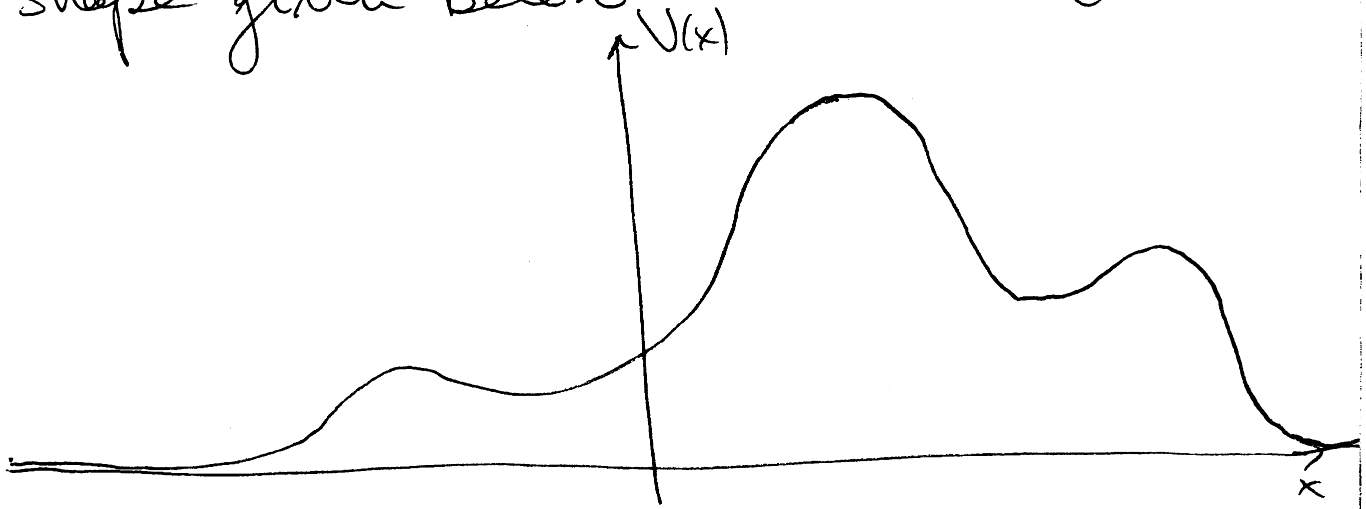
II. Applications In One-Dimension

2.1 Scattering off a Potential Step

In potential scattering we consider particle states, initially prepared in regions of space where the potential vanishes, impinging on regions of non-zero potential. The measured quantities in such an experiment are the probability that the particle is reflected from the potential or otherwise transmitted. In general the potential, in our one-dimensional case, is assumed to vanish as $x \to \pm\infty$ with a generic shape given below



The incident beam of particles is prepared in a region of zero potential, say in the region to the far left. Since the particles are not interacting with anything we prepare them in a state of well defined energy and momentum. Indeed, since $V=0$ in this region the particle's wavefunction obeys the free Schrödinger equation, hence the incident wave can be taken as a plane wave

$$\psi_{inc}(x,t) = \psi_{inc}(x) e^{-iEt/\hbar}$$

with $\psi_{inc}(x) = N e^{ikx}$ where

N is a constant. This corresponds to a wave propagating in the $+\hat{x}$ direction. Since ψ_{inc} obeys the free Schrödinger equation

$E = \frac{\hbar^2 k^2}{2m}$ is the energy of the incident particle and $p = \hbar k$ is its momentum.

As the incident beam of particles enters the region of non-zero potential, scattering will occur. Besides the incident wave function there will be superimposed on it a scattered wave function so that the sum $\psi = \psi_{inc} + \psi_{scatt}$ will obey the Schrödinger equation with appropriate boundary conditions. The scattered wave function will contain a piece due to reflection of the incident wave, $\psi_{reflection}$, back into the region to the left of the potential and a piece due to transmission, $\psi_{transmission}$, of the incident wave into the region to the right of the potential. In the laboratory we will measure the ratio of the scattered probability fluxes to the incident probability flux. Recall that the probability current in one-dimension is

$$S = \frac{\hbar}{2im}\left(\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right).$$

Thus the incident particle's probability current density is simply

$$S_{inc} = \frac{\hbar}{2im}\left(\psi^*_{inc}\frac{d\psi_{inc}}{dx} - \frac{d\psi^*_{inc}}{dx}\psi_{inc}\right)$$

with $\psi_{inc} = N e^{ikx}$ which yields

$$S_{inc} = |N|^2 \frac{\hbar k}{m}. \quad \text{As expected}$$

the incident probability current density is just the probability density $\rho = |\psi_{inc}|^2 = |N|^2$ times the free particle velocity $\frac{\hbar k}{m}$.

We can measure the probability current density that is reflected or transmitted by measuring the particle flux in the region to the left of the potential and to the right of the potential (i.e. put particle counters at $x = \pm\infty$), That is we can measure the reflection coefficient

$$R = \left| \frac{S_{\text{reflection}}}{S_{\text{incident}}} \right|$$

and transmission coefficient

$$T = \left| \frac{S_{\text{transmission}}}{S_{\text{incident}}} \right| ,$$

where

$$S_{\text{reflec.}} = \frac{\hbar}{2im}\left(\psi^*_{\text{reflec}} \frac{d\psi_{\text{reflec}}}{dx} - \frac{d\psi^*_{\text{reflec}}}{dx}\psi_{\text{reflec}} \right),$$

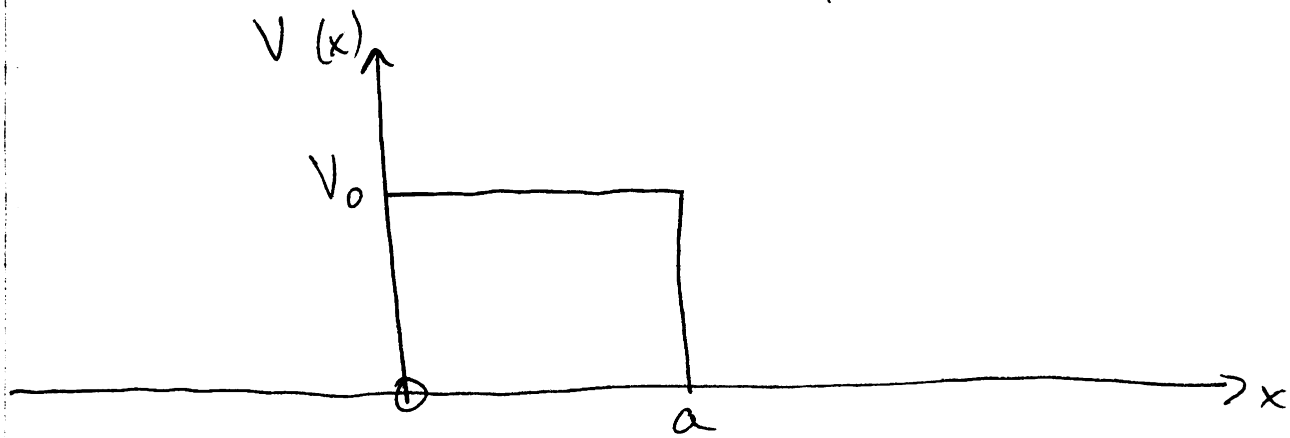
$$S_{\text{trans.}} = \frac{\hbar}{2im}\left(\psi^*_{\text{trans}} \frac{d\psi_{\text{trans}}}{dx} - \frac{d\psi^*_{\text{trans}}}{dx}\psi_{\text{trans}} \right)$$

are the reflected and transmitted wavefunction probability current densities respectively.

As an example of one-dimensional scattering consider the scattering of a particle of mass m and energy E

off the potential (step) barrier

$$V(x) = \begin{cases} 0 & , x<0 \\ V_0>0 & , 0\le x\le a \\ 0 & , x>a \end{cases} .$$



The time independent Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad , \text{for } \begin{matrix} x<0 \\ x>a \end{matrix}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi \quad , \text{for } 0\le x\le a .$$

We have two cases depending on whether the incident particle's energy $E > V_0$ or $E < V_0$.

Case 1) $E > V_0$: Define

$$k = \sqrt{\frac{2mE}{\hbar^2}} > 0 \quad \left(\text{i.e. } E = \frac{\hbar^2 k^2}{2m}\right),$$

$$q = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} > 0,$$

so that the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi + k^2\psi = 0 \quad , \text{for } x<0 \;\&\; x>a$$

$$\frac{d^2\psi}{dx^2} + q^2\psi = 0 \quad , \text{for } 0 \le x \le a$$

The solution to these equations in the 3 regions is

$$\psi(x) = N \begin{cases} e^{ikx} + r\, e^{-ikx} & , \text{for } x<0 \\ A e^{iqx} + B e^{-iqx} & , \text{for } 0 \le x \le a \\ t\, e^{ikx} + C e^{-ikx} & , \text{for } x>a \end{cases}$$

Since e^{ikx} corresponds to a wave travelling in the $+\hat{x}$ direction and e^{-ikx} to a wave travelling in the $-\hat{x}$ direction, we interpret

The incident particle's wavefunction as

$$\psi_{inc}(x) = N e^{ikx}$$

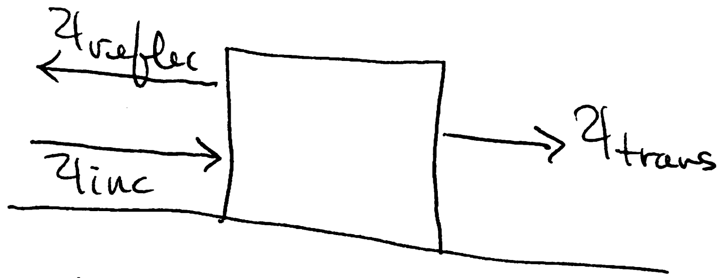
where we take the incident particle to come in from the $x \to -\infty$ direction. The reflected wavefunction would then correspond to $\psi - \psi_{inc}$ on the left side of the potential, that is

$$\psi_{reflec} = N r e^{-ikx},$$

travelling back to $x \to -\infty$. Likewise any wave transmitted through the potential will be travelling to the right on the right of the potential. That is the transmitted wavefunction is identified with

$$\psi_{trans.} = N t e^{ikx}.$$

Since we prepared the initial particle to be incident from the left there should be no wave travelling to the left on the right side of the potential. Thus we impose the boundary condition $C = 0$ corresponding to the physical preparation of our experiment. Thus we have the schematic



Thus to determine A, B, r, t (and C) we apply our boundary conditions

$$C=0$$

1) at $x=0$

$$\psi(x=0^-)=\psi(x=0^+) \Rightarrow 1+r=A+B$$

$$\frac{d}{dx}\psi(x=0^-)=\frac{d}{dx}\psi(x=0^+) \Rightarrow k(1-r)=q(A-B)$$

That is

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left(1+\tfrac{k}{q}\right)+\tfrac{r}{2}\left(1-\tfrac{k}{q}\right) \\ B &= \tfrac{1}{2}\left(1-\tfrac{k}{q}\right)+\tfrac{r}{2}\left(1+\tfrac{k}{q}\right) \end{aligned}}$$

2) at $x=a$

$$\psi(x=a^-)=\psi(x=a^+) \Rightarrow Ae^{iqa}+Be^{-iqa}=te^{ika}$$

$$\frac{d}{dx}\psi(x=a^-) = \frac{d}{dx}\psi(x=a^+)$$

$$\Rightarrow q\left(Ae^{iqa} - Be^{-iqa}\right) = kte^{ika}$$

That is

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left(1+\tfrac{k}{q}\right)te^{i(k-q)a} \\ B &= \tfrac{1}{2}\left(1-\tfrac{k}{q}\right)te^{i(k+q)a} \end{aligned}}$$

Eliminating A, B from these 2 sets of equations yields the r & t coefficients

$$r = \frac{i(q^2-k^2)\sin qa}{2kq\cos qa - i(q^2+k^2)\sin qa}$$

$$t = \frac{2kq\, e^{-ika}}{2kq\cos qa - i(q^2+k^2)\sin qa}.$$

Recalling our discussion of the ψ_{inc}, $\psi_{reflec.}$, $\psi_{trans.}$ wavefunctions and the expression for the probability current density for a plane wave we find

The reflection coefficient

$$R = \left|\frac{S_{refl.}}{S_{inc.}}\right| = |r|^2 = \frac{(q^2-k^2)^2 \sin^2 qa}{4k^2q^2 + (q^2-k^2)^2 \sin^2 qa}$$

and the transmission coefficient

$$T = \left|\frac{S_{trans.}}{S_{inc.}}\right| = |t|^2 = \frac{4k^2q^2}{4k^2q^2 + (q^2-k^2)^2 \sin^2 qa}.$$

Remarks: 1) R and T are independent of N, the normalization of the incident plane wave.

2) $R + T = 1$.

3) Using our original definitions for

$$k^2 \equiv \frac{2mE}{\hbar^2}, \quad q^2 \equiv \frac{2m(E-V_0)}{\hbar^2}$$

The reflection and transmission coefficients become

$$R = \frac{V_0^2 \sin^2\left(\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, a\right)}{4E(E-V_0) + V_0^2 \sin^2\left(\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, a\right)}$$

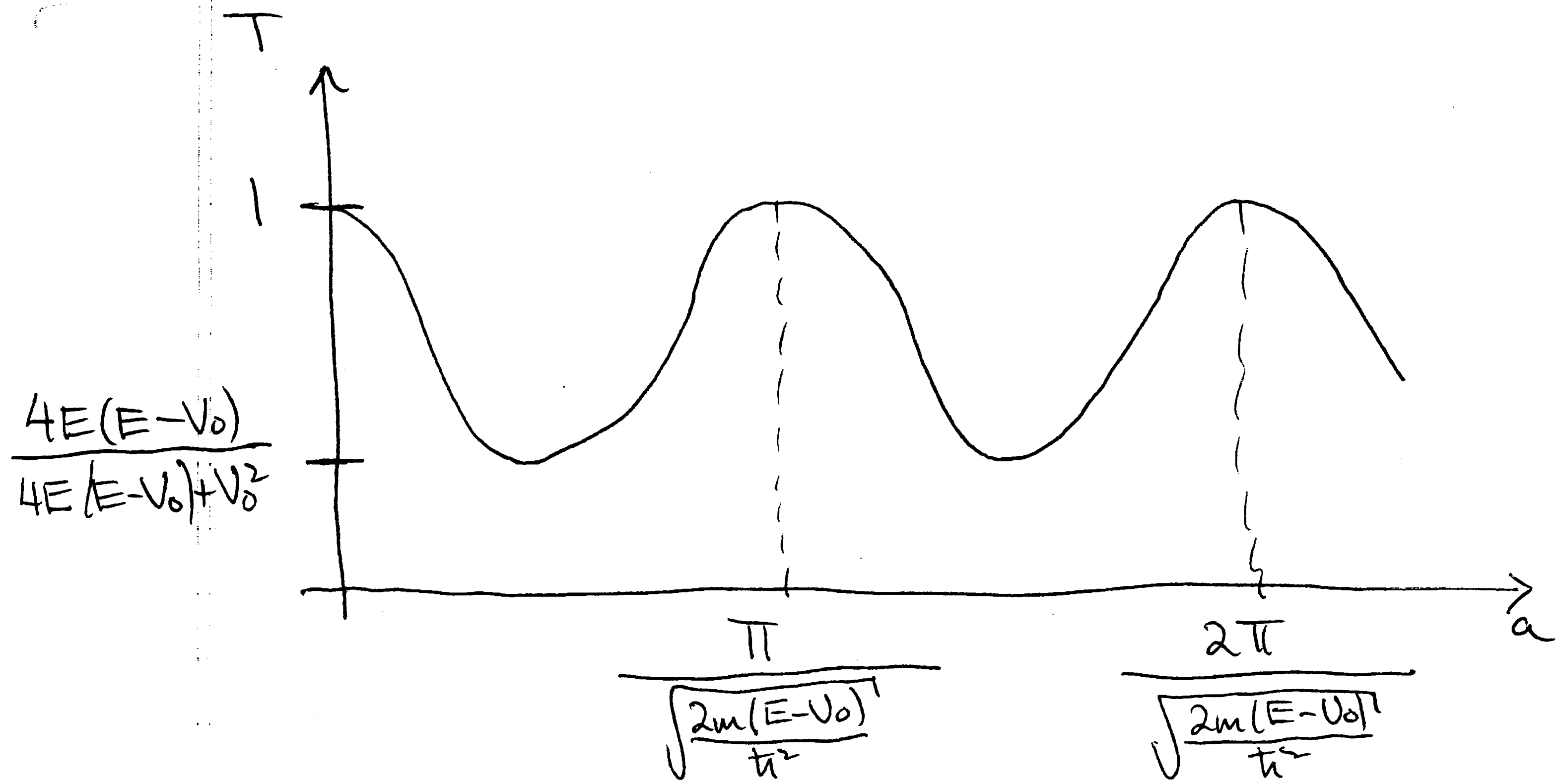
$$T = \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2 \sin^2\left(\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, a\right)}.$$

Plotting T as a function of a, its maxima occur at $\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, a = n\pi$, $n = 0, 1, 2, \ldots$, at which $T = 1$ and, hence, $R = 0$

The minima of T occur at $\sqrt{\frac{2m(E-V_0)}{\hbar^2}}\, a = \left(n+\frac{1}{2}\right)\pi$, $n = 0, 1, 2, \ldots$, where

$$T = \frac{4E(E-V_0)}{4E(E-V_0) + V_0^2}$$ and hence

$$R = \frac{V_0^2}{4E(E-V_0) + V_0^2}.$$



At the series of peaks for $T=1$, the particle is said to undergo resonance scattering.

Case 2) $V_0 > E > 0$, Barrier Penetration (Tunnelling)

For this case we define

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}} > 0 \quad \text{still, but now}$$

$$\kappa \equiv \sqrt{\frac{2m(V_0-E)}{\hbar^2}} > 0.$$

With these the Schrödinger equation becomes

$$\frac{d^2}{dx^2}\psi + k^2\psi = 0 \quad , \text{ for } x<0,\ x>a$$

$$\frac{d^2}{dx^2}\psi - \kappa^2\psi = 0 \quad , \text{ for } 0 \le x \le a .$$

As previously we can find the solutions using the boundary conditions on ψ and $\frac{d}{dx}\psi$. Equivalently we note that the previous (case 1 problem) is converted into this case 2 by the replacement $q \to -i\kappa$. Using the fact that

$$\sin qa \to \sin(-i\kappa a) = -i \sinh \kappa a$$

we have $\sin^2 qa \to -\sinh^2 \kappa a$
and $q^2 \to -\kappa^2$. Thus the transmission coefficient in case 2 is

$$T = \frac{4k^2\kappa^2}{4k^2\kappa^2 + (\kappa^2+k^2)^2 \sinh^2(\kappa a)}$$

$$= \frac{4E(V_0-E)}{4E(V_0-E) + V_0^2 \sinh^2\left(\sqrt{\frac{2m(V_0-E)}{\hbar^2}}\, a\right)}$$

while the reflection coefficient is $R = 1 - T$.
Note that for $\kappa a = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}\, a \gg 1$,
the transmission coefficient becomes

$$T \approx \frac{16E(V_0 - E)}{V_0^2}\, e^{-2\sqrt{\frac{2m(V_0-E)}{\hbar^2}}\, a}.$$

<u>Comments</u>: We see that quantum mechanically $T \neq 0$, there is a nonzero probability that the particle appears to the right of the barrier $x > a$ even when its energy $E < V_0$. The particle is said to have penetrated the barrier or tunnelled through the barrier. Of course classically the particle would never appear in the region $x > a$ when its energy $E < V_0$. There are many examples of this tunnelling phenomenon in nature; they <u>include</u> the tunnel diode, the Josephson effect, the α-decay of nuclei.

It is instructive to determine the value of T for two different types of particles. First consider incident electrons $\quad \frac{1}{\kappa} = \frac{\hbar}{\sqrt{2m(V_0-E)}} = \frac{1.96\,\text{Å}}{\sqrt{V_0-E}}$

with V_0, E in eV. Typical atomic physics values for V_0, E are $E = 1\,eV$, $V_0 = 2\,eV$, which gives

$\frac{1}{\kappa} = 1.96\,\text{Å}$, which combined with $a = 1\,\text{Å}$ implies $\kappa a = \frac{1}{1.96}$.

Plugging these numbers into T yields $T = 0.78$, quite a large probability that the e^- tunnel through the barrier.

On the other hand for incident protons the value of T is much smaller since

$\frac{m_{e^-}}{m_p} \simeq \frac{1}{1836}$ and hence

$$\frac{1}{\kappa} = \frac{1.96}{\sqrt{1836}\sqrt{V_0-E}}\,\text{Å} = \frac{4.6\times10^{-2}\,\text{Å}}{\sqrt{V_0-E}},$$

with V_0, E in eV. For the above values for E, V_0, a this gives $\kappa a = \frac{\sqrt{1836}}{1.96} \gg 1$,

and

$$T \simeq 4\times10^{-19}, \text{ quite negligible.}$$