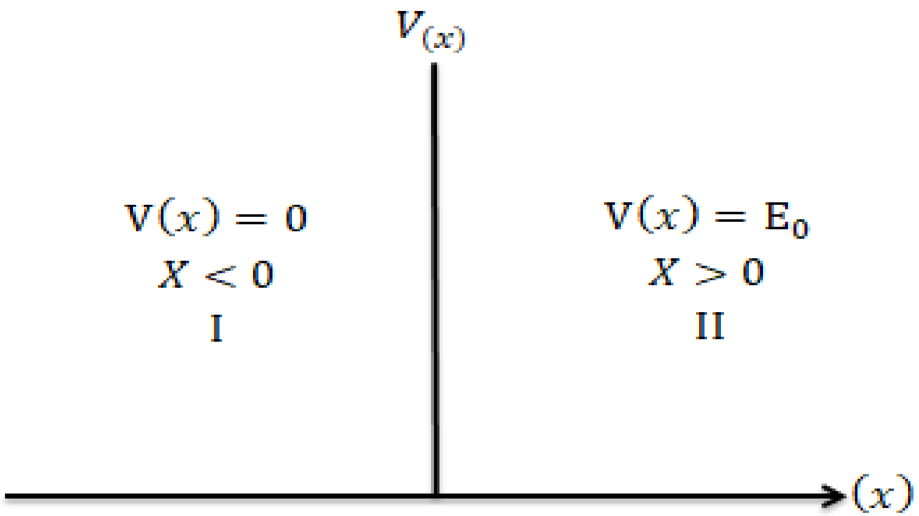
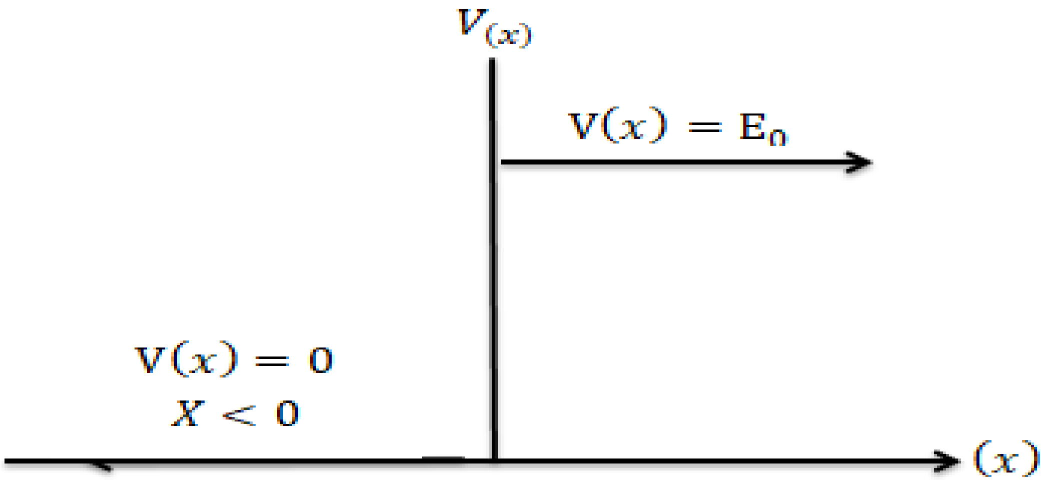
3.3.2 Potential Step

Two regions separated by potential barrier, therefore the potential energy for any particle inside this region equals to zero(v=0), and in the other region equal to quantity(v=E) as shown in figure (3.1)



Figure(3.1) potential step

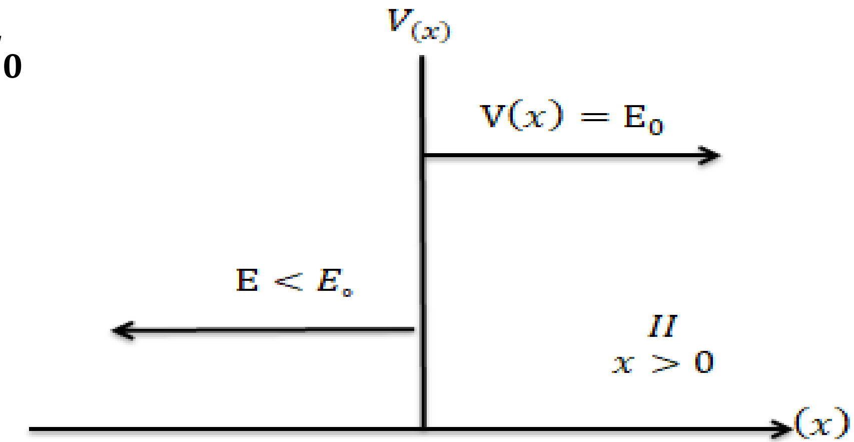
For example variation of free electron potential in metal when it is close to the surface



To discussion this potential step carefully can be separated into
two situations

When $E < E_0$

$E < E_0$



According to the classical mechanic was found that the particle has total energy less than the potential energy in region II. Based on this hypothesis all the particles cannot across any particle from region I to region II because of the energy is negative in II.

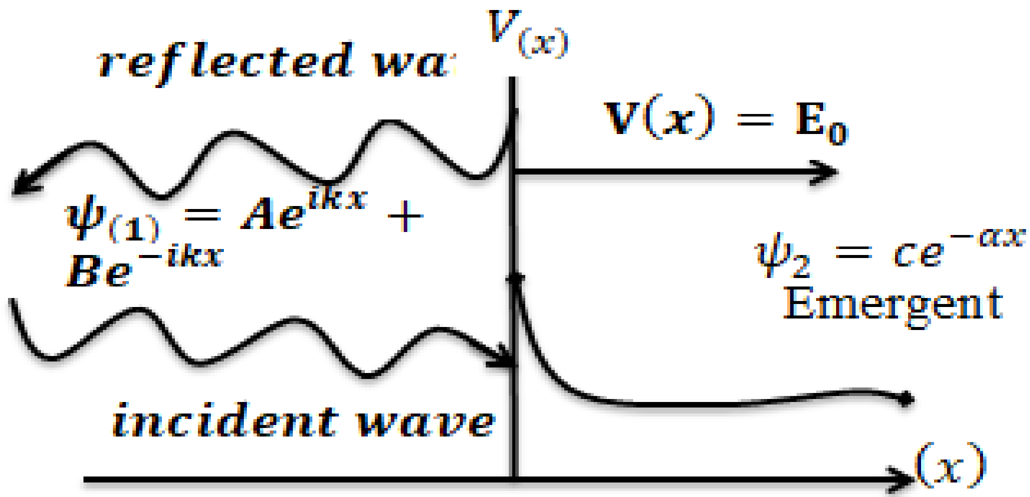
$$E = T + V$$
$$T = E - V \; Negative \; when \; E < V$$

In quantum mechanics the across of particle from I to II can be take place in the tiny probability and to prove that we solve (O.D.T.I.S.E) in the two regions (I and II).

- **Solution of Schrodinger equation in** $(\boldsymbol{V = 0} \;\&\; \boldsymbol{E < E_0})$
- $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + v\psi = E\psi$
- $\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} = 0$ ....(i)
- $E = T + V = T + 0 = T = \frac{1}{2}mv^2$
- $E = \frac{p^2}{2m} \rightarrow p^2 = 2mE = h^2k^2$
- $\therefore k^2 = \frac{2mE}{h^2} \quad substitute\ \ in\ equation$ (i)
- $\frac{d^2\psi}{dx^2} + k^2\psi = 0$
- The general solution is
- $\psi_{(x)} = Ae^{ikx} + Be^{-ikx}$ ....(ii)

- In the R.H. the first term Ae^{ikx} represents the material wave that is Accompanying with the particle that moves to right side with P=ħk the term A: is the amplitude of this wave; in the other words it represents the dynamic state of the particle that fall on the boundaries between the two regions.
- The second termBe^{-ikx} represents the material wave that accompanying with the particle that moves to left side with P=ħk (this term represent the dynamic state to reflect the particle to first region(I).
- The difference between A and B $(A \neq B)$ means the part for incident particle penetrate to second region (II).

- **Solution of Schrodinger equation in region II.**
- $-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2}+v\psi_2=E\psi_2$
- In II $(V=E_0)$
- $\frac{d^2\psi_2}{dx^2}-\frac{2m}{\hbar^2}(E_0-E)\psi_2=0$
- $Suppose$
- $\alpha^2=\frac{2m}{\hbar^2}(E_0-E)$
- $\therefore \frac{d^2\psi}{dx^2}-\alpha^2\psi_2=0$
- $\therefore \psi_2=Ce^{-\alpha x}+De^{\alpha x}$
- ψ_2 must be limited for any value of x and it is forbidden to be close to ∞ When $x=\infty$ D must be equal to zero (D=0) then
- $\psi_2=ce^{-\alpha x}$
- Since $\psi_2\neq 0$ this means the probability of particle returned to region I in spite of the barrier $(E<E_0)$ is exist.



Figure(3.2) The waves in potential step

A: The amplitude of incident wave.
B: The amplitude of reflected wave.
C: The amplitude of emergent wave.
The intensity of incident wave $= |A|^2$
The intensity of reflected wave $= |B|^2$
The intensity of emergent wave $= |C|^2$

- **The relation between A,B and C**
- To determine The relation between A, B and C
- $\psi_1 = Ae^{ikx} + Be^{-ikx}, \ \psi_2 = Ce^{-\alpha x}$
- $\psi_1 \ = \psi_2 \ at \ x = 0 \Longrightarrow A + B = C$
- $\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x} \ at \ x = 0 \ \Longrightarrow i\, kA - i\, kB = -\alpha c$
- $B = \frac{ik + \alpha}{ik - \alpha} \ A$
- $C = \frac{2ik}{ik - \alpha} A$
- $\psi_1(x) \ = Ae^{ikx} + Be^{-ikx} \Longrightarrow Ae^{ikx} + \frac{ik + \alpha}{ik - \alpha} Ae^{-ikx}$
- $\therefore \psi_1 = A(e^{ikx} + \frac{ik + \alpha}{ik - \alpha} e^{-ikx}) \ , \quad \psi_2(x) = \frac{2ik}{ik - \alpha} Ae^{-\alpha x}$

- by comparing the number of incident and reflected particles , the following equations can be written.
- $|B|^2 = B^*. B = \frac{-ik+\alpha}{-ik-\alpha} . \frac{ik+\alpha}{ik-\alpha} A^*. A$
- $|B|^2 = \frac{k^2+\alpha^2}{K^2+\alpha^2} |A|^2$
- $\therefore |B|^2 = |A|^2$

- $|B|^2 = |A|^2$
- **From the above equation can be concluded that :**The number of incident particles equals to number of reflected particles which includes the emergent particles.
- $IF\ E_0 = \infty \Longrightarrow \alpha\text{: } very\ high\ value \Longrightarrow \psi_2 = 0$
- $\therefore$ Then the quantity $\frac{ik+\alpha}{ik-\alpha} = -1$
- $\therefore \psi_1(x)$ becomes
- $\psi_1(x) = A\left(e^{ikx} - e^{-ikx}\right)$
- $= A[(Cos\ kx + i\sin kx) - (Cos\ kx - i\sin kx)]$
- $= A(2\, i \sin kx)$
- $\boxed{\therefore \psi_1\ (x) = 2\, i\, A \sin kx}$

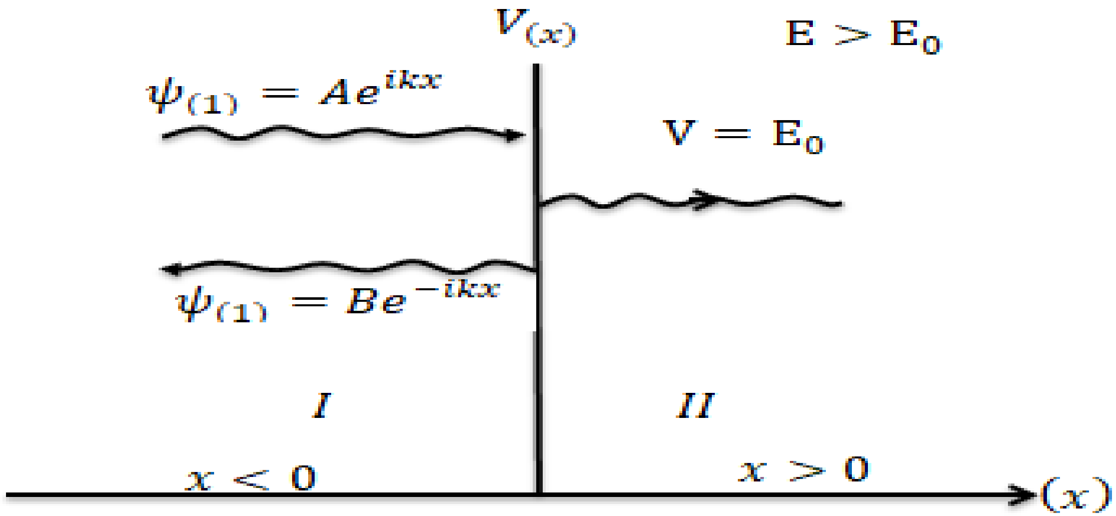


Figure (3.3) incident and reflected wave in potential step

According to the classical mechanic all particles are crossing from region I to region II while the quantum mechanic is effecting on some of these particles which will be defected at the boundary between the two regions (x=0). To prove that we can solve.(TISE)

Note:

A: Amplitude of incident material wave.

B: Amplitude of the reflected material wave.

But $B \neq 0 \Longrightarrow$ reflected some particle inspite of the total energy is greater than the potential energy $(V = E_o)$ in region II.

- **solution of TISE in region II**
- $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{dx^2} + v\psi_2 = E\psi_2$
- $V = E_0 \therefore -\frac{\hbar^2}{2m}\ \frac{\partial^2\psi_2}{dx^2} + E_0\psi_2 = E\psi_2$
- $\frac{\partial^2\psi_2}{dx^2} + \ \frac{2m\ (E-E_0)}{\hbar^2}\psi_2 = 0$
- $E = T + E_0$
- $E - E_0 = T$
- $T = \frac{P^2}{2m} \Longrightarrow P^2 = 2mT = 2m(E - E_0)$
- $\hbar^2\acute{k}^2 = 2m(E - E_0)$
- $\acute{k}^2 = \frac{2m(E-E_0)}{\hbar^2}$
- $\therefore \frac{\partial^2\psi_2}{dx^2} + k^2\psi_2 = 0$
- The general solution for this equation

- $\psi_2(x) = Ce^{i\acute{k}x} + De^{-i\acute{k}x}$
- $Ce^{i\acute{k}x}$: represents the moving wave to the right
- $De^{-i\acute{k}x}$:represent the moving wave to the left and refers to the reflected wave but in region II can not found reflected wave because, of absence boundary in this region ; then $De^{-i\acute{k}x} = 0$.
- $\therefore \psi_2(x) = Ce^{i\acute{k}x}$
- To find relation between A,B and C we can go
- $\psi_1 = \psi_2 \; at \; x = 0 \; \Longrightarrow A + B = C$
- $\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x} \; at \; x = 0 \Longrightarrow i\,kA - i\,kB = i\,\acute{k}C$

- $\boxed{B = \frac{k-\acute{k}}{k+\acute{k}} A}$ $\boxed{C = \frac{2k}{k+\acute{k}} A}$
- $\psi_1(x) = Ae^{ikx} + Be^{-ikx}$
- $\psi_1(x) = A(e^{ikx} + \frac{k-\acute{k}}{k+\acute{k}} e^{-ikx})$
- $\psi_2(x) = \frac{2k}{k+\acute{k}} Ae^{ikx}$

- **3.4 Normalized condition**
-
- $\int_{-\infty}^{\infty} \psi^* \psi \, \partial x = 1$ ……..(3.9)
- Means the total probability of the presence of particle =1 or 100% in a certain region
- **3.5 Orthogonal condition**
- $\int_{-\infty}^{\infty} \psi_m^* \psi_n \, \partial x = 0 \quad m \neq n$ …….(3.10)
- Means the particle can't presence in two different state at the same time
- $\int_{all\ space} \psi_m^* \ \psi_n \, \partial x = \delta_{mn}$ ……..(3.11)
- $\delta_{mn}: koncdcer\ Delta$
- $\delta_{mn} = 1 = if\ m = n$
- $\delta_{mn} = 0\ if\ m \neq n$

- *Thank you for listening*