

1(a) The Schrodinger Equation for a quantum Particle of mass m in a potential $V(x)$ is,

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x,t) \Psi(x,t)$$

Now to apply separation of variable method,
we choose,

$$\Psi(x,t) = \psi(x) \phi(t)$$

Putting this into the Schrodinger equation yields,

$$i\hbar \frac{d\phi(t)}{dt} \psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} \phi(t) + V(x,t) \psi(x) \phi(t)$$

We divide the above equation by Ψ to get,

$$i\hbar \frac{d\phi(t)}{dt} \frac{1}{\phi(t)} = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} \frac{1}{\psi(x)} + V(x,t)$$

Now we obtained a function where LHS is only function of time and on the right hand side we have only function of position, except for the potential V .

Now to solve this we assume that the potential is independent of time.

$$\text{i.e. } V(x,t) = V(x)$$

\therefore we have

$$i\hbar \frac{d\phi(t)}{dt} \frac{1}{\phi(t)} = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} \frac{1}{\psi(x)} + V(x)$$

Now since each side depends only on one variable the these are independent, then it must be true that each side equals a constant.

$$\therefore i\hbar \frac{d\phi(t)}{dt} \frac{1}{\phi(t)} = E \quad \text{and}$$

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

Now we have to solve the two ODE's

$$i\hbar \frac{d\phi(t)}{dt} = E \phi(t) \quad \text{and}$$

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

Now

$$i\hbar \frac{d\phi(t)}{dt} = E \phi(t)$$

$$\Rightarrow \frac{d\phi(t)}{\phi(t)} = \frac{-iE}{\hbar} dt$$

$$\Rightarrow \int \frac{d\phi(t)}{\phi(t)} = \int -\frac{iE}{\hbar} dt$$

$$\Rightarrow \log\{\phi(t)\} = \frac{-iE}{\hbar} t + c$$

$$\Rightarrow \phi(t) = e^{-(iE/\hbar)t + c} = e^{-\frac{iE}{\hbar}t} + e^c = e^{-\frac{iE}{\hbar}t} c$$

Since we are looking for solutions to $\Psi = \phi\psi$, we will incorporate the constant c into ψ and give the solution ϕ as,

$$\phi(t) = e^{-\frac{iE}{\hbar}t}$$

Thus the general solution to the time-dependent wave equation is,

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

b) Solution of the Schrodinger equation,

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

If we have an even potential then $V(x) = V(-x)$ then $\psi(x)$ can be taken as even or odd. This followed by considering Schrodinger Equation with a x replaced by $-x$

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

Thus $\psi(-x)$ satisfies the same equation as $\psi(x)$ for an even potential, so another pair of solution must be $\psi(-x) \pm \psi(x)$

(i) Even

$$\psi_+(x) = \psi(-x) + \psi(x)$$

x replaced by $-x$

$$\psi_+(-x) = \psi(x) + \psi(-x) = \psi_+(x)$$

(ii) odd

$$\psi_-(x) = \psi(-x) - \psi(x)$$

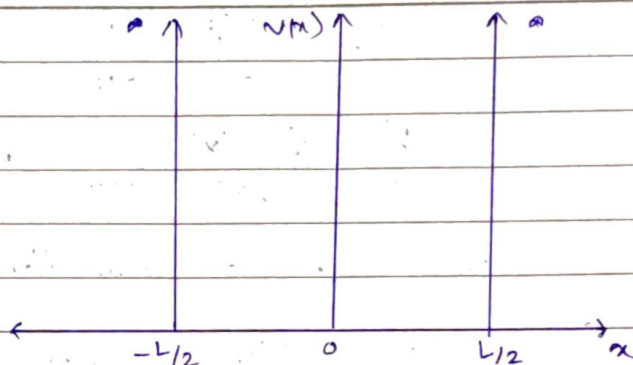
x replacing by $-x$

$$\psi_-(-x) = \psi(x) - \psi(-x) = -[\psi(-x) - \psi(x)]$$

$$\psi_-(-x) = -\psi_-(x)$$

Thus the general solution is a linear combination of even and odd functions.

c)



we have,

$$V(x) = \begin{cases} 0 & , |x| < \frac{L}{2} \\ \infty & , \text{otherwise} \end{cases}$$

Now, the 1-D Schrodinger Equation is,

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} E \psi(x) = 0 \quad , \quad \text{for } |x| < \frac{L}{2}$$

Since the particle is free inside the box, we can write the general solution as the sum of the two plane waves propagating in opposite directions, which is equivalent to the sum of a cosine and a sine, with wave number k

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

$$; \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

The wave function must be zero at both walls of well to satisfy the boundary conditions.

$$\therefore A \cos\left(k \frac{L}{2}\right) + B \sin\left(k \frac{L}{2}\right) = 0 \quad \text{and}$$

$$A \cos\left(-k \frac{L}{2}\right) + B \sin\left(-k \frac{L}{2}\right) = 0$$

$$\Rightarrow A \cos\left(k \frac{L}{2}\right) - B \sin\left(k \frac{L}{2}\right) = 0$$

$$\therefore \text{A} \cos\left(k \frac{L}{2}\right) = 0 \text{ and}$$

$$B \sin\left(k \frac{L}{2}\right) = 0$$

Now we can conclude from above

$$A = 0 ; \quad \frac{KL}{2} = (2n-1) \frac{\pi}{2} ; \quad n = 1, 2, \dots$$

$$B = 0 ; \quad \frac{KL}{2} = n\pi , \quad n = 1, 2, 3, \dots$$

here the top solution will lead to odd parity wavefunctions and the bottom one to even parity wavefunctions.

Normalizing;

$$\int_{-L/2}^{L/2} |A|^2 \cos^2\left(\frac{(2n-1)\pi}{L} x\right) dx = 1$$

$$\Rightarrow \frac{A^2}{2} \int_{-L/2}^{L/2} \left(1 + \cos\left[\frac{2(2n-1)\pi x}{L}\right]\right) dx = 1$$

$$\Rightarrow \frac{A^2}{2} \left[x + \sin\left\{\frac{2(2n-1)\pi x}{L}\right\} \cdot \frac{L}{2(2n-1)\pi} \right]_{-L/2}^{L/2} = 1$$

$$\Rightarrow \frac{A^2}{2} \left[\left(\frac{L}{2}\right) - \left(-\frac{L}{2}\right) \right] = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

and

$$\int_{-L/2}^{L/2} |B|^2 \sin^2\left(\frac{2n\pi x}{L}\right) dx = 1$$

$$\Rightarrow \frac{|B|^2}{2} \int_{-L/2}^{L/2} \left[1 - \cos\left\{\frac{4n\pi x}{L}\right\}\right] dx = 1$$

$$= \frac{B^2}{2} \left[x - \frac{L}{4n\pi} \sin\left(\frac{4n\pi x}{L}\right) \right]_{-L/2}^{L/2} = 1$$

$$*) \frac{B^2}{2} \left[\left(\frac{L}{2} \right) - \left(-\frac{L}{2} \right) \right] = 1$$

$$\Rightarrow B = \sqrt{\frac{2}{L}}$$

\therefore the solution becomes

$$\Psi(x) = \sqrt{\frac{2}{L}} \cos \left\{ \frac{(2n+1)\pi x}{L} \right\} + \frac{\sqrt{2}}{L} \sin \left(\frac{2n\pi x}{L} \right)$$

d) we have,

$$\frac{d^2 \Psi(x)}{dx^2} + \frac{2m}{\hbar^2} E \Psi(x) = 0 \rightarrow (1)$$

To make the equation dimensionless we take,

$$\xi = \frac{x}{L}$$

$$\frac{d\xi}{dx} = \frac{1}{L}$$

$$\frac{d\Psi}{dx} = \frac{d\Psi}{d\xi} \frac{d\xi}{dx} = \frac{1}{L} \frac{d\Psi}{d\xi}$$

$$\begin{aligned} \frac{d^2 \Psi}{dx^2} &= \frac{d}{dx} \left(\frac{1}{L} \frac{d\Psi}{d\xi} \right) \\ &= \frac{1}{L} \frac{d^2 \Psi}{dx d\xi} + \frac{d\Psi}{d\xi} \frac{d}{dx} \left(\frac{1}{L} \right) \end{aligned}$$

$$\frac{d^2 \Psi}{dx^2} = \frac{1}{L} \frac{d}{d\xi} \left(\frac{d\Psi}{dx} \right)$$

$$= \frac{1}{L} \frac{d}{d\xi} \left(\frac{d\Psi}{d\xi} \frac{d\xi}{dx} \right)$$

$$= \frac{1}{L^2} \frac{d^2 \Psi}{d\xi^2}$$

Now, we define

$$\epsilon = \frac{2mL^2}{\hbar^2} E$$

$\frac{\hbar^2}{2mL^2}$ is the unit of energy

So the equation (1) becomes

$$\frac{1}{L^2} \frac{d^2 \psi}{d\xi^2} + \epsilon \psi(\xi) = 0$$

The energy eigenvalue for the potential well

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

$$\therefore \frac{2mL^2}{\hbar^2} E_n = n^2 \pi^2$$

$$\epsilon = n^2 \pi^2$$

to obtain E in physical form

$$E = \frac{\epsilon \hbar^2}{2mL^2} \text{ eV}$$