These are the d.E. of matter waves. When a particle moves the wave are always associated to the particle such waves are called ~~as~~ Matter waves.

The wave function ψ represents the probability of finding the particle in entire space.

There are two types of SWE :-

i) Time dependent SWE
ii) Time Independent SWE (Stationary State eq^n)

Time Dependent SWE

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When a particle moves the waves are always associated to the particle if ψ is a wave f^n ψ_0 is its amplitude then the eq^n of wave is given by :-

$$\psi = \psi_0 e^{-i\omega\left(t - \frac{x}{v}\right)}$$

but $\omega = 2\pi\nu$.

$$v = \nu\lambda$$

$$\psi = \psi_0 e^{-2\pi i\nu\left(t - \frac{x}{\nu\lambda}\right)}$$

$$\psi = \psi_0 e^{-2\pi i\left(\nu t - \frac{x\nu}{\nu\lambda}\right)}$$

$$\psi = \psi_0 e^{-2\pi i\left(\frac{E}{h}t - \frac{Px}{h}\right)}$$

$$\psi = \psi_0 e^{-\frac{2\pi i}{h}(Et - Px)}$$

$$\boxed{\psi = \psi_0 e^{-\frac{i}{\hbar}(Et - Px)}} \quad \text{---} (i)$$

Since particle is moving so total energy

$$E = K.E. + P.E.$$

$$E = \frac{P^2}{2m} + V$$

$$E\psi = \frac{P^2}{2m}\psi + V\psi \quad \text{---} (ii)$$

from (i)

$$\frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} E \psi_0 e^{-\frac{i}{\hbar}(Et - Px)}$$

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = E\psi}$$

Again diffn (i) with respect to 'x'

$$\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} P \psi_0 e^{-\frac{i}{\hbar}(Et - Px)}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{i}{\hbar}P\right)^2 \psi$$

$$\boxed{-\hbar^2 \frac{\partial^2 \psi}{\partial x^2} = P^2 \psi}$$

from (ii)

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi}$$

in 3-D

$$E\psi = \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi$$

$$\boxed{E\psi = H\psi}$$

where

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V$$

Hamiltonian operator

** Time Independent SWE

(Stationary State eq^n)

When a particle moves the waves are always associated to the particle. If ψ is a wave function and ψ_0 is its amplitude then the eq^n of wave independent of position is given by:-

$$\psi = \psi_0 e^{-\omega i t}$$

but $\omega = 2\pi \nu$

$v = \nu \lambda$

$$\psi = \psi_0 e^{-2\pi i \nu t} \quad \text{—— (i)}$$

but the classical diff^n eq^n is given by:-

$$\frac{d^2\psi}{dt^2} = v^2 \frac{d^2\psi}{dx^2} \quad \text{—— (ii)}$$

On diff^n (i) w.r.t. (t)

$$\frac{d\psi}{dt} = -2\pi i \nu \psi_0 e^{-2\pi i \nu t}$$

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$$\frac{d^2\psi}{dt^2} = -4\pi^2\nu^2\psi$$

then from (2)

$$-4\pi^2\nu^2\psi = v^2\frac{\partial^2\psi}{dx^2}$$

$$\frac{d^2\psi}{dx^2} + 4\pi^2\frac{\nu^2}{v^2}\psi = 0$$

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2}{\lambda^2}\psi = 0 \qquad \text{(3)}$$

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Since particle is moving, so the total energy of the particle is

$$E = K.E + P.E.$$

$$E = \frac{1}{2}mv^2 + V$$

$$2m(E-V) = m^2v^2$$

$$mv = \sqrt{2m(E-V)}$$

but

$$\lambda = \frac{h}{mv}$$

$$\lambda = \frac{h}{\sqrt{2m(E-V)}}$$

from (3).

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2}{h^2} 2m(E-V)\psi = 0$$

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

Normalization of Wave function

A wave function is said to be normalized if it follows the condⁿ

$$\int \psi\psi^* \, dV = 1$$

where ψ^* is called complex conjugate of ψ. if it is not in the case then it is called unnormalized wave function.

Physical significance of ψ

A wave function ψ is a quantum mechanical operator, By knowing ψ we can determine energy & momentum of a particle. It is complex quantity so it have its complex conjugate. if ψ is a wave function and ψ^* is its complex conjugate then

$\psi\psi^* \, dV$ give the probability of finding the particle in entire space.

Orthogonal Wave function

A wave function is said to be orthogonal if it follows the condⁿ

$$\int \psi_1 \psi_2^* dv = \int \psi_2 \psi_1^* dV = 0$$

Applications of SWE

There are three appst

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1. Particle in a box

Consider a particle of mass (m) is placed inside the box, the walls of the box is so much high. that the probability of finding the particle outside of the box is zero.

W.r.t. the time independent SWE is given by:

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

The total energy of the particle is only the K.E. then $V=0$.

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

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

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{----------} \rightarrow (1)$$

this is the second order d.E., let the solⁿ becomes

$$\psi = A\sin kx + B\cos kx \quad \text{———} \ (2)$$

where A and B are the constants by using the boundary condⁿ i.e.,

at $x = 0, \psi = 0$

~~using~~ $x = a, \psi = 0$

using (1)st B.C. in (2)

$$B = 0$$

again

$$\psi = A\sin kx$$

$$0 = A\sin ka$$

$$\sin ka = \sin n\pi$$

$$ka = n\pi$$

$$\boxed{k = \frac{n\pi}{a}}$$

$$\boxed{\psi = A\sin\frac{n\pi}{a}x}$$

for <u>Normalization of wave function</u>

$$\int_0^a |\psi|^2 dx = 1$$

$$\int_0^a A^2\sin^2\frac{n\pi}{a}x\, dx = 1$$

$$A^2 \int_0^a \frac{\left(1 - \cos \frac{2n\pi x}{a}\right)}{2} dx = 1$$

$$\frac{A^2}{2} a = 1$$

$$\boxed{A = \sqrt{\frac{2}{a}}}$$

then $$\boxed{\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}}$$

then

$$K = \frac{2\pi}{\lambda} = \frac{n\pi}{a}$$

$$\boxed{\lambda = \frac{2a}{n}}$$

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

$$\frac{n^2\pi^2\hbar^2}{a^2} = 2mE$$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

If $n=1$

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

$n=2$

$E_2 = 2^2 E_1$

$n=3$

$E_3 = 3^2 E_1$

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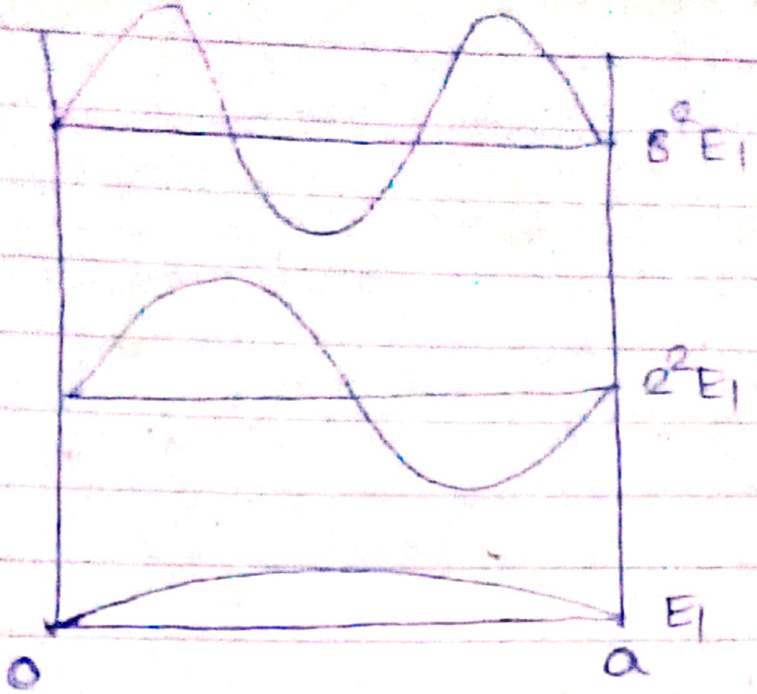
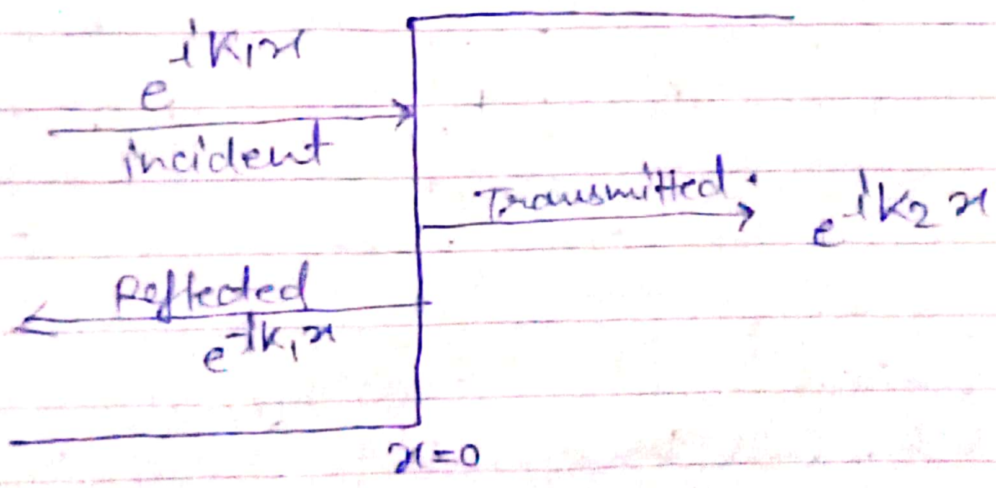


2. Rectangular potential ~~strip~~ Step



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Consider a particle of mass m moving along (+)ve x-direction striking the potential barrier. If its energy is less than the barrier it will be reflected back. If its energy is greater than the Barrier it will be transmitted i.e.,

$$V = 0 \qquad x < 0$$
$$V = V_0 \qquad x > 0$$

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Now time independent s.w.e. is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{---} (1)$$

If $V=0$ $\quad x<0$

$$\frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2}\psi_1 = 0$$

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

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0 \quad \text{---} (1)$$

This is second order d.E., let its sol^n become

$$\psi_1 = Ae^{iK_1x} + Be^{-iK_1x} \quad \text{---} (2)$$

If $V=V_0$ $\quad , x>0$
then

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

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

$$\frac{d^2\psi_2}{dx^2} + K_2^2\psi_2 = 0 \quad \text{---} (4)$$

This is second order d.E., let its sol^n become

$$\psi_2 = Ce^{iK_2x} \quad \text{---} (3)$$

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where A, B & C are constants. By using the boundary condⁿ i.e.

i) at $x=0$, $\psi_1 = \psi_2$

ii) at $x=0$, $\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x}$

Applying Iˢᵗ BC.

$$A e^{ik_1 \times 0} + B e^{-ik_1 \times 0} = C e^{ik_2 \times 0}$$

$$A = C - B \quad \text{—— } \cancel{6}\ (4)$$

$$\frac{\partial \psi_1}{\partial x} = ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x}$$

$$\frac{\partial \psi_2}{\partial x} = ik_2 C e^{ik_2 x}$$

Using 2ⁿᵈ B.C.

$$ik_1 A - ik_1 B = ik_2 C$$

$$ik_1 A = ik_2 C + ik_1 B$$

$$A = \frac{k_2 C + k_1 B}{k_1} \quad \text{—— } \cancel{7}\ (5)$$

Adding (4) & (5)

$$2A = C - B + \frac{k_2 C + k_1 B}{k_1}$$

$$2Ak_1 = Ck_1 - \cancel{Bk_1} + k_2 C + \cancel{k_1 B}$$

$$\boxed{C = \frac{2Ak_1}{k_1 + k_2}}$$

from ④

$$A = \frac{2AK_1 - BK_1 - K_2B}{(K_1+K_2)}$$

$$\boxed{B = \left(\frac{K_1-K_2}{K_1+K_2}\right)A}$$

Now to show the sum of reflected and transmitted coefficient is equal to one. We will use the probability function i.e.,

$$P = \frac{\hbar}{2mi}\left[\psi^* \nabla\psi - \psi\nabla\psi^*\right]$$

Now

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_1^* = A^* e^{-ik_1x} + B^* e^{ik_1x}$$

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$$\frac{\partial\psi_1}{\partial x} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}$$

$$\frac{\partial\psi_1^*}{\partial x} = -ik_1A^*e^{-ik_1x} + ik_1B^*e^{ik_1x}$$

then

$$P = \frac{\hbar}{2mi}\Big[(A^*e^{-ik_1x} + B^*e^{ik_1x})(ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x}) - (Ae^{ik_1x} + Be^{-ik_1x})(-ik_1A^*e^{-ik_1x} + ik_1B^*e^{ik_1x})\Big]$$

$$= \frac{\hbar}{2mi}\Big[ik_1AA^* - \cancel{ik_1A^*Be^{-2ik_1x}} + \cancel{ik_1AB^*e^{2ik_1x}} - ik_1BB^* + ik_1AA^* - \cancel{ik_1AB^*e^{2ik_1x}} + \cancel{ik_1A^*Be^{-2ik_1x}} - ik_1BB^*\Big]$$

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$$P = \frac{\hbar}{2mi} 2iK_1 \left[|A|^2 - |B|^2 \right]$$

$$P = \frac{\hbar K_1}{m} \left[|A|^2 - |B|^2 \right]$$

Now incident wave $= \frac{\hbar K_1}{m} |A|^2$

Reflected wave $= \frac{\hbar K_1}{m} |B|^2$

Transmitted " $= \frac{\hbar K_2}{m} |C|^2$

Reflected Coefficient $= \frac{\text{Reflected wave}}{\text{incident wave}}$

$$R = \frac{\frac{\hbar K_1}{m} |B|^2}{\frac{\hbar K_1}{m} |A|^2}$$

$$= \frac{|B|^2}{|A|^2} = \frac{(K_1 - K_2)^2}{(K_1 + K_2)^2}$$

Transmitted Coefficient $= \frac{\frac{\hbar K_2}{m} |C|^2}{\frac{\hbar K_1}{m} |A|^2}$

$$= \frac{K_2 \, 4K_1^2}{K_1 (K_1 + K_2)^2}$$

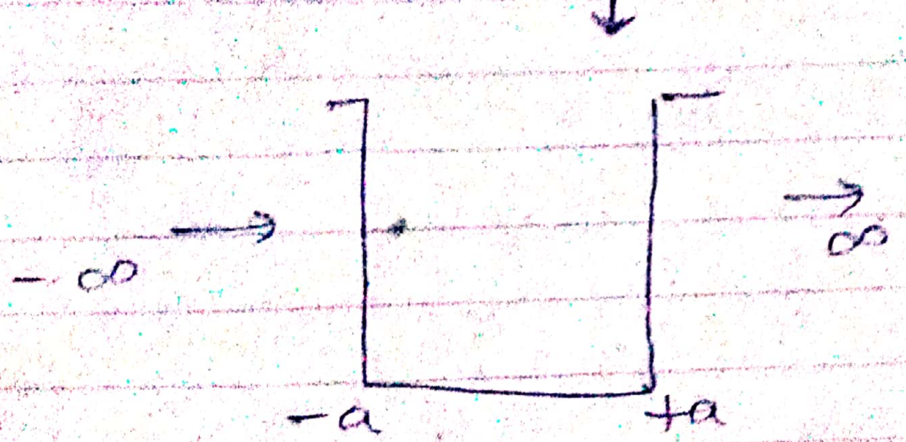
$$\boxed{T = \frac{4K_1 K_2}{(K_1 + K_2)^2}}$$

$$R+T = \frac{(k_1-k_2)^2 + 4k_1k_2}{(k_1+k_2)^2}$$

$$\text{"} = \frac{(k_1+k_2)^2}{(k_1+k_2)^2}$$

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

3. <u>Square well Potential</u>



consider a particle of mass (m) moving along (+)ve x-dir^n then there are 3 regions

1) $V = V_0 \quad -\infty < x < -a$

$V = 0 \quad -a < x < a$

$V = V_0 \quad a < x < \infty$

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w.r.t. time independent SWE is given by:

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{——(1)}$$

$e^{-Va}(C+D) = 2B\cos\beta a$ — (9)

$Ve^{-Va}(D-C) = 2A\beta\cos\beta a$ — (10)

$-2A\sin\beta a = e^{Va}(D-C)$ — (11)

$V(D+C)e^{-Va} = 2B\beta\sin\beta a$ — (12)

If $V = V_0$ $\quad -\infty < x < -a$

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_1 = 0$$

Put

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

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

This is the second order diff^n eq^n let sol^n of this eq^n:

$$\psi_1 = Ce^{-i\alpha x} + De^{i\alpha x}$$

at $x = -\infty$ $\quad Ce^{-i\alpha x}$ does not exist

$$\psi_1 = De^{i\alpha x} \quad \text{— (2)}$$

at $V = 0$, $\quad -a < x < a$

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

Put $\quad \dfrac{2mE}{\hbar^2} = \beta^2$

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

This is 2nd order d.E.

let Sol^n becomes

$$\psi_2 = A\sin\beta x + B\cos\beta x \quad \text{— (3)}$$

at $V = V_0$, $\quad a < x < \infty$

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

This is 2nd d.E., let sol^n becomes :

9 (5-7) (6-8) 10 9/10 11/12 (5-7) (6-8) 12 (11)

$$\psi_3 = Ce^{-i\alpha x} + De^{i\alpha x}$$

at $x = \infty$ then $De^{i\alpha x}$ does not exist

$$\psi_3 = Ce^{-i\alpha x} \quad \text{—— (4)}$$

where A, B, C & D are the constants, by using the boundary condⁿ :

1) $\psi_1 = \psi_2$ at $x = -a$

2) $\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x}$ at $x = -a$

3) $\psi_2 = \psi_3$ at $x = a$

4) $\frac{\partial \psi_2}{\partial x} = \frac{\partial \psi_3}{\partial x}$ at $x = a$

Using 1st B.C.

$$De^{-i\alpha a} = -A\sin\beta a + B\cos\beta a \quad \boxed{i\alpha = \nu}$$

$$De^{-\nu a} = -A\sin\beta a + B\cos\beta a \quad \text{—— (5)}$$

$$\frac{\partial \psi_1}{\partial x} = i\alpha De^{i\alpha x}$$

$$\frac{\partial \psi_2}{\partial x} = A\beta\cos\beta x - B\beta\sin\beta x$$

Using 2nd B.C, Put $i\alpha = \nu$

$$\nu De^{-\nu a} = A\beta\cos\beta a + B\beta\sin\beta a \quad \text{—— (6)}$$

Using III rd B.C.

$$Ce^{-\nu a} = A\sin\beta a + B\cos\beta a \quad \text{—— (7)}$$

Using IV th B.C.

$$-\nu Ce^{-\nu a} = A\beta\cos\beta a - B\beta\sin\beta a \quad \text{—— (8)}$$

Adding (5), (7) and (6) & (8)

$$(D+C)\, e^{-\nu a} = 2B\cos\beta a \quad \text{(9)}$$

$$\nu(D-C)\, e^{-\nu a} = 2A\beta\cos\beta a \quad \text{(10)}$$

Substracting (5), (7) & (6) & (8)

$$(D-C)\, e^{-\nu a} = -2A\sin\beta a \quad \text{(11)}$$

$$\nu\,(D+C)\, e^{-\nu a} = 2B\beta\sin\beta a \quad \text{(12)}$$

Dividing (9) by (12), (10) by (11)

$$\frac{1}{\nu} = \frac{1}{\beta}\cot\beta a \quad \text{(13)}$$

$$\nu = -\beta\cot\beta a \quad \text{(14)}$$

from (13) & (14)

$$-\frac{1}{\beta\cot\beta a} = \frac{1}{\beta}\cot\beta a$$

$$\boxed{\tan^2\beta a = -1}$$