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Solution of the one-dimensional Schrödinger equation for a heterostructure with a triangular potential function by the power series method

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Abstract. In the work by the power series method the one-dimensional Schrödinger equation is solved with a triangular potential function which is applied in various modern heterostructures, in particular for GaAs and the others. By varying available parameters it is possible to obtain the desired precision of the numerical solution of the Schrödinger equation with any type of potential function for modern heterostructures. For the original Schrödinger equation are obtained wave functions in the form Airy functions and the analytical formula for the energy levels through the zeros of the Airy function. The values energy levels from this analytical formula agree with its results obtained by direct power series method with precision up to 10^{-4} percents, that is, up to 5 decimal signs. However, it is more rational and easier to use the Schrödinger equation solution, because the numerical calculations zeros of Airy function present separate complex and complicated numerical problem. But in order to achieve high numerical accuracy, it is necessary to set the Digits flag to several dozen significant digits and increasing the number of power series, that leads to an increasing in the time spent on the computer.

Key words and phrases: Schrödinger equation, triangular potential function, heterostructures, energy levels, wave functions, the Airy equation, zeros of the Airy function, power series, mathematical modeling, the Maple computer system

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1. Introduction

In this work, the one-dimensional Schrödinger equation with a triangular potential function has been solved using the power series method [1–4], which is used in the study of semiconductor nano-dimensional structures in the field of modern advanced microelectronics for the creation of new devices and devices in various fields of technology [5–16]. However, heterostructures are complex quantum systems with many quantum features. For example, the heterostructure between the layers GaAs and $Al_xGa_{1-x}As$ electrons are in the triangular potential well [13, 17, 18].

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A very promising direction is their use in the field of the new generation of microelectronics for the creation of devices and devices that will become elements of large integrated circuits capable of storing huge amounts of information and processing them at high speed and will form the basis of a new generation of electronic and optoelectronic machines of small sizes [6, 12, 15]. Motion of electrons in these structures is essentially described by the laws of quantum mechanics, and various quantum models have been developed to describe them [5–10, 12, 13, 15].

2. Solving of the basic equations

In our work, we solved the Schrödinger equation with the triangular potential function as

$$V(x) = \begin{cases} \alpha x, & \alpha = |e| \cdot |\vec{E}|, x > 0, \\ \infty, & x \leq 0. \end{cases} \quad (1)$$

In the atomic system of units ($m = e = \hbar = 1$), the Schrödinger equation has the form

$$\left[-\frac{1}{2} \cdot \frac{d^2}{dx^2} + V(x) \right] \psi(x) = E\psi(x), \quad (2)$$

where

$$\psi(0) = 0, \quad \psi(\infty) \rightarrow 0. \quad (3)$$

Is boundary condition. Here e is the elementary charge, \vec{E} is the electric field strength. The integration of equation (1)–(2) is performed on the segment $[R_{\text{left}}; R_{\text{right}}]$ with the help of a developed computer program [1] in the Maple system. Our maple program have three parameters R_{left} ; R_{right} , and n -number of member in power series. By variation of these parameters one can achieved desirable exactness.

The optimal cut-off values of segment select in our calculations by variation method and it are equal $R_{\text{left}} = -0.28 \cdot 10^{-26}$ и $R_{\text{right}} = 13.5$ and with the number of members in the power series equal to $n = 200$. As it know, the power series method first calculates two linearly independent solutions and, which depend on the total energy as a parameter. Their linear combination gives the general solution of the Schrödinger equation (2). Consideration of the boundary conditions (3) leads to a homogeneous algebraic system, the nontrivial solutions of which are given by the allowable energy levels and the corresponding wave functions. The following lower energy levels were calculated. The optimal cut-off values were the target of selection and in our calculations are equal and with the number of members in the power series equal. As know, in the power series method first calculates two linearly independent solutions $\psi_1(x, E)$ and $\psi_2(x, E)$, which depend on the total energy as a parameter. Their linear combination gives the general solution of the Schrödinger equation (2). Taking into account the boundary conditions (3) leads to a homogeneous algebraic system, the nontrivial solutions of which are given by the allowable energy levels and the corresponding wave functions. If $\alpha = 1$ the following lower energy levels were calculated:

$$E_k = 1.855575; 3.24446; 4.381671; 5.386613; 6.305263.$$

and the corresponding wave functions, which because of their bulkiness are represented in the following form:

$$\begin{aligned}
\psi_1(x) &= 0.61139759 \cdot 10^{-5}x - 0.142163116 \cdot 10^{-30}x^2 - 0.0000169241805x^3 + \dots \\
&\quad - 0.593525574 \cdot 10^{-15}x^{25} + 0.590773946 \cdot 10^{-16}x^{26} + 0.171191325 \cdot 10^{-31}x^{27} \\
\psi_2(x) &= 0.136823205 \cdot 10^{-6}x - 0.31814343910 \cdot 10^{-32}x^2 - 0.378742190 \cdot 10^{-6}x^3 + \dots \\
&\quad - 0.132823670 \cdot 10^{-16}x^{25} + 0.132207889 \cdot 10^{-17}x^{26} + 0.383104973 \cdot 10^{-33}x^{27} \\
\psi_3(x) &= 0.353019093 \cdot 10^{-9}x - 0.820845473 \cdot 10^{-35}x^2 - 0.977196991 \cdot 10^{-9}x^3 + \dots \\
&\quad - 0.198239895 \cdot 10^{-17}x^{22} + 0.999308236 \cdot 10^{-18}x^{23} - 0.131621212 \cdot 10^{-19}x^{24} - \\
&\quad - 0.342699846 \cdot 10^{-19}x^{25} + \dots
\end{aligned}$$

It is shown also, that initial problem admit the analytical solution. Indeed, rewrite equation (2) in the form

$$\psi''_{xx} - 2\alpha \left(x - \frac{E}{\alpha} \right) \psi(x) = 0$$

and do following substitution:

$$z = \beta \left(x - \frac{E}{\alpha} \right), \quad \left(x - \frac{E}{\alpha} \right) = \frac{z}{\beta}.$$

Then by $\beta^3 = 2\alpha$ initial equation (2) bring to [19-21]:

$$\psi''_{zz} - z\psi(z) = 0. \quad (4)$$

Solution of this equation (4) will be known function Airy and solution initial problem (2) - (3) will be following wave function:

$$\psi(x) = \text{const} \cdot \text{Ai} [z(x)] = \text{const} \cdot \text{Ai} \left[\beta \left(x - \frac{E}{\alpha} \right) \right]. \quad (5)$$

From (5) and (3) obtain equality $\beta \cdot E = -\alpha \cdot z_k$, where z_k are zeros of Airy function $\text{Ai}(z_k) = 0$. And thus we have analytical expression for energy levels in atomic units:

$$E_k = -(z_{k+1}) \cdot \sqrt[3]{\frac{\alpha^2}{2}}, \quad k = 0, 1, 2, \dots \quad (6)$$

The values energy levels from formula (6) agree with its results obtained by direct power series method with precision up to $10^{-4}\%$. However, it is more rational and faster to calculate the energy levels with the help of direct solution of the Schrödinger's equation by some known method [2].

3. Results

A computer program of symbolic-numerical solution of the one-dimensional Schrödinger equation is developed, and calculations of energy levels and wave functions of a perspective gallium arsenide semiconductor with a triangular potential function are carried out, which is experimentally detected for electrons at the boundary between layers of this semiconductor.

4. Discussion

It is shown that the Schrödinger equation with a triangular potential function admits analytical solutions, both for wave functions and for the energy spectrum. In particular, an analytical formula for energy levels is obtained, which uses the zeros of the Airy function. In the calculations, it was found that the energy levels obtained by direct numerical calculation of the Schrödinger equation practically coincide with their values calculated by the analytical formula (five decimal places coincide). It should be pointed out that the developed method for solving the Schrödinger equation is quite applicable for calculations with other types of potential functions in other heterostructures. It can be hoped that the results of the calculations and the developed program will be applied in the field of modern research on semiconductors.

5. Conclusions

Thus, this program finds the solution of the Schrödinger equation with high precision by variations of its three parameters: $(R_{\text{left}}, R_{\text{right}}, n)$ and the `Digits` commands from the Maple system provide high precision in solving the Schrödinger equation with other potential functions that are used in heterostructures. Thus, it has been shown that the developed method of solving the Schrödinger equation allows for high numerical accuracy and our program can be made available to interested parties.

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Решение одномерного уравнения Шрёдингера для гетероструктур с треугольной потенциальной функцией методом степенных рядов

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Аннотация. В работе методом степенных рядов решается одномерное уравнение Шрёдингера с треугольной потенциальной функцией, которая применяется в различных современных гетероструктурах, в частности для GaAs и других. Варьируя доступные параметры, можно получить желаемую точность численного решения уравнения Шрёдингера с любым типом потенциальной функции для современных гетероструктур. Для исходного уравнения Шрёдингера получены волновые функции в виде функций Эйри и аналитическая формула для уровней энергии с помощью нулей функции Эйри. Значения энергетических уровней из этой аналитической формулы согласуются с результатами, полученными методом прямых степенных рядов, с точностью до 10^{-4} процентов, то есть до 5 десятичных знаков. Однако рациональнее и проще использовать решение уравнения Шрёдингера. Но для достижения высокой точности вычислений необходимо установить флажок Digits на несколько десятков значащих цифр и увеличить количество членов степенного ряда, что приводит к увеличению времени счета на компьютере.

Ключевые слова: уравнение Шрёдингера, треугольная потенциальная функция, гетероструктуры, энергетические уровни, волновые функции, уравнение Эйри, нули функции Эйри, степенные ряды, математическое моделирование, компьютерная система Maple