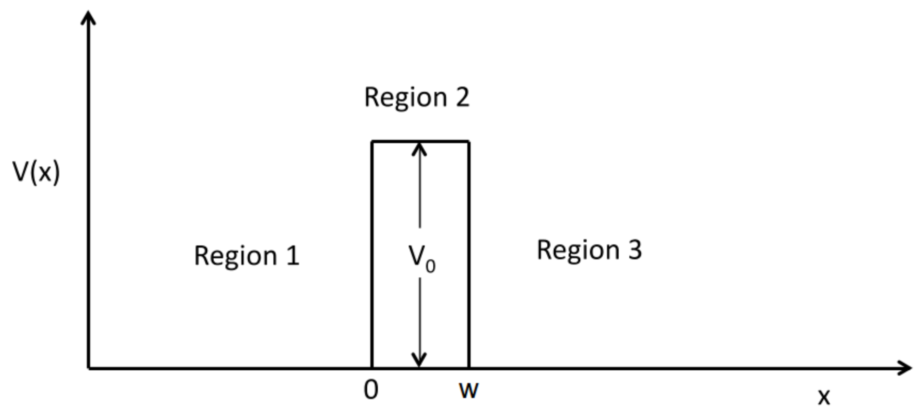
Quantum-mechanical tunneling

One of the fun features of quantum mechanics is that a particle can be found on the other side of a potential barrier even if it does not have enough energy to get over the barrier (see figure below). This is called *quantum-mechanical tunneling*, and is important in high resolution microscopy, chemical kinetics, flash memory, protein mechanisms, and many other fields. In this typical problem we will arrive at the probability of finding the particle on the other side of the barrier.



V(x) = 0	x<0	(Region 1)
V(x) = V_0	0<x<w	(Region 2)
V(x) = 0	w <x	(Region 3)

(a) We will find the wavefunction for the entire problem by finding a solution for each of the three regions and then "stitching" them together. Write down the time independent Schrödinger equation (TISE) for each of the three regions. Note that the energy of the particle is less than V_0 ($E < V_0$).

(b) Using your answers from (a), show that the following guesses are solutions to the TISE for their corresponding regions.

$$\Psi_1(x) = A\, e^{ik_1x} + Be^{-ik_1x} \text{ (region 1)}$$
$$\Psi_2(x) = C\, e^{k_2x} + De^{-k_2x} \text{ (region 2)}$$
$$\Psi_3(x) = F\, e^{ik_1x} + Ge^{-ik_1x} \text{ (region 3)}$$

To show this, you will have to find what k_1 and k_2 are in terms of m, E, and V_0.

(c) Now that we have wavefunctions each region, we have to combine them into one wavefunction which works for the whole problem. We do this by invoking two rules of quantum mechanics:

- Ψ must be continuous, i.e., $\Psi_1(0) = \Psi_2(0)$ and $\Psi_2(a) = \Psi_3(a)$
- $d\Psi/dx$ also must be continuous from region to region

After some math, it's possible to obtain the overall wavefunction in terms of the parameters of the Hamiltonian and A, the coefficient in Ψ_1. In Region 3, we assume G=0, because the particle is coming from Region 1 and is moving in the positive x direction.

The resulting wavefunction is complicated. Rather than writing down the expression, let's examine how it, or more specifically $\Psi^*\Psi$, behaves using the provided Mathematica notebook. Indicate how the amplitude in region 3 changes with:

1. A taller barrier?
2. A wider barrier?
3. A higher energy particle?
4. A heavier particle?

Why do you think the value of $\Psi^*\Psi$ in Region 3 is a constant?

(d) The variable A^*A corresponds to the probability density of the incoming wave, and F^*F is the probability density of the wave on the other side of the barrier (see part (b) to see where these coefficients come from). We can define the transmission coefficient (the probability of the particle passing through the barrier), as $T = \left|\frac{F}{A}\right|^2$, which we can obtain from our wavefunction as

$$T = \frac{16}{16 + \frac{(k_1^2 + k_2^2)^2}{k_1^2 k_2^2}(e^{k_2 w} - e^{-k_2 w})^2}$$

write this expression in terms of V_0, E, and m using your values of k_1 and k_2 from earlier. Assuming that the barrier is large (V_0 >>E), show that $T \propto e^{-\frac{2\sqrt{2m(V_0-E)}}{\hbar}w}$.

This approximation is commonly used and the result that the transmission coefficient decreases exponentially with the width of the barrier has applications in many areas of chemistry.

(e) One application that involves quantum tunneling is the scanning tunneling microscope (STM), a microscope with atomic resolution that won its inventors the Nobel Prize in 1986. The STM works by measuring the rate at which electrons tunnel from a sharp metal tip to a sample held in vacuum, creating a tunneling current.

According to our model for tunneling, which region corresponds to the tip, and which corresponds to the sample? What in the experiment determines the width of the barrier? How would the tunneling current change if you moved across a bump in the surface (such as an atom)?

NOTE: If we placed a particle between two tunneling barriers and made those barriers infinitely high and wide, we would get our familiar result – particle in a box.