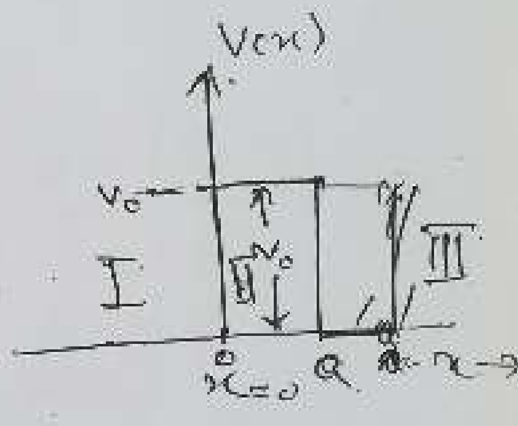
The Rectangular Potential Barrier and Well:

Consider a particle of mass "m" moving in a +ve x-direction in an infinite well, the potential at the boundaries are given as.

$$V(x) = \begin{cases} 0 & , x < 0 \\ V_0 & , 0 \leq x \leq a \\ 0 & , x > a \end{cases}$$



Now we consider the two cases

1) $\underline{E > V_0}$

The time-independent S.W.E is

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi$$

Region I $\underline{x < 0}$, $V = 0$.

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 = E\psi_1$$

$$\frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0.$$

$$k_1^2 = \frac{2mE}{\hbar^2}$$

Region II $0 \leq x \leq a$ $V = V_0$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} + K_2^2\psi_2 = 0$$

$$\because K_2^2 = \frac{2m(E-V_0)}{\hbar^2}$$

Region III $x > a$ $V = 0$

$$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$$

$$\frac{d^2\psi_3}{dx^2} + K_1^2\psi_3 = 0$$

$$\because K_1^2 = \frac{2mE}{\hbar^2}$$

The solution of the S.W.E in these regions are

I: $\psi_1 = Ae^{iK_1x} + Be^{-iK_1x}$

II $\psi_2 = Ce^{iK_2x} + De^{-iK_2x}$

III $\psi_3 = Ee^{iK_1x} + Fe^{-iK_1x}$

In region III ($x>a$), the term Fe^{-ik_1x} represents the reflected wave in the -ve-x-direction. Since, there is no such wave, therefore, $F=0$, so the solution in region III ($x>a$) will becomes

III: $\psi_3 = E e^{ik_1x}$

The matching conditions are

$\psi_1(0) = \psi_2(0)$ — ①

$$\frac{d\psi_1(0)}{dx} = \frac{d}{dx}\psi_2(0) \quad \text{— ②}$$

and

$$\psi_2(a) = \psi_3(a) \quad \text{— ③}$$

$$\frac{d\psi_2(a)}{dx} = \frac{d}{dx}\psi_3(a) \quad \text{— ④}$$

These equation gives us

$$A+B = C+D \quad \text{— ⑤}$$

$$ik_1(A-B) = ik_2(C-D) \quad \text{— ⑥}$$

$$Ce^{ik_2a} + De^{-ik_2a} = Ee^{ik_1a} \quad \text{— ⑦}$$

$$ik_2\left(Ce^{ik_2a} - De^{-ik_2a}\right) = ik_1Ee^{ik_1a} \quad \text{— ⑧}$$

By adding (7) and (8), one gets

$$C = E\left[\frac{K_2+K_1}{2K_2}\,e^{iK_1a-iK_2a}\right] \quad (9)$$

Now, by subtracting (7) and (8), one gets

$$D = E\left[\frac{K_2-K_1}{2K_2}\,e^{ia(K_1+K_2)}\right] \quad (10)$$

Now, by adding (5) and (6)

$$A = \frac{K_1+K_2}{2K_1}C + \frac{K_1-K_2}{2K_1}D.$$

by putting the value of "C and D" from (9) and (10), respectively,

$$A = E\,e^{iK_1a}\left[\cos(K_2a) - i\,\frac{K_1^2+K_2^2}{2K_1K_2}\times \sin(K_2a)\right]$$

Now, by substracting (5) and (6)

$$B = \frac{K_1-K_2}{2K_1}C + \frac{K_1+K_2}{2K_1}D.$$

19

By putting the value of "C and "D"

$$B = -iE\, e^{ik_1 a} \frac{k_1^2-k_2^2}{2k_1k_2} \sin(k_2 a)$$

Now.

$$\frac{B}{A} = \frac{-i\cancel{E}\cancel{e^{ik_1 a}} \frac{k_1^2-k_2^2}{2k_1k_2}\sin(k_2 a)}{\cancel{E}\cancel{e^{ik_1 a}}\left[\cos(k_2 a) - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2 a)\right]}$$

$$= \frac{-i\frac{k_1^2-k_2^2}{2k_1k_2}\sin(k_2 a)}{\cos(k_2 a) - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2 a)}$$

multiply and divided by $2i\frac{k_2}{k_1}$ on RHS

$$\frac{B}{A} = \frac{\left(1-\frac{k_2^2}{k_1^2}\right)\sin(k_2 a)}{2i\frac{k_2}{k_1}\cos(k_2 a) + \left(1+\frac{k_2^2}{k_1^2}\right)\sin(k_2 a)}$$

Now.

$$A = E\, e^{ik_1 a}\left[\cos(k_2 a) - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2 a)\right]$$

$$\frac{E}{A} = \frac{1}{e^{ik_1 a}\left[\cos(k_2 a) - i\frac{k_1^2+k_2^2}{2k_1k_2}\sin(k_2 a)\right]}$$

$$\frac{E}{A} = \frac{2e^{-ik_1 a}}{2\cos(k_2 a) - i\,\frac{k_1^2+k_2^2}{k_1 k_2}\sin(k_2 a)}$$

The various Current densities are

$$J_i = \cancel{\frac{\hbar}{2mi}}\ \cancel{C}$$

Incident Current Density:

$$J_i = \frac{\hbar}{2mi}\left(\psi_i^* \frac{\partial \psi_i}{\partial x} - \psi_i \frac{\partial \psi_i^*}{\partial x}\right)$$

$$\psi_i = A e^{ik_1 x}, \quad \psi_i^* = A^* e^{-ik_1 x}$$

$$\frac{\partial \psi_i}{\partial x} = ik_1 A e^{ik_1 x}$$

and

$$\frac{\partial \psi_i^*}{\partial x} = -ik_1 A^* e^{-ik_1 x}$$

then

$$\boxed{J_i = \frac{k_1 \hbar}{m} A^* A} = \frac{k_1 \hbar}{m} |A|^2$$

Transmitted Current Density:

$$J_t = \frac{\hbar}{2mi}\left[\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x}\right]$$

$$\psi_t = E e^{ik_1x}, \quad \psi_t^* = E e^{ik_1x}$$

$$\frac{\partial \psi_t}{\partial x} = ik_1 E e^{-ik_1x}, \quad \frac{\partial \psi_t^*}{\partial x} = ik_1 E e^{ik_1x}$$

then

$$\boxed{J_t = \frac{\hbar k_1}{m}|E|^2 = \frac{\hbar k_1}{m} E^* E}$$

Reflected Current Density:

$$J_r = \frac{\hbar}{2mi}\left(\psi_r^* \frac{\partial \psi_r}{\partial x} - \psi_r \frac{\partial \psi_r^*}{\partial x}\right)$$

$$\psi_r = B e^{-ik_1x}, \quad \psi_r^* = B e^{ik_1x}$$

$$\frac{\partial \psi_r}{\partial x} = -ik_1 B e^{-ik_1x}, \quad \frac{\partial \psi_r^*}{\partial x} = ik_1 B e^{ik_1x}$$

then

$$J_r = -\frac{\hbar k_1}{m}|B|^2$$

$$\boxed{J_r = -\frac{\hbar k_1}{m} B^* B}$$

Reflection Co-efficient R:

The reflection Co-efficient "R" can be calculated as:

$$R = \left|\frac{J_r}{J_i}\right| = \left|\frac{-\frac{\hbar k_1}{m} B^* B}{\frac{\hbar k_1}{m} A^* A}\right|$$

$$R = \frac{B^* B}{A^* A} = \left|\frac{B}{A}\right|^2 =$$

$$R = \left|\frac{\left(1 - \frac{k_2^2}{k_1^2}\right)\sin(k_2 a)}{\left(1 + \frac{k_2^2}{k_1^2}\right)\sin(k_2 a) \mp 2i\frac{k_2}{k_1}\cos(k_2 a)}\right|^2$$

$$= \frac{\left(1 - \frac{k_2^2}{k_1^2}\right)^2 \sin^2(k_2 a)}{\left(1 + \frac{k_2^2}{k_1^2}\right)^2 \sin^2(k_2 a) + 4\frac{k_2^2}{k_1^2}\cos^2(k_2 a)}$$

$$\boxed{R = \frac{\left(k_1^2 - k_2^2\right)^2 \sin^2(k_2 a)}{\left(k_1^2 + k_2^2\right)^2 \sin^2(k_2 a) + 4k_1^2 k_2^2 \cos^2(k_2 a)}}$$

Transmission Co-efficient "T":

The transmission co-efficient can be calculated as.

$$T = \left|\frac{J_t}{J_i}\right| = \left|\frac{-\hbar k_1/m \, E^* E}{\hbar k_1/m \, A^* A}\right|$$

$$= \left|\frac{E}{A}\right|^2$$

$$= \frac{4}{4\cos^2(k_2 a) + \left(\frac{k_2^2}{k_1} + \frac{k_1^2}{k_2}\right)^2 \sin^2 k_2 a}$$

$$= \frac{4}{4(1-\sin^2 k_2 a) + \left(\frac{k_2^2}{k_1} + \frac{k_1^2}{k_2}\right)^2 \sin^2 k_2 a}$$

$$= \frac{4}{4 - \left[4 - \frac{(k_2^2 + k_1^2)^2}{k_1^2 k_2^2}\right] \sin^2 k_2 a}$$

$$= \frac{4}{4 + \left[\frac{(k_1^2 - k_2^2)^2}{k_1^2 k_2^2}\right] \sin^2 k_2 a}$$

$$T = \left[1 + \frac{1}{4}\left(\frac{K_1^2 - K_2^2}{K_1 K_2}\right)^2 \sin^2 K_2 a\right]^{-1}$$

Classical mechanics tells us that the particle of energy $E > V_0$ should cross the barrier i.e there is no reflection. But according to the Q.M. there is some probability of the particle reflected back in region I $(x < 0)$.

As

$$R + T = 1$$

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

If there is no reflection then

$\underline{\underline{T = 1}}$, which can be only if

$$\left(\frac{K_1^2 - K_2^2}{K_1 K_2}\right)^2 \sin^2 K_2 a = 0$$

~~One~~ 1st possibility

i) $\sin^2 k_2 a = 0$

ii) $\dfrac{k_1^2}{k_1 k_2} - \dfrac{k_2^2}{k_1 k_2} = 0$

or $\dfrac{k_1}{k_2} - \dfrac{k_2}{k_1} = 0$

(ii) gives

$k_1 = k_2$, we know that

$$k_1 = \sqrt{\frac{2mE}{\hbar}}, \quad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$k_1 = k_2$ only if $E >>> V_0$.

(i) gives

$$\sin^2 k_2 a = 0$$

$$\therefore \quad k_2 a = n\pi$$

$$k_2 = \frac{n\pi}{a}$$

$$\sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \frac{n\pi}{a}$$

$$\frac{2m(E-V_0)}{\hbar^2} = \frac{n^2\pi^2}{a^2}$$

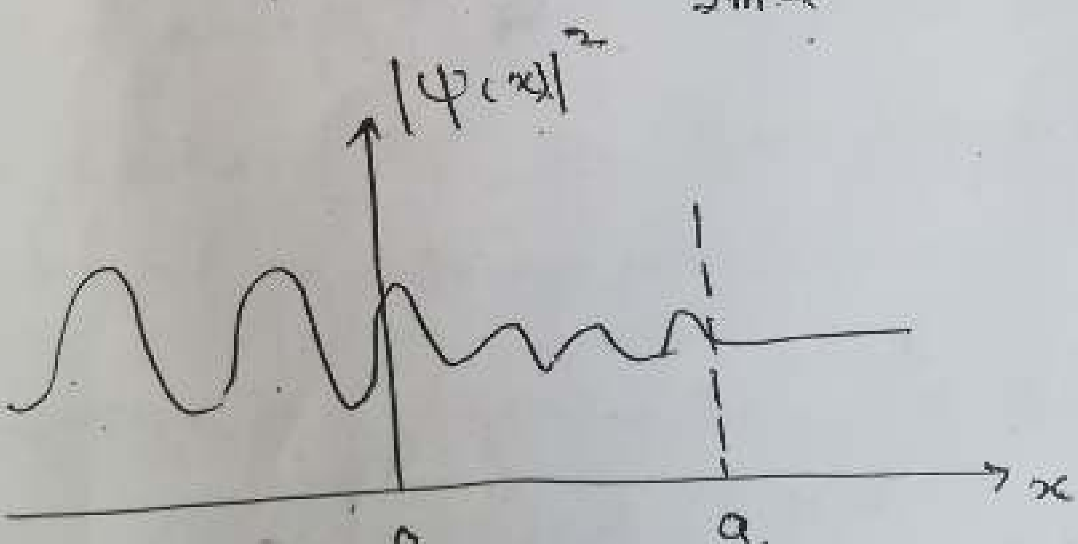
$$E - V_0 = \frac{n^2\pi^2\hbar^2}{a^2}$$

$$\frac{E}{V_0} - 1 = \frac{n^2\pi^2\hbar^2}{2ma^2V_0}$$

$$\frac{E}{V_0} = \frac{n^2\pi^2\hbar^2}{2ma^2V_0} + 1$$

The incident energy of the particle is

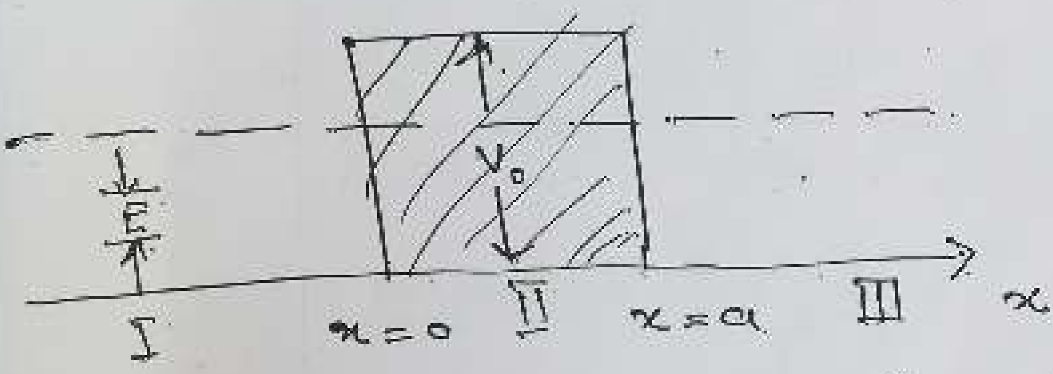
$$E_n = V_0 + \frac{n^2\pi^2\hbar^2}{2ma^2}, \quad n = 1, 2, 3, \ldots$$



$E > V_0$.

(3) E < V_0: Tunneling (21)

Classically, no particle penetrate the barrier, which have less incident energy at that of the barrier height V_0. Hence, one would expect total reflection, no transmission.



But the quantum mechanical predictions differ sharply from the classical ones. The solution of the Schroedinger wave equation in three regions are

(I) $x<0$, $\psi_1(x) = Ae^{iK_1x} + Be^{-iK_1x}$

(II) $0 \le x \le a$, $\psi_2(x) = Ce^{K_2'x} + De^{-K_2'x}$

(III) $x>a$, $\psi_3(x) = Ee^{iK_1x} + Fe^{-iK_1x}$

where $K_1 = \frac{\sqrt{2mE}}{\hbar}$, and $K_2' = \frac{\sqrt{2m(V_0-E)}}{\hbar}$

Since, there is no reflection wave in region III ($x > a$), so we set $F = 0$.

The matching conditions of the wave fns at $x = 0$ and $x = a$ are

$$\psi_1(0) = \psi_2(0)$$

$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx}$$

$$\psi_2(a) = \psi_3(a)$$

$$\frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx}$$

yields

$$A + B = C + D \quad \text{--- (1)}$$

$$iK_1(A - B) = K_2'(C - D) \quad \text{--- (2)}$$

$$C e^{K_2' a} + D e^{-K_2' a} = E e^{iK_1 a} \quad \text{--- (3)}$$

$$K_2'(C e^{K_2' a} - D e^{-K_2' a}) = iK_1 E e^{iK_1 a} \quad \text{--- (4)}$$

By adding (3) and (4), one gets

$$C = \frac{E}{2}\left(1 + i\frac{k_1}{k_2'}\right) e^{(ik_1 - k_2')a}$$

and by subtracting (3) and (4), we get

$$D = \frac{E}{2}\left(1 - i\frac{k_1}{k_2'}\right) e^{(ik_1 + k_2')a}$$

Inserting the values of "C" and "D" from above eqns in (1) and (2) and dividing by A, we will get

$$1 + \frac{B}{A} = \frac{E}{A} e^{ik_1 a}\left[\cosh(k_2' a) - i\frac{k_1}{k_2'}\sinh(k_2' a)\right] \to (5)$$

$$1 - \frac{B}{A} = \frac{E}{A} e^{ik_1 a}\left[\cosh(k_2' a) + i\frac{k_2}{k_1}\sinh(k_2' a)\right] \to (6)$$

Solving the equ. (5) and (6) for B/A and E/A, one can obtained.

$$\left[\begin{array}{l} \sinh x = \dfrac{e^{x} - e^{-x}}{2} = \dfrac{e^{2x} - 1}{2e^{x}} = \dfrac{1 - e^{-2x}}{2e^{-x}} \\ \cosh x = \dfrac{e^{x} + e^{-x}}{2} = \dfrac{e^{2x} + 1}{2e^{x}} = \dfrac{1 + e^{-2x}}{2e^{-x}} \end{array}\right.$$

$$\frac{B}{A} = -i\,\frac{k_1^2 + k_2'^2}{k_1 k_2'}\sin(k_2' a)\left[2\cosh(k_2' a) + i\,\frac{k_2'^2 - k_1^2}{k_1 k_2'}\sinh(k_2' a)\right]^{-1}$$

and

$$\frac{E}{A} = 2\,e^{-ik_1 a}\left[2\cosh(k_2' a) + i\,\frac{k_2'^2 - k_1^2}{k_1 k_2'}\sinh(k_2' a)\right]^{-1}$$

Thus, the reflection and Transmission coefficients are

$$R = \frac{|B|^2}{|A|^2} = \left(\frac{k_1^2 + k_2'^2}{k_1 k_2'}\right)^2 \sinh^2(k_2' a) \times \left[4\cosh^2(k_2' a) + \left(\frac{k_2'^2 - k_1^2}{k_1 k_2}\right)^2 \times \sinh^2(k_2' a)\right]^{-1}$$

$$T = \frac{|E|^2}{|A|^2} = 4\left[4\cosh^2(k_2' a) + \frac{k_2'^2 - k_1^2}{k_1 k_2'} \times \sinh^2(k_2' a)\right]^{-1}$$

we can re-write "R" in terms of "T" as

$R + T = 1$

$R = T - 1$

$$R = \frac{1}{4} T \left(\frac{k_1^2 + k_2'^2}{k_1 k_2} \right) \sinh^2(k_2' a)$$

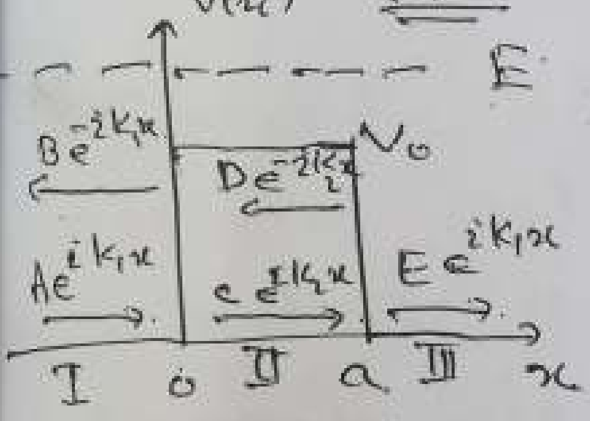
since $\cosh^2(k_2' a) = 1 + \sinh^2(k_2' a)$, then "T" will becomes

$$T = \left[1 + \frac{1}{4} \left(\frac{k_1^2 + k_2'^2}{k_1 k_2} \right) \sinh^2(k_2' a) \right]^{-1}$$

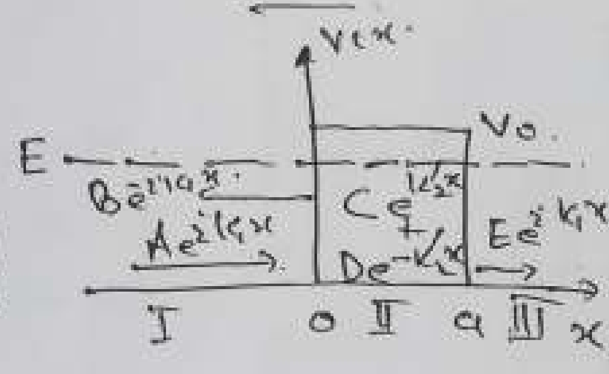
One can see that "T" is finite, which means that the probability for the transmission of the particles into the region $x \geq a$ is not zero. This is a purely quantum mechanical effect which is due to the wave aspect of microscopic objects; it is known as the tunneling effect: quantum mechanical objects can tunnel through classically forbidding or regions.

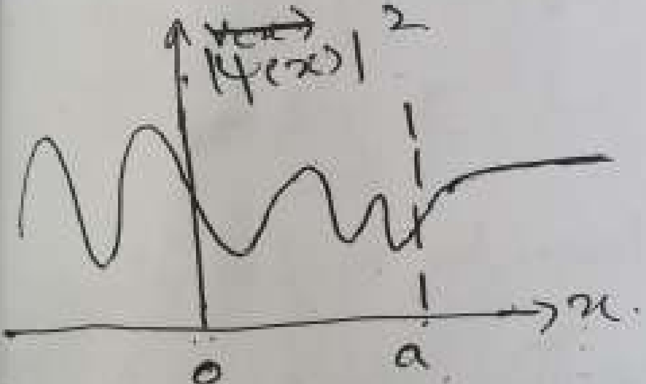
This barrier penetration effect has important applications in various branches of modern physics ranging from particle and nuclear physics to semiconductor devices.

$\underline{E > V_0}$

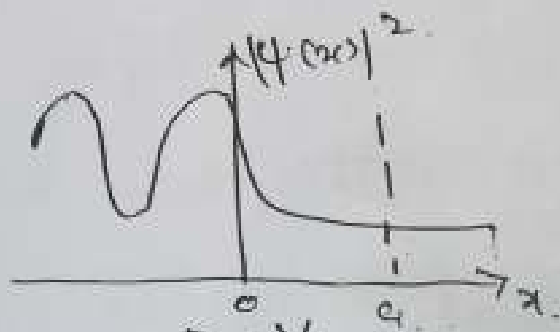


$\underline{E < V_0}$





$\underline{E > V_0}$



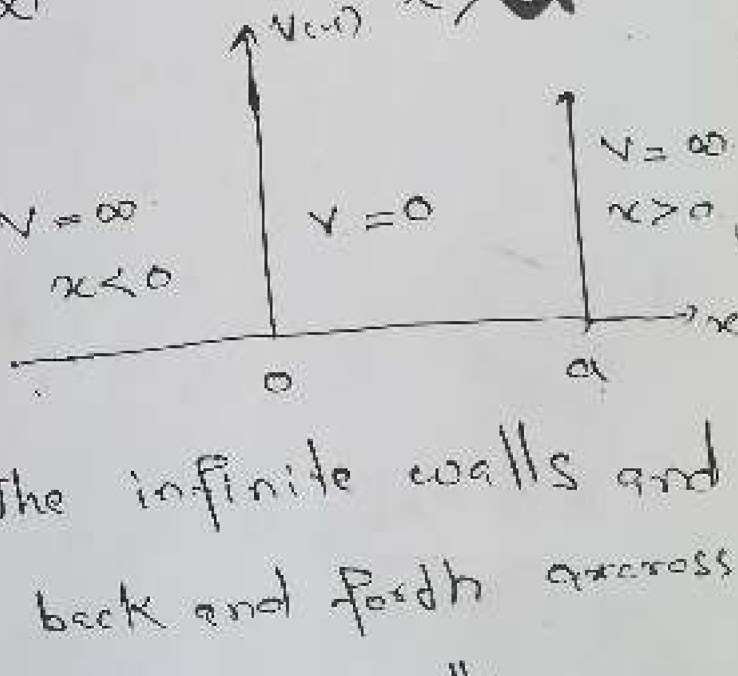
$\underline{E < V_0}$

The Infinite Square Well Potential.

The Asymmetric Square Well:

The infinite square well potential is defined as

$$V(x) = \begin{cases} +\infty & x < 0 \\ 0 & 0 \leq x \leq a \\ +\infty & x > a \end{cases}$$



Classically, it is assumed that a particle is trapped with energy E by the infinite walls and therefore travels back and forth across the well. Quantum mechanically, we assumed that the particle to have only bound state solutions and a discrete non-degenerate energy spectrum.

Since, the particle can not exist outside the well due to the infinite barrier and also outside the well $V(x)$ is infinite for $0 \leq x \leq a$. i.e $\psi_{out} = 0$.

The wavefn must be zero at the outside the boundary (i.e. $x>0, x<0$). Hence, we will get the solution only inside the well as:

The S.W.E for the particle inside the well $(V=0)$ can be written as.

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi = 0$$

$$\because V(x) = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0, \quad K = \frac{\sqrt{2mE}}{\hbar}$$

The general solution is

$$\psi(x) = A' e^{ikx} + B' e^{-ikx}$$

$$= A'(\cos kx + i\sin kx) + B'(\cos kx - i\sin kx)$$

$$= (A'+B')\cos kx + i(A'-B')\sin kx$$

$$\psi(x) = A\cos kx + B\sin kx \quad \text{--- (1)}$$

In order to meet the boundary conditions that $\psi(x) = 0$ at the walls i.e at $x \leq 0$, $x \geq a$, so

i) $\psi(0) = 0$

ii) $\psi(a) = 0$

then (i) gives

$\boxed{A = 0}$, therefore equ 1 becomes

$$\psi(x) = B \sin kx$$

(ii) boundary condition gives

$$\psi(a) = 0$$

$$B \sin(ka) = 0$$

which means

$$k_n a = n\pi, \quad n = 1, 2, 3, \ldots$$

as $$k^2 = \frac{2mE}{\hbar^2}$$

then $$E_n = \frac{\hbar^2 k_n^2}{2m}$$

$$E_n = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \cdot n^2,$$

$$n = 1, 2, 3, \ldots$$

The energy is quantized, and only certain values are permitted.

- The states of a particle which is confined to a limited regions of space are bound states and the energy spectrum is discrete

- Sharp contrast to classical physics where the energy of the particle, given by $E = p^2/2m$, takes any value, the classical energy evolves continuously.

So $\quad K_n = n\pi/a$

then $\quad \psi_n(x) = B \sin\left(\frac{n\pi x}{a}\right)$

Normalization condition gives,

$$\int_0^a B^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1$$

one will gets

$$B = \sqrt{\frac{2}{a}}$$

Hence,

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

There is an infinite sequence of discrete energy levels corresponding to the positive integer values of quantum number n.

For $n = 0$, $\psi_0(x) = 0$

$n = 1$, $\psi_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$

$n = 2$, $\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$

$n = 3$, $\psi_3(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)$