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Electronic energy state and transmission properties study of parabolic double quantum well using Non-Equilibrium Green function method

M. Batı[1,*]

[1]Department of Physics, Recep Tayyip Erdoğan University, Rize, Turkey

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*Correspondence E-mail: mehmet.bati@erdogan.edu.tr

ABSTRACT We apply the non-equilibrium Green's function method based on the finite difference method to the parabolic double quantum well structure. In particular, we examine the effect of system parameters on transmission coefficient. The properties of the electronic state also studied as a function of the system parameters, such as, the well widths and depth. We also tested energy electronic state with calculating density of states.

Keywords: Non-equilibrium Green Functions; Finite Difference Method; Parabolic Double Well; Transmission.

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1. INTRODUCTION

According to Moore's famous law [1], states that the number of transistors on integrated circuits doubles every year. Last decades semiconductor devices already reached the limit to the nano-scale. The non-equilibrium Green's function (NEGF) method [2] are extensively used method for finding transmission properties in nanoscale devices.

Quantum wells are semiconductor structures in which we can observe and control many quantum mechanical effects. Recent developments in nanofabrication technologies have allowed us to fabricate variety type of wells. Such as, parabolic quantum wells (PQWs) which are related the development of high performance semiconductor devices (infrared detectors, cascade lasers, etc.) [3-6].
The properties of the electronic state in the PQW were studied in experimentally and theoretically [7,9]. Because of the unique properties (equally spaced electronic spectrum, radiative transitions at the same oscillator frequency etc.), researchers [10, 11] studied the electronic state in the PQW by using different methods to derive the energy levels. PQW has been widely investigated and some new properties of electrons are obtained [12, 13]. PQWs have been applied to study non-linear optical properties [14], the quantum Hall effect [15], charge, spin oscillations [16], magnetic properties and photoluminescence measurements [17, 18]. Capasso and Kiehl proposed a resonant-tunneling bipolar transistor with a smooth parabolic well [19, 20].

The aim of the present work is to study transmission properties and electronic states in one dimensional double GaAs/AlGaAs PQW using NEGF method.

2. MODEL AND METHOD

We apply the NEGF method to find electronic eigen-state and transmission characteristic of parabolic double quantum well (PDQW). As depicted in Fig. 1, L_i denotes the region boundary of the structure.

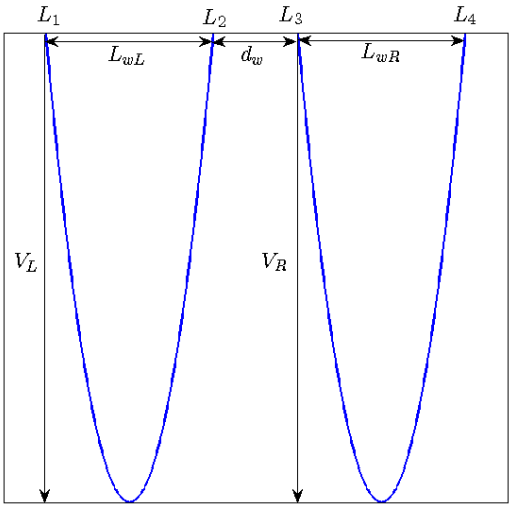

Fig. 1. Schematic representation of one-dimensional parabolic double quantum well.

An ideal parabolic potential well represents a "Harmonic oscillator well" which is described in quantum mechanics textbooks. One-dimensional PDQW potential can be written as

$$\boldsymbol{U(x)} = \begin{cases} \boldsymbol{a_L(x-(L_1+L_2))^2 - V_L}, & \boldsymbol{L_1 \le x \le L_2} \\ \boldsymbol{a_R(x-(L_3+L_4))^2 - V_R}, & \boldsymbol{L_3 \le x \le L_4} \\ \boldsymbol{0}, & \boldsymbol{odher\ wise} \end{cases} \quad (1)$$

where, $\boldsymbol{a_L} = \frac{\boldsymbol{V_L}}{\boldsymbol{(L_{wL})^2}}$, $\boldsymbol{a_R} = \frac{\boldsymbol{V_R}}{\boldsymbol{(L_{wR})^2}}$, left well width is $\boldsymbol{L_{wL}} = \boldsymbol{|L_2 - L_1|}$, and right well width is $\boldsymbol{L_{wR}} = \boldsymbol{|L_4 - L_3|}$ and distance between two well is $\boldsymbol{d_w} = \boldsymbol{|L_3 - L_2|}$. We use dimensionless form of the Schrödinger equation by using the Effective Bohr radius ($\mathbf{a_0^*}$) and Hartree energy ($\mathbf{E_H^*}$) for scales. So, Schrödinger equation becomes

$$-\frac{1}{2}\frac{d^2\psi}{d\tilde{x}^2} + \tilde{U}(\tilde{x})\psi = \tilde{E}\psi \quad (2)$$

Finite difference discretization method applied to the equation (2) as follows [2]:

$$-\tilde{t}\psi_{n-1} + \left(2\tilde{t} + \tilde{U}_n\right) - \tilde{t}\psi_{n+1} = E\psi_n \quad (3)$$

where $\tilde{t} = \frac{1}{2\Delta\tilde{x}^2}$ is the hopping parameters, and we use abbreviation $\tilde{U}_n = \tilde{U}(\tilde{x}_n)$. Including self-energies and considering matrix representations, the new form of Eq.2 becomes

$$[EI - H - \Sigma_L - \Sigma_R]\{\psi\} = \{S\} \quad (4)$$

where [H] is the Hamiltonian matrix [I] is the identity matrix, $\{\psi\}$ is the wave function vector and $\{S\}$ is scattering term vector. Σ_L and $\Sigma_R$are corresponding to the self-energies of the left and right contacts, respectively. Accordingly, [H] takes form as:

$$\begin{pmatrix} 2\tilde{t}+\tilde{U}_1 & -\tilde{t} & 0 & \cdots & 0 & 0 \\ -\tilde{t} & 2\tilde{t}+\tilde{U}_2 & -\tilde{t} & \cdots & 0 & 0 \\ 0 & -\tilde{t} & 2\tilde{t}+\tilde{U}_3 & \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & \ddots & -\tilde{t} & 0 \\ \vdots & \vdots & \ddots & -\tilde{t} & 2\tilde{t}+\tilde{U}_{N-1} & -\tilde{t} \\ 0 & \cdots & 0 & 0 & -\tilde{t} & 2\tilde{t}+\tilde{U}_N \end{pmatrix}$$

In addition, self-energy terms $[\Sigma_L]$, $[\Sigma_R]$ and source term $\{S\}$ are given by

$$[\Sigma_L] = \begin{pmatrix} -\tilde{t}e^{i\tilde{k}_L\Delta\tilde{x}} & 0 & \cdots & 0 \\ 0 & 0 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & & \cdots & 0 \end{pmatrix},$$

$$[\Sigma_R] = \begin{pmatrix} 0 & \cdots & & 0 \\ \vdots & \ddots & & \vdots \\ 0 & & 0 & 0 \\ 0 & \cdots & 0 & -\tilde{t}e^{i\tilde{k}_R\Delta\tilde{x}} \end{pmatrix},$$

$$\{S\} = \begin{pmatrix} -\tilde{t}(e^{i\tilde{k}_L\Delta\tilde{x}} - e^{-i\tilde{k}_L\Delta\tilde{x}} \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

There are several methods for finding the energy eigenvalues corresponding to a particular potential. One can use eigenvalues of [H] matrix to find energy eigenvalues. The retarded Green's function of the system is

$$[G^r] = [(E + i\lambda)I - H - \Sigma_L - \Sigma_R]^{-1} \quad (5)$$

where λ is an infinitesimally small positive number. Transmission coefficient T can be computed as

$$T = Tr[\Gamma_L G^r \Gamma_R G^{r+}] \quad (6)$$

Here, $\Gamma_L = i[\Sigma_L - \Sigma_L^+]$ and $\Gamma_R = i[\Sigma_R - \Sigma_R^+]$ are broadening functions. Finally, density of states (DOS) can be computed as follows

$$DOS = -\frac{1}{\pi} Im(Tr[G^r]). \quad (7)$$

3. RESULTS

Here, transmission coefficient (T) in parabolic quantum well structure is investigated, we assume the effective mass of the electron $0.067m_0$ to be constant through the system. The transmission coefficients are numerically evaluated across PDQW structure with different structure parameter. Lowest ten energy states for different structure parameters are presented in Tables. There are bound states and scattering state. Number of energy states is altering with changing structure parameters.

We examine the dependence of the transmission coefficient on the well width as depicted in Fig.2. We can see in Fig. 2 and also Table 1 number of energy levels (bound and scattering states) increases with increasing well width. We see that in Table2 because of the increment of well depth, the confinement becomes stronger and so number of bound state increases.

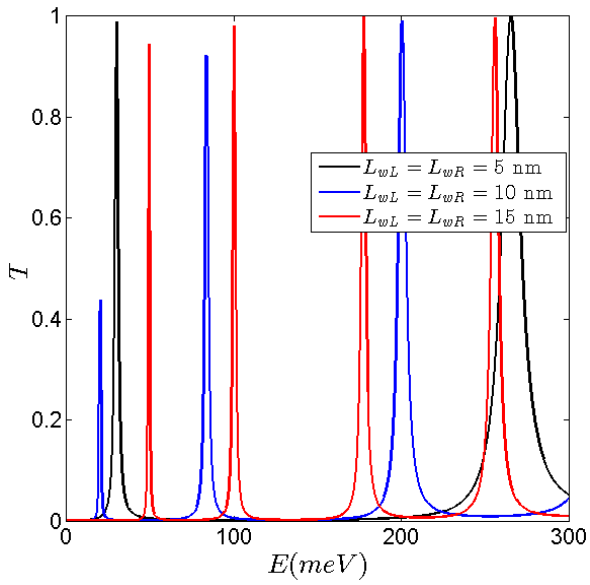

Fig. 2. Transmission probability versus electron energy. Structure parameter is V_L=V_R=150 meV 〖,d〗_w=1 nm

In order to illustrate the effect of well separation, we plot Fig.3 for $V_L = V_R = 150$ meV, $L_{wL} = L_{wR} =$ 10 nm. We can see that in Fig.3 and Table 3 energy level decreases with increasing well separation.

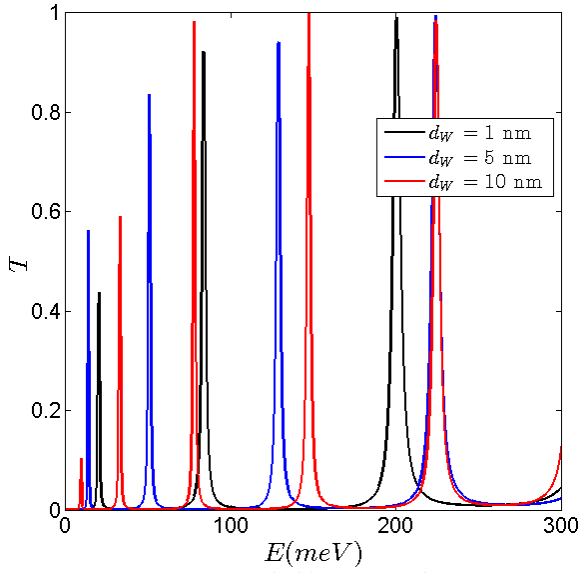

Fig. 3. Transmission probablity versus electron energy. Structure parameter is V_L=V_R=150 meV, L_wL=L_wR=10 nm

Density of states (DOS) is calculated for 5 nm, 10 nm and 15 nm symmetrical well width structures by calculating the diagonal elements of retarded Green's function. As shown in Fig.4 the first peak in the DOS for all structure is sharp and high. Energy level position is consistent to the T(E) in Fig.2. Existence of sharp resonance states are reported form the knowledge of density of states [16]. DOS also helps to predict the device performance.

Table 1. Eigen states of PDQW with different well width for V_L=V_R=150 meV, d_w=1 nm

$L_{wL} = L_{wR} = 5\ nm$ Eigen-states (E-S) (meV)	$L_{wL} = L_{wR} = 10\ nm$ E-S (meV):	$L_{wL} = L_{wR} = 15\ nm$ E-S (meV):	$L_{wL} = L_{wR} = 20\ nm$ E-S (meV):
-46.5	-93.7	-111.2	-120.7
-44.1	-80.3	-108.6	-120.1
295.3	242	-36.1	-63.1
579.6	213.3	-15.5	-56.9
965.4	341.2	52.6	-5.6
1427.3	502.6	105.8	17.9
1974.9	682.7	185.2	68.7
2607.1	890.1	266.7	112.3
3321.5	918.0	365.2	171.1
4122.4	1120.0	471.4	230.8

Table 2. Eigen states of PDQW with different well depth for L_wL=L_wR=10 nm, 〖d〗_w=1 nm

$V_L = V_R = 150\ meV$ Eigen-states (E-S) (meV)	$V_L = V_R = 300\ meV$ E-S (meV):	$V_L = V_R = 600\ meV$ E-S (meV):	$V_L = V_R = 900\ meV$ E-S (meV):
-93.7	-217.7	-482.7	-756.3
-80.3	-211.9	-481.2	-755.8
24.2	-58.8	-250.6	-469.4
91.8	-13.6	-233.2	-462.4
213.3	129.8	-25.7	-190.0
341.2	245.7	52.4	-146.1
502.6	413.7	246.5	92.7
682.7	590.0	405.7	221.3
890.1	799.3	622.9	454.9
1120.0	1028.0	845.8	665.5

Table 3. Eigen states of PDQW with different well separation for 〖V_L=V〗_R=150 meV, L_wL=L_wR=10 nm

$d_w = 1\ nm$ Eigen-states (E-S)(meV)	$d_w = 5\ nm$ E-S(meV):	$d_w = 10\ nm$ E-S(meV):	$d_w = 20\ nm$ E-S(meV):
-93.7	-88.6	-87.4	-87.2
-80.3	-85.8	-86.9	-87.2
24.2	16.5	10.9	5.5
91.8	56.0	36.4	19.7
213.3	136.3	82.7	41.4
341.2	235.6	153.5	74.2
502.6	343.3	233.9	119.3
682.7	475.2	321.0	173.2
890.1	621.8	424.0	231.8
1120.0	784.7	540.4	294.9

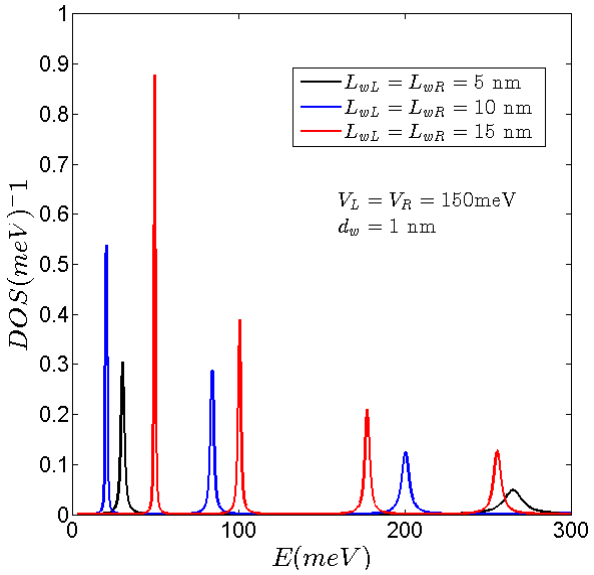

Fig. 4. DOS

4. CONCLUSION

Numerical results of the transmission coefficient are obtained for several parabolic double quantum well structures. We are found that the energy states and resonant peaks shift towards the lower energy region as the distance between wells increases. New resonant peaks emerge when the well widths or depths become wider. These structures are useful for the design of electronic devices.

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Biographies

Mehmet BATI was born on March 01, 1984 in Midyat, Turkey. In 2001, he graduated the high school "Kemalpaşa Lisesi" in İzmir, in 2006, he graduated from Dokuz Eylül University with first-degree in faculty of art and science. He earned a master degree in Physics from the Erciyes University and a Ph.D. degree from the Dokuz Eylül University. He is married and has two children.