POTENTIAL STEPS & BARRIERS

One very efficient way of obtaining information about <u>microobjects</u> is by <u>bombarding</u> them with other particles and checking how the bombarded objects and the "projectiles" behave.

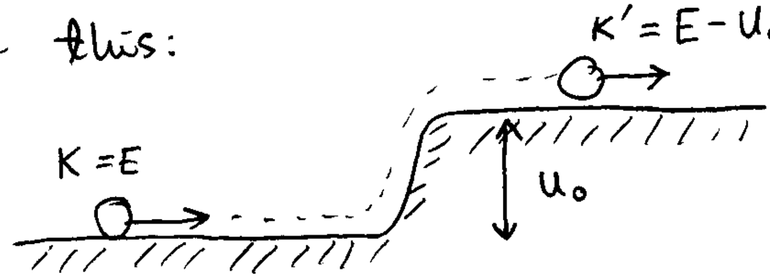
The topic "potential steps and barriers" is an introduction to the "bombarding theory", more appropriately termed as "<u>the scattering theory</u>".

The "real" scattering theory, of course, deals with 3-dimensional situations.

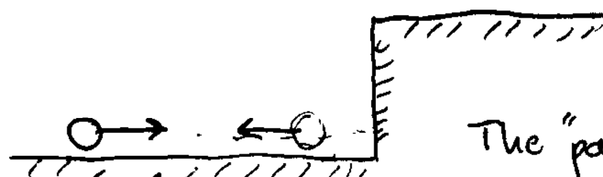
In this course, we talk only about some 1-D examples – but you will get familiar with some basic notions and concepts of the scattering theory.

First example: a potential step, $E > U_0$

In classical mechanics, it would be something like this:

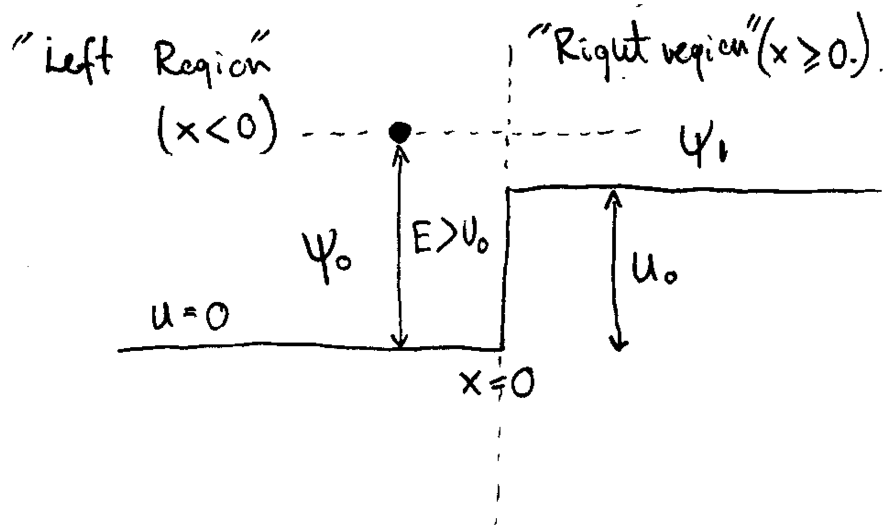


Or, if the step is "sharp":



The "particle" would be bounced back with the same kinetic energy.

In the microworld, of course, there are no real "walls". We will not specify what causes the sudden change of the potential energy – let's just consider an idealized situation that a particle approaches from a region where the potential energy is zero, and at $x = 0$ it sharply changes to $U_0 > 0$:



The Schrödinger Eq. in the "left region":

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_0}{dx^2} = E\psi$$

and in the "right" one $(x \geq 0)$ it is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} + U_0\psi = E\psi$$

Or, we can write:

"Left region": $\dfrac{d^2\psi_0}{dx^2} = -k_0^2\,\psi_0$ with $k_0 = \sqrt{\dfrac{2mE}{\hbar^2}}$

"Right region": $\dfrac{d^2\psi_1}{dx^2} = -k_1^2\,\psi_1$ with $k_1 = \sqrt{\dfrac{2m(E-U_0)}{\hbar^2}}$

Both equations have the same mathematical form that we know from the free-particle problem.

Hence —
We can seek solutions of the same form as in that problem:

$$\psi_0 = A\sin(k_0 x) + B\cos(k_0 x) \qquad (x<0)$$

and

$$\psi_1 = C\sin(k_1 x) + D\cos(k_1 x) \qquad (x \geq 0)$$

which are simple waves...

BUT!!! WAIT A MOMENT!!!

We are talking about a particle encountering a potential step.
And only a few days ago Dr. Tom told in class that a simple wave is not a good physical description of a particle.

Rather, A realistic description of a particle is a packet constructed by adding ("superposing") many simple waves with a Gaussian distribution of amplitudes — isn't that what Dr Tom said?

So, shouldn't we rather seek solutions in the form of wave packets?

WELL – in a fully rigorous approach this is indeed what ought to be done.

But... the truth is that in most situations the wave packets describing particles are constructed from waves whose wevenumbers k belong to a <u>narrow</u> Δk <u>range</u>.

So, in order to find out what happens to the particle considered, it is sufficient to consider only the "mean", or the "central" k value of the packet.

Therefore, using a solution in the form of a <u>simple wave</u> is O.K. for reaching some conclusions.
(valuable)

Well, to proceed with the solution procedure, it is convenient to switch from the "sine & cosine" convention to the <u>complex exponential function</u> convention, based on the known Euler equation: $e^{i\varphi} = \cos\varphi + i\sin\varphi$

It is easy to check that the solution of the Schr. Equations for the two regions can also be written as:

$$\psi_0(x) = A' e^{ik_0 x} + B' e^{-ik_0 x} \qquad (x<0)$$

and

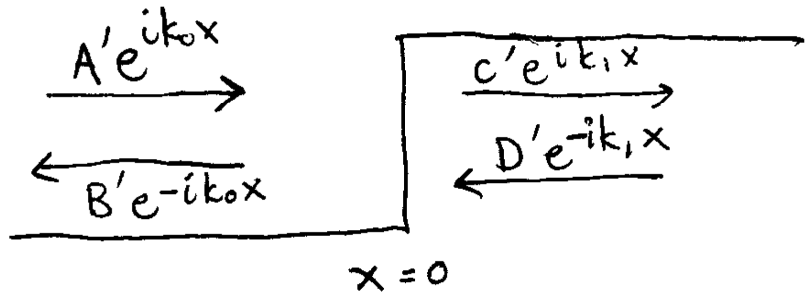
$$\psi_1(x) = C' e^{ik_1 x} + D' e^{-ik_1 x} \qquad (x \geqslant 0)$$

The solutions in this form have the advantage that each term has a clear meaning:

$A' e^{ik_0 x}$ and $C' e^{ik_1 x}$ are waves with a <u>positive</u> wavenumber – they represent waves propagating from <u>left</u> to <u>right</u>.

$B' e^{-ik_0 x}$ and $D' e^{-ik_1 x}$ are waves propagating from <u>right</u> to <u>left</u>

Which can be schematically presented as:



$A'e^{ik_0x}$ can be clearly identified as the wavefunction representing the <u>incident particle</u>.

What happens if the incident particle encounters the potential step? Well, it may either be "backreflected" or become "transmitted" to the high-potential region.

So, $B'e^{-ik_0x}$ represent the <u>backreflected wave</u>

$C'e^{ik_1x}$ " " <u>transmitted wave</u>

But what is $D'e^{-ik_1x}$?

It represent a wave coming <u>from the right</u>!

But there is no such a wave !!!
So, the term $D'e^{-ik_1x}$ <u>has no physical meaning</u> and we have to put $\underline{D'=0}$.

Then, our solutions reduce to:

$$\psi_0(x) = A'e^{ik_0x} + B'e^{-ik_0x} \qquad (x<0)$$
$$\psi_1(x) = C'e^{ik_1x} \qquad (x \geq 0)$$

What next? We have to use the continuity conditions for the function, and its first derivative, at $x=0$:

$$\begin{cases} \psi_0(x=0) = \psi_1(x=0) \\ \psi_0'(x=0) = \psi_1'(x=0) \end{cases}$$

By carrying out calculations that are tedious, but rather straightforward, from the above conditions one can obtain the values of the B'/A' and C'/A' ratios.

Note that $|A'|^2$, $|B'|^2$ and $|C'|^2$ have the physical meaning of <u>probabilities</u> of finding the particles

$|B'|^2$ represent the probability of finding the particle being "bounced back";
$|C'|^2$ represent the probability of finding the particle moving to the right in the $x>0$ region.

So:

$$R = \frac{|B'|^2}{|A'|^2} \text{ is the "backreflection coefficient"}$$

$$T = \frac{|C'|^2}{|A'|^2} \text{ is the "transmission coefficient"}$$

With increasing U_0, R increases, and T decreases. Finally when $U_0 = E$, $T=0$ – there is no more transmission, the particle can only be reflected back.