SIMULATION OF ELECTRON MOVEMENT IN QUANTUM NANOSTRUCTURES

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Abstract. *The article discusses the modeling of electron motion in a one-dimensional potential well. Analytical and numerical methods and results for solving the Schrödinger equation for the problem considered are presented. The results of the numerical solution of the Schrödinger equation for rectangular, triangular, quadratic and exponential potentials are also presented.*

Keywords*: electron, potential well, Schrödinger equation, transmission and reflection coefficients.*

Introduction

If initially quantum mechanics was perceived as a new natural philosophy, causing numerous disputes about its foundations and methods, then in the 21st century it is increasingly viewed as an applied science, making it possible to study effects of interest for applications, simulate physical processes, calculate new electronic devices, et al [1, 2].

In the study of quantum mechanics, a special role belongs to problems that have an exact solution, when the solution to the Schrödinger equation is represented in the form of algebraic expressions and functions. At the same time, it is known that the number of precisely solvable problems is very limited. In fact, an exact solution can only be found for systems with high symmetry. In this case, the system has a complete set of operators commuting with the Hamiltonian, and such a system is integrable. For real physical systems, and especially many partial ones (atoms, molecules, solids), the Schrödinger equation is non-integrable, therefore, for its analysis it is necessary to use approximate and numerical methods [3, 4].

At the dawn of quantum mechanics, people dealt only with atomic systems. At the end of the last century, semiconductor technology reached such a level that it became possible to produce structures whose dimensions are comparable to the characteristic de Broglie wavelength of electrons. Let's try to understand why this became possible and what we can “order” from technologists who produce systems with ultra-small dimensions [5, 6].

From a general theoretical point of view, the calculation of electronic states in layered structures should be carried out by solving the corresponding three-dimensional problem on the band structure of the material. Currently, sophisticated methods have been developed for computer calculation of quantum states in nanostructures, based on microscopic models of pseudo potential or strong coupling. Nevertheless, these methods are not yet omnipotent and not omnipotent, and in specific work it is the approximate methods that turn out to be more convenient and effective [7, 8].

In approximate approaches, the solution inside each layer of a multilayer structure is written in the form of a linear combination of independent volumetric solutions, and for matching

at hetero boundaries, boundary conditions are introduced for the envelopes of the electron wave function and their derivatives along the normal coordinate.

Calculations of electronic states in semiconductor nanostructures, performed using the effective mass method, are based on solving the stationary Schrödinger equation, which is one-dimensional for the movement of electrons in the direction perpendicular to the plane of the layers:

$$-\frac{\hbar^3}{2m}\frac{\partial^2\Psi(z,E)}{\partial z^2}+U(z)\Psi(z,E)=E\Psi(z,E) \qquad (1)$$

here m - is the effective mass of the electron, E- is its total energy, $U(z)$- is the potential relief for the electron along the z axis directed in the direction perpendicular to the plane of the layers. The solution to this Schrödinger equation is the z-component of the envelope of the wave function $\Psi(z,E)$, which characterizes the motion of electrons in the direction perpendicular to the plane of the layers and determines, up to normalization, the probability of finding an electron with energy E moving along the Oz axis at a point with the coordinate z.

For a simple band structure, the boundary conditions at the interface between layers A and B in the general case have the form:

$$\begin{cases}\Psi_A=t_{11}\Psi_B+t_{11}\widehat{\Psi}_B,\\ \widehat{\Psi}_A=t_{21}\Psi_B+t_{22}\widehat{\Psi}_B,\end{cases}$$

where $\Psi_{A,B}$ - are the values of the wave function envelope at the interface from the side of layer A and from the side of layer B, respectively,

$$\widehat{\Psi}_A=l\frac{\partial\Psi}{\partial z}|_A,\quad \widehat{\Psi}_B=l\frac{m_A}{m_B}\frac{\partial\Psi}{\partial z}|_B \qquad (2)$$

$m_{A,B}$ -effective masses of electrons in layers A and B, respectively, l- is an arbitrary parameter with the dimension of length, introduced so that the elements of the matrix t_{ij} are dimensionless. The choice of t_{ij} values is usually postulated or carried out by comparison with the results of an experiment or calculation within the framework of some microscopic model. The boundary conditions associated with the name Bastard are used most often:

$$\begin{cases}\Psi/_A=\Psi/_B,\\ \frac{1}{m_A}\frac{\partial\Psi}{\partial z}|_A=\frac{1}{m_B}\frac{\partial\Psi}{\partial z}|_B\end{cases} \qquad (3)$$

By solving equation (1) with boundary conditions (3), it is possible to construct the envelopes of the wave functions of electrons with different energy values E. If you form a thin layer of narrow-gap material between two sufficiently thick layers of wide-gap material, then for an electron moving in a direction transverse to the planes of the layers, a potential relief can be formed, which is called a rectangular potential well [10].

For describe scattering processes in a quantum medium, it is necessary to solve the Schrödinger equation with the corresponding boundary conditions. For a one-dimensional quantum well, i.e. for

$$U(z)=\begin{cases}0, & |z|\le L,\\ -U_0, & |z|>L\end{cases} \qquad (4)$$

The solution to the Schrödinger equation has the form

$$\Psi(x)=\begin{cases} e^{ikx}+re^{-ikx}, & x<0 \\ ae^{iqx}+be^{-iqx}, & 0\le x\le L \\ te^{ik(x-L)}, & x>L \end{cases} \quad (5)$$

where $q^2 = 2\,m\,(E + V_0)$, $k^2 = 2\,mE$.

Coefficients a, b, r, t are determined from the boundary conditions, i.e. conditions for the continuity of the wave function and its derivative at $x = 0$ and at $x=L$

$\psi(0)=1+r,\ \psi'(0)=ik(1-r),$ (6)

$\psi'(L)-ik\psi(L) = 0$ (7)

From here you can determine reflections and transmissions:

$r = -1 + \psi(0),\ t = \psi(L)$ (8)

Let us consider a method for numerically solving the Schrödinger equation. Let us write the Schrödinger equation for the wave function $\psi_n=\psi(x_n)\ (n = 0, 1,..,N)$, given in a set of discrete $x_n = n\Delta$ points:

$\psi_n+\psi_n+u_n\psi_n=0$ (9)

where

$u_n = -2 + 2m\Delta^2(E - V_n)/\hbar^2,\ V_n=V(x_n)$ (10)

Then the boundary conditions take the form

$\psi_1 + (u_0/2 + ik\Delta)\psi_0 = 2ik\Delta,$ (11)

$\psi_{n+1}=R_n\psi_n$ (12)

From here we obtain a recurrence relation for the auxiliary functions R_n

$R_{N-1}=-1/(u_N/2+ik\Delta)$ (13)

Now the functions $R_{N-2}, R_{N-3}, \ldots, R_1, R_0$ are determined starting from R_{N-1} in the opposite direction. After determining R_0

$\psi_0 = 2ik\Delta/[R_0 + (u_0/2 + ik\Delta)]$ (14)

ψ_0 is determined, and then $\psi_1, \psi_2, \ldots, \psi_N$ are determined from (12), then the reflection and transmission coefficients are determined from expression (8).

Results and discussions

Using the above expressions for the analytical and numerical solution of the Schrödinger equation, a visual basic program was created for studying the energy dependence of the electronic transition and reflection coefficients for potential quantum wells of arbitrary shape. A special feature of the program is that it allows you to solve the Schedinger equation for any potential, and the results are automatically sent to MS Excel and graphs are plotted [9].

For example, in Fig. Figure 1 shows the dependence of the squared modulus of the wave function of electrons with different energies for a rectangular quantum well, and Fig. Figure 2 shows the dependence of the transition and reflection coefficients on the electron energy. This figure also shows the results of the wave function expression obtained by the analytical method.

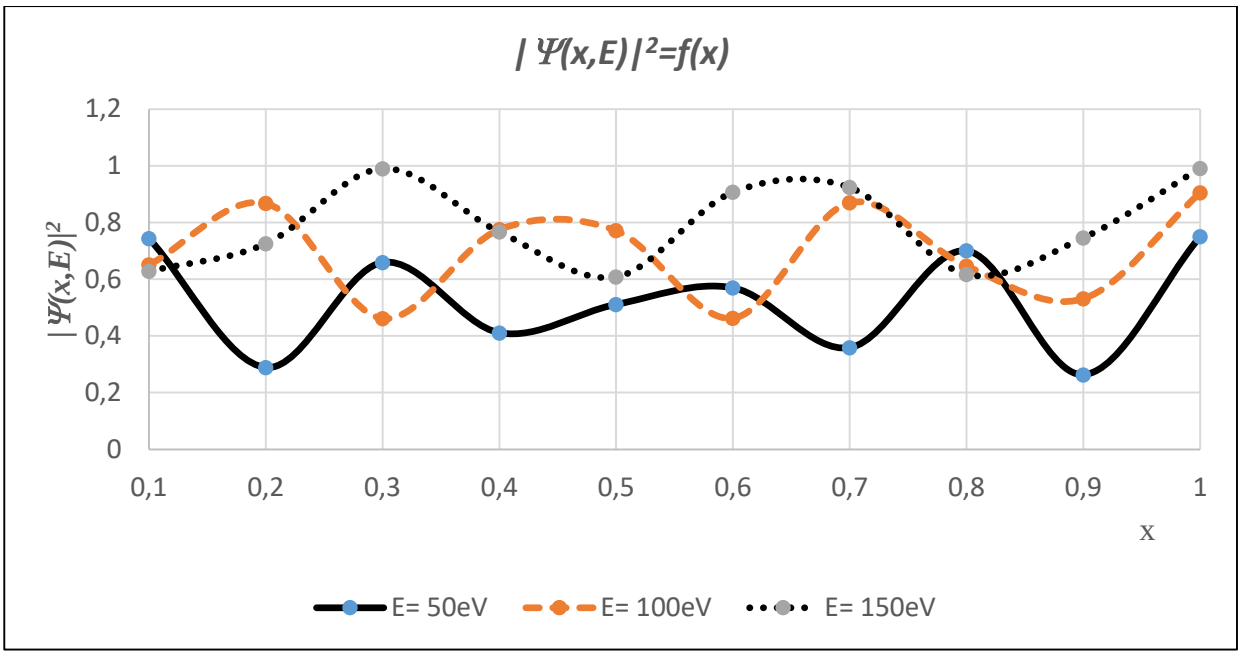

Fig. 1. Dependence of the squared modulus of the wave function of electrons with different energies for a rectangular quantum well. (Dots – approximate calculation, lines – analytical solutions).

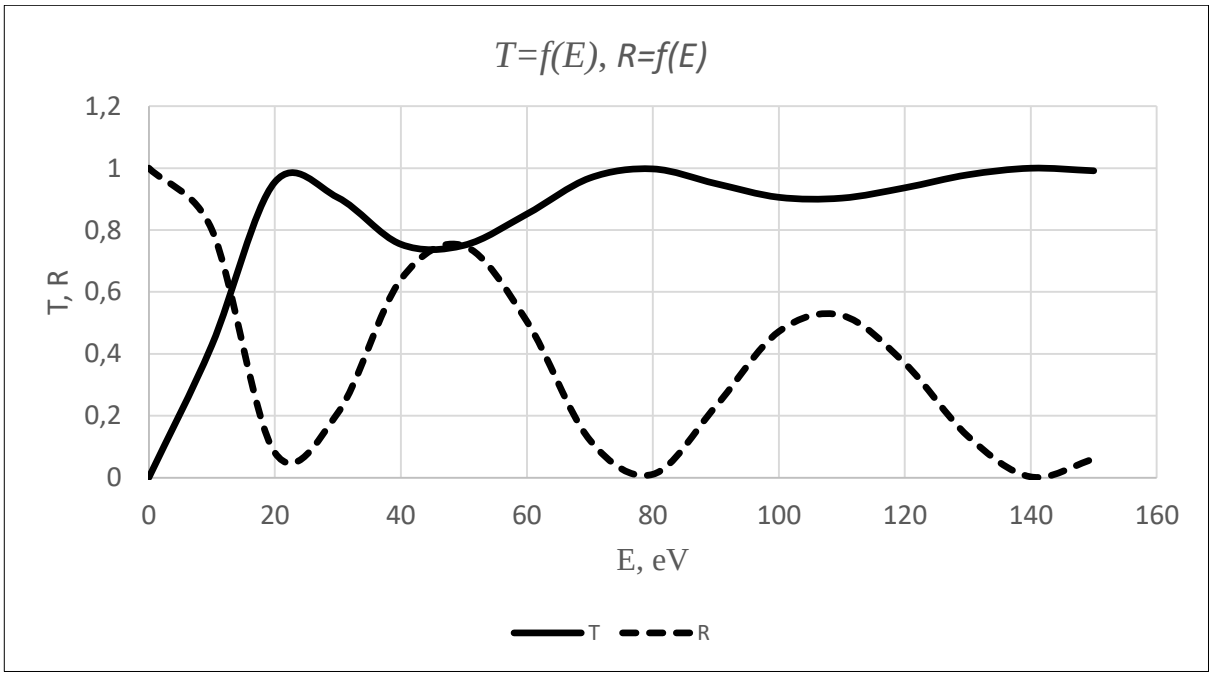

Fig. 2. Dependence of the reflection and transmission coefficients of electrons on energy.

In Fig. 3 shows graphs of the energy dependence of transmission coefficients for rectangular, triangular, quadratic and exponential potentials. The figure shows that the transparency coefficients for rectangular, triangular and quadratic potentials are almost the same, and for exponential potential the growth is slower.

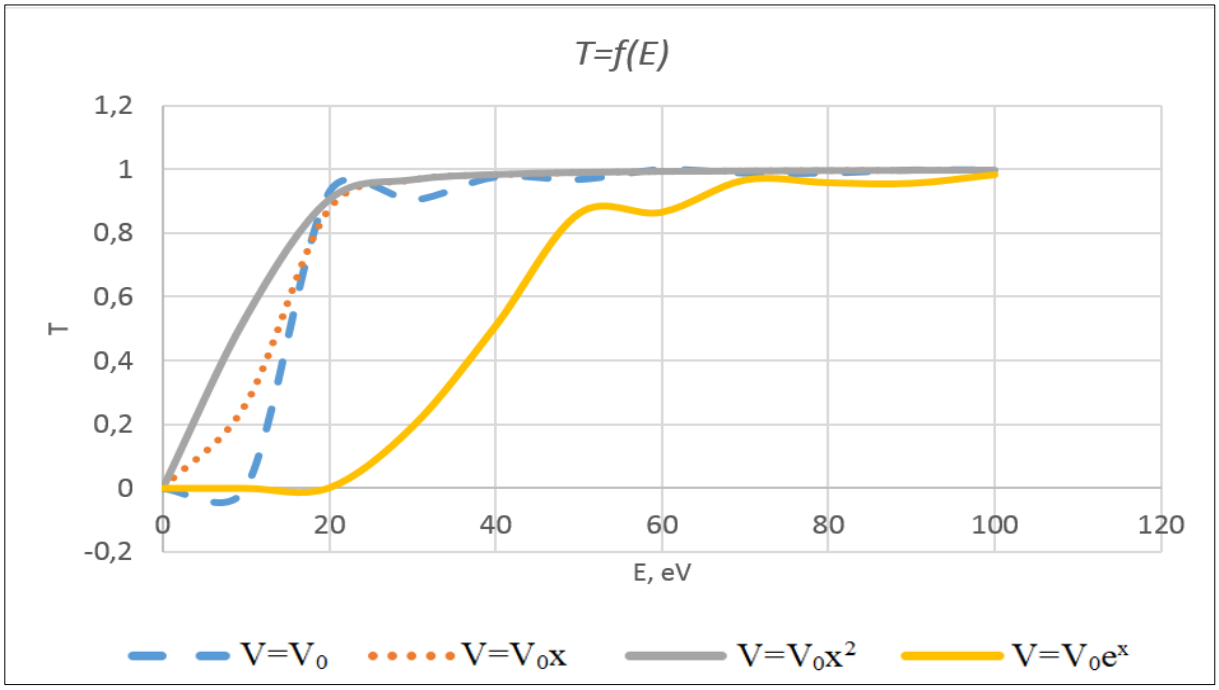

Fig.3. Graphs of energy dependence of transmission coefficients for rectangular, triangular, quadratic and exponential potentials.

Conclusions

Thus, in this work, a program was created to simulate the motion of an electron in a one-dimensional potential well. A special feature of the program is that it allows you to solve the Schrödinger equation for any potential, and the results are automatically sent to MS Excel and graphs are plotted.

The most special aspect of the program, that is, the method for numerically solving the Schrödinger equation, is that it allows you to calculate the wave function, as well as transmission and reflection coefficients, not only for rectangular, but also for arbitrary potentials. As can be seen from the results obtained, the smaller the calculation step, the closer the approximate results are to the analytical solution. This program also allows you to simulate the behavior of electrons in multilayer quantum nanostructures.

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