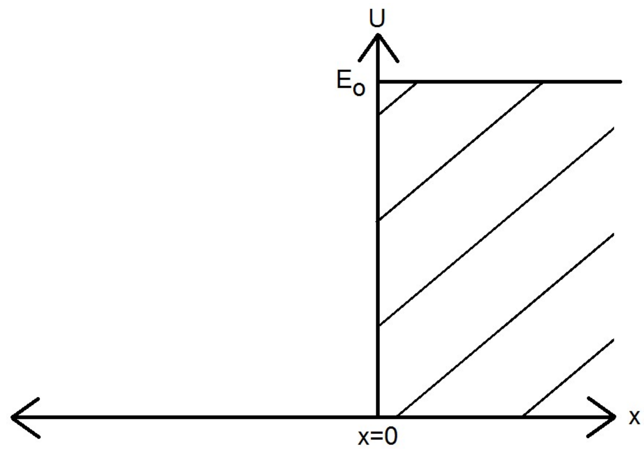
Section 12 - Penetration and Tunneling

One of the more useful properties of quantum systems is the *tunneling effect*. Let's explore some specific examples of one dimensional wave functions in a little more depth.

Consider a potential barrier U(x) that is not infinitely high at x = 0, extending off to infinity in the +x direction. From a classical mechanics point of view, a particle of total energy $E < E_o$ coming from the left could never pass over the barrier, much like a swinging pendulum bob can never rise above a particular height.



In the modern view, such a particle can pass through such a barrier. Let's see how.

The potential for negative x is zero. Consider a particle of energy $E < E_o$ coming from the left. Schrödinger's time-independent equation is

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U(x)\psi = E\psi\,.$$

We'll re-arrange this to

$$\frac{\partial^2\psi}{\partial x^2} = \frac{2m(U-E)}{\hbar^2}\psi\,.$$

The nature of the solution in each region depends on U relative to E. For x < 0, U = 0 and the equation becomes

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi$$

with solution of either sine or cosine:

$$\psi = A\sin\left(\frac{\pm\sqrt{2mE}}{\hbar}x + \phi\right).$$

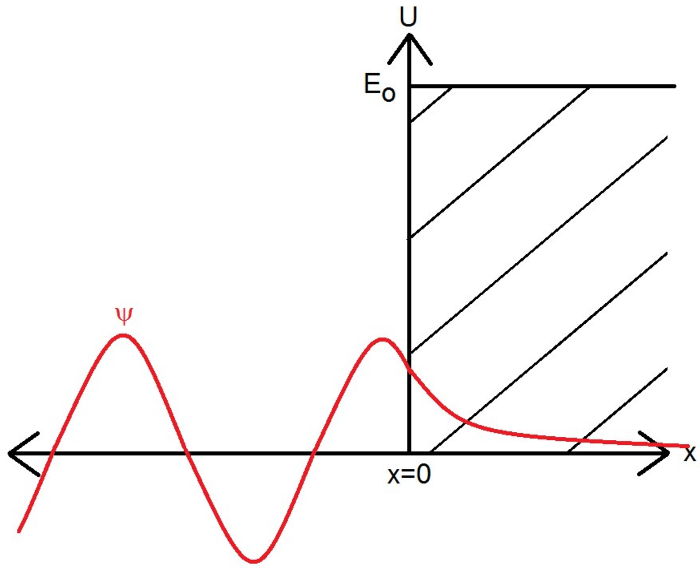
On the other hand, when x > 0, the equation becomes

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

with solution

$$\psi = A \exp\left(\frac{\pm\sqrt{2m(E_o - E)}}{\hbar} x\right).$$

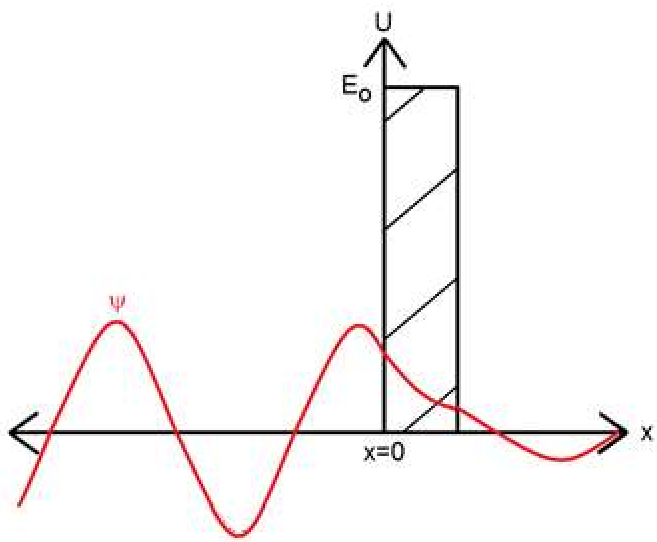
Since the function can't be allowed to increase to infinity as x goes to infinity (the probability of being somewhere can't exceed 100%), we must take the solution with the negative sign:



$$\psi = A \exp\left(-\frac{\sqrt{2m(E_o - E)}}{\hbar} x\right).$$

Note that, unlike for the infinitely high wall, there is a non-zero wavefunction for x > 0, and therefor some probability that the object is actually inside the barrier!

Now, suppose that the barrier is not infinitely thick, but instead has width L. Since, at x = L, the wave function has not exponentially 'decayed' to zero, there is some probability that the particle exists at locations to the right of the barrier. The particle has 'tunneled' through a barrier over which it could never pass classically.



Insert Classical Analog.

All analogies fall apart eventually, and here is the problem with this one: For the light waves, some of the light is reflected and some is transmitted. Obviously we can't have some fraction of an electron be reflected and the rest transmitted; there is however a certain probability that the electron is completely reflected and the complementary probability that it is transmitted. If a large number of identical electrons were to be launched at the barrier, the numbers of each sharing a fate would agree with these probabilities. Let's see if we can estimate the probability of transmission.

One again, the Schrödinger Equation can be written as

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

Let's assume solutions of the following type, much as we did in Section V-3.

$$\psi = e^{+ik} \quad and/or \quad e^{-ikx} \;,$$

where we have again omitted the oscillating time dependence. The quantity k is the magnitude of the wave vector (= 2π/λ) and i is the root of negative one, in which case,

$$k = \sqrt{\frac{2m(E - E_o)}{\hbar^2}} \;.$$

We have two terms for each region (x < 0, 0 < x <L, and x > L) in order to account for incoming and reflected waves, although we expect no reflected waves for x>L. The solutions in the three regions then are:

$$\psi(x < 0) = Ae^{+i\sqrt{\frac{2mE}{\hbar^2}}x} + Be^{-i\sqrt{\frac{2mE}{\hbar^2}}x}$$

$$\psi(0 < x < L) = Ce^{-i\sqrt{\frac{2m(E-E_o)}{\hbar^2}}x} + De^{+i\sqrt{\frac{2m(E-E_o)}{\hbar^2}}x} = Ce^{+\sqrt{\frac{2m(E_o-E)}{\hbar^2}}x} + De^{-\sqrt{\frac{2m(E_o-E)}{\hbar^2}}x}$$

$$\psi(x > L) = Fe^{+i\sqrt{\frac{2mE}{\hbar^2}}x} \;.$$

What we would like to know is the *transmission coëfficient* T, the ratio of the probability of the outgoing wave for x > L to that of the incoming wave from x < 0:

$$T = \frac{F^*F}{A^*A} \;.$$

Here are the constraints placed on the coëfficients. We required our wave functions to be continuous. Therefore, at x = 0:

$$Ae^{+i\sqrt{\frac{2mE}{\hbar^2}}0} + Be^{-i\sqrt{\frac{2mE}{\hbar^2}}0} = Ce^{+\sqrt{\frac{2m(E_o-E)}{\hbar^2}}0} + De^{-\sqrt{\frac{2m(E_o-E)}{\hbar^2}}0} \rightarrow \; A + B = C + D \;.$$

At x = L:

$$Ce^{+\sqrt{\frac{2m(E_o-E)}{\hbar^2}}L} + De^{-\sqrt{\frac{2m(E_o-E)}{\hbar^2}}L} = Fe^{+i\sqrt{\frac{2mE}{\hbar^2}}L} \;.$$

But, you may remember, we also required, in general, that the wave function's derivative *d*ψ/*d*x must be continuous when U≠ infinity, so:

$$-Ai\sqrt{\frac{2mE}{\hbar^2}}\,e^{-i\sqrt{\frac{2mE}{\hbar^2}}0}+Bi\sqrt{\frac{2mE}{\hbar^2}}\,e^{+i\sqrt{\frac{2mE}{\hbar^2}}0}$$
$$=C\sqrt{\frac{2m(E_o-E)}{\hbar^2}}\,e^{+\sqrt{\frac{2m(E_o-E)}{\hbar^2}}0}-D\sqrt{\frac{2m(E_o-E)}{\hbar^2}}\,e^{-\sqrt{\frac{2m(E_o-E)}{\hbar^2}}0}$$

or,

$$-Ai\sqrt{\frac{2mE}{\hbar^2}}+Bi\sqrt{\frac{2mE}{\hbar^2}}=C\sqrt{\frac{2m(E_o-E)}{\hbar^2}}-D\sqrt{\frac{2m(E_o-E)}{\hbar^2}}\quad ,$$

Then, at x = L,

$$C\sqrt{\frac{2m(E_o-E)}{\hbar^2}}\,e^{+\sqrt{\frac{2m(E_o-E)}{\hbar^2}}L}-D\sqrt{\frac{2m(E_o-E)}{\hbar^2}}\,e^{-\sqrt{\frac{2m(E_o-E)}{\hbar^2}}L}=Fi\sqrt{\frac{2mE}{\hbar^2}}\,e^{+i\sqrt{\frac{2mE}{\hbar^2}}L}\quad .$$

Lots of math I'll add later…..

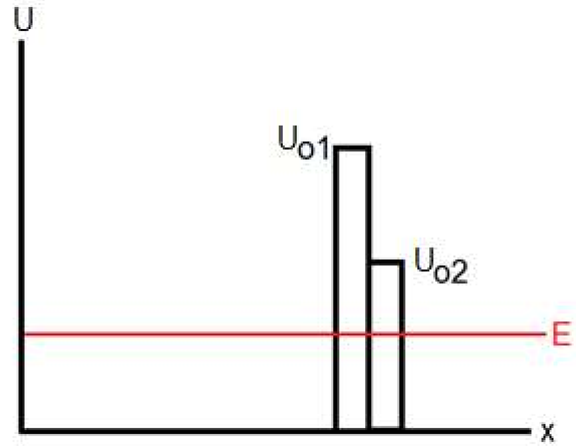
$$T=\left(1+\frac{sinh^2\left(\sqrt{\frac{2mU_oL^2}{\hbar^2}\left(1-\frac{E}{U_o}\right)}\right)}{4\frac{E}{U_o}\left(1-\frac{E}{U_o}\right)}\right)^{-1}\quad .$$

When the barrier is quite thick, or when $E \ll E_o$, this can be approximated with

$$T=16\,\frac{E}{U_o}\left(1-\frac{E}{U_o}\right)e^{-\sqrt{8mU_o\left(1-\frac{E}{U_o}\right)}\,L/\hbar}\quad .$$

The tunneling effect is seen in many physical systems, and forms the basis for many technological devices.

Now, what if we have a non- rectangular barrier? Let's start with two rectangular barriers that are back to back, one of height U_{o1} and the other of height U_{o2}. Any particle making it through the combined barrier must have passed through the first one and the second. If T_1 is the probability of making it through the first and T_2 is the probability of making it through the second, the probability of making it though both is



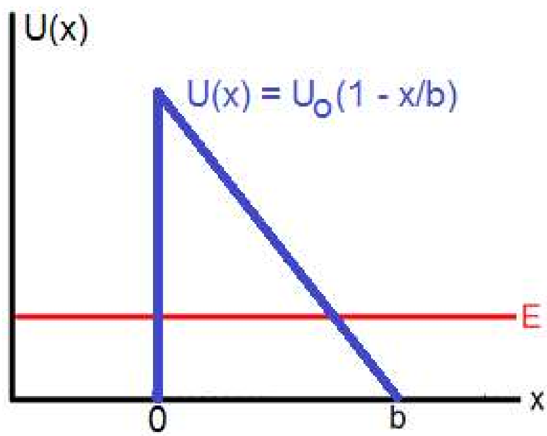
$$T = T_1 T_2 \ .$$

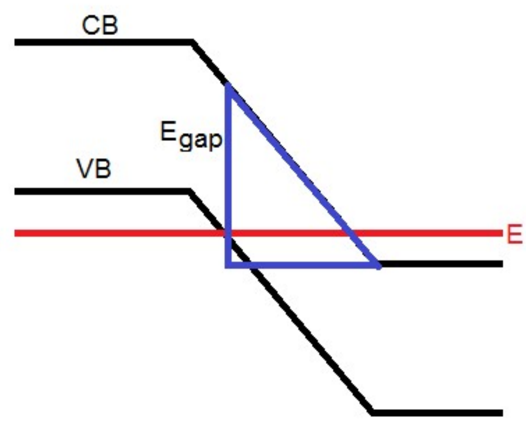
If that's OK, then what if we have N barriers?

$$T = T_1 T_2 T_3 \ldots T_N \ .$$

EXAMPLE

Let's use this idea to see if we can find the transmission coefficient for a triangular barrier as shown in the figure; this corresponds roughly to what an electron in a reverse-biased diode would experience. The barrier is formed by the *energy gap* between the valence and conduction bands.



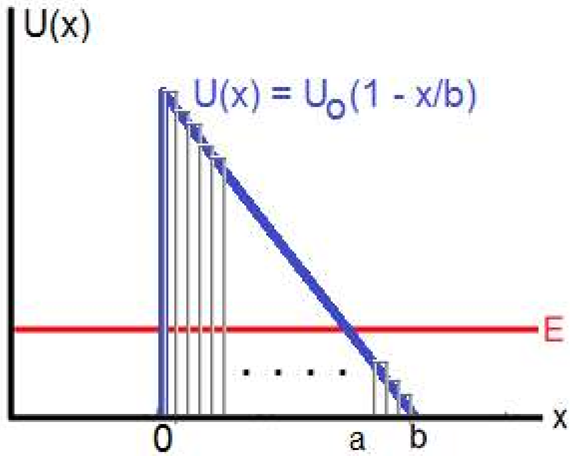


We're going to make a lot of approximations and hope to get an order of magnitude value. We'll model the barrier as a series of rectangular barriers whose heights follow the relationship

$$U(x) = U_o\left(1 - \frac{x}{b}\right) \ .$$

First, let's look again at the approximate result from above for one barrier:

$$T = 16\,\frac{E}{U_o}\left(1 - \frac{E}{U_o}\right) e^{-\sqrt{8mU_o\left(1-\frac{E}{U_o}\right)}\,L/\hbar} \ .$$



The variable here appears to be E/U$_o$. It seems clear that the exponential term will vary much more quickly than the terms in front, which are probably on the order of one, anyway. So, let's drop them, leaving

$$T_n = e^{-\sqrt{8m(U_{on} - E)}\,L_n/\hbar} .$$

Let's let each barrier have thickness dx and substitute in the potential function U(x) to obtain

$$T(x) \approx e^{-\sqrt{8m(U(x) - E)}\,dx/\hbar} .$$

Remembering that the transmission coefficient for all the barriers combined is the product of the individual coefficients, and that the product of exponentials is the exponential of the sum, we obtain

$$T \approx e^{-\int \frac{\sqrt{8m(U(x)-E)}}{\hbar}dx} = e^{-\sqrt{\frac{8m}{\hbar^2}}\int\sqrt{U_o\left(1-\frac{x}{b}\right)-E}\,dx} = e^{-\sqrt{\frac{8mU_o}{\hbar^2}}\int\sqrt{1-\frac{E}{U_o}-\frac{x}{b}}\,dx} .$$

Let's concentrate for now on just the integral:

$$\int\sqrt{1-\frac{E}{U_o}-\frac{x}{b}}\,dx$$

We'll need limits; the lower limit is clearly 0, but the upper limit a depends on U$_o$ and E. Specifically, we'll set U(a) = U$_o$(1-a/b) = E and find that a = (1- E/U$_o$)b:

$$\int_0^{\left(1-\frac{E}{U_o}\right)b}\sqrt{1-\frac{E}{U_o}-\frac{x}{b}}\,dx .$$

We'll use the substitution z = 1 - E/U$_o$ - x/b and dz = -dx/b, and change the limits:

$$-b\int_{1-\frac{E}{U_o}}^{0} z^{1/2}\,dz = b\int_0^{1-\frac{E}{U_o}} z^{1/2}\,dz = \frac{2b}{3}\left(1-\frac{E}{U_o}\right)^{3/2} .$$

Replacing this result into the exponential term above,

$$T \approx exp\left(-\sqrt{\frac{32m}{9\hbar^2}}\frac{b}{U_o}(U_o - E)^{\frac{3}{2}}\right).$$

Next, we'll do two things. We might expect the energy of the electrons to be quite a bit smaller than the band gap energy, so U$_o$ – E ≈ U$_o$. The second thing is a bit weaslier. The potential difference U_o can be thought of as being due to an electric field, ε; certainly, we can modify the barrier (primarily its width) by applying our own E-field within the diode.

$$U_o = q\,\Delta V = q\,\mathcal{E}\,b \quad \rightarrow \quad \frac{b}{U_o} = \frac{b}{q\mathcal{E}} = \frac{1}{q\mathcal{E}}$$

$$T \approx exp\left(-\sqrt{\frac{32mU_o^3}{9q^2\hbar^2}}\,\frac{1}{\mathcal{E}}\right) \quad .$$

Since we may naïvely think that the current through a p-n junction would be proportional to the tunneling probability, we predict that

$$\log\big(I(\mathcal{E})\big) \sim -\frac{1}{\mathcal{E}} \,.$$

Here is a graph of real data. The agreement is O.K. for weak electric fields.