

CHAPTER 10 PARTICLE IN POTENTIAL BARRIER

A. Introduction

In this chapter it will be studied important thing about particle in potential barrier i.e.:

1. Particle in step potential with energy $E < V_0$.
2. Particle in step potential with energy $E > V_0$.
3. Particle in barrier potential with energy $E < V_0$.
4. Particle in barrier potential with energy $E > V_0$.

To study this topics it is required comprehension about Schrodinger equation, continuity of wave function, and its physical interpretation. Analysis is conducted by describe eigen function in each area and determinate the transmission coefficient (transmutation) T.

B. Particle in Step Potential with Energy $E < V_0$

In Figure 10.1 is described particle in step potential with energy $E < V_0$:

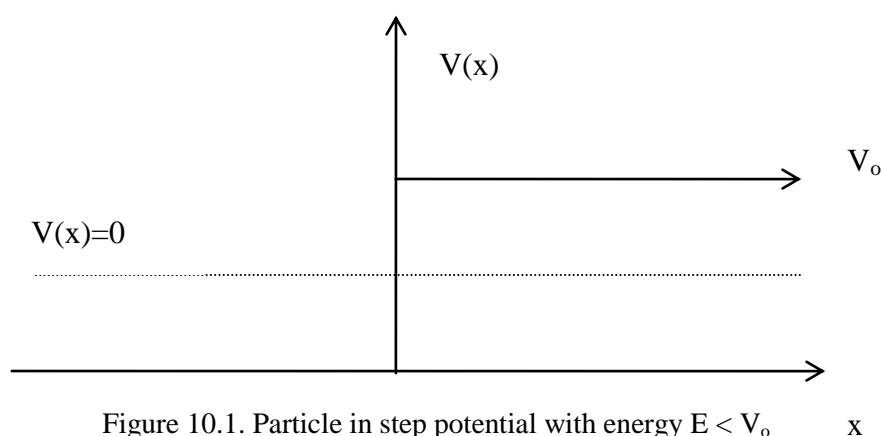


Figure 10.1. Particle in step potential with energy $E < V_0$

According to classical mechanics, particle with energy $E < V_0$ will be reflected in left direction. Based on this view, particle is not possible in area of $x > 0$.

According quantum mechanics, in area $x < 0$ with $V(x)=0$ full filled equation:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (10.1)$$

It has general solution:

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad (10.2)$$

where $k_1 = \frac{1}{\hbar} \sqrt{2mE}$

In area $x > 0$ with $V(x) = V_o$ full filled:

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

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

$$\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = (V_o - E)\psi(x) \text{ where } V_o - E > 0. \quad (10.3)$$

Equation (10.3) has general solution:

$$\psi(x) = Ce^{k_2x} + De^{-k_2x} \quad (10.4)$$

where $k_2 = \frac{1}{\hbar} \sqrt{2m(V_o - E)}$

Then at $\psi(x)$ is applied boundary condition in order to the wave function has well behave in all interval of x .

1. $\psi(x)$ finite, hence $C=0$. If $C \neq 0$ then $\psi(x) = \infty$ for $x \rightarrow \infty$.
2. $\psi(x)$ continue at $x=0$, it full filled relation among the coefficients:
 $A + B = D$ (10.5)
3. $\psi'(x)$ also continue at $x=0$:

In area $x < 0$ it is obtained: $\psi'(x) = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}$

In area $x > 0$ it is obtained: $\psi'(x) = -k_2De^{-k_2x}$

Continuity condition at $x=0$ produce:

$$ik_1A - ik_1B = -k_2C \quad (10.6)$$

Based on equation (10.5) and (10.6) it can be obtained coefficient A and B which stated in D as follow:

Multiply equation (10.5) with ik_1 then add with equation (10.6):

$$ik_1A + ik_1B = ik_1D$$

$$ik_1A - ik_1B = -k_2C$$

It is obtained:

$$2ik_1A = D(ik_1 - k_2)$$

$$A = \frac{D}{2} \left(\frac{ik_1 - k_2}{ik_1} \right)$$

$$A = \frac{D}{2} \left(1 - \frac{k_2}{ik_1} \right)$$

$$A = \frac{D}{2} \left(1 - \frac{k_2}{ik_1} \frac{i}{i} \right)$$

$$A = \frac{D}{2} \left(1 + \frac{ik_2}{k_1} \right) \tag{10.7}$$

Coefficient of B is determined by this way:

$$B = D - A = D - \frac{D}{2} \left(1 + \frac{ik_2}{k_1} \right)$$

$$B = D - \frac{D}{2} \left(\frac{k_1 + ik_2}{k_1} \right)$$

$$B = \frac{2k_1D - (k_1 + ik_2)D}{2k_1}$$

$$B = \frac{k_1D - ik_2D}{2k_1}$$

$$B = \frac{D(k_1 - ik_2)}{2k_1}$$

$$B = \frac{D}{2} \left(1 - \frac{ik_2}{k_1} \right) \tag{10.8}$$

Boundary condition that $\psi(x)$ must be *well behaved function* give solution:

1. In area $x \leq 0$ it has wave function:

$$\psi(x) = \frac{D}{2} \left(1 + \frac{ik_2}{k_1} \right) e^{ik_1x} + \frac{D}{2} \left(1 - \frac{ik_2}{k_1} \right) e^{-ik_1x} \tag{10.9}$$

2. In area $x \geq 0$ it has wave function:

$$\psi(x) = De^{-k_2x} \quad (10.10)$$

Total wave function:

$$\Psi(x,t) = \psi(x)e^{\frac{iEt}{\hbar}}$$

Total wave function in area $x \leq 0$ is:

$$\Psi(x,t) = \frac{D}{2} \left(1 + \frac{ik_2}{k_1} \right) e^{i(k_1x - \omega t)} + \frac{D}{2} \left(1 - \frac{ik_2}{k_1} \right) e^{-i(k_1x + \omega t)} \quad (10.11)$$

where $\omega\hbar = E$

The first part of equation (10.11) represents wave which propagates in right direction (incident wave). The second part of equation (10.11) represent wave which propagates in left direction (reflected wave).

Solution for area $x \geq 0$ give total wave function:

$$\Psi(x,t) = De^{-k_2x} e^{-i\omega t} \quad (10.12)$$

Reflection Coefficient:

$$R = \frac{B^*B}{A^*A} = \frac{\frac{D^*}{2} \left(1 + \frac{ik_2}{k_1} \right) \frac{D}{2} \left(1 - \frac{ik_2}{k_1} \right)}{\frac{D^*}{2} \left(1 - \frac{ik_2}{k_1} \right) \frac{D}{2} \left(1 + \frac{ik_2}{k_1} \right)} = 1 \quad (10.13)$$

This is according to classical description, all incident particle will be reflected all.

In left side of $x=0$ or area $x \geq 0$, it is full filled:

$$\Psi^*(x,t)\Psi(x,t) = D^*De^{-2k_2x} \quad (10.14)$$

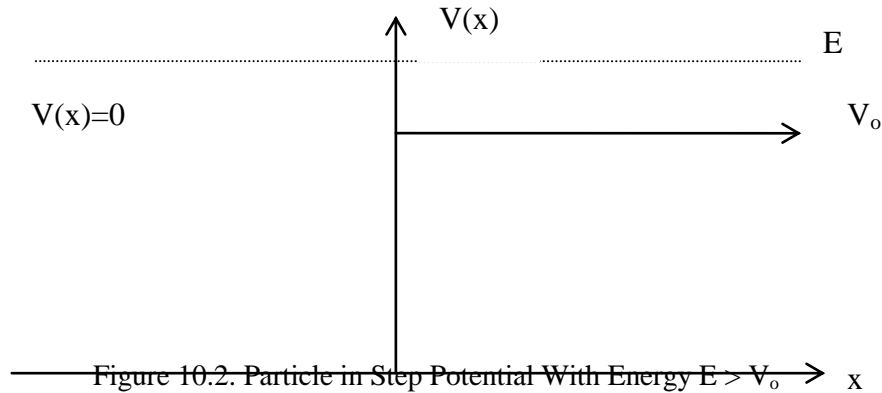
This will give approximation value of zero for $x \rightarrow \infty$. In area near $x=0$, there is value of $\Psi^*(x,t)\Psi(x,t)$. This is very different from classical view that reject the attendance of particle in area $x > 0$.

$$\Psi^*(x,t)\Psi(x,t) > 0 \quad (10.15)$$

Equation (10.15) has a meaning that it will be penetration of potential wall (penetration effect) if Δx is small enough.

C. Particle in Step Potential With Energy $E > V_o$

In Figure 10.2 is described particle in step potential with energy $E > V_o$.



According to quantum mechanics, in area $x < 0$ with $V(x) = 0$ full filled time independent of Schrodinger equation:

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

It has general solution:

$$\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

where $k_1 = \frac{1}{\hbar} \sqrt{2mE}$

in area $x > 0$ with $V(x) = V_o$ full filled:

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

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = (E - V_o)\psi(x) \tag{10.16}$$

Equation (10.16) has general solution:

$$\psi(x) = Ce^{ik_2x} + De^{-ik_2x} \tag{10.17}$$

where $k_2 = \frac{1}{\hbar} \sqrt{2m(E - V_o)}$

Then in $\psi(x)$ is applied boundary condition in order wave function has well behave in all interval of x .

1. Particle come from left side to the right side of step potential at $x=0$ may be undergoes resistance, hence reflection is happen. But in $x>0$ there is no wave which propagate in left direction, hence coefficient D in equation (10.17) equals to zero ($D=0$).
2. Condition of well behave function is $\psi(x)$ continue at $x=0$, it is obtained:

$$A + B = C \quad (10.18)$$
3. Condition of well behave function $\psi'(x)$ also continue at $x=0$:

In area $x<0$ it is obtained: $\psi'(x) = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}$

In area $x>0$ it is obtained: $\psi'(x) = ik_2Ce^{ik_2x}$

Continuity condition at $x=0$ produce:

$$\begin{aligned} ik_1A - ik_1B &= ik_2C \\ k_1(A - B) &= k_2C \end{aligned} \quad (10.19)$$

Based on equation (10.18) and (10.19), it can be determined coefficient B and C which are stated in A as follow:

$$\begin{aligned} B - C &= -A \\ k_1B + k_2C &= k_1A \end{aligned}$$

The equation can be written:

$$\begin{aligned} k_2B - k_2C &= -k_2A \\ k_1B + k_2C &= k_1A \end{aligned}$$

Sum of both equation produce:

$$\begin{aligned} (k_1 + k_2)B &= (k_1 - k_2)A \\ B &= \frac{(k_1 - k_2)}{(k_1 + k_2)}A \end{aligned} \quad (10.20)$$

Furthermore coefficient C can be determined:

$$\begin{aligned} C &= A + B \\ C &= A + \frac{(k_1 - k_2)}{(k_1 + k_2)}A \\ C &= \frac{(k_1 + k_2)A + (k_1 - k_2)A}{(k_1 + k_2)} \end{aligned}$$

$$C = \frac{2k_1}{(k_1 + k_2)} A \quad (10.21)$$

The eigen function which determined are:

1. In area $x < 0$:

$$\psi(x) = A e^{ik_1 x} + A \left(\frac{k_1 - k_2}{k_1 + k_2} \right) e^{-ik_1 x}$$

2. In area $x > 0$:

$$\psi(x) = A \left(\frac{2k_1}{k_1 + k_2} \right) e^{ik_2 x}$$

Reflection Coefficient R:

$$R = \frac{v_1 B^* B}{v_1 A^* A} = \frac{(k_1 - k_2)^* A^* (k_1 - k_2) A}{(k_1 + k_2)^* A^* (k_1 + k_2) A}$$

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \quad (10.22)$$

where v_1 is velocity of particle which has the same value with group velocity

Transmission Coefficient T:

$$T = \frac{v_2 C^* C}{v_1 A^* A} = \frac{k_2 \left(\frac{2k_1}{k_1 + k_2} \right)^* A^* \left(\frac{2k_1}{k_1 + k_2} \right) A}{A^* A}$$

$$T = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (10.23)$$

Sum of R and T produce:

$$R + T = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} + \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

$$R + T = \frac{k_1^2 - 2k_1 k_2 + k_2^2 + 4k_1 k_2}{(k_1 + k_2)^2}$$

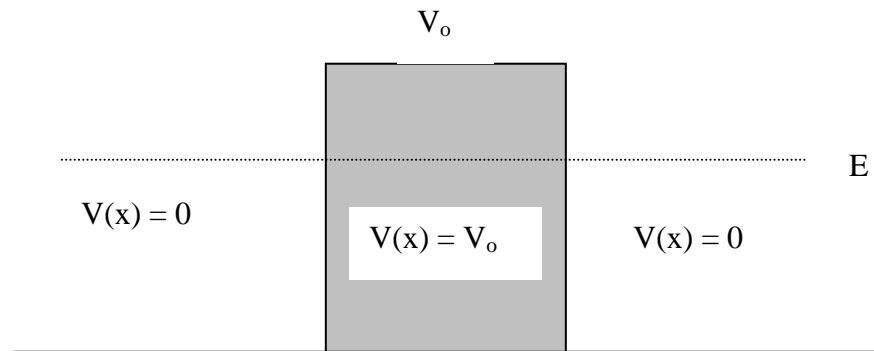
$$R + T = \frac{k_1^2 + 2k_1 k_2 + k_2^2}{(k_1 + k_2)^2}$$

$$R + T = \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2} = 1 \quad (10.24)$$

Equation (10.24) shows the conservation of probability.

D. Particle in Barrier Potential with $E < V_0$

In Figure 10.3 is presented illustration about particle in barrier potential with $E < V_0$. Potential barrier has wide of a and height of V_0 .



Area in a axis is divided in 3 part with $x = 0$ and $x = a$

Figure 10.3. Particle in Barrier Potential With $E < V_0$

1. Area I, $x < 0$: $\psi(x) = Ae^{ik_1x} + Be^{-ik_1x}$ where $k_1 = \frac{1}{\hbar}\sqrt{2mE}$
2. Area II, $0 < x < a$: $\psi(x) = Ce^{k_2x} + De^{-k_2x}$ where $k_2 = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$
3. Area III, $x > a$: $\psi(x) = Fe^{ik_1x} + Ge^{-ik_1x}$ where $k_1 = \frac{1}{\hbar}\sqrt{2mE}$

In order to $\psi(x) \neq \infty$ at $x \rightarrow \infty$ then coefficient $G = 0$, hence it is obtained:

$$\psi(x) = Fe^{-ik_1x}$$

Continuity condition $\psi(x)$ and $\psi'(x)$ at $x = 0$ and $x = a$, will give relation among coefficients of A, B, C, D, and F. Based on the relation, we can determine transmission coefficient T as follow:

$$T = \frac{v_1}{v_1} \frac{F^* F}{A^* A} = \left[1 + \frac{(e^{k_2a} - e^{-k_2a})^2}{16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right)} \right]^{-1}$$

$$T = \left[1 + \frac{\sinh^2 k_2 a}{4 \frac{E}{V_o} \left(1 - \frac{E}{V_o} \right)} \right]^{-1} \quad (10.25)$$

$$\text{where } k_2 a = \left[\frac{2mV_o^2 a^2}{\hbar^2} \left(1 - \frac{E}{V_o} \right) \right]^{1/2}$$

Based on equation (10.25) show that quantum analysis for particle with energy less than barrier potential prove the existence of particle in area III. It means that penetration effect is occurred in barrier potential. In quantum view, less particle is reflected in area I. This phenomenon is very different from classical analysis that it does not probable particle in area III for energy of particle less than barrier potential. According to classical mechanics, all particle will be deflected in area I.

E. Particle in Potential Barrier with $E > V_o$

In Figure 10.4 is presented illustration about particle in barrier potential with $E > V_o$. Potential barrier has wide of a and height of V_o .

1. Area I, $x < 0$: $\psi(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$ where $k_1 = \frac{1}{\hbar} \sqrt{2mE}$
2. Area II, $0 < x < a$: $\psi(x) = Ce^{k_2 x} + De^{-k_2 x}$ where $k_2 = \frac{1}{\hbar} \sqrt{2m(E - V_o)}$
3. Area III, $x > a$: $\psi(x) = Ee^{ik_1 x} + Fe^{-ik_1 x}$ where $k_1 = \frac{1}{\hbar} \sqrt{2mE}$

In order to $\psi(x) \neq \infty$ at $x \rightarrow \infty$ then $E = 0$, hence it is obtained:

$$\psi(x) = Fe^{-ik_1 x}$$

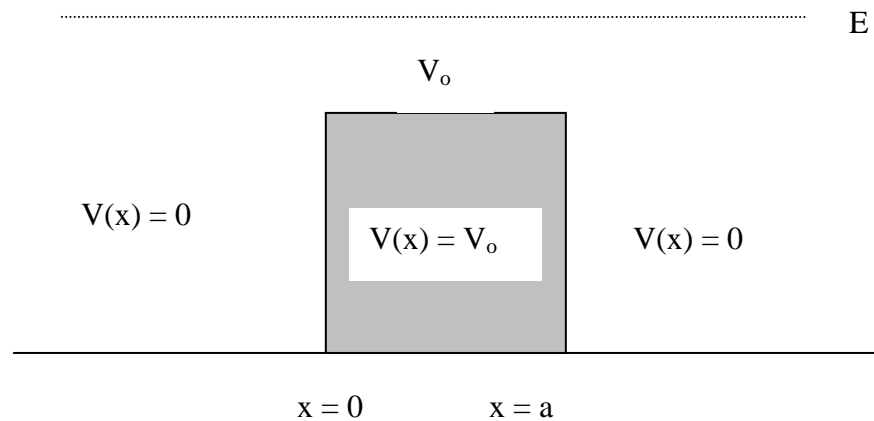


Figure 10.4. Particle in Barrier Potential With $E > V_o$

By applied continuity condition of $\psi(x)$ and $\psi'(x)$ at $x = 0$ and at $x = a$, it will give relation among coefficients of A, B, C, D, and F. Based on the relation, we can determine transmission coefficient T as follow:

$$T = \frac{v_1}{v_1} \frac{F^* F}{A^* A} = \left[1 + \frac{(e^{ik_2 a} - e^{-ik_2 a})^2}{16 \frac{E}{V_o} \left(1 - \frac{E}{V_o}\right)} \right]^{-1}$$

$$T = \left[1 + \frac{\sin^2 k_2 a}{4 \frac{E}{V_o} \left(1 - \frac{E}{V_o}\right)} \right]^{-1} \quad (10.26)$$

$$\text{where } k_2 a = \left[\frac{2mV_o^2 a^2}{\hbar^2} \left(1 - \frac{E}{V_o}\right) \right]^{1/2}$$

Analysis of classical mechanics and quantum for particle with energy $E > V_o$ can be explained as followt:

- According to classical mechanics, particle with energy $E > V_o$ always pass through potential barrier.
- According to quantum mechanics, particle with energy $E > V_o$, part of particles will be reflected and other parts will be transmitted. When particle pass through barrier potential, kinetic energy of particle will decrease $E - V_o$. As consequence momentum of particle decrease and de Broglie wave length of particle increase.

G. Problems

1. Electron and proton have the same energy (E), move close to step potential which has height of V larger than E. Are both particle have the same probability for passing through the barrier? Which particle does have bigger probability?
2. Electron with energy of 4 eV come to barrier potential which has height of 5 eV and wide of 0,1 nm. Determine the probability of electron to penetrate the barrier!
3. Electron beam comes to barrier potential which has height of 5 eV and wide of 0,2 nm. Determine energy of electron in order to the electron can penetrate the barrier!

H. Reference

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