Transfer Matrix Method for Computation of Electron Transmission Through Aperiodic MQW

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Abstract— **This paper presents the Eigen values and corresponding Eigen functions for the electron states in an aperiodic and asymmetric Multiple Quantum Well structure. A faster, simpler, and accurate algorithm based on Transfer Matrix method has been introduced for solving time independent Schrödinger equation in the most general case of aperiodic and asymmetric MQW structure. The MQWs are aperiodic with varying well and barrier widths and asymmetric i.e., having different materials and effective masses for the different regions of the wells and barriers. Adjacent wells are coupled through the barriers. Effect of barrier width on the tunneling properties has also been investigated. The theoretical results are compared with experimental results of Giorgetta et all [1]. Results of the computation based on the general model agree well with experimental data.**

Keywords **- *Multiple Quantum wells, Optical Devices,***

Transfer Matrix method, Quantum Tunneling.

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I. INTRODUCTION

The quantum mechanical tunneling through multiple quantum wells is a long-standing and well-known problem. Three methods proposed earlier for calculating the tunneling probabilities and energy splitting i.e., (1). Instanton Method (2) WKB Approximation and (3) Numerical Calculation. Instaton method is helpful having a physical insight of quantum tunneling but the validity is restricted to the case of large separation between the two potential minima. WKB approximation is widely used in its simple mathematical form, but the result is inaccurate due to its inherent defect in connection formula. Recently WKB approximation has been developed by changing the phase loss at the classical turning points but none of the above approximations have provided the perfect result. Using numerical methods, one can get the solution up to the desired accuracy, but a considerable deal of physical insight is lost in this process. In this paper a general model for multiple quantum wells or barriers have been developed without over simplistic assumptions by using analytical Transfer matrix method (ATMM), which has been applied to any arbitrary potential well and barrier sequence successfully.

In recent times low dimensional carrier systems in the semiconductor heterostructures are gaining much importance due to the potential use of their unique properties in applications ranging from optoeltronics to high speed devices [1-4]. Perpendicular transport of the carriers in semiconductor heterostructures has attracted much attention [1-7]. The MQW structures are becoming very important due to their potential use in the device design and fabrication of quantum cascade lasers, Quantum Infra-red photo-detectors (QWIP), Quantum cascade detector (QCD), resonant photodetectors, resonant tunneling diodes, single electron tunneling transistors [8] etc. Recently much research is carried out in the field of semiconductor QWIP and QCD [1-5]

In this paper a general mathematical model has been developed that helps in evaluating the tunneling probability and energy Eigen values inside asymmetric and aperiodic MQW structures. The model is tested on the experimental data for a 16.5 μm QCD of reference [1]. This model will also help in studying the tunneling of carriers one well to another through a quantum barrier. Tunneling depends significantly on the barrier width. Scaling of structure dimension affects this variation very sharply. The theory has been based on the 'transfer matrix' method [5-8].

The mathematical model is tested is an array of $In_{.53}Gs_{.47}As/In_{.52}Al_{.48}As$ layers of thicknesses 157/**55**/69/**26**/90/**43**/94/**40**/95/**38**/96/**28 in A^0** [1]. The first two wells have widely different widths and the barriers that separate them and flank the pair on either side are of unequal width. The effective mass of the carriers are different inside the well and in the barrier, which are made of different materials. The model is tested on this well pair to match the computed result of coupled energy states with those obtained experimentally.
The wells widths are varying very slightly with the barrier width. The wells and barriers widths 90/**43**/94/**40**/95/**38**/96 can be approximated by a periodic pattern. Under this circumstance the general model can be simplified and the energies are computed. The comparison with experimental data proves encouraging.

II. THEORY

Numerical device simulation is an important procedure for the design and optimization of novel semiconductor devices. In this paper we have started with most generalized case where the well widths and barrier widths are all unequal, the well and barrier materials can be different with different barrier heights and effective electron masses. If we assume that the barrier widths are such that adjacent wells are coupled through the barriers then we will have to deal with five wave functions; the wave functions of the electrons inside the wells and the electron wave functions for the barriers on either side of these wells. We had considered the general quantum structure as shown in Fig. 1 where a series of three barriers of widths 2d, 2b and 2f with wells of width 2a and 2c between the barriers 2d and 2b and 2f respectively. The well barrier combination is shown below.

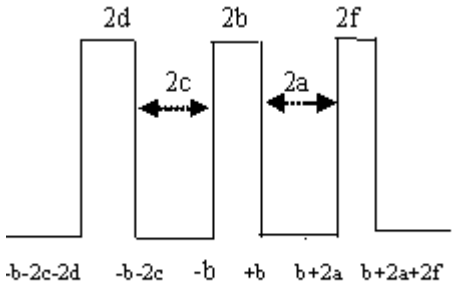

Figure 1: Array of MQWs.

The Schrödinger wave equation according to the effective mass theory for the finite potential barrier and the well regions on either side take on the well known form

$$(\hbar^2/2m^*)\, d/dx\{d\Psi/dx\} + (E-V)\,\Psi = 0 \qquad (1)$$

where m* is the effective mass, h, is the Planck's constant E, is the energy Eigen values and v is the potential energies for the region where the equation is defined. The effective mass $m^* = m_B$ inside the the barrier region with potential energy is V_o , and $m^* = m_w$ outside the barrier and potential energy is zero.

The general solution of the Schrödinger equation for the Quantum well and barrier region obtained are given by Equations (2) to (6).

$\Psi_{B1}(x) = A_{B1} \exp(ik_{B1}x) + B_{B1} \exp(-ik_{B1}x)$ (2)
for $-(b-2c-2d) < x < -(b+2c)$ in the first barrier

$\Psi_{W1}(x) = A_{W1} \exp(ikw_1x) + B_{W1}\exp(-ik_{W1}x)$ (3)
for $-(b+2c) < x < -b$ inside the first well

$\Psi_{B2}(x) = A_{B2} \exp(ik_{B2}x) + B_{B2} \exp(-ik_{B2}x)$ (4)
for $-b < x < +b$ in the second barrier.

$\Psi_{W2}(x) = A_{W2} \exp(ikw_2x) + BW_2 \exp(-ik_{W2}x)$ (5)
for $b < x < b+2a$ inside the second well

$\Psi_{B3}x) = A_{B3} \exp(ik_{B3}x)$ (6)
for $(b+2a) < x < (b+2a+2f)$ in the second barrier

Where $k_{Bn} = (2m_n [Vo_n - E]/\hbar^2)^{1/2}$ and $k_{Wi} = (2m_{Wi}E/\hbar^2)^{1/2}$ with m_{wi} and m_{Bn} are the electron effective masses in the well and barrier regions respectively.

In the most general case the barrier heights Vo_n and electron effective masses m_{wi} and m_{Bn} in the different regions are assumed to be all different.

Now we apply boundary conditions, the continuity of the wave functions $\Psi_{Bn}(x) = \Psi_{Wi}(x)$ at each boundary and Ben Daniel Duke (BDD) boundary condition relates the flux of electrons incident on the barrier to that which penetrates it:

$(1/m_{wi})[d\Psi_{Wi}(x)/dx] = (1/m_{Bn})\,[d\Psi_{Bn}(x)/dx]$ (7)
at well-barrier interface.

The implementation of the transfer matrix method has been carried by Appling appropriate boundary conditions as described above.

$$\begin{bmatrix} A_j \\ B_j \end{bmatrix} = \begin{bmatrix} M_{11}^{[j]} & M_{12}^{[j]} \\ M_{21}^{[j]} & M_{22}^{[j]} \end{bmatrix} \begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} \qquad (8)$$

Using equation (3) we obtained the coefficients of the wave function at the leftmost slab to those of the right most slab

$$\begin{bmatrix} A^j \\ B^j \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -ik_w^{-1} \\ 1 & ik_w^{-1} \end{bmatrix} [M_j] \begin{bmatrix} 1 & 1 \\ ik_w & -ik_w \end{bmatrix} \begin{bmatrix} A_{j+1} \\ B_{j+1} \end{bmatrix} \qquad (9)$$

Where M_J is the jth transfer matrix corresponding to the jth junction written as:

$$M_j = M_b(b_j)M_w(a_j)M_b(b_{j+1}) \qquad (10)$$

Applying the boundary conditions we find in the above equations we find the following result involving the coefficients that define the wave functions.

$$A_{B1} = \frac{m_b}{2k_1}\left(\frac{k_1}{m_b} + \frac{k_2}{m_w}\right) e^{i(k_1 - k_2)(b+2c)} A_{w1} + \frac{m_b}{2k_1}\left(\frac{k_1}{m_b} - \frac{k_2}{m_w}\right) e^{i(k_1 + k_2)(b+2c)} B_{w1} \qquad (11)$$

$$B_{B1} = \frac{m_b}{2k_1}\left(\frac{k_1}{m_b} - \frac{k_2}{m_w}\right)e^{-i(k_1+k_2)(b+2c)}A_{w1} + \frac{m_b}{2k_1}\left(\frac{k_1}{m_b} + \frac{k_2}{m_w}\right)e^{-i(k_1-k_2)(b+2c)}B_{w1} \quad (12)$$

Which can be written in the Matrix form as:

$$U_1 = T^1 U_2 \ , \ U_i = \begin{bmatrix} a_i \\ b_i \end{bmatrix}, \ i = 1, 2 \text{ etc} \quad (13)$$

$$\text{With } T^1 = \frac{m_b}{2k_1}\begin{bmatrix} T^{11} & T^{12} \\ T^{21} & T^{22} \end{bmatrix} \quad (14)$$

Where

$$T^{11} = \left(\frac{k_1}{m_b} + \frac{k_2}{m_w}\right)e^{i(k_1-k_2)(b+2c)}$$

$$T^{12} = \left(\frac{k_1}{m_b} - \frac{k_2}{m_w}\right)e^{i(k_1+k_2)(b+2c)}$$

$$T^{21} = \left(\frac{k_1}{m_b} - \frac{k_2}{m_w}\right)e^{-i(k_1-k_2)(b+2c)}$$

$$T^{22} = \left(\frac{k_1}{m_b} + \frac{k_2}{m_w}\right)e^{-i(k_1-k_2)(b+2c)}$$

In completely, we obtained the transfer matrix T^2at the slice x = 2c and $U_2 = T^2 U_3$

$$\gg U_1 = T^1 U_2 = T^1 T^2 U_3 \quad (15)$$

Doing this for all the slices X_1…….X_N, we obtained the complete transfer matrix M that connect the wave function on the left side of the potential with one of the right side,

$$U_1 = MU_{N+1} \quad (16)$$

Where $M = T^1 T^2 \ldots\ldots\ldots\ldots T^N$

If it is assumed that there is no reflected wave in the region N and the amplitude of the incident wave is unity, then we find:

$$\begin{pmatrix} A_{BN} \\ 0 \end{pmatrix} = M\begin{pmatrix} 1 \\ B_{B1} \end{pmatrix} \quad (17)$$

Using these above equations we obtained the value of coefficient of wave functions.

The Matrix equation is very complex and involves a large number of terms. By putting $\tau = 1$ we get the coupling energy between two adjacent wells . This iterative method will yield the energy for which electrons may be coupled to both the wells by penetrating through the intervening barrier.

This mathematical model is tested on an array of $In_{.53}Gs_{.47}As/In_{.52}Al_{.48}As$ layers of thicknesses 157/**55**/69/**26**/90/**43**/94/**40**/95/**38**/96/**28 in A^0** [1]. The first two wells have widely different widths and the barriers that separate them and flank the pair on either side are of unequal width. The effective mass of the carriers are the same in both the wells ($m_{w1}=m_{w2}=m_w$) but different from that in the barriers, which are made of the same material so that $m_{B1}=m_{B2}=m_{B3}=m_B$. The barrier hights in all the barrier regions are same and equal to V_o. The expression for the transmission coefficient simplifies and becomes

$$\tau = 16(k_B k_W)^2 / [(m_B m_W)^2\{(k_B/m_B) + (k_W/m_W)\}^4 + \{(k_W/m_W) - (k_B/m_B)\}^4 - 2\{(k_W/m_W)^2 - (k_B/m_B)^2\}^2\cos(4ck_B)\}] \quad (18)$$

The Eigen value energy equation takes the form

$$(m_W k_B)/(m_B k_W) = \tan(ck_B)/\tan(ck_W) \quad (19)$$

Where c is the well width.

The coupling energies obtained from equation (19) when the transmission coefficients given by equation (18) will tend to unity.

III. RESULTS AND DISCUSSIONS:

The general model of AMQW structure is tested on the MQW structure of a 16.5µm quantum cascade detector proposed by Giorgetta et al [1]. The effective electron mass of the well material $In_{.53}Gs_{.47}As$ is taken to be $m_W = 0.043m_o$ [18] and that of the barrier layer of $In_{.52}Al_{.48}As$ is $m_B = 0.072m_o$. The well and barrier widths that alternate are given in Angstroms as 157/**55**/69/**26**/90/**43**/94/**40**/95/**38**/96/**28** [1]. The conduction band offset for $In_{.53}Gs_{.47}As/In_{.52}Al_{.48}As$ pair is 0.51eV. [8-11]

The energy values obtained from the computation agrees well with the experimental data. The comparison is given in table-1 and the wave functions for the structure are shown in figure 2. This compares well with the experimental data given in figure 3.

At the Eigen values the transmission probabilities are unity are shown in table-01. These computed values agree quite well with the experimental values given in figure 2. Tunnelling at around 0.2eV is very clearly indicated.

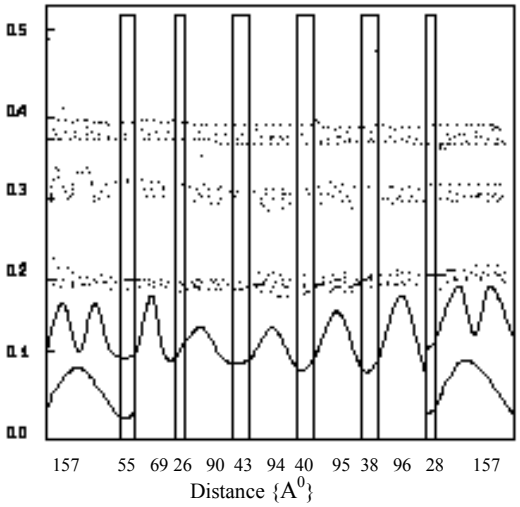

Fig 2. Calculated Band structure 16.5 µm QCD

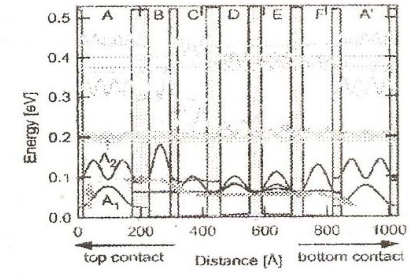

FIG. 1. Band structure of one period of the 16.5 μm QCD. $In_{53}Ga_{47}As/In_{52}Al_{48}As$ layer thicknesses in angstrom from left to right: 157/55/69/26/90/43/94/40/95/38/96/28. The arrows show the photocurrent path.

Fig 3. Band structure of experimental data of Giorgetta [1].

Table-1

Experimental Results (R. Giorgetta et al)	Theoretical results (Computed)
E1 = 0.02 eV	E1= 0.02 eV
E2 = 0.10 eV	E2 = 0.1014eV
E3 = 0.20 eV	E3 = 0.1959eV
E4= 0.30 eV	E4 = 0.2899eV
E5 = 0.40 eV	E5 = 0.3910eV
E6 = 0.45eV	E6 = 0.495eV

In this computation the transmission coefficient is 0.999 at 0.205 eV. For the other energies transmission coefficients are high but less than what we have for 0.205eV. The transmission coefficients at these energies are around 0.97.

The model is applied to the last three wells. Here the array of $In_{.53}Gs_{.47}As/In_{.52}Al_{.48}As$ pair is 90/**43**/94/**40**/95/**38** Angstroms. The well widths of 90**,** 94 and 95 Angstroms are quite close. So are the barrier widths of 43, 40 and 38 Angstroms. Here the simpler expressions represented by equations 13 and 14 may be applied without much error. The energies computed are 0.06 eV and 0.205eV with transmission coefficients 0.99.

IV. ACKNOWLEDGEMENT

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