College of Science
Department of Physics
Fourth Class
Lecture 15

Quantum Mechanics

2023-2024

Lecture 15: Rectangular potential barrier

Preparation

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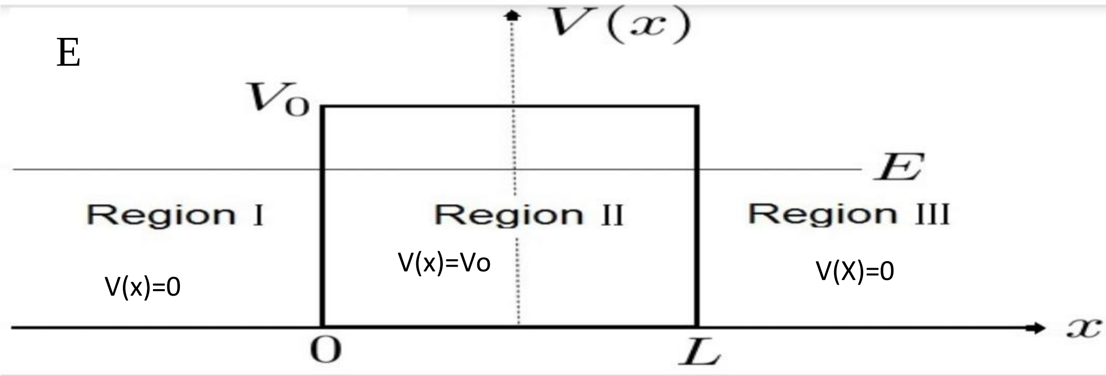
7.2 Rectangular potential barrier



$$V(x) = \left.\begin{matrix} 0 & for \quad x < 0 \\ V_0 & for \quad 0 < x < a \\ 0 & x > a \end{matrix}\right\} ------33$$

We have a potential barrier between x=0 and x=a.

If a particle having energy less than V_o i.e. $\underline{\boldsymbol{E < V_o}}$ approaches this barrier from left i.e. from region I, classically, the particle will always be reflected. However, quantum mechanics predicts that, the particle has some probability of penetrating to region III, the probability of penetrating being greater if (V_o – E) and (a) are smaller. While if $\underline{\boldsymbol{E > V_o}}$ classical mechanic predicts that the particle will always be transmitted, while according to wave mechanics the particle has a finite probability of transmission and hence it is not certain that the particle will penetrate the barrier. To solve the problem,

The schr$\ddot{o}$dinger eq. for **region I** is

$$\frac{\partial^2\Psi_1}{\partial x^2} + \frac{2m}{\hbar^2}\, E\Psi_1 = 0 ------34$$

The schr$\ddot{o}$dinger eq. for **region II** is

$$\frac{\partial^2\Psi_2}{\partial x^2} + \frac{2m}{\hbar^2}\, (E - V_o)\Psi_2 = 0 ------35$$

The schr$\ddot{o}$dinger eq. for **region III** is

$$\frac{\partial^2\Psi_3}{\partial x^2} + \frac{2m}{\hbar^2}\, E\Psi_3 = 0 ------36$$

Ψ_1,Ψ_2 and Ψ_3 are wave functions for I, II, & III regions respectively .

The general solutions of eqs. (34,35,36) are

$$\Psi_1 = A_1\, e^{\frac{iP_1x}{\hbar}} + B_1 e^{-\frac{iP_1x}{\hbar}} \;-----\; 37$$

$$\Psi_2 = A_2\, e^{\frac{iP_2x}{\hbar}} + B_2 e^{-\frac{iP_2x}{\hbar}} \;------38$$

$$\Psi_3 = A_3\, e^{\frac{iP_1x}{\hbar}} + B_3 e^{-\frac{iP_1x}{\hbar}} \;------39$$

P_1 and P_2 , the momenta of particles in the corresponding regions, are given by

$$P_1 = \sqrt{2mE} \quad , \quad P_2 = \sqrt{2m(E - V_o)} \;-----\; 40$$

A_1, B_1, A_2, B_2, A_3 & B_3 are constants to be determined by boundary conditions.

In eq. 37

1st term represents the incident wave in region I and 2nd term represents the reflected wave in region I at x = 0.

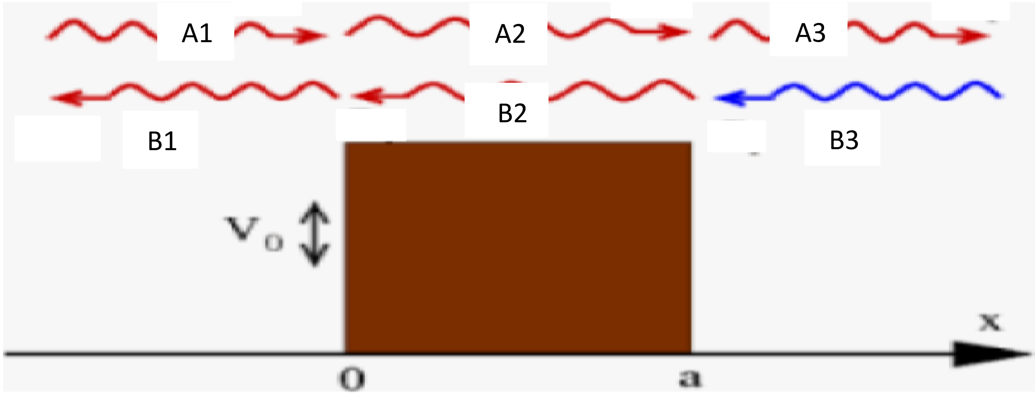
In eq. 38

The 1st term represents the transmitted wave at x = 0 in region II and 2nd term represents the reflected wave in region II at x = a.

In eq. 39

The 1st term represents the transmitted wave into region III at x=a , but no wave travels back from infinity in region III. Consequently B_3=0, so that eq.39 can be written as

$$\Psi_3 = A_3\, e^{\frac{iP_1x}{\hbar}} \;-------\; 41$$



For evaluating the constants A1, B1, A2, B2 and A3 we shall apply the condition at two boundaries x = 0 and x = a.

One condition is that Ψ must be continuous at the boundaries, i.e

$$\left.\begin{array}{l} \Psi_1 = \Psi_2 \;\; at\ x = 0 -------(i) \\ \Psi_2 = \Psi_3\ at\ x = a --------(ii) \end{array}\right\} --42$$

The other condition is that $\frac{\partial \Psi}{\partial x}$ must be continuous at the boundaries.

$$\left.\begin{array}{l} \frac{\partial \Psi_1}{\partial x} = \frac{\partial \Psi_2}{\partial x} \;\; at\ x = 0 --- (i) \\ \frac{\partial \Psi_2}{\partial x} = \frac{\partial \Psi_3}{\partial x} \;\; at\ x = a --- (ii) \end{array}\right\} --- 43$$

Applying boundary condition 42(i) to eq. 37 & 38 we have

$A_1 + B_1 = A_2 + B_2$ at x=0 ---------44

Applying boundary condition 42(ii) to eqs.38&41 we get

$$A_2\, e^{\frac{iP_2 a}{ħ}} + B_2 e^{-\frac{iP_2 a}{ħ}} = A_3\, e^{\frac{iP_1 a}{ħ}} \quad at\ x = a --- 45$$

Differentiating eqs. 37,38 & 41, we get

$$\frac{\partial \Psi_1}{\partial x} = \frac{iP_1}{ħ}\left[A_1\, e^{\frac{iP_1 x}{ħ}} - B_1 e^{-\frac{iP_1 x}{ħ}}\right] ----46$$

$$\frac{\partial \Psi_2}{\partial x} = \frac{iP_2}{ħ}\left[A_2\, e^{\frac{iP_2 x}{ħ}} - B_2 e^{-\frac{iP_2 x}{ħ}}\right] ----47$$

$$\frac{\partial \Psi_3}{\partial x} = \frac{iP_1}{ħ}\left[A_3\, e^{\frac{iP_1 x}{ħ}}\right] ----48$$

Applying the boundary condition 43(i) & (ii) to these eqs., we get

$P_1[A_1 - B_1] = P_2[A_2 - B_2]$ at x = 0

And $P_2\left[A_2\, e^{\frac{iP_2a}{\hbar}} - B_2 e^{-\frac{iP_2a}{\hbar}}\right] = P_1\left[A_3\, e^{\frac{iP_1a}{\hbar}}\right] - - - - x = a$

Or $\quad A_1 - B_1 = \frac{P_2}{P_1}(A_2 - B_2) - - - - - 49$

$$A_2\, e^{\frac{iP_2a}{\hbar}} - B_2 e^{-\frac{iP_2a}{\hbar}} = \frac{P_1}{P_2} A_3\, e^{\frac{iP_1a}{\hbar}} - - - - 50$$

Solving eqs.44 &49for A_1 & B_1, we get

$$A_1 = \frac{A_2}{2}\left(1 + \frac{P_2}{P_1}\right) + \frac{B_2}{2}\left(1 - \frac{P_2}{P_1}\right) - - - - 51$$

$$B_1 = \frac{A_2}{2}\left(1 - \frac{P_2}{P_1}\right) + \frac{B_2}{2}\left(1 + \frac{P_2}{P_1}\right) - - - - 52$$

Solving eqs.45 &50 for A_2 &B_2 we get

$$A_2 = \frac{A_3}{2}\left(1 + \frac{P_1}{P_2}\right) e^{\frac{i(P_1 - P_2)a}{\hbar}} - - - - 53$$

$$B_2 = \frac{A_3}{2}\left(1 - \frac{P_1}{P_2}\right) e^{\frac{i(P_1 + P_2)a}{\hbar}} - - - - 54$$

Substituting values of A_2 & B_2 from these eqs. Into eqs.51&52, we get

$$A_1 = \frac{A_3}{4} e^{\frac{iP_1a}{\hbar}}\left[\left(1 + \frac{P_2}{P_1}\right)\left(1 + \frac{P_1}{P_2}\right) e^{-\frac{iP_2a}{\hbar}} + \left(1 - \frac{P_2}{P_1}\right)\left(1 - \frac{P_1}{P_2}\right) e^{\frac{iP_2a}{\hbar}}\right] 55$$

$$B_1 = \frac{A_3}{4} e^{\frac{iP_1a}{\hbar}}\left[\left(1 - \frac{P_2}{P_1}\right)\left(1 + \frac{P_1}{P_2}\right) e^{-\frac{iP_2a}{\hbar}} + \left(1 + \frac{P_2}{P_1}\right)\left(1 - \frac{P_1}{P_2}\right) e^{\frac{iP_2a}{\hbar}}\right] 56$$

Eq.55 may be written as

$$\frac{A_3}{A_1} = \frac{4e^{\frac{-iP_1a}{\hbar}}}{\left[\left(1 + \frac{P_2}{P_1}\right)\left(1 + \frac{P_1}{P_2}\right) e^{-\frac{iP_2a}{\hbar}} + \left(1 - \frac{P_2}{P_1}\right)\left(1 - \frac{P_1}{P_2}\right) e^{\frac{iP_2a}{\hbar}}\right]}$$

$$\frac{A_3}{A_1} = \frac{2P_1P_2e^{\frac{-iP_1a}{\hbar}}}{(P_1^2 + P_2^2)\sinh\left(\frac{iP_2a}{\hbar}\right) + 2P_1P_2\cosh\left(\frac{iP_2a}{\hbar}\right)}$$

$$\frac{A_3}{A_1} = \frac{2P_1P_2e^{\frac{-iP_1a}{\hbar}}}{[(P_1^2 + P_2^2)\tanh\left(\frac{iP_2a}{\hbar}\right) + 2P_1P_2]\cosh\left(\frac{iP_2a}{\hbar}\right)}$$

$$\frac{A_3}{A_1} = \frac{2P_1P_2 sech\left(\frac{iP_2a}{\hbar}\right)e^{\frac{-iP_1a}{\hbar}}}{[(P_1^2 + P_2^2)\tanh\left(\frac{iP_2a}{\hbar}\right) + 2P_1P_2]} \quad ----57$$

The complex conjugate of above eq. is written as

$$\frac{A_3^*}{A_1^*} = \frac{2P_1P_2^* sech\left(\frac{-iP_2^*a}{\hbar}\right)e^{\frac{+iP_1a}{\hbar}}}{[(P_1^2 + P_2^{*2})\tanh\left(\frac{-iP_2^*a}{\hbar}\right) + 2P_1P_2^*]} ----58$$

Here $P_2 = \sqrt{2m(E - V_o)}$ is imaginary since $E < V_o$, therefore iP_2 is real, Since

$$P_2 = \sqrt{2m(E - V_o)} = \sqrt{-2m(V_o - E)} = i\sqrt{2m(V_o - E)}$$

so that we have

$$P_2^* = -i\sqrt{2m(V_o - E)} = -P_2$$

$$\therefore P_2^{*2} = P_2^2$$

Then eq.58 becomes

$$\frac{A_3^*}{A_1^*} = \frac{-2P_1P_2 sech\left(\frac{iP_2a}{\hbar}\right)e^{\frac{+iP_1a}{\hbar}}}{[(P_1^2 + P_2^2)\tanh\left(\frac{iP_2a}{\hbar}\right) - 2P_1P_2]}$$

The transmittance or the transmission coefficient is given by

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

$$T = \frac{(A_3A_3^*)\frac{P_1}{m}}{(A_1A_1^*)\frac{P_1}{m}} = \frac{(A_3A_3^*)}{(A_1A_1^*)}$$

Using eq.57 & 59

$$T = \frac{\left[2P_1P_2 sech\left(\frac{iP_2a}{\hbar}\right)e^{\frac{-iP_1a}{\hbar}}\right]\left[-2P_1P_2 sech\left(\frac{iP_2a}{\hbar}\right)e^{\frac{+iP_1a}{\hbar}}\right]}{\left[(P_1^2+P_2^2)\tanh\left(\frac{iP_2a}{\hbar}\right)+2P_1P_2\right]\left[(P_1^2+P_2^2)\tanh\left(\frac{iP_2a}{\hbar}\right)-2P_1P_2\right]}$$

Or

$$\boxed{T = \frac{-4P_1^2P_2^2 sech^2\left(\frac{iP_2a}{\hbar}\right)}{(P_1^2+P_2^2)^2\tanh^2\left(\frac{iP_2a}{\hbar}\right)-4P_1^2P_2^2}} ------60$$

Here P_2 is imaginary, i.e.iP_2 is real and so P_2^2 is real therefore T is real.

The reflectance of the barrier or the reflected coefficient is given by

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

$$R = \frac{B_1B_1^*}{A_1A_1^*} ---------61$$

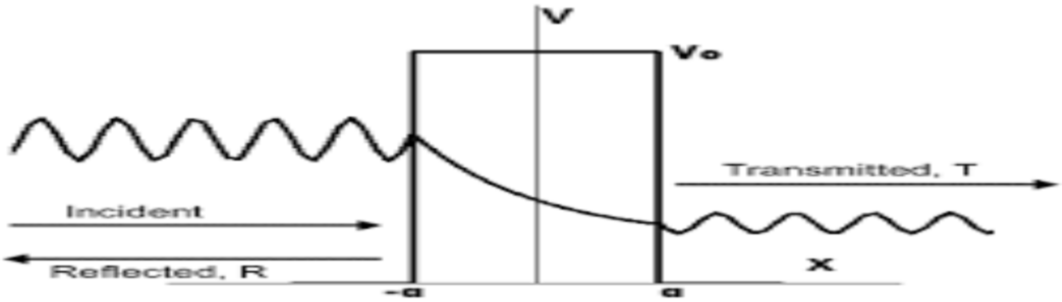
Using eqs.55 and 56 and remembering the $P_2^* = -P_2$ eq.61, after simplification yield

$$\boxed{R = \frac{(P_1^2-P_2^2)^2\tanh^2\left(\frac{iP_2a}{\hbar}\right)}{(P_1^2+P_2^2)^2\tanh^2\left(\frac{iP_2a}{\hbar}\right)-4P_1^2P_2^2}} ------62$$

The reflection coefficient R may be obtained by the fact

R + T = 1 i.e. R = 1- T -------------63

The property of the barrier penetration is entirely due to the wave nature of matter and is very similar to the total internal reflection of light waves. If two plates of glass are placed close to each other with a layer of air as a medium between them, the light will be transmitted from one plate to another, even though the angle of incident is greater than the critical angle. However, the intensity of transmitted wave will decrease exponentially with thickness of the layer of air. In this case the intensity of electron waves decreases exponentially with the thickness of the barrier. The wave function has the form "more or less" as shown in Fig



Let us consider a special case when the barrier is thick i.e. $iP_2a > ħ$ as (a) is very large or $V_o > E$

<u>In this case</u> $\tanh\left(\frac{iP_2a}{ħ}\right) = 1$ & $sech\left(\frac{iP_2a}{ħ}\right) = 2\,e^{\frac{iP_2a}{ħ}}$

It is to be noted that P_2 is imaginary and so iP_2 and P^2_2 are real and negative than eq.60 yield

$$T = \frac{-16P_1^2P_2^2e^{\frac{2iP_2a}{ħ}}}{(P_1^2+P_2^2)^2 - 4P_1^2P_2^2}$$

Or $$\boxed{T = \frac{-16P_1^2P_2^2e^{\frac{2iP_2a}{ħ}}}{\left(P_1^2-P_2^2\right)^2}} ------64$$

And substituting values of $P_1 = \sqrt{2mE}$, $P_2 = \sqrt{2m(E-V_o)}$

In eq.64 gives

$$T = \frac{-16(2mE)2m(E-V_o)\exp\left(2i\sqrt{\frac{2m(E-V_o)}{ħ^2}}\,a\right)}{[2mE-2m(E-V_o)]^2}$$

$$\boxed{T = \frac{16E(V_o-E)}{V_o^2}\exp\left[-2\sqrt{\frac{2m(V_o-E)}{ħ^2}}\,a\right]} ------65$$

This is the expression for transmission coefficient for a very large barrier. The phenomenon of the particles (electrons, ray) penetrating the potential barrier is called "tunnel effect" and is especially important in thermionic and field emission