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Behavior of Transmission Probability in a Single Rectangular Potential Barrier at Constant Barrier Height–Barrier Width Product

[1,] Rupam Goswami, [2,] Basab Das
[1,2,]Department of Electronics & Communication Engineering, National Institute of Technology Silchar

Abstract

The application of Time Independent Schrodinger's Wave Equation to understand the behavior of a particle in a single rectangular potential barrier in one dimension has remained as one of the fundamental theories of potential barrier problems in quantum physics. This work chiefly focuses on the transmission of a particle, basically an electron, in such a barrier from a different perspective- behavior of transmission probability at constant barrier height (energy)-barrier width product. Three basic cases of relationship between energy of the particle and barrier potential energy have been discussed: energy of particle greater than barrier energy, energy of particle equal to barrier energy and energy of particle less than barrier energy, where appropriate approximations have been utilized to calculate the transmission probability in each case. The results have led to major observations: if the energy of barrier is scaled by a constant and its width is scaled by the same constant such that the barrier height-barrier width product always remains constant, then for a particular value of particle energy, the transmission probability remains constant for the first and third case whereas in the second case, the transmission probability reduces with decreasing energy and vice versa.

Keywords– Barrier height-barrier width product, rectangular potential barrier, scaling parameter, Schrodinger's Wave Equation, transmission probability

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1. INTRODUCTION

The rectangular potential barrier problem is a basic problem in modeling and studying various semiconductor device interfaces (for example, oxide films). This work takes up a single rectangular potential barrier in one dimension with a defined barrier height (energy) and barrier width. Thereafter, the barrier height and barrier width are scaled to new values using a common scaling parameter such that their product always remains same - this product has been referred to as barrier height-barrier width product during the course of the paper. The purpose of this work is to express transmission probability of a particle (basically an electron) in terms of the energy-width product of the potential barrier and study its variation with varying scaling parameter.
Although there are numerous models of single rectangular potential barrier where transmission probabilities of particles are calculated and applied, the approach introduced in this work is another process of studying the transmission probability in such barriers by identifying a new factor: barrier height-barrier width product. In this work, the nature of the barrier height-barrier width product is at first defined. Using Time Independent Schrodinger's Wave Equation in one dimension to the single barrier introduced, the transmission probabilities for three cases are derived: particle energy greater than barrier height, particle energy equal to barrier height and particle energy less than barrier height. The expressions are then modified applying proper approximations wherever required and calculations, to express transmission probabilities as functions of barrier height-barrier width product. Necessary graphs are plotted to verify the analytical results.

2. PROPOSED PROCESS

A single rectangular barrier is taken into consideration as shown in Fig. 1, where the barrier height (energy) is given by V_o and the barrier extends from x = 0 to x = a_o. So, we have the barrier height- barrier width product:

$$A = V_o a_o \quad (1)$$

Now, if we divide the barrier height by a non-zero real number p so that it becomes $V = V_o/p$ and multiply the barrier width by the same amount to get $a = pa_o$, then from (1) we have the barrier height-barrier width product:

$$A_p = \left(\frac{V_o}{p}\right)(pa_o) = V_o a_o = A \quad (2)$$

From (2), it is seen that the barrier height-barrier width product remains constant if the above procedure of scaling is used. This has been shown in Fig. 2.

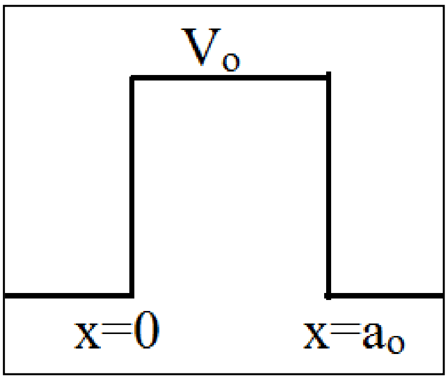

Fig. 1: A simple rectangular potential barrier

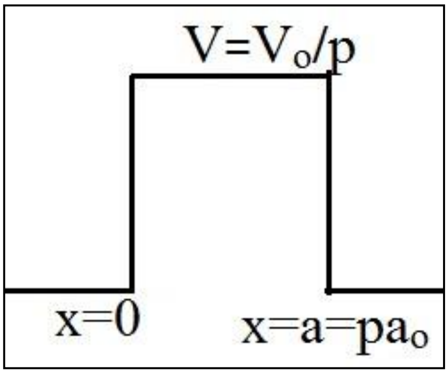

Fig. 2: Rectangular potential barrier using defined scaling

The Time Independent Schrodinger's Wave Equation (TISWE) in one dimension [1] for a particle is given by:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \qquad (3)$$

In equation (3), we have
Ψ = Wave function
m = mass of the particle
E = total energy of the particle
V = scaled barrier height = Vo/p
ħ = h/2π

The transmission probability of a particle in the rectangular barrier of Fig. 2 is found with the help of equation (3) for three cases: E > V, E = V and E < V, where we consider the particle to be incident on the barrier from left at x = 0, keeping the barrier height-barrier width product constant by using the scaling as discussed in the preceding part. Thereafter we apply appropriate approximations wherever necessary to obtain the transmission probabilities for the three cases in terms of barrier height-barrier width product.

3. EXPRESSIONS OF TRANSMISSION PROBABILITY

The single rectangular potential barrier [2] can be divided into three regions: Region I (x < 0), Region II (0 < x < a) and Region III (x > 0) as shown in Fig. 3 and then TISWE is applied to each of the regions separately for the three cases described.

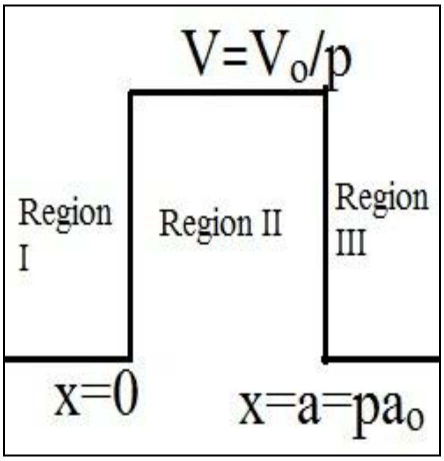

Fig. 3: Three regions of the rectangular potential barrier to which TISWE is applied separately

The three cases under consideration are:

3.1 Case I: E > V

When the particle energy is lesser than the barrier energy, we have the solution of equation (3) in the three regions as:

$$\psi = \begin{cases} Ae^{jKx} + Be^{-jKx} & (x < 0) & (4) \\ Ce^{jK'x} + De^{-jK'x} & (0 < x < a) & (5) \\ Fe^{jKx} & (x > a) & (6) \end{cases}$$

Here,

$$K^2 = \frac{2mE}{\hbar^2}$$

$$K'^2 = \frac{2m\,(E - V)}{\hbar^2}$$

The solution of wave function given by expression (6) consists of only one term in the positive x-direction because in Region III, there is no barrier present to reflect the particle.

The boundary conditions for this problem are:

$$\psi_{x<0}(0) = \psi_{0<x<a}(0) \qquad (7)$$

$$\psi'_{x<0}(0) = \psi'_{0<x<a}(0) \qquad (8)$$

$$\psi_{0<x<a}(a) = \psi_{x>a}(a) \qquad (9)$$

$$\psi'_{0<x<a}(a) = \psi'_{x>a}(a) \qquad (10)$$

Using one dimensional TISWE solutions (4), (5), (6) and boundary conditions (7), (8), (9), (10) we at first express the constant A in terms of F. The transmission probability of a particle in this case will be given by its relationship with the constant associated with the transmission of the particle in Region III and the constant associated with incidence of the particle in Region I. Hence the transmission probability for E > V is:

$$T = \frac{|F|^2}{|A|^2} = \frac{4K^2K'^2}{4K^2K'^2 + (K^2 - K'^2)^2 \sin^2(K'a)} = \frac{1}{1 + \frac{(K^2 - K'^2)^2 \sin^2(K'a)}{4K^2K'^2}} \qquad (11)$$

3.2 Case II: E=V

For a particle incident on the barrier in Region I with energy equal to the barrier energy, the solution of the TISWE in one dimension of equation (3) is given by:

$$\psi = \begin{cases} Ae^{jKx} + Be^{-jKx} & (x < 0) & (12) \\ C + Dx & (0 < x < a) & (13) \\ Fe^{jKx} & (x > a) & (14) \end{cases}$$

The boundary conditions of this case are exactly similar to those of Case I and are given by boundary conditions (7), (8), (9) and (10). Using solutions of one-dimensional TISWE (12), (13), (14) and following the same procedure as in Case I, we get the transmission probability as:

$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \frac{mEa^2}{2\hbar^2}} \qquad (15)$$

3.3 Case III: E < V

In case of a particle with energy less than the barrier energy, the solutions of TISWE in one dimension are given by:

$$\psi = \begin{cases} Ae^{jKx} + Be^{-jKx} & (x < 0) & (16) \\ Ce^{K'x} + De^{-K'x} & (0 < x < a) & (17) \\ Fe^{jKx} & (x > a) & (18) \end{cases}$$

where,

$$K^2 = \frac{2mE}{\hbar^2}$$

$$K'^2 = \frac{2m\,(V - E)}{\hbar^2}$$

Using one-dimensional TISWE solutions (16), (17), (18) and boundary conditions (7), (8), (9), (10), and following the same calculation steps as in Cases I and II, we get the transmission probability:

$$T = \frac{|F|^2}{|A|^2} = \frac{4K^2K'^2}{4K^2K'^2 + (K^2 + K'^2)^2 \sinh^2(K'a)} = \frac{1}{1 + \frac{(K^2 + K'^2)^2 \sinh^2(K'a)}{4K^2K'^2}} \quad (19)$$

4. Transmission Probability (T) In Terms Of Constant Barrier Height-Barrier Width Product (A)

It has been derived under proposed process that in a rectangular potential barrier, when the barrier height (V_o) is reduced by 'p' times and the barrier width (a_o) is increased by 'p' times, the barrier height-barrier width product (A) is a constant independent of 'p'. We can express transmission probability (T) of a particle in a rectangular potential barrier in one dimension in terms of barrier height-barrier width product (A) for the three cases under consideration using appropriate approximations in whichever case, applicable.

4.1 Case I: E > V

From equation (11), the transmission probability is:

$$T = \frac{1}{1 + \frac{(K^2 - K'^2)^2 \sin^2(K'a)}{4K^2K'^2}} \quad (20)$$

Since $K'a$ in equation (20) is very small, so, from Taylor's series expansion of sin ($K'a$), we can approximate:

$$\sin(K'a) \approx K'a \quad (21)$$

Hence, using approximation (21) in equation (20), we get:

$$T = \frac{1}{1 + \frac{(K^2 - K'^2)^2 (K'a)^2}{4K^2K'^2}}$$

$$= \frac{1}{1 + \frac{(K^2 - K'^2)^2 a^2}{4K^2}} \quad (22)$$

Substituting the values of K^2 and K'^2 in equation (22), we get:

$$= \frac{1}{1 + \frac{\left(\frac{2mV}{\hbar^2}\right)^2 a^2}{4\frac{2mE}{\hbar^2}}}$$

$$= \frac{1}{1 + \frac{mV^2a^2}{2\hbar^2 E}}$$

$$= \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}}$$

Therefore, transmission probability in terms of barrier height-barrier width product for E > V is:

$$T = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}} \quad (23)$$

4.2 Case II: E = V

Equation (15) gives:

$$T = \frac{1}{1 + \frac{mEa^2}{2\hbar^2}}$$

$$= \frac{1}{1 + \frac{mEVa^2}{2\hbar^2 V}}$$

$$= \frac{1}{1 + \frac{mV^2a^2}{2\hbar^2 V}} \qquad [\because E = V]$$

$$= \frac{1}{1 + \frac{mA^2}{2\hbar^2 V}}$$

$$= \frac{1}{1 + \frac{pmA^2}{2\hbar^2 V_0}} \qquad [\because V = \frac{V_o}{p}]$$

$$= \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}} \qquad \left[\because E = V = \frac{V_o}{p}\right]$$

So, transmission probability in terms of barrier height-barrier width product for E = V is:

$$T = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}} \qquad (24)$$

4.3 Case III: E < V

From equation (19), the transmission probability is:

$$T = \frac{1}{1 + \frac{(K^2 + K'^2)^2 \sinh^2(K'a)}{4K^2K'^2}}$$

Since $K'a$ is very small, so, from Taylor's series expansion of sin ($K'a$), we can approximate:

$$\sinh(K'a) \approx K'a \qquad (25)$$

So, using approximation (25) in equation (19), we have:

$$T \approx \frac{1}{1 + \frac{(K^2 + K'^2)^2 (K'a)^2}{4K^2K'^2}}$$

$$= \frac{1}{1 + \frac{(K^2 + K'^2)^2 a^2}{4K^2}}$$

$$= \frac{1}{1 + \frac{(K^2 + K'^2)^2 a^2}{4K^2}} \qquad (26)$$

Using the values of K^2 and K'^2 in expression (26), we get:

$$T = \frac{1}{1 + \frac{\left(\frac{2mV}{\hbar^2}\right)^2 a^2}{4\frac{2mE}{\hbar^2}}}$$

$$= \frac{1}{1 + \frac{mV^2a^2}{2\hbar^2 E}}$$

$$= \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}}$$

So, transmission probability in terms of barrier height-barrier width product for E < V is:

$$T = \frac{1}{1 + \frac{mA^2}{2\hbar^2 E}} \quad (27)$$

5. Results And Discussion

The results obtained during the calculation and approximations applied to the general expressions of transmission probability for the three cases under consideration are discussed here.

5.1 Case I: E > V

5.1.1. Interpretation

Equation (23) shows the transmission probability (T) of a particle in terms of constant barrier height-barrier width product (A) when the particle energy is greater than barrier height. In equation (23), the variables m, A and $\hbar$ are constants. So, T is a function of E only. Hence, observing the equation, we can conclude that: For a particle with a particular value of energy E greater than scaled barrier height V, the transmission probability is constant.

5.1.2. Table

In order to derive a simpler interpretation that transmission probability for Case I is constant for a particular E, it is required to depict that the term $\frac{mA^2}{2\hbar^2 E}$ in the denominator of expression (23) is a constant for a specific value of E. Hence, equation (23) can be written as:

$$\mathbf{L = \frac{1 - T}{T} = \frac{mA^2}{2\hbar^2 E}} \quad \mathbf{(28)}$$

Table 1

E	p	L
10 eV	2	2.635×10^{-20}
	4	
	6	
	8	
	10	
15 eV	3	
	4	1.757×10^{-20}
	7	
	8	
	10	
20 eV	1	1.318×10^{-20}
	4	
	5	
	8	
	9	
25 eV	2	1.054×10^{-20}
	3	
	6	
	9	
	10	

For calculations in Table 1, the following values are considered:

$V_o = 5$ eV
$a_o = 1$ angstrom
$\hbar = 6.582 \times 10^{-16}$ eV − s
m = mass of electron $= 9.1 \times 10^{-31}$ kg

Hence, barrier height-barrier width product, A = 5×10^{-10} eV − angstrom

We know that the barrier height or barrier width is varied by varying the scaling parameter p. From equations (1) and (2), it is seen that the barrier height-barrier width is constant for any value of p. So, by plotting a curve between L and scaling parameter p for different values of E greater than scaled barrier height V as listed in Table 1, the result obtained in section 5.1.1 is proved.

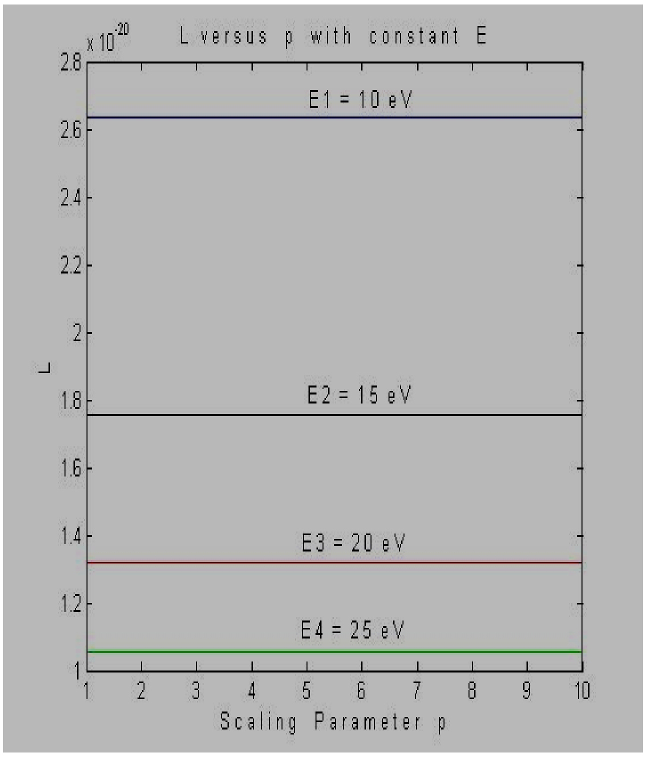

Fig. 4: Plotof L versus p for Case I (E > V) with constant E

For a constant E, L is a constant. We have:

$$T = \frac{1}{1 + L} \qquad (29)$$

From the curve, L is a constant for a particular value of E. Hence from equation (29), T is constant for a particular value of particle energy E.

5.2. Case II: E = V

5.2.1. Interpretation

Equation (24) expresses the transmission probability of Case II in terms of barrier height-barrier width product when particle energy (E) is equal to scaled barrier height (V). Equation (24) is exactly similar to that of equation (23). However, here since E = V = V_o/p, E is a function of scaling parameter p unlike in Case I and Case III. Hence, there exists one curve between L and p for varying E. From equation (24), it is easily observed that with increase in p, E (= V) decreases due to which the transmission probability reduces and vice-versa.

5.2.2. Table

As in the previous case we can modify equation (23) and write it as:

$$L = \frac{1 - T}{T} = \frac{mA^2}{2\hbar^2 E} = \ = \frac{pmA^2}{2\hbar^2 V_0} \qquad (30)$$

$$T = \frac{1}{1 + L} \qquad (31)$$

Table 2

p	$E = V_o/p$	L
2	25 eV	1.054×10^{-18}
4	12.5 eV	2.108×10^{-18}
6	8.33 eV	3.162×10^{-18}
8	6.25 eV	4.216×10^{-18}
10	5 eV	5.27×10^{-18}

For calculations in Table 2, the following values are considered:

$V_o = 50$ eV

$a_o = 1$ angstrom

$\hbar = 6.582 \times 10^{-16}$ eV − s

m = mass of electron $= 9.1 \times 10^{-31}$ kg

Hence, barrier height-barrier width product,

A = 5×10^{-9} eV − angstrom

5.2.3 Curve

The plot between L and scaling parameter p is shown in Fig. 4. It can be observed that with increase in p, L increases. From equation (31), since T is inversely related to L, hence, T reduces with increasing p and vice-versa- this establishes the interpretation in section 5.2.1.

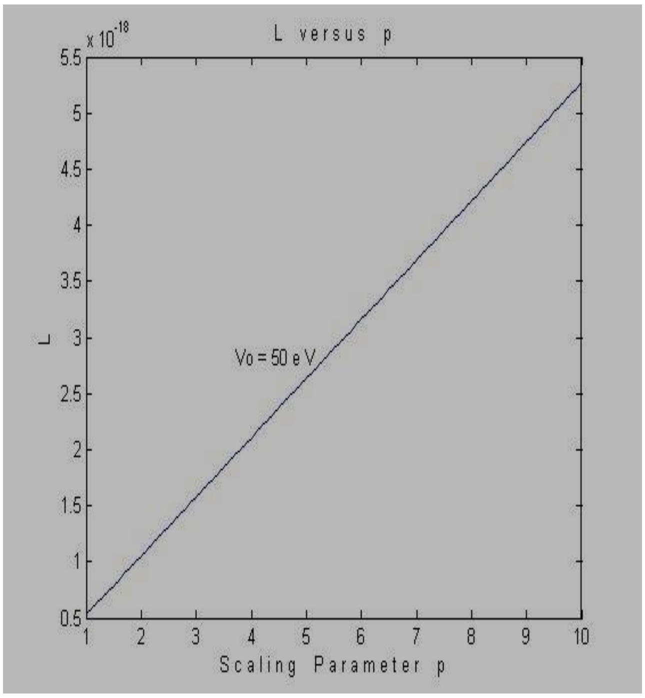

Fig. 5: Plot of L versus p for Case II (E = V)

5.3. Case III: E < V

5.3.1. Interpretation

This case is exactly similar to that of Case I except that whenever particle energy is considered in curve plots, it is kept below V. This is well depicted in the table and curve.

5.3.2. Table

Table 3

E	p	L
2 eV	2	13.18×10^{-18}
	4	
	6	
	8	
	10	
4 eV	3	6.588×10^{-18}
	4	
	7	
	8	
	10	
6 eV	1	4.392×10^{-18}
	4	
	5	
	8	
	9	
8 eV	2	3.294×10^{-18}
	3	
	6	
	9	
	10	

For calculations in Table 3, the following values are considered:
$V_o = 50$ eV
$a_o = 1$ angstrom
$\hbar = 6.582 \times 10^{-16}$ eV − s
m = mass of electron $= 9.1 \times 10^{-31}$ kg

Hence, barrier height-barrier width product,
A = 5×10^{-9} eV − angstrom

5.3.3. Curve

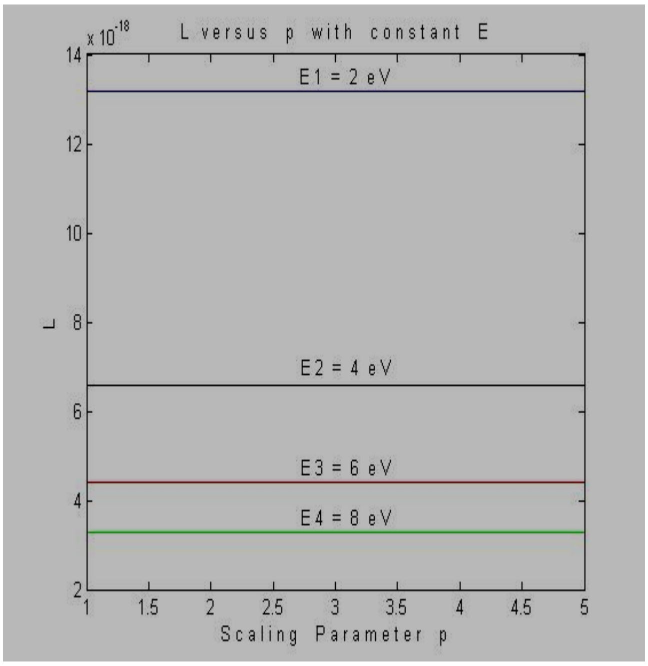

Fig. 6: Plot of L versus p for Case I (E < V) with constant E

6. CONCLUSION

This work clearly depicts how transmission probability in a single rectangular potential barrier can be studied in terms of barrier height-barrier width product. A new parameter is introduced to project the variation of transmission probabilities in such barriers, which is important keeping in view the highest chances of exercising these relationships in understanding semiconductor device mechanisms. The advantage of this work is the simplicity in approach and deriving the expressions to obtain important properties of rectangular potential barriers. As in Cases I and III, the transmission probabilities remain constant for a constant barrier height-barrier width product for a particular value of energy E. Such results may be used in modeling barriers in devices where constant transmission probability is to be achieved by varying the barrier height and barrier width appropriately. On the other hand, results of Case II show that the transmission probability reduces with increasing scaling parameter, p when particle energy is equal to scaled barrier height V. Rectangular potential barriers find applications in designing conduction models of polycrystalline Silicon [3] and gate oxide-buried oxide in Silicon-on-insulator (SOI) [4]. The results obtained in this work may be applied on such barriers present in devices.

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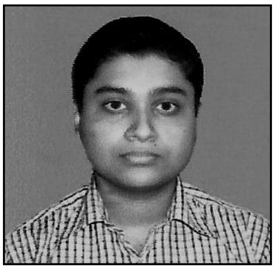
Authors:



Rupam Goswami,
Studying Master of Technology,
Department of Electronics & Communication Engineering,
National Institute of Technology Silchar, Silchar – 788010, Assam, India
Specialization: Microelectronics & VLSI Design.

Basab Das,
Studying Master of Technology,
Department of Electronics & Communication Engineering,
National Institute of Technology Silchar, Silchar – 788010, Assam, India
Specialization: Microelectronics & VLSI Design.