

Chapter 13. Potential Surfaces and the Heisenberg Uncertainty Principle.

Inarguably the most recognized statement in quantum mechanics is, “You can’t know where something is and how fast it is going.” However, the real meaning and implications of the Heisenberg uncertainty principle could not be made less clear. At the heart is the statistical nature of quantum, and the fact that different properties are correlated by the operators that describe them. Furthermore, the Heisenberg uncertainty principle is dynamic. For example, let’s say that you localize a quantum particle to a spot that you know absolutely. As a result, you can’t know the speed at all, and this requires that the speed is actually quite high. After all, if you know where something is and you know it’s not moving, then you have completely upended the principle! Last, there are actually several uncertainty principles, such as you can’t know where something is and its energy at the same time.

13.1 Potential Energy Surfaces.

13.1.1 The step potential. We have discussed the most simple potential surface possible in the previous chapter- the one dimension “freewave” potential that never ends. Unfortunately, the Universe (at times) can be quite a bit more complicated. So, introduced here quite literally the first step towards understanding more complex problems: the step potential shown in Figure 13.1. Now that potential energy has entered into the equation, we define the Schrodinger equation which now has two parts depending on whether the particle is to the left or right of the barrier:

$$x < 0: \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_I(x) = E \cdot \psi_I(x)$$

$$x > 0: \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{II}(x) + V_0 \cdot \psi_{II}(x) = E \cdot \psi_{II}(x)$$

Clearly there must be two solutions, one for the left side with no potential and another for the right. By “solution” we mean the wavefunction, and from the wavefunctions we can determine the energy of the

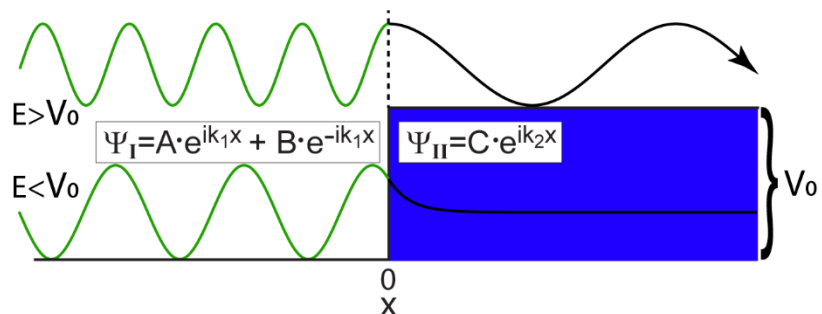


Figure 13.1. The step potential problem demonstrates how a quantum object reflects off a barrier.

system and many other properties. Since we have already discussed the solution to the flat potential “free wave”:

$$\psi_I = A \cdot e^{ik_1x} + B \cdot e^{-ik_1x}$$

Now as for the 2nd region, it turns out that since the potential energy is finite but flat that the same solution applies albeit with a different wavevector k_2 :

$$\psi_{II} = C \cdot e^{ik_2x} + D \cdot e^{-ik_2x}$$

Here, the wavevectors are as defined in the previous chapter: $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ and: $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$.

The second wavevector can be found by simply rearranging the Schrodinger equation in region II as: $\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi_{II}(x) = (E - V_0) \cdot \psi_{II}(x)$, and thus one can see that where we had “E” in k_1 is now replaced with $(E - V_0)$ in k_2 . Furthermore, $k_2 < k_1$, which makes sense since the k ’s are related to the kinetic energy, which is the difference in the total energy minus the potential energy. Hence, the particle in region II must be moving slower and has a correspondingly lower k_2 .

The next step is to question what are we solving any of this for? The original freewave problem is great for developing a fundamental understanding of wavefunctions and operators, but it is also very unrealistic. As for the step potential, its utility is that it shows what happens when a quantum mechanical particle encounters a barrier. A classical (Newtonian) particle will only do two things, bounce off the barrier if the energy is lower than the potential or cross over otherwise. As we will see here, a quantum particle is very different.

13.1.2 Reflection and Transmission. Up until now, you have been told that if a particle has enough energy, perhaps by a statistical process as described by the Boltzmann distribution, it certainly traverses over the energy hill. Here, we will show you a quantum particle isn’t as cooperative. The next two topics will introduce how quantum particles interact with barriers. This is literally the definition of dynamics, and here we show that quantum particles such as electrons in light atoms do new things that a “classical” particle such as a pickup truck doesn’t.

As for the utility of the step potential, we can create a phenomenological model whereby a 1-dimensional universe is created with a particle to the right of the barrier. The particle is designed with kinetic energy and leftwards momentum, for which the correct wavefunction is:

$$\psi_I(x) = A \cdot e^{ik_1x}$$

If the particle reflects off the barrier, it must move to the left with the same kinetic energy and momentum due to conservation of energy. Thus, the wavefunction in region I is actually:

$$\psi_I(x) = A \cdot e^{ik_1x} + B \cdot e^{-ik_1x}$$

We can refer to the “A” wave as the incoming particle and the “B” wave as the reflected particle. This is because the probability amplitude of the incoming wave is:

$$|A \cdot e^{ik_1x}|^2 = |A|^2 \cdot e^{-ik_1x} \cdot e^{ik_1x} = |A|^2 \cdot e^0 = |A|^2$$

Likewise the probability amplitude of the reflecting wave is $|B|^2$. If the particle transmits over the barrier it can only continue to the right, since there will not be any more walls to bound off of:

$$\psi_{II}(x) = C \cdot e^{ik_2x}$$

Hence we refer to the “C” wave as the transmitted wave. We set “D” equal to 0 because the quantum particle cannot turn left if it goes over the barrier (i.e. it forever more moves to the right).

The nature of the utility of the finite step potential is that it demonstrates the probability that a quantum object with transmit or reflect off a barrier. Clearly this is related to the coefficients A, B, and C, so we seek to solve these constants as a function of energy. Due to the fact that the absolute value of a wavefunction is related to probability, it is true that the probability of reflection (R) is: $R = \frac{|B|^2}{|A|^2}$ and thus $\sqrt{R} = \frac{B}{A}$. Hence, the reflection is the probability that a wave turns left divided that it was moving right to begin with (hopefully this makes sense). We will solve for \sqrt{R} first. To do so, we invoke a stipulation from the previous chapter that wavefunctions be continuous and smooth. There would only be a potential problem at the step, $x=0$, because this is where the two different solutions meet. Thus:

$$\psi_{I,(x=0)} = \psi_{II,(x=0)} \text{ (continuous) and: } \frac{\partial\psi_{I,(x=0)}}{\partial x} = \frac{\partial\psi_{II,(x=0)}}{\partial x} \text{ (smooth)}$$

These equations will allow us to solve all the coefficients, and in fact it turns out there is a great shortcut to this problem. That is to equate the log derivative: $\partial \ln(\psi) = \frac{\psi'}{\psi}$ of each side at $x=0$:

$$\frac{\psi_I'(x=0)}{\psi_I(x=0)} = \frac{\psi_{II}'(x=0)}{\psi_{II}(x=0)}$$

Hence:

$$\frac{A \cdot ik_1 e^0 - B \cdot ik_1 e^0}{A \cdot e^0 + B \cdot e^0} = \frac{C \cdot ik_2 e^0}{C \cdot e^0}$$

$$k_1 A - k_1 B = k_2 A + k_2 B$$

This can be simplified to:

$$\sqrt{R} = \frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

Using a similar analysis one can find that:

$$\sqrt{T} = \frac{2\sqrt{k_1 k_2}}{k_1 + k_2}$$

Now that we have these relationships, what we do with them is calculate the values of k 's as a function of energy for a realistic system. By "realistic",

first consider that a car is not very quantum mechanical but an electron is. So, we will

describe an electron using a mass of 9.109×10^{-31} kg. The only other parameter of the model is the potential step V_0 . For this, we will use $V_0 = 1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$, which is an electron volt (the energy an electron experiences travelling through a 1 Volt potential). Plotted in Figure 13.2 are the reflections and transmissions, where you can see that having enough energy to get over a barrier, does not mean that you go over the barrier! It's likely, but not assured. The particle hitting the barrier with greater energy helps, which is about the only thing that makes sense.

13.1.3 Tunneling. The next step up in complexity is the finite barrier shown in Figure 13.3. This is just the step potential that steps back down after a length of L . As before, we should ask ourselves what lessons can be learned from this system, which as can be seen in the figure we might find that a particle, with an energy less than the potential, may not decay to 0 before it reaches the end of the barrier. What happens then? As we show here, the particle can continue to the right (forevermore), meaning that the particle has gone through a barrier even though it doesn't have enough energy to do so. Imagine a pickup truck with an idling engine suddenly going over

As in the previous example the waves are the "A" on-coming wave and the "B" reflected one.

There is a "C" and "D" that represent transmission through the barrier and reflection off the

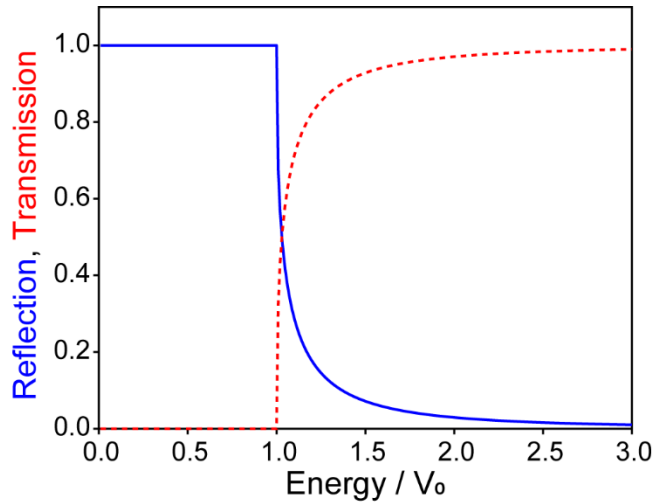


Figure 13.2. Reflection and transmission as a function of the particle's energy.

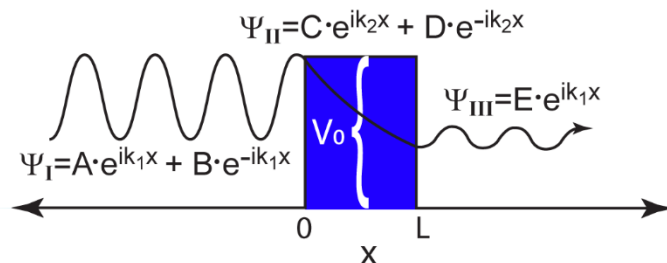


Figure 13.3. The finite barrier problem demonstrates the process of tunneling through a barrier.

interface at $x=L$, respectively. The “E” wave is fully transmitted. You might wonder why there is a “D” wave, after all, the particle isn’t encountering a higher potential barrier (rather, quite the opposite!). The reason that the “D” wave exists is because all interfaces cause reflection, even when one traverses from a higher potential to a lower one. For example, you can see your reflection in a car with new black paint, right? This is the same idea.

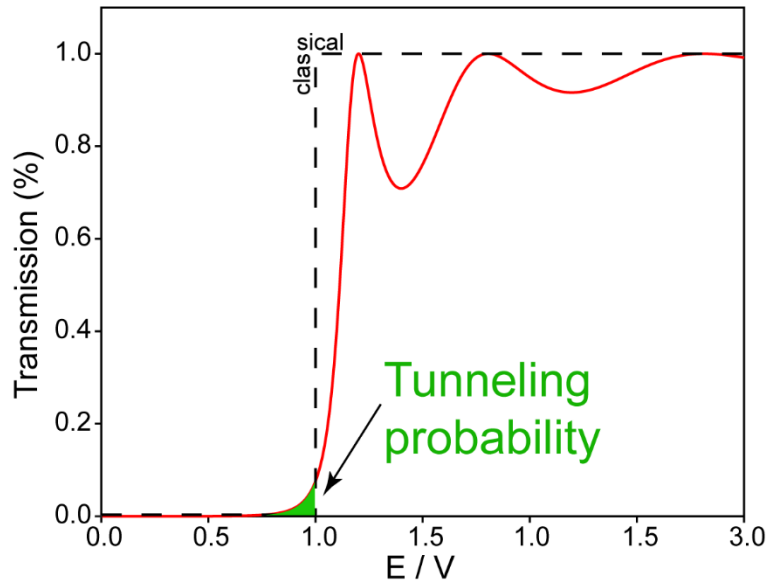


Figure 13.4. The %Transmission of a quantum particle through a barrier reveals some probability of passing through despite not having enough energy to do so!

For this problem the main lesson to be learned is to examine the %transmission, $|E|^2$, as a function of energy as shown in Figure 13.4. Here we see structure in the %T as a function of increasing energy. These are called “resonances”, and they are observed because the electron’s wavelength perfectly matches the size of the barrier. Next, we see that there is some area under the curve for energies below the barrier. This is quantum tunneling, a phenomenon that has been experimentally verified countless times. This means that the particle penetrates through the barrier despite the fact that it doesn’t classically have enough energy to do so. This is also where students state that quantum mechanics stipulates that a person can walk through a door; correct, but highly improbable!

13.1.4 The particle in a box. The next potential energy surface on our list is the “particle-in-a-box”, which has $V(x)=\infty$ at $x \leq 0$ and $x \geq L$ and $V(x)=0$ everywhere in-between. This model system can be applied to understand many real phenomena and can also be used to describe electrons in atoms. For the latter case, this works because an electron sees a hydrogen’s proton like a trap- Coulomb’s law keeps it close by since there is a huge energy penalty to be far away. Shown in Figure 13.5 is the particle in a box’s potential energy surface and first two wavefunctions, which due to the fact that the potential is flat can be described using:

$$\psi_{II}(x) = A \cdot e^{ik_1x} + B \cdot e^{-ik_1x}$$

Given the infinite potentials at the boundaries it must be true that: $\psi_{x=0} = 0$ and: $\psi_{x=L} = 0$, which are boundary conditions. If these conditions weren't true then the particle can technically escape the box, which requires a nominal infinite amount of energy. These also allow us to solve the wavefunction by satisfying the boundary conditions. Given that, at $x=0$:

$$A \cdot e^{ik_1x} + B \cdot e^{-ik_1x} = 0$$

Then $A + B = 0$ and $A = -B$. We recognize that the symmetry imparted by the fact that means:

$$\psi(x) = \sin(k_1x)$$

Now we have to apply the second boundary condition at $x=L$:

$$\sin(k_1L) = 0$$

which can only be true if $k_1L = n\pi$, allowing us to solve for the wave vector:

$$k_1 = \frac{n\pi}{L}$$

where n is an integer that goes from 1,2,3...

As a result, the wavefunction is $\psi(x) = N \cdot \sin\left(\frac{n\pi}{L}x\right)$ and 0 everywhere else due to the infinite potential. Also N is the normalization constant. Notice how we have solved the wavefunction without worrying about normalization? To find that part we note that:

$$N^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

We can use the internet to find that, and solving for N yields:

$$\psi_{II}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

Last, we can calculate the energy either using the eigenvalue or expectation value methods; you should try that for an exercise. The result is:

$$E = \frac{n^2 \hbar^2 \pi^2}{2mL^2} = \frac{n^2 h^2}{8mL^2}$$

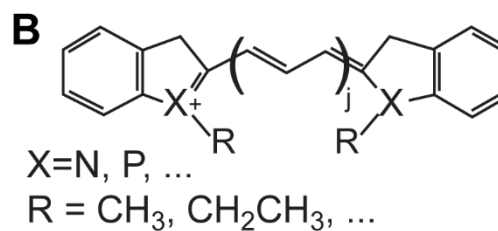
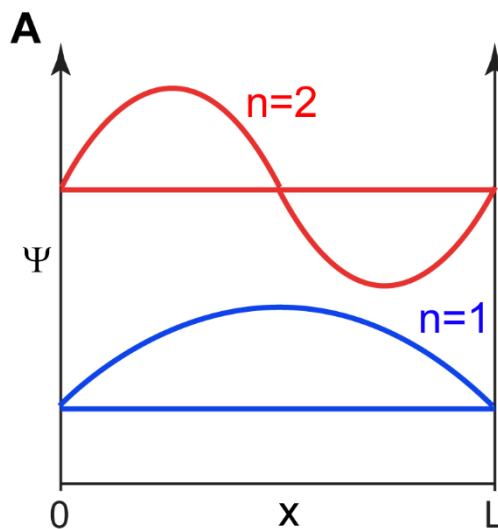


Figure 13.5 A. The particle in a box potential and first two states. **B.** The potential is a good model for cyanine dyes.

where we used the fact that $\hbar^2 = \frac{h^2}{4\pi^2}$.

The particle in a box describes many things. Shown in Figure 13.5B are cyanine dyes, where the length of the alternating double bonds in the center of the molecule represents the length of the box. Lengthening this part of the molecule causes a red-shift in the dye absorption and emission. Shown in Figure 13.6 is a more dramatic example using nanotechnology, specifically semiconductor CdSe quantum dots. The emission of the particles can be tuned by changing the diameter on the order of just a few nanometers. And as solid-state materials, these particles are significantly more robust against degradation from the environment, which is why they are being incorporated into displays, including television sets!



Figure 13.6. Semiconductor quantum dots change their emission color based on the size of the nanoparticle. Typical sizes are 2→10 nm.

13.1.5 The particle in the finite box. The following is the same as the infinite box without the potential energy going to infinity outside the trap area as shown in Figure 13.7A. A better analogy is an upside-down finite barrier, mostly because the problem is unfortunately difficult to solve. Note that we have centered the box at $x=0$ for mathematical convenience as you will see later. There are two issues to consider, namely that there are three regions each of which has a different wavefunction. As in the finite box, we will use boundary conditions to solve for the allowed energy levels as there are bound solutions for $E < V_0$. For $E > V_0$, the solutions are unbound, meaning that the wavefunctions are just waves and any energy is allowed. We won't consider that situation and will instead only study the case where $E < V_0$.

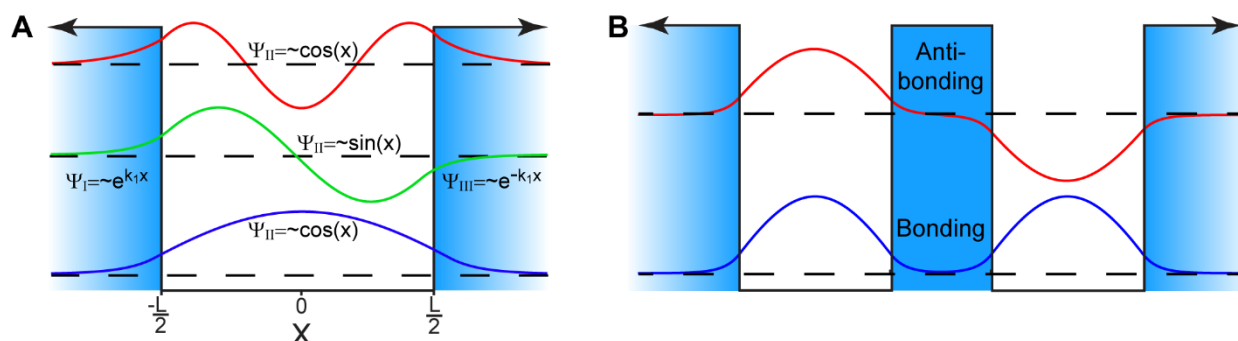


Figure 13.7A. The finite box problem is centered at $x=0$, and has alternating even- and odd-symmetric solutions. **B.** The ground and 1st excited state of a particle between two finite boxes look like bonding and antibonding orbitals.

It is possible to spend quite a bit of time on this system, so we will limit the discussion to an analysis of the ground state. We assume that the trap region has an even symmetry wavefunction, i.e. $\psi_{II} = B \cdot \cos(k_2 x)$, where $k_2 = \sqrt{\frac{2mE}{\hbar^2}}$ since there is no potential energy in that region. If the particle somehow breaks out on the left it will continue in that direction, implying $\psi_I = A \cdot e^{k_1 x}$ where $k_1 = \sqrt{\frac{2m(V-E)}{\hbar^2}}$. Using the same logic $\psi_{III} = C \cdot e^{-k_1 x}$. As per the boundary conditions, the wavefunctions must be continuous and smooth at the region I/II boundary:

$$A \cdot e^{-k_1 \cdot L/2} = B \cdot \cos\left(-k_2 \frac{L}{2}\right) \quad \text{and} \quad k_1 \cdot A \cdot e^{-k_1 \cdot L/2} = -k_2 \cdot B \cdot \sin\left(-k_2 \frac{L}{2}\right)$$

and likewise for region II/III:

$$B \cdot \cos\left(k_2 \frac{L}{2}\right) = C \cdot e^{-k_1 \cdot L/2} \quad \text{and} \quad -k_2 \cdot B \cdot \sin\left(k_2 \frac{L}{2}\right) = -k_1 \cdot C \cdot e^{-k_1 \cdot L/2}$$

Solving using log boundary conditions yields what is called a “transcendental” equation for k_1 and k_2 :

$$\tan\left(k_2 \frac{L}{2}\right) = \frac{k_1}{k_2}$$

This is an equation which requires you to search for an energy which satisfies the above, given your potential energy descriptors (length of the box, potential height, and mass of the particle). You have to use a computer in this regard, and once you know the allowed energies you can determine the A, B etc. coefficients and then plot the wavefunctions as shown in Figure 13.7A.

One last interesting point is that the finite box is a very good representation of an atom and can even give us an idea about chemical bonds if we allow two finite boxes to get close to each other. Shown in Figure 13.7B are the ground and 1st excited states for a particle between two finite boxes. Due to the way the wavefunction “bunches” between the two traps in the ground state while a node prevents the same in the excited state, we can say that these look just like bonding and antibonding orbitals!

13.2. Complex Potential Energy Surfaces: Vibration. We will take our first step into a non-flat potential surface by looking at harmonic oscillators, also known as springs. Also known as chemical bonds.

13.2.1 Turning points. An interesting aspect of quantum mechanics is revealed by the vibrational potential energy surface.

13.3 Superposition: Wavefunctions as Waves. We will first demonstrate the idea of uncertainty in quantum mechanics using the well-known position / momentum version. To begin, we will start with a wavefunction, and while any old wavefunction will do let's use a Gaussian (bell-shaped) one that is centered inside a box that goes from $0 \leq x \leq L$:

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-L/2)^2}{4\sigma^2}}$$

We will consider two wavefunctions, one that is “delocalized” and thus wide and another that is narrow that we call “localized”. Hopefully it is intuitively clear that there is more certainty in the position of the localized state vs. the delocalized state.

In the previous chapter we introduced the idea that an eigenfunction of one operator, ψ , can be expressed as a linear combination of the eigenfunctions of another, Φ_n :

$$\psi = \sum c_n \cdot \Phi_n$$

and for our purposes we will make all the Φ_n 's the particle in a box states:

$$\Phi_n = \sqrt{\frac{2}{L}} \cdot \sin\left(n\pi \frac{x}{L}\right)$$

This is referred to as a superposition of states. These functions are all graphed in Figure 13.8.

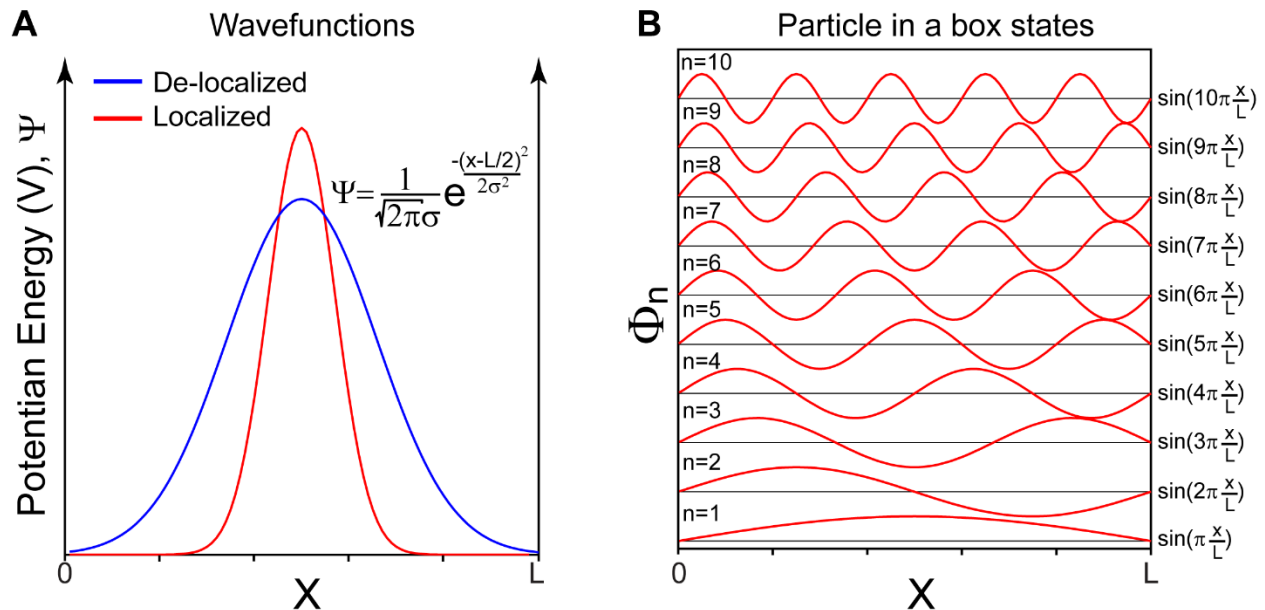


Figure 13.8. A. Localized (red) and delocalized (blue) Gaussian-type wavefunctions have different kinetic energies due to the uncertainty principle. **B.** Particle in a box states can be summed into a superposition that equates to any other function, such as the localized and delocalized states shown in A.

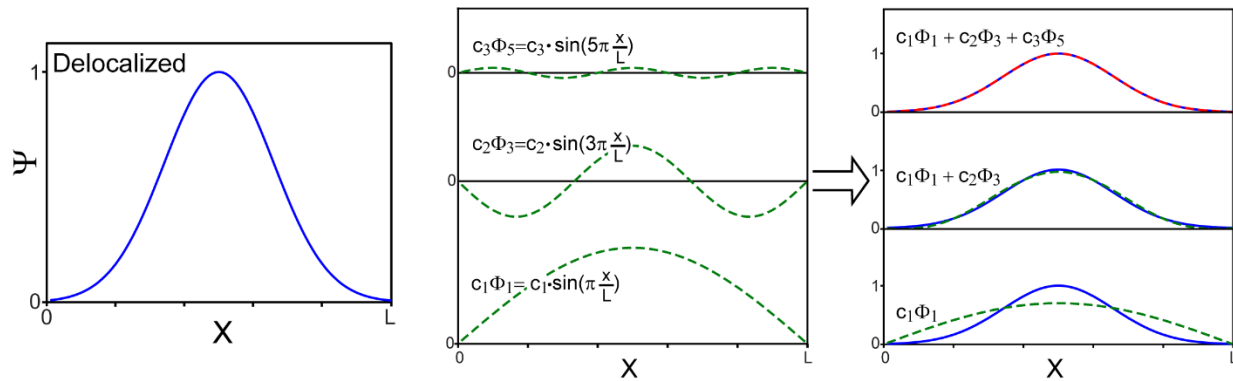


Figure 13.9. A delocalized (blue) Gaussian-type wavefunctions can be constructed by summing several particle in a box states times appropriate weighing functions. The states have to have even symmetry. A sum of just three states can provide a near-perfect representation of the delocalized state.

Now for the superposition. In Figure 13.9 we show that the wider bell-shaped state on the left can be equated to a sum of particle in a box wavefunctions of even symmetry ($n=1, 3, 5$, etc.) weighted by an appropriate amount. Technically, this delocalized function or any other can have perfect overlap with a superposition of particle in a box states so long as an infinite number of those states are summed. However, just adding three particle in a box states does such a good job that it is hard to discern any difference between them as shown here:

A very different result is observed with the localized state shown in Figure 13.10. Here, it is necessary to sum at least 5 particle in a box states to provide a reasonable representation of the original function. Even then the overlap isn't as good as observed with the delocalized state in Figure 13.9 even though more functions are used!

Now you are probably asking what any of this has to do with the uncertainty principle. To answer, let's now measure other properties such as the momentum. The measurement will require us to do an experiment, and any good experimentalist the measurement will be repeated several times to statistically quantify the average value and standard deviation of the results. This is necessary because the same momentum won't be measured in every experiment. In fact, we contend that each measurement will return the momentum of one of the particle in a box's states, which is $\hbar k = \hbar \cdot \frac{n\pi}{L}$, with a probability $|c_n|^2$. Thus, measuring the momentum from the delocalized state will return one of the three composing particle in a box's state's momentum with corresponding probabilities of $|c_1|^2$, $|c_2|^2$, or $|c_3|^2$, which would have an average value of:

$$\langle p \rangle = |c_1|^2 \cdot \hbar \frac{\pi}{L} + |c_2|^2 \cdot \hbar \frac{3\pi}{L} + |c_3|^2 \cdot \hbar \frac{5\pi}{L}$$

In contrast, when the same experiment is repeated on the localized state, each measurement may return one of five values of momentum with corresponding probabilities of $|c_1|^2$, $|c_2|^2$, $|c_3|^2$, $|c_4|^2$, or $|c_5|^2$. Now here is a good question, which result has greater certainty? Of course, there is greater certainty in making measurements off the delocalized state since each measurement returns one of just three values, and probably we won't have to make too many measurements before we are comfortable with the resultant average value. However, measuring properties from the localized state is more problematic since the variations from our multiple measurements are greater. This is due to the fact that five particle in a box eigenfunctions equate to the localized state, and thus we will have to make more measurements to have the confidence in an average value. We conclude that the certainty in position is anticorrelated to the certainty in other properties such as momentum. This is in fact the Heisenberg uncertainty principle, "you can't know something is and how fast it's going at the same time." Clearly there is more certainty in position for the localized state shown in Figure 13.1.A, and correspondingly less knowledge of the position of the delocalized one. Mathematically, this is expressed by the variance in the function, the square root of which is the standard deviation (σ) you may recall from your first introduction into statistics; more on this later.

The above demonstration isn't really that exact and was meant to give the reader a graphical description of uncertainty in quantum mechanics. Now, we must slog through the more rigorous mathematics. First, let's define uncertainty via the variance, and we will start with position:

$$\text{Var}(x) = \frac{1}{N-1} \sum_{i=1}^N (x_i - \bar{x})^2 = \langle x^2 \rangle - \langle x \rangle^2$$

You are probably familiar with the summation from an introduction to statistics in high school. The second expression might also be familiar to you, these are expectation values. Let's calculate the variance in the position for our bell-shaped wavefunction $\psi(x) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-L/2)^2}{2\sigma^2}}$.

$$\langle \hat{x} \rangle = \int_{\text{lower}}^{\text{upper}} \psi_n^* \hat{x} \psi_n \cdot d\tau \approx \int_{-\infty}^{\infty} \left(\frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-L/2)^2}{4\sigma^2}} \right)^* \cdot x \cdot \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-L/2)^2}{4\sigma^2}} \cdot dx =$$

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x \cdot e^{-\frac{(x-\frac{L}{2})^2}{2\sigma^2}} \cdot dx = \frac{L}{2}$$

Next we calculate

$$\langle \widehat{x^2} \rangle = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} x^2 \cdot e^{-\frac{(x-\frac{L}{2})^2}{2\sigma^2}} \cdot dx = \sigma^2 + \left(\frac{L}{2}\right)^2$$

As a result $\langle \widehat{x^2} \rangle - \langle \widehat{x} \rangle^2 = \sigma^2 + \left(\frac{L}{2}\right)^2 - \left(\frac{L}{2}\right)^2 = \sigma^2$. This is a perfectly sensible result, and in fact it is a standard statistical definition that the variance of a bell-shaped curve is σ^2 . Better yet, we know that we did the integrals correctly!

Now let's look at momentum; this is shall we say a bit more arduous:

$$\begin{aligned} \langle \widehat{p} \rangle &= \int_{\text{lower}}^{\text{upper}} \Psi_n^* \widehat{p} \Psi_n \cdot d\tau \approx \int_{-\infty}^{\infty} \left(\frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \right)^* \cdot \frac{\hbar}{i} \frac{\partial}{\partial x} \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot dx = \\ &= \frac{\hbar}{i\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot \frac{\partial}{\partial x} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot dx = \frac{\hbar}{i\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot \frac{(x-\frac{L}{2})}{2\sigma^2} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot dx = \\ &= \frac{\hbar}{i\sqrt{8\pi\sigma^3}} \int_{-\infty}^{\infty} \left(x - \frac{L}{2}\right) \cdot e^{-\frac{(x-\frac{L}{2})^2}{2\sigma^2}} \cdot dx = 0 \end{aligned}$$

No average momentum. The average of the momentum squared takes a bit more algebra:

$$\begin{aligned} \langle \widehat{p^2} \rangle &= \int_{\text{lower}}^{\text{upper}} \Psi_n^* \widehat{p^2} \Psi_n \cdot d\tau \approx -\hbar^2 \int_{-\infty}^{\infty} \left(\frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \right)^* \cdot \frac{\partial^2}{\partial x^2} \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot dx = \\ &= \frac{-\hbar^2}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot \frac{\partial^2}{\partial x^2} e^{-\frac{(x-\frac{L}{2})^2}{4\sigma^2}} \cdot dx = \frac{-\hbar^2}{\sqrt{32\pi\sigma^5}} \int_{-\infty}^{\infty} \left(\frac{L^2}{4} - 2\sigma^2 - Lx + x^2 \right) \cdot e^{-\frac{(x-\frac{L}{2})^2}{2\sigma^2}} \cdot dx = \frac{\hbar^2}{4\sigma^2} \end{aligned}$$

As a result, the variance in momentum is: $\langle \widehat{p^2} \rangle - \langle \widehat{p} \rangle^2 = \frac{\hbar^2}{4\sigma^2}$

To summarize, we see that the uncertainty in position and momentum are anticorrelated; the position uncertainty scales as σ^2 , however, the same for momentum is inversely proportional to σ^2 .

It turns out that there is a theorem in geometry that can assist us with understanding the Heisenberg Uncertainty Principal. It's called the Cauchy-Schwartz inequality, and using it we can do a short derivation to show that:

$$\text{Var}(\hat{x}) \cdot \text{Var}(\hat{p}) \geq \frac{1}{4} |[\hat{x}, \hat{p}]|^2$$

Where we introduce a new mathematical entity called a commutator:

$$[\hat{x}, \hat{p}] = \hat{x} \cdot \hat{p} - \hat{p} \cdot \hat{x}$$

NOT DONE YET!

There are several meanings to unpack here.

$$\text{Therefore: } \left(\frac{\hbar^2 L^2}{2\sigma^4} \right) (\sigma^2) = \frac{\hbar^2 L^2}{2\sigma^2}.$$

Problems: Numerical

1. If the uncertainty principal for position and momentum is: $\sigma_x^2 \cdot \sigma_p^2 \geq \frac{1}{4} |[\hat{x}, \hat{p}]|^2$

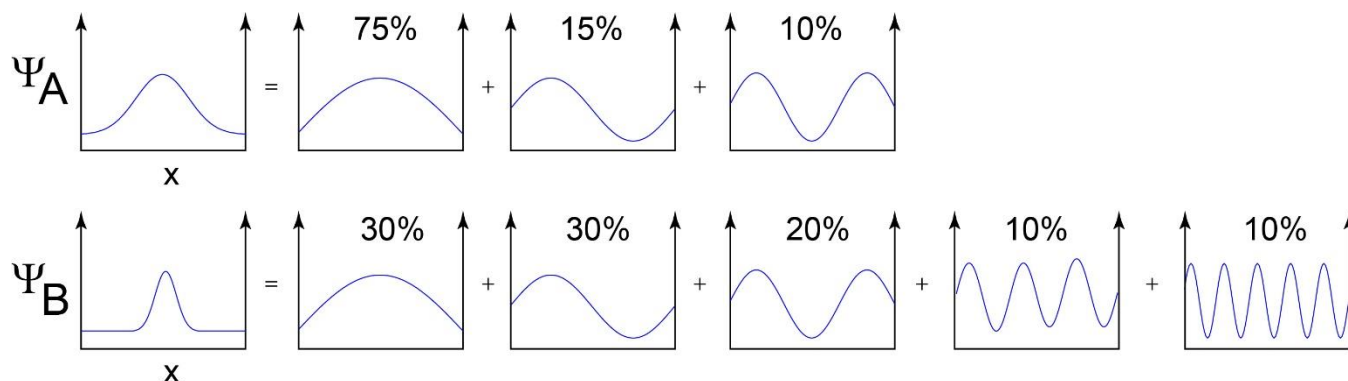
And since we showed in class that: $\frac{1}{4} |[\hat{x}, \hat{p}]|^2 = \frac{1}{4} \left| \frac{\hbar}{i} \right|^2 = \frac{\hbar^2}{4}$, therefore:

$$\sigma_x^2 \cdot \sigma_p^2 \geq 0.25 \cdot \hbar^2$$

Can you show that this principle is consistent with the σ_x^2 and σ_p^2 determined in problems 4 and 5 for $\Psi(x) = \frac{2}{L} \cdot \sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)$? **(3 pts)**

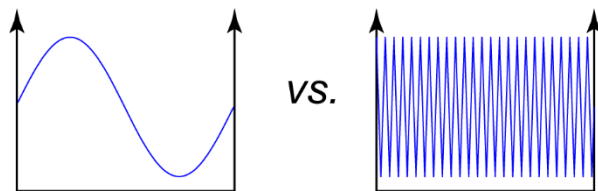
2. In class, I mentioned that the uncertainty principal “does things”. Here is what I mean:

We decomposed the particle in a box wavefunctions shown below (A & B) into momentum wave eigenstates (i.e. e^{ikx}) as shown below:



Recall that, as the “A” state has more uncertainty in position, it can be decomposed into just a few momentum waves. However, the “B” state requires more momentum waves, perhaps ~ 100 of them. Also look at the handout for a definitive example that was done with computer analysis.

a. How does the energy of the momentum waves change? Better yet, just tell me which momentum wave below has more energy and why: **(2 pts)**



b. Given your answer in pt. a, which of the two wavefunctions (the delocalized state “A” or more localized state “B”) have more kinetic energy and why? **(8 pts)**

Hint: I have made up a table of components 1 \rightarrow 5 that have respective energies of 1 J \rightarrow 5 J, and the percent that each contributes to states A and B. Use these data to find the average

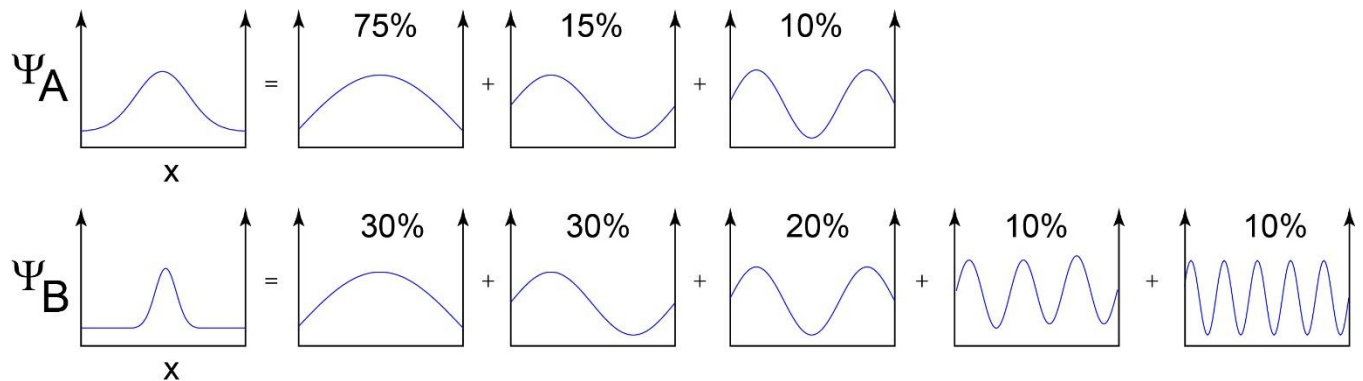
values of energies for states A and B, which should give you some insight into how to answer this problem.

Energy (eV)	%A	%B
1	75%	30%
2	15%	30%
3	10%	20%
4	0%	10%
5	0%	10%

This should help you understand how increasing the percent of higher energy states will affect the total energy.

3. In class, I mentioned that the uncertainty principal “does things”. Here is what I mean:

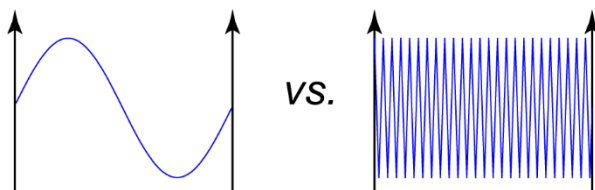
We decomposed the particle in a box wavefunctions shown below (A & B) into momentum wave eigenstates (i.e. $e^{ik \cdot x}$) as shown below:



Recall that, as the “A” state has more uncertainty in position, it can be decomposed into just a few momentum waves. However, the “B” state requires more momentum waves, perhaps ~100 of them. Also look at the handout for a definitive example that was done with computer analysis.

a. How does the energy of the momentum waves change? Better yet, just tell me which momentum wave below has more energy and why:

(2 pts)



b. Given your answer in pt. a, which of the two wavefunctions (the delocalized state “A” or more localized state “B”) have more kinetic energy and why?

(8 pts)

Hint: I have made up a table of components 1→5 that have respective energies of 1 J →5 J, and the percent that each contributes to states A and B. Use these data to find the average values of energies for states A and B, which should give you some insight into how to answer this problem.

Energy (eV)	%A	%B
1	50%	30%
2	30%	20%
3	20%	20%
4	0%	15%
5	0%	15%

This should help you understand how increasing the percent of higher energy states will affect the total energy.

4. HCl gas has an absorption at 2990 cm^{-1} ; this is one of the highest frequencies that is known in the infrared spectrum (the IR range is $200 \rightarrow 13,000\text{ cm}^{-1}$). Using this information can you estimate the force constant k_f of the spring (bond) that connects the H and Cl? Recall that the energy of a harmonic oscillator is $E = \left(v + \frac{1}{2}\right) \hbar\omega =$

$\left(v + \frac{1}{2}\right) \hbar \sqrt{\frac{k_f}{\mu}}$, where μ is the reduced mass: $\mu = \frac{m_1 m_2}{m_1 + m_2}$. **Hint:** The ground state has $v = 0$, and $1\text{ cm}^{-1} = 1.986 \times 10^{-23}\text{ J}$. The mass of H is 1 amu and Cl is 35.5 amu. **(7 pts)**
 Hint-hint: Did you get $\sim 2050\text{ N/m}$? Then you forgot that absorption wavelength is due to the **difference in energy** between the 1st excited and ground state (final energy – initial energy).

5. Deuterium chloride (DCl) gas has an absorption at 2144 cm^{-1} in the infrared (the IR range is $200 \rightarrow 13,000\text{ cm}^{-1}$). Using this information can you estimate the force constant k_f of the spring (bond) that connects the D and Cl? Recall that the energy of a harmonic oscillator is $E = \left(v + \frac{1}{2}\right) \hbar\omega = \left(v + \frac{1}{2}\right) \hbar \sqrt{\frac{k_f}{\mu}}$, where μ is the reduced mass: $\mu = \frac{m_1 m_2}{m_1 + m_2}$.

Hint: The ground state has $v = 0$, and $1\text{ cm}^{-1} = 1.986 \times 10^{-23}\text{ J}$. The mass of D is 2 amu and Cl is 35.5 amu. Hint-hint: Did you get $\sim 2050\text{ N/m}$? Then you forgot that absorption wavelength is due to the **difference in energy** between the 1st excited and ground state (final energy – initial energy). **(7 pts)**

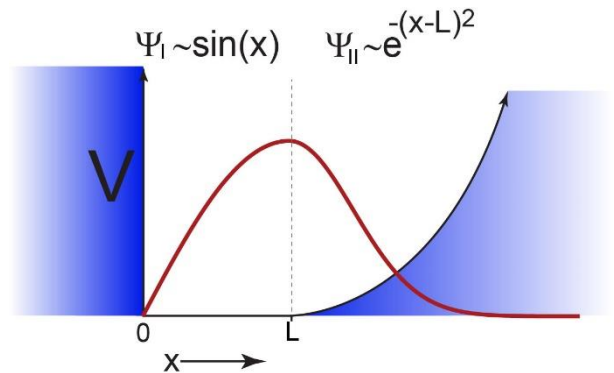
Problems: Theoretical or Explain in Words

1. If I have a potential energy surface as shown on the right, then the solution to the Schrodinger equation to the left of $x=L$ is:

$$\Psi_I(x) = A \cdot \sin\left(\pi \cdot \frac{x}{2L}\right)$$

To the right of $x=L$ is:

$$\Psi_{II}(x) = B \cdot e^{-(x-L)^2}$$



a. Why is the wavefunction in region I a sine function? (3 pts)

Why not a cosine function?

b. What is the relationship between constants A and B? (3 pts)

Hint: This is a derivation question, and the wavefunctions must be continuous. Thus, the “right” wavefunction must equal the “left” one at $x=L$.

c. Show that the wavefunctions are smooth at $x=L$. (3 pts)

Hint: Now that you know how A is related to B, you can show that the derivatives of the wavefunctions are equal at $x=L$.

2. If I have a potential energy surface as shown on the right, then the solution to the Schrodinger equation to the left of $x=0$ is:

$$\Psi_I(x) = A \cdot \cos\left(\pi \cdot \frac{x}{2L}\right)$$

To the right of $x=0$ is:

$$\Psi_{II}(x) = B \cdot e^{-x^2}$$

a. Why is the wavefunction in region I a cosine function? Why not a sine function? (3 pts)

b. What is the relationship between constants A and B? (3 pts)

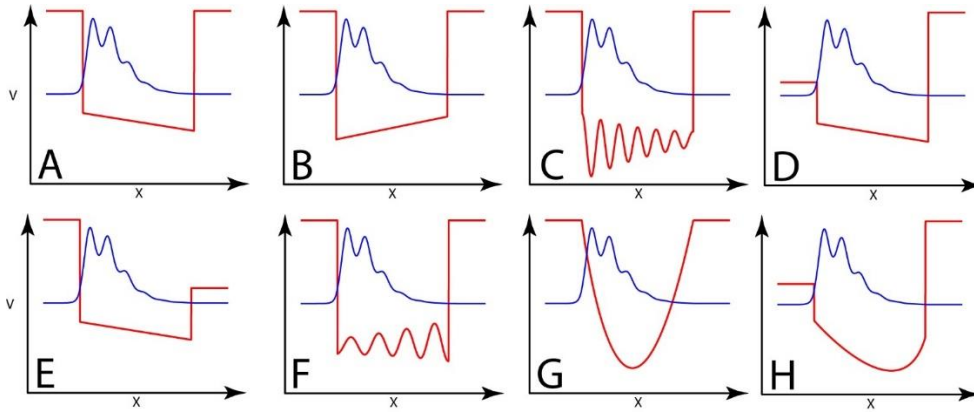
Hint: This is a derivation question, and the wavefunctions must be continuous. Thus, the “right” wavefunction must equal the “left” one at $x=0$.

c. Show that the wavefunctions are smooth at $x=0$. (3 pts)

Hint: Now that you know how A is related to B, you can show that the derivatives of the wavefunctions are equal at $x=0$.

3. I have calculated a wavefunction, in blue, for one of the potential surfaces (red) below. Only one of them is correct- can you identify which potential function is correct and please state why?

(7 pts)



4. For a free wave hitting a barrier:

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

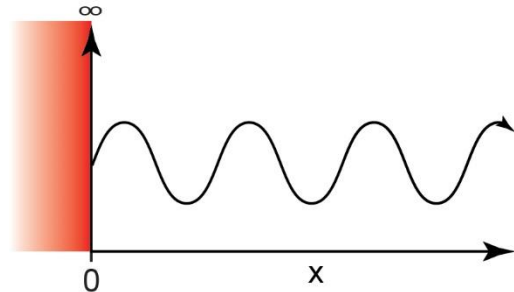
where k_1 is real since $k_1 = \frac{\sqrt{2mE}}{\hbar}$ and E is a positive number. However, if $E < V$, then: $k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$

and is imaginary and can be expressed as $k_2 = i \cdot k'_2 = i \cdot \frac{\sqrt{2m(V-E)}}{\hbar}$ (note how V and E have

switched place when "i" is added). The equation for reflection is then: $\frac{B}{A} = \frac{k_1 - i \cdot k'_2}{k_1 + i \cdot k'_2}$. Since the percent

reflection is actually $\frac{|B|^2}{|A|^2} = \frac{B^* B}{A^* A}$, please show that reflection is always 100% if $E < V$. **(5 pts)**

5. Consider the following potential energy surface that has an infinite potential at $x=0$:



a. Which of the wavefunctions below is the correct for region I and why?

1. $\cos(k \cdot x)$ 2. $\sin(k \cdot x)$ 3. E^{ikx} 4. E^{-ikx}

(5 pts)

b. Is there any boundary condition that dictates what k is? In other words, can k take on any value so long as the correct form (question a) is determined? **(3 pts)**

c. If there is no boundary condition that limits the value of k , are there limits on the energy? Please explain, and hint: this is basically a freewave problem. **(3 pts)**

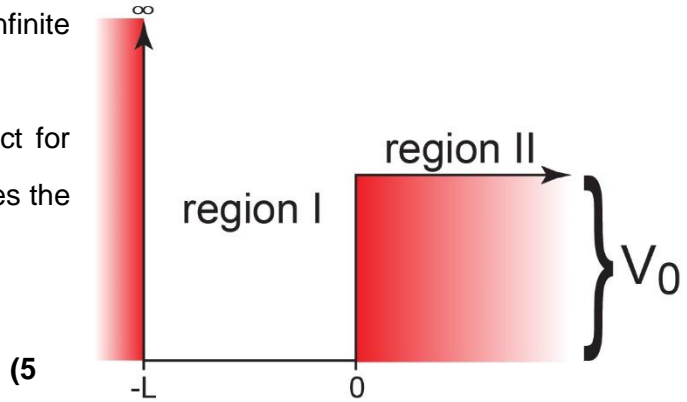
6. The “quantum” in quantum mechanics describes when only certain energy levels are allowed. Thus, there are finite energy differences between the ground state and other excited states. Not all systems have quantized energy levels. **(9 pts)**

a. For the free wave: is energy quantized? **b.** What about the particle in a box? **c.** What about the particle in a finite box, if the energy is $> V_0$ (like the blue wave)?

7. The “half-baked well” potential has infinite potential energy at $x=-L$, and a step at $x=0$:

a. Which wavefunction below is the correct for region I and why? Hint: what stipulation does the infinite potential place on the wavefunction?

1. $\cos\left(k_1\left\{x + L\right\} - \frac{\pi}{2}\right)$ 2. $\sin(k_1 \cdot x)$
 3. e^{ik_1x} 4. e^{-ik_1x}



(5 pts)

b. In the 1st region, since $V=0$ the Schrodinger equation is:

$$\frac{\hbar^2 k_1^2}{2m} \cdot \Psi_I(x) = E \cdot \Psi_I(x)$$

Solve for k_1 . Hint: this is just an algebra problem.

(2 pts)

c. In the 2nd region where the potential step $V=V_0$ exists:

$$\frac{\hbar^2 k_2^2}{2m} \cdot \Psi_{II}(x) = (E - V_0) \cdot \Psi_{II}(x)$$

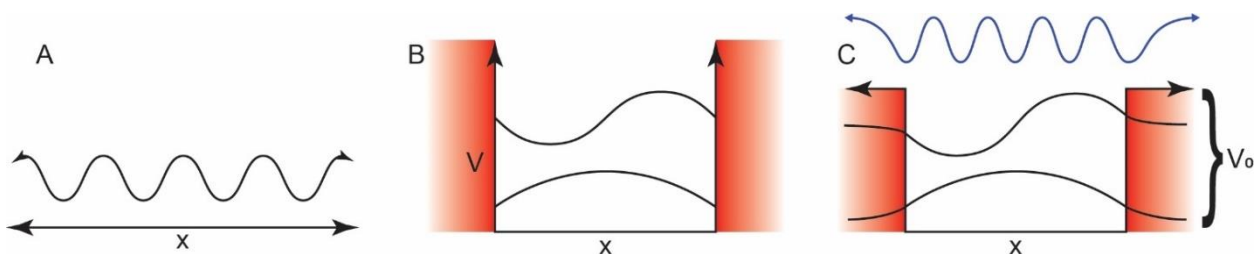
Solve for k_2 in this case.

(2 pts)

d. The wavefunction $\Psi_{II}(x)$ is in a region of constant potential, therefore possible wavefunctions are:

1. $\cos\left(k_2\left\{x + L\right\} - \frac{\pi}{2}\right)$ 2. $\sin(k_2 \cdot x)$ 3. e^{ik_2x} 4. e^{-ik_2x}

Figuring out which one is correct is a bit harder. Here is how you reason through it: if a particle passes through the wall from region 1 into region 2, it will continue moving to the right and do so



forever since there are no more walls to bounce off of. Therefore, which of the functions above (1-4) correctly describe a particle always moving right? **(5 pts)**

e. Now unfortunately we run into two possible solutions for region 2. Let's say that in region 2:

$k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$, and thus the two possibilities are that the particle has more energy than the potential barrier ($E > V_0$) or it has less ($E < V_0$). In the former case ($E > V_0$), $\Psi_{II}(x) = e^{i\frac{\sqrt{2m(E-V_0)}}{\hbar}x}$ which is a wave that travels to the right forever.

If the energy is less than the potential energy, can you justify substituting $k_2 = i\frac{\sqrt{2m(V_0-E)}}{\hbar}$ for $\frac{\sqrt{2m(E-V_0)}}{\hbar}$? Please explain. **(2 pts)**

f. If you plug $k_2 = i\frac{\sqrt{2m(V_0-E)}}{\hbar}$ into $\Psi_{II}(x) = e^{ik_2x}$, does the wavefunction continue to oscillate like a sine or cosine or does it behave differently? Please explain your answer. **(4 pts)**

8. I have drawn here two wavefunctions that are solutions to the half-baked well if the energy of the particle is less than V_0 . Obviously, the wavefunctions are continuous and smooth, which is due to using the "right" energies. To show that this is the case, let's do the following:

a. Set:

$$\Psi_I(x) = \cos\left(\frac{\sqrt{2mE}}{\hbar}\left\{x + L\right\} - \frac{\pi}{2}\right)$$

and:

$$\Psi_{II}(x) = e^{-\frac{\sqrt{2m(V_0-E)}}{\hbar}x}$$

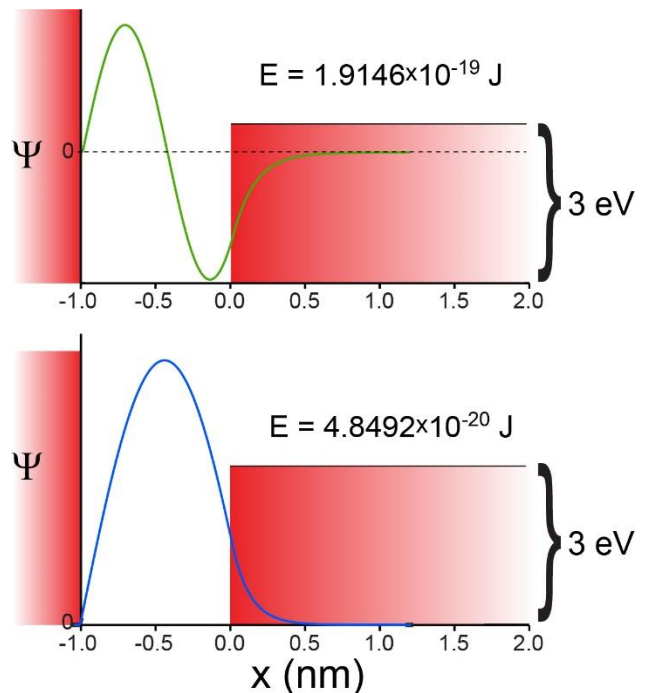
equal at $x=0$.

(2 pts)

b. Calculate the derivative of $\Psi_I(x)$ and $\Psi_{II}(x)$, and set the two derivatives equal at $x=0$. **(6 pts)**

c. Divide the equation in **b** by the equation in **a** to derive the relationship:

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}L - \frac{\pi}{2}\right) = \frac{\sqrt{V_0 - E}}{\sqrt{E}}$$



This equation does not allow one to solve for E analytically. Basically, you have to plug in numbers for L, m, and V_0 and then determine what energy E makes the left side equals the right side.

(6 pts)

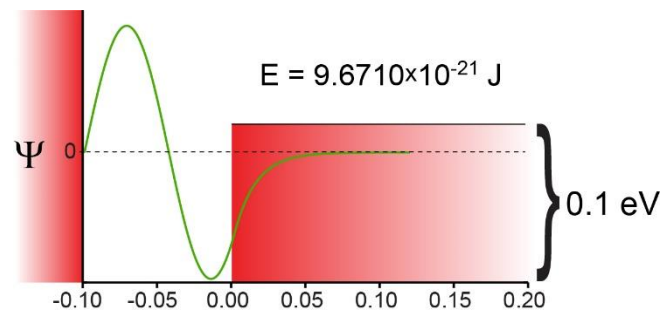
d. If the mass of the particle is that of an electron, L is 1 nm, and the barrier is 3 eV, can you show that energies E of 4.8492×10^{-20} J and 1.9146×10^{-19} J (the same shown in the figure) satisfy the relationship in pt. c?

(4 pts)

e. Drawn above are the two wavefunctions for the states with $E = 4.8492 \times 10^{-20}$ J and the other with $E = 1.9146 \times 10^{-19}$ J. How would you describe these two states to a student in freshman chemistry?

(4 pts)

9. I have drawn here two wavefunctions that are solutions to the half-baked well if the energy of the particle is less than V_0 . Obviously, the wavefunctions are continuous and smooth, which is due to using the “right” energies. To show that this is the case, let’s do the following:



a. Set:

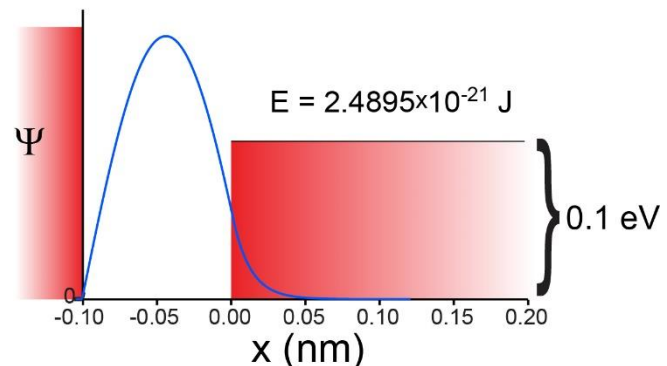
$$\Psi_I(x) = \cos\left(\frac{\sqrt{2mE}}{\hbar}\{x + L\} - \frac{\pi}{2}\right)$$

and:

$$\Psi_{II}(x) = e^{-\frac{\sqrt{2m(V_0 - E)}}{\hbar} \cdot x}$$

equal at $x=0$.

(2 pts)



b. Calculate the derivative of $\Psi_I(x)$ and

$\Psi_{II}(x)$, and set the two derivatives equal at $x=0$. **(6 pts)**

c. Divide the equation in **b** by the equation in **a** to derive the relationship:

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}L - \frac{\pi}{2}\right) = \frac{\sqrt{(V_0 - E)}}{\sqrt{E}}$$

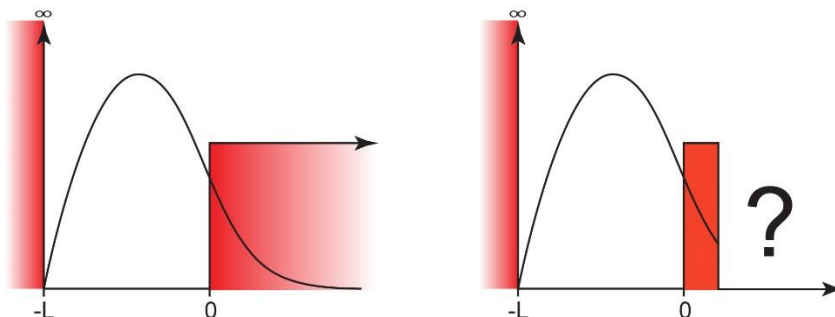
This equation does not allow one to solve for E analytically. Basically, you have to plug in numbers for L, m, and V_0 and then determine what energy E makes the left side equals the right side.

(6 pts)

d. If the mass of the particle is that of a proton, L is 0.1 nm, and the barrier is 0.1 eV, can you show that energies E of 2.4895×10^{-21} J and 9.6710×10^{-21} J (the same shown in the figure) satisfy the relationship in pt. c? **(4 pts)**

e. Draw above are the two wavefunctions for the states with $E = 2.4895 \times 10^{-21}$ J and the other with $E = 9.6710 \times 10^{-21}$ J. How would you describe these two states to a student in freshman chemistry? **(4 pts)**

10. In the particle-in-a-half-baked-well problem, you see that the wavefunction decayed exponentially into the barrier when $E < V$ as shown on the left. Now the question is- what do you think



happens if the right barrier was “thin”, such that the wavefunction doesn’t decay to 0 before the end of the barrier as shown here? Please draw and explain your result. **(5 pts)**

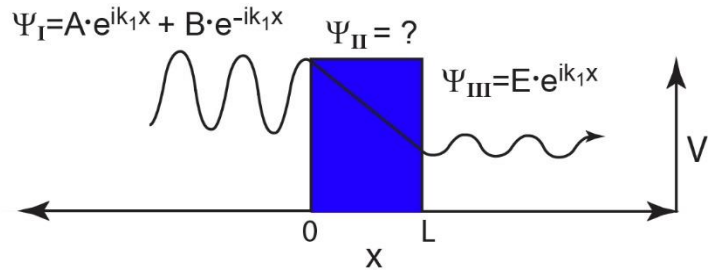
11. Units! a. In problem set 6, question 6 (a copy is at the end of this problem set), an electron (mass = 9.109×10^{-31} kg) was trapped in a 1 nm ($L = 1 \times 10^{-9}$ m), 3 eV ($V_0 = 4.807 \times 10^{-19}$ J) potential well. I gave you the ground and excited state energies (4.85×10^{-20} J and 1.91×10^{-19} J), which I found with: $\tan\left(\frac{\sqrt{2\text{mass}\cdot E}}{\hbar} \cdot L - \frac{\pi}{2}\right) = \frac{\sqrt{(V_0 - E)}}{\sqrt{E}}$ using the [Wolfram zeros calculator](#).

Now you do the same- please use the equation, with SI units inputted to find the energies that solve the expression above. ($\hbar = 1.0546 \times 10^{-34}$ J · s)

Hint: to answer just send us a screen clip of the website, and most important the website won’t work so don’t try too hard! **(3 pts)**

b. The website won’t return any values because the input parameters are too small. To resolve the problem you are going to use atomic units, in which $\hbar = 1$, $\frac{1}{4\pi\epsilon_0} = 1$, $e^2 = 1$ (the charge of an electron), length is in Bohrs ($= 0.0529$ nm), and the mass of an electron is: $m_e = 1$. In this system of units energy is in Hartrees, where 1 Hartree = 27.2114 eV = 4.36×10^{-18} J. So, if you do the conversions, and re-insert into the $\tan\left(\frac{\sqrt{2\text{mass}\cdot E}}{\hbar} \cdot L - \frac{\pi}{2}\right) = \frac{\sqrt{(V_0 - E)}}{\sqrt{E}}$ equation, the website should return the correct answers; please send us a screen shot and verify that the energies are the same as the ones I gave. **Hint:** the website can crash if you put in more than three significant figures. **(7 pts)**

12. Concerning the finite barrier problem, let's think about what happens when a particle hits a barrier (region II) with the same amount of energy as the potential energy barrier, i.e. $E=V$.



Free wavefunctions in the presence of a flat potential are the solution to:

$$\hat{H}\Psi = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) + V \cdot \Psi(x) = E \cdot \Psi(x)$$

which is simplified into:

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) = (E - V) \cdot \Psi(x)$$

For region II, the wavefunction has a general solution of the form: $\Psi(x) = C \cdot e^{i \cdot k_2 \cdot x} + D \cdot e^{-i \cdot k_2 \cdot x}$, where C and D are constants and k_2 is defined as: $k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$.

It turns out that, if $E=V$, then $\Psi_{II}(x) = C + D \cdot x$. Can you show that this wavefunction is a solution to $\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x) = (E - V) \cdot \Psi(x)$? **(5 pts)**

13. Going back to #8, the problem of the finite barrier when $E=V$, we need to solve what is the probability of reflection and transmission. To do so, we must solve a system of four equations—the continuity and smoothness of the wavefunctions Ψ_I & Ψ_{II} at $x=0$ and the same for Ψ_{II} and Ψ_{III} at $x=L$.

a. If $\Psi_I(x) = A \cdot e^{i \cdot k_1 \cdot x} + B \cdot e^{-i \cdot k_1 \cdot x}$ and $\Psi_{II}(x) = C + D \cdot x$, what are the two equations that stipulate that the wavefunction is continuous and smooth at $x=0$? **(4 pts)**

b. Now if $\Psi_{II}(x) = C + D \cdot x$ and $\Psi_{III}(x) = E \cdot e^{i \cdot k_1 \cdot x}$, what are the two equations that stipulate that the wavefunction is continuous and smooth at $x=L$? **(4 pts)**

14. Now let's solve the equations we derived in question 9 by insert values. We have already assumed that $E=V$, and let's use a finite value for $k_1 = \frac{4\pi}{L}$. This gives us four equations to work with:

$$\begin{aligned} A + B &= C \\ i \cdot \frac{4\pi}{L} \cdot A - i \cdot \frac{4\pi}{L} \cdot B &= D \\ C + D \cdot L &= E \cdot e^{i \cdot 4\pi} \\ D &= i \cdot \frac{\pi}{L} \cdot E \cdot e^{i \cdot 4\pi} \end{aligned}$$

While we can use and note that $e^{i \cdot 4\pi} = 1$ to simplify the above, unfortunately, this system of four equations has 5 unknowns (A, B, C, D, and E). However, if we want the (reflection)^{1/2}, that is equal to the ratio of B/A. Likewise, (transmission)^{1/2} is the ratio of E/A. Using this information, we can rewrite the system of equations as:

$$\begin{aligned} 1 + r &= C \\ i \cdot \frac{4\pi}{L} - i \cdot \frac{4\pi}{L} \cdot r &= D \\ C + D \cdot L &= t \\ D &= i \cdot \frac{4\pi}{L} \cdot t \end{aligned}$$

where $r=B/A$ (the square root of the reflectance) and $t=E/A$ (the square root of the transmission).

Now you can plug these into the Mathematica Online system of equations solver found here:

<http://www.wolframalpha.com/widgets/view.jsp?id=ae438682ce61743f90d4693c497621b7>

and determine what r and t are.

When you do, note that you need to take the absolute value of the results for r and t to get the real values like you did in question 3. For example, if you find that $r = \frac{2\pi}{2\pi+i}$, then:

$$|r|^2 = \left(\frac{2\pi}{2\pi+i}\right)^* \left(\frac{2\pi}{2\pi+i}\right) = \left(\frac{2\pi}{2\pi-i}\right) \left(\frac{2\pi}{2\pi+i}\right) = \frac{4\pi^2}{4\pi^2+1} = 0.975, \text{ which is } \sim 97.5\%. \text{ Note that } 1-|r|^2 = |t|^2.$$

(8 pts)

Hint: Show me what the web site returns of r and t, and then determine the absolute values. Also I found that the Wolfram web site can hang, if so, hit the equal sign as indicated here.

15. Now let's solve the equations we derived in question 9 by insert values. We have already assumed that $E=V$, and let's use a finite value for $k_1 = \frac{2\pi}{L}$. This gives us four equations to work with:

$$\begin{aligned} A + B &= C \\ i \cdot \frac{2\pi}{L} \cdot A - i \cdot \frac{2\pi}{L} \cdot B &= D \\ C + D \cdot L &= E \cdot e^{i \cdot 2\pi} \\ D &= i \cdot \frac{\pi}{L} \cdot E \cdot e^{i \cdot 2\pi} \end{aligned}$$

While we can use and note that $e^{i \cdot 2\pi} = 1$ to simplify the above, unfortunately, this system of four equations has 5 unknowns (A, B, C, D, and E). However, if we want the (reflection)^{1/2}, that is equal to the ratio of B/A. Likewise, (transmission)^{1/2} is the ratio of E/A. Using this information, we can rewrite the system of equations as:

$$1 + r = C$$

$$i \cdot \frac{2\pi}{L} - i \cdot \frac{2\pi}{L} \cdot r = D$$

$$C + D \cdot L = t$$

$$D = i \cdot \frac{2\pi}{L} \cdot t$$

where $r=B/A$ (the square root of the reflectance) and $t=E/A$ (the square root of the transmission). Now you can plug these into the Mathematica Online system of equations solver found here:

<http://www.wolframalpha.com/widgets/view.jsp?id=ae438682ce61743f90d4693c497621b7>

and determine what r and t are. When you do, note that you need to take the absolute value of the results for r and t to get the real values like you did in question 3. For example, if you find that $r = \frac{\pi}{\pi+i}$, then:

$$|r|^2 = \left(\frac{\pi}{\pi+i}\right)^* \left(\frac{\pi}{\pi+i}\right) = \left(\frac{\pi}{\pi-i}\right) \left(\frac{\pi}{\pi-i}\right) = \frac{\pi^2}{\pi^2+1} = 0.908, \text{ which is } \sim 91\%. \text{ Note that } 1-|r|^2 = |t|^2. \quad (8 \text{ pts})$$

Hint: Show me what the web site returns of r and t , and then determine the absolute values. Also I found that the Wolfram web site can hang, if so, hit the equal sign as indicated here.

16. For a wavefunction of the form: $\Psi(x) = \frac{2}{L} \cdot \sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)$, what is the variance in momentum $\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$?

a. First determine: $\left(\frac{\hbar}{i}\right) \frac{\partial}{\partial x} \left(\frac{2}{L} \sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)\right)$ (6 pts)

b. Set up the $\langle p \rangle$ as: (4 pts)

$$\langle p \rangle = \frac{4}{L^2} \int_0^L \left(\sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)\right)^* \left(\frac{\hbar}{i}\right) \frac{\partial}{\partial x} \left(\sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)\right) \cdot \partial x$$

And using your answer from pt. a you should be able to find the answer in the list of identities.

c. Now as for:

$$\langle p^2 \rangle = \frac{4}{L^2} \int_0^L \left(\sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)\right)^* \left(\frac{\hbar^2}{i^2}\right) \frac{\partial^2}{\partial x^2} \left(\sqrt{x} \cdot \sin\left(\frac{\pi}{L}x\right)\right) \cdot \partial x$$

Unfortunately, this one requires the professional form of Mathematica to solve. I used it to determine that $\langle p^2 \rangle \approx \frac{11\hbar^2}{L^2}$. From this you can now calculate $\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2$. (2 pts)