Study on Transmission Probabilities for Some Rectangular Potential Barriers

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ABSTRACT

In this research, we apply the time independent Schrödinger equation for a particle moving in one dimensional potential barrier of finite width and height. We study the two cases which corresponds to the particle energies being respectively larger and smaller than the potential barrier. Then, we calculate transmission coefficient (T) as a function of particle energy (E) for a potential barrier by changing the barrier height (V₀) and width (L) using Propagation Matrix Method. If we keep the barrier width constant and varying the height, we see that the passing limit is shifting towards the higher energies when barrier height is increased. If we keep the barrier height constant and change the barrier width, we see significance change in oscillations.

KEYWORDS: Rectangular Potential Barrier, Propagation Matrix Method

INTRODUCTION

A differential equation for the wave function Ψ actually for the variation of wave function with space and time is called Schrödinger equation which describes the behavior of particles like electron, proton, neutron etc. We apply the Schrödinger equation for a particle moving in one dimensional potential barrier of finite width and height V₀. We consider a beam of particles of mass m along the x-axis from left to right on a potential barrier. According to classical physics, if a beam of particles with energy E < V₀ is incident on the potential barrier, it will be reflected. It cannot go through the potential barrier[1]. However, according to quantum mechanics there is finite probability that a particle with energy less than the height of potential barrier can penetrate it. Transmission occur with finite probability for all values of E except in some special cases. We consider the following two cases which correspond to the particle energies being respectively larger and smaller than the potential barrier.

A. Case I (E > V₀)

We divide the whole space into three regions: Region I (x < 0), Region II (0 < x < L) and Region III (x > L). In region I and III the particle is free[2]. According to classical physics, if a beam of particles with energy E > V₀ approaches the potential barrier from the left, all of the particles in the beam will go over the barrier to region III. The time independent Schrödinger equation for each region is

\[
\frac{d^2}{dx^2} \psi_1(x) = 0 \quad (x < 0)
\]

\[
\frac{d^2}{dx^2} \psi_2(x) = 0 \quad (0 < x < L)
\]

\[
\frac{d^2}{dx^2} \psi_3(x) = 0 \quad (x > L)
\]

The solutions of the Schrödinger equation in the three regions are
We need only to calculate \( L \). The potential barrier and propagation directions of the incident, reflected and transmitted waves are shown in Fig. (1) for \( E > V_0 \). The wave function will display an oscillatory pattern in all three regions; its amplitude reduces every time the particle enters a new region. The constants \( B, C, D \) and \( F \) can be obtained in terms of \( A \) from the boundary conditions. The wave functions and their first derivatives must have continuous values [3]. Solving for \( F \), we obtain

\[
F = 4k_1 k_2 A e^{-ik_1 L} \left[ (k_1 + k_2)^2 e^{-ik_1 L} - (k_1 - k_2)^2 e^{ik_2 L} \right]^{-1}
\]

The potential barrier and the energy \( E \)

\[
F = 4k_1 k_2 A e^{-ik_1 L} \left[ 4k_1 k_2 \cos(k_2 L) - 2i(k_1^2 + k_2^2) \sin(k_2 L) \right]
\]

The probability of transmission is given by the transmission coefficient \( T \).

\[
T = \frac{|F|^2}{|A|^2} \left[ 1 + \frac{4(k_1^2 - k_2^2)^2}{k_1 k_2} \sin^2(k_2 L) \right]^{-1} \quad (E > V_0) \quad (7)
\]

We note that \( T \) is finite. This means that the probability for the transmission of the particles into the region \( 0 \leq x \leq L \) is not zero as expected from classical physics. This is a purely quantum mechanical effect which is due to the wave aspect of microscopic objects; it is known as the tunneling effect: quantum mechanical objects can tunnel through classically impenetrable barriers.

\[ T = \frac{|F|^2}{|A|^2} \left[ 1 + \frac{4(k_1^2 - k_2^2)^2}{k_1 k_2} \sin^2(k_2 L) \right]^{-1} \quad (8) \]

where \( k_1^2 = 2mE/\hbar^2 \) and \( k_2^2 = 2m(V_0 - E)/\hbar^2 \). The potential barrier and propagation directions of the incident, reflected and transmitted waves are shown in Fig. (2) for \( E < V_0 \). The wave function has an exponential form in the forbidden region inside the barrier. But there is also an oscillator wave to the right of barrier. To find transmission coefficients \( T = \frac{|F|^2}{|A|^2} \), we need only to calculate \( F \) in terms of \( A \). The wave functions and their first derivatives must have continuous values. Solving equation for \( F/A \), we obtain

\[
F = 2e^{-ik_1 L} \left[ 2 \cosh(k_2 L) + i \frac{k_2^2 - k_1^2}{k_1 k_2} \sinh(k_2 L) \right]^{-1}
\]

Fig. (2) The potential barrier and the energy \( E \).
may be calculated by multiplying together the appropriate $2 \times 2$ matrices. We can solve for a particle moving in an arbitrary potential by dividing the potential into a number of potential energy steps. The following four basic parts are needed. We may use the propagation matrix method to calculate the probability of the electron emerging on the right-hand side of the barrier. The method is best approached by dividing it into small, easy-to-understand, logical parts.

The Step Propagation Matrix

We calculate the propagation matrix $p_{\text{step}}$ for transmission and reflection of the wave function representing a particle of energy $E$ incident on a single potential step. The potential step we consider is at position $x_{j+1}$ in Fig.(3).

Fig.3 Approximation of a smoothly varying one dimensional potential $V(x)$ with a series of potential steps

In this approach, the potential between position $x_j$ and $x_{j+1}$ in region $j$ is approximated by a value $V_j$. Associated with the potential step at $x_j$ and free propagation distance $L_j = x_{j+1} - x_j$ is a $2 \times 2$ matrix which carries all of the amplitude and phase information on the particle. Fig.(4) shows detail of the potential step at position index $j + 1$. The coefficients $A$ and $C$ correspond to waves traveling left to right in region $j$ and $j+1$, respectively.

Fig.4 A one dimensional potential step. In region $j$ the potential energy is $V_j$ and in region $j+1$ the potential energy is $V_{j+1}$.

The transition between region $1$ and region $2$ occurs at position $x = x_{j+1}$. The electron (or particle) has wave vector $k_j = \frac{(2m(E - V_j))^{1/2}}{\eta}$ in region $j$, and the wave functions, which are solutions to the Schrödinger equation in regions $j$ and $j+1$, are

$$\psi_j = A_j e^{i k_j x} + B_j e^{-i k_j x}$$

$$\psi_{j+1} = C_{j+1} e^{i k_{j+1} x} + D_{j+1} e^{-i k_{j+1} x}$$

Following the convention we have adopted in this paper, $A$ and $C$ are coefficients for the wave function traveling left-to-right in regions $j$ and $j+1$, respectively, and $B$ and $D$ are the corresponding right-to-left traveling-wave coefficients. The two wave functions given by Eq.(13) and (14) are related to each other by the constraint that $\psi$ and $d\psi/dx$ must be continuous. This means that at the potential step that occurs at the boundary between regions $j$ and $j+1$ we require
\[
\psi_j \bigg|_{x=x_j} = \psi_{j+1} \bigg|_{x=x_{j+1}} \tag{15}
\]

and
\[
\frac{d \psi_j}{dx} \bigg|_{x=x_{j+1}} = \frac{d \psi_{j+1}}{dx} \bigg|_{x=x_{j+1}} \tag{16}
\]

Substituting Eq. (13) and (14) into Eq. (15) and (16) gives two equations

\[
A_j e^{ik_j x} + B_j e^{-ik_j x} = C_{j+1} e^{ik_{j+1} x} + D_{j+1} e^{-ik_{j+1} x} \tag{17}
\]

\[
A_j e^{ik_j x} - B_j e^{-ik_j x} = \frac{k_{j+1}}{k_j} C_{j+1} e^{ik_{j+1} x} - \frac{k_{j+1}}{k_j} D_{j+1} e^{-ik_{j+1} x} \tag{18}
\]

By organizing into rows and columns the terms that contain left to right traveling waves of the form \(e^{ikx}\) and right-to-left traveling waves of the form \(e^{-ikx}\), we may write Eq. (17) and (18) for a potential step at position \(x_{j+1} = 0\) as a matrix equation:

\[
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\begin{bmatrix}
A_j \\
B_j
\end{bmatrix}
= \frac{1}{k_j}
\begin{bmatrix}
\frac{1}{k_j+1} & -\frac{1}{k_j+1} \\
-\frac{1}{k_j} & \frac{1}{k_j}
\end{bmatrix}
\begin{bmatrix}
C_{j+1} \\
D_{j+1}
\end{bmatrix} \tag{19}
\]

We would much prefer a simple equation of the type

\[
\begin{bmatrix}
A_j \\
B_j
\end{bmatrix}
= \begin{bmatrix}
p_{j\text{step}} & C_{j+1} \\
D_{j+1}
\end{bmatrix} \tag{20}
\]

where \(p_{j\text{step}}\) is the 2×2 matrix describing wave propagation at a potential step. To obtain this expression, we need to eliminate the 2×2 matrix on the left-hand side of Eq. (19). We simply use from basic linear algebra that the inverse of a 2×2 matrix

\[
A = \begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{bmatrix}
is \quad A^{-1} = \frac{1}{|A|} \begin{bmatrix}
a_{22} & -a_{12} \\
-a_{21} & a_{11}
\end{bmatrix}
\]

where the determinant of \(A\) is given by

\[
|A| = a_{11} a_{22} - a_{12} a_{21} \]

Hence, the inverse of

\[
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
is \frac{1}{2} \begin{bmatrix}
1 & -1 \\
1 & -1
\end{bmatrix} = \frac{1}{2} \begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\]

so that we may write

\[
\begin{bmatrix}
A_j \\
B_j
\end{bmatrix}
= \frac{1}{2}
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix}
\begin{bmatrix}
\frac{1}{k_j+1} & -\frac{1}{k_j+1} \\
-\frac{1}{k_j} & \frac{1}{k_j}
\end{bmatrix}
\begin{bmatrix}
C_{j+1} \\
D_{j+1}
\end{bmatrix} = \begin{bmatrix}
p_{j\text{step}} & C_{j+1} \\
D_{j+1}
\end{bmatrix} \tag{21}
\]

where the step matrix is

\[
p_{j\text{step}} = \frac{1}{2}
\begin{bmatrix}
1 + \frac{k_{j+1}}{k_j} & 1 - \frac{k_{j+1}}{k_j} \\
1 - \frac{k_{j+1}}{k_j} & 1 + \frac{k_{j+1}}{k_j}
\end{bmatrix} \tag{22}
\]

This is our result for the step potential that will be used later. We continue the development of the matrix method by considering the propagation between steps.

**The Propagation between Steps**

We calculate the propagation matrix \(p_{\text{free}}\) for propagation of the wave function between steps. The free propagation we consider is between positions \(x_i\) and \(x_{i+1}\) in Fig. (3). The distance of this free propagation is \(L_j\). Propagation between potential steps separated by distance \(L_j\) carries phase information only so that \(A_j e^{ik_j L_j} = C_{j+1}\) and \(B_j e^{-ik_j L_j} = D_{j+1}\). This may be expressed in matrix form as

\[
\begin{bmatrix}
e^{ik_j L_j} & 0 \\
0 & e^{-ik_j L_j}
\end{bmatrix}
\begin{bmatrix}
A_j \\
B_j
\end{bmatrix}
= \begin{bmatrix}
C_{j+1} \\
D_{j+1}
\end{bmatrix} \tag{23}
\]

Or, alternatively,

\[
\begin{bmatrix}
A_j \\
B_j
\end{bmatrix}
= p_{j\text{free}}
\begin{bmatrix}
C_{j+1} \\
D_{j+1}
\end{bmatrix} \tag{24}
\]

where

\[
p_{j\text{free}} = \begin{bmatrix}
e^{-ik_j L_j} & 0 \\
0 & e^{ik_j L_j}
\end{bmatrix} \tag{25}
\]
The Propagation Matrix $P_j$ for the $j$-th Region
We calculate the propagation matrix for the $j$-th region in Fig.(3). This is achieved if we multiply $p_{\text{step}}$ and $p_{\text{free}}$ to obtain the propagation matrix $P_j$ for the $j$-th region of the discretized potential. To find the combined effect of $p_{\text{free}}$ and $p_{\text{step}}$ we simply multiply the two matrices together. Hence, propagation across the complete $j$-th element consisting of a free propagation region and a step is

$$P_j = p_{\text{free}} P_{\text{step}} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \quad (26)$$

When we multiply out the matrices $p_{\text{free}} p_{\text{step}}$ given by Eq.(25) and (22), respectively, it gives us the propagation matrix for the $j$-th region:

$$p_j = \frac{1}{2} \begin{bmatrix} 1 & \frac{k_{j+1}}{k_j} & e^{-ik_j L_j} & \left(1 - \frac{k_{j+1}}{k_j}\right) & e^{-ik_j L_j} \\ 1 & \frac{k_{j+1}}{k_j} & e^{ik_j L_j} & \left(1 + \frac{k_{j+1}}{k_j}\right) & e^{ik_j L_j} \end{bmatrix} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \quad (27)$$

Propagation through an Arbitrary Series of Step Potentials
We calculate the total propagation matrix $P$ for the complete potential by multiplying together the propagation matrices for each region of the discretized potential. For the general case of $N$ potential steps, we write down the propagation matrix for each region and multiply out to obtain the total propagation matrix,

$$P = p_1 p_2 \ldots p_j \ldots p_N = \prod_{j=1}^{N} p_j \quad (28)$$

The total propagation matrix $P$ satisfies continuity in $\Psi$ and $d\Psi/dx$ between adjacent regions. Since the particle is introduced from the left, we know that $A = 1$, and if there is no reflection at the far right then $D = 0$. We may then rewrite

$$\begin{bmatrix} A \\ B \end{bmatrix} = \prod_{j=1}^{N} p_j \begin{bmatrix} C \\ D \end{bmatrix} = P \begin{bmatrix} C \\ D \end{bmatrix} \quad (29)$$

as

$$\begin{bmatrix} 1 \\ B \end{bmatrix} = \begin{bmatrix} p_{11} & p_{12} \\ p_{21} & p_{22} \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} \quad (30)$$

In this case, because $1 = p_{11} C$, the transmission probability $|C|^2$ is simply

$$|C|^2 = \frac{1}{p_{11}} \quad (31)$$

Eq.(20) is a particularly simple result. We will make use of this when we calculate the transmission probability of a particle through an essentially arbitrary one-dimensional potential.

Transmission Probability for a Rectangular Potential Barrier
Fig.(5) is a sketch of the rectangular potential barrier we will consider. The thickness of the barrier is $L$. A particle of mass $m$ incident from the left of energy $E$ has wave vector $k_1$. In the barrier region, the wave vector is $k_2$. The wave vectors $k_1$ and $k_2$ are related through $k_1^2 = k_2^2 + 2mV_0/\eta^2$. 

![Fig.5 The potential of a one dimensional rectangular barrier of energy $V_0$](image-url)
A wavy particle incident on the barrier from the left with amplitude $A$ sees a potential step-up in energy of $V_0$ at $x = 0$, a barrier propagation region of length $L$, and a potential step-down at $x = L$. A particle of energy $E$, mass $m$, and charge $e$ has wave number $k_1$ outside the barrier and $k_2$ in the barrier region $0 < x < L$. We consider a particle impinging on a step change in potential between two regions in which the wave vector changes from $k_1$ to $k_2$ due to the potential step up shown in Fig.(3). The corresponding wave function changes from $\psi_1$ to $\psi_2$. Solutions of the Schroedinger equation for an step change in potential are

$$\psi_1 = \frac{A}{\sqrt{k_1}} e^{ik_1x} + \frac{B}{\sqrt{k_1}} e^{-ik_1x}$$

(32)

$$\psi_2 = \frac{C}{\sqrt{k_2}} e^{ik_2x} + \frac{D}{\sqrt{k_2}} e^{-ik_2x}$$

(33)

Applying the condition that the wave function is continuous at the potential step $\psi_1 |_{step} = \psi_2 |_{step}$, and that the derivative of the wave function is continuous

$$\frac{d\psi_1}{dx} |_{step} = \frac{d\psi_2}{dx} |_{step}$$

(34)

To eliminate the $2 \times 2$ matrix on the left-hand side of this equation, we must find and multiply by its inverse matrix. The determinant of the left-hand matrix is $(-1 - 1)/k_1 = -2/k_1$, so the inverse of the left-hand matrix is $k_1/2\sqrt{k_1} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$. Hence, we may rewrite Eq. (36) as

$$\begin{bmatrix} A \\ B \end{bmatrix} = \frac{1}{2\sqrt{k_1k_2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} k_1 + k_2 \\ k_1 - k_2 \end{bmatrix} \begin{bmatrix} k_1 + k_2 \\ k_1 - k_2 \end{bmatrix} \begin{bmatrix} C \\ D \end{bmatrix}$$

(37)

Since the rectangular potential barrier consists of a step up and a step down, we can make use of this symmetry and immediately calculate the $2 \times 2$ matrix for the step down by simply interchanging $k_1$ and $k_2$. The total propagation matrix for the rectangular potential barrier of thickness $L$ consists of the step-up $2 \times 2$ matrix multiplied by the propagation matrix from the barrier thickness $L$ multiplied by the step-down matrix. Hence, our propagation matrix become

$$P = \frac{1}{2\sqrt{k_1k_2}} \begin{bmatrix} k_1 + k_2 & k_1 - k_2 \\ k_1 - k_2 & k_1 + k_2 \end{bmatrix} \begin{bmatrix} e^{-ik_2L} \\ 0 \end{bmatrix} \frac{1}{2\sqrt{k_1k_2}} \begin{bmatrix} k_2 + k_1 & k_2 - k_1 \\ k_2 - k_1 & k_2 + k_1 \end{bmatrix}$$

$$P = \frac{1}{4k_1k_2} \begin{bmatrix} (k_1 + k_2)e^{-ik_2L} & (k_1 - k_2)e^{ik_2L} \\ (k_1 - k_2)e^{-ik_2L} & (k_1 + k_2)e^{ik_2L} \end{bmatrix} \begin{bmatrix} k_2 + k_1 \\ k_2 - k_1 \end{bmatrix}$$

(38)

To find the matrix elements of $P$, we just multiply out the matrices in Eq.(38). For example $P_{12}$ becomes

$$P_{12} = -\frac{k_2^2 - k_1^2}{4k_1k_2} (e^{ik_2L} - e^{-ik_2L})$$

(39)
The next step we want to take is to calculate the transmission probability for a particle incident on the barrier. We already know that the transmission of a particle incident from the left is given by \( \frac{1}{p_{11}} \), so that we will be interested in obtaining \( p_{11} \) from Eq. (38)

\[
p_{11} = \frac{(k_2 + k_1)(k_1 + k_2)e^{-ik_2L} + (k_1 - k_2)(k_2 - k_1)e^{ik_2L}}{4k_1k_2}
\]

(40)

\[
p_{11} = \frac{(k_2^2 + k_1^2 + 2k_1k_2)e^{-ik_2L} - (k_2^2 + k_1^2 - 2k_1k_2)e^{ik_2L}}{4k_1k_2}
\]

(41)

\[
p_{11} = \frac{(k_2^2 + k_1^2)(e^{-ik_2L} - e^{ik_2L})}{4k_1k_2} + \frac{2k_1k_2(e^{-ik_2L} + e^{ik_2L})}{4k_1k_2}
\]

(42)

\[
p_{11} = -\frac{1}{2} \frac{(k_2^2 + k_1^2)(e^{ik_2L} - e^{-ik_2L})}{2k_1k_2} + \frac{1}{2} (e^{-ik_2L} + e^{ik_2L})
\]

(43)

\[
p_{11} = -\frac{1}{2} \frac{(k_2^2 + k_1^2)(e^{ik_2L} - e^{-ik_2L})}{2k_1k_2} + \frac{1}{2} (e^{-ik_2L} + e^{ik_2L})
\]

(44)

**The Result and Discussion**

We use the propagation matrix approach to calculate the transmission coefficient \( T \) of a rectangular potential barrier with width \( L = 1 \) nm and height \( V_0 = 0.3 \) eV as shown in Fig.(5). Matrix technique in transmission calculations means that we express every region of barrier as a propagation matrix \( P \). The transmission coefficient can be expressed

\[
T = \frac{1}{|p_{11}|^2}
\]

Using this principle, transmission coefficient \( T \) dependence on electron energy for a rectangular potential barrier was numerically calculated in Fig.(6). We vary barrier width while keeping barrier height constant. Transmission probabilities \( T(E) \) for barrier height \( V_0 = 0.3 \) eV and width \( L = 0.2 \) nm to \( 3.2 \) nm by increasing twice of initial value are shown in Fig.(7) to Fig.(11) respectively. Fig.(12) shows the transmission probability \( T(E) \) for barrier height \( V_0 = 0.3 \) eV and different barrier width.

**Fig.(5) The transmission coefficient \( T \) for a barrier of width \( L = 1 \) nm and height \( V_0 = 0.3 \) eV.**

**Fig.(6) The transmission coefficient \( T \) for a barrier of width \( L = 1 \) nm and height \( V_0 = 0.3 \) eV.**

**Fig.(7) Numerical calculation of transmission coefficient for a barrier of height \( V_0 = 0.3 \) eV and width \( L = 0.2 \) nm.**

**Fig.(8) Numerical calculation of transmission coefficient for a barrier of height \( V_0 = 0.3 \) eV and width \( L = 0.4 \) nm.**
Fig. (9) Numerical calculation of transmission coefficient for a barrier of height $V_0 = 0.3$ eV and width $L = 0.8$ nm.

Fig. (10) Numerical calculation of transmission coefficient for a barrier of height $V_0 = 0.3$ eV and width $L = 1.6$ nm.

Fig. (11) Numerical calculation of transmission coefficient for a barrier of height $V_0 = 0.3$ eV and width $L = 3.2$ nm.

When a beam of particles of fixed energy is incident on a potential barrier, a certain fraction of the incident particles is transmitted while the remaining fraction is reflected. This is in contrast to classical mechanics. Classically, there must be total transmission if the energy of the incident particle is more than the height of the barrier, and total reflection if the energy of the incident particle is less than the height of the barrier. Fig. (12) shows the transmission probability $T(E)$ for barrier height $V_0 = 0.3$ eV and different barrier width. If we keep the barrier height constant and change the barrier width, we see significance change in oscillations. When barrier width is narrow, even electron with lower energy can pass through the barrier by quantum tunneling. The wider the barrier will be the less observable the tunneling is, which is expectation from classical approach as well.

**Conclusion**

We have found that the transmission coefficient ($T$) depends upon potential barrier height ($V_0$) and barrier width ($L$). The transmission coefficient ($T$) is a measure of the probability that the particle will be transmitted through the barrier. Thus, we conclude that there is finite probability of particle penetrating the barrier and appearing on the other sides. The ability of particle to penetrate the barrier when $E < V_0$ is a quantum mechanical result and is known as tunnel effect. In nuclear physics, there are nuclei that decay into an α particle and daughter nucleus. This α decay process can be explained by tunnel effect.

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