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Topic:

Nanoscale system (2): Quantum Mechanical Scattering and Tunnelling in One Dimension-across a Step Potential

Elements of Modern Physics (2):

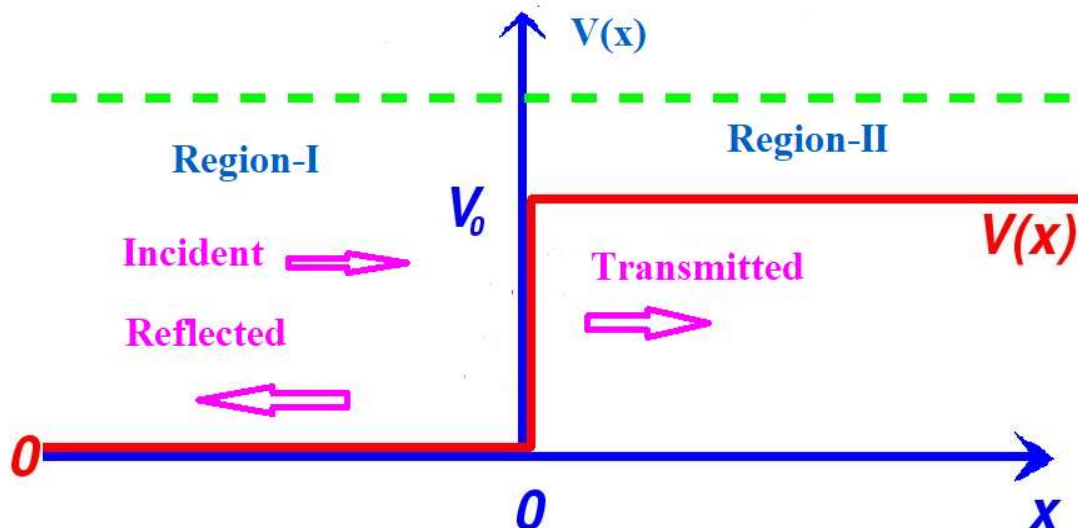
One Dimensional Step Potential:

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

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 $V(x) = V_0, \text{ for } x > 0$, 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-



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

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

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

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

For Region-II

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

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

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

$$\text{The solution of equation (1) becomes- } \psi_1 = A e^{i\alpha x} + B e^{-i\alpha x} \dots \dots \dots (3)$$

$$\text{And } \psi_2 = C e^{i\beta x} + D e^{-i\beta x} \dots \dots \dots (4)$$

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 $D e^{-i\beta x}$ is neglected.

$$\text{And } \psi_2 = C e^{i\beta x} \dots \dots \dots (5)$$

Putting the boundary condition,

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

Using the boundary condition

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

$$\text{and, } \alpha A - \alpha B = \beta C$$

By solving we get,



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$J_r + J_t = J_i$$



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Reflection and Transmission Coefficient:

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

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

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

Case B ($E < V_0$):

For region I ($x < 0$) the schoredinger equation becomes-

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

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

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

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

For Region-II

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

$$\text{Or, } \frac{d^2\psi_2}{dx^2} - \gamma^2\psi_2 = 0 \dots\dots\dots(2)$$

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

$$\text{The solution of equation (1) becomes- } \psi_1 = A e^{i\alpha x} + B e^{-i\alpha x} \dots\dots\dots(3)$$

$$\text{And } \psi_2 = C e^{\gamma x} + D e^{-\gamma x} \dots\dots\dots(4)$$

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

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

$$\text{Therefore, } \psi_2 = D e^{-\gamma x}$$

Applying the boundary conditions,

$$1. \psi_1 \text{ at } x = 0 = \psi_2 \text{ at } x = 0$$



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

Using the boundary condition

$$\text{we get, } A + B = 0$$

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

By solving we get,

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

$$\text{And also, } |B|^2 = |A|^2$$

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

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

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

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

Reflection and Transmission Coefficient:

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

(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 $\psi_2 = D e^{-\gamma x}$ i.e. ψ_2 is exponentially damped.
This leads to finite probability of finding the particle in region II

Frequently Asked Questions/Numerical:



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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 Jyotirmoy Guha, 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- Jyotirmoy Guha, 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 Distinguished Professors of Indian & Foreign Universities:

- (1) <https://www.youtube.com/watch?v=vj39m0Ul38M><https://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>