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Study of tunneling and oscillation in a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice: using transfer matrix method

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ABSTRACT

The study of superlattice (SL) system in lower dimensions, which shows tunneling and oscillation of particles, is very interesting from the point of view of fundamental physics and is important for devices. Here, we present results of our calculations related to tunneling/oscillations in a general SL system using a Symmetrical Quadruple Well (SQW) potential. This class of problems is handled using a transfer matrix (T-matrix), which is obtained by taking the solution of Schrodinger equation with appropriate boundary conditions on either side of SQW and then repeatedly applying it for the SL system. The electron wave functions in the system are found to be either in a symmetric or an anti-symmetric state with a very small energy difference between the two, leading to oscillations between these states. In this study, probability density and period of oscillation of the particle in SQW is calculated. The result is useful for high frequency operations in devices using SL.

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1. Introduction

A superlattice (SL) can be modeled by a set of quantum wells, spaced sufficiently close, in which electrons can tunnel between the wells. The potential profile of the SL is analogous to the Kronig-Penney model [1,2]. The SL system has a variety of applications in devices such as resonant tunneling structure and far-infrared detector. If the quantum wells are periodically coupled, new phenomena may arise because carriers from one quantum well may tunnel through an intervening layer to the next well. By varying the number of wells and controlling the strength of interaction between wells there is a possibility of making semiconductor devices with tailored band gap. This will enable devices sensitive to and operating at energies in the range of our interest.

The idea of semiconductor SL was first proposed by Esaki and Tsu in 1970 [3]. Semiconductor SL is formed by layered fabrication of two or more semiconductors of different band gaps (e.g. *GaAs* and *Al_{0.3}Ga_{0.7}As*) in a nanometer scale. It has been studied for different applications by several groups for their optical and transport properties [4-6]. Photoluminescence measurement was performed in SL with parabolic bands, such as *GaAs/AlGaAs*[7]. *AlGaAs/GaAs* SL mini-band detectors, which operate at very low or zero bias voltage, have been discussed and their peak spectral response in the range from 4 to 10 μm has also been reported [8,9]. Bloch oscillations in *AlGaAs/GaAs* SL in terahertz region using Monte Carlo method have also been studied [10], in which, the effective mass approximation was used in two dimensional model and studied electron miniband transport. Renk et al. [11] have done experimental study on semiconductor SL oscillator in the frequency range of 60GHz.

High frequency devices have been an important research area for many years. The application of resonant tunneling diode (RTD) in 1980's was not very successful in the terahertz (THz) region due to the extrinsic design manner, which relied on external circuit elements to induce oscillation. A new theory for the origin of intrinsic oscillation due to inter sub-band coupling in a multi sub-band system in the terahertz frequency region has been developed (for example, current oscillation in a Double Barrier Quantum Well Structure [DBQWS] based oscillators) [12,13]. The relationship between oscillation frequency and sub-band structure can be used as design criteria for new types of intrinsic oscillators.

The tunneling calculations on sawtooth and rectangular SL of *AlGaAs/GaAs* using transfer matrix was previously done [14]. Hence, the concept of the transfer matrix on SL of *AlGaAs/GaAs*, as done by Forrest et al. [14] is used to study tunneling, oscillatory behavior and the frequency of oscillation. In the present work a SL of *GaAs* and *Al_{0.3}Ga_{0.7}As* is studied. An accurate

form of solution is offered by transfer matrix method [15]. We first solve a Symmetric Quadruple Wells (SQW) (with three barriers in between) problem exactly and find the matrix which associates the wave function in the first well with the wave function of the fourth well. This matrix is then used to develop the Transfer Matrix (T-matrix) which relates the wave function in the first well of the SL with the wave function of the last well.

In this paper, we derive a theoretical formalism for a general SL, utilizing the methods of T-matrix. First we find the solution of the Schrödinger equation as applied to an SQW with suitable boundary conditions and then repeating the obtained result for the whole SL system. In the first part of Section 2 we develop a general theory of a SL and derive T-matrix by finding first the solution of the Schroedinger equation as applied to a SQW with suitable boundary conditions and then repeating the obtained result for the whole SL system.

In the second part, we use the T-matrix method to find solution in the SQW. A SQW is a four well structure bounded by vacuum levels at the either ends in the growth directions. Due to spatial symmetry the electron wave function in the system is either symmetric or anti-symmetric with a small energy difference between the levels [16].

To simplify the problem, time evolution of combined symmetric and anti-symmetric lowest lying state is taken which gives the frequency of oscillation in the SQW. The probability density of finding a particle in the SQW is also calculated and shown graphically.

2. Theoretical Formulation

2.1 A general superlattice (SL)

Consider a general SL system of $(n + 1)$ layers having $n/2$ barriers and $(n/2 + 1)$ wells, Fig. 1(a). We explore the tunneling of electrons through a single barrier to find the transfer coefficient.

Schrodinger equations for an electron with energy $E < V_0$, (V_0 being the height of the barrier) and effective masses m_w and m_b in the well and in the barrier regions respectively of the SL are:

for the well region,

$$\frac{d^2\psi_w(z)}{dz^2} + \frac{2m_w E}{\hbar^2} \psi_w(z) = 0 \quad (1a)$$

for the barrier region,

$$\frac{d^2\psi_b(z)}{dz^2} - \frac{2m_b(V_0 - E)}{\hbar^2} \psi_b(z) = 0 \quad (1b)$$

The corresponding wave vectors are:

$$k_w = \sqrt{2m_w E / \hbar^2}, \text{ and } k_b = \sqrt{2m_b(V_0 - E) / \hbar^2}.$$

The solutions of the equations above are:

For the well region:

$$\psi_w(z) = A_w \sin(k_w z) + B_w \cos(k_w z) \quad (2a)$$

For the barrier region:

$$\psi_b(z) = A_b \sinh(k_b z) + B_b \cosh(k_b z) \quad (2b)$$

The applicable boundary conditions are continuity of the wave function and equality of the effective mass-weighted slope of the wave functions (Ben Daniel Duke condition) at the interface [17]. Applying this for the $(p-1)^{th}$ well, p^{th} barrier and $(p+1)^{th}$ well we get

$$\begin{pmatrix} A_{p+1} \\ B_{p+1} \end{pmatrix} = M_w^{-1}(z)|_{z=z_p} M_b(z)|_{z=z_p} M_b^{-1}(z)|_{z=z_{p-1}} M_w(z)|_{z=z_{p-1}} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} = T^{p+1 \leftarrow p-1} \begin{pmatrix} A_{p-1} \\ B_{p-1} \end{pmatrix} \quad (3)$$

where,

$$M_w(z)|_{z=z_p} = \begin{bmatrix} \sin(k_w z_p) & \cos(k_w z_p) \\ \left(\frac{k_w}{m_w}\right) \cos(k_w z_p) & \left(-\frac{k_w}{m_w}\right) \sin(k_w z_p) \end{bmatrix} \quad (4a)$$

$$M_b(z)|_{z=z_p} = \begin{bmatrix} \sinh(k_b z_p) & \cosh(k_b z_p) \\ \left(\frac{k_b}{m_b}\right) \cosh(k_b z_p) & \left(\frac{k_b}{m_b}\right) \sinh(k_b z_p) \end{bmatrix} \quad (4b)$$

and

$$T^{p+1 \leftarrow p-1} = M_w^{-1}(z)|_{z=z_p} M_b(z)|_{z=z_p} M_b^{-1}(z)|_{z=z_{p-1}} M_w(z)|_{z=z_{p-1}} \quad (5)$$

$T^{p+1 \leftarrow p-1}$ is the transfer matrix, which is a product of four matrices and connects the coefficients of the wave functions of the $(p+1)^{th}$ and $(p-1)^{th}$ well.

The idea of transfer matrix can be extended to envelope the whole SL system. Therefore,

$$\begin{pmatrix} A_{2n+1} \\ B_{2n+1} \end{pmatrix} = T^{(2n+1) \leftarrow 1} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} \quad (6)$$

2.2 Symmetric quadruple well (SQW)

Consider a SQW, a system formed by four alternate wells and three barriers between them using, for example, alternating layers of GaAs and $Al_{0.3}Ga_{0.7}As$ in such a way that the central barrier divides the system into symmetric left and right halves as shown in Fig. 1(b). R and L in the Fig. 1(b) are the extreme right and extreme left high potential barriers going into vacuum level. The wave functions in R and L regions have a single exponentially decreasing term. The width of the barrier and the wells are taken to be l_b and l_w respectively. The odd Greek numerals as subscript on ψ represent, from right, the four wells and even numbered subscripts give the three barriers.

Since the potential is symmetric, the solutions of the Schrodinger equations 2(a) and 2(b) separate into symmetric and anti-symmetric wave functions.

Symmetric solutions are given by

$$\left. \begin{aligned} \psi_R(z) &= D_R e^{-k_D z} \\ \psi_{VII}^s(z) &= A_7^s \sin(k_w z) + B_7^s \cos(k_w z) \\ \psi_{VI}^s(z) &= A_6^s \sinh(k_b z) + B_6^s \cosh(k_b z) \\ \psi_V^s(z) &= A_5^s \sin(k_w z) + B_5^s \cos(k_w z) \\ \psi_{IV}^s(z) &= C^s \cosh(k_b z) \end{aligned} \right\} \quad (7)$$

Here, k_w and k_b were defined earlier and $k_D = \sqrt{2m_w(V_D - E) / \hbar^2}$, where V_D is the vacuum level. The symmetric solutions $\psi_{III}^s(z)$, $\psi_{II}^s(z)$, $\psi_I^s(z)$ and $\psi_L^s(z)$ are obtained by changing z to $-z$ in $\psi_V^s(z)$, $\psi_{VI}^s(z)$, $\psi_{VII}^s(z)$ and $\psi_R^s(z)$ respectively and without changing the sign of $\psi(z)$.

The anti-symmetric solutions are obtained in an analogous manner and are denoted by superscript 'a'. The solution in the central barrier is given by a sinh rather than a cosh. Change of sign of z is accompanied by simultaneous change in the sign of the corresponding ψ .

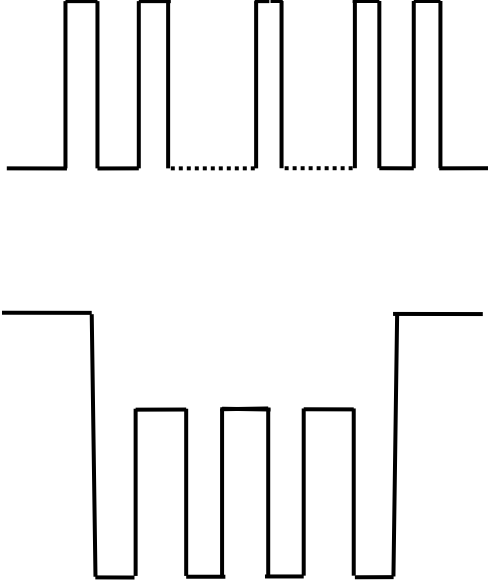


Fig. 1: (a) Rectangular superlattice of equal barrier height V_0 . (b) Spatially Symmetric Quadruple Well (SQW) with a barrier in the center.

The boundary conditions are applied at each point separating a barrier and a well and also at R and at L to obtain expressions for the energy levels corresponding to the symmetric and anti-symmetric states. All the coefficients in different regions can be related to the coefficient C^s or C^a in the central region (barrier region IV). After some tedious algebra we get

$$\tan(k_w^s z_4) = \frac{\left(-\frac{B_1^s}{A_1^s}\right) \left[1 + \left(\frac{k_w^s}{k_D}\right) \left(\frac{m_b}{m_w}\right) \frac{A_1^s}{B_1^s}\right]}{\left[1 - \left(\frac{k_w^s}{k_D}\right) \left(\frac{m_b}{m_w}\right) \frac{B_1^s}{A_1^s}\right]} = \left(-\frac{B_1^s}{A_1^s}\right) F\left(A_1^s, B_1^s, \frac{k_w^s}{k_D}\right),$$

which gives, $k_w^s z_4 = n\pi +$

$$\tan^{-1} \left[\left(-\frac{B_1^s}{A_1^s}\right) F\left(A_1^s, B_1^s, \frac{k_w^s}{k_D}\right) \right] \quad (8)$$

Since V_D is very large in comparison to V_0 , the wave vector ratio $\frac{k_w^s}{k_D}$ is small. This leads the function $F\left(A_1^s, B_1^s, \frac{k_w^s}{k_D}\right)$ to converge to 1 [14]. The final relation is,

$$k_w^s \left(\frac{3}{2} l_b + 2 l_w\right) = n\pi + \tan^{-1} \left(-\frac{B_1^s}{A_1^s}\right) = n\pi + \tan^{-1} \left(-\frac{\beta_1^s}{\alpha_1^s}\right) \quad (9)$$

where $\frac{B_n^s}{A_n^s} = \frac{\beta_n^s}{\alpha_n^s}$

Left hand side relation in (9) is a function of energy assuming the barrier parameters are known and the right hand side is accessible in terms of energy. Thus, by plotting left hand and right hand side functions with energy the intersecting points would give the symmetric energy eigen values. The evaluation of the right hand side function can be done using the value of $\frac{B_1^s}{A_1^s}$ in (8).

Let T be the transfer matrix that connects the wave function coefficients of region I to region III.

$$\begin{pmatrix} A_3^s \\ B_3^s \end{pmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{pmatrix} A_1^s \\ B_1^s \end{pmatrix}$$

On solving and rearranging the terms we arrive at the following relation,

$$\begin{pmatrix} B_1^s \\ A_1^s \end{pmatrix} = \frac{\begin{bmatrix} T_{11} - T_{21} \frac{A_3^s}{B_3^s} \\ T_{22} \frac{A_3^s}{B_3^s} - T_{12} \end{bmatrix}}{\quad} \quad (10)$$

Furthermore, the evaluation of C^s can be done by normalization condition for the system as,

$$\begin{aligned} |C^s|^2 & \left\{ \int_{-z_4}^{-z_3} |-\alpha_1^s \sin(k_w z) + \beta_1^s \cos(k_w z)|^2 dz + \int_{-z_3}^{-z_2} |-\alpha_2^s \sinh(k_b z) + \beta_2^s \cosh(k_b z)|^2 dz + \int_{-z_2}^{-z_1} |-\alpha_3^s \sin(k_w z) + \beta_3^s \cos(k_w z)|^2 dz + \int_{-z_1}^{z_1} |\cosh(k_b z)|^2 dz + \int_{z_1}^{z_2} |\alpha_3^s \sin(k_w z) + \beta_3^s \cos(k_w z)|^2 dz + \int_{z_2}^{z_3} |\alpha_2^s \sinh(k_b z) + \beta_2^s \cosh(k_b z)|^2 dz + \int_{z_3}^{z_4} |\alpha_1^s \sin(k_w z) + \beta_1^s \cos(k_w z)|^2 dz \right\} = 1 \quad (11) \end{aligned}$$

The replication of similar technique for anti-symmetric states leads to the solution of energy value and wave function coefficient C^a for the particles in this state. Calculations on concrete systems, detailed later, show that consecutive symmetric and anti-symmetric energy levels are very close, resulting in oscillations between the levels.

The total travelling wave solution in the SQW is

$$\psi(z, t) = \frac{1}{\sqrt{2}} \left[\psi^s \exp\left(-i \frac{2\pi}{h} E_s t\right) + \psi^a \exp\left(-i \frac{2\pi}{h} E_a t\right) \right] \quad (12)$$

where E_s and E_a are nearby symmetric and anti-symmetric energy values.

$$P(z, t) = \frac{1}{2} \left[\psi^{s^2} + \psi^{a^2} + \psi^s \psi^a \left(\exp \left(-i \frac{2\pi}{h} (E_a - E_s) t \right) + \exp \left(i \frac{2\pi}{h} (E_a - E_s) t \right) \right) \right]$$

$$P(z, t) = \frac{1}{2} \left[\psi^{s^2} + \psi^{a^2} + \left\{ \psi^s \psi^a \left(\exp \left(-i \frac{2\pi}{h} \Delta E t \right) + \exp \left(i \frac{2\pi}{h} \Delta E t \right) \right) \right\} \right]$$

Therefore,

$$P(z, t) = \frac{1}{2} \left[\psi^{s^2} + \psi^{a^2} + 2\psi^s \psi^a \cos \left(\frac{2\pi}{h} \Delta E t \right) \right]$$

This equation gives the probability to find the particle at time ‘t’ in the neighborhood of spatial region z and can be used to study the time evolution of system including its tunneling behavior in SQW.

3. Results and Discussion

We consider $GaAs$ and $Al_x Ga_{(1-x)} As$ SL system with SQW potential in which the width of the well and barrier are 4 nm and 5 nm respectively. The height of barrier depends on the concentration of Al in $Al_x Ga_{(1-x)} As$ and is given by $0.067 + 0.083x$. With $x = 0.3$, the height of barrier is taken to be $228 meV$ [17]. Effective masses of electrons in the well (m_w) and in the barrier (m_b) regions are taken as $0.067m_e$ and $0.091m_e$ [18] respectively. Fig. 2(a) shows the graphical solution for energy levels in symmetric state corresponding to the value of the right and of the left sides of the Eq. (9). The plot of $Y_1 = k_w^s \left(\frac{3}{2} l_b + 2 l_w \right)$ is in solid (black) line and $Y_2 = n\pi + \tan^{-1} \left[\left(-\frac{B_1^s}{A_1^s} \right) \right]$ is plotted in dash (red), dot (blue), dash dot (magenta) and short dash dot (navy) styles color (color online) for $n=1, 2, 3$ and 4 respectively. The eigen values of energy for the symmetric states for $n=1, 2$ and 3, in eV, are 0.0147000839, 0.136077023 and 0.156888216 respectively. Fig. 2(b) shows similar plots of Y_1 and Y_2 in the same colors and styles for $n=1$ to 4 for

The probability to find particle at any time t is given by:

$$P(z, t) = |\psi(z, t)|^2$$

anti-symmetric states. The anti-symmetric energy eigen values are 0.0147488590, 0.137090183 and 0.15718252 in eV the states $n=1, 2$ and 3 respectively.

For simplicity, only the lowest symmetric and anti-symmetric state for $n=1$ are considered in the calculation. The energy of the lowest anti-symmetric state is slightly higher as compared to the symmetric state, which is clearly seen in inset of the Fig. 2(c). The difference ΔE is 0.0000487751 eV and is also referred as ‘energy ting’ [16].

Fig. 3 shows the variation of the lowest ($n = 1$) lying anti-symmetric dash (red) and symmetric dot (blue) wave functions as a function of the width of the SQW. It shows the amplitude of the two waves, which are in phase in the right half and amplitude peaks in this region. They are out of phase in the left hand side and cancel each other.

The time evolution of the combined wave function is displayed in Fig. 4.(a), (b) and (c), which show the probability of finding a particle with position within the SQW at different instants of time. At $t=0$, Fig. 4(a) shows higher probability in the right half of the system. It gradually decreases and becomes nearly equal in both half at $t = T/4$, as shown in Fig. 4(b). Then, the peak starts to increase in the left half of the SQW. $t = T/2$, the probability of finding the particle in the left half of the system

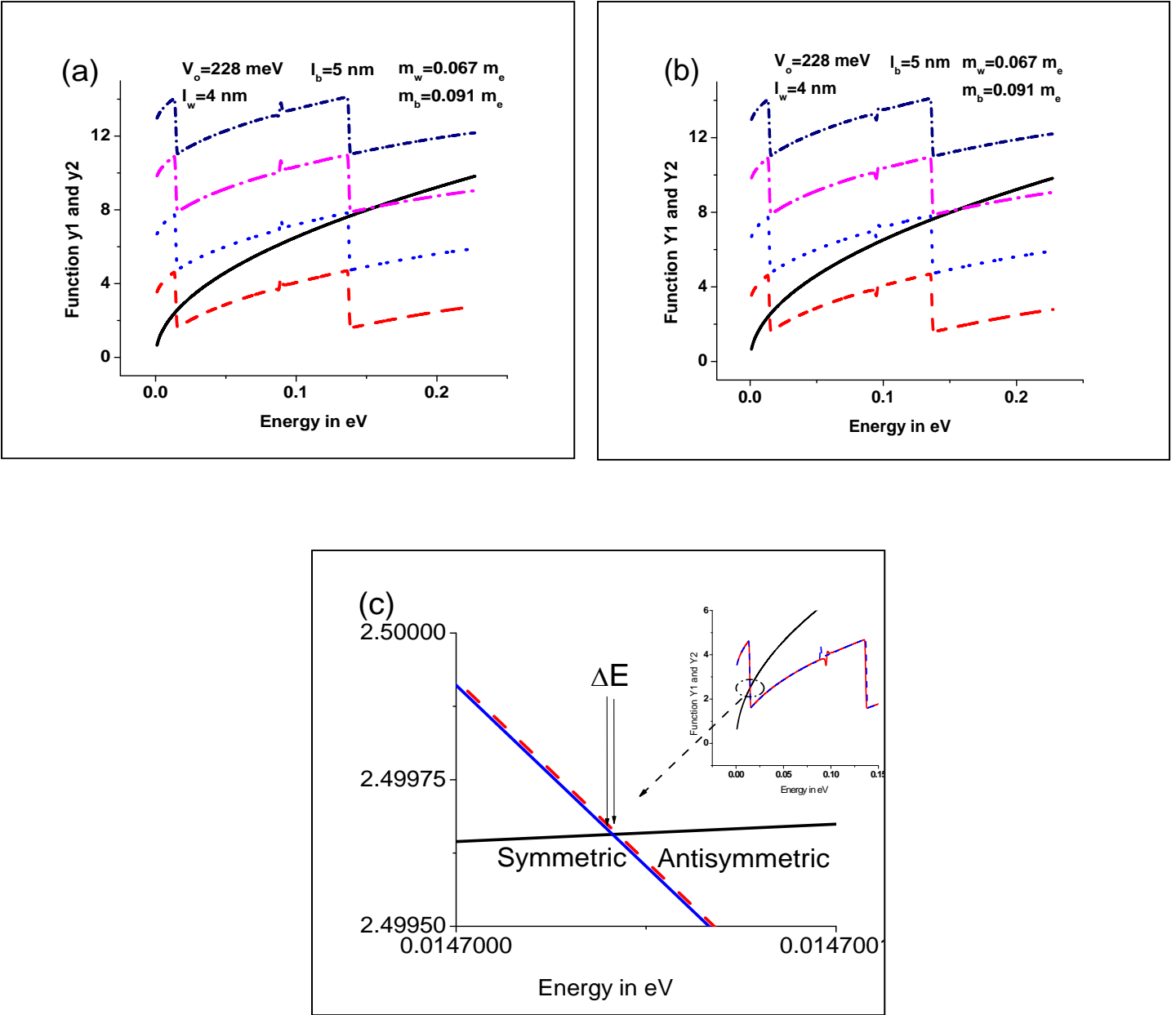


Fig. 2: (a) Plot of $Y_1 = k_w^s \left(\frac{3}{2} l_b + 2 l_w \right)$ in solid (black) line and $Y_2 = n\pi + \tan^{-1} \left[\left(-\frac{B_1^s}{A_1^s} \right) \right]$ in dash (red), dot (blue), dash dot (magenta) and short dash dot (navy) styles color (color online) for $n=1, 2, 3$ and 4 respectively for symmetric states. The intersecting values of abscissa give the energy of symmetric states. (b) Similar plot of Y_1 in solid (black) line and Y_2 in different style and color line showing the energy of anti-symmetric states. (c) Expanded view of the lowest symmetric in dash (red) and anti-symmetric in solid (blue) states (online) of the curves are shown in the inset view.

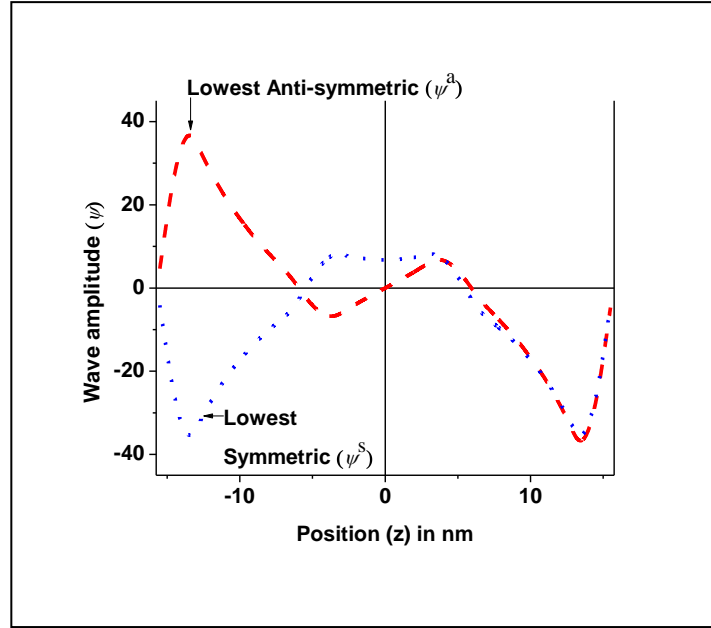


Fig. 3: The lowest symmetric and anti-symmetric wave functions, shown by solid (blue) and dash (red) line (color online) respectively versus the net width of the SQW. Here, $V_0=228$ meV, width of each barrier region (l_b)=5 nm and width of each well region (l_w)=4 nm.

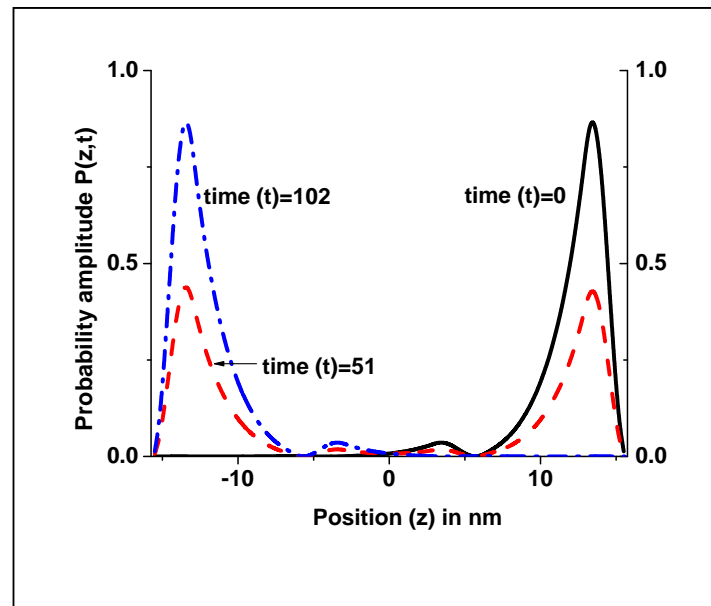


Fig. 4: Probability distribution of finding a charged particle in different spatial region within the SQW with height of barrier region $V_0= 228$ meV, width of barrier region $l_b=5$ nm at time(t)=0, $t= T/4$ and $t=T/2$ shown by solid (black), dash (red) and dash-dot (blue) (color online) line respectively.

becomes the largest, as shown in Fig. 4(c). Thus, the particle which initially was in the left region of system tunneled through all the barriers to reach to the right part of the system, giving rise to tunneling-oscillation phenomenon. The time taken by particle to tunnel through the barrier is found to be 102 units of time, which is half of the time period of oscillation measured in the units of $\left(\frac{h}{e*10^{-2}}\right)$. The total time period of oscillation is $T = 2 * 102 * \left(\frac{h}{e*10^{-2}}\right)$ i.e. $8.479 * 10^{-11}$ s. It corresponds to the tunneling frequency equal to 11.79 GHz.

The tunneling behavior of electron in symmetric double well has been studied by E.P. Lopez 2006 [16] with the barrier height (V_0) as 108 meV and barrier width (l_b) as $0.2 A^0$ and the width of the well (l_w) as $0.6 A^0$ also. The authors have calculated the frequency of oscillations to be 25.356 GHz.

It is found that as the barrier height is increased, the difference in energy values decreases. This increases the time period and the time taken by the particle to tunnel through it. For sufficiently high barriers the particle may not tunnel through, because the frequency of tunneling decays to a very small value. In case of very high barrier quantum well structures in which the frequency of oscillation is almost zero.

This model of tunneling oscillation is expected to be useful for the study of the strength of the barrier and oscillation behavior of electron in symmetric quantum well/barrier systems. In addition, the fast switching semiconductor devices and high frequency oscillators can be studied by the proposed method and using the related results.

4. Conclusion

A method of exact solution for energy level and wave function of the particle in SL is studied using T-matrix. The tunneling behavior of the electron in SQW is described with the help of time evolution. The value of energy and tunneling frequency for the electron described in SQW are estimated to be $\nabla E^1 = 0.0000487751 eV$ and $\nu_T = 11.79$ GHz

respectively. The method can be extended for larger number of wells as well for fast switching semiconductor devices in GHz region.

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