folder of the device, while ActiveSync defines, during the installation, the folder in a PC where the synchronized versions of all necessary files from My Documents folder in a PocketPC were stored. When a device is connected to the PC over the USB cable, ActiveSync compares the corresponding files from both devices, and automatically updates their versions, including the Program.ini file.

Install Creator was used to create installations for both devices. Also during the development of the application MWSnap was used for creation of the screenshots, as well as some high-performance program for image processing (like Adobe Photoshop) [10].

III. INTERFACE AND THE APPLICATION OF THE PROGRAM

With the appearance of a new Visual Studio a new and redesigned graphical controls arrived, that resemble to those used in Office 2007 and 2010 versions. These changes are the most noticeable in menu bars, toolbars and command buttons.

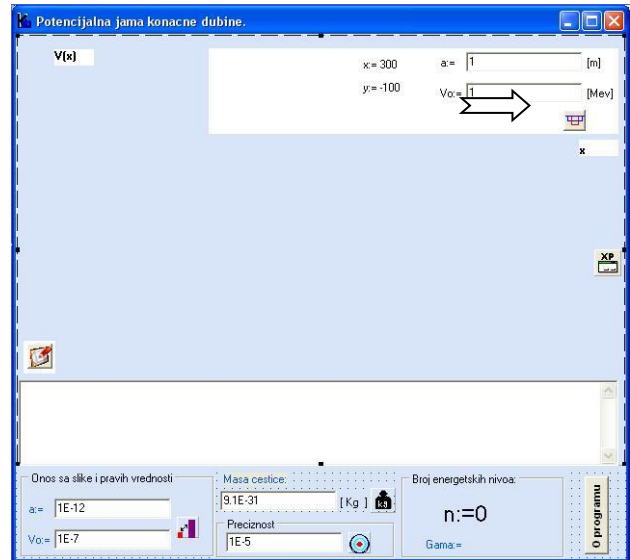


Fig. 6. Interface of the main program

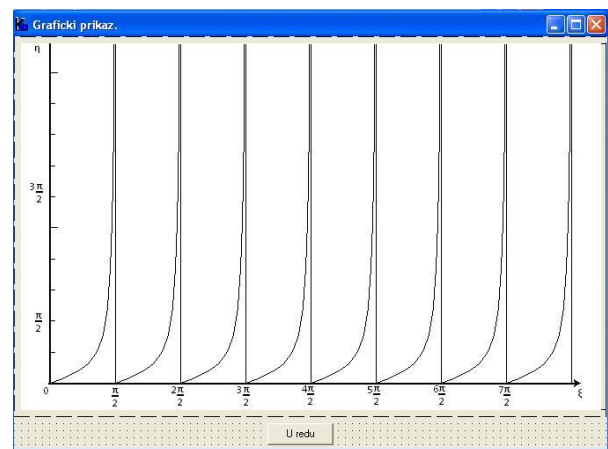


Fig. 7. Graphical illustration

The interface of the main program can be divided into several sections:

- 1) The main – initial line – where the program name is written;
- 2) Icons of the components – that are used for displaying graphics in a Dekart coordinate system, and for the visualization of the increase and the decrease of the width and depth of the well (shown in Fig. 10);

- 3) Toolbar – contains shortcuts toward some menu command;

For command tasters and buttons on the toolbar, tooltip function is implemented. It is a kind of help to the user of the program.

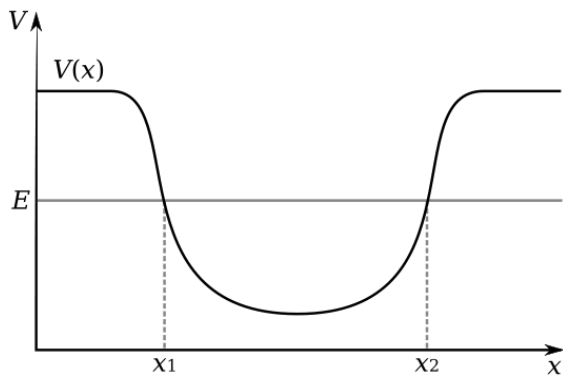


Fig. 8. The visualization of the increase and the decrease of the width and depth of the well

IV. CONCLUSION

According to the presented results, it is obvious that a complicated mathematical apparatus is required and used to describe phenomena in quantum-mechanics. These methods must be correctly adjusted to meet the mathematical knowledge and understanding of a typical secondary school student. Because of the students' knowledge limitation, the obtained visual results are very close to the correct value and are based on a classical theory, that are sometimes not applicable on a quantum mechanics cases. The correct mathematical calculations require additional mathematical models. In this paper we have tried to bridge the gap between the abstract quantitative formalism of quantum mechanics and the qualitative understanding necessary to clarify and predict different physical phenomena [12]. At the end we can conclude that during the physics education a special attention should be paid to cognitive issues since visualization tools can help students build qualitative representation about different and difficult quantum phenomena.

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