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Topic:

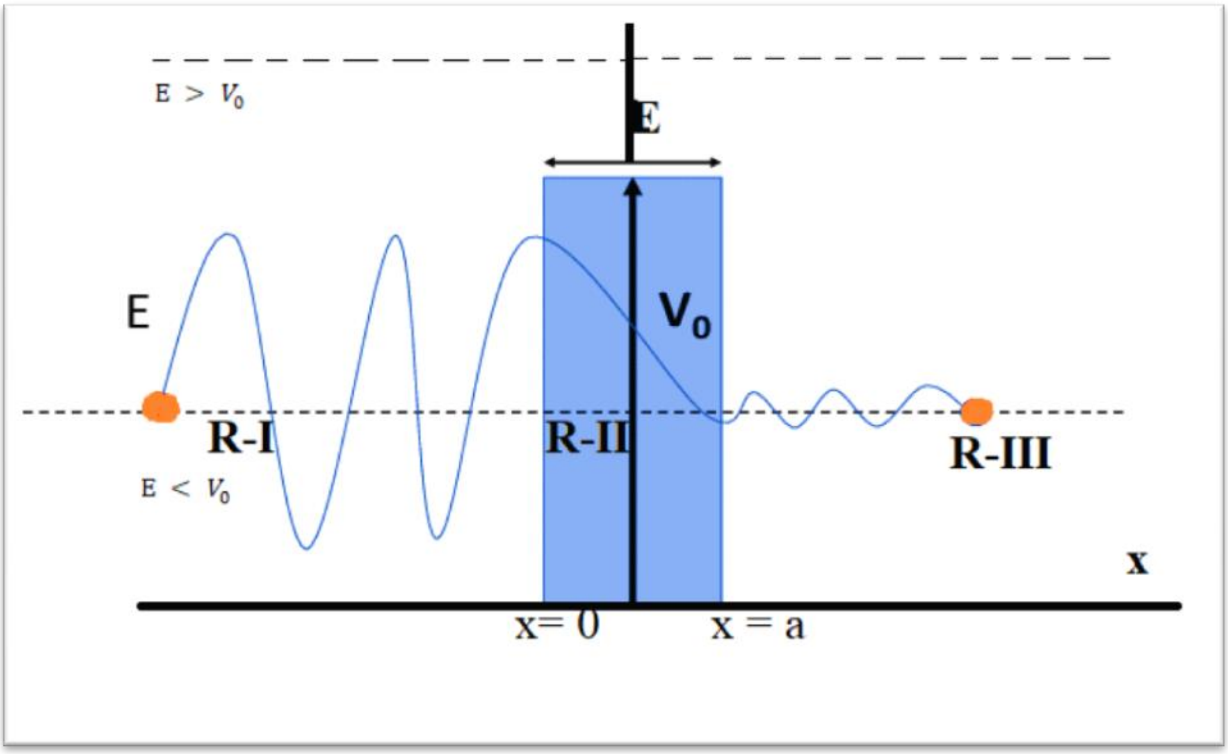
Elements of Modern Physics (3): Quantum Mechanical Scattering and Tunnelling in One Dimension-across Rectangular Potential Barrier

Elements of Modern Physics (3):

One Dimensional Rectangular Potential Barrier:

The potential function V(x) is a one dimensional rectangular potential barrier where, i.e. $V(x) = 0, x < 0$ and $x \geq 0$ as well as $V(x) =, V_0, for 0 \leq x \leq a$.

Let us consider a particle of mass m and K.E. $= E$ is travelling parallel to the x-axis and is incident from left of the barrierat $x = 0$.



The following two cases may arise-

(1) $E > V_0$, then according to classical mechanics, the particle will be wholly transmitted; as well as no reflection is possible. However, in quantum mechanically, we see that there will be a finite probability for the particles to be reflected at $x = 0$ and $x = a$

(2) If, $E < V_0$, then classically the particles will be wholly reflected and hence penetration through the barrier is impossible. However, in quantum mechanically, we see that there will be a finite probability of penetration of particles through the barrier and appearance of particle in region-III. The finite probability of transmission through the barrier in case of the condition, $E < V_0$, is called the *Quantum Mechanical Tunnelling Effect*.

CASE (i) $E > V_0$

The time dependent Schrödinger equation for region-I ($x < 0$) where $V(x) = 0$ becomes-

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1$$

Or, $\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0$

Or, $\frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0$…………………..(1)

Where, $\alpha = \sqrt{(\frac{2m}{\hbar^2}E)}$

For Region-II

We get, $\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$

Or, $\frac{d^2\psi_2}{dx^2} + \beta^2\psi_2 = 0$…………………..(2)

Where, $\beta = \sqrt{\frac{2m}{\hbar^2}}(E - V_0)$

The solution of equation (1) becomes-$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x}$………………..(3)

And $\psi_2 = Ce^{i\beta x} + De^{-i\beta x}$……………………(4)

Where A, B, C, D are constants of integration.

The term $e^{i\alpha x}$ represent the wave travelling + ve x direction. The term $e^{-i\alpha x}$ represent the wave travelling - ve x direction, i.e. reflected wave. Also, $e^{i\beta x}$ represents the wave travelling + ve x direction and term $e^{-i\beta x}$ represent the wave travelling - ve x direction, i.e. reflected wave.

For Region-III

$\frac{d^2\psi_3}{dx^2} + \alpha^2\psi_3 = 0$……………………(5)

Where, $\alpha = \sqrt{(\frac{2m}{\hbar^2}E)}$

The solution of equation (5) becomes-$\psi_3 = Fe^{i\alpha x} + Ge^{-i\alpha x}$…………………(6)

There is no wave reflected from region-III. Therefore,

The solution of equation (5) becomes-$\psi_3 = Fe^{i\alpha x}$…………………(7)

Putting the boundary condition,

1. $\psi_1 atx = 0 = \psi_2$ at $x = 0$
2. $\frac{d\psi_1}{dx}\ atx = 0 = \frac{d\psi_2}{dx}\ atx = 0$
3. $\psi_2 atx = a = \psi_3$ at $x = a$
4. $\frac{d\psi_2}{dx}\ atx = a = \frac{d\psi_3}{dx}\ atx = a$

Using the boundary condition

we get, $A + B = C$…………………(8)

and, $\alpha A - \alpha B = \beta C$- βD…………….(9)

$Ce^{i\beta x} + De^{-i\beta x} = Fe^{i\alpha a}$…………………(10)

$Ce^{i\beta x} + De^{-i\beta x} = \frac{\alpha}{\beta} e^{i\alpha a}$…………………(11)

Now, solving the equations (8 and 9) we get,

By solving we get,

$A = \frac{C}{2}\left(1 + \frac{\beta}{\alpha}\right) + \frac{D}{2}\ (1 - \frac{\beta}{\alpha})$………… … ….(12)

$B = \frac{C}{2}\left(1 - \frac{\beta}{\alpha}\right) + \frac{D}{2}\ (1 + \frac{\beta}{\alpha})$…………… ……(13)

Now, solving the equations (10 and 11) we get,

$C = \frac{F}{2}\left(1 + \frac{\beta}{\alpha}\right) e^{-i(\alpha-\beta)a}$………………………(14)

$D = \frac{F}{2}\left(1 - \frac{\beta}{\alpha}\right) e^{i(\alpha-\beta)a}$………………………..(15)

Substituting the values of C and D from (14, 15) in (12, 13) we get,

$$A = \frac{F}{4}e^{i\alpha a}[\left(1-\frac{\beta}{\alpha}\right)\left(1+\frac{\beta}{\alpha}\right)e^{-i\beta a} + \left(1-\frac{\beta}{\alpha}\right)\left(1-\frac{\alpha}{\beta}\right)e^{i\beta a} \ldots\ldots\ldots\ldots(14)$$

$$B = \frac{F}{4}e^{i\alpha a}[\left(1-\frac{\beta}{\alpha}\right)\left(1+\frac{\beta}{\alpha}\right)e^{-i\beta a} + \left(1+\frac{\beta}{\alpha}\right)\left(1-\frac{\alpha}{\beta}\right)e^{i\beta a} \ldots\ldots\ldots\ldots(15)$$

From these equations, we find-

$$\frac{F}{A} = \frac{4e^{-i\alpha a}}{\left(1+\frac{\beta}{\alpha}\right)\left(1+\frac{\alpha}{\beta}\right)e^{-i\beta a} + \left(1+\frac{\beta}{\alpha}\right)\left(1-\frac{\alpha}{\beta}\right)e^{i\beta a}}$$

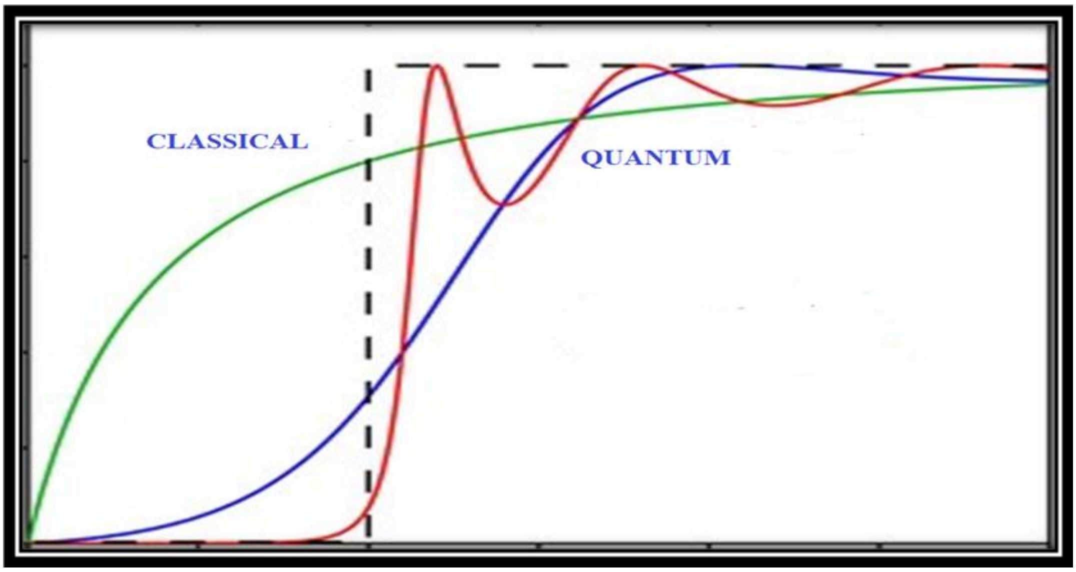
$$\frac{F}{A} = \frac{2\alpha\beta e^{-i\alpha a}}{2\alpha\beta Cos\beta a - i(\alpha^2-\beta^2)Sin\,\beta a}$$

Hence, transmission coefficient,

Transmission Coefficient (T) $=\frac{Transmitted\ Flux\ (J_t)}{Incident\ Flux\ (J_i)} = \frac{|F|^2}{|A|^2} = \frac{4\alpha^2\beta^2}{4\alpha^2\beta^2 Cos^2\beta a + (\alpha^2+\beta^2)^2 Sin^2\beta a}$

Therefore, (T) $=\frac{1}{1+\frac{V_0^2}{4E(E-V_0)}Sin^2\beta a}$…………………..(16)

From equation (16) T=1, if $Sin^2\beta a = 0$ or, $\beta a = n\pi, n = 1,2,3$; Then, $\frac{n\pi}{\beta} = a$



If barrier region contains an integral multiple of half de Broglie wavelength, then the barrier transmission is complete. This is known as Ramsauer-Townsend Effect.

Hence, reflection coefficient,

Reflection Coefficient (R) $=\frac{Reflected\ Flux\ (J_r)}{Incident\ Flux\ (J_i)} = \frac{|B|^2}{|A|^2} = \frac{\frac{(\alpha^2-\beta^2)^2}{4\alpha^2\beta^2}Sin^2\,\beta a}{1+\frac{(\alpha^2-\beta^2)^2}{4\alpha^2\beta^2}Sin^2\,\beta a}$

Therefore, (R) $=\frac{\frac{V_0^2}{4E(E-V_0)}Sin^2\,\beta a}{1+\frac{V_0^2}{4E(E-V_0)}Sin^2\,\beta a}$……………………(17)

CASE (i) $E < V_0$

The time dependent Schrödinger equation for region-I ($x < 0$) where $V(x) = 0$ becomes-

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1$$

Or, $\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0$

Or, $\frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0$…………………..(2.1)

Where, $\alpha = \sqrt{(\frac{2m}{\hbar^2}E)}$

For Region-II

We get, $\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0$

Or, $\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0$……………………(2.2)

Where, $\beta = \sqrt{\frac{2m}{\hbar^2}}(E - V_0)$

The solution of equation (1) becomes-$\psi_1 = Ae^{i\alpha x} + Be^{-i\alpha x}$………………..(2.3)

And $\psi_2 = Ce^{\beta x} + De^{-\beta x}$……………………(2.4)

Where A, B, C, D are constants of integration.

The term $e^{i\alpha x}$ represent the wave travelling + ve x direction. The term $e^{-i\alpha x}$ represent the wave travelling - ve x direction, i.e. reflected wave. Also, $e^{i\beta x}$ represents the wave travelling + ve x direction and term $e^{-i\beta x}$ represent the wave travelling - ve x direction, i.e. reflected wave.

For Region-III

$\frac{d^2\psi_3}{dx^2} + \alpha^2\psi_3 = 0$……………………(2.5)

Where, $\alpha = \sqrt{(\frac{2m}{\hbar^2}E)}$

The solution of equation (5) becomes-$\psi_3 = Fe^{i\alpha x} + Ge^{-i\alpha x}$………………..(2.6)

There is no wave reflected from region-III. Therefore,

The solution of equation (5) becomes-$\psi_3 = Fe^{i\alpha x}$………………..(2.7)

Putting the boundary condition,

1. $\psi_1 atx = 0 = \psi_2$ at $x = 0$

2. $\frac{d\psi_1}{dx}$ $atx = 0 = \frac{d\psi_2}{dx}$ $atx = 0$

3. $\psi_2 atx = a = \psi_3$ at $x = a$

4. $\frac{d\psi_2}{dx}$ $atx = a = \frac{d\psi_3}{dx}$ $atx = a$

Using the boundary condition

we get, $A + B = C$……………… …(2.8)

and, $-i\alpha A - i\alpha B = \beta C$- βD………… …..(2.9)

$Ce^{\beta a} + De^{-\beta a} = Fe^{\alpha a}$…………… …..(2.10)

$\beta Ce^{\beta a} - D\beta e^{-\beta a}$ =$i\alpha F\ e^{i\alpha a}$…………… …..(2.11)

Now, solving the equations (2.8 and 2.9) we get,

By solving we get,

$A = \frac{C}{2}\left(1 - \frac{i\beta}{\alpha}\right) + \frac{D}{2}\ (1 + \frac{i\beta}{\alpha})$………… … ….(2.12)

$B = \frac{C}{2}\left(1 + \frac{i\beta}{\alpha}\right) + \frac{D}{2}\ (1 - \frac{i\beta}{\alpha})$…………… ……(2.13)

Now, solving the equations (2.10 and 2.11) we get,

$C = \frac{F}{2}\left(1 + \frac{i\alpha}{\beta}\right) e^{(i\alpha - \beta)a}$………………………(2.14)

$D = \frac{F}{2}\left(1 - \frac{i\alpha}{\beta}\right) e^{(i\alpha + \beta)a}$………………………..(2.15)

Substituting the values of C and D from (14, 15) in (12, 13) we get,

$A = \frac{F}{4} e^{i\alpha a}[\left(1 + \frac{i\beta}{\alpha}\right)\left(1 + \frac{\alpha}{i\beta}\right) e^{-\beta a} + \left(1 - \frac{i\beta}{\alpha}\right)\left(1 - \frac{\alpha}{i\beta}\right) e^{\beta a}$………………………(2.16)

$B = \frac{F}{4} e^{i\alpha a}[\left(1 - \frac{i\beta}{\alpha}\right)\left(1 + \frac{\alpha}{i\beta}\right) e^{-\beta a} + \left(1 + \frac{i\beta}{\alpha}\right)\left(1 - \frac{\alpha}{i\beta}\right) e^{\beta a}$………………………(2.17)

From these equations, we find-

$$\frac{F}{A} = \frac{4e^{-i\alpha a}}{\left(1 + \frac{\beta}{\alpha}\right)\left(1 + \frac{\alpha}{\beta}\right) e^{-i\beta a} + \left(1 + \frac{\beta}{\alpha}\right)\left(1 - \frac{\alpha}{\beta}\right) e^{i\beta a}}$$

$$\frac{F}{A} = \frac{4}{e^{i\alpha a}\ [\left(1 + \frac{i\beta}{\alpha}\right)\left(1 + \frac{\alpha}{i\beta}\right) e^{-\beta a} + \left(1 - \frac{i\beta}{\alpha}\right)\left(1 - \frac{\alpha}{i\beta}\right) e^{\beta a}]}$$

Hence, transmission coefficient,

Transmission Coefficient (T) =$\frac{Transmitted\ Flux\ (J_t)}{Incident\ Flux\ (J_i)} = \frac{|F|^2}{|A|^2}$=$1/(1 + \frac{(\beta^2 - \alpha^2)^2}{16\beta^4\alpha^4}\ \ Sin^2\ \beta a)$

Therefore, (T) $=\frac{1}{1+\frac{V_0^2}{4E(V_0-E)}Sinh^2\beta a}$…………………..(2.18)

Reflection and Transmission Coefficient:

Hence, reflection coefficient,

Reflection Coefficient (R) $=\frac{Reflected\ Flux\ (J_r)}{Incident\ Flux\ (J_i)}=\frac{|B|^2}{|A|^2}=\frac{\frac{(\alpha^2+\beta^2)^2}{4\alpha^2\beta^2}Sinh^2\beta a}{Cosh^2\beta a+\frac{(\beta^2-\alpha^2)^2}{4\alpha^2\beta^2}Sin^2\beta a}$

Therefore, (R) $=\frac{\frac{(\alpha^2+\beta^2)^2}{4\alpha^2\beta^2}Sinh^2\beta a}{Cosh^2\beta a+\frac{(\beta^2-\alpha^2)^2}{4\alpha^2\beta^2}Sinh^2\beta a}$…………………..(2.19)

Quantum Mechanical Tunnelling:

Quantum Mechanical Tunnelling is the phenomenon of transmission of particle through the potential barrier of finite height and width when its energy is less than the barrier height.

The transmission probability depends on V_0 and width a such that T is small if V_0 and a are large.

When $a \longrightarrow large\ value\ of\ \beta a \longrightarrow \infty$

Therefore, $Sinh^2\beta a=\frac{e^{2\beta a}}{4}>>1$

Therefore, (T) $=\frac{16\alpha^2\beta^2}{(\alpha^2+\beta^2)}e^{-2\beta a}$…………………..(2.20)

Therefore, (T) $=\frac{16(V_0-E)}{{V_0}^2}e^{-2\beta a}$…………………..(2.21)

From, (17 & 19), we get, $R+T=1$

Frequently Asked Questions/Numerical:

For theoretical questions and problems in this section of 1D Potential Well, students can solve the problems of Concept of Atomic Physics, Author- S. P. Kuila, Published by NCBA (2018 Ed.) and Quantum Mechanics by JyotirmoyGuha, Published by Books & Allied Pvt. Ltd. (2018 Ed.).

References:

(i) *Concept of Atomic Physics, Author- S. P. Kuila, Published by NCBA (2018 Ed.).*

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(ii) *Refresher Course in Physics, Author- C. L. Arora, Published by S. Chand (2018 Ed.).*
(iii) *Quantum Mechanics- Author- JyotirmoyGuha, Published by Books & Allied Pvt. Ltd. (2018 Ed.).*
(iv) https://en.wikipedia.org/wiki/Rectangular_potential_barrier*https://quantummechanics.ucsd.edu/ph130a/130_notes/node149.html (Images are taken only for class note)*

Link to Audio visual Lectures (e-Lectures) on this topic given by Distinguish Professors of Indian &Foreign Universities:

(1) *https://www.youtube.com/watch?v=6B1EI2npnighttps://www.youtube.com/watch?v=4PnmKYR9_uM*
(2) *https://www.youtube.com/watch?v=gBsj_i5hB6U*
(3) *https://www.youtube.com/watch?v=wqettJHPaWY*
(4) *https://nptel.ac.in/courses/115102023/*
(5) *https://nptel.ac.in/courses/122106034/*