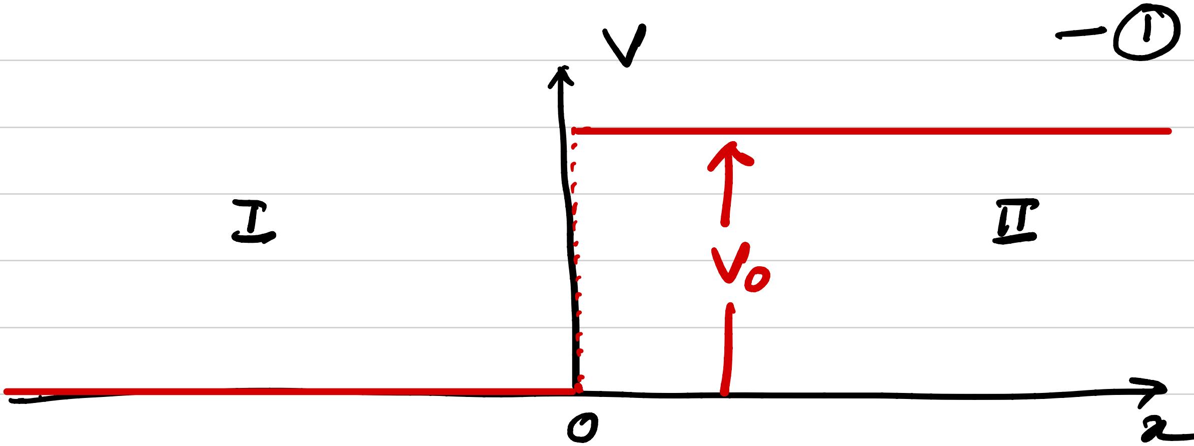
8/10/2025

Day 25: The Step Potential and QM Tunneling

Consider a potential energy function:

$$V(x) = \begin{cases} 0 & , x < 0 \quad \text{rg. I} \\ V_0 > 0 & , x > 0 \quad \text{rg. II} \end{cases} \quad \text{—(1)}$$



A classical particle with energy $E < V_0$, starting out from a pt. $x = -a$ and moving towards the right will simply bounce back upon reaching the origin. This is because it does not have enough energy to overcome the potential barrier at $x = 0$.

On the other hand if $E > V_0$, it would simply go past the origin without much influence from the barrier.

The quantum case is not so straightforward. Herein, we will look at the case of $E < V_0$. (For other cases, please refer to §5.4 R. Shankar)

$\underline{E < V_0}$:

$$\hat{H} = \begin{cases} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} & \text{in reg. I} \\ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0 & \text{in reg. II} \end{cases} \quad \text{— (2)}$$

Let's first solve the TISE.

Reg. I resembles the free particle case, But since there is a boundary at $x=0$, we have to write the general solution as:

$$\psi_I(x) = A e^{ikx} + B e^{-ik} \quad \text{— (3)}$$

where $$k = \sqrt{\frac{2m}{\hbar^2} E} \quad — (3)$$

& A, B are constants to be determined.

In reg. II, we have to solve.

$$\frac{d^2\psi_{II}(x)}{dx^2} + \underbrace{\frac{2m}{\hbar^2}(E - V_0)}_{\equiv -K^2 \; (\because E < V_0)} \psi_{II}(x) = 0 \quad — (4)$$

$$\Rightarrow \frac{d^2\psi_{II}(x)}{dx^2} - K^2 \psi_{II}(x) = 0 \quad — (5)$$

This is readily solved finding (see this before)

$$\psi_{II}(x) = C e^{-Kx} + D e^{Kx} \quad — (6)$$

At $x \to \infty$ the second term explodes. To keep ψ_{II} finite, we must have that $D = 0$ — (7)

$$\therefore \quad \psi_{II}(x) = C e^{-Kx} \quad — (8)$$

Now we apply the boundary condition to determine A, B & C. Note that the jump in $V(x)$ at $x=0$ is finite. Therefore derivative of ψ also needs to continuous at $x=0$, along with ψ itself.

Thus, we have.

$$\left.\begin{aligned} \psi(x=0^-) &= \psi(x=0^+) \\ \psi'(x=0^-) &= \psi'(x=0^+) \end{aligned}\right\} \quad (9)$$

$$\psi' \rightarrow \frac{d\psi}{dx}$$

i.e.

$$\left.\begin{aligned} \psi_I(0) &= \psi_{II}(0) \\ \frac{d\psi_I(0)}{dx} &= \frac{d\psi_{II}(0)}{dx} \end{aligned}\right\} \quad (10)$$

Using (7) & (8) we get

$$A + B = C \quad \text{—(11)}$$
$$ik(A - B) = -\kappa C \quad \text{—(12)}$$

This system of equations is readily solved to yield.

$$\frac{C}{A} = \left(\frac{2k}{k+i\kappa}\right) \quad \text{—(13)}$$

$$\frac{B}{A} = \left(\frac{k-i\kappa}{k+i\kappa}\right) \quad \text{—(14)}$$

$$\therefore \psi(x) = \begin{cases} A\left[e^{ikx} + \left(\frac{k-i\kappa}{k+i\kappa}\right)e^{-ikx}\right] \\ A\left(\frac{2k}{k+i\kappa}\right)e^{-\kappa x} \end{cases} \quad \text{—(15)}$$

A can be determined by normalization

The important thing to note here is that $A \neq 0$. This means that the probability of finding a particle with energy $E < V_0$ in region II is,

$$P_{II}(x) = |\psi_{II}(x)|^2$$

$$= |C|^2 e^{-2Kx}$$

$$= |A|^2 \frac{4k^2}{k^2+K^2} e^{-2Kx}$$

$$= 4|A|^2 \left(E/V_0\right) \exp\left(-2\sqrt{\frac{2m}{\hbar^2}(V_0-E)}\, x\right) \quad — (16)$$

So unlike the classical case, the particle can actually cross the origin although its energy is less than the barrier height.

This phenomenon is known as QM tunneling.

In reg-I, $\psi_I(x) = \underbrace{A e^{ikx}}_{\text{right travelling}} + \underbrace{B e^{-ikx}}_{\text{left-travelling}}$.

Apparently, a right travelling wave can also be reflected at the boundary and pick up a left-travelling companion.

What is the probability current density for left & right?
We saw in the previous lecture that it makes sense to do this separation.

First we note that in region II, since the wavefunction is real, there is no current density and no net flow.
$\therefore$ all contribution to $\vec{j}$ comes from reg. I.

$$j_I(x,t) = \frac{\hbar k}{m} |A|^2 \quad — (17)$$ also called incident current

$|||^{ly}$ left current or reflected current is

$$j_R(x,t) = \frac{\hbar k}{m} |B|^2 \quad — (18)$$

The current density moving right from $x=0$ onwards (region II) is called the transmitted current

In the present case $(E < V_0)$, this is zero since ψ_{II} is real.

$$\therefore \; j_T(x,t) = 0 \quad — (19)$$

We can define two quantities two ratios to measure the efficiency of "barrier transmission".

Reflection coefficient

$$R = \frac{j_R}{j_I} \quad -(20)$$

Transmission coefficient

$$T = \frac{j_T}{j_I} \quad -(21)$$

Presently,

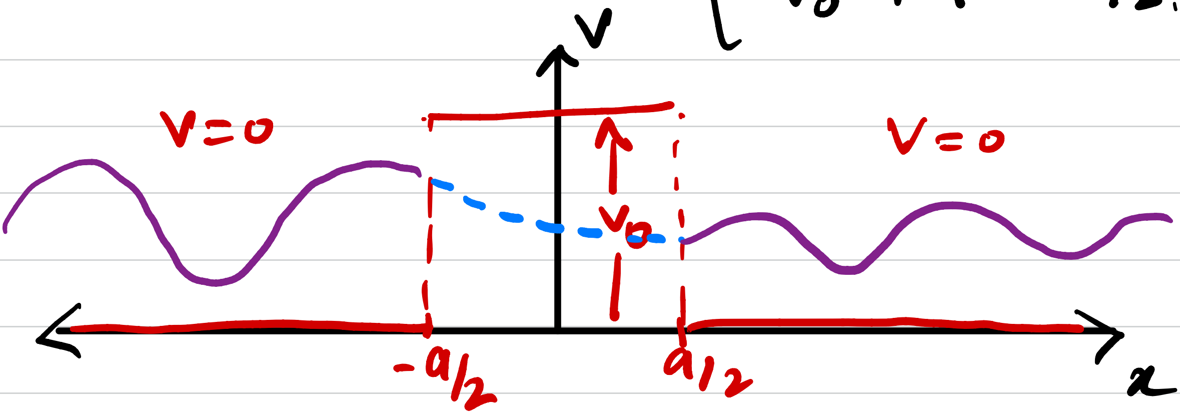
$$R = \left|\frac{B}{A}\right|^2 = \frac{k^2+K^2}{k^2+K^2} = 1 \quad -(22)$$

$$T = 0 \quad -(23)$$

i.e. there is no steady flow (propagating current) into the barrier region. This is despite there being a finite probability in that region

Tunneling raises interesting possibility.
Suppose,

$$V(x) = \begin{cases} 0 & |x| > a/2 \\ V_0 & |x| < a/2. \end{cases}$$



Then, it could happen, that, depending the energy of the approaching particle, it's probability current is transmitted to the right side of the barrier.

Indeed such an effect is seen in many physical instances and can only be explained as a consequence of Q.M.