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Topic:

Elements of Modern Physics (2): Quantum Mechanical Scattering and Tunnelling in One Dimension-across a Step Potential

Elements of Modern Physics (2):

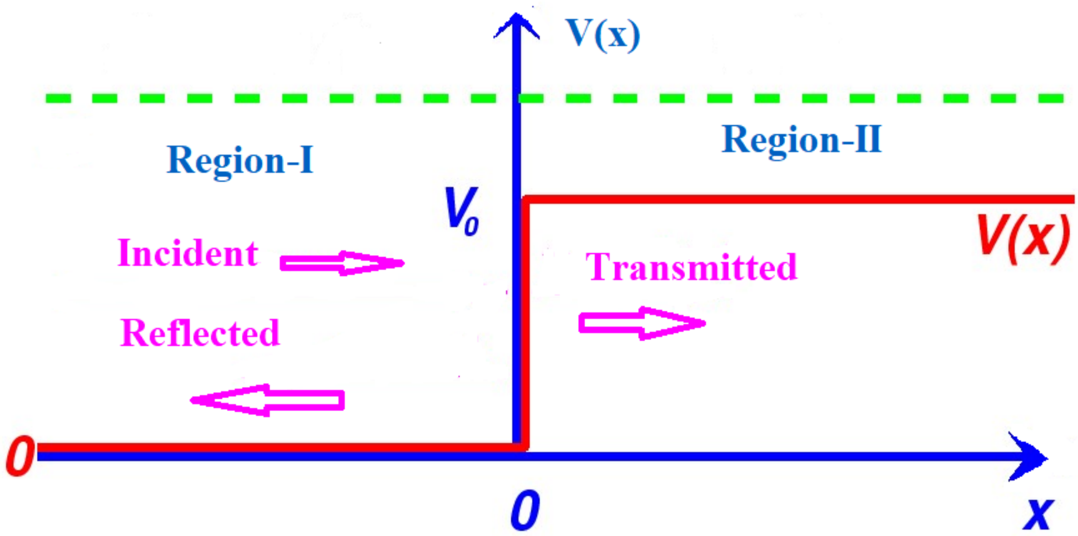
One Dimensional Step Potential:

The potential function V(x) is a one dimensional single step potential function where, i.e. $V(x) = 0, x < 0$and $V(x) =, V_0, for x > 0$.

Let us consider a particle of mass m and K.E. $= E$ is travelling parallel to the x-axis and is incident on the potential step at $x = 0$. Since, $V(x) = 0, x < 0$and $V(x) = V_0, for x > 0.$, the energy of the particle is wholly kinetic for $x < 0$ and partially kinetic and partially potential for $x > 0$.

From classical point of view in Region –I the particle can move freely as $V(x) = 0$. But in the region-II, $E <, V_0$, the particle will remain in region-I for ever and will be reflected back at $x = 0$. However, $E >, V_0$, the particle will be partly reflected and partly transmitted.

Therefore we shall find two case (i) $E <, V_0$ and (ii)$E >, V_0$



CASE (i) $E > V_0$

The time dependent Schrödinger equation for region-I 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. However, no wave should in $e^{-i\beta x}$ the wave travelling - ve x direction, i.e. reflected wave in region-II. Therefore, the term $De^{-i\beta x}$ is neglected.

And $\psi_2 = Ce^{i\beta x}$ … … … … … … . (5)

Putting the boundary condition,

1. ψ_1 $\boldsymbol{at x} = 0 = \psi_2$ at $\boldsymbol{x} = \boldsymbol{0}$
2. $\frac{d\psi_1}{\text{dx}}$ $\boldsymbol{at x} = 0 = \frac{d\psi_2}{\text{dx}}$ $\boldsymbol{at x} = 0$

Using the boundary condition

we get, $\boldsymbol{A + B = C}$

and, $\alpha A - \alpha B = \beta C$

By solving we get,

$B = \frac{\alpha-\beta}{\alpha+\beta} A$ and $C = \frac{2\alpha}{\alpha+\beta} A$

$$\psi_1 = A \left[e^{i\alpha x} + \left(\frac{\alpha - \beta}{\alpha + \beta}\right) e^{-i\alpha x}\right]$$

$$\psi_2 = \left(\frac{2\alpha}{\alpha + \beta}\right) A\, e^{i\beta x}$$

The probability current density for the incident beam of particle in region-I is-

For Incident beam $J_i = \frac{\hbar\alpha}{m}(A\, e^{i\alpha x})\,(Ae^{i\alpha x})^*$

i.e. $J_i = \frac{\hbar\alpha}{m} A^2$

The probability current density for the reflected beam-$J_r = \frac{\hbar\alpha}{m}(B\, e^{-i\alpha x})\,(Be^{-i\alpha x})^*$

$$J_r = \frac{\hbar\alpha}{m} |B|^2$$

The net probability current density in the direction from left to right

$J = J_i - J_r = \frac{\hbar\alpha}{m}\left(|A|^2 - |B|^2\right)$

But, $B^2 = \left(\frac{\alpha-\beta}{\alpha+\beta}\right)^2 A^2$

Therefore, $J = \frac{4\alpha\beta}{(\alpha+\beta)}\frac{\hbar\alpha}{m}\, |A|^2$

Again the probability current density for the incident beam of particle in region-II

$J_t = \frac{\hbar\beta}{m}(C\, e^{i\beta x})\,(Ce^{-i\beta x})^* = \frac{\hbar\beta}{m}\,|C^2|$

But, $C = \frac{2\alpha}{\alpha+\beta} A$

Hence, $J_t = \frac{\hbar\beta}{m}(C\, e^{i\beta x})\,(Ce^{-i\beta x})^* = \frac{\hbar\beta}{m}\,|C^2| = \frac{\hbar\beta}{m}\left|\left(\frac{2\alpha}{\alpha+\beta} A\right)^2\right|$

$$J_t = \frac{4\alpha^2}{(\alpha + \beta)^2}\frac{\hbar\beta}{m}\,|A^2|$$

The net current density becomes-$J_r + J_t = \frac{\hbar\alpha}{m}(\frac{\alpha-\beta}{\alpha+\beta})^2 A^2 + \frac{4\alpha^2}{(\alpha+\beta)^2}\frac{\hbar\beta}{m}|A^2| = \frac{\hbar\alpha}{m}A^2 = J_i$

$J_r + J_t = J_i$

Reflection and Transmission Coefficient:

Reflection Coefficient (R) $= \frac{Reflected\ Flux\ (J_r)}{Incident\ Flux\ (J_i)} = \frac{\frac{\hbar\alpha}{m}|B|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{|B|^2}{|A|^2} = (\frac{\alpha-\beta}{\alpha+\beta})^2$

Transmission Coefficient (T) $= \frac{Transmitted\ Flux\ (J_t)}{Incident\ Flux\ (J_i)} = \frac{\frac{\hbar\beta}{m}|C|^2}{\frac{\hbar\alpha}{m}|A|^2} = \frac{\beta}{\alpha}\frac{|C|^2}{|A|^2} = \frac{4\alpha\beta}{(\alpha+\beta)^2}$

Therefore, R+T= $(\frac{\alpha-\beta}{\alpha+\beta})^2 + \frac{4\alpha\beta}{(\alpha+\beta)^2} = 1$

Case B (E<V_0):

For region I$(x < 0)$ the schoredinger equation 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, $\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_2 = 0$Here, $V_0 > E$

Or, $\frac{d^2\psi_2}{dx^2} - \gamma^2\psi_2 = 0$…………………..(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 $\psi_2 = Ce^{\gamma x} + De^{-\gamma x}$……………………(4)

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

Here, $e^{\gamma x} \longrightarrow \infty$ as $x \longrightarrow \infty$

Therefore, $\psi_2 = De^{-\gamma x}$

Applying the boundary conditions,

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

Using the boundary condition

we get, $A + B = 0$

and, $i\alpha A - i\alpha B = -\gamma D$

By solving we get,

$D = \frac{2i\alpha}{i\alpha - \gamma} A$, and $B = \frac{2i\alpha}{i\alpha - \gamma} A$

And also, $|B|^2 = |A|^2$

The probability current density for the incident beam of particle in region-I is-

$J_t = -\frac{i\hbar}{2m} [\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx}]$

$J_t = -\frac{i\hbar}{2m} [D^* e^{-\gamma x} D(-\gamma) e^{-\gamma x} - De^{-\gamma x} D^*(-\gamma) e^{-\gamma x}]$

$J_t = \frac{i\hbar}{2m} DD^* \gamma [e^{-2\gamma x} - e^{-2\gamma x}] = 0$

Reflection and Transmission Coefficient:

Reflection Coefficient (R) $= \frac{Reflected\ Flux\ (J_r)}{Incident\ Flux\ (J_i)} = \frac{|B|^2}{|A|^2} = 1$

(Since, $|B|^2 = |A|^2$) for $V_0 > E$,

Therefore, $R = 1$

But for Region II, $J_t = 0$

Therefore, $T = 0$

The conclusions become-

(1) The incident wave is totally reflected at the potential step, $R = 1$

(2) In region II, the probability current density is zero, $J_t = 0$

(3) In region II, the wave function $\psi_2 = De^{-\gamma x}$ i.e. ψ_2 is exponentially damped. This leads to finite probability of finding the particle in region II

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.).*

(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://dradchem.files.wordpress.com/2015/09/particle-in-box.png (Images are taken only for class note)*

(v) *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=vj39m0Ul38Mhttps://nptel.ac.in/courses/115106086/*

(2) *https://www.youtube.com/watch?v=0ABYYJSvkVk*

(3) *https://www.youtube.com/watch?v=hszLM5k7aNY*

(4) *https://www.youtube.com/watch?v=QOsy-1J5w-Y*