Physics 486

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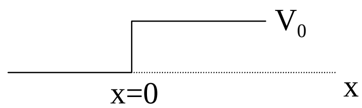
Lecture 7

<u>The step potential</u>



There are several simple one-dimensional potentials that are of interest because they approximate certain real physical situations. In addition, they make evident non-classical behavior. We have already discussed one of these, the infinite square well. Now we look at the one-dimensional potential step defined by

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

where V_0 is a positive constant.

The time-independent Schrödinger equation for this case reads

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

We define

$$k^2 \equiv \frac{2mE}{\hbar^2} \qquad q^2 \equiv \frac{2m(E - V_0)}{\hbar^2}$$

The most general solution to the left of the step (where $V(x)=0$) is $e^{\pm ikx}$, and to the right of the step is $e^{\pm iqx}$. Note that we have made no assumptions about the relative magnitude of V_0 and the particle energy E. If E is greater than V_0 then we get an oscillatory solution and if E is less that V_0 then we get an exponentially decaying solution.

As we have noted on several occasions, these solutions have the flaw that they are not normalizable. For the infinite square well, they were because we had boundaries at *0, a*. Here that is not the case. One way to handle this difficulty is to solve the entire problem in terms of the wave packets we developed to solve the normalization problem. That certainly works, but there is an easier way. We can sidestep this problem in the following way. The physics we are interested in here is the probability that a particle be reflected at the potential step (or equivalently, that it be transmitted past it). Thus we will never be asking for the probability that the particle be localized in some region of space. We can think of the problem as consisting of a certain *flux* of particles impinging on the step, and our job is to find what fraction of them are reflected. In this way, the density of particles in space is a constant on either side of the step (though not the same from one side to the other!) which is consistent with the fact that the magnitude squared of the wave function is a constant. The flux of particles is naturally given, in terms of the wave function, by the probability current we defined in Lecture 4

$$J(x) = \frac{i\hbar}{2m}\left[\frac{d\psi^*(x)}{dx}\psi(x) - \psi^*(x)\frac{d\psi(x)}{dx}\right]$$

So defined, the flux for a wave function $Ae^{\pm ikx}$ is $\pm|A|^2\,\hbar k/m$.

Let's define the problem as a flux of particles approaching the step from the left with $E>V_0$. For $x<0$ we have $V(x)=0$ and the solution contains both incident and reflected waves

$$\psi(x) = e^{ikx} + Be^{-ikx}$$

The positive exponential corresponds to right moving particles and the negative to left moving particles. We are free to use just a single constant, B, because we only care about the fraction of reflected waves (we are defining the incident amplitude to be "1").
For $x>0$ we can write

$$\psi(x) = Fe^{iqx}$$

Note that e^{-iqx} is also a solution, but we've set up the problem so that there is nothing travelling left from $x>0$.

The next step is to apply the boundary conditions, which are as usual, the continuity of the wave function and its first derivative at the boundary ($x=0$)

$$\begin{aligned}
&\psi_<(0) = \psi_>(0) \Rightarrow \\
&1 + B = F \\
&\frac{d\psi_<(0)}{dx} = \frac{d\psi_>(0)}{dx} \Rightarrow \\
&ik(1-B) = iqF
\end{aligned}$$

The two equations in two unknowns, B,F, can be solved as follows

$$\begin{aligned}
&F = \frac{k}{q}(1-B) = 1 + B \\
&\frac{k}{q} - 1 = B\left(1 + \frac{k}{q}\right) \\
&k - q = B(k+q) \\
&B = \frac{k-q}{k+q} \qquad F = \frac{2k}{k+q}
\end{aligned}$$

The flux $J(x)$ to the left of the barrier is given by

$$J(x<0) = \frac{\hbar k}{m}\left(1 - |B|^2\right)$$

where the first term is the incident flux and the second the reflected flux. To the right of the barrier the flux is

$$J\left(x>0\right)=\frac{\hbar q}{m}\left|F\right|^2$$

The reflection coefficient is the ratio of the incident to reflected flux

$$\frac{\frac{\hbar k}{m}\left|B\right|^2}{\frac{\hbar k}{m}}=\left|B\right|^2=\left(\frac{k-q}{k+q}\right)^2$$

and the transmission coefficient is the ratio of the transmitted to incident flux

$$\frac{\frac{\hbar q}{m}\left|F\right|^2}{\frac{\hbar k}{m}}=\frac{q}{k}\left|F\right|^2=\sqrt{\frac{E-V_0}{E}}\left|F\right|^2$$

Note the factor of q/k here. This is a result of the fact that the particle travels at a different speed on the left and right side of the step.

It is easy to show that incident flux minus the reflected flux is equal to the transmitted flux, in fact this follows in general from the continuity equation. The continuity equation tells us

$$\frac{\partial}{\partial t}\wp(x,t)+\frac{\partial}{\partial x}J(x,t)=0$$

but since the problem has no time dependence, we must have

$$\frac{\partial J(x)}{\partial x}=0$$

that is, the flux is independent of x. If this is the case, then the flux to the left of the barrier must be equal to the flux to the right of the barrier, or

$$\frac{\hbar k}{m}\left(1-\left|B\right|^2\right)=\frac{\hbar q}{m}\left|F\right|^2$$

Let's investigate some features of these solutions.

1) Classically, for $E>V_0$ there is no reflection at the step, just a loss of kinetic energy so that the total energy remains constant. Quantum mechanically we have discovered that a certain amount of the wave, which depends on E-V_0, is reflected.
2) For $E>>V_0$, the transmission coefficient approaches 1 as expected classically.
3) For $E<V_0$, q is imaginary, thus

$$\psi_>\left(x\right)=Fe^{-|q|x}$$

(note we cannot have the positive exponential solution because it blows up as $x\rightarrow\infty$).

$$k^2 \equiv \frac{2mE}{\hbar^2} \qquad q^2 \equiv \frac{2m(E-V_0)}{\hbar^2}$$

Returning to the case where $E<V_0$, we see that q becomes imaginary, and the wavefunction to the right of the step becomes $\psi_>(x) = Fe^{-|q|x}$
(note we cannot have the positive exponential solution because it blows up as $x\to\infty$).

In this case, we can repeat the algebra from the last lecture to get

$$B = \frac{k-i|q|}{k+i|q|} \text{ and}$$

$$|B|^2 = \frac{k-i|q|}{k+i|q|} \bullet \frac{k+i|q|}{k-i|q|} = 1$$

so that the entire wave is reflected. This agrees with our classical intuition, but there is a very important quantum mechanical effect going on here. Check out the transmitted amplitude

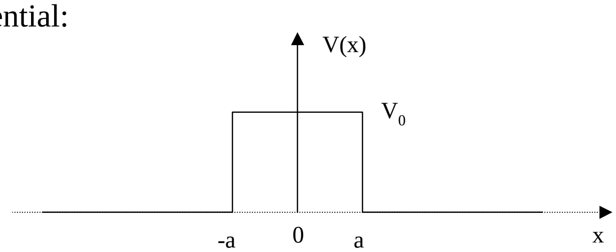
$$F = \frac{2k}{k+i|q|} \qquad |F|^2 = \frac{4k^2}{k^2+q^2}$$

The non-zero transmitted amplitude means that the wave penetrates past $x=0$. At first glance, this would seem to contradict a reflection coefficient of 1. However, the flux to the right of the barrier is

$$J(x>0) = \frac{i\hbar}{2m}\left(-|q||F|^2 e^{-2|q|x} + |q||F|^2 e^{-2|q|x}\right) = 0$$

so that the transmission coefficient (as opposed to the transmitted amplitude) *is* equal to zero. The point is that although some of the wave does penetrate past $x=0$, eventually it turns around and is reflected. This is a result of the fact that the potential is constant for $x>0$. If instead the potential returned to zero at some positive x, the penetration past $x=0$ would allow some transmission through the barrier. This is the phenomenon of *tunneling*. Let's examine this phenomenon by looking at the solutions to the one-dimensional square barrier potential:

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



The solution goes along the same lines as the step function with the difference that we now have two boundaries to deal with. We are interested (for the moment) in the case $0<E<V_0$. We define

$$k^2 \equiv \frac{2mE}{\hbar^2} \qquad \kappa^2 \equiv \frac{2m(V_0-E)}{\hbar^2}$$

where *both* constants are real for $E<V_0$ (note the sign change of κ^2 compared to q^2. The solution for $|x|<a$ is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

Again, we assume that the particle is incident from the left, in which case we have for $x<-a$

$$\psi(x) = e^{ikx} + Ce^{-ikx}$$

and for $x>a$ there is only the transmitted wave

$$\psi(x) = De^{ikx}$$

For $x<-a$ the flux J is identical in form to the solution for the step potential

$$J(x<-a) = \frac{\hbar k}{m}\left(1-|C|^2\right)$$

Similarly for $x>a$ we get our previous solution except that $q \rightarrow k$, since $V_0 = 0$ for $x>a$.

$$J(x>a) = \frac{\hbar k}{m}|D|^2$$

Since we are interested in the transmission coefficient, i.e. the ratio of incident to transmitted flux through the barrier, we will not need the form of the flux within the barrier. We must solve for R and T using the boundary conditions at $x=a, -a$.

$$e^{-ika} + Ce^{ika} = Ae^{\kappa a} + Be^{-\kappa a} \qquad \{\psi \text{ @ } x=-a\}$$

$$ik\left(e^{-ika} - Ce^{ika}\right) = \kappa\left(Be^{-\kappa a} - Ae^{\kappa a}\right) \qquad \left\{\frac{d\psi}{dx} \text{ @ } x=-a\right\}$$

$$Ae^{-\kappa a} + Be^{\kappa a} = De^{ika} \qquad \{\psi \text{ @ } x=+a\}$$

$$\kappa\left(Be^{\kappa a} - Ae^{-\kappa a}\right) = ikDe^{ika} \qquad \left\{\frac{d\psi}{dx} \text{ @ } x=+a\right\}$$

With *lots* of algebra, this can be solved to find

$$D = e^{-2ika}\frac{2k\kappa}{2k\kappa\cosh(2\kappa a) + i\left(k^2-\kappa^2\right)\sinh(2\kappa a)}$$

$$\Rightarrow |D|^2 = \frac{(2k\kappa)^2}{(2k\kappa)^2 + \left(k^2+\kappa^2\right)^2\sinh^2(2\kappa a)}$$

In this case, since the velocity factor $\hbar k/m$ is the same on both sides of the barrier, the transmission coefficient is just $|D|^2$, and quantum mechanics tells us that there is transmission through the barrier even for $E<V_0$. This is tunneling, which is crucial to our understanding of many physical phenomena.

For κa large, the transmission coefficient becomes

$$|D|^2 \approx \left(\frac{4k\kappa}{k^2+\kappa^2}\right)^2 e^{-4\kappa a}$$

where (1)

$$\kappa a = \sqrt{\frac{2ma^2}{\hbar^2}(V_0 - E)}$$

from which it is clear that the transmission coefficient is a very sensitive function of the barrier width, *2a*, and *$(V_0$-$E)$*.

Many of the applications we will want to study contain not square barriers, but barriers of some other (hopefully smooth) shape. A rigorous treatment of this problem involves something called the WKB approximation (Wentzel, Kramers and Brillouin). It is dealt with in Chapter 8 of Griffiths, and we will cover it in 387. Nevertheless, we can use the results above and an approximation or two to get at the main result that we can then apply to some interesting physical systems. For those of you who want more rigor, I include a more rigorous derivation in the appendix to this lecture.

We note that the transmission coefficient in eq. (1) consists of an exponential term that dominates

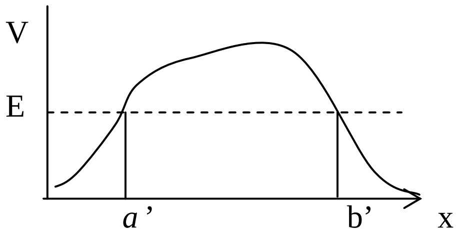
$$\ln|D|^2 \approx -4\kappa a + 2\ln\frac{2k\kappa a^2}{(ka)^2+(\kappa a)^2}$$

For reasonable κa the first term (which comes from the exponential) dominates. Given this, we write the transmission coefficient as

$$|\mathrm{D}|^2 \sim e^{-4\kappa a} = e^{-4\sqrt{\frac{2Ma^2}{\hbar^2}}(V_0-E)}$$

$$= e^{-2\sqrt{2M/\hbar^2 (V_0-E)}\bullet 2a}$$

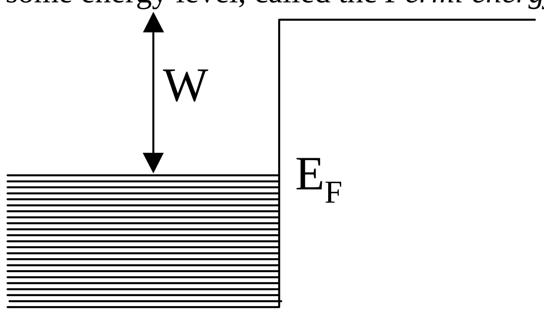
The factor of *2a* in the exponent is the width of the barrier. Suppose now that we have a barrier whose height depends on *x* in a smooth way. We can think of this as a superposition of a large number of very thin square barriers, and the solution above for the transmission coefficient becomes an integral in the exponent



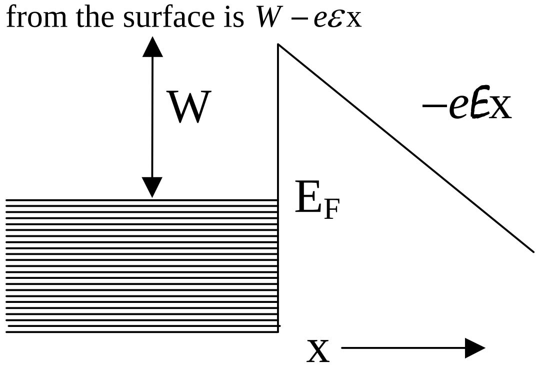
$$|D|^2 \approx e^{-2\int_{a'}^{b'}\sqrt{\frac{2M}{\hbar^2}(V_0-E)}\,dx}$$

Field Emission (aka Cold Emission):

As we will see later on, the photoelectric effect can be explained by considering the electrons in a metal to be in a potential well of finite depth. Electrons have the property that you can put two of them in each energy state in the well (one with spin up and one with spin down, but we'll get to that). Thus we can describe a metal as a well filled up to some energy level, called the *Fermi energy*, E_F



W is the work function, familiar from the photoelectric effect as the amount of energy necessary to free an electron from the metal. We now view this as the depth, from the top of the well, of an electron at the Fermi energy. In this picture an electron can never escape from the well without the addition of energy from, say, a photon (of course this is an idealized picture, in reality there are thermal excitations, etc.). However, if an external electric field, $\mathcal{E}$, is applied, the potential seen by an electron as a function of distance x from the surface is $W - e\mathcal{E}$x



Now an electron at the *Fermi surface* (i.e. with energy E_F) can tunnel through the barrier to freedom. In this simple picture, the transmission coefficient for an electron at the

Fermi surface is (we are using our approximation – we don't expect quantitatively exactly correct solutions)

$$|D|^2 = e^{-2\int_0^a \sqrt{2m[W - e\varepsilon x]/\hbar^2}\,dx}$$

where the lower limit of integration is taken as the position of the metal surface (right side of the well), and the upper limit, *a*, is the value of *x* for which $W\text{-}e\varepsilon x=0$. Integrating we find

$$|D|^2 = e^{-\left(\frac{4}{3}\frac{W}{e\varepsilon}\frac{\sqrt{2mW}}{\hbar}\right)} \equiv e^{-\varepsilon_0/\varepsilon}$$

Note that there is a strong dependence on the value of the work function at the surface. This transmission coefficient is a tunneling probability for a single electron. The electron current due to quantum tunneling should be directly proportional to this probability

$I = I_0 e^{-\varepsilon_0/\varepsilon}$

The original experiments on this effect were done in 1926 by Millikan and Eyring and the results agree quite well with this formula.

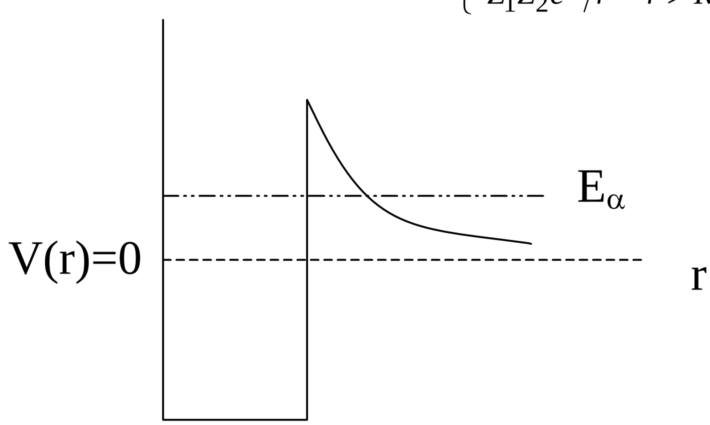
Alpha decay of nuclei:

In the alpha decay of nuclei, a heavy nucleus decays to a lighter one by the emission of an alpha particle, i.e. the nucleus of a helium atom with two neutrons and two protons:

$$^{Z}_{N}X^{A} \rightarrow {}^{(Z-2)}_{(N-2)}Y^{(A-4)} + {}^{2}_{2}He^{4}$$

Where *Z* is the number of protons, *N* the number of neutrons, and $A=Z+N$. We model this process by assuming the parent nucleus *X* to be made up of an alpha particle, plus the daughter nucleus *Y*, with the alpha particle trapped inside the daughter nucleus by the Coulomb barrier. Thus the alpha particle moves in the potential of the daughter nucleus, which is a combination of an attractive square well, plus a repulsive Coulomb potential:

$$V(r) = \begin{cases} -V_0 & r < R \\ Z_1 Z_2 e^2/r & r > R \end{cases}$$



We use $Z_1=Z_\alpha=2$, and $Z_2=Z-2$, where Z is the charge of the parent nucleus. As you can see from the figure, we have to assign the alpha particle a positive energy, E_α, in order for there to be a possibility of tunneling. The probability that the alpha particle will tunnel through the barrier *on each approach* is given by

$$|D|^2 = e^{-G}$$

where

$$G = 2\sqrt{\frac{2m}{\hbar^2}}\int_a^b \sqrt{\frac{Z_1 Z_2 e^2}{r} - E_\alpha}\, dr$$

Here a is the radius of the daughter nucleus (i.e. the size of the well) and b is the classical turning point given by

$$b = \frac{Z_1 Z_2 e^2}{E_\alpha}$$

The mass, m, is the mass of the alpha particle. The integration can be done in closed form, giving

$$G = 2\sqrt{\frac{2mZ_1Z_2e^2b}{\hbar^2}}\sqrt{b}\left[\cos^{-1}\left(\frac{a}{b}\right)^{\frac{1}{2}} - \left(\frac{a}{b} - \frac{a^2}{b^2}\right)^{\frac{1}{2}}\right]$$

For relatively low alpha particle energies, such that E_α is close to zero, $a/b<<1$, and we have

$$G \approx -2\sqrt{\frac{2mZ_1Z_2e^2b}{\hbar}}\frac{\pi}{2}$$

Using $b = Z_1Z_2e^2/E_\alpha = 2Z_1Z_2e^2/mv^2$, where v is the velocity of the alpha particle inside the nucleus, the exponent G becomes

$$G \approx \frac{-2\pi Z_1 Z_2 e^2}{\hbar v}$$

And the transmission probability is

$$|D|^2 \approx e^{-\frac{2\pi Z_1 Z_2 e^2}{\hbar v}}$$

To find a formula for the lifetime, we imagine the alpha particle rattling around inside the nucleus with an average velocity v. For a nucleus of size a, the average time between collisions with the Coulomb barrier will be a/v, thus the probability of emission per unit time is

$$\frac{v}{a}e^{-G}$$

The lifetime of the parent nucleus is the reciprocal of this factor

$$\tau = \frac{a}{v}e^{G}$$

We don't know the velocity very well, however, this doesn't matter much as the variation in lifetimes is completely dominated by the exponential factor, relative to which the velocity factor in front is nearly constant.

Appendix:

This is just here for your enjoyment.

Tunneling through barriers of arbitrary shape (The WKB Approximation)

Motivated by the plane wave solutions for flat potentials (i.e. constant over some region), we look for solutions to the Schrödinger equation of the form

$$\psi(x) = A(x)e^{iF(x)/\hbar}$$

Plugging this form into the time-independent Schrödinger equation, we get

$$A(x)\left[\frac{1}{2m}\left(\frac{dF(x)}{dx}\right)^2 - \left(E - V(x)\right)\right]$$
$$-\hbar\left(\frac{i}{2m}\right)\left[2\frac{dA(x)}{dx}\frac{dF(x)}{dx} + A(x)\frac{d^2F(x)}{dx^2}\right]$$
$$-\hbar^2\left[\frac{1}{2m}\frac{d^2A(x)}{dx^2}\right] = 0$$

Now, $\hbar$ is a small number, so we will neglect the last term which is proportional to $\hbar^2$. This leaves us with a real term (the first) and an imaginary term (the second) which must independently give zero. Thus, from the real term we have

$$\frac{dF(x)}{dx} = \pm\sqrt{2m\left(E - V(x)\right)} \equiv \pm p(x)$$

and, integrating we get

$$F(x) = \pm\int^{x} p(x)dx$$

where *p(x)* is just the classical momentum. The imaginary term then gives

$$2\frac{dA(x)}{dx}p(x) + A(x)\frac{dp(x)}{dx} = 0$$

Multiplying both sides by $A(x)$ we get

$$\left(2A(x)\frac{dA(x)}{dx}\right)p(x) + A^2(x)\frac{dp(x)}{dx} = \frac{d}{dx}\left[A^2(x)p(x)\right] = 0$$

or

$$A^2(x)p(x) = C$$

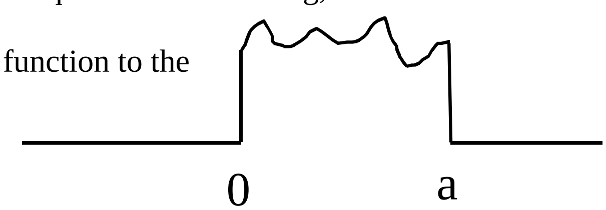
where C is a constant. We then have two independent solutions, corresponding as usual to right (+) and left (-) moving waves

$$\psi^{\pm}(x) = \frac{C_{\pm}}{\sqrt{p(x)}} e^{\pm i \int^{x} p(x)dx \big/ \hbar}$$

Note that when *E<V(x)*, then *p(x)* becomes imaginary, and the solution is exponential instead of oscillatory

$$\psi^{\pm}(x) = \frac{C_{\pm}}{\sqrt{p(x)}} e^{\pm\sqrt{2m/\hbar^2}\int^{x}\sqrt{V(x)-E}dx}$$

Now, let's apply such a wave function to the question of tunneling, this time for a barrier with a smooth, but not flat, potential.



As we saw before, for a barrier, the wave function to the left of the barrier is

$$\psi(x) = e^{ikx} + Re^{-ikx}$$

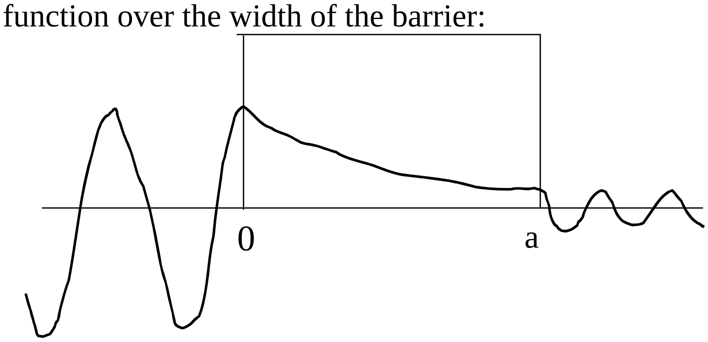
and to the right of the barrier it is

$$\psi(x) = Te^{ikx}$$

The tunneling probability is just $|T|^2$ which we found on page 2 above for a rectangular barrier (n.b. we are still assigning the incident amplitude =1). In the tunneling region, the WKB approximation gives us

$$\psi(x) \approx \frac{C}{\sqrt{|p(x)|}} e^{\frac{1}{\hbar}\int_0^x |p(x')|dx'} + \frac{D}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}$$

If the barrier is very high or wide, i.e. the probability of tunneling is small, then the coefficient of the exponentially increasing term can be set equal to zero. The relative amplitudes of the incident and transmitted waves are given by the exponential decrease of the wave function over the width of the barrier:



Then we have

$$|T| \sim e^{-\frac{1}{\hbar}\int_0^a |p(x)|dx}$$

so that the tunelling probability is

$$|T|^2 \approx e^{-2\int_0^a |p(x)|dx / \hbar}$$

Note that this is the same as the exponential factor in the tunneling probability calculated on page 2. Now we are in a position to calculate tunneling probabilities for an arbitrarily shaped, smooth potential.