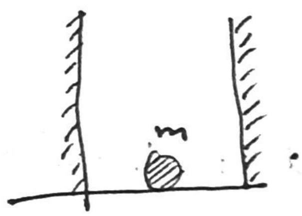
Recall: Infinite square well: 22nd January 2024



$$V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

Time independent Schroedinger equation:

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

The equation is well behaved if we use well behaved potentials.

General solution: $\boxed{\psi(x) = Ae^{iKx} + Be^{-iKx}}$

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

(*) If $V(x)$ blows up, $\psi(x)$ must go to zero.

We now need to fix the constants A and B.

$\psi(x=0^-) = 0$ (particle cannot be there - potential is infinity)

$\Rightarrow \boxed{A+B=0} \Rightarrow \boxed{B=-A}$

Similarly,

$\psi(x=a^+) = 0$

$\Rightarrow Ae^{iKa} - Ae^{-iKa} = 0$ → Does not allow us to fix A.

We impose a condition,

$e^{i2Ka} = 1 = e^{i2n\pi} \Rightarrow Ka = n\pi$

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

$\therefore E = \frac{\hbar^2 K^2}{2m} = \boxed{\frac{\hbar^2 n^2\pi^2}{2ma^2} = E_n}$ Energy eigenvalues that are allowed

Now, the n^{th} wave function,

$$\Psi_n(x) = Ae^{i\frac{n\pi x}{a}} - Ae^{-i\frac{n\pi x}{a}}$$

$$\Rightarrow \boxed{\Psi_n(x) = D\sin\left(\frac{n\pi x}{a}\right)} \rightarrow \text{Energy eigenfunc/ eigenstate.}$$

We can verify,

$$\boxed{\hat{H}\Psi_n = E_n\Psi_n} \rightarrow \text{Eigenvalue equation.}$$

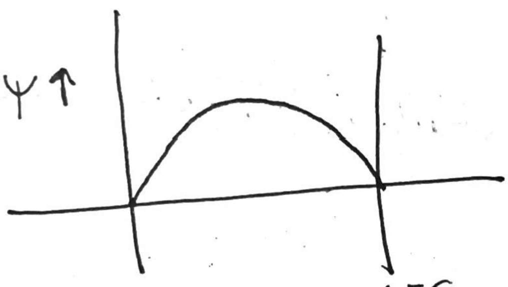
now,

$n=1$:

$$E_1 = \frac{\hbar^2\pi^2}{2ma^2} \rightarrow \text{Noground state.}$$

(minimumenergy configuration)

$$\Psi_1 = D\sin\left(\frac{\pi x}{a}\right)$$



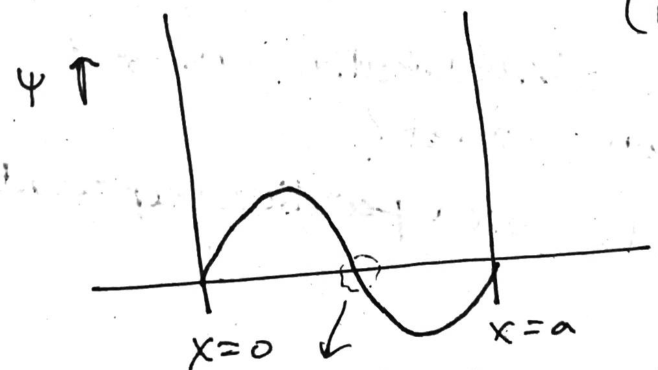
Quantum mechanical ground state.

If $\Delta p = 0$, uncertainty would be violated.

$n=2$:

$$\boxed{E_2 = \frac{4\pi^2\hbar^2}{2ma^2}} \rightarrow \boxed{\Psi_2 = D\sin\left(\frac{2\pi x}{a}\right)}$$

(Firstexcited state)



Node (1) → Exactlyone node.

State canbe determined bycounting non-boundary nodes.

(*) Time-dependant part of the Schroedinger eqn $\longrightarrow$

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

We have solved $\psi(x)$,

$$\boxed{\hat{H}\,\psi_n(x) = E_n\,\psi_n(x)}$$

Now,

$$i\hbar\,\frac{dT(t)}{dt} = E_n\,T(t)$$

Solution is,

$$\boxed{T = T_0\,e^{-i\frac{E_n t}{\hbar}}}$$

Therefore, the full solution to the Schroedinger equation,

$$i\hbar\,\frac{\partial \psi(x,t)}{\partial t} = \hat{H}\,\psi(x,t)$$

$$\boxed{\Psi_n(x,t) = \psi_0\,e^{-i\frac{E_n t}{\hbar}}\,\sin\left(\frac{n\pi x}{a}\right)}$$

We have a non-trivial solution (non-zero)

(*) Is this a wave, or not?

Does $\Psi_n(x,t)$ for a particle represent any wave?

Now, put $\frac{E}{\hbar} = \omega$, $n\pi = kx$

$$\Psi = \Psi_0 e^{-i\omega t} \left(\frac{e^{ikx} - e^{-ikx}}{2i} \right)$$ → sin x using Euler's identity.

$$\Rightarrow \boxed{\Psi(x,t) = C_1 e^{i(kx-\omega t)} + C_2 e^{i(kx+\omega t)}}$$

$C_1 e^{i(kx-\omega t)}$ → wave moving to the right

$C_2 e^{i(kx+\omega t)}$ → wave moving to the left.

What does the wave function Ψ represent for a particle? (open question)

Maxwell's equations —

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\varepsilon_0}, \quad \vec{\nabla} \times \vec{B} = \mu_0 \left(\vec{J} + \varepsilon_0 \frac{\partial \vec{E}}{\partial t} \right)$$

$\rho = \rho(x,t)$ → Charge density

$\vec{J} = \vec{J}(x,t)$ → current vector..

Now, we use the identity $\vec{\nabla} \cdot (\vec{\nabla} \times \vec{A}) = 0$

$$\vec{\nabla} \cdot (\vec{\nabla} \times \vec{B}) = 0 = \vec{\nabla} \cdot \vec{J} + \varepsilon_0 \vec{\nabla} \cdot \left(\frac{\partial \vec{E}}{\partial t} \right)$$

$$\Rightarrow \boxed{\vec{\nabla} \cdot \vec{J} + \frac{\partial \rho}{\partial t} = 0}$$ → Charge conservation equation.

$$\underbrace{\frac{d}{dt} \int_V d^3x \, \rho(x,t)}_{Q} = \underbrace{-\int_V d^3x \, (\vec{\nabla} \cdot \vec{J})}_{= -\int_S \vec{J} \cdot d\vec{S}}$$

→ If no charge is leaking through the surface S, $\int_S \vec{J} \cdot d\vec{S} = 0$, then total charge Q is conserved as $\boxed{\frac{dQ}{dt} = 0}$

The SE also admits situations like this.

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \quad -①$$

$\psi \rightarrow$ complex valued function.

So we can write a conjugate equation,

<u>Conjugate:</u>

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V(x)\psi^* \quad -②$$

(Assume V real)

$\psi^* \times ① - \psi \times ② \Rightarrow$

$$i\hbar\left(\psi^*\frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}\right) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right)$$

$$\Rightarrow \cancel{i\hbar}\frac{\partial}{\partial t}(\psi^*\psi) = -\vec{\nabla}\left[\frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\cdot\psi - \psi\vec{\nabla}\cdot\psi^*\right)\right]$$

So analogously,

$$\rho = \psi^*\psi \quad , \quad \vec{J} = \frac{\hbar}{2mi}\left(\psi^*\vec{\nabla}\cdot\psi - \psi\vec{\nabla}\cdot\psi^*\right)$$

$$\Rightarrow \boxed{\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J} = 0} \rightarrow$$ Conservation equation implied by Schroedinger eqn

$\rightarrow \int d^3x\, \psi^*\psi \rightarrow$ is a conserved quantity

if $\int_S \vec{J}\cdot d\vec{S} = 0$

⊛ At boundary if ψ is zero, then $\vec{J} = 0$.