College of Science
Department of Physics
Fourth Class
Lecture 14

Quantum Mechanics

2023-2024

Lecture 14: Step and Barrier Potentials

Preparation

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Unit 7

Step and Barrier Potentials

7.1 Potential step

In potential step, the potential function goes only one discontinuous change, and the potential function may be represented as Fig (1)

$$V(x) = \begin{cases} 0 & for\ x < 0 \\ V_o & for\ x > 0 \end{cases}$$

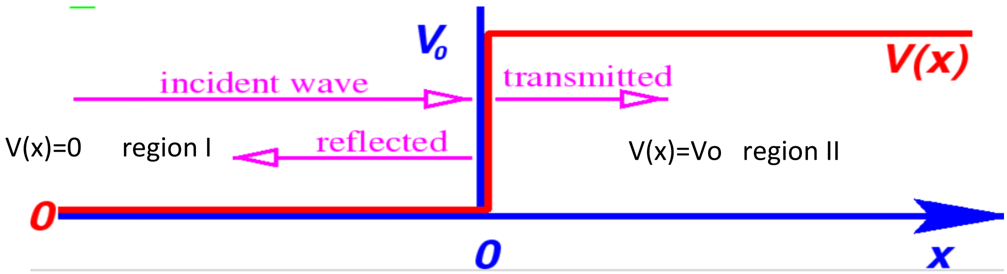


Fig (1) potential step

Let the electrons of energy E move along the positive direction of x-axis. Let us apply Q.M. to the problem, according to which the electrons behave like a wave moving from left to right and face a sudden shift in the potential at x=0.

The problem is similar when light strikes a sheet of glass where there is a shift in the index of reflection and the wave is partly transmitted. Hence in potential step problem the electrons will be partly reflected and partly transmitted at the discontinuity.

To solve the problem let us write the schrödinger equation for two regions.

The schrödinger equation for region I is given by

$$\frac{\partial^2 \Psi_1}{\partial x^2} + \frac{2m}{\hbar^2} E\Psi_1 = 0 - - - - - 1$$

As V(x)=0 in region I

The schrödinger equation for region II is given by

$$\frac{\partial^2 \Psi_2}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_o)\Psi_2 = 0 - - - - - 2$$

The general solution of eq.1 and 2 may be written as

$$\Psi_1 = A\, e^{\frac{iP_1x}{\hbar}} + Be^{-\frac{iP_1x}{\hbar}} ------3$$

And $$\Psi_2 = C\, e^{\frac{iP_2x}{\hbar}} + De^{-\frac{iP_2x}{\hbar}} ------4$$

Where $P_1 \& P_2$ are the momentum in regions I&II respectively and are given by

$$P_1 = \sqrt{2mE} \quad , \quad P_2 = \sqrt{2m(E - V_o)} ------5$$

$\Psi_1 \& \Psi_2$ are the wave functions fore I &II regions respectively. A,B,C & D are constants and may be determined by boundary condition .

In equation 3

the first term represents the wave travelling along +ve x-axis in region I, i.e. the incident wave, and the 2nd term represents the wave travelling along –ve x-axis in region-I ,i.e. The reflected wave.

In equation 4

The first term represents the wave travelling along +ve x-axis in region II, i.e. the transmitted wave. While the 2nd term represents the wave travelling a long –ve x-axis in region II, but there is no reflection of electrons in region II and hence there will be no wave travelling along –ve x-axis.

Consequently D=0 , so that eq. 4 may be written as

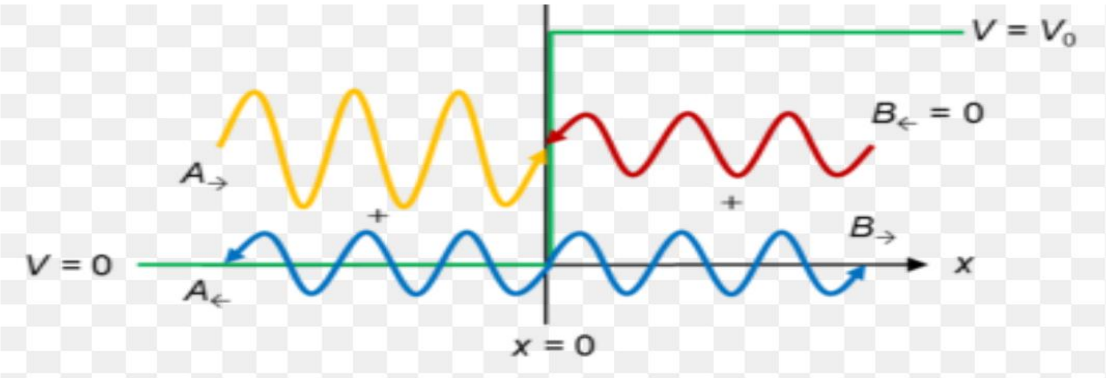
$$\Psi_2 = C\, e^{\frac{iP_2x}{\hbar}} ------6$$

According to probability interpretation the wave function Ψ must be finite ,whereas E and V must be finite , because infinite energies do not exist in nature.

Then from schrödinger equation we conclude that $\frac{\partial^2 \Psi_2}{\partial x^2}$ is everywhere finite but not necessarily continuous.

But $\frac{\partial^2 \Psi_2}{\partial x^2}$ can only be finite if $\frac{\partial \Psi}{\partial x}$ is continuous everywhere. This is first boundary condition .

If $\frac{\partial \Psi}{\partial x}$ is continuous everywhere then Ψ must be continuous. This is 2nd boundary condition.



Now the boundary conditions, in this case may be represented as follows

a- The continuity of Ψ implies $\Psi_1 = \Psi_2$ at x=0
b- The continuity of $\frac{\partial \Psi}{\partial x}$ implies $\frac{\partial \Psi_1}{\partial x} = \frac{\partial \Psi_2}{\partial x}$ at x=0

Applying boundary condition (a)in eq.3 &6, we get

$$A\, e^{\frac{iP_1 x}{\hbar}} + Be^{-\frac{iP_1 x}{\hbar}} = C\, e^{\frac{iP_2 x}{\hbar}} \qquad at\ x = 0$$

A+B = C ----------7

Differentiating eg.3&6 , we get

$$\frac{\partial \Psi_1}{\partial x} = \frac{iP_1}{\hbar}\left[A\, e^{\frac{iP_1 x}{\hbar}} - Be^{-\frac{iP_1 x}{\hbar}}\right] - - - - - - 8$$

$$\frac{\partial \Psi_2}{\partial x} = \frac{iP_2}{\hbar}\, C\, e^{\frac{iP_2 x}{\hbar}} - - - - 9$$

Applying boundary condition (b) in eqs(7,8 &9) we get

$P_2\,C = P_1[A-B]$ -------------10

$B= C - A$ from eq.7

$P_2C= P_1[\,A- C +A]$, $P_2\,C + P_1\,C = 2\,P_1\,A$

$$\therefore \boxed{C = \frac{2P_1A}{P_1 + P_2}} - - - - - - - - 11$$

Now sub. C from eq.7 into eq10

$P_2(A + B) = P_1[A - B]$, $P_2A + P_2B = P_1A - P_1B$

$B(P_1 + P_2) = A(P_1 - P_2)$

$$\frac{B}{A} = \frac{(P_1 - P_2)}{(P_1 + P_2)}$$

$\therefore \boxed{B = \frac{(P_1 - P_2)}{(P_1 + P_2)} A}$ & $\boxed{A = \frac{(P_1 + P_2)}{(P_1 - P_2)} B}$ ------------12

Where B & C represents the amplitudes of the reflected and transmitted beam respectively in terms of the amplitude of incident wave.

The reflectance (or reflectivity or reflection coefficient) and the transmittance or(transmissivity or transmission coefficient) at the potential discontinuity may be define as follows :

The reflectance, i.e. the fraction of electrons reflected is equal to the ratio of reflected current to the incident current:

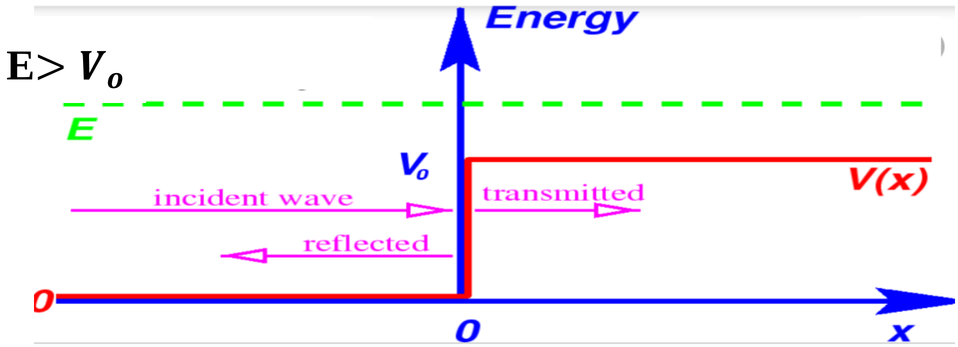
$\boxed{Reflecttance\ (R) = \frac{magnitude\ of\ reflected\ current}{magnitude\ of\ incident\ current}}$ --------13

The transmittance,i.e. the fraction of electrons transmitted, is equal to the ratio of transmitted current to the incident current:

$\boxed{Transmittance\ (T) = \frac{magnitude\ of\ transmitted\ current}{magnitude\ of\ incident\ current}}$ -----14

There may be two cases:

1- **Case I (E> V_o)**



$\Psi_1 = A\, e^{\frac{iP_1x}{\hbar}} + Be^{-\frac{iP_1x}{\hbar}}$ ---------15

It is complex conjugate Ψ_1^* is given by

$$\Psi_1^* = A^* \, e^{\frac{-iP_1 x}{\hbar}} + B^* e^{\frac{iP_1 x}{\hbar}} ----16$$

So, we have

$$\frac{\partial \Psi_1}{\partial x} = \frac{iP_1}{\hbar}\left[A \, e^{\frac{iP_1 x}{\hbar}} - Be^{-\frac{iP_1 x}{\hbar}}\right] ----17$$

$$\frac{\partial \Psi_1^*}{\partial x} = -\frac{iP_1}{\hbar}\left[A^* \, e^{\frac{-iP_1 x}{\hbar}} - B^* e^{\frac{iP_1 x}{\hbar}}\right] ----18$$

The probability current is defined as

$$\boxed{J = \frac{\hbar}{2im}\left[\Psi^* \nabla \Psi - \Psi \nabla \Psi^*\right]}$$

This expression for region I become

$$(J_x)_I = \frac{\hbar}{2im}\left[\Psi_1^* \frac{\partial \Psi_1}{\partial \mathrm{x}} - \Psi_1 \frac{\partial \Psi_1^*}{\partial \mathrm{x}}\right] ----19$$

Since in this case the particles are moving only along x-axis, using eq. 15,16,17 and 18 we have

$$(J_x)_I = \frac{\hbar}{2im}\left[\left\{\left(A^* \, e^{\frac{-iP_1 x}{\hbar}} + B^* e^{\frac{iP_1 x}{\hbar}}\right)\frac{iP_1}{\hbar}\left(A \, e^{\frac{iP_1 x}{\hbar}} - Be^{-\frac{iP_1 x}{\hbar}}\right)\right\} - \left\{\left(A \, e^{\frac{iP_1 x}{\hbar}} + Be^{-\frac{iP_1 x}{\hbar}}\right)\left(-\frac{iP_1}{\hbar}\right)\left(A^* \, e^{\frac{-iP_1 x}{\hbar}} - B^* e^{\frac{iP_1 x}{\hbar}}\right)\right\}\right]$$

$$\boxed{(J_x)_I = \frac{P_1(AA^* - BB^*)}{m} = \frac{P_1}{m}\left[|A|^2 - |B|^2\right]} ----20$$

From this expression it is clear that the current in the first region(**region I)** is made up of the difference between two terms ,of which the first proportional to $P_1|A|^2$ and represents the wave travelling from left to right i.e. the incident wave , while the second is proportional to $P_1|B|^2$ and represents the wave travelling from right to left i.e. The reflected wave.

The probability current of the incident beam =$|A|^2 \frac{P_1}{m}$ -------21

The probability current of the reflected beam = $|B|^2 \frac{P_1}{m}$ -------22

In region II we have

$$\Psi_2 = C\, e^{\frac{iP_2 x}{ħ}} \rightarrow \quad \frac{\partial \Psi_2}{\partial x} = \frac{iP_2}{ħ}\, C\, e^{\frac{iP_2 x}{ħ}}$$

$$\Psi_2^* = C^* e^{\frac{-iP_2 x}{ħ}} \rightarrow \quad \frac{\partial \Psi_2^*}{\partial x} = -\frac{iP_2}{ħ}\, C^*\, e^{\frac{-iP_2 x}{ħ}} \text{ ---------23}$$

The probability current in this case is

$$(J_x)_{II} = \frac{ħ}{2im}\left[\Psi_2^* \frac{\partial \Psi_2}{\partial \mathrm{x}} - \Psi_2 \frac{\partial \Psi_2^*}{\partial \mathrm{x}}\right]$$

Using eqs.23 , we get

$$(J_x)_{II} = \frac{ħ}{2im}\left[\left\{C^* e^{\frac{-iP_2 x}{ħ}}\left(\frac{iP_2}{ħ}\, C\, e^{\frac{iP_2 x}{ħ}}\right)\right\} - \left\{C\, e^{\frac{iP_2 x}{ħ}}\left(-\frac{iP_2}{ħ}\, C^*\, e^{\frac{-iP_2 x}{ħ}}\right)\right\}\right]$$

$$\boxed{(J_x)_{II} = \frac{P_2}{2m}[CC^* + CC^*] = \frac{P_2}{m}(CC^*) = \frac{|C|^2 P_2}{m}} \text{--------24}$$

In region II, there is only transmitted wave, therefore eq.24 represents the transmitted current.

Now we can obtain the expression for reflectance and transmittance in this case i.e. **(** **E**$>$ $\boldsymbol{V_o}$) or P_2 is real.

<u>The reflectance</u>

R=$\frac{magnitude\ of\ reflected\ current}{magnitude\ of\ incident\ current}$

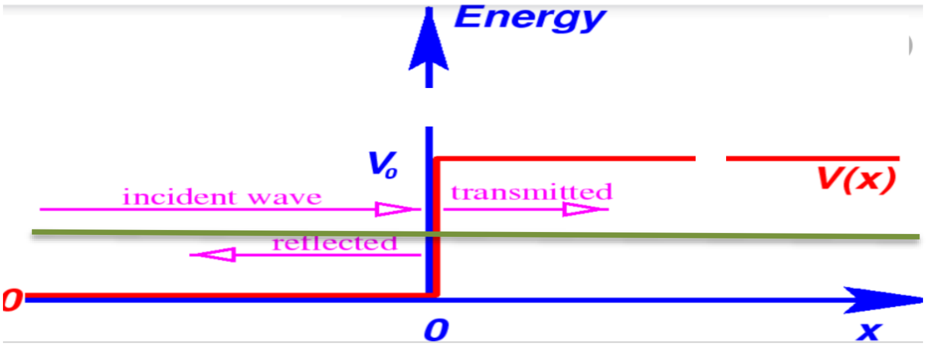
R=$\frac{|B|^2 \frac{P_1}{m}}{|A|^2 \frac{P_1}{m}} = \frac{|B|^2}{|A|^2} = \frac{(P_1 - P_2)^2}{(P_1 + P_2)^2} \qquad E > V_o$

<u>The transmittance</u>

T=$\frac{magnitude\ of\ transmited\ current}{magnitude\ of\ incident\ current}$

T=$\frac{|C|^2 \frac{P_2}{m}}{|A|^2 \frac{P_1}{m}} = \left(\frac{2P_1}{P_1 + P_2}\right)^2 \frac{P_2}{P_1} = \frac{4P_1 P_2}{(P_1 + P_2)^2}$

2- Case two (E< V_o)



E< V_o

$$\frac{\partial^2 \Psi_1}{\partial x^2} + \frac{2m}{\hbar^2} E\Psi_1 = 0 \qquad x < 0$$

$$\frac{\partial^2 \Psi_2}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_o)\Psi_2 = 0 \qquad x > 0 \text{ ------------25}$$

$$\Psi_1 = A\, e^{\frac{iP_1 x}{\hbar}} + Be^{-\frac{iP_1 x}{\hbar}} \qquad P_1 = \sqrt{2mE} \quad x < 0 \; ----26$$

$$\Psi_2(x) = Ce^{\mathcal{K}x} + De^{-\mathcal{K}x} ------27$$

Note: $\mathcal{K} = \frac{\sqrt{2m(V_o - E)}}{\hbar} \quad E < V_o$

$$p = \sqrt{2m(E - V_o)} \qquad E > V_o$$

The arbitrary constants A, B, C and D must be chosen as

Ψ(x) & $\frac{\partial \Psi(x)}{\partial x}$ must be finite & continuous every where

As $x \to \infty$ the solution of the schrödinger equation given in eq.27, will diverge because of the first term. To prevent this, we must set the coefficient of the first term equal to zero thus

C = 0 , $\Psi_2(x) = De^{-\mathcal{K}x}$ because $\boldsymbol{e}^{-\infty} = \mathbf{1}$ & $\boldsymbol{e}^{\infty} = \infty$---28

Now at x=0 Ψ(x) & $\frac{\partial \Psi(x)}{\partial x}$ must be continuous so

$\Psi_1 = \Psi_2$ & $\frac{\partial \Psi_1}{\partial x} = \frac{\partial \Psi_2}{\partial x}$

$$(De^{-\mathcal{K}x})_{x=0} = A\left(e^{\frac{iP_1 x}{\hbar}}\right)_{x=0} + B\left(e^{-\frac{iP_1 x}{\hbar}}\right)_{x=0}$$

This yield D = A+ B ----------29

Continuity of the derivative of the solution is obtained if the relation

$$-\mathcal{K}D(e^{-\mathcal{K}x})_{x=0} = \frac{iP_1}{\hbar}\left[A\, e^{\frac{iP_1x}{\hbar}} - Be^{-\frac{iP_1x}{\hbar}}\right]_{x=0}$$

-$\mathcal{K}$D = $\frac{iP_1}{\hbar}$ (A- B) ----------30 B= D – A from eq.29

Adding eq.29&30 gives

D + $\frac{i\mathcal{K}\hbar}{P_1}D = 2A \quad \rightarrow \boxed{A = \frac{D}{2}(1 + \frac{i\mathcal{K}\hbar}{P_1})} - - - - 31$

Subtracting gives $2B = D - \frac{ik\hbar}{p_1}\ D$

$$\therefore \boxed{B = \frac{D}{2}(1 - \frac{i\mathcal{K}\hbar}{P_1})} - - - 32$$

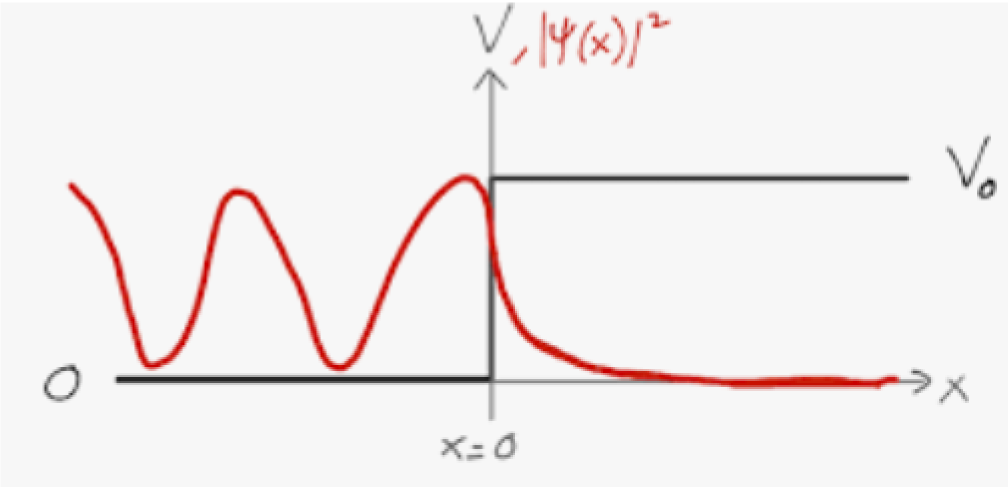
Thus $\Psi_1(x) = \frac{D}{2}\left(1 + \frac{i\mathcal{K}\hbar}{P_1}\right) e^{\frac{iP_1x}{\hbar}} + \frac{D}{2}(1 - \frac{i\mathcal{K}\hbar}{P_1})e^{-\frac{iP_1x}{\hbar}}$

$\Psi_2(x) = De^{-\mathcal{K}x}$

In region II the probability of finding the particle

$$\Psi_2^*\Psi_2 = D^*De^{-2\mathcal{K}x}$$

Although this decrease rapidly with increasing x, there is a finite probability of finding the particle in region II.



The step potential and proba...