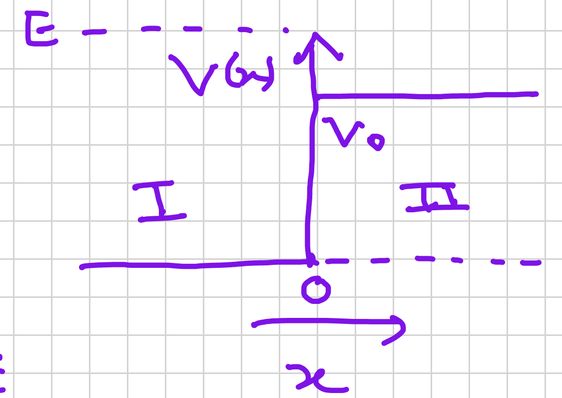
Step Potential

Case I. $E > V_0$



$$\psi_I(x) = e^{ikx} + A e^{-ikx}$$

$$\psi_{II}(x) = B e^{iqx}$$

$$\begin{cases} k = \sqrt{\dfrac{2mE}{\hbar^2}} \\ q = \sqrt{\dfrac{2m(E-V)}{\hbar^2}} \end{cases}$$

Continuity of $\psi(x)$ & $\psi'(x)$ at $x = 0$, implies,

$$1 + A = B.$$

$$ik(1-A) = iqB.$$

$$\Rightarrow \begin{cases} 1 + A = B \\ 1 - A = \dfrac{q}{k} B. \end{cases}$$

$$\therefore A = \left(\frac{k-q}{2k}\right) B$$

$$\& \quad 2 = \frac{k+q}{k} B.$$

$$\Rightarrow \boxed{\begin{aligned} A &= \left(\frac{k-q}{k+q}\right) \\ B &= \left(\frac{2k}{k+q}\right) \end{aligned}} \quad \text{I}$$

$$J_x = \frac{i\hbar}{2m}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^* \frac{\partial \psi}{\partial x}\right)$$

$$\Rightarrow J_I(x) = \frac{i\hbar}{2m}\Big[-ik(e^{-ikx} - A^* e^{ikx})(e^{ikx} + A e^{-ikx}) - ik(e^{-ikx} + A^* e^{ikx})(e^{ikx} - A e^{-ikx})\Big]$$

$$= \frac{i\hbar}{2m}\Big[-ik(1 + A e^{-2ikx} - A^* e^{2ikx} - |A|^2) - ik(1 - A e^{-2ikx} + A^* e^{2ikx} - |A|^2)\Big]$$

$$= \frac{(i\hbar)(-2ik)}{2m}\left[1 - A^2\right] = \frac{\hbar k}{m}(1 - |A|^2).$$

$$= J_{inc.}(x) - J_{ref.}(x).$$

Similarly,

$$J_{II}(x) = \frac{\hbar q}{m}|B|^2 = J_{trans.}(x)$$

$$\therefore \quad r = \frac{J_{ref.}(x)}{J_{inc.}(x)} = |A|^2 = \frac{(k-q)^2}{(k+q)^2} = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2$$

$$t = \frac{J_{trans.}(x)}{J_{inc.}(x)} = \frac{q}{k}|B|^2 = \frac{4kq}{(k+q)^2} = \frac{4\sqrt{E(E-V_0)}}{(\sqrt{E}+\sqrt{E-V_0})^2}$$

Note

- classically, for $E > V_0$, $r = 0$.

  But quantum mechanically, $r = \left(\frac{k-q}{k+q}\right)^2 \neq 0$.

  Here, $r \to 0$ for $k \to q$, i.e., when $V_0 \ll E$,

  or, when $E \to \infty$.

- **Conservation of particle number:**

$$\frac{\hbar k}{m}(1-|A|^2) = \frac{\hbar q}{m}|B|^2$$

$$\Rightarrow \quad J_I(x) = J_{II}(x).$$

$$\therefore \quad J_{inc.}(x) = J_{ref.}(x) + J_{tran.}(x).$$

Case II

$(E < V_0)$

$$\psi_I(x) = e^{ikx} + Ae^{-ikx}$$

$$\psi_{II}(x) = Be^{-Kx} \quad , \quad q = iK = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

$$\left(K = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} \; . \right)$$

$\because E < V_0$

$$\therefore \quad A = \frac{k-iK}{k+iK} .$$

$$B = \frac{2k}{k+iK} .$$

Note:

$$|A|^2 = 1 \implies r = 1.$$

$$\therefore \quad t = 1 - r = 0$$

Also, $$J_{II}(x) = \frac{i\hbar}{2m}\left[\frac{\partial \psi_{II}^*}{\partial x}\psi_{II} - \psi_{II}^* \frac{\partial \psi_{II}}{\partial x} \right]$$

$$= \frac{i\hbar}{2m}\left[-K|B|^2 e^{-2Kx} + K|B|^2 e^{-2Kx} \right]$$

$$= 0.$$

$\therefore$ Although particles penetrate to a depth $\sim \frac{1}{K}$, the net particle flux to the right is zero.

(Such a scenario happening on the right side is known as evanescent wave generation.).

$$\psi(x) = \psi_{I}(x)\,\Theta(-x) + \psi_{II}(x)\,\Theta(x).$$

$$\Rightarrow \psi(x) = \left(e^{ikx} + \frac{k - iK}{k + iK}\, e^{-ikx}\right)\Theta(-x)$$

$$+ \frac{2k}{k + iK}\, e^{-Kx}\,\Theta(x).$$

$$= \frac{(k + iK_{\circ})\, e^{ikx} + (k - iK_{\circ})\, e^{-ikx}}{k + iK_{\circ}}\,\Theta(-x)$$

$$+ \frac{2k}{k + iK_{\circ}}\, e^{-K_{\circ}x}\,\Theta(x).$$

$$= \left[\frac{2k}{k + iK_{\circ}}\cos kx - \frac{2K_{\circ}}{k + iK_{\circ}}\sin kx\right]\Theta(-x)$$

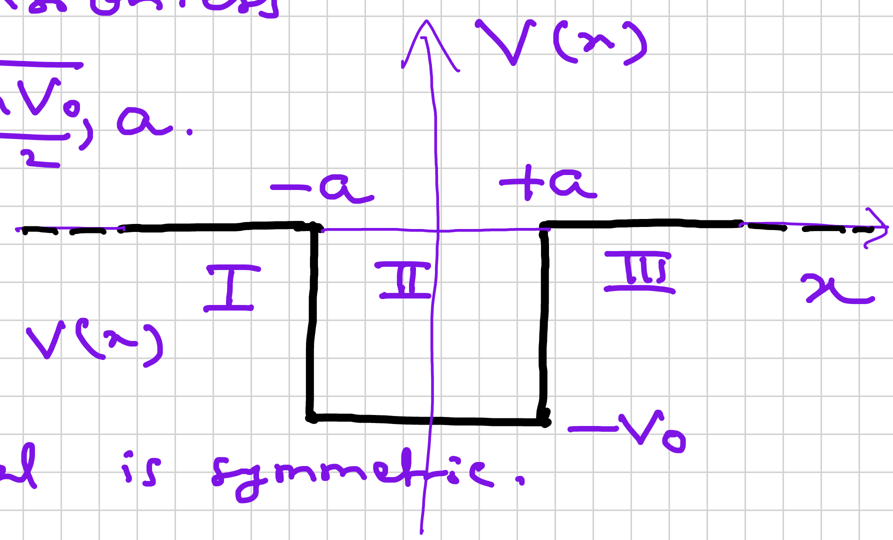
$$+ \frac{2k}{k + iK_{\circ}}\, e^{-K_{\circ}x}\,\Theta(x).$$

$$\therefore \psi(x) = \left\{\left(\cos kx - \left(\frac{K_{\circ}}{k}\right)\sin kx\right)\Theta(-x) + e^{-K_{\circ}x}\,\Theta(x)\right\}\frac{2}{\left(1 + \frac{iK_{\circ}}{k}\right)}.$$

Finite Potential Well

$$V(x) = \begin{cases} -V_0 & \forall \; x \in [-a, a] \\ 0 & \text{otherwise} \end{cases}$$

Construct a dimensionless parameter, $\alpha = \sqrt{\left(\frac{2mV_0}{\hbar^2}\right)}\, a$.



We observe, $V(-x) = V(x)$

i.e., the potential is symmetric.

$\therefore$ Parity, P is relevant operator.

$\updownarrow$

$P f(x) = f(-x)$.

Brief primer on $\hat{P}$.

Note that, $\hat{P}\psi(x) = \pm\psi(x)$

positive parity

−ve parity

$\therefore \hat{H}\hat{P}\psi(x) = \hat{P}\hat{H}\psi(x)$.

$\Rightarrow [\hat{H}, \hat{P}] = 0$.

$\therefore \psi(x)$ is a simultaneous eigenstate of $\hat{P}$ and $\hat{H}$.

Also, we must consider either positive parity solutions or, negative parity solutions (only) for all the regions I, II and III.

Bound states $(-V_0 \leq E \leq 0)$

In regions I & III,

$$\frac{d^2\psi}{dx^2} - K^2\psi = 0, \qquad K = \sqrt{\frac{-2mE}{\hbar^2}}.$$

In region II,

$$\frac{d^2\psi}{dx^2} + q^2\psi = 0, \qquad q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Positive parity solution (even symmetry)

$$\psi(x) = \begin{cases} A\cos qx & x \in [-a, a] \\ Be^{-Kx} & x > a \\ Be^{+Kx} & x < a \end{cases}$$

Negative parity solution (odd symmetry)

$$\psi(x) = \begin{cases} A\sin qx & x \in [-a, a] \\ Be^{-Kx} & x > a \\ -Be^{Kx} & x < a \end{cases}$$

Let's consider positive parity (even symmetry) solutions,

Continuity of ψ at $x = a$

$$\Rightarrow A\cos qa = Be^{-\kappa a}.$$

Continuity of ψ' at $x = a$

$$\Rightarrow -qA\sin qa = -\kappa Be^{-\kappa a}.$$

Taking ratio's,

$$\Rightarrow \boxed{\tan qa = \frac{\kappa}{q}}$$

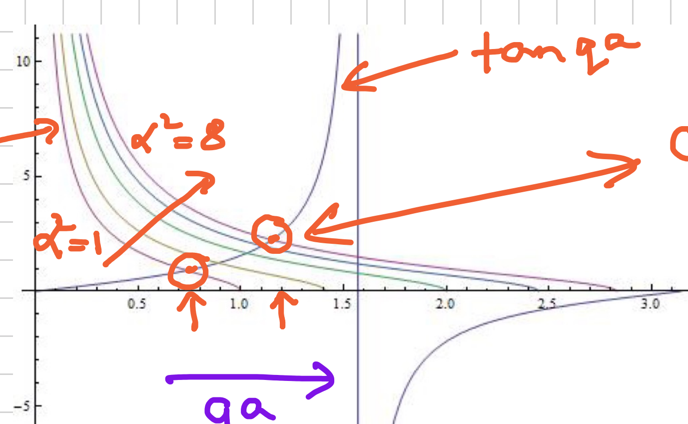
we need to express the R.H.S. in terms of qa.

we had, $q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$, $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$ and $\alpha = \sqrt{\left(\frac{2mV_0}{\hbar^2}\right)}\, a$

$$\Rightarrow \kappa a = [\alpha^2 - (qa)^2]^{1/2}.$$

$$\therefore \boxed{\tan qa = \frac{[\alpha^2 - (qa)^2]^{1/2}}{qa}}.$$

$\frac{[\alpha^2 - (qa)^2]^{1/2}}{qa}$



Condition for bound states

For a particular α (corresponding V_0 and a) there is a unique qa. Using this qa value, E can be estimated.