Chapter 5 - The Schrodinger Equation (Part II): Finite Potential Well and Step Potential

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5.9 Finite Potential Well

In this example we modify the infinite potential well problem by "softening" the sides of the box. Rather than assuming the potential is infinite at the edges of the box, we will assume it has a value U_0:

$$U(x) = \begin{cases} U_0 & \text{for } x \leq -L/2 \qquad \text{(Region I)} \\ 0 & \text{for } -L/2 < x < L/2 \quad \text{(Region II)} \\ U_0 & \text{for } x \geq L/2 \qquad \text{(Region III)} \end{cases}$$

We divide space into three regions: region II is inside the well, and regions I and III are outside it. We set up (but not completely solve) this problem by following the steps outlined in section 5.6.

You could imagine this potential as being a very crude approximation to the potential well of an atom. In this case, the force trapping the electron would be the electric force. If the electron absorbs a photon with energy greater than U_0, then it would escape the potential well and become a free electron. Alternately, this potential could describe the potential felt by a proton or neutron trapped inside an atomic nucleus. In this case, the force would be the strong nuclear force (which we will return to in a few weeks).

Step 1. Plug potential into the S.E. Inside the well in region II, $U(x) = 0$ so the Schrodinger equation may be written as

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi(x). \qquad \text{(Region II)}$$

In regions I and III the potential is $U(x) = U_0$ and the Schrodinger equation is

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2m(U_0 - E)}{\hbar^2}\psi(x). \qquad \text{(Region I and III)}$$

We assume $E < U_0$ so that the particle is trapped inside the potential well.

Step 2. Solve the S.E. The general solution in region II is the same as the infinite potential well:

$$\psi_{II}(x) = A\sin(kx) + B\cos(kx) \qquad \text{where } k = \frac{\sqrt{2mE}}{\hbar}.$$

In regions I and III we are in the classically forbidden region where $E < U_0$ and the general solution is

$$\psi_I(x) = Ce^{k'x} + De^{-k'x} \qquad \text{where } k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

and

$$\psi_{III}(x) = Ee^{k'x} + Fe^{-k'x} \qquad \text{where } k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar}.$$

Step 3. Boundary Conditions. Because we will be matching up solutions across three regions, we will have lots of boundary constraints.

- **Left side of Region I**. This region extends to $-\infty$, so the condition

  $$\psi_I(x = -\infty) = 0$$

  implies that $D = 0$. This means that the region I solution simplifies to

  $$\psi_I(x) = Ce^{k'x}.$$

- **Right side of Region III**. This region extends to $+\infty$, so the condition

  $$\psi_{III}(x = \infty) = 0$$

  implies that $E = 0$. This means that the region III solution simplifies to

  $$\psi_{III}(x) = Fe^{-k'x}.$$

- **Region I-II Interface**. This interface occurs at position $x = -L/2$. We require the wave function to be both continuous and smooth at the interface. First the continuity condition:

  $$\begin{aligned} \psi_I(-L/2) &= \psi_{II}(-L/2) \\ Ce^{-k'L/2} &= A\sin(-kL/2) + B\cos(-kL/2). \end{aligned}$$

  Now for the smoothness condition:

  $$\begin{aligned} \left.\frac{\partial \psi_I}{\partial x}\right|_{x=-L/2} &= \left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=-L/2} \\ k'Ce^{-k'L/2} &= kA\sin(-kL/2) - kB\cos(-kL/2). \end{aligned}$$

- **Region II-III Interface**. This interface occurs at position $x = L$. We require the wave function to be both continuous and smooth at the interface. First the continuity condition:

  $$\begin{aligned} \psi_{II}(L/2) &= \psi_{III}(L/2) \\ Ce^{k'L} &= A\sin(kL/2) + B\cos(kL/2). \end{aligned}$$

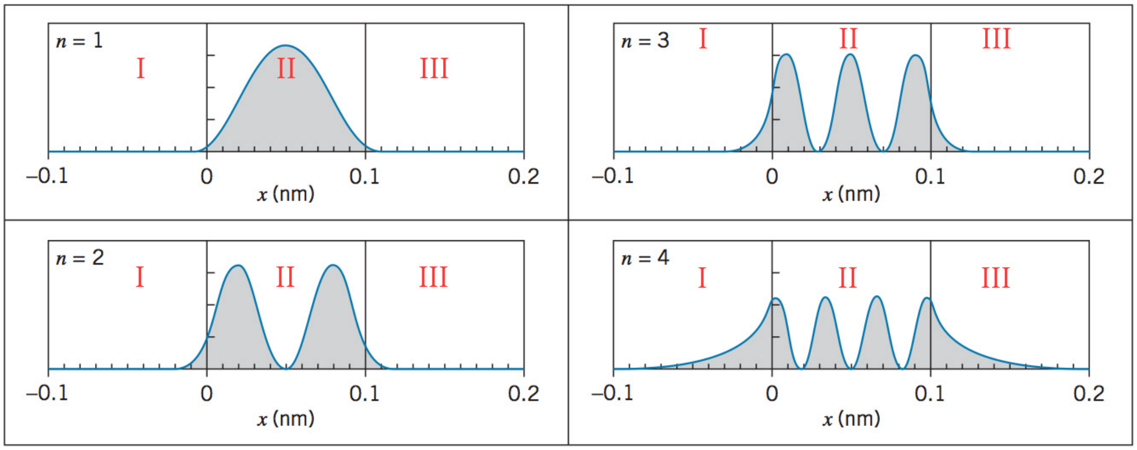

Figure 1: Plots of $|\psi(x)|^2$ for the finite potential well for quantum numbers $n = 1, 2, 3, 4$.

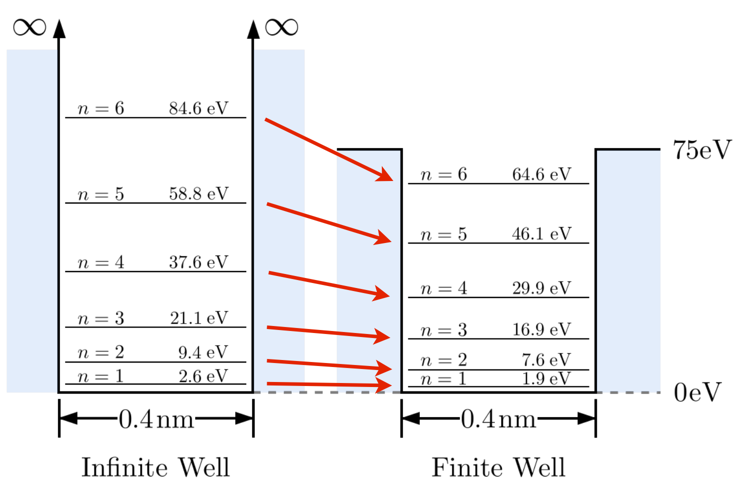

Figure 2: Comparison of energy level diagrams for the infinite potential well and finite potential well.

Now for the smoothness condition:

$$\left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=L/2} = \left.\frac{\partial \psi_{III}}{\partial x}\right|_{x=L/2}$$
$$k'Ce^{k'L/2} = kA\sin(kL/2) - kB\cos(kL/2)$$

We will stop here in the quantitative derivation of this problem, since it requires a numerical solution and you will return to solve this problem in detail when you take Quantum Mechanics. However, we'll look at the results qualitatively. Figure 1 shows the probability density $|\psi(x)|^2$ for the first four quantum numbers $n = 1, 2, 3, 4$. Compare this solution to the solution for the infinite potential well. Notice that the number of "bumps" in the probability density equals the quantum number n. Notice also that the wave function penetrates into the forbidden regions I and II. As the energy E approaches the top of the well U_0, the particle is more likely to be found in the forbidden region. Figure 2 shows the energy level diagram for the finite potential well with width $L = 0.4$ nm. The energy levels of the finite potential well are lower than those of the infinite potential well due to the spreading out of the wave function into the classically forbidden region.

5.10 Step Potential, $E > U_0$

In this example, we imagine a stream of particles traveling through free space. At position $x = 0$, they experience an obstacle that requires some energy U_0 to overcome. You could imagine a ball rolling along a flat surface. A steep hill is present at $x = 0$. If the ball has enough kinetic energy to overcome the hill, it will keep going (but at a slower velocity once it is on the higher plateau). The potential is:

$$U(x) = \begin{cases} 0 & \text{for } x \leq 0 \qquad \text{(Region I)} \\ U_0 & \text{for } 0 \qquad \text{(Region II)} \end{cases}$$

We divide space into two regions: region I is to the left of the step with $U(x) = 0$ and region region II is to the right where $U(x) = U_0$. We set up this problem and leave the rest for you to solve in problem 28.

Step 1. Plug potential into the S.E. In Region I where $U(x) = 0$ so the Schrodinger equation may be written as

$$\frac{\partial^2 \psi_I(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi_I(x). \qquad \text{(Region I)}$$

In regions II the potential is $U(x) = U_0$ and the Schrodinger equation is

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} = \frac{2m(E - U_0)}{\hbar^2}\psi_{II}(x). \qquad \text{(Region II)}$$

We assume $E > U_0$ so that the particle is free to move past the barrier into Region II.

Step 2. Solve the SE Because the particle's energy is greater than the potential in both regions, the solutions will be harmonic waves. It turns out to be easier to deal with complex exponentials in this case rather than sines and cosines. The Solutions are:

$$\psi_I(x) = A'e^{ik_1x} + B'e^{-ik_1x} \qquad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad \text{(Region I)}$$

and

$$\psi_{II}(x) = C' e^{ik_2 x} + D' e^{-ik_2 x} \qquad \text{where } k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar} \qquad \text{(Region II).}$$

We can understand the physical meaning behind these solutions if we look at the full time-dependent solutions by multiplying each by $e^{-i\omega t}$:

$$\Psi_I(x,t) = \psi_I(x)e^{-i\omega t} = \underbrace{A' e^{i(k_1 x - \omega t)}}_{\text{wave moving right}} + \underbrace{B' e^{-i(k_1 x + \omega t)}}_{\text{wave moving left}} \qquad \text{(Region I)}$$

and

$$\Psi_{II}(x,t) = \psi_{II}(x)e^{-i\omega t} = \underbrace{C' e^{i(k_2 x - \omega t)}}_{\text{wave moving right}} + \underbrace{D' e^{-i(k_2 x + \omega t)}}_{\text{wave moving left}} \qquad \text{(Region II)}$$

We see that the terms with the A' and C' coefficients correspond to harmonic waves traveling to the right and the terms with the B' and D' coefficients correspond to harmonic waves traveling to the left.

Step 3. Boundary conditions. Let's first interpret each of the terms of the solution:

- A' term: incident wave in Region I moving to the right toward the barrier. We can think of A' as the amplitude of the incident wave and treat it as a free parameter.
- B' term: wave reflected from the barrier moving back to the left in Region I.
- C' term: transmitted wave in Region II moving to the right
- D' term: This would be a wave in Region II moving to the left. But there is no physical way this wave could be generated by the incident wave A', so we rule it out as nonphysical, i.e. $D' = 0$.

Our only boundary conditions are the ones at $x = 0$. The continuity condition is:

$$\psi_I(0) = \psi_{II}(0).$$

The smoothness condition is:

$$\left.\frac{\partial \psi_I}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=0}$$

We leave the rest up to you (see problem 28 on your homework).

After evaluating the boundary conditions, you can solve for the reflection coefficient R and the transmission coefficient T. The results are:

$$R = \frac{|B'|^2}{|A'|^2} = \left[\frac{1 - k_2/k_1}{1 + k_2/k_1}\right]^2$$

and

$$T = \frac{|C'|^2}{|A'|^2} = \frac{4k_2/k_1}{(1 + k_2/k_1)^2}.$$

where

$$\frac{k_2}{k_1} = \sqrt{1 - \frac{U_0}{E}}.$$

The reflection coefficient R is the probability that a particle will be reflected by the barrier. The transmission coefficient T is the probability that it will be transmitted, i.e. pass over the barrier. Because R and T are probabilities, they must add up to unity, i.e. $R+T=1$. Remember that while the wave function contains both a reflected and a transmitted part, when you make an observation the particle will just be found on one side of the barrier or the other. It will never be observed on both sides!

Example 1. Find the reflection and transmission probabilities if the particle's energy is double the potential barrier, i.e. $E = 2U_0$.

Solution. We first calculate

$$\frac{k_2}{k_1} = \sqrt{1 - \frac{U_0}{E}} = \sqrt{1 - \frac{1}{2}} \approx 0.707.$$

The reflection probability is

$$R = \left[\frac{1 - k_2/k_1}{1 + k_2/k_1}\right]^2 = \left[\frac{1 - \sqrt{2}/2}{1 + \sqrt{2}/2}\right]^2 \approx 0.029 \text{ or } 2.9\%.$$

and the transmission probability is

$$T = \frac{4k_2/k_1}{(1 + k_2/k_1)^2} = \frac{4\sqrt{2}/2}{(1 + \sqrt{2}/2)^2} = 0.971 \text{ or } 97.1\%.$$

In classical physics, we would expect the particle to pass from Region 1 to Region II 100% of the time. It would just slow down since $K = E - U_0$ is smaller. The fact that the particle has a chance of being reflected is due to the fact that is has a wave nature.

As the energy is lowered, less particles will make it past the barrier and more will be reflected.

Example 2. Find the reflection and transmission probabilities if the particle's energy is double the potential barrier, i.e. $E = 1.01U_0$.

Solution. We first calculate

$$\frac{k_2}{k_1} = \sqrt{1 - \frac{U_0}{E}} = \sqrt{1 - \frac{1}{1.01}} \approx 0.0995.$$

The reflection probability is

$$R = \left[\frac{1 - k_2/k_1}{1 + k_2/k_1}\right]^2 = \left[\frac{1 - 0.0995}{1 + 0.0995}\right]^2 \approx 0.67 \text{ or } 67\%.$$

and the transmission probability is

$$T = \frac{4k_2/k_1}{(1+k_2/k_1)^2} = \frac{40.0995}{(1+0.0995)^2} = 0.33 \text{ or } 33\%.$$

With the energy closer to the potential barrier, we see that there is a higher chance of the particle to be reflected.

5.11 Step Potential, $E < U_0$

Now let's lower the energy of the particle so that it is lower than the potential barrier U_0.

The solution in Region I is the same as before, i.e.

$$\psi_I(x) = A'e^{ik_1x} + B'e^{-ik_1x} \qquad \text{where } k_1 = \frac{\sqrt{2mE}}{\hbar} \qquad \text{(Region I)}$$

Because we now have $U_0 - E > 0$ in Region II, the solutions are exponentials:

$$\psi_{II}(x) = C'e^{k_2'x} + D'e^{-k_2'x} \qquad \text{where } k_2' = \frac{\sqrt{2m(U_0-E)}}{\hbar} \qquad \text{(Region II).}$$

As before, let's look at the meaning of each of the four terms:

- A' term: incident wave in Region I moving to the right toward the barrier. We can think of A' as the amplitude of the incident wave and treat it as a free parameter.
- B' term: wave reflected from the barrier moving back to the left in Region I.
- C' term: exponential function diverges to ∞ as $x \to \infty$. We can rule this solution out because it is nonphysical, i.e. we want $\psi \to 0$ as $x \to \infty$. Thus, $C' = 0$.
- D' term: decaying exponential. This term satisfies our condition that $\psi \to 0$ as $x \to \infty$.

Because we set $C' = 0$, we can write the wave function in Region II as

$$\psi_{II}(x) = C'e^{k_2'x} \qquad \text{where } k_2' = \frac{\sqrt{2m(U_0-E)}}{\hbar} \qquad \text{(Region II).}$$

As before, we apply the boundary conditions at $x = 0$:

$$\psi_I(0) = \psi_{II}(0).$$

and

$$\left.\frac{\partial \psi_I}{\partial x}\right|_{x=0} = \left.\frac{\partial \psi_{II}}{\partial x}\right|_{x=0}$$

After evaluating the boundary conditions and doing some algebra, you would find

$$\frac{B'}{A'} = \frac{1+ik_2'/k_1}{1-ik_2'/k_1} \quad \longrightarrow \quad R = \left|\frac{B'}{A'}\right|^2 = 1$$

and

$$\frac{D'}{A'} = \frac{2}{1 - ik_2'/k_1} \quad \longrightarrow \quad T = \left|\frac{D'}{A'}\right|^2 = 0$$

Thus, we see that when the particle's energy is less than the potential barrier, the transmission probability is zero so it will always be reflected back to the left. Notice, however, that the coefficient $D' \neq 0$. This means that there is a nonzero probability of finding the particle to the right of the barrier in the classically forbidden zone.

5.12 Step Barrier, $E < U_0$

In this example, we imagine a stream of particles traveling to the right through space. At position $x = 0$, they experience an obstacle that requires some energy U_0 to overcome. The barrier has width L, after which the potential drops back down to $U(x) = 0$. We will find that even though it is not possible for a classical particle to "hop over" the barrier, that quantum particles have a non-zero probability of tunneling through it.

The potential is:

$$U(x) = \begin{cases} 0 & \text{for } x \leq 0 & \text{(Region I)} \\ U_0 & \text{for } 0 < x \leq L & \text{(Region II)} \\ 0 & \text{for } x > L & \text{(Region III)} \end{cases}$$

Step 1. Plug potential into the S.E. In Region I where $U(x) = 0$ so the Schrodinger equation may be written as

$$\frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi(x). \qquad \text{(Regions I and III)}$$

In regions II the potential is $U(x) = U_0$ and the Schrodinger equation is

$$\frac{\partial^2 \psi_{II}(x)}{\partial x^2} = \frac{2m(E - U_0)}{\hbar^2}\psi_{II}(x). \qquad \text{(Region II)}$$

Step 2. Solve the SE Because the particle's energy is greater than the potential in both regions, the solutions will be harmonic waves. It turns out to be easier to deal with complex exponentials in this case rather than sines and cosines. The Solutions are:

$$\psi_I(x) = A'e^{ikx} + B'e^{-ikx} \qquad \text{where } k = \frac{\sqrt{2mE}}{\hbar} \qquad \text{(Region I)}$$

$$\psi_{II}(x) = C'e^{k'x} + D'e^{-k'x} \qquad \text{where } k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar} \qquad \text{(Region II).}$$

$$\psi_{III}(x) = E'e^{ikx} + F'e^{-ikx} \qquad \text{where } k = \frac{\sqrt{2mE}}{\hbar} \qquad \text{(Region III)}$$

Problem 30 in the homework asks you to set up the boundary conditions. There are four: conditions of continuity and smoothness at $x = 0$ and $x = L$. You should also consider which (if any) of the coefficients can be set to zero because you determine them to be nonphysical.

It turns out that the tunneling probability (i.e. the probability of the particle making though the barrier and "popping out" in region III) is

$$T = \left|\frac{E'}{A'}\right|^2 = \frac{1}{1 + \left(\frac{k^2+k'^2}{2k'k}\right)^2 \sinh^2(k'L)} \tag{5.1}$$

Since $k'L \gg 1$ in most cases we can approximate $\sinh^2(k'L) \approx e^{2k'L}$. Furthermore, since $e^{2k'L} \gg 1$ the transmission probability simplifies to

$$T \approx \left(\frac{k^2 + k'^2}{2k'k}\right)^2 e^{-2k'L} \tag{5.2}$$

or

$$T \approx \frac{16E(U_0 - E)}{U_0^2} e^{-2k'L}. \tag{5.3}$$

As we will in see in the next example, the exponential factor is an *incredibly* small number for any macroscopic problem. However it can become significant on the atomic scale.

Example 3. Find the tunneling probability for a particle with mass $m = 1$ gm to tunnel through a barrier with width $L = 1$ cm and $U_0 - E = 1$ erg $= 10^{-7} J$.

Solution. We first calculate

$$k' = \frac{\sqrt{2m(U_0 - E)}}{\hbar} = \frac{\sqrt{2 \cdot 10^{-3} \text{ kg } \cdot 10^{-7} \text{ J}}}{1.055 \times 10^{-34} \text{ J s}} \approx 10^{29} \text{ m}^{-1}$$

so

$$2k'L = 2(10^{29} \text{ m}^{-1})(10^{-2} \text{ m}) \approx 10^{27}$$

To order of magnitude, we can ignore the leading coefficient that depends on E and U_0 to estimate the tunneling probability to be about

$$T \approx e^{-2k'L} \approx e^{10^{-27}}.$$

Again, to order of magnitude, we find

$$T \approx \frac{1}{10^{10^{27}}} = \frac{1}{10^{1000000000000000000000000000}}$$

which is so small, we can safely say that this has never happened in the lifetime of our visible universe.