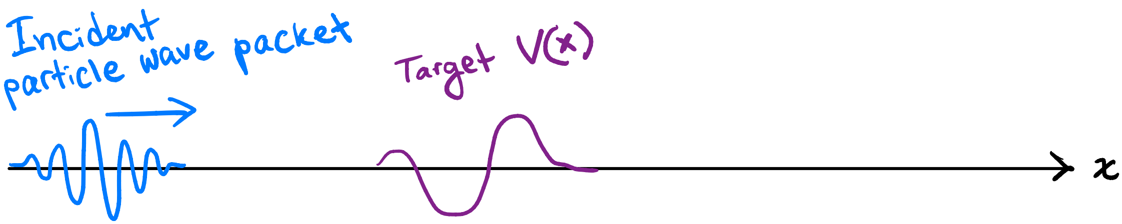
Discussion 10: Scattering in 1D

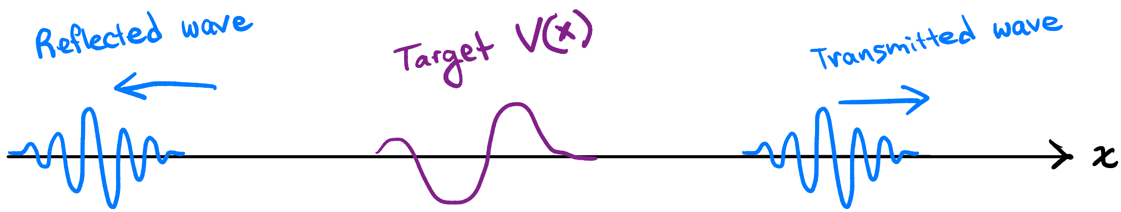
The "harmonic oscillator" and the "infinite square well" are examples of situations where the particle is bound: that is, confined within some region of space.

Today we consider how to handle the situation where the particle is free to roam anywhere. In a laboratory, this most commonly occurs in a scattering expiriment, where a particle is fired at a target, interacts with the target somehow, and then bounces off.

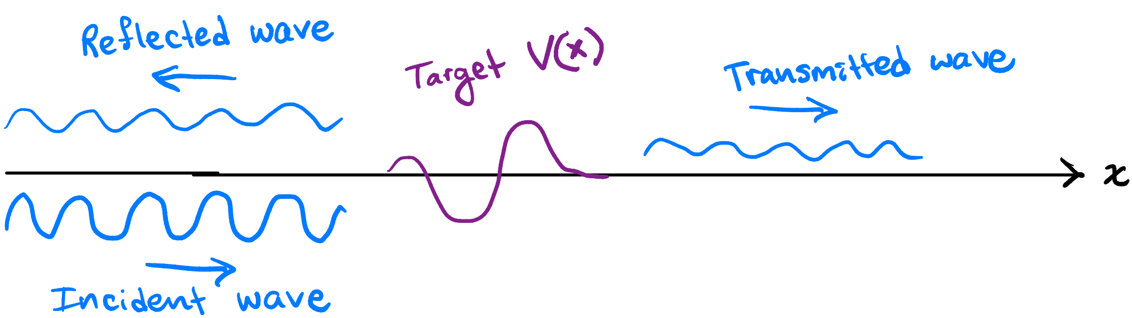
In this case, the particle is allowed to have any energy - the energy is not quantized. Rather, you pick the energy by picking the initial speed of the particle.

The quantity of interest then becomes the final velocity of the particle. In one dimension, there are only two options: either the particle is reflected by the target, or it is transmitted by the target. The particle cannot be 'absorbed' by the target so long as the target is described by a conservative force.





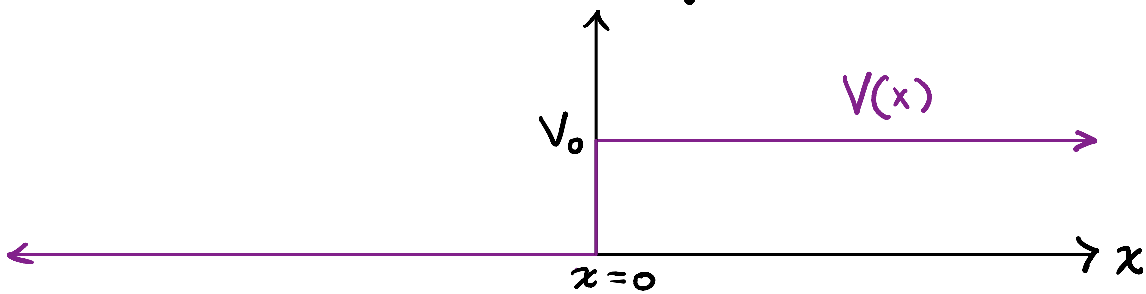
In a realistic scenario, the incoming particle is described by a wave packet, which is a linear combination of many energy eigenstates, and which is somewhat localized in space. However, because time evolution is linear, we can get away with approaching this problem in a slightly less realistic way, where the particle is in an energy eigenstate.



The question is now: how do we determine the probability that the particle is reflected vs. transmitted? This is best addressed by example.

Example: One Small Step (for a particle)

Consider the potential energy step:



Explicitly:

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

We will proceed by finding the <u>energy eigenstates</u> $\psi_E(x)$ such that:

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

These are of course just the solutions to the time-independent Schrodinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi_E(x) = E\,\psi_E(x)$$

We solve it piece-wise now.

* To the left of the barrier the TISE reads:

$$-\frac{\hbar^2}{2m}\psi_E''(x) = E\psi_E(x)$$

This is just the free particle equation. The most general solution is:

$$\psi_E(x) = \underbrace{Ae^{ikx}}_{\text{Incident wave}} + \underbrace{Be^{-ikx}}_{\text{Reflected wave}} \qquad (x<0)$$

where for convenience we define

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$

* To the right of the barrier, the TISE reads

$$-\frac{\hbar^2}{2m}\psi_E''(x) + V_0\psi_E(x) = E\psi_E(x)$$

$$\psi_E''(x) = \frac{2m}{\hbar^2}(V_0 - E)\psi_E(x)$$

This is basically the same equation as before, but now there are two cases, depending on the sign of $V_0 - E$.

<u>Case 1</u> $E > V_0$

The particle's energy is greater than the potential step V_0. Then ⟶

the solutions are oscillatory, with the most general solution being:

Transmitted wave

$$\psi_E(x) = C e^{ik'x} + D e^{-ik'x} \qquad (x > 0)$$

Left-moving wave

where

$$k' \equiv \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

We cannot generate left-moving particles in the region $x > 0$, supposing we start out by launching particle in from the left. So, we demand that

$$D = 0$$

on physical grounds.

* Now we finish things off by stitching the two solutions together at $x = 0$, using the following two requirements:

$$\begin{cases} (1)\ \psi_E(x) \text{ is continuous at } x = 0. \\ (2)\ \psi_E'(x) \text{ is continuous at } x = 0. \end{cases}$$

Both are required for the Schrodinger equation to be satisfied.

Write our general solution:

$$\psi_E(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik'x} & x > 0 \end{cases}$$

Continuity implies that:

$$A + B = C \qquad (1)$$

Continuity of $\psi_E'(x)$ implies that

$$Aik - Bik = Cik' \qquad (2)$$

Combining these equations gives:

$$k(A-B) = k'(A+B)$$

Solve for B:

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

and now solve for C:

$$C = A + B = \left(\frac{k+k'}{k+k'}\right)A + \left(\frac{k-k'}{k+k'}\right)A = \frac{2k}{k+k'} A$$

$$\hookrightarrow \quad C = \frac{2k}{k+k'} A$$

Therefore, our solution to the TISE (assuming $E > V_0$) is:

$$\boxed{\psi_E(x) = A \begin{cases} e^{ikx} + \left(\frac{k-k'}{k+k'}\right) e^{-ikx} & (x<0) \\ \frac{2k}{k+k'} e^{ik'x} & (x>0) \end{cases}}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \qquad k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}.$$

Note that the remaining factor of A is just a normalization constant, so it cannot be solved for. This wavefunction is not normalizable.

Similarly, the energy E is unconstrained. It can take any value $E > V_0$. It is not quantized, but rather just determined by the initial speed it is launched at.

Transmission and reflection probabilities

The question remains: how do we determine the probabilities of reflection and transmission from knowing the wave function?

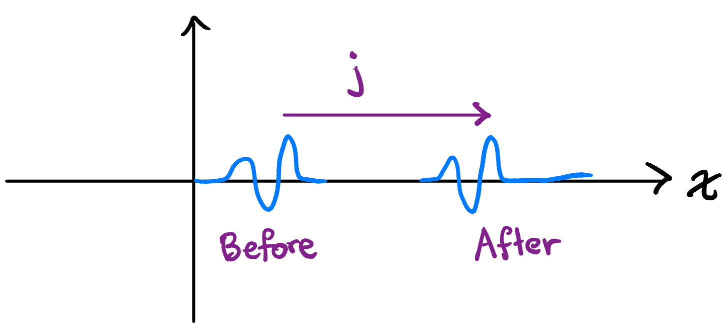
This is properly answered by using the probability current:

$$j \equiv \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

This quanitity (which is in the homework) gives the rate of flow of probability past the point x. In particular,

$$\frac{d}{dt}\int_a^b dx\, |\psi(x,t)|^2 = -j(b,t) + j(a,t)$$

which just says that the probability density $|\psi(x,t)|^2$ is like a conserved fluid: Any change in the probability at one location must be due to a flow into or out of that location



Let's evaluate j for our wavefunction. For $x<0$, we have:

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

$$= \frac{\hbar}{2mi}\Big(\left(A^* e^{-ikx} + B^* e^{ikx}\right)\left(ikA e^{ikx} - ikB e^{-ikx}\right)$$

$$- \left(A e^{ikx} + B e^{-ikx}\right)\left(-ikA^* e^{-ikx} + ikB^* e^{ikx}\right)\Big)$$

$$= \frac{\hbar}{2mi}\Big(ik|A|^2 - \cancel{ikA^*B e^{-2ikx}} + \cancel{ikAB^* e^{2ikx}} - ik|B|^2$$

$$+ ik|A|^2 + \cancel{ikA^*B e^{-2ikx}} - \cancel{ikAB^* e^{2ikx}} - ik|B|^2 \Big)$$

$$\boxed{j = \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right) \qquad (x<0)}$$

and similarly

$$\boxed{j = \frac{\hbar k'}{m}|C|^2 \qquad (x>0)}$$

We intepret these as:

$$j_{inc} = \frac{\hbar k}{m}|A|^2$$ incident probability current.

$$j_{refl} = -\frac{\hbar k}{m}|B|^2$$ reflected probability current.

$$j_{trans} = \frac{\hbar k'}{m}|C|^2$$ transmitted probability current.

Then the probability of reflection is:

$$R = \left| \frac{j_{refl}}{j_{inc}} \right| = \frac{|B|^2}{|A|^2} = \boxed{\left(\frac{k - k'}{k + k'} \right)^2}$$

The probability of transmission is

$$T = \left| \frac{j_{trans}}{j_{inc}} \right| = \frac{k'}{k} \frac{|C|^2}{|A|^2} = \boxed{\frac{4kk'}{(k + k')^2}}$$

Note that

$$R + T = 1$$

as it must for probability to be conserved.