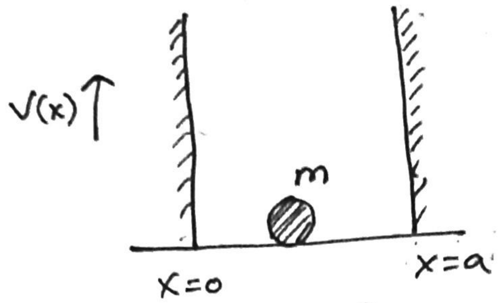
19th January 2024

⊛ Infinite square well → (1+1 D)

Suppose potential $V(x)$ is given as $V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & \text{otherwise} \end{cases}$



(i) The particle is free inside the box
↳ No force acting on it.

$$\boxed{F = -\frac{\partial V}{\partial x} = 0} \quad \text{for } \cancel{0 \leq x \leq a} \; 0 < x < a$$

(ii) What about the force at the boundary?

$$F(a_+) = -\lim_{h \to 0^+} \frac{V(a+h) - V(a)}{h}$$

$$= -\infty$$

$$F(a_-) = -\lim_{h \to 0} \frac{V(a-h) - V(a)}{h} = 0$$

The particle experiences an infinite force if it tries to move to the right at $x=a$

At $x=0$, opposite situation arises.

(iii) Within the wall : Total ~~ene~~ energy of the particle,

$$E = \frac{1}{2}mv^2 + V^{\to 0} = \frac{p^2}{2m} \geq 0$$

either 0 or positive

$E=0$ is called the minimum energy configuration.

(Ground state)

Now we solve it using <u>Quantum Mechanics</u> →

Schrodinger equation (Time independent)

$$\hat{H}\,\Psi(x) = \frac{\hat{P}^2}{2m}\,\Psi(x) = E\,\Psi(x)$$

Again, this is an <u>operator</u>.

$$\hat{P} = -i\hbar\frac{d}{dx}$$

$$\Rightarrow \boxed{\hat{H}\,\Psi(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\left(\Psi(x)\right) = E\,\Psi(x)}$$

2nd order ODE

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

<u>Ansatz</u>: $\Psi(x) = e^{mx}$

$$\Rightarrow m^2 + K^2 = 0 \Rightarrow m = \pm iK$$

(Auxilliary eqn)

<u>General Solution</u>: $\boxed{\Psi(x) = Ae^{iKx} + Be^{-iKx}}$

How do we determine the constants A and B?

(In Newtonian case, it was intuitive as x_0 and $\dot{x}_0$)

Time independent Schroedinger equation -

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

It is a law of nature and it should remain well defined for all physically plausible domain (i.e, $-\infty < x < \infty$) and for all physically plausible potential

(i.e $\underline{V(x) < \infty}$) → physically plausible

(Think of $V(x) = \infty$ as a limit to infty, not infty)

(*) Well-defined means that the values involved are finite.

Integrating (1), over a small interval around $x = a$

$$\int_{a-\varepsilon}^{a+\varepsilon} \frac{d}{dx}\left(\frac{d\psi}{dx}\right) dx = \int_{a-\epsilon}^{a+\epsilon} (V - E)\,\psi(x)\,dx$$

why? It must not blow up

as $\epsilon \to 0$

$$\Rightarrow \left.\frac{d\psi}{dx}\right|_{x=a+\epsilon} - \left.\frac{d\psi}{dx}\right|_{x=a-\epsilon} = L < \infty \text{ (finite)}$$

(Say)

Now, $$\left.\frac{d\psi}{dx}\right|_{x=a+\epsilon} = \frac{\psi(a+\epsilon) - \psi(a)}{\epsilon}$$

So, $$\Rightarrow \psi(x)\big|_{x=a+\epsilon} - \psi(x)\big|_{x=a-\epsilon} = L\epsilon$$

$= 0$

(as $\epsilon \to 0$)

$$\Rightarrow \boxed{\psi(a+\epsilon) = \psi(a-\epsilon)}$$

$\psi(x)$ is continuous at $x = a$ (???)

(A) If $V(x)$ is continuous,

$\Rightarrow \psi'(x)$ is also continuous.

(B) If $\boxed{V(x) = V_0\,\delta(x-a)}$

$\psi'(x)$ has a finite discontinuity at $x = a$

(C) $V \to \infty$

$$\int_{a-\epsilon}^{a+\epsilon} V\,\psi(x)\,dx < L$$

$\to \infty$ (What??)

$$\Rightarrow \psi(a) \int_{a}^{a+\epsilon} V(x)\,dx < L$$