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One-dimensional Stationary Schrödinger Equation with the Fourier Transformation

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The paper describes a new numerical method for solving of one-dimensional stationary Schrödinger equation. The method is based on the Fourier transformation of the wave equation. Wave function is obtained by using a reverse Fourier transformation. Discrete energy levels are split and form the forbidden and allowed zones for a one-dimensional finite crystal.

Keywords: Fourier transformation, Energy levels, Schrödinger equation.

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1. INTRODUCTION

Quantum wells are often studied since their physical effects can be seen at room temperature and can be exploited in real devices [1, 2]. An analysis of devices based on quantum wells requires the solution of the Schrödinger stationary equation. Precise solutions of one-dimensional stationary Schrödinger equation have been obtained only for a small number of functional dependencies of the potential well [3]. The search solutions of one-dimensional Schrödinger stationary equation continues for this reason [4]. It should be noted that the known methods of searching the discrete levels of energy are based on the solution of the wave equation in the coordinate's area. The relevant wave functions and the primary derivatives of coordinate x to $\pm\infty$ are equal to zero for discrete levels of energy. Therefore, there is a Fourier image [5] for the wave function and the relevant wave equation can be translated into the frequency domain by means of a Fourier transformation.

The objective of this study is to develop a new numerical method to solve the Schrödinger one-dimensional stationary equation using the Fourier transformation

2. RESULTS AND DISCUSSIONS

2.1 Schrödinger Wave Equation and its Fourier Transform

The one-dimensional stationary Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x) \qquad (1)$$

Dimensionless equation frequently in quantum mechanics, which is obtained by replacing the variables. The dimensionless equation (1) can be presented as follows:

$$-\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x) \qquad (2)$$

Function $\psi(x)$ is a solution of the stationary Schrödinger equation, which corresponds to discrete levels of energy, and their primary derivatives tend to zero if $x\to\pm\infty$. Therefore, a Fourier transformation exists for these functions as well as for their primary and secondary derivatives. Let us write the appropriate proportions for $\psi(x)$. Thus, the Fourier transformation of $\psi(x)$ and their primary and secondary derivatives $\psi(x)$ is equal to [5] and can be written as follows:

$$\psi(u)=\int_{-\infty}^{\infty}\psi(x)\exp(-i2\pi ux)dx, \qquad (3)$$

$$i2\pi u\psi(u)=\int_{-\infty}^{\infty}\frac{d\psi(x)}{dx}\exp(-i2\pi ux)dx, \qquad (4)$$

$$-(2\pi u)^2\psi(u)=\int_{-\infty}^{\infty}\frac{d^2\psi(x)}{dx^2}\exp(-i2ux)dx. \qquad (5)$$

In addition, functions for which a Fourier transformation exists satisfied by following relations:

$$\begin{aligned}&F\{g(x)\}=G(u),\ F\{h(x)\}=H(u),\\ &F\{g(x)h(x)\}=\int_{-\infty}^{\infty}G(u-v)H(v)dv,\end{aligned} \qquad (6)$$

where $F\{...\}$ denotes the Fourier transformation. Eq. (6) describes the contents of the convolution theorem.

Let us execute the Fourier transformation of the left and right parts of Eqs. (2), by using (3), (5) and (6). As a result we obtain:

$$4\pi^2u^2\psi(u)+\int_{-\infty}^{\infty}U(u-v)\psi(v)dv=E\psi(u) \qquad (7)$$

Therefore, we proceed from the differential equation (2) for eigenfunctions and eigenvalues toward the integral one (7). We can replace the integral with the sum, while the continuous u and v can be replaced with discrete variables, as follows:

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$$4\pi^2(s\Delta)^2\psi(s\Delta)+\sum_{p=-(N-1)/2}^{(N-1)/2}U(s\Delta-p\Delta)\psi(p\Delta)\Delta=E\psi(s\Delta), \qquad (8)$$

where $\Delta=u_{\max}/N$, $u_s=s\Delta$, $v_p=p\Delta$, $-(N-1)/2\le s$, $p\le(N-1)/2$, s, p are integers; $|u|\ge u_{\max}/2$; values of $\psi(x)$ are almost equal to zero. N must be large and preferably have an odd value.

Let us write the equation for all discrete spatial frequencies $u_s=s\Delta$, where s are changes between $-(N-1)/2$ and $(N-1)/2$ then a set of equations in the amount of N can be written in the form of a matrix equation, where E is common for all s:

$$(\mathbf{P}+\mathbf{U})\psi=E\psi, \qquad (9)$$

where $\mathbf{P}$ is a diagonal matrix with elements equal to $4(\pi s\Delta)^2$, $\mathbf{U}$ is a square symmetric matrix with elements equal to $U(s\Delta-k\Delta)$, ψ is a vector with elements equal to $\psi(s\Delta)$.

Therefore, in the latter case the problem has been reduced to the eigenvalues (energy) and eigenvectors (a discrete Fourier image $\psi(x)$) problem, which corresponds to the given value of energy. We can have multiple eigenvalues and corresponding eigenvectors. Having made an inverse discrete Fourier transformation of eigenvector, we can obtain the eigenfunction $\psi(x)$. All eigenvalues (discrete levels of energy) are determined inside the potential well for quantum-mechanical problems. If the potential well of finite depth then the precision is determined by N and Δ. If the potential energy varies from zero to infinity (for example $U=x^2$) then in this method is limit the potential energy, i.e. it serves up to a certain value as $U(x)$, and further acquires a constant value. Obviously, in this case, the lowest levels of energy can be determined with the highest level of accuracy.

2.2 Numerical Simulation of One-dimensional Crystal

One-dimensional crystal consists of periodic placement of potential wells, which are described by the following analytical function:

$$U(x)=a-a\exp(-\pi x^2), \qquad (10)$$

where a is a certain positive number determining the depth of a potential well.

If we have a N_1 number of periodically placed (N_1-odd) potential wells at a distance Λ from each other, we will receive a one-dimensional crystal, whose potential energy will be described as following expression:

$$U(x)_{kr}=a-a\sum_{n=(N_1-1)/2}^{(N_1-1)/2}\exp\left[-\pi(x-n\Lambda)^2\right]. \qquad (11)$$

Following simple mathematical transformations we obtain the Fourier image of the function (12):

$$F\{U(x)_{kr}\}=a\delta(u)-a\exp(-\pi u^2)\frac{\sin[\pi N_1\Lambda u]}{\sin(\pi\Lambda u)}. \qquad (12)$$

Figure 1 demonstrates the potential energies and energy levels for a singular potential well and the one-dimensional crystal. The scales of figure 2 and 2b are vertically the same; the starting point of the coordinates for both pictures is combined. The lowest level splits to the least degree, while $E_{0,10}=16.533261$. Level E_3 splits the most: $E_{3,0}=87.157709$, $E_{3,10}=93.704412$.

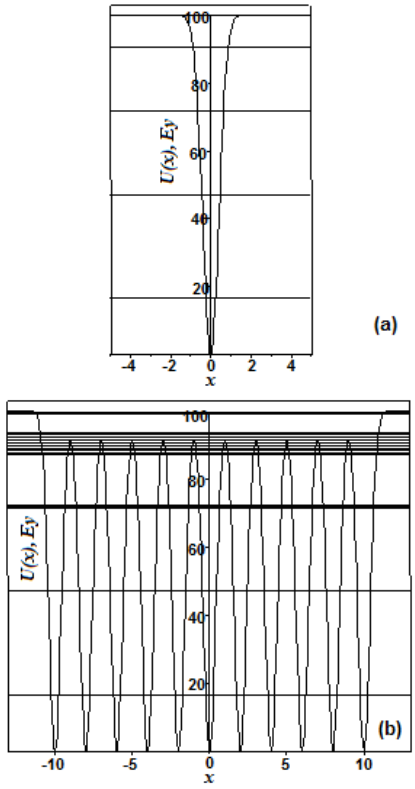

Fig. 1 – Dependence of potential energy of the coordinates and energy level (horizontal line): (a) single potential pit; (b) one-dimensional crystal.

3. CONCLUSION

The new numerical method for solving stationary Schrödinger equation, based on a Fourier transformation has been developed. The integral equation is obtained as a result of mathematical manipulation. The method has been tested in a number of examples and shows high accuracy of the energy levels for a singular potential energy. The method is characterized by numerical stability.

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