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Ground state quantum modes in the triangular nanowires using by finite differencing technique

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ABSTRACT

In this study, the ground state energies of a right-angle equilateral triangular cross-section nanowire have been calculated. Symmetrical geometry cross-section of nanowire helps us to find correct Eigen energy when we drawing probability function of the electron by the finite differencing method. We found that this drawing method with our computational code give us ground state energies in a good precision in order to $0.1(meV)$ *and this result is better than similar researches. Therefore, probability function symmetry would be disappeared by more deviation of this value. Moreover, the maximum of the probability function occurs in the* $\frac{11}{18}$ *of Height from the vertex of the triangular.*

Keywords: *nanowires, ground state energies, finite differencing method, sparse matrices*

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INTRODUCTION

Nanowires (NWs) or one-dimensional (1D) materials are classified in a group of materials with size <100 nm in two out of three dimensions and, for owning encouraging properties, are an outstanding zone in current nanotechnology research. We have come along with this kind of material since the 1950s, just after electron microscope invention. Despite that, just in the last few years, examining this type of material has become possible with more details by means of enhanced characterization techniques and achieving better control in growth processes.
This paper aims the introduction of a simple, virtually analytical and numerical technique in order to approximate the solutions in triangular cross-section [3,4]. The preceding trend corresponds forming the required multidimensional solutions to Schrodinger's equation from combinations of decoupled one-dimensional quantum which have been taken into consideration as the best solution. These approximated solutions which have been risen from combining of the simple and the best ones, can be improved by adding of an appropriate term by considering the probability function. This will play roll as rapid and proper method for every sort of Schrödinger equation for the motion along the x direction, which can be solved analytically, and is given by

$$\frac{-\hbar^2}{2m^*}\frac{\partial^2\psi(x)}{\partial x^2} = E_x\psi(x) \quad , (2)$$

and a two-dimensional Schrödinger equation for the confinement within the cross- section of the wire which is our main concern, given by

potential energy and nanostructure, in respect to other methods such as KP theory [1], plane wave expansion[2] and Fourier expansion[3].

THEORY: FINITE DIFFERENCE EXPANSION
The system which is going to be examined has a simplified feasible geometry. It is formed of an infinitely deep rectangular cross-sectional wire. Although this geometry could not be practical indeed, it provides us with a good starting point since should be in a form that could play as a source of solutions for any cross-section and any potential[8-10].
In this primitive research, we will concentrate on the general constant effective mass given by Schrödinger equation and in three directions:

$$\frac{-\hbar^2}{2m^*}\nabla^2\psi(x,y,z) + V(x,y,z)\psi(x,y,z) = E\psi(x,y,z) \quad , (1)$$

Note that m∗ is the electron effective mass, and V (x, y, z) the potential energy. If the potential is defined only on y-z plane by putting x component equal to zero, then the motion along the x axis of the wire can take an infinitely large magnitude [8], therefore we will face to a one-dimensional

$$\frac{-\hbar^2}{2m^*}\left[\frac{\partial^2\psi(y,z)}{\partial y^2} + \frac{\partial^2\psi(y,z)}{\partial z^2}\right] = \left(E_{y,z} - V(y,z)\right)\psi(y,z) \quad , (3)$$

Where the full solution to Eq. (1) is given by

$$\psi(x,y,z) = \psi(x)\psi(y,z) \quad , (4)$$

Expanding Eq. (3) in terms of finite differences, while ensuring that the step lengths δy and δz are small in magnitude so that the approximation is valid, yields

, (5)

In order to solve Eq. (5) numerically for ψ(y, z), it is necessary to divide the cross-section of the wire into blocks of

$$(\delta y)^2\left[\psi(y,z+\delta z)+\psi(y,z-\delta z)\right]+(\delta z)^2\left[\psi(y+\delta y,z)+\psi(y-\delta y,z)\right]-\left[\frac{-2m^*}{\hbar^2}\left(E_{y,z}-V(y,z)\right)(\delta y\delta z)^2+2\left((\delta y)^2+(\delta z)^2\right)\right]\psi(y,z)=0.$$

, (5)

In order to solve Eq. (5) numerically for ψ(y, z), it is necessary to divide the cross-section of the wire into blocks of

is now characterized by its corresponding row and column indices, i.e. (i, j). Rewriting Eq. (5) in terms of these indices yields

$$(\delta y)^2\left[\psi_{i,j+1}+\psi_{i,j-1}\right]+(\delta z)^2\left[\psi_{i-1,j}+\psi_{i+1,j}\right]-k\psi_{i,j}=0.$$

, (6)

Where

$$k=\frac{-2m^*}{\hbar^2}\left(E_{y,z}-V\right)(\delta y\delta z)^2+2\left((\delta y)^2+(\delta z)^2\right)$$

, (7)

Eq. (6) idicates that the value of the wave function at each point correspond to the four surrounding grid point.

Hence, the wave function can be calculated for any energy by solving the sets of simultaneous equations created by Eq. (6), if an appropriate fluctuating value is chosen. This fluctuation has to own a non-zero value; otherwise the solution to this system of linear equations cloud be uniformly zero. Since energy eigenvalues are independent of scaling the wave function by a constant factor, we can select the following perturbation value

$$\psi_{1,1}=1.$$, (8)

The current method is associated with the ability to write the simultaneous equations into a single matrix equation.

The matrix equation has the following form:

$\boldsymbol{A}.\boldsymbol{\Psi}=\boldsymbol{S}$, (9)

Where A is the wave function coefficient matrix and $\boldsymbol{\Psi}$ is a column vector of the wave function that corresponds to points take part in oscillation. S is a column vector consisting of the source terms. They are called the source terms because of a duality between the current equation and heat transfer equation which is solved in a same manner. In the current equation the source is replaced by the perturbation value. The standard boundary conditions, given below, are satisfied with all solutions.

ψ(y, z)→0 as z→±∞, (10)

ψ(y, z)→0 as y→±∞. (11)

This can be done by putting all the outermost array elements equal to zero (indicated as the dashed lines in Fig. 2). The computational domain was selected to be such large to ensure us that the derivatives and the eigenvalues do not vary with computational domain. Thus, it is only necessary to calculate the internal points of the array,as a result of that we reduce the number of unknowns to [n1 ×n2]. Also, since $\psi_{1,1}$ is defined by the fluctuation value of Eq. (8), there exist only

infinitesimal length δz and height δy. The wave function is now mapped to the elements of this two-dimensional array.

These array elements can now be characterized in the typical way. The value of δz is chosen so that the total width of the wire, Lz, is indicated by the total number of columns, n1 + 2. Similarly, δy is selected so that the total height of the wire, Ly , is indicated by the total number of rows, n2 + 2. For simplicity in notes,the value of the wave function at each array point

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[n1×n2]−1 points which are supposed to calculate. In order to simplify the problem more, δz = δy is supposed.

Thus the column vector $\boldsymbol{\Psi}$ is going to consist of n = [n1 × n2] − 1 elements, which is the total number of unknown elements and is given by Eq. (12). It is composed of a total number of n2 blocks such that each of them have length of n1 elements, with this assumption that, first block which consists of n1−1 elements ,for $\psi_{1,1}$ is already characterized

$$\Psi=\begin{pmatrix}\psi_{1,2}\\ \psi_{1,3}\\ \vdots\\ \psi_{1,n_1}\\ \psi_{2,1}\\ \vdots\\ \psi_{n_2,n_1}\end{pmatrix}$$, (12)

Then the matrix A will be a (n × n) scattering matrix. The best way to indicate this matrix, is employing the associated sub-matrices. Here, there are n2 blocks or sub-matrices, which can be written as follows:

$$A=\overbrace{\begin{pmatrix}\beta_1 & I_1 & 0 & \cdots & \cdots & 0\\ I_2 & \beta & I & 0 & \cdots & 0\\ 0 & I & \beta & I & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & \ddots & 0\\ 0 & \ddots & 0 & I & \beta & I\\ 0 & \cdots & \cdots & 0 & I & \beta\end{pmatrix}}^{n_2\ Blocks}$$, (13)

Where the sub-matrices β_1, β, I_1, I_2 and I, have been used from the references[5-10]. Finally, the matrix S is a column vector of n elements and takes the following form:

$$S = \begin{pmatrix} -\psi_{1,1} \\ 0 \\ \vdots \\ 0 \\ -\psi_{1,1} \\ 0 \\ \vdots \\ 0 \end{pmatrix} , (14)$$

The general forms of the preceding matrices which have been developed here, created here by using the MATHEMATICA package like several other computer softwares available, which can be employed to solve this system of equations. For these calculations the preceding package was used.

TRIANGULAR NANOWIRE MODEL

The infinitely deep rectangular cross-section wire for testing the finite differences technique has studied in literature [9]. The analytical results of this model would be calculated easily and using it ensures us for every potential geometry cross section type. The model is considered here will be a nanowire with right-angle equilateral triangular cross section that has been studied in some researches (Fig. 1). The purpose of this model is the development of the numerical method and its performance on other potentials. The potential energy in the NW, around it, in the cube and outside the cube will be considered zero, 5000 (meV) and infinity, respectively as the Fig. 1.

In association with potential energy we can introduce k factors in the two part of the model, k_1 inside the nanowire with $V_1 = 0$ and k_2 outside the nanowire due $V_2 = 5000(meV)$ in the cube and k sum of k_1 and k_2 as the forms;

$$k_1 = \frac{-2m^*}{\hbar^2}\left(E_{y,z} - V_1\right)\left(\delta y \delta z\right)^2 + 2\left(\left(\delta y\right)^2 + \left(\delta z\right)^2\right) \quad (15)$$

$$k_2 = \frac{2m^*}{\hbar^2}\left(V_2\right)\left(\delta y \delta z\right)^2 , (16)$$

$$k = k_1 + k_2 \quad (17)$$

In the above equations, parametric constants of models involves electron effective mass and step lengths δy and δz will be considered; $m^* = 0.067m$ and $\delta y = \delta z = 1(A)$. The ranks of Matrices that are obtained by schorodinger equation are 435 to 1635. Essential part of finding the right energy occurs when the wave function is obtained with the highest symmetry(Fig2). Deviation of the actual amount of energy, equivalent to $0.1(meV)$ creates a turbulence at the beginning of the probability function(Fig3).

By these definitions and finite difference approach the ground state energy has been calculated. These amounts to 8 NWs consecutive linearly increases in size in Table 1 were obtained. According to these values, it can be seen that by increasing the size of the wire cross-section area decreases the energy that is in accord with other similar works [5-10]. In addition, with increasing wire size also reduced the gap between energy levels, which is consistent with our expectation in quantum systems (Fig 5).

An illustration of nearby symmetrical probability function is shown in Fig. 4 at the $y = 11$ plane that it occurs in the correct energy. These energies are decreasing when the dimensions of NWs are increasing also we expect and this is shown in Fig. 5. Furthermore, it is found that the runtime by Computer CPU verses nanowire dimensions are not linear when dimensions increased linearly (Fig. 6).

Another interesting topic that comes from drawing an analogy with the well-Delta wave at the apex of the triangle. Because in the apex of triangle, the width of the well is dropped to the Dirac delta function (Fig.7). Calculations for these NWs obtained by a PC with Core i7 CPU and 8 GB RAM.

CONCLUSION

In this paper the Schrödinger equation for a quantum wire with triangular cross-section is solved using finite difference approach. The ground state energy is obtained with a good approximation. At this value, the wave and probability functions have the best symmetry resulted from the geometrical symmetry. Deviating as much as $0.1(meV)$ from the exact ground state eigenvalue, the probability function symmetry is destroyed and perturbation will be appearing. The maximum of the probability function occurs on the height of the triangular at $\frac{11}{18}H$ from the vertex which the height H is drawn. Furthermore, by leaving the vertex and approaching to base, the width of probability function increases. This justifies our expectation that the quantum well width would be increased.

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Fig1. Nanowire with right-angle equilateral triangular cross section and potential energy in differences parts.

Fig2. Cross-sections of Probability function by y plans from 1 to 18 of a nanowire with $n_1 = 33$ and $n_2 = 17$, respectively. The symmetry takes place in the exact value of $E_{gs} = 3155.2\ (meV)$.

Fig3. Cross-sections of Probability function in by y planes from 1 to 18 of a nanowire with $n_1 = 33$ and $n_2 = 17$, respectively. The $0.1(meV)$ deviation from exact value shows perturbation in the beginning of the Probability function

at $E_{gs} = 3155.1\ (meV)$.
Fig4. Cross-section of Probability function in $y = 11$ plane of a nanowire with $n_1 = 33$ and $n_2 = 17$. The symmetry takes place in the exact value of $E_{gs} = 3155.2\ (meV)$.
Fig5. Black curve shows variation of GS Energy level while n_1 increases linearly. Horizontal lines shows variation energy gaps between consecutive NWs.
Fig6. Runtime by computer when n_1 is increasing linearly will not linear.
Fig7. Cross-section of Probability function in $y = 3$ plane of a nanowire with $n_1 = 33$ and $n_2 = 17$. Because of the potential well width is trivial at the vertex of triangular the Probability function behaves like delta function potential.

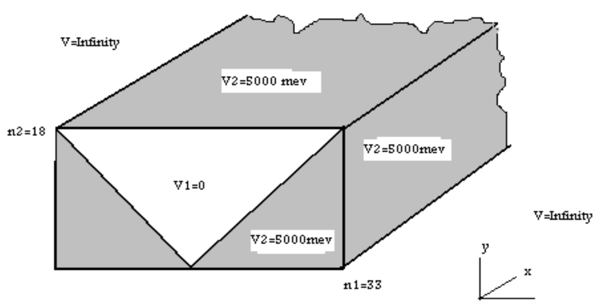

Fig1

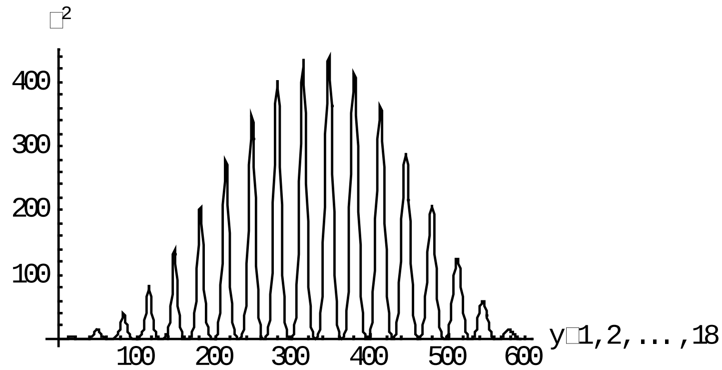

Fig2

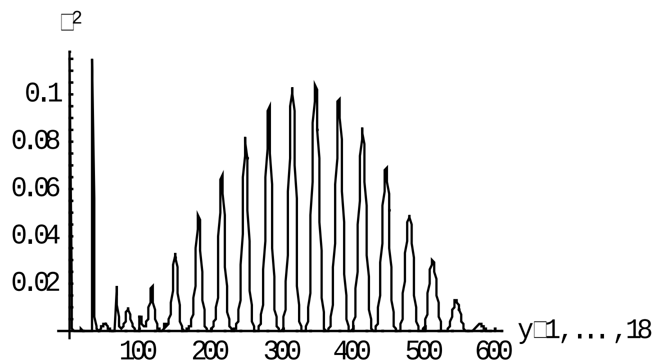

Fig3

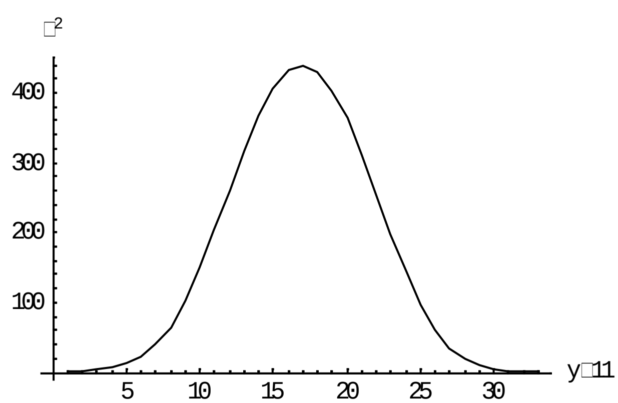

Fig4

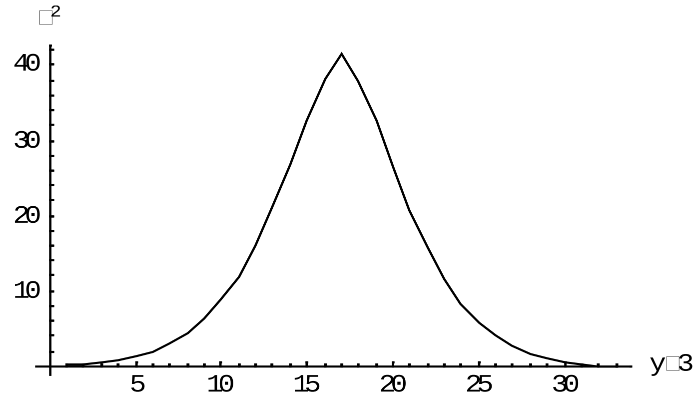

Fig7

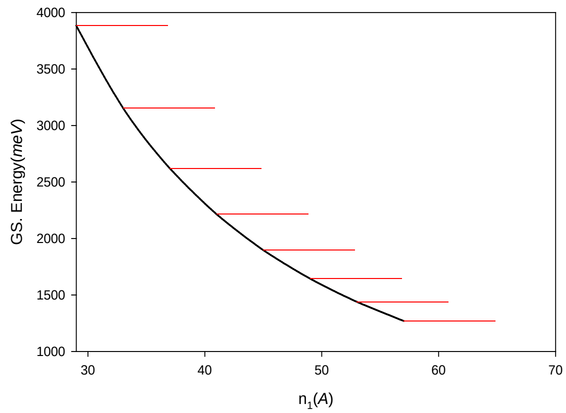

Fig5

n_1	n_2	$n_1.n_2$	E_{gs}	Run time(s)
29	15	435	3883.4	53
33	17	561	3155.2	99
37	19	703	2620.8	175
41	21	861	2214.6	295
45	23	1035	1896.7	465
49	25	1225	1644.4	714
53	27	1431	1439.5	1206
57	29	1635	1270.2	1965

Table1: GS energies, runtimes, dimensions and triangular areas of NWs.

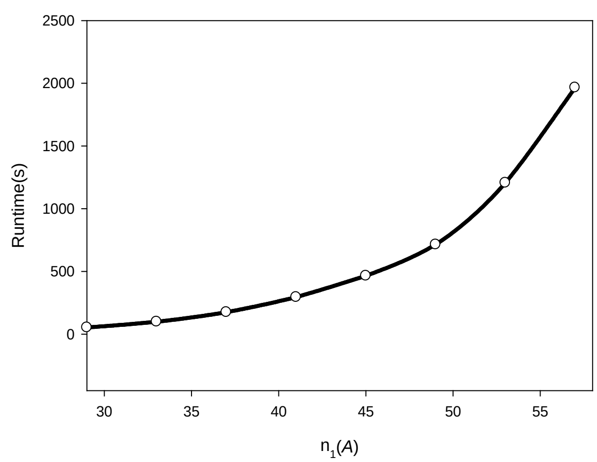

Fig6