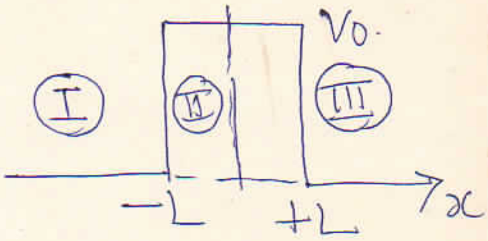
Square barrier (1/8)
Reflection and Transmission
Computational Details.

Consider a beam of particles incident on a target which may be represented by a potential

$$V(x) = \begin{cases} 0 & x < -L \\ V_0 & -L < x < L \\ 0 & x > L \end{cases}$$



For positive V_0, we call such a potential as square barrier.

Classically we expect that

$E < V_0$ the particles will get reflected.

$E > V_0$ the particles will get transmitted.

We want to solve the Schrodinger equation and obtain energy eigenfunctions. We shall write the solutions in the three regions

I : $x < -L$ II $-L < x < L$ III $x > L$

separately. The solutions are given by, <u>for $E < V_0$</u>

$$u_I(x) = Ae^{ikx} + Be^{-ikx}$$

$$u_{II}(x) = Ce^{\beta x} + De^{-\beta x} \quad , \quad \beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$u_{III}(x) = Fe^{ikx} + Ge^{-ikx} \quad ; \quad k^2 = \frac{2mE}{\hbar^2}$$

We the incident beam is coming from $-\infty$, there will be no particles travelling to the left in region III. So we set <u>$G = 0$</u>.

Impose the boundary conditions at $x=L$ that the wave function is and its derivative must be continuous. This means

$$u_{II}(L) = u_{III}(L) \quad , \quad u'_{II}(L) = u'_{III}(L)$$

or $$Ce^{\beta L} + De^{-\beta L} = Fe^{ikL} + Ge^{-ikL} \quad \text{---- ①}$$

$$\beta Ce^{\beta L} - \beta De^{-\beta L} = Fike^{ikL} - ikGe^{-ikL} \quad \text{---- ②}$$

Set $G=0$; multiply ① by ik and subtract from (2) to get

$$(\beta - ik)Ce^{\beta L} - (\beta + ik)De^{-\beta L} = 0$$

or $$\frac{D}{C} = \left(\frac{\beta - ik}{\beta + ik}\right)e^{2\beta L} \quad \text{------ ③}$$

—— x ——

Boundary conditions at $x=-L$ are

$$u_{I}(L) = u_{II}(L) \; ; \; u'_{I}(L) = u'_{II}(L) \quad \text{---- ④}$$

These equations give

$$Ce^{-\beta L} + De^{\beta L} = Ae^{-ikL} + Be^{ikL} \quad \text{---- ⑤}$$

$$C\beta e^{-\beta L} - D\beta e^{\beta L} = Aike^{-ikL} - Bike^{ikL} \quad \text{---- ⑥}$$

We will solve these equations for $\underline{\underline{B/A}}$. Multiply ⑤ by ik. and add ⑥ to get

$$C(\beta + ik)e^{-\beta L} - D(\beta - ik)e^{\beta L} = 2Aike^{-ikL} \quad ⑦$$

Next multiply ⑤ by ik and subtract from ⑥

⑥ − ik × ⑤

$$C(\beta - ik)e^{-\beta L} - D(\beta + ik)e^{\beta L} = -2ikBe^{ikL} \quad ⑧$$

Use (3) to eliminate D from ⑦. This gives

$$2Aike^{-ikL} = C(\beta+ik)e^{-\beta L} - \frac{(\beta-ik)^2}{(\beta+ik)} e^{3\beta L} C$$

$$= C \frac{(\beta+ik)^2 e^{-\beta L} - (\beta-ik)^2 e^{3\beta L}}{(\beta+ik)}$$

$$= \frac{Ce^{\beta L}}{(\beta+ik)}\left[(\beta+ik)e^{-2\beta L} - (\beta-ik)e^{2\beta L}\right]$$

$$= \frac{Ce^{\beta L}}{(\beta+ik)}\Big((\beta^2-k^2)(e^{-2\beta L}-e^{2\beta L}) + 2i\beta k(e^{-2\beta L}+e^{2\beta L})\Big)$$

$$= \frac{Ce^{\beta L}}{(\beta+ik)}\left(-2(\beta^2-k^2)\sinh 2\beta L + 4i\beta k\cosh 2\beta L\right) \quad —⑨$$

Next use (3) again, this time to eliminate D from ⑧. This gives

$$2ikBe^{ikL} = D(\beta+ik)e^{\beta L} - C(\beta-ik)e^{-\beta L}$$

$$= \left(\frac{\beta-ik}{\beta+ik}\right)C(\beta+ik)e^{3\beta L} - C(\beta-ik)e^{-\beta L}$$

$$= C(\beta-ik)e^{\beta L}(e^{2\beta L}-e^{-2\beta L})$$

$$= C(\beta-ik)e^{\beta L}\, 2\sinh 2\beta L \quad — ⑩$$

Divide ⑨ ⑩ by ⑨ to get

$$e^{2ikL}\left(\frac{B}{A}\right) = \frac{2(\beta-ik)(\beta+ik)\sinh 2\beta L}{-2(\beta^2-k^2)\sinh 2\beta L + 4i\beta k\cosh 2\beta L}$$

$$\text{or} \left(\frac{B}{A}\right) = \frac{(\beta^2+k^2)\sinh 2\beta L\, e^{-2ikL}}{(k^2-\beta^2)\sinh 2\beta L + 2i\beta k\cosh 2\beta L} \quad ⑪$$

Consider Eq (1) and 5 and solve for (C/A) and (F/C)

Eq (1) with $G=0$

$$Ce^{\beta L}+De^{-\beta L}=Fe^{ikL} \qquad (12)$$

Eq 5

$$Ce^{-\beta L}+De^{\beta L}=Ae^{-ikL}+Be^{+ikL} \qquad (13)$$

(12) gives

$$Fe^{ikL}=Ce^{\beta L}+De^{-\beta L}$$

$$=Ce^{\beta L}+\left(\frac{\beta-ik}{\beta+ik}\right)Ce^{\beta L} \qquad \text{|| use (3) and eliminate } D$$

$$F=Ce^{\beta L}\frac{2\beta}{(\beta+ik)}e^{-ikL} \qquad (14)$$

Next solve for C/A:

LHS of (13)

$$=Ce^{-\beta L}+De^{\beta L}$$

$$=Ce^{-\beta L}+C\left(\frac{\beta-ik}{\beta+ik}\right)e^{3\beta L} \qquad \text{|| use (3) and eliminate } D$$

$$=\frac{Ce^{\beta L}}{(\beta+ik)}\left((\beta+ik)e^{-2\beta L}+(\beta-ik)e^{2\beta L}\right)$$

$$=\frac{Ce^{\beta L}}{(\beta+ik)}\left(\beta\left(e^{-2\beta L}+e^{2\beta L}\right)-ik\left(e^{2\beta L}-e^{-2\beta L}\right)\right)$$

$$=\frac{Ce^{\beta L}}{(\beta+ik)}\left(2\beta\cosh 2\beta L-2ik\sinh 2\beta L\right) \qquad (15)$$

R.H.S. of (13) gives

$$Ae^{-ikL}+Be^{ikL}= \qquad \text{substitute for } B \text{ from (11)}$$

$$=Ae^{-ikL}+Ae^{-ikL}\frac{(\beta^2+k^2)\sinh 2\beta L}{(k^2-\beta^2)\sinh 2\beta L+2i\beta k\cosh 2\beta L}$$

$$= Ae^{-ikL}\left(1+\frac{(\beta^2+k^2)\sinh 2\beta L}{(k^2-\beta^2)\sinh 2\beta L+2i\beta k\cosh 2\beta L}\right)$$

$$= Ae^{-ikL}\frac{2k^2\sinh 2\beta L+2i\beta k\cosh 2\beta L}{(k^2-\beta^2)\sinh 2\beta L+2\beta ik\cosh 2\beta L} \quad (16)$$

Equating L.H.S. of (13) and RH.S of (13) using expressions (15) and (16) gives

$$\frac{Ce^{\beta L}}{(\beta+ik)}(2\beta\cosh 2\beta L-ik\sinh 2\beta L)$$

$$= Ae^{-ikL}\frac{(ik)(2\beta\cosh 2\beta L-2ik\sinh 2\beta L)}{(k^2-\beta^2)\sinh 2\beta L+2i\beta k\cosh 2\beta L}$$

$$\text{or } \frac{C}{A} = (\beta+ik)\,e^{-(\beta+ik)L}\times\frac{ik}{(k^2-\beta^2)\sinh 2\beta L+2i\beta k\cosh 2\beta L} \quad (17)$$

From (14)

$$\frac{F}{C} = e^{(\beta-ik)L}\frac{2\beta}{(\beta+ik)} \quad ---- (18)$$

multiplying (17) and (18) gives.

$$\frac{F}{A} = \frac{2i\beta k\, e^{-2ikL}}{(k^2-\beta^2)\sinh(2\beta L)+2i\beta k\cosh(2\beta L)} \quad (19)$$

Transmission coefficient is $|F/A|^2$ and we get

$$T=|F/A|^2 = \left(1+\frac{(\beta^2+k^2)^2}{2\beta^2k^2}\sinh^2 2\beta L\right)^{-1} \quad — (20)$$

Square barrier ... continued.

$E < V_0$: Very high barrier

Transmission Coefficient.

$$= \left(1 + \frac{(\beta^2 + k^2)^2}{4\beta^2 k^2} \sinh^2 2\beta L \right)^{-1}$$

$$\beta^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

$$\beta^2 + k^2 = \frac{2mV_0}{\hbar^2}$$

$$k^2 = \frac{2mE}{\hbar^2}.$$

$$2\beta^2 k^2 = \frac{8(V_0 - E)E m^2}{\hbar^4}$$

$E \ll V_0$

$$T = \left(1 + \frac{V_0^2}{\cancel{4}(V_0 - E)(E)} \frac{e^{+4\beta L}}{4} \right)^2$$

$\sinh \beta L 2$

$= \cancel{\sin} \frac{1}{2} e^{2\beta L}$.

$\cong \frac{1}{2}$

$$\cong \frac{16E(V_0 - E)}{V_0^2} e^{-4\beta L}$$

$\cancel{E \gg V_0}$ $E \simeq V_0$ $\quad \beta L \approx 0$

$\sinh 2\beta L \approx 2\beta L$

$$T = \left(1 + \frac{V_0^2}{4(V_0 - E)E} 4\beta^2 L^2 \right)^{-1}$$

$$= \left(1 + \frac{V_0}{4(V_0 - E)E} \times 4 \frac{2m(V_0 - E)}{\hbar^2} L^2 \right)^{-1}$$

$$= \left(1 + \frac{V_0^2 L^2 2m}{E\hbar^2} \right)^{-1} = \left(1 + \frac{V_0^2}{E\Delta}\right)^{-1}$$

$$\Delta = \hbar^2 / 2mL^2$$

Square barrier

$E > V_0$

$$\beta^2 = \frac{2m(V_0 - E)}{\hbar^2} = -\alpha^2$$

$$\alpha^2 = \frac{2m(E - V_0)}{\hbar^2} \qquad \beta \to i\alpha.$$

$$\sinh 2\beta L = \frac{e^{2\beta L} - e^{-2\beta L}}{2}$$

$$= \frac{e^{2i\alpha L} - e^{-2i\alpha L}}{2}$$

$$= i \sin 2\alpha L$$

$$\sinh^2 2\beta L = -\sin^2 2\alpha L$$

$$\therefore T = \left(1 + \frac{V_0^2}{4(V_0 - E)E} \times (-)\sin^2 2\alpha L\right)^{-1}$$

$$= \left(1 + \frac{V_0^2}{4(E - V_0)E} \sin^2 2\alpha L\right)^{-1}$$

maximum when $2\alpha L = n\pi$

$$\alpha^2 = \frac{2m(E - V_0)}{\hbar^2} = \frac{p^2}{\hbar^2} = \frac{4\pi^2}{\lambda^2}$$

$$\alpha = \frac{2\pi}{\lambda}$$

$$\frac{(2L)}{\lambda} = n\pi$$

$$(2L)\left(\frac{2\pi}{\lambda}\right) = n\pi$$

$$(2L) = n \cdot \left(\frac{\lambda}{2}\right).$$

Integral multiples of $n(\lambda/2)$ fit into the well range. then $T = 1$.

$E < V_0$

$$T = \left(1 + \frac{\sinh^2 \beta L}{E/V_0 \,(1 - E/V_0)}\right)^{-1}$$

When $E < V_0$ T increases monotonically with E.

$\beta L >> 1 \quad \sinh^2 \beta L \simeq \frac{1}{4} e^{\beta L} >> 1$

$$T = 16 \frac{E}{V_0}\left(1 - \frac{E}{V_0}\right) e^{-\beta L}$$

$$= 16 \left(\frac{E}{V_0}\right)\left(1 - \frac{E}{V_0}\right) e^{-4\sqrt{\frac{V_0 - E}{\Delta}}}$$

$\Delta = \frac{\hbar^2}{2mL^2}$ uncertainty energy for particle confined to length L.

$\beta L >> 1 \quad V_0 - E >> \Delta$

$E > V_0 \quad \beta \to q$

R

$$T(E) = \left(1 + \frac{\sin^2 \alpha L}{4 E/V_0 (1 - E/V_0)}\right)^{-1}$$

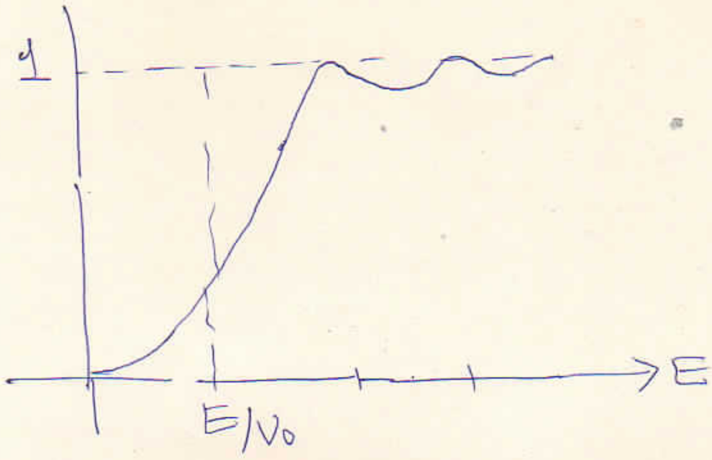
$$\alpha^2 = \frac{2m}{\hbar^2} (E - V_0) L$$

$T(E) = 1$ when $\sin \alpha L = 0$

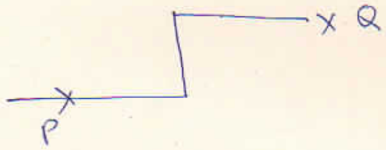
$$\alpha L = n\pi$$

$$\Rightarrow \quad \frac{2\pi}{\lambda} . L = n\pi , \quad \lambda = n . \lambda/2$$

8



Definition of transmission and reflection coefficient when potential does not go to zero at infinity.



No of particles received at a point P per sec

= N

$N e^{ikx}$

$= v_i \rho = |N|^2 v_i$

$T = \left|\frac{N_2}{N_1}\right|^2 \left(\frac{v_2}{v_1}\right)$