A Solution of One-Dimensional Stationary Schrödinger Equation by the Fourier Transform

V. M. Fitio [1], I. Y. Yaremchuk [1], V. V. Romakh [1], and Y. V. Bobitski [1,2]

[1] Department of Photonics
Lviv Polytechnic National University, Lviv, 79013, Ukraine
polyana@polynet.lviv.ua, yaremchuk@polynet.lviv.ua, vladykv@gmail.com

[2] Institute of Technology
University of Rzeszów, Rzeszów, 35959, Poland
bobitski@polynet.lviv.ua

Abstract — In this paper, a new numerical method for solving of one-dimensional stationary Schrödinger equation has been presented. The method is based on the Fourier transform of a wave equation. It is shown that, as a result we obtain an integral equation where integral is replaced by sum. A main problem is transformed in the eigenvalue/eigenvector problem which corresponds to discrete energy levels as well as the Fourier transform of wave functions. Wave function is obtained by usage of the inverse Fourier transform. Discrete energy levels are split and form the forbidden and permitted zones for the one-dimensional finite crystal. The method is tested in many examples, and it is characterized by high accuracy and stability of search of the discrete energy levels.

Index Terms — Convolution, energy levels, Fourier transform, Schrödinger equation.

I. INTRODUCTION

Quantum wells [1] emerging in semiconductor heterostructures have recently become the subject of significant scientific interest. They are often studied since their physical effects can be seen at room temperature and can be exploited in real devices [2]; for example, as a primary component of a number of optoelectronic devices such as: photo-detectors in infrared spectral range [3], quantum cascade lasers [4] and other optoelectronic devices [5]. A detailed theory of optoelectronic devices based on quantum wells is offered by Bastard in [6].

An analysis of devices based on quantum wells requires a solution of the stationary Schrödinger equation solution is reduced to the transcendental equation if a potential well has a rectangular form. In case of two or more rectangular wells, the obtained transcendental equation becomes much more complicated. In addition, a solution becomes more difficult if the potential well hasn't a rectangular barrier. Precise solutions of one-dimensional stationary Schrödinger equation [7] have been obtained only for a small number of functional dependencies of a well potential. For this reason, search of solutions of one-dimensional Schrödinger stationary equation continues; moreover, there are attempts to form potential energy in such a way to obtain a precise analytical solution of the corresponding equation [8-10].

A similar problem exists at the finding of propagation constants of waveguide modes in the gradient planar waveguides [11-16]. The methods described in [12-16] can be used for solving the Schrödinger equation as a structure of the wave equation is identical to the one-dimensional stationary Schrödinger equation for planar waveguides. On the other hand, the approaches developed in quantum mechanics, for instance, the WKB approximation [11], can be used to search propagation constants of gradient planar waveguides.

The current state of computer technologies and the sophistication of software allow applied numerical methods to solve equations of the various types. The numerical method ensures high accuracy, and it is relatively simple. It enables its application in quantum mechanics and waveguide technologies. A well-known numerical method to find propagation constants of waveguide modes [16] is based on replacing the second derivative of the wave equation by the difference operator. The solution is reduced to the eigenvalue/eigenvector problem in this method. This method also can be used to search discrete energy levels of the stationary Schrödinger equation. However, it doesn't offer high accuracy. In addition, the evidence of

Submitted On: July 2, 2014
Accepted On: April 8, 2015

numerical differentiation is found as a source of noise due to approximation in the numerical process.

It should be noted that, the known methods of searching the discrete levels of energy (searching of propagation constants of waveguide modes) are based on the solution of a wave equation in a coordinate domain. The relevant wave functions and the primary derivatives of coordinate x at $\pm\infty$ are zero for discrete levels of energy. Therefore, there is the Fourier transform [17] of a wave function, and the appropriate wave equation can be transformed into a frequency domain by the Fourier transform. At the same time, integral equation will be obtained and also can be solved by numerical methods.

The aim of this study is to develop a new numerical method to solve the Schrödinger one-dimensional stationary equation using the Fourier transform, and demonstrate some advantages in comparison with the known methods. The second section of this paper is devoted to numerical implementation of the method proposed. The third section presents the results of the numerical analysis of the stationary Schrödinger equation for certain functional dependencies of the potential energy. The fourth section presents the results of the solution of the Schrödinger one-dimensional stationary equation in accordance with the method proposed for the one-dimensional crystal which has several periods.

II. ONE-DIMENSIONAL SCHRÖDINGER WAVE EQUATION AND ITS FOURIER TRANSFORM

The one-dimensional stationary Schrödinger equation is:

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

where $U(x)$ is a potential energy of particle which has only discrete values, $\psi(x)$ is a wave function.

Dimensionless equation is used [7] frequently in quantum mechanics, which is obtained by replacing the variables. The dimensionless equation (1) can be presented as:

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

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 at $x \to \pm\infty$. Therefore, the Fourier transform for these functions as well as for their primary and secondary derivatives exists. Let's write the appropriate proportions for $\psi(x)$. Thus, the Fourier transform of $\psi(x)$ and its primary and secondary derivatives are zero [17], and it can be written as follows:

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

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

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

In addition, for functions for which a Fourier transform exists, the next conditions are satisfied [17]:

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

where $F\{...\}$ is the Fourier transform. Expression (6) describes the content of the convolution theorem.

Let's execute the Fourier transform of left and right parts of equation (2) by using equations (3), (5) and (6). As a result we obtain:

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

Therefore, we have moved from the differential equation (2) for eigenfunctions and eigenvalues to the integral one equation (7). In the last equation we can replace integral by sum, so the continuous values u and v can be replaced by discrete ones:

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

where $\Delta=u_{\max}/N$, $u_s=s\Delta$, $v_p=p\Delta$, $-(N-1)/2\le s$, $p\le(N-1)/2$, s and p are integers; $|u|\ge u_{\max}/2$; values of $\psi(x)$ are almost equal to zero. Value of N must be large and preferably unpaired. Obviously, sum in equation (8) should have N elements.

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

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

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

Therefore in the last case, the problem is reduced to the problem of eigenvalues (energy) and eigenvectors (the discrete Fourier transform of $\psi(x)$) which corresponds to the given value of energy. We can have many eigenvalues and its corresponding eigenvectors. By carrying out the inverse discrete Fourier transform of eigenvector, we 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 has 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 the potential energy is limited; 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 accuracy. In our numerical calculations whose results are presented below, we used the simplest way to replace integral by sum.

III. EXAMPLES OF NUMERICAL SIMULATION

Example 1. Schrödinger equation according to equation (2), for which potential energy is:

$$U = \begin{cases} x^2, & |x| \le a, \\ a^2, & |x| > a = 7 \end{cases}.$$

Numerical process parameters are: sampling number $N = 1001$, maximum frequency $u_{\max} = 8.0$. The 25 eigenvalues of energy are obtained by numerical calculations. There are 13 lowest energy levels which have next values: $E_0 = 1.00000000025$, ..., $E_6 = 13.00000000025$, ..., $E_{12} = 24.999999971$, and they accurately fit the data of [7], where $E_n = 2n+1$. However, error is large enough at potential energy $U(x) = x^2$ for $E_{24} = 48.64036656$, which is sufficiently accurate for our model potential. Figure 1 shows the wave functions (not normalized) for the three lowest values of energy. One can see well that points fit with continuous curves.

Example 2. Schrödinger equation according to equation (2) where potential energy is:

$$U = \begin{cases} x^4, & |x| \le a, \\ a^4, & |x| > a = 3 \end{cases}.$$

Numerical process parameters are next: $N = 1001$, $u_{\max} = 25$. The 11 smallest eigenvalues E_n are found at these data, there are: $E_0 = 1.0603646$, ..., $E_5 = 21.238375$, ..., $E_{10} = 50.256257$. This quantum problem is not solved precisely by analytical methods, therefore the value of the lowest level of energy is found by approximation at which $E_0 \approx 1.156194$ [7]. In other words, the approximate value is found with a large error. In addition, this problem can be solved by the numerical difference method [16], however, it offers solutions with low accuracy: $E_0 = 1.0603593$, ..., $E_5 = 21.237897$, ..., $E_{10} = 50.253695$.

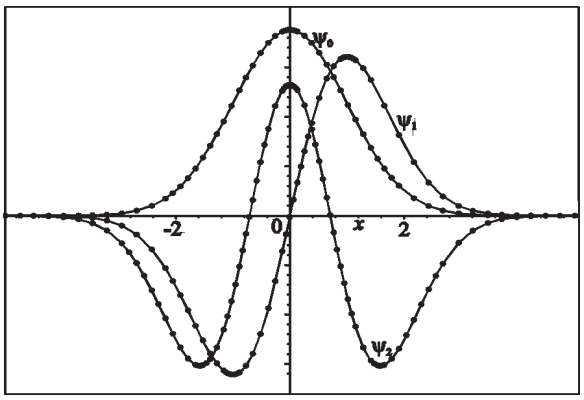

Fig. 1. Wave functions of the three lowest energy levels. The continuous curves correspond to exact wave functions, while the points correspond to the results of calculation obtained by the method proposed in this study.

IV. NUMERICAL SIMULATION OF ONE-DIMENSIONAL CRYSTAL

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

$$U(x) = a - a\exp(-\pi x^2), \tag{10}$$

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

The Fourier transform of this function is:

$$F\{U(x)\} = a\delta(u) - a\exp(-\pi u^2). \tag{11}$$

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

$$U(x)_{kr} = a - a\sum_{n=(N_1-1)/2}^{(N_1-1)/2} \exp\left[-\pi(x - n\Lambda)^2\right]. \tag{12}$$

After simple mathematical transformations we obtain the Fourier transform of equation (12):

$$F\{U(x)_{kr}\} = a\delta(u) - a\exp(-\pi u^2)\frac{\sin[\pi N_1 \Lambda u]}{\sin(\pi \Lambda u)}. \tag{13}$$

The five energy levels are found ($a = 100$): $E_0 = 16.539595$, $E_1 = 47.036248$, $E_2 = 72.011285$, $E_3 = 90.446940$, $E_4 = 99.832730$ for the potential energy according to equation (10) at parameters of the numerical process $N = 1001$ and $u_{\max} = 10 \div 20$.

A more detailed dependence of the calculated energy levels as function on $u_{\max}$ is presented in Table 1. Table 2 shows the dependence of the calculated energy levels on N at $u_{\max} = 15$. Analysis of Table 1 indicates

that there is a frequency range at sufficiently large N in which values of energy are constant (these values of energy in the Tables are shown in bold).

Four levels are split into 11 sublevels and form the permitted zones, but level E_4 splits only into two sublevels: $E_{4,0} = 99.041696$ and $E_{4,1} = 99.551008$.

The widths of permitted zones increase with the increase of energy. The fact that the fourth level splits into two sublevels only can be understood from Fig. 2.

Table 1: The dependence of the calculated energy levels on $u_{\max}$ at $N = 1001$

$u_{\max}$	4	6	10	14	20	24	28
E_0	16.54607358	16.53959718	16.53959510	16.53959509	16.53959509	16.53959509	16.53959510
E_1	47.08219239	47.03626733	47.03624767	47.03624767	47.03624767	47.03624767	47.03624768
E_2	72.15044578	72.01136385	72.01128540	72.01128540	72.01128540	72.01128540	72.01128541
E_3	90.66025796	90.44709161	90.44693968	90.44693968	90.44693968	90.44693968	90.44693969
E_4	99.88445912	99.83277513	99.83272955	99.83272955	99.83272955	99.83272950	99.832729002

Table 2: The dependence of the calculated energy levels on N at $u_{\max} = 15$

N	101	201	401	601	801	1001	1501
E_0	16.53959512	16.53959510	16.53959511	16.53959509	16.53959509	16.53959509	16.53959509
E_1	47.03624768	47.03624766	47.03624768	47.03624767	47.03624767	47.03624767	47.03624767
E_2	72.01128540	72.01128539	72.01128542	72.01128540	72.01128540	72.01128540	72.01128540
E_3	90.44694122	90.44693968	90.44693970	90.44693968	90.44693968	90.44693968	90.44693968
E_4	99.76898968	99.82787662	99.83270759	99.83272945	99.83272955	99.83272955	99.83272955

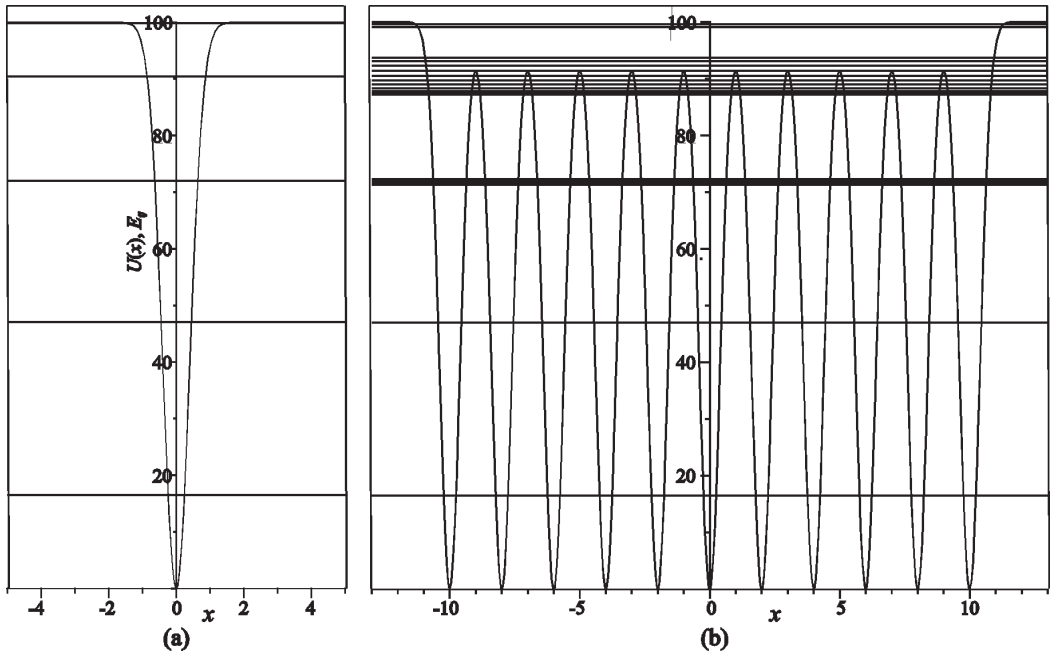

Fig. 2. Dependence of potential energy on the coordinate and energy level (horizontal line): (a) single potential well, and (b) one-dimensional crystal.

The numerical analysis of one-dimensional crystal was carried out at the following parameters: $N = 1001$, $u_{\max} = 25$, $\Lambda = 2$.

Figure 2 demonstrates the potential energies and energy levels for single potential well and one-dimensional crystal. The scales of Figs. 2 (a) and 2 (b)

are vertically the same; the starting point of the coordinates for both pictures is combined. The lowest level is split to the least degree: $E_{0,10} = 16.533261$. Level E_3 is split at most: $E_{3,0} = 87.157709$, $E_{3,10} = 93.704412$.

Table 2 leads to a conclusion that the calculated energy tends toward a certain value at increase of *N* for certain frequencies.

V. CONCLUSION

The new numerical method for solving stationary Schrödinger equation based on the Fourier transform is developed. The integral equation is obtained as a result of mathematical manipulations. The next step is to obtain the eigenvalue/eigenvector problem by replacing integral by sum and to write the corresponding equation for a set of discrete frequencies, where the eigenvalues correspond to energy levels and eigenvectors do to the discrete Fourier transforms of wave functions. Carrying out the inverse Fourier transform of the eigenvector, the wave function in a coordinate domain is obtained. The method is tested on a number of examples, and it shows high accuracy of the energy levels for a single potential energy. The method is characterized by numerical stability.

The discrete levels of energy have been determined for one-dimensional crystal, consisting of 11 regularly placed potential wells. It demonstrates that discrete levels are split and form permitted zones during the formation of one-dimensional crystal, and the multiplicity of splitting equals to a number of potential wells that form one-dimensional crystal. The energy width of the permitted zone expands at the increase of energy of corresponding discrete level of a single potential well. This conclusion is consistent with the data of [18].

ACKNOWLEDGMENT

This work was supported by the Ministry of Education and Science of Ukraine (DB/Microlaser, DB/Tekton).

REFERENCES

[1] L. C. West and S. J. Eglash, "First observation of an extremely large dipole infrared band of a GaAs quantum well," *Appl. Phys. Lett*., vol. 46, pp. 1156-1158, 1985.

[2] J. Faist, F. Capasso, A. L. Hutchnson, L. Pfeiffer, and K. W. West, "Suppression of optical absorption by electric-field-induced quantum interference in coupled potential wells," *Phys. Rev. Lett*., vol. 71, pp. 3573-3576, 1993.

[3] B. F. Levine, "Quantum-well infrared photodetectors," *J. Appl. Phys*., vol. 74, pp. R1-R81, 1993.

[4] J. Faist, P. Capasso, D. L. Sivco, C. Sirtori, A. L. Hutchnson, and A. Y. Cho, "Quantum cascade laser," *Science*, vol. 264, pp. 553-556, 1994.

[5] S. Noda, T. Yamashita, M. Ohya, Y. Muromoto, and A. Sasaki, "All-optical modulation for semiconductor lasers by using three energy levels in n-doped quantum wells," *IEEE J. Quantum Electron*., vol. 29, no. 6, pp. 1640-1647, 1993.

[6] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures*, Les editions de physique, Les Ulis, France, 1988.

[7] I. O. Vakarchuk, *Quantum Mechanics*, Second edition, Ivan Franko Lviv National University, Lviv, 2004.

[8] A. Caticha, "Construction of exactly soluble double-well potentials," *Physical Review A*, vol. 51, pp. 4264-4267, 1995.

[9] A. S. Dutra, "Conditionally exactly soluble class of quantum potentials," *Physical Review A*, vol. 47, pp. R2435-2437, 1993.

[10] V. M. Tkachuk and T. V. Fityo, "Multidimensional quasi-exactly solvable potentials with two known eigenstates," *Phys. Lett. A*, vol. 309, pp. 351-356, 2003.

[11] A. Gedeon, "Comparison between rigorous theory and WKB-analysis of modes in graded-index waveguides," *Opt. Commun*., vol. 12, no. 3, pp. 329-332, 1974.

[12] R. E. Smith, S. N. Houde-Walter, and G. W. Forbes, "Mode determination for planar waveguide using the four-sheeted dispersion relation," *J. Quantum Electronics*, vol. 26, no. 4, pp. 627-630, 1990.

[13] E. Anemogiannis and E. N. Glytsis, "Multilayer waveguides: efficient numerical analysis of general structures," *J. Lightwave Technol*., vol. 10, no. 10, pp. 1344-1351, 1992.

[14] A. K. Chatak, K. Thyaagarajan, and M. R. Shenoy, "Numerical analysis of planar optical waveguides using matrix approach," *J. Lightwave Technol*., vol. 5, no. 5, pp. 660-667, 1987.

[15] T. Baba and Y. Kokubun, "Dispersion radiation loss characteristics of antiresonant reflecting optical waveguides-numerical results and analytical expressions," *J. Quantum Electronics*, vol. 28, no. 7, pp. 1689-1700, 1992.

[16] A. G. Rganov and S. E. Grigas, "Numerical algorithm for waveguide and leaky modes determination in multilayer optical waveguides," *Technical Physics*, vol. 55, pp. 1614-1618, 2010.

[17] J. W. Goodman, *Introduction to Fourier Optics*, McGraw-Hill Book Company, 1968.

[18] C. Kittel, *Introduction to Solid State Physics*, Fourth edition, John Wiley and Sons, Inc., 1978.

Fitio Volodymyr was born in Lviv, Ukraine, in 1950. He graduated from the Department of Radiophysics and Radioelectronics, Ivan Franko National University of Lviv in 1974, and received the both Ph.D degree in 1998 and Doctor habilitation in Optics and Laser Techniques from the Institute of Physics of NAS of Ukraine in 2009.

His research interests include holography, diffraction by periodical and chaotic structures, distribution light by waveguide, feedback lasers and the application of numerical methods for the analysis and design of optic elements and devices. He has more than 150 papers in international journals and proceedings of international and national symposia.

Yaremchuk Iryna was born in Lviv, Ukraine, in 1980. She graduated from the Department of Semiconductors, Ivan Franko National University of Lviv in 2004, and received the Ph.D degree in Optoelectronics Systems from the Institute of Semiconductors Physics of NAS of Ukraine in 2009.

Her research interests include diffraction by periodical structures, plasmonics and the numerical methods for the analysis and design elements to some engineering optical applications. She has more than 50 papers in international journals and proceedings of international and national symposia.

Romakh Volodymyr was born in Lviv, Ukraine in 1991. He received the M.Sc. in Laser and Optoelectronics Engineering from the Lviv Polytechnic National University, Ukraine. He is currently working towards his PhD Degrees at the Photonics Department.

His research interests include design and analysis of distribution of electromagnetic wave in active and passive waveguides.

Yaroslav Bobitski was born in Lviv, Ukraine, in 1951. He graduated from the Department of Automated Control Systems, Lviv Polytechnic National University in 1974, and received the both Ph.D degree in 1980 and Professor Habilitation in Technology of materials for electronic devices from the Lviv Polytechnic National University in 1991. He is the head of the Photonics Department.

His research interests include distribution light by nanostructured systems, interaction laser irradiation with layered media. He has more than 150 papers in international journals and proceedings of international and national symposia.