Weds 6.1, 6.2

Particles at step and barrier potentials

So far we have applied quantum theory to completely free particles and also bound particles. We now consider situations where particles encounter steps or barriers. These will demonstrate unusual properties of quantum theory that are absent in classical physics. We can illustrate the classical via a cart sliding along a track.

First consider a step. Here there are two possibilities

~~ead~~ earlier | later

moves freely with slower speed

later definitely returns with certainty moves freely

never enters this region

OR

earlier | later

moves freely with a faster speed

never returns to this region

definitely enters this region, moves freely

Second consider <u>a barrier</u>

earlier

moves freely with slower speed

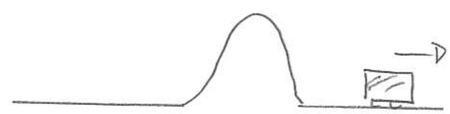
later

later definitely returns with certainty

never enters this region

OR

moves freely with higher speed



never returns.

later moves freely

definitely enters this region

We shall analyse these situations in quantum theory and see that the "never", "definitely" and "certainty" terms no longer apply.

The procedure will be to:

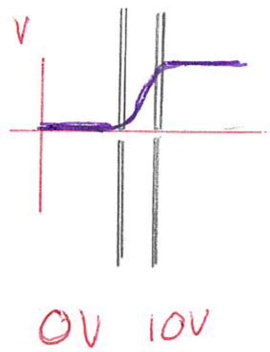
1) provide a potential that describes the step / barrier

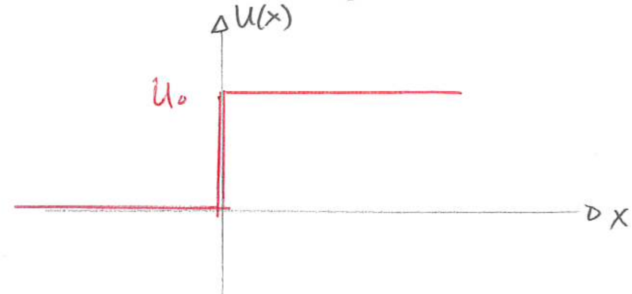
2) solve the TISE for the potential

3) interpret the solutions in terms of "transmission" and "reflection."

The barrier potential particularly has many technical and fundamental applications.

We could imagine creating such potentials with various electrodes that are charged. For example a step potential might involve. Mathematically this may be describe in terms of potentials that are piecewise constant with sudden jumps.





Free particle solutions

In classical physics in any region where the potential is constant the particle is free and moves with constant momentum. In one dimension this can either be left or right. This is described by the sign of the momentum.

In quantum theory the simplest such case occurs when $U(x) = 0$. Then the TISE gives

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi(x)$$

The possible solutions to this are

$$\psi(x) = Ae^{ikx} \quad \text{OR} \quad \psi(x) = Ae^{-ikx}$$

where we require $k \geq 0$

Quiz 1 → Type - partials

Substitution gives

$$-\frac{\hbar^2}{2m}(\pm ik)^2 = E \Rightarrow \frac{\hbar^2 k^2}{2m} = E \Rightarrow k = \sqrt{\frac{2mE}{\hbar^2}}$$

But $E = \frac{p^2}{2m} \Rightarrow p^2 = \hbar^2 k^2 \Rightarrow |p| = \hbar k$

We need to resolve the sign of the momentum. We will have to stipulate how this is implemented. By convention we will always operate with $k \geqslant 0$.

Consider the momentum operator acting on each. Thus

$$\hat{p}\psi = -i\hbar \frac{\partial \psi}{\partial x}$$

If $\psi = Ae^{ikx}$ then this gives

$$\hat{p}\psi = -i\hbar(ik)\psi = \hbar k\psi \longrightarrow$$ suggests momentum is positive $\hbar k$

If $\psi = Ae^{-ikx}$ then this gives

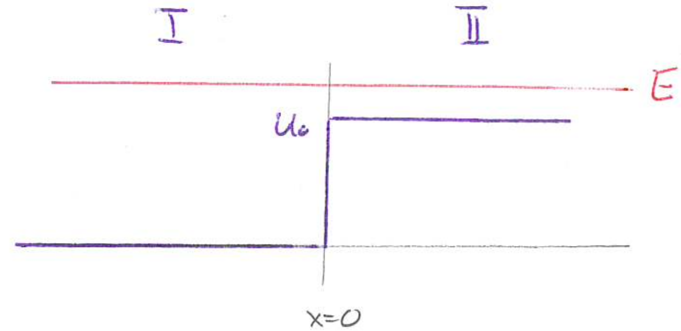
$$\hat{p}\psi = -i\hbar(-ik)\psi = -\hbar k\psi \rightarrow$$ suggests momentum is negative: $-\hbar k$.

Thus

Free particles with energy E are described by (here $k=\sqrt{\frac{2mE}{\hbar^2}}$)	
$\psi(x) = Ae^{ikx}$	$\psi(x) = Ae^{-ikx}$
momentum $p = \hbar k$	momentum $p = -\hbar k$
travels right	travels left

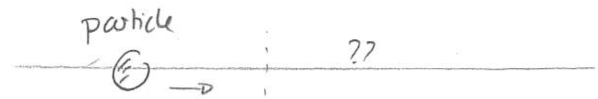
Quantum theory for a step potential (energy greater than step)

A step potential has the form



$$U(x) = \begin{cases} 0 & x<0 \\ U_0 & x>0 \end{cases}$$

We consider the situation where the total energy $E > U_0$. We assume that the particle is



incident from the left. In classical physics we expect that it will definitely move right beyond the step but with reduced momentum.

In quantum theory we solve the TISE in each region:

Region I $(x<0)$ $$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} = E\psi_I$$

Region II $(x>0)$ $$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + U_0\psi_{II} = E\psi_{II}$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = (E-U_0)\psi_{II}$$

We will also require that, at the boundary

1) $\Psi_I(0) = \Psi_{II}(0)$ (wavefunctions match)

2) $\left.\frac{d\psi_I}{dx}\right|_0 = \left.\frac{d\psi_{II}}{dx}\right|_0$ (slopes match)

Then the generic solutions are:

Region I	Region II
$\Psi_I = \underbrace{Ae^{ikx}}_{\text{moves right}} + \underbrace{Be^{-ikx}}_{\text{moves left}}$	$\Psi_{II} = \underbrace{Ce^{ik'x}}_{\text{moves right}} + \underbrace{De^{-ik'x}}_{\text{moves left}}$
(incident) (reflected)	transmitted (inc. left)
$k = \sqrt{\frac{2mE}{\hbar^2}}$	$k' = \sqrt{\frac{2m(E-U_0)}{\hbar^2}}$

We assume that particles are incident from the left. Thus $D=0$. So

$$\Psi_I = Ae^{ikx} + Be^{-ikx} \qquad k = \sqrt{2mE/\hbar^2}$$

$$\Psi_{II} = Ce^{+ik'x} \qquad k' = \sqrt{2m(E-U_0)/\hbar^2}$$

Now we match at the boundary.

Quiz 2 → change $-ik'$ to ik'

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

Linear algebra gives:

$$\boxed{B = \frac{k-k'}{k+k'} A \qquad C = \frac{2k}{k+k'} A}$$

→ some particles will be reflected back

→ some particles (not all) will be transmitted.