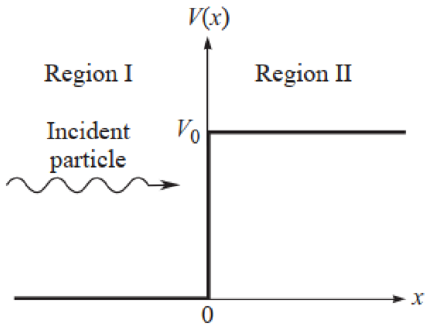
Chapter Three

Scattering of Particles by Barriers and Wells

5.1 The Potential Step

It is an infinite-width potential barrier given by,



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} \quad \ldots(5.1)$$

Suppose, a particle of mass m is incident on the step from the left with energy E. Since the potential does not depend on time, the motion of the particle is described by the wave function $\psi(x,t) = \psi(x)e^{-iEt/\hbar}$, where $\psi(x)$ satisfies the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \quad \ldots(5.2)$$

According to classical mechanics, we shall discuss the solution of this equation separately for the two cases,

- If $E < V_0$, then the particle would be reflected back at $x = 0$ because it does not have sufficient energy to climb the barrier.
- If $E > V_0$, then the particle would not be reflected; it would keep moving towards the right with reduced energy.

Case 1: $E > V_0$

Region I (x < 0): the time-independent Schrödinger equation is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$$

or $$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \qquad k^2 = \frac{2mE}{\hbar^2} \qquad \ldots(5.3)$$

The general solution of this equation is

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

Ae^{ikx}: a plane wave of amplitude A incident on the potential step from the left.

Be^{-ikx}: a plane wave of amplitude B reflected from the step.

Thus, according to quantum mechanics, the particle may be reflected back at $x = 0$ even though $E > V_0$. This is not possible classically.

Region II (x > 0): the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi = E\psi$$

or $$\frac{d^2\psi}{dx^2} + k'^2\psi(x) = 0, \qquad k'^2 = \frac{2m(E - V_0)}{\hbar^2} \qquad \ldots(5.4)$$

Since $E > V_0$, the quantity k'^2 is positive. Therefore, the general solution of this equation is

$$\psi(x) = Ce^{ik'x} + D\,e^{-ik'x}$$

$Ce^{i\acute{k}x}$: Incident wave on the barrier from the left. (*transmitted wave*)

$De^{-i\acute{k}x}$: Reflected wave in *region II,* But there is nothing in this region which can cause a reflection. Therefore, we must put $D = 0$. Thus the complete eigenfunction is given by,

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik'x} & x > 0 \end{cases} \qquad \ldots(5.5)$$

The eigenfunction consists of:

- In ***region I***: An Incident wave of amplitude *A* and a reflected wave of amplitude *B* with wave number *k*
- In ***region II***: Atransmitted wave of amplitude *C* with wave number $\acute{k}$.

Continuity of $\psi(x)$ and $d\psi/dx$ at $x = 0$ (H.W)

$$A + B = C$$

and

$$k(A - B) = k'C$$

from which we obtain,

$$\frac{B}{A} = \frac{k - k'}{k + k'} \qquad \ldots(5.6)$$

and

$$\frac{C}{A} = \frac{2k}{k + k'} \qquad \ldots(5.7)$$

H.W.: Prove equations (5.6) and (5.7).

5.1 Probability current densities

From the relation, $j = Re\left[\psi^* \frac{\hbar}{im}\frac{\partial\psi}{\partial x}\right]$ we can obtain the probability current densities associated with the incident, the reflected and the transmitted waves., **(H.W)**

- For incident waves $j_{in} = \frac{\hbar k}{m}|A|^2$ …(5.8)
- For reflected waves $j_{re} = \frac{\hbar k}{m}|B|^2$ …(5.9)
- For transmitted waves $j_{tr} = \frac{\hbar \acute{k}}{m}|C|^2$ …(5.10)

A particle incident on the step will either be reflected or transmitted.

The probability of reflection is given by the ***reflection coefficient R***:

$$R = \frac{j_{re}}{j_{in}} = \left|\frac{B}{A}\right|^2 = \left(\frac{k - k'}{k + k'}\right)^2 \qquad \ldots(5.11)$$

Substituting the values of k and k' and simplifying this becomes

$$R = \left[\frac{1-(1-V_0/E)^{1/2}}{1+(1-V_0/E)^{1/2}} \right]^2, \quad E > V_0 \qquad \ldots(5.12)$$

The probability of transmission is given by the ***transmission coefficient T***:

$$T = \frac{j_{\text{tr}}}{j_{\text{in}}} = \frac{k'}{k} \left| \frac{C}{A} \right|^2 = \frac{4kk'}{(k+k')^2} \qquad \ldots(5.13)$$

Substituting the values of k and k',

$$T = \frac{4(1-V_0/E)^{1/2}}{[1+(1-V_0/E)^{1/2}]^2}, \quad E > V_0 \qquad \ldots(5.14)$$

Note:

- $\boldsymbol{R}$ and $\boldsymbol{T}$ depend only on the ratio V_0/E.
- $\boldsymbol{R + T = 1}$ because the probability is conserved.

It can be easily shown that

$$k(|A|^2 - |B|^2) = k'|C|^2 \qquad \ldots(5.15)$$

- This shows that the net current incident on the step from the left is equal to the transmitted current.

Case 2: $\boldsymbol{E < V_0}$

In region I : The Schrödinger equation, its solution and interpretation remain the same as in Case 1 $E > V_0$.

In region II: the equation becomes,

$$\frac{d^2\psi(x)}{dx^2} - K^2\psi(x) = 0, \quad K^2 = \frac{2m(V_0 - E)}{\hbar^2} \qquad \ldots(5.16)$$

Since $V_0 > E$, the quantity K^2 is *positive*. Therefore, the general solution of this equation is,

$$\psi(x) = Ce^{-Kx} + De^{Kx}$$

Now, the wave function should not become infinite at $x \to \infty$. Since $\exp(Kx)$ diverges in that limit, we must choose $D = 0$. Thus the complete eigenfunction is given by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{-Kx} & x > 0 \end{cases} \qquad \ldots(5.17)$$

In region II we note that:

- The wave function is not zero in the classically forbidden region. It decreases rapidly as x increases. There is a finite and small, probability of finding the particle in region II.
- This phenomenon is called **barrier penetration**.
- Barrier penetration observed experimentally in various atomic and nuclear systems.
- The barrier penetration illustrates a fundamental difference between classical and quantum physics.

Note that $k' = iK$, therefore the reflection coefficient can be written as, (using (5.11))

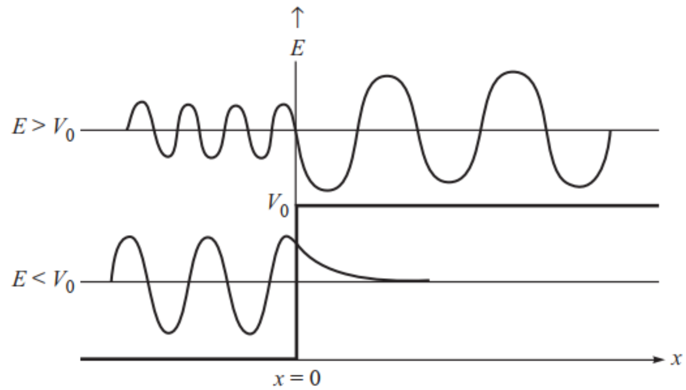
$$R = \left| \frac{k - iK}{k + iK} \right|^2 = 1 \qquad \ldots(5.18)$$

Since the eigenfunction is now real in region II, the transmitted probability current is zero according to Equation , $j = Re\left[\psi^* \frac{\hbar}{im}\frac{\partial\psi}{\partial x}\right]$. Therefore, the transmission coefficient is zero:

$$T = 0 \qquad \ldots(5.19)$$

These results show that although there is a finite probability of finding the particle in the classically-forbidden region II, there is no permanent penetration. It means that there is continuous reflection in region II until all the incident particles are ultimately returned to region I.

Figure of eigenfunctions for the step potential

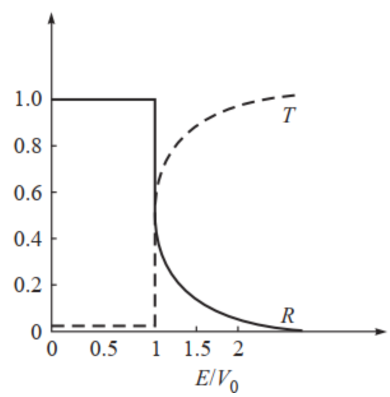


Note that for the cases, $E > V_0$:

- The amplitude of the wave is larger in region II. The reason is that the velocity of the particle is smaller in this region and, therefore, it spends more time there.
- The wavelength is also larger in region II because the kinetic energy is lower in this region.

Note that for the cases, $E < V_0$:

- The eigenfunction is exponentially decaying but nonzero in region II.



Variation of reflection and transmission coefficients with $\boldsymbol{E/V_0}$

Problem.1: For a particle scattered by a potential step show that the sum of the reflection and transmission coefficients is one.

Solution: For $E > V_0$,

$$R + T = \frac{(k-k')^2}{(k+k')^2} + \frac{4kk'}{(k+k')^2} = \frac{(k+k')^2}{(k+k')^2} = 1$$

For $E < V_0$,

$$R + T = 1 + 0 = 1$$

Problem 2: A particle of kinetic energy *9 eV* is incident on a potential step of height *5 eV*. Calculate the reflection coefficient.

Solution:

$$R = \left(\frac{k-k'}{k+k'}\right)^2$$

$$k - k' = \frac{\sqrt{2m}}{\hbar}\left(\sqrt{E} - \sqrt{E-V_0}\right)$$

$$k + k' = \frac{\sqrt{2m}}{\hbar}\left(\sqrt{E} + \sqrt{E-V_0}\right)$$

So

$$\frac{k-k'}{k+k'} = \frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}} = \frac{\sqrt{9}-\sqrt{9-5}}{\sqrt{9}+\sqrt{9-5}} = \frac{1}{5}$$

$$R = \left(\frac{1}{5}\right)^2 = \frac{1}{25} = \boxed{0.04}$$

Problem 3: An electron of energy E is incident on a potential step of height $V_0=10$ *eV*. Calculate the reflection coefficient R and the transmission coefficient T when (a) $E=5$ *eV*, (b) $E=15$ *eV*, and (c) $E=10$ *eV*. In the Case 1: $E > V_0$ and again in the Case 2: $E < V_0$

Solution: (a) Here $E < V_0$. Therefore

$$R = \boxed{1},\ T = \boxed{0}$$

(b) $E > V_0$

$$R = \left[\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}}\right]^2 = \left[\frac{\sqrt{15} - \sqrt{15 - 10}}{\sqrt{15} + \sqrt{15 - 10}}\right]^2$$

$$= \left[\frac{\sqrt{15} - \sqrt{5}}{\sqrt{15} + \sqrt{5}}\right]^2$$

$$= \left(\frac{3.873 - 2.236}{3.873 + 2.236}\right)^2$$

$$= \left(\frac{1.637}{6.109}\right)^2 = \boxed{0.072}$$

$$T = 1 - R = 1 - 0.072 = \boxed{0.928}$$

(c) Here $E = V_0$. Therefore,

$$R = \boxed{1}, \quad T = \boxed{0}$$