



Quantum Mechanical Reflection and Transmission Coefficients for a Particle through a One-Dimensional Vertical Step Potential

Rohit Gupta, Tarun Singhal, Dinesh Verma

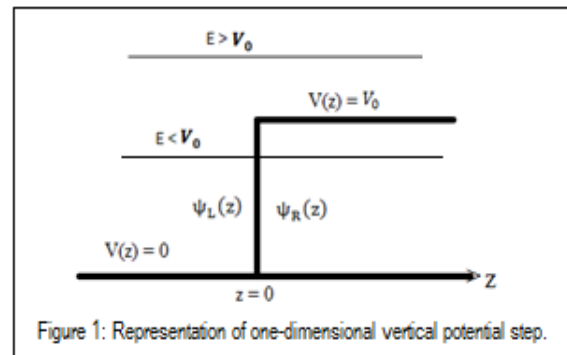
Abstract: In this paper, we illustrate an application of the Laplace transformation for finding the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential. Quantum mechanics is one of the branches of physics in which the physical problems are solved by algebraic and analytic methods. By applying the Laplace transformation, we can find the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential. Generally, the Laplace transformation has been applied in different areas of science and engineering and makes it easier to solve the problems in engineering applications. It is a mathematical tool which has been put to use for solving the differential equations without finding their general solutions. It has applications in nearly all science and engineering disciplines like analysis of electrical circuits, heat and mass transfer, fluid dynamics, nuclear physics, process controls, quantum mechanical problems, etc.

Index terms: Quantum mechanical Reflection and Transmission coefficients, one-dimensional vertical step potential, Laplace transformation.

I. INTRODUCTION

Consider a particle of mass m and total energy E which is moving from a region where the potential is zero to a region where the potential is constant, then the potential function is represented as $V(z) = 0$ for $z < 0$ and $V(z) = V_0$ for $z > 0$. It is clear that the potential function undergoes only one discontinuous change at $z = 0$ as shown in figure 1. The potential function of this type is known as a vertical step potential. Hence when the force field acting on a particle is zero everywhere except in the limited region, it is known as a potential step or single step barrier or vertical step potential [1-2]. If we consider a beam of particles (say electrons) of energy E moving from left to right, i.e. along the positive direction of Z -axis and impinging from the left on a vertical step potential at $z = 0$, then according to quantum mechanics, the particles behave like a wave moving from left to right and face a sudden shift in the potential at $z = 0$. The problem is analogous when light strikes a sheet of glass where there is a shift in the index of refraction and the wave is partially transmitted.

Hence in this problem, the electrons will be partially reflected and partially transmitted at the discontinuity.



In this paper, an application of the Laplace transformation is illustrated for finding the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential. The reflection coefficient R is a measure of the fraction of electrons reflected at the potential discontinuity i.e. it is a measure of the probability that the particle will be reflected at the potential discontinuity and is defined as the ratio of reflected probability flux to the incident probability flux. The transmission coefficient T is a measure of the fraction of electrons transmitted through the potential discontinuity i.e. it is a measure of the probability that the particle will be transmitted through the potential discontinuity and is defined as the ratio of transmitted probability flux to the incident probability flux. The probability flux is defined as the product of velocity of the particle in the given region and the probability density of particle in that region [3-4].

II. DEFINITION OF LAPLACE TRANSFORMATION

The Laplace transformation [5] of $g(z)$, which is defined for real numbers $z \geq 0$, is denoted by $L\{g(z)\}$ or $G(r)$ and is defined as $L\{g(z)\} = G(r) = \int_0^\infty e^{-rz} g(z) dz$, provided that the integral exists, i.e. convergent. If the integral is convergent for some value of r , then the Laplace transform of $g(z)$ exists otherwise not, where r is the parameter which may be a real or complex number and L is the Laplace transform operator.

1.1. Laplace Transformation of Elementary Functions

- $L\{1\} = \frac{1}{r}, r > 0$
- $L\{z^n\} = \frac{n!}{r^{n+1}}, r > 0$

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*Correspondence Author(s)

Mr. Rohit Gupta, Lecturer, Department of Physics (Applied Sciences), Yogananda College of Engineering and Technology, Gurha Brahmana (Patoli), Akhnoor Road, Jammu (J&K, India).

Dr. Tarun Singhal, Assistant Professor, Department of Applied Sciences, CGC College of Engineering, Landran Mohali, Chandigarh, India.

Dr. Dinesh Verma, Associate Professor, Department of Mathematics, Yogananda College of Engineering and Technology, Gurha Brahmana (Patoli), Akhnoor Road, Jammu (J&K, India).

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where $n = 0, 1, 2, \dots$

c. $L\{e^{cz}\} = \frac{1}{r-c}, r > c$

d. $L\{\text{sinc}z\} = \frac{c}{r^2+c^2}, r > 0$

e. $L\{\text{cos}cz\} = \frac{r}{r^2+c^2}, r > 0$

1.2. Laplace Transformation of Derivative of a function

If the function $g(z), z \geq 0$ is having an exponential order, that is if $g(z)$ is a continuous function and is a piecewise continuous function on any interval, then the Laplace transform of derivative [6-7] of $g(z)$ i.e. $L\{g'(z)\}$ is given by

$$L\{g'(z)\} = \int_0^\infty e^{-rz} g'(z) dz$$

Integrating by parts, we get

$$L\{g'(z)\} = [0 - g(0)] - \int_0^\infty -re^{-rz} g(z) dz,$$

$$\text{Or } L\{g'(z)\} = -g(0) + r \int_0^\infty e^{-rz} g(z) dz$$

$$\text{Or } L\{g'(z)\} = rL\{g(z)\} - g(0)$$

$$\text{Or } L\{g'(z)\} = rG(r) - g(0)$$

Since $L\{g'(z)\} = rL\{g(z)\} - g(0)$, therefore,

$$L\{g''(z)\} = rL\{g'(z)\} - g'(0)$$

Or

$$L\{g''(z)\} = r\{rL\{g(z)\} - g(0)\} - g'(0)$$

Or

$$L\{g''(z)\} = r^2L\{g(z)\} - rg(0) - g'(0)$$

Or

$$L\{g''(z)\} = r^2G(r) - rg(0) - g'(0),$$

And so on.

1.3. Inverse Laplace Transformation

The inverse Laplace transform [6-7] of the function $G(r)$ is denoted by $L^{-1}\{G(r)\}$ or $g(z)$.

If we write $L[g(z)] = G(r)$, then $L^{-1}\{G(r)\} = g(z)$, where L^{-1} is called the inverse Laplace transform operator.

1.3.1. Inverse Laplace Transformations of Some Functions

a. $L^{-1}\{\frac{1}{r}\} = 1$

b. $L^{-1}\{\frac{1}{(r-c)}\} = e^{cz}$

c. $L^{-1}\{\frac{1}{r^2+c^2}\} = \frac{1}{c} \sin cz$

d. $L^{-1}\{\frac{r}{r^2+c^2}\} = \cos cz$

e. $L^{-1}\{\frac{1}{r^n}\} = \frac{z^{n-1}}{(n-1)!}, n > 0$

III. METHODOLOGY

The time - independent Schrodinger equation [8] in one-dimension is written as:

$$D_z^2\psi(z) + \frac{2m}{\hbar^2}[E - V(z)]\psi(z) = 0 \dots(1) D_z \equiv \frac{d}{dz}$$

This equation is second order linear differential equation. In this equation $\psi(z)$ is probability wave function of the particle incident from left on the one-dimensional vertical step potential of height V_0 (a positive constant) at $z = 0$, E is the total energy of the particle and $V(z)$ is the potential energy of the particle.

If $\psi_L(z)$ and $\psi_R(z)$ are the probability wave functions to the left and the right side of the vertical step potential at $z = 0$, then these wave functions and their first order derivatives are continuous [4, 9] at $z = 0$ i.e.

$$\psi_L(0) = \psi_R(0) = A \text{ (say)}$$

$$\text{and } D_z\psi_L(0) = D_z\psi_R(0) = B \text{ (say),}$$

where A and B are constants.

In the region, $z < 0$, $V(z) = 0$, therefore, in this region the time - independent Schrodinger equation in one-dimension is written as

$$D_z^2\psi_L(z) + \frac{2mE}{\hbar^2}\psi_L(z) = 0 \dots\dots(3)$$

Taking Laplace transforms of equation (3), we get

$$r^2\overline{\psi}_L(r) - r\psi_L(0) - D_z\psi_L(0) + \frac{2mE}{\hbar^2}\overline{\psi}_L(r) = 0,$$

Or

$$r^2\overline{\psi}_L(r) - rA - B + \frac{2mE}{\hbar^2}\overline{\psi}_L(r) = 0.$$

Rearranging the equation, we get

$$\overline{\psi}_L(r) = \frac{rA+B}{r^2+k_1^2}; k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\text{Or } \overline{\psi}_L(r) = \frac{rA}{r^2+k_1^2} + \frac{B}{r^2+k_1^2}$$

Taking inverse Laplace transform, we get

$$\psi_L(z) = A \cos k_1z + \frac{B}{k_1} \sin k_1z \dots\dots(4)$$

Writing $\cos k_1z$ and $\sin k_1z$ in terms of exponentials, we get

$$\psi_L(z) = A \frac{e^{ik_1z} + e^{-ik_1z}}{2} + \frac{B}{k_1} \frac{e^{ik_1z} - e^{-ik_1z}}{2i}$$

Or

$$\psi_L(z) = \left(\frac{A}{2} + \frac{B}{2ik_1}\right)e^{ik_1z} + \left(\frac{A}{2} - \frac{B}{2ik_1}\right)e^{-ik_1z}$$

Or

$$\psi_L(z) = \left(\frac{A}{2} - i\frac{B}{2k_1}\right)e^{ik_1z} + \left(\frac{A}{2} + i\frac{B}{2k_1}\right)e^{-ik_1z} \dots(5)$$

In equation (5), the first term and the second term on R.H.S. i.e. $\left(\frac{A}{2} - i\frac{B}{2k_1}\right)e^{ik_1z}$ and $\left(\frac{A}{2} + i\frac{B}{2k_1}\right)e^{-ik_1z}$ represent the incident and the reflected waves in the region $z < 0$ i.e.

$$\psi_{in}(z) = \left(\frac{A}{2} - i\frac{B}{2k_1}\right)e^{ik_1z}$$

and

$$\psi_{re}(z) = \left(\frac{A}{2} + i\frac{B}{2k_1}\right)e^{-ik_1z}.$$

Now, in the region, $z > 0$, depending on the values of E and V_0 , two possibilities arise: either $V(z) = V_0 < E$ or $V(z) = V_0 > E$.

Case I: $E > V_0$

In this case, in the region, $z > 0$, $V(z) = V_0 < E$, therefore, the time-independent Schrodinger equation in one-dimension is written as

$$D_z^2\psi_R(z) + k_2^2\psi_R(z) = 0 \dots\dots(6), \text{ where } k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \text{ is real.}$$

Taking Laplace transforms of equation (3), we get

$$r^2\overline{\psi}_R(r) - r\psi_R(0) - D_z\psi_R(0) + k_2^2\overline{\psi}_R(r) = 0,$$

$$\text{Or } r^2\overline{\psi}_R(r) - rA - B + k_2^2\overline{\psi}_R(r) = 0.$$

Rearranging the equation, we get

$$\overline{\psi}_R(r) = \frac{rA+B}{r^2+k_2^2}$$

$$\text{Or } \overline{\psi}_R(r) = \frac{rA}{r^2+k_2^2} + \frac{B}{r^2+k_2^2}$$



Taking inverse Laplace transform, we get

$$\Psi_R(z) = A \cos k_2 z + \frac{B}{k_2} \sin k_2 z \dots\dots (4)$$

Writing $\cos k_2 z$ and $\sin k_2 z$ in terms of exponentials, we get

$$\Psi_R(z) = A \frac{e^{ik_2 z} + e^{-ik_2 z}}{2} + \frac{B}{k_2} \frac{e^{ik_2 z} - e^{-ik_2 z}}{2i}$$

Or

$$\Psi_R(z) = \left(\frac{A}{2} + \frac{B}{2ik_2}\right)e^{ik_2 z} + \left(\frac{A}{2} - \frac{B}{2ik_2}\right)e^{-ik_2 z}$$

Or

$$\Psi_L(z) = \left(\frac{A}{2} - i\frac{B}{2k_2}\right)e^{ik_2 z} + \left(\frac{A}{2} + i\frac{B}{2k_2}\right)e^{-ik_2 z} \dots (7)$$

In equation (7), the first term on R.H.S. i.e. $\left(\frac{A}{2} - i\frac{B}{2k_2}\right)e^{ik_2 z}$ represents the transmitted wave in the region $z > 0$ i.e.

$$\Psi_{tr}(z) = \left(\frac{A}{2} - i\frac{B}{2k_2}\right)e^{ik_2 z}$$

Since $\left(\frac{A}{2} + i\frac{B}{2k_2}\right)$ represents the coefficient of a beam incident from right on the potential step, which is not physical, therefore, $\left(\frac{A}{2} + i\frac{B}{2k_2}\right) = 0$

$$\text{Or } \frac{A}{2} + i\frac{B}{2k_2} = 0$$

$$\text{Or } B = ik_2 A \dots\dots (8)$$

Using equations (8), we can write

$$\Psi_{in}(z) = \frac{A}{2} \left(1 + \frac{k_2}{k_1}\right) e^{ik_1 z}$$

$$\Psi_{re}(z) = \frac{A}{2} \left(1 - \frac{k_2}{k_1}\right) e^{-ik_1 z}$$

and

$$\Psi_{tr}(z) = A e^{ik_2 z}$$

The quantum mechanical reflection coefficient R is given by^[8-9]

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

or $R = \frac{v_1 \Psi_{re} \Psi_{re}^*}{v_1 \Psi_{in} \Psi_{in}^*}$, where v_1 is the velocity of particle in the region $z < 0$ and Ψ_{re}^* is the complex conjugate of Ψ_{re} and Ψ_{in}^* is the complex conjugate of Ψ_{in} .

$$\text{Or } R = \frac{\frac{A}{2} \left(1 - \frac{k_2}{k_1}\right) e^{-ik_1 z} \frac{A}{2} \left(1 - \frac{k_2}{k_1}\right) e^{ik_1 z}}{\frac{A}{2} \left(1 + \frac{k_2}{k_1}\right) e^{ik_1 z} \frac{A}{2} \left(1 + \frac{k_2}{k_1}\right) e^{-ik_1 z}}$$

$$\text{Or } R = \frac{\left(1 - \frac{k_2}{k_1}\right) \left(1 - \frac{k_2}{k_1}\right)}{\left(1 + \frac{k_2}{k_1}\right) \left(1 + \frac{k_2}{k_1}\right)}$$

On simplifying, we get

$$R = \left[\frac{k_1 - k_2}{k_1 + k_2}\right]^2 \dots\dots\dots (9)$$

It is clear that the value of R is positive and less than one. The equation (9) provides the expression for the quantum mechanical reflection coefficient at the vertical step potential with $E > V_0$.

The quantum mechanical transmission coefficient T is given by^[8-9]

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

or $T = \frac{v_2 \Psi_{tr} \Psi_{tr}^*}{v_1 \Psi_{in} \Psi_{in}^*}$, where v_2 is the velocity of particle in the region $z < 0$ and Ψ_{tr}^* is the complex conjugate of Ψ_{tr} .

$$T = \frac{v_2 A e^{-ik_2 z} A^* e^{ik_2 z}}{v_1 \frac{A}{2} \left(1 + \frac{k_2}{k_1}\right) e^{ik_1 z} \frac{A}{2} \left(1 + \frac{k_2}{k_1}\right) e^{-ik_1 z}}$$

$$T = \frac{4v_2}{v_1 \left(1 + \frac{k_2}{k_1}\right)^2} \dots\dots\dots (10)$$

Using the relation [10] between the momentum (or velocity) and the propagation constant, we can write

$$\frac{p_2}{p_1} = \frac{mv_2}{mv_1} = \frac{\hbar k_2}{\hbar k_1}$$

$$\text{Or } \frac{v_2}{v_1} = \frac{k_2}{k_1}$$

Hence we can re write equation (10) as

$$T = \frac{4k_2}{k_1 \left(1 + \frac{k_2}{k_1}\right)^2}$$

On simplifying the equation, we get

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2} \dots\dots (11)$$

The equation (11) provides the expression for the quantum mechanical transmission coefficient at the vertical step potential with $E > V_0$. On adding equations, (9) and (11), we can find that the sum of R and T is one which shows that the sum of the number of electrons reflected at the potential discontinuity and the number of electrons transmitted through the potential discontinuity is equal to number of electrons incident on the potential discontinuity with $E > V_0$.

Case II: $E < V_0$

In this case, in the region, $z < 0$, the solution remains the same. In the region, $z > 0$, $V(z) = V_0 < E$, therefore, the time – independent Schrodinger equation in one dimensions is written as

$$D_z^2 \Psi_R(z) + k_3^2 \Psi_R(z) = 0 \dots (12), \text{ where}$$

$$k_3 = i \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = ik \text{ is complex}; k = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Taking Laplace transforms of equation (12), we get

$$r^2 \overline{\Psi_R}(r) - r \Psi_R(0) - D_z \Psi_R(0) + k_3^2 \overline{\Psi_R}(r) = 0, \text{ where } \overline{\Psi_R}(r) \text{ is the Laplace transform of } \Psi_R(z).$$

Or

$$r^2 \overline{\Psi_R}(r) - r A - B + k_3^2 \overline{\Psi_R}(r) = 0.$$

Rearranging the equation, we get

$$\overline{\Psi_R}(r) = \frac{r A + B}{r^2 + k_3^2}$$

$$\text{Or } \overline{\Psi_R}(r) = \frac{r A}{r^2 + k_3^2} + \frac{B}{r^2 + k_3^2}$$

Taking inverse Laplace transform, we get

$$\Psi_R(z) = A \cos k_3 z + \frac{B}{k_3} \sin k_3 z \dots\dots (13)$$

Writing $\cos k_3 z$ and $\sin k_3 z$ in terms of exponentials, we get

$$\Psi_R(z) = A \frac{e^{ik_3 z} + e^{-ik_3 z}}{2} + \frac{B}{k_3} \frac{e^{ik_3 z} - e^{-ik_3 z}}{2i}$$

Or

$$\Psi_R(z) = \left(\frac{A}{2} + \frac{B}{2ik_3}\right)e^{ik_3 z} + \left(\frac{A}{2} - \frac{B}{2ik_3}\right)e^{-ik_3 z}$$

Or

$$\Psi_R(z) = \left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3 z} + \left(\frac{A}{2} + i\frac{B}{2k_3}\right)e^{-ik_3 z} \dots (14)$$



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In equation (14), $\left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3z}$ represents the transmitted wave in the region $z > 0$ i.e.

$$\psi_{tr}(z) = \left(\frac{A}{2} - i\frac{B}{2k_3}\right)e^{ik_3z} \dots\dots (15)$$

Since $\left(\frac{A}{2} + i\frac{B}{2k_3}\right)$ represents the coefficient of a beam incident from right on the potential step, which is not physical, therefore, $\left(\frac{A}{2} + i\frac{B}{2k_3}\right) = 0$

$$\text{Or } \frac{A}{2} + i\frac{B}{2k_3} = 0$$

$$\text{Or } B = ik_3A \dots\dots (16)$$

Using equations (16), we can write

$$\psi_{in}(z) = \frac{A}{2} \left(1 + \frac{k_3}{k_1}\right) e^{ik_1z},$$

$$\psi_{re}(z) = \frac{A}{2} \left(1 - \frac{k_3}{k_1}\right) e^{-ik_1z} \text{ and}$$

$$\psi_{tr}(z) = Ae^{ik_3z}.$$

The quantum mechanical reflection coefficient R is given by^[8-9]

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

Or $R = \frac{v_1\psi_{re}\psi_{re}^*}{v_1\psi_{in}\psi_{in}^*}$, where v_1 is the velocity of particle in the region $z < 0$ and ψ_{re}^* is the complex conjugate of ψ_{re} and ψ_{in}^* is the complex conjugate of ψ_{in} .

Or $R = \frac{\frac{A}{2} \left(1 - \frac{k_3}{k_1}\right) e^{-ik_1z} \frac{A^*}{2} \left(1 - \frac{k_3^*}{k_1^*}\right) e^{ik_1z}}{\frac{A}{2} \left(1 + \frac{k_3}{k_1}\right) e^{ik_1z} \frac{A^*}{2} \left(1 + \frac{k_3^*}{k_1^*}\right) e^{-ik_1z}}$, where A^* and k_3^* are the complex conjugates of A and k_3 .

$$\text{Or } R = \frac{\left(1 - i\frac{k}{k_1}\right) \left(1 + i\frac{k}{k_1}\right)}{\left(1 + i\frac{k}{k_1}\right) \left(1 - i\frac{k}{k_1}\right)}$$

$$\text{Or } R = 1 \dots\dots (17)$$

The equation (17) provides the expression for the quantum mechanical reflection coefficient at the vertical step potential with $E < V_0$.

The quantum mechanical transmission coefficient T is given by^[8-9]

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

Or $T = \frac{v_2\psi_{tr}\psi_{tr}^*}{v_1\psi_{in}\psi_{in}^*}$, where v_2 is the velocity of particle in the region $z < 0$ and ψ_{tr}^* is the complex conjugate of ψ_{tr} .

$$T = \frac{v_2Ae^{-ik_3z}A^*e^{ik_3^*z}}{v_1\frac{A}{2} \left(1 + \frac{k_3}{k_1}\right) e^{ik_1z} \frac{A^*}{2} \left(1 + \frac{k_3^*}{k_1^*}\right) e^{-ik_1z}}$$

$$\text{Or } T = \frac{v_2Ae^{kz}A^*e^{-kz}}{v_1\frac{A}{2} \left(1 + i\frac{k}{k_1}\right) e^{ik_1z} \frac{A^*}{2} \left(1 - i\frac{k}{k_1}\right) e^{-ik_1z}}$$

$$\text{Or } T = \frac{4v_2}{v_1 \left[1 + \left(\frac{k}{k_1}\right)^2\right]} \dots\dots\dots (18)$$

Using the relation [10] between the velocity and the propagation constant, we can write

$$\frac{v_2}{v_1} = \frac{k_3}{k_1}$$

$$\text{Or } \frac{v_2}{v_1} = i\frac{k}{k_1}$$

Hence we can rewrite equation (18) as

$$T = \frac{4ik}{k_1 \left[1 + \left(\frac{k}{k_1}\right)^2\right]}, \text{ which is complex whose real part is given}$$

by

$$\text{Real}(T) = 0 \dots\dots (19)$$

The equation (9) provides the expression for the quantum mechanical reflection coefficient at the vertical step potential with $E < V_0$.

Again, on adding equations (17) and (19), we can find $R + T = 1$ which shows that the sum of the number of electrons reflected at the potential discontinuity and the number of electrons transmitted through the potential discontinuity is equal to number of electrons incident on the potential discontinuity with $E < V_0$.

IV. RESULT AND DISCUSSION

In this paper, we have discussed the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential through the Laplace transformation method. It is revealed that the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential can be obtained easily through the application of Laplace transformation. This method results out a new technique in discussing the quantum mechanical Reflection and Transmission coefficients for a particle through a one-dimensional vertical step potential, and it served well to illustrate the application of the Laplace transformation tool.

V. CONCLUSION

It is concluded that sum of **R** and **T** (whether $E > V_0$ or $E < V_0$) is one which shows that the sum of the number of electrons reflected at the potential discontinuity (i.e. the flux of reflected particles) and the number of electrons transmitted through the potential discontinuity (i.e. the flux of transmitted particles) is always equal to number of electrons incident on the potential discontinuity (i.e. the flux of incident particles) which means that no particle is lost at the potential discontinuity.

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AUTHORS PROFILE



Mr. Rohit Gupta is currently Lecturer, Department of Physics (Applied Sciences), Yogananda College of Engineering and Technology, Gurha Brahmna (Patoli), Akhnoor Road, Jammu (J&K, India). He has done M.Sc. Physics from University of Jammu (J&K) in the year 2012. He has been teaching UG Classes for well over six and half years. He has to his credit Sixteen Research Papers. He has attended three Workshop/Conferences/FDP during his six and half years' experience of teaching.



Dr. Tarun Singhal is currently Assistant Professor, Department of Applied Sciences, CGC College of Engineering, Landran Mohali, Chandigarh, India. He has done Ph. D. in Electronics and Communication Engineering from Maharishi Dayanand University Rohtak Haryana, India. He has been teaching UG and PG Classes for well over Thirteen years. He has to his credit Eleven Research Papers. He has attended Twenty five Workshop/Conferences/FDP during his Thirteen years' experience of teaching.



Dr. Dinesh Verma is currently Associate Professor, Department of Mathematics, Yogananda College of Engineering and Technology, Gurha Brahmna (Patoli), Akhnoor Road, Jammu (J&K, India). He has done Ph.D. at M.J.P. Rohilkhand University, Bareilly (U.P.) in 2004. He has been teaching UG Classes for well over two decades. He has to his credit four books for Engineering and Graduation level which are used by students of various universities. He has to his credit Twenty Two Research Papers. He has attended Seventeen Workshop/Conferences/FDP during his Twenty years' experience of teaching. Also, he has a membership with ISTE (Indian Society for Technical Education) and ISCA (Indian Science Congress Association).