

Quantum Tunneling

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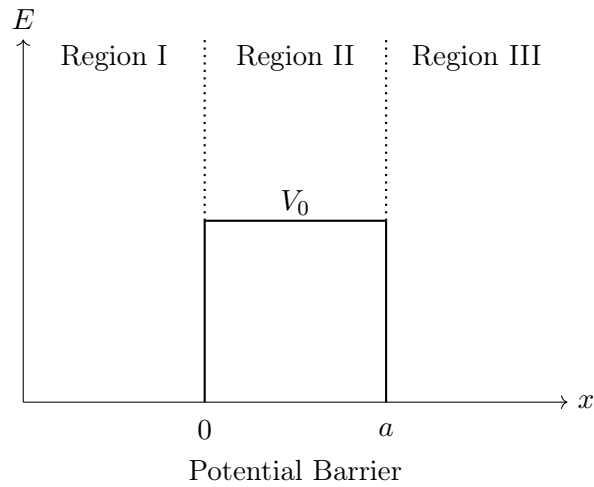
1. Introduction

This article explores the quantum tunneling phenomenon through a finite potential barrier, with full derivations for all energy regimes and a discussion on continuity of the transmission and reflection coefficients. It is written as a reference for students or anyone curious about the mathematics behind tunneling.

Consider the potential $V(x)$ defined by:

$$V(x) = \begin{cases} V_0 & (> 0) & 0 \leq x \leq a \\ 0 & & \text{otherwise} \end{cases}$$

The given potential could be sketched as follows:



Here we have divided the space into three regions with Region II containing the potential barrier of height V_0 and width a . We will consider a quantum particle to be moving towards positive x direction in Region I and solve one dimensional time independent Schrödinger Equation for the following three mutually exclusive and exhaustive cases:

1. $0 < E < V_0$
2. $E = V_0$
3. $E > V_0$

where E is the particle's energy.

This classic quantum mechanical problem is typically introduced in standard texts such as Griffiths [1], but often without explicit treatment of continuity at the energy threshold.

2. Solving Schrödinger Equation

The time independent Schrödinger Equation is given as:

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)} \quad (1)$$

A detailed discussion of the Schrödinger equation and its solutions for piecewise constant potentials can be found in Shankar [2].

2.1 Case I: $0 < E < V_0$

In Region I and Region III, (1) reduces to the following equation:

$$\frac{d^2}{dx^2} \psi(x) = -k^2 \psi(x), \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar} \quad (2)$$

The solution to (2) is oscillatory and is given as:

$$\text{Region I: } \psi_1(x) = Ae^{ikx} + Be^{-ikx} \quad (3)$$

$$\text{Region III: } \psi_3(x) = Ce^{ikx} + De^{-ikx} \quad (4)$$

In (4), De^{-ikx} represents a particle reflected in Region III and hence travelling along negative x direction. Since there is no potential barrier in Region III, a particle having transmitted through the potential barrier in Region II and travelling along positive x direction in Region III cannot be reflected back. Hence $D = 0$. Therefore (4) reduces to the following equation:

$$\text{Region III: } \psi_3(x) = Ce^{ikx} \quad (5)$$

In Region II, (1) reduces to the following equation:

$$\frac{d^2}{dx^2} \psi(x) = \kappa^2 \psi(x), \quad \text{where } \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (6)$$

The solution to (6) is exponential and is given as:

$$\text{Region II: } \psi_2(x) = Fe^{\kappa x} + Ge^{-\kappa x} \quad (7)$$

Using continuity of $\psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi_2(a) = \psi_3(a) \quad (8)$$

$$\Rightarrow A + B = F + G \quad \text{and} \quad Fe^{\kappa a} + Ge^{-\kappa a} = Ce^{ika} \quad (9)$$

Using continuity of $\frac{d}{dx} \psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\left. \frac{d}{dx} \psi_1(x) \right|_{x=0} = \left. \frac{d}{dx} \psi_2(x) \right|_{x=0} \quad \text{and} \quad \left. \frac{d}{dx} \psi_2(x) \right|_{x=a} = \left. \frac{d}{dx} \psi_3(x) \right|_{x=a} \quad (10)$$

$$\Rightarrow ikA - ikB = \kappa F - \kappa G \quad \text{and} \quad \kappa Fe^{\kappa a} - \kappa Ge^{-\kappa a} = ikCe^{ika} \quad (11)$$

Since we have five constants A, B, C, F, G and only four equations given by (9) and (11), the system is underdetermined.

Now note that Ae^{ikx} represents a particle (wave) travelling along positive x direction in Region I, Ce^{ikx} represents a particle (wave) travelling along positive x direction in Region III after having transmitted through the potential barrier and Be^{-ikx} represents a particle (wave) travelling along negative x direction after getting reflected from the wall of the potential barrier at $x = 0$. Accordingly we can write:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx} = \psi_{1,\text{right}} + \psi_{1,\text{left}} \quad (12)$$

$$\psi_3(x) = Ce^{ikx} = \psi_{3,\text{right}} \quad (13)$$

2.1.1 Finding Transmission and Reflection coefficients

Probability of finding a particle travelling right in Region I:

$$P_{1,\text{right}} = \psi_{1,\text{right}}^* \psi_{1,\text{right}} = (A^* e^{-ikx})(Ae^{ikx}) = A^* A \quad (14)$$

Probability of finding a particle travelling left in Region I:

$$P_{1,\text{left}} = \psi_{1,\text{left}}^* \psi_{1,\text{left}} = (B^* e^{ikx})(Be^{-ikx}) = B^* B \quad (15)$$

Probability of finding a particle travelling right in Region III:

$$P_{3,\text{right}} = \psi_{3,\text{right}}^* \psi_{3,\text{right}} = (C^* e^{-ikx})(Ce^{ikx}) = C^* C \quad (16)$$

The transmission coefficient T and reflection coefficient R are defined as follows:

$$T = \frac{P_{3,\text{right}}}{P_{1,\text{right}}} \quad \text{and} \quad R = \frac{P_{1,\text{left}}}{P_{1,\text{right}}} \quad (17)$$

Using (14), (15) and (16), (17) could be written as:

$$T = \frac{C^* C}{A^* A} = t^* t \quad (\text{say}) \quad \text{and} \quad R = \frac{B^* B}{A^* A} = r^* r \quad (\text{say}) \quad (18)$$

Now for notational simplicity, let $\frac{B}{A} = r$, $\frac{F}{A} = f$, $\frac{G}{A} = g$ and $\frac{C}{A} = t$. We have already found the four sets of equations given by (9) and (11) using boundary conditions and continuity of wavefunction and its first derivative. On dividing each of these four equations by A and using the notations as mentioned above, we get:

$$1 + r = f + g \quad (19)$$

$$ik - ikr = \kappa f - \kappa g \quad (20)$$

$$fe^{\kappa a} + ge^{-\kappa a} = te^{ika} \quad (21)$$

$$\kappa fe^{\kappa a} - \kappa ge^{-\kappa a} = ikte^{ika} \quad (22)$$

Multiplying (21) by κ and adding it to (22), we get:

$$2\kappa f e^{\kappa a} = i k t e^{i k a} + \kappa t e^{i k a} \quad (23)$$

Dividing (23) by $2\kappa e^{\kappa a}$ and then simplifying, we get:

$$f = \frac{t e^{(i k - \kappa) a} (i k + \kappa)}{2\kappa} \quad (24)$$

Multiplying (21) by κ and then subtracting it from (22), we get:

$$-2\kappa g e^{-\kappa a} = i k t e^{i k a} - \kappa t e^{i k a} \quad (25)$$

Dividing (25) by $-2\kappa e^{-\kappa a}$ and then simplifying, we get:

$$g = \frac{t e^{(i k + \kappa) a} (i k - \kappa)}{-2\kappa} \quad (26)$$

Multiplying (19) by $i k$ and then adding it to (20) we get:

$$2i k = (i k + \kappa) f + (i k - \kappa) g \quad (27)$$

Using (24), (26) in (27) and then simplifying, we get:

$$2i k = [e^{-\kappa a} (i k + \kappa)^2 - e^{\kappa a} (i k - \kappa)^2] \frac{t e^{i k a}}{2\kappa} \quad (28)$$

Simplifying (28) further, we get:

$$2i k = [(-k^2 + \kappa^2)(e^{-\kappa a} - e^{\kappa a}) + (2i k \kappa)(e^{-\kappa a} + e^{\kappa a})] \frac{t e^{i k a}}{2\kappa} \quad (29)$$

The hyperbolic $\sinh(x)$ and $\cosh(x)$ are given as:

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \quad \text{and} \quad \cosh(x) = \frac{e^x + e^{-x}}{2} \quad (30)$$

Using (30), we can write (29) as:

$$2i k = [-(-k^2 + \kappa^2) 2 \sinh(\kappa a) + (2i k \kappa) 2 \cosh(\kappa a)] \frac{t e^{i k a}}{2\kappa} \quad (31)$$

Solving (31) for t , we get:

$$t = \frac{4i k \kappa e^{-i k a}}{(k^2 - \kappa^2) 2 \sinh(\kappa a) + (2i k \kappa) 2 \cosh(\kappa a)} \quad (32)$$

The complex conjugate of t can be written as:

$$t^* = \frac{-4i k \kappa e^{i k a}}{(k^2 - \kappa^2) 2 \sinh(\kappa a) - (2i k \kappa) 2 \cosh(\kappa a)} \quad (33)$$

Using (18), we have:

$$T = t^* t = \frac{-4i k \kappa e^{i k a}}{(k^2 - \kappa^2) 2 \sinh(\kappa a) - (2i k \kappa) 2 \cosh(\kappa a)} \times \frac{4i k \kappa e^{-i k a}}{(k^2 - \kappa^2) 2 \sinh(\kappa a) + (2i k \kappa) 2 \cosh(\kappa a)} \quad (34)$$

$$\Rightarrow T = \frac{16k^2\kappa^2}{4(k^2 - \kappa^2)^2 \sinh^2(\kappa a) + 16k^2\kappa^2 \cosh^2(\kappa a)} \quad (35)$$

$$\Rightarrow T = \frac{1}{\frac{(k^2 - \kappa^2)^2}{4k^2\kappa^2} \sinh^2(\kappa a) + \cosh^2(\kappa a)} \quad (36)$$

Using the identity $\cosh^2(x) - \sinh^2(x) = 1$ in (36), it can be written as:

$$T = \frac{1}{1 + \left[\frac{(k^2 - \kappa^2)^2}{4k^2\kappa^2} + 1 \right] \sinh^2(\kappa a)} \quad (37)$$

Now we will first simplify the denominator of (37) as follows:

$$\frac{(k^2 - \kappa^2)^2}{4k^2\kappa^2} + 1 = \frac{k^2}{4\kappa^2} + \frac{\kappa^2}{4k^2} + \frac{1}{2} \quad (38)$$

Using the expression for k and κ from (2) and (6) respectively, we can write (38) as:

$$\frac{(k^2 - \kappa^2)^2}{4k^2\kappa^2} + 1 = \frac{V_0^2}{4E(V_0 - E)} \quad (39)$$

Substituting (39) in (37) and letting $\eta = \frac{E}{V_0}$, we can write:

$$T = \left[1 + \frac{\sinh^2(\kappa a)}{4\eta(1 - \eta)} \right]^{-1}, \quad \eta \in (0, 1) \quad (40)$$

The particle could either be transmitted through the barrier or be reflected from the barrier. Hence we must have:

$$T + R = 1 \quad \Rightarrow \quad R = T - 1 \quad (41)$$

Using expression for κ from (6) and the notation of η , we can rewrite κ as:

$$\kappa = \frac{\sqrt{2mV_0(1 - \eta)}}{\hbar} \quad (42)$$

2.2 Case II: $E = V_0$

In this case the solution in Region I and Region III will remain same as given by (3) and (5) respectively, i.e.,

$$\text{Region I: } \psi_1(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (43)$$

$$\text{Region III: } \psi_3(x) = Ce^{ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (44)$$

In Region II, (1) reduces to the following equation:

$$\frac{d^2}{dx^2}\psi_2(x) = 0 \quad (45)$$

The solution to (45) is linear and is given by:

$$\psi_2(x) = P + Qx \quad (46)$$

Using continuity of $\psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi_2(a) = \psi_3(a) \quad (47)$$

$$\Rightarrow A + B = P \quad \text{and} \quad P + Qa = Ce^{ika} \quad (48)$$

Using continuity of $\frac{d}{dx}\psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\left.\frac{d}{dx}\psi_1(x)\right|_{x=0} = \left.\frac{d}{dx}\psi_2(x)\right|_{x=0} \quad \text{and} \quad \left.\frac{d}{dx}\psi_2(x)\right|_{x=a} = \left.\frac{d}{dx}\psi_3(x)\right|_{x=a} \quad (49)$$

$$\Rightarrow ikA - ikB = Q \quad \text{and} \quad Q = ikCe^{ika} \quad (50)$$

Since we have five constants A, B, C, P, Q and only four equations given by (48) and (50), the system is underdetermined.

2.2.1 Finding Transmission and Reflection coefficients

Note that (12), (13), (14), (15), (16), (17) and (18) still holds in this case.

Now for notational simplicity, let $\frac{B}{A} = r$, $\frac{P}{A} = p$, $\frac{Q}{A} = q$ and $\frac{C}{A} = t$. We have already found the four sets of equations given by (48) and (50) using boundary conditions and continuity of wavefunction and its first derivative. On dividing each of these four equations by A and using the notations as mentioned above, we get:

$$1 + r = p \quad (51)$$

$$ik - ikr = q \quad (52)$$

$$p + qa = te^{ika} \quad (53)$$

$$q = ikte^{ika} \quad (54)$$

Multiplying (54) by a and subtracting it from (53), we get:

$$p = (1 - ika)te^{ika} \quad (55)$$

Multiplying (51) by ik and adding it to (52), we get:

$$2ik = pik + q \quad (56)$$

Using (54) and (55) in (56), we get:

$$2ik = (2 - ika)kte^{ika} \quad (57)$$

Solving (57) for t , we get:

$$t = \frac{2e^{-ika}}{2 - ika} \quad (58)$$

The complex conjugate of t can be written as:

$$t^* = \frac{2e^{ika}}{2 + ika} \quad (59)$$

Using (18), we have:

$$T = t^*t = \frac{2e^{ika}}{2 + ika} \times \frac{2e^{-ika}}{2 - ika} = \frac{4}{4 + k^2a^2} \quad (60)$$

$$\Rightarrow T = \left[1 + \left(\frac{ka}{2} \right)^2 \right]^{-1}, \quad k = \frac{\sqrt{2mE}}{\hbar} = \frac{\sqrt{2mV_0}}{\hbar} \quad (61)$$

Note that $\eta = \frac{E}{V_0} = 1$ in this case.

The particle could either be transmitted through the barrier or be reflected from the barrier. Hence we must have:

$$T + R = 1 \quad \Rightarrow \quad R = 1 - T \quad (62)$$

2.3 Case III: $E > V_0$

In this case the solution in Region I and Region III will remain same as given by (3) and (5) respectively, i.e,

$$\text{Region I: } \psi_1(x) = Ae^{ikx} + Be^{-ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (63)$$

$$\text{Region III: } \psi_3(x) = Ce^{ikx}, \quad k = \frac{\sqrt{2mE}}{\hbar} \quad (64)$$

In Region II, (1) reduces to the following equation:

$$\frac{d^2}{dx^2}\psi_2(x) = -\alpha^2\psi_2(x), \quad \text{where } \alpha = \frac{\sqrt{2m(E - V_0)}}{\hbar} \quad (65)$$

The solution to (65) is oscillatory and is given by:

$$\psi_2(x) = Me^{i\alpha x} + Ne^{-i\alpha x} \quad (66)$$

Using continuity of $\psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\psi_1(0) = \psi_2(0) \quad \text{and} \quad \psi_2(a) = \psi_3(a) \quad (67)$$

$$\Rightarrow A + B = M + N \quad \text{and} \quad Me^{i\alpha a} + Ne^{-i\alpha a} = Ce^{ika} \quad (68)$$

Using continuity of $\frac{d}{dx}\psi(x)$ at $x = 0$ and at $x = a$, we have:

$$\left. \frac{d}{dx}\psi_1(x) \right|_{x=0} = \left. \frac{d}{dx}\psi_2(x) \right|_{x=0} \quad \text{and} \quad \left. \frac{d}{dx}\psi_2(x) \right|_{x=a} = \left. \frac{d}{dx}\psi_3(x) \right|_{x=a} \quad (69)$$

$$\Rightarrow kA - kB = \alpha M - \alpha N \quad \text{and} \quad \alpha Me^{i\alpha a} - \alpha Ne^{-i\alpha a} = kCe^{ika} \quad (70)$$

Since we have five constants A, B, C, M, N and only four equations given by (68) and (70), the system is underdetermined.

2.3.1 Finding Transmission and Reflection coefficients

Note that (12), (13), (14), (15), (16), (17) and (18) still holds in this case.

Now for notational simplicity, let $\frac{B}{A} = r$, $\frac{M}{A} = m$, $\frac{N}{A} = n$ and $\frac{C}{A} = t$. We have already found the four sets of equations given by (68) and (70) using boundary conditions and continuity of wavefunction and its first derivative. On dividing each of these four equations by A and using the notations as mentioned above, we get:

$$1 + r = m + n \quad (71)$$

$$k - kr = \alpha m - \alpha n \quad (72)$$

$$me^{i\alpha a} + ne^{-i\alpha a} = te^{ika} \quad (73)$$

$$\alpha me^{i\alpha a} - \alpha ne^{-i\alpha a} = kte^{ika} \quad (74)$$

Multiplying (73) by $i\alpha$ and adding it to (74), we get:

$$2\alpha me^{i\alpha a} = kte^{ika} + \alpha te^{ika} \quad (75)$$

Dividing (75) by $2\alpha e^{i\alpha a}$ and then simplifying, we get:

$$m = \frac{te^{(ik-i\alpha)a}(k+\alpha)}{2\alpha} \quad (76)$$

Multiplying (73) by α and then subtracting it from (74), we get:

$$-2\alpha ne^{-i\alpha a} = kte^{ika} - \alpha te^{ika} \quad (77)$$

Dividing (77) by $-2\alpha e^{-i\alpha a}$ and then simplifying, we get:

$$n = \frac{te^{(ik+i\alpha)a}(k-\alpha)}{-2\alpha} \quad (78)$$

Multiplying (71) by k and then adding it to (72) we get:

$$2k = (k + \alpha)m + (k - \alpha)n \quad (79)$$

Using (76), (78) in (79) and then simplifying, we get:

$$2k = [e^{-i\alpha a}(k + \alpha)^2 - e^{i\alpha a}(k - \alpha)^2] \frac{te^{ika}}{2\alpha} \quad (80)$$

Simplifying (80) further, we get:

$$2k = [(k^2 + \alpha^2)(e^{-i\alpha a} - e^{i\alpha a}) + (2k\alpha)(e^{-i\alpha a} + e^{i\alpha a})] \frac{te^{ika}}{2\alpha} \quad (81)$$

The hyperbolic $\sinh(x)$ and $\cosh(x)$ are given as:

$$\sinh(x) = \frac{e^x - e^{-x}}{2} \quad \text{and} \quad \cosh(x) = \frac{e^x + e^{-x}}{2} \quad (82)$$

Using (82), we can write (81) as:

$$2k = [-(-k^2 + \alpha^2)2\sinh(i\alpha a) + (2k\alpha)2\cosh(i\alpha a)] \frac{te^{ika}}{2\alpha} \quad (83)$$

But $\sinh(ix) = i\sin(x)$ and $\cosh(ix) = \cos(x)$. Therefore we have from (83):

$$2k = [-i(-k^2 + \alpha^2)2\sin(\alpha a) + (2k\alpha)2\cos(\alpha a)] \frac{te^{ika}}{2\alpha} \quad (84)$$

Solving (84) for t , we get:

$$t = \frac{4k\alpha e^{-ika}}{-i(k^2 + \alpha^2)2\sin(\alpha a) + (2k\alpha)2\cos(\alpha a)} \quad (85)$$

The complex conjugate of t can be written as:

$$t^* = \frac{4k\alpha e^{ika}}{i(k^2 + \alpha^2)2\sin(\alpha a) + (2k\alpha)2\cos(\alpha a)} \quad (86)$$

Using (18), we have:

$$T = t^*t = \frac{4k\alpha e^{ika}}{i(k^2 + \alpha^2)2\sin(\alpha a) + (2k\alpha)2\cos(\alpha a)} \times \frac{4k\alpha e^{-ika}}{-i(k^2 + \alpha^2)2\sin(\alpha a) + (2k\alpha)2\cos(\alpha a)} \quad (87)$$

$$\Rightarrow T = \frac{16k^2\alpha^2}{4(k^2 + \alpha^2)^2\sin^2(\alpha a) + 16k^2\alpha^2\cos^2(\alpha a)} \quad (88)$$

$$\Rightarrow T = \frac{1}{\frac{(k^2 + \alpha^2)^2}{4k^2\alpha^2}\sin^2(\alpha a) + \cos^2(\alpha a)} \quad (89)$$

Using the identity $\cos^2(x) + \sin^2(x) = 1$ in (89), it can be written as:

$$T = \frac{1}{1 + \left[\frac{(k^2 + \alpha^2)^2}{4k^2\alpha^2} - 1 \right] \sin^2(\alpha a)} \quad (90)$$

Now we will first simplify the denominator of (90) as follows:

$$\frac{(k^2 + \alpha^2)^2}{4k^2\alpha^2} - 1 = \frac{k^2}{4\alpha^2} + \frac{\alpha^2}{4k^2} - \frac{1}{2} \quad (91)$$

Using the expression for k and α from (64) and (65) respectively, we can write (91) as:

$$\frac{(k^2 + \alpha^2)^2}{4k^2\alpha^2} - 1 = \frac{V_0^2}{4E(E - V_0)} \quad (92)$$

Substituting (92) in (90) and letting $\eta = \frac{E}{V_0}$, we can write:

$$T = \left[1 + \frac{\sin^2(\alpha a)}{4\eta(\eta - 1)} \right]^{-1}, \quad \eta \in (1, \infty) \quad (93)$$

The particle could either be transmitted through the barrier or be reflected from the barrier. Hence we must have:

$$T + R = 1 \quad \Rightarrow \quad R = 1 - T \quad (94)$$

Using expression for α from (65) and the notation of η , we can rewrite α as:

$$\alpha = \frac{\sqrt{2mV_0(\eta - 1)}}{\hbar} \quad (95)$$

3. Continuity of Transmission coefficient function $T(\eta)$ and Reflection coefficient function $R(\eta)$

Since we have already found the Transmission and Reflection coefficients, we will now inspect their continuity.

Let us define $T : (0, \infty) \rightarrow [0, 1]$ by

$$T(\eta) = \begin{cases} \left[1 + \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)}\right]^{-1}, & \kappa = \frac{\sqrt{2mV_0(1-\eta)}}{\hbar} & \forall \eta \in (0, 1) \\ \left[1 + \left(\frac{ka}{2}\right)^2\right]^{-1}, & k = \frac{\sqrt{2mV_0}}{\hbar} & \text{if } \eta = 1 \\ \left[1 + \frac{\sin^2(\alpha a)}{4\eta(\eta-1)}\right]^{-1}, & \alpha = \frac{\sqrt{2mV_0(\eta-1)}}{\hbar} & \forall \eta \in (1, \infty) \end{cases}$$

We note that 1 , $\sinh^2(\kappa a)$ and $4\eta(1-\eta)$ are positive smooth functions when $\eta \in (0, 1)$. Also note that 1 and $4\eta(\eta-1)$ are positive smooth functions and $\sin^2(\alpha a)$ is non-negative smooth function when $\eta \in (1, \infty)$. Hence $T(\eta)$ is continuous when $\eta \in (0, 1) \cup (1, \infty)$. Now we will inspect the continuity of $T(\eta)$ at $\eta = 1$.

Note that $\frac{d}{d\eta}\kappa = \frac{-mV_0}{\hbar\sqrt{2mV_0(1-\eta)}}$ and $2\sinh(\kappa a)\cosh(\kappa a) = \sinh(2\kappa a)$. The limit of $T(\eta)$ as $\eta \rightarrow 1^-$ is given as:

$$\lim_{\eta \rightarrow 1^-} T(\eta) = \frac{1}{1 + \lim_{\eta \rightarrow 1^-} \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)}} \quad (96)$$

Since the limit in (96) gives an indeterminate form $(\frac{0}{0})$, we have using L'Hôpital's Rule:

$$\lim_{\eta \rightarrow 1^-} \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)} = \lim_{\eta \rightarrow 1^-} \frac{2a \sinh(\kappa a) \cosh(\kappa a) \frac{d}{d\eta}\kappa}{4 - 8\eta} = \frac{mV_0 a}{4\hbar} \lim_{\eta \rightarrow 1^-} \frac{\sinh(2\kappa a)}{\sqrt{2mV_0(1-\eta)}} \quad (97)$$

The limit in (97) again gives an indeterminate form $(\frac{0}{0})$. Using L'Hôpital's Rule again gives:

$$\lim_{\eta \rightarrow 1^-} \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)} = -\frac{mV_0 a}{4\hbar} \cdot \frac{4a}{2mV_0} \lim_{\eta \rightarrow 1^-} \cosh(2\kappa a) \sqrt{2mV_0(1-\eta)} \frac{d}{d\eta}\kappa \quad (98)$$

$$\Rightarrow \lim_{\eta \rightarrow 1^-} \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)} = \frac{mV_0 a^2}{2\hbar^2} \lim_{\eta \rightarrow 1^-} \cosh(2\kappa a) \quad (99)$$

Since $\kappa \rightarrow 0$ as $\eta \rightarrow 1^- \Rightarrow \cosh(2\kappa a) \rightarrow 1$ as $\eta \rightarrow 1^-$. Therefore we have from (99):

$$\lim_{\eta \rightarrow 1^-} \frac{\sinh^2(\kappa a)}{4\eta(1-\eta)} = \frac{mV_0 a^2}{2\hbar^2} \quad (100)$$

Using (100) in (96), we have:

$$\lim_{\eta \rightarrow 1^-} T(\eta) = \left[1 + \frac{mV_0 a^2}{2\hbar^2} \right]^{-1} \quad (101)$$

Now note that $\frac{d}{d\eta} \alpha = \frac{mV_0}{\hbar \sqrt{2mV_0(\eta-1)}}$ and $2 \sin(\alpha a) \cosh(\alpha a) = \sin(2\alpha a)$. The limit of $T(\eta)$ as $\eta \rightarrow 1^+$ is given as:

$$\lim_{\eta \rightarrow 1^+} T(\eta) = \frac{1}{1 + \lim_{\eta \rightarrow 1^+} \frac{\sin^2(\alpha a)}{4\eta(\eta-1)}} \quad (102)$$

Since the limit in (102) gives an indeterminate form $(\frac{0}{0})$, we have using L'Hôpital's Rule:

$$\lim_{\eta \rightarrow 1^+} \frac{\sin^2(\alpha a)}{4\eta(\eta-1)} = \lim_{\eta \rightarrow 1^+} \frac{2a \sin(\alpha a) \cos(\alpha a) \frac{d}{d\eta} \alpha}{8\eta - 4} = \frac{mV_0 a}{4\hbar} \lim_{\eta \rightarrow 1^+} \frac{\sin(2\alpha a)}{\sqrt{2mV_0(\eta-1)}} \quad (103)$$

The limit in (103) again gives an indeterminate form $(\frac{0}{0})$. Using L'Hôpital's Rule again gives:

$$\lim_{\eta \rightarrow 1^+} \frac{\sin^2(\alpha a)}{4\eta(\eta-1)} = \frac{mV_0 a}{4\hbar} \cdot \frac{4a}{2mV_0} \lim_{\eta \rightarrow 1^+} \cos(2\alpha a) \sqrt{2mV_0(\eta-1)} \frac{d}{d\eta} \alpha \quad (104)$$

$$\Rightarrow \lim_{\eta \rightarrow 1^+} \frac{\sin^2(\alpha a)}{4\eta(\eta-1)} = \frac{mV_0 a^2}{2\hbar^2} \lim_{\eta \rightarrow 1^+} \cos(2\alpha a) \quad (105)$$

Since $\alpha \rightarrow 0$ as $\eta \rightarrow 1^+ \Rightarrow \cos(2\alpha a) \rightarrow 1$ as $\eta \rightarrow 1^+$. Therefore we have from (105):

$$\lim_{\eta \rightarrow 1^+} \frac{\sin^2(\alpha a)}{4\eta(\eta-1)} = \frac{mV_0 a^2}{2\hbar^2} \quad (106)$$

Using (106) in (102), we have:

$$\lim_{\eta \rightarrow 1^+} T(\eta) = \left[1 + \frac{mV_0 a^2}{2\hbar^2} \right]^{-1} \quad (107)$$

At $\eta = 1$, we have:

$$T(1) = \left[1 + \left(\frac{ka}{2} \right)^2 \right]^{-1} = \left[1 + \frac{mV_0 a^2}{2\hbar^2} \right]^{-1} \quad (108)$$

From (101), (107) and (108), we have:

$$\lim_{\eta \rightarrow 1^-} T(\eta) = \lim_{\eta \rightarrow 1^+} T(\eta) = T(1) = \left[1 + \frac{mV_0 a^2}{2\hbar^2} \right]^{-1} \quad (109)$$

Hence $T(\eta)$ is also continuous at $\eta = 1$. Therefore $T(\eta)$ is continuous on $(0, \infty)$.

Now define $R : (0, \infty) \rightarrow [0, 1]$ by

$$R(\eta) = 1 - T(\eta) \quad \forall \quad \eta \in (0, \infty) \quad (110)$$

Since both 1 and $T(\eta)$ are continuous on $(0, \infty) \Rightarrow R(\eta)$ is continuous on $(0, \infty)$.

4. Plotting Transmission and Reflection coefficients vs η using Python

Let us consider an electron moving along positive x direction in Region I. It will encounter a potential barrier of height 1 eV and of width 1 nm. Let us plot the values of Transmission and Reflection coefficients vs η . We will use the expressions for T , R , κ , k and α as determined in this article.

4.1 Python Code

```
import numpy as np
import matplotlib.pyplot as plt

# Constants
m = 9.11 * 10**(-31)           # mass of electron (kg)
hbar = 1.055 * 10**(-34)       # reduced Planck's constant (Js)
V0 = 1 * 1.6 * 10**(-19)       # barrier height in Joules (1 eV)
a = 10**(-9)                   # barrier width (m)

# Tunneling region : eta <= 1
eta_tunnel = np.linspace(0,1,500)[1:-1] # exclude 0 and 1
kappa = np.sqrt(2 * m * V0 * (1 - eta_tunnel)) / hbar
sinh_term = np.sinh(kappa * a)**2
T_kappa = 1 / (1 + (sinh_term / (4 * eta_tunnel * (1 - eta_tunnel))))
R_kappa = 1 - T_kappa

# E=V0 : eta=1
eta=np.array([1])
k=np.sqrt(2 * m * V0) / hbar
T=np.array([1 / (1 + ((k * a) / 2)**2)])
R=1-T

# Over-barrier region : eta > 1
eta_above = np.linspace(1,7,3000)[1:] # exclude 1
alpha = np.sqrt(2 * m * V0 * (eta_above - 1)) / hbar
sin_term = np.sin(alpha * a)**2
T_alpha = 1 / (1 + (sin_term / (4 * eta_above * (eta_above - 1))))
R_alpha = 1 - T_alpha

# Plotting
plt.plot(eta_tunnel, T_kappa, color='red', label=r'Transmission Coefficient $T$')
plt.plot(eta_tunnel, R_kappa, color='blue', label=r'Reflection Coefficient $R$')
plt.plot(eta, T, 'r,')
plt.plot(eta, R, 'b,')
plt.plot(eta_above, T_alpha, color='red')
plt.plot(eta_above, R_alpha, color='blue')
plt.title('Quantum Tunneling')
plt.xlabel(r'$\eta = \dfrac{E}{V_0}$')
plt.ylabel('Coefficient Value')
plt.legend()
plt.grid()
plt.ylim(-0.05, 1.05)
plt.xlim(0, 7)
plt.show()
```

4.2 Plot

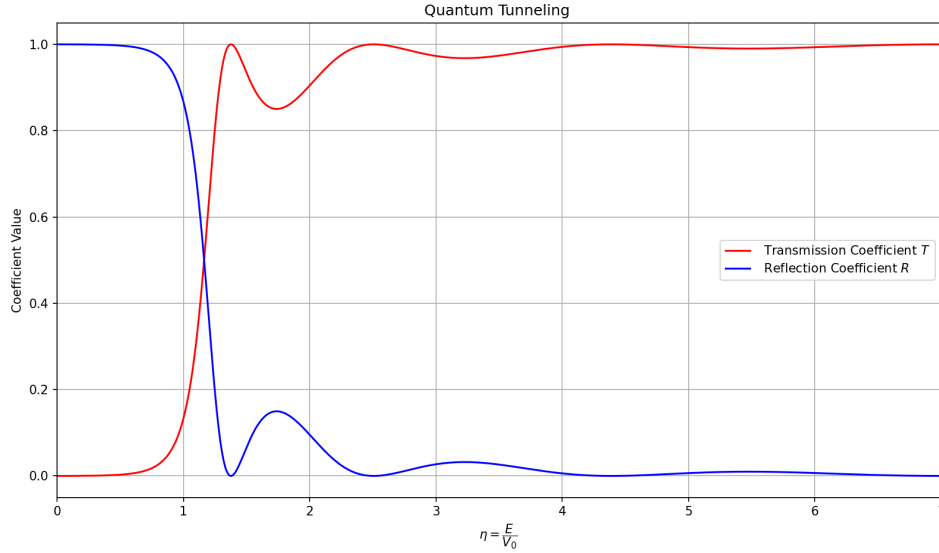


Figure 1: Plot of transmission coefficient $T(\eta)$ and reflection coefficient $R(\eta)$ as functions of the dimensionless energy parameter $\eta = E/V_0$. The plot illustrates continuity at $\eta = 1$ and the transition from tunneling to oscillatory behavior.

4.3 Inference from the Plot

The graph depicting the transmission coefficient $T(\eta)$ and reflection coefficient $R(\eta)$ as functions of the dimensionless parameter $\eta = \frac{E}{V_0}$ reveals the nuanced behavior of quantum particles interacting with a potential barrier.

For $\eta < 1$, we observe that $T(\eta)$ remains strictly non-zero as $\eta \rightarrow 1^-$, indicating that particles with energy less than the barrier height still possess a finite probability of tunneling through the barrier. This behavior arises from the continuity of the wavefunction and its derivative across the potential barrier. As $\eta \rightarrow 0$, $T(\eta) \rightarrow 0$, and $R(\eta) \rightarrow 1$, which agrees with intuitive expectations of nearly total reflection at very low energies.

At $\eta = 1$, a critical threshold, the function $T(\eta)$ is shown to be continuous, as confirmed by analytical limits using L'Hôpital's Rule. This reflects the smooth transition between classically forbidden and allowed energy regimes in quantum mechanics.

For $\eta > 1$, the particle energy exceeds the potential of the barrier. In this regime, $T(\eta)$ exhibits oscillatory behavior due to constructive and destructive interference between forward and backward traveling waves. As $\eta \rightarrow \infty$, $T(\eta) \rightarrow 1$ and $R(\eta) \rightarrow 0$, aligning with the classical limit of full transmission at high energies.

5. Comparison with Classical Mechanics

For $E < V_0$ ($\eta < 1$), classical mechanics predicts total reflection, as the particle cannot overcome the potential barrier, implying $T = 0$ and $R = 1$. However, in quantum mechanics, the wave-like nature of particles allows for non-zero penetration into the classically forbidden region, governed by the exponential solution to the Schrödinger equation in the barrier region (Region II). The continuity of the wavefunction and its derivative enforces boundary conditions that yield a non-zero transmission probability, a distinctly quantum phenomenon known as tunneling.

At $E = V_0$ ($\eta = 1$), classical mechanics predicts total reflection, since the particle has zero kinetic energy at the barrier and cannot proceed. In quantum mechanics, however, the continuity of the wavefunction and its derivative still allows for a non-zero transmission probability. Although the wavefunction is linear in the barrier region (Region II) at this energy, the boundary conditions ensure that partial transmission occurs even at this critical point.

For $E > V_0$ ($\eta > 1$), classical mechanics predicts total transmission. Quantum mechanics, in contrast, introduces partial reflection due to abrupt changes in the potential in a region. The wavefunction in the barrier region (Region II) undergoes interference due to its complex exponential form, resulting in oscillatory behavior of both T and R . These oscillations encode the resonant and anti-resonant conditions determined by the phase relation between waves, a concept entirely absent in classical particle dynamics.

Thus, the quantum description not only accommodates classically forbidden phenomena (tunneling), but also provides richer structure in classically allowed regimes, revealing the fundamentally wave-like nature of microscopic systems.

References

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