Step-wise change in potential — a "simple" model for various interactions

We will consider two types of problems

a) Bound ~~ne~~ states — particle is localized
→ Descrete energy spectrum
only specific values of energy give stationary states
→ we find them by solving

① $\hat{H}\psi = E\psi$

② $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1$

$|\psi(x)|^2$ describes the probability density

b) Unbound states — particle flux
~~Total~~ $|\psi(x)|^2 \Delta x$ describes the probability to find a particle b/w x and $x+\Delta x$
but $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx \to \infty$ since there should be a source of particles somewhere

Energy spectrum is continuous → any E is possible
Instead, ~~we~~ in such problems we are interested in ratios b/w fluxes

reflected ←

→ incident

$$\left| \frac{\text{amplitude of reflected}}{\text{amplitude of incident}} \right|^2 = R$$

Finite potential barrier

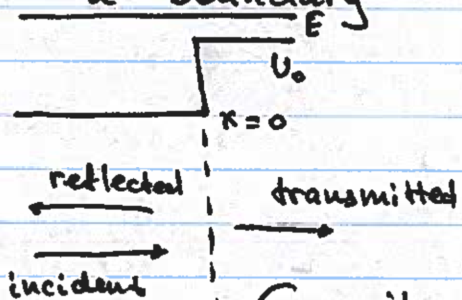
1. "Low" potential barrier $E > U_0$

<u>Classical particle</u> can exist in both regions,

$x<0$ $\quad K_0 = P_0^2/2m = E \quad \Rightarrow \quad p_0 = \sqrt{2mE} \quad k_0 = P_0/\hbar = \dfrac{\sqrt{2mE}}{\hbar}$

$x>0$ $\quad K+U = E = P^2/2m \quad \Rightarrow \quad p = \sqrt{2m(E-U_0)} \quad k = \dfrac{P_0}{\hbar} = \dfrac{\sqrt{2m(E}}{\hbar}$

<u>Classical wave analogue</u> : light travelling through a boundary of two transparent materials



Wave function will have different functional form for $X<0$ and $X>0$

$$\psi(x) = \begin{cases} \underbrace{Ae^{ik_0x}}_{\text{incident}} + \underbrace{Be^{-ik_0x}}_{\text{reflected}} & x<0 \\ \underbrace{Ce^{ikx}}_{\text{transmitted}} & x>0 \end{cases}$$

Boundary conditions : a wave function in a finite potential must be continuous and smooth

Continuous : $\psi(x-0) = \psi(x+0)$ $\quad A+B = C$

Smooth: $\psi'(x-0) = \psi'(x+0)$ $\quad ik_0A - ik_0B = ikC$

$\cancel{i}k_0A - \cancel{i}k_0B = \cancel{i}kA + \cancel{i}kB$

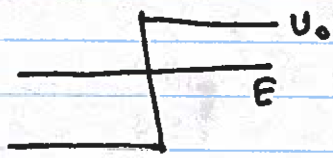
$$\frac{B}{A} = \frac{k_0-k}{k_0+k}$$

Reflection probability: $R = \left|\frac{B}{A}\right|^2 = \left(\frac{k_0 - k}{k_0 + k}\right)^2$

if $B/A < 0$ $(k_0 - k) < 0$ then there will be a $180°$ phase shift upon reflection

Transmission probability $T = 1 - R = \frac{4k_0 k}{(k_0+k)^2}$
(same expressions as in optics!)

2. "High" potential barrier $E < U_0$
Classical particle can only be in $x<0$;
$x>0$ – classically forbidden region
Classical wave analogue: total internal reflection, real wave for $x<0$, evanescent wave for $x>0$



$x<0$: $\psi_{x<0} = A e^{ik_0 x} + B e^{-ik_0 x}$

$x>0$ Schrodinger equation

$$-\frac{\hbar^2}{2m} \psi''_{x>0} + U_0 \psi_{x>0} = E \psi_{x>0}$$

$$\psi''_{x>0} = \frac{2m}{\hbar^2}(U_0 - E)\psi_{x>0} = q^2 \psi_{x>0}$$

Possible solutions: $e^{\pm qx}$

Since classical particle cannot exist at $x>0$ region, the probability of finding it there should fall down, thus $\psi_{x>0}(x) = C e^{-qx}$

$$\psi(x) = \begin{cases} A e^{ik_0 x} + B e^{-ik_0 x} & x<0 \\ C e^{-qx} & x>0 \end{cases}$$

Boundary conditions
Continuous: $A + B = C$
Smooth $ik_0 A - ik_0 B = -qC = -qA - qB$

$$\frac{B}{A} = \frac{ik_0 + q}{ik_0 - q}$$

Reflection probability $R = \left|\frac{B}{A}\right| = \left|\frac{ik_0+q}{ik_0-q}\right| = 1$

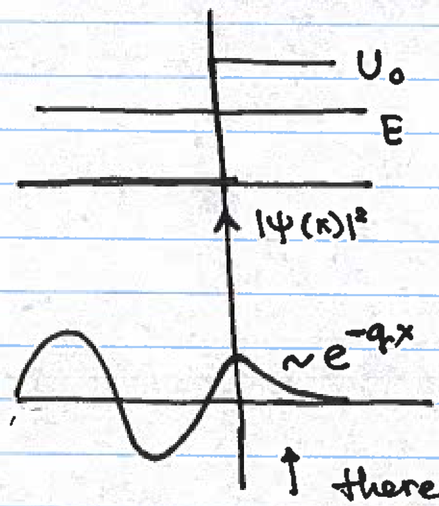
as expected

$\frac{B}{A} = e^{i\varphi}$ φ = phase shift

$$\varphi = \sin^{-1}\left(\frac{2k_0q}{q^2-k_0^2}\right)$$

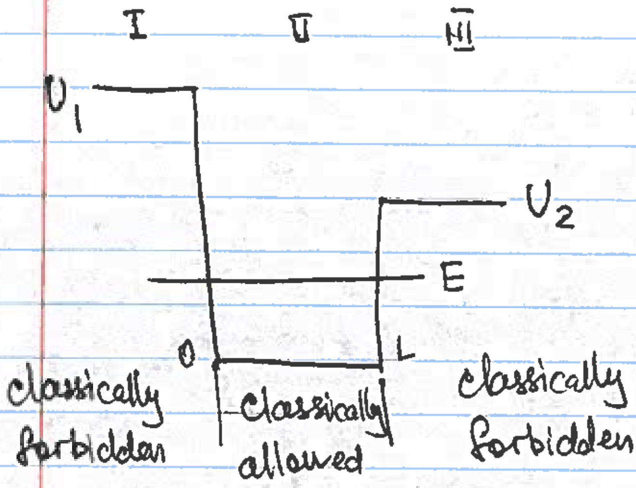
If we can measure this phase shift (by, for example, interfering it with the original wave) we can get information about the height of the barrier

(~~Why do you think~~



↑ there is non-zero probability to find the particle beyond the barrier, although it's decaying exponentially with distance

Finite potential well



Classical particle motion in finite well and infinite well are identical (bouncing back and forth)

However, we found that reflection off a finite potential wall affects the phase of the reflected wave ⟹ thus, the conditions for standing wave would be affected as well

$$\psi(x) = \begin{cases} D e^{+q_1 x} & x<0 \\ A\cos k_0 x + B\sin k_0 x & 0<x<L \\ C e^{-q_2(x-L)} & x>L \end{cases}$$

$$q_1 = \frac{\sqrt{2m(U_1-E)}}{\hbar}$$

$$q_2 = \frac{\sqrt{2m(U_2-E)}}{\hbar}$$

$$k_0 = \frac{\sqrt{2mE}}{\hbar}$$

[Infinite square well $\psi=0$ $x<0$ & $x>L$]

Boundary conditions for <u>both</u> boundaries

<u>$x=0$</u>

$\psi(x \overset{=0}{-} 0) = \psi(x \overset{=0}{+} 0)$ $\qquad D = A$

$\psi'(x \overset{=0}{-} 0) = \psi'(x \overset{=0}{+} 0)$ $\qquad q_1 D = k_0 B$

$x=L$

$\psi(x=L-0) = \psi(L+0)$ $\qquad A\cos k_0 L + B\sin k_0 L = C$

$\psi'(L-0) = \psi'(L+0)$ $\qquad k_0 A\sin k_0 L - k_0 B\cos k_0 L = -q_2 C$

5 unknowns A,B,C,D coeff + energy E

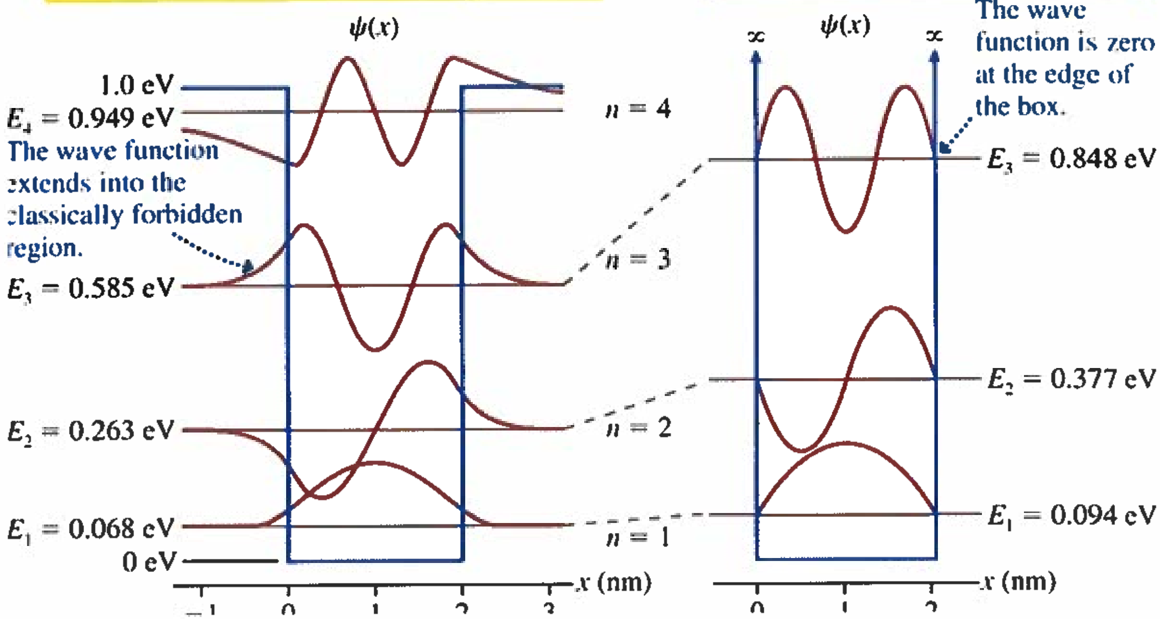
Get rid of coefficients, to get a transcendental equation for energy. Solutions will provide the spectrum of eigen energies

Usually, we will have only <u>finite</u> # of stationary states

Comparison of infinite and finite potential wells

Electron in finite square well
(a=2 nm and V=1.0 eV)

Infinite potential well
(a = 2 nm and V = ∞)



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

in numbers

$$E_n = \frac{(\hbar c)^2 \pi^2 n^2}{2(mc^2) L^2} = \frac{(197\ eV \cdot nm)^2 \pi^2 n^2}{2 \cdot 0.51 \cdot 10^6 eV \cdot (2nm)^2}$$

$$= 0.094\, eV \cdot n^2$$