

## Unit 11: Quantum Waves in One Dimension

In this unit, we will expand on this notion of particles acting as waves. We will find that aside from not allowing us to say anymore *where* a particle is, we will also find that in many situations that we are not even allowed to give the particle an arbitrary amount of energy. This is in stark contrast to conventional mechanics according to  $F=ma$ , but you will be able to derive some of these peculiar energy restrictions from your understanding of wave properties.

The quantum mechanical waves are a bit different from the sorts of waves you have considered thus far, such as sound. Quantum waves have more complicated oscillations, and the standard mathematical analysis involves the use of imaginary numbers. To enable us to gain some conceptual insight into the behavior of these waves without taking a course in complex functions (functions with real and imaginary parts), we need to develop a graphical model that lets us *see* these waves. The “waving” can occur in two inter-related ways (hence the need for real and imaginary parts), so we will use color and brightness in computer renderings to convey this information. Then, with this model in mind, we can develop useful intuition about how these waves operate.

### Session 1: Free Quantum Waves and the Color Analogy

The primary motivation for the development of quantum mechanics was to explain some rather mysterious features of atoms. Physicists attempted to explain an atom by a classical planetary model that had a point nucleus which was heavy and the source of an attractive force (like the sun in our solar system) and was surrounded by many light satellites which are the electrons (and are analogous to the planets in our solar system). These efforts were complete failures. The reason for this failure is that the wavelengths of the electrons in these atoms are typically about the size of the atom, roughly  $1 \text{ \AA}$ , or  $10^{-10} \text{ m}$ , and so one needs to apply the rules of wave motion to atoms, and not the rules of particle motion.

So that we can draw pictures of these waves, and ultimately pictures in two dimensions that represent quantum waves in two and three dimensions, we need to have a new way of drawing these waves. When we needed to represent waves in 2 and 3d space, we used the grayscale capabilities of the Macintoshes to draw pictures of plane and circle waves. We will do the same sort of thing, except now we need a way to represent an extra quantity, or degree of freedom as physicists like to say, at each point in space. We will use color for this purpose.

#### *Guidebook Entry 11.1: Our Quantum Palette*

The program "Quantum Palette" shows the set colors that I chose for drawing most of our quantum waves. Double click on "Quantum Palette" in the "Quantum Programs 11.1" folder. The shows the time evolution, but allows you to pause to examine the colors carefully. Describe how they are laid out in the table.

The colors are arranged in a particular order from left to right. Write down what colors you see and in what order.

The rules that govern quantum waves are more complicated than the rules that govern most classical waves like sound waves. For example, the shape of a wave does not necessarily stay the same as a function of time. However, we will still see the familiar features of oscillations in time and in space. For a special set of quantum waves, the waves that are associated with well-resolved energies, the rules are very simple. "Quantum Palette" animates the colors in that way. Describe the time evolution of the colors in your own words.

You probably described the apparent motion across the screen. However, the rules can be defined for a single point without knowing anything about the neighboring points (for this special class of wave functions, that is). In the words of our color analogy, the color at any point changes into the next hue in the rainbow as time progresses. The brightness remains unchanged. If this is not the way you described it, start the program again, and see if this makes sense. What is the order of color changes?

Now that we see how we will represent these wave functions, and how they will evolve in time, we need to apply it to something closer to reality. The first thing to try is to represent a single particle moving with a particular momentum. Remember that we learned in the last unit that the wavelength of a quantum wave is given by the deBroglie relation

$$\lambda = h / p, \text{ where}$$

$$h = 6.626 \times 10^{-34} \text{ J sec.}$$

In many of the following exercises you will need to make predictions of what a color wave will look like. If you like you can bring colored pencils or markers to class, but in general I will simply expect you to mark areas with the following letters to represent the hues of the "color wheel:"

R for Red  
 O for Orange  
 Y for Yellow  
 G for Green  
 B for Blue  
 V for Violet

which matches the Roy G. Bv acronym that many of you know.

*Guidebook Entry 11.2: A First Quantum Wave*

If this particle (perhaps it is an electron) has a particular momentum  $p$ , can you express its kinetic energy in terms of the momentum? Give that expression as a mathematical equation.

Since we can know the energy of this particle (assuming there are no forces acting on it), it is presumably one of these special wave functions where the time evolution is just given by the rotation through the colors. Let's make the further assumption that this oscillation in time is the same as the oscillation we expect to see in space. In the band I have drawn below, make letter marks for the colors you would expect to see along the band. Don't hesitate to ask for help if need it!

Now, use the recipe that the colors move backwards through the list we gave earlier, that is R goes to O, O goes to Y, Y goes G, etc. Using this, fill in the bands below for the next few time steps.

Now start the program "1dQWave" which animates just what you sketched above. Describe what you see. Does it do what you expected?

Does it make qualitative sense that this wave corresponds to a particle with momentum? In what way does it? In what way doesn't it? Discuss this with an instructor.

Consider now the first band in which you specified colors on the previous page. What would this look like if the wave traveled in the opposite direction? Check your result by looking at 1dQWaveRev.

One way of summarizing the behavior of quantum waves is to say that the "waving" occurs in the hue part of the wave function, and not in the intensity part. [For those of you who have had some experience with complex numbers, the "waving" consists

of a rotation through the complex plane; the phase changes with time, while the amplitude stays constant.]

But an important hallmark of a true wave is the notion of superposition. How do we add two colors together? The answer is that we add these colors just as we learned to do in elementary school. If we add colors that are close together on the color wheel (e.g. yellow and green) we get an intermediate color of reasonable brightness (e.g. greenish yellow). If we add colors that are nearly opposite on the color wheel (e.g. red and green), we get a dark brownish black color. This is the sense in which we can superpose colors. To be specific, we will assign the following to be opposite colors for the purposes of our exercises:

R is opposite to G  
 O is opposite to B  
 Y is opposite to V

While this is not strictly true, having six colors makes it easier to do some of our analyses.

*Guidebook Entry 11.3: Superposition of Left- and Right-going Waves*

In the following bands, fill in the appropriate colors for left- and right-going waves, starting with R on the far left, as shown.

R									
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R									
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In the band below, mark where there will be constructive interference, and mark with appropriate letters what colors you expect to see there. Shade in the regions of destructive interference.

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Now let the waves progress one tick of time (i.e. enough time for O to change to R, etc.). Mark the colors in the two waves in the bands below.

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In the band below, mark the constructive and destructive interference points.

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How do you think the superposition of the two waves behaves as a function of time?

Now check your guess by looking at the program "1dQStandWave." Does this do what you predicted? Describe what you see, and how it compares to what you predicted.

We found that a backwards traveling wave resulted when a wave on a rope reached the end of the rope. What kind of wave resulted from the superposition of the forward and backward going waves?

Are there similarities between the quantum superposition and the rope superposition? Describe them.

The standing waves that result in our rope wave were most like the quantum version you just investigated when you made the end of the rope move in a circle, rather than just up and down. The resulting wave moved like a jump rope, except perhaps with multiple bumps in the rope. If this analogy appeals to you, you must think of the rope angle as being indicative of the color, and the displacement as the brightness. **BE CAREFUL NOT TO THINK OF THE ROPE MOTION AS INDICATING PARTICLE MOTION!** Although an electron has wave properties, it does not mean that the particle moves in an oscillatory pattern. The meaning of the wave function is much more subtle than that, and we will discuss it in the next session. But before we end this session, let's once again touch base with the Heisenberg uncertainty principle that we learned about in the last unit.

*Guidebook Entry 11.4: The Uncertainty Principle Revisited.*

Look once again at our basic one dimensional wave simulation "1d Q. Wave." Is there any way to tell *where* the particle might be? Explain.

Remember that we developed this wave by assuming a perfectly well-determined momentum  $p$ . The Heisenberg Uncertainty Principle tells us

$$\Delta p \Delta x > h,$$

that is, that the better we know the momentum of an object, the more we must sacrifice information about where the particle is. If the momentum of the wave is given *exactly* by  $p$ , how big is  $\Delta p$ ?

How big then does the uncertainty principle say  $\Delta x$  must be?

To produce a quantum wave that is localized, we must do just as we did with our Excel simulation; we must add together a number of sinusoidal functions that are carefully phased with one another to form a pulse. This wave function then does *not* have a well defined momentum, *nor* a well defined kinetic energy. This then means that the time development of such a wave, even in the absence of forces, is mathematically complicated. Although we will not do this, you should not be surprised to know that if one does create such a pulse, it moves coherently with a velocity that is given by the average momentum divided by the mass

$$v = p/m$$

and the kinetic energy is given approximately by the expression

$$E = p^2/2m$$

just as one gets with classical mechanics. However, the width of the pulse grows as a function of time, which is a purely quantum effect.

## Session 2: Quantization in One Dimension

In the last session, you found that you could produce standing waves from these strange color waves just as you could produce standing waves in a string. This is extremely useful, as the behavior of quantum waves confined to a region of space is qualitatively the same as the behavior of waves on a string that is fixed at both ends, like a string on a violin or guitar. Just as in the case of the string we found only certain frequencies were allowed, we will now have the case where only certain quantum frequencies (which correspond to only certain energies) are allowed.

### *Guidebook Entry 11.5: Energy of a Quantum Wave*

Since a particle is no longer represented by a location, we cannot rely on using its time derivatives (velocity and acceleration) to find the properties of a particle, such as its kinetic energy. However, since we know the momentum is related to the wavelength, we can use the momentum to calculate other quantities.

If we assume that the kinetic energy is related to the momentum of a quantum particle just as it is for a classical, write an equation that gives the kinetic energy  $E$  in terms of the momentum  $p$  and the mass  $m$  of a particle. Although you have done this before, it is so central a concept, it won't hurt to review this.

Now substitute the deBroglie expression  $\lambda = h/p$  to find an expression for the kinetic energy in terms of the wavelength of the wave function and the mass of the particle.

### *Guidebook Entry 11.6: A Quantum Particle "in a Box"*

In this exercise, we will be considering what happens when we confine a quantum wave to a limited region of space. Since we are still working only with waves in one dimension, this is completely analogous to the case of a string with limited extent. In that case, we wanted to have a node at either end of the string. Here, we will want exactly the same boundary conditions: a node at each end of the region. While this may seem rather artificial, it makes a fair approximation of what happens for shared electrons in some long-chain molecules.

First, what is the spacing between nodes in terms of the wavelength for a conventional standing wave (e.g. a wave on a rope)?

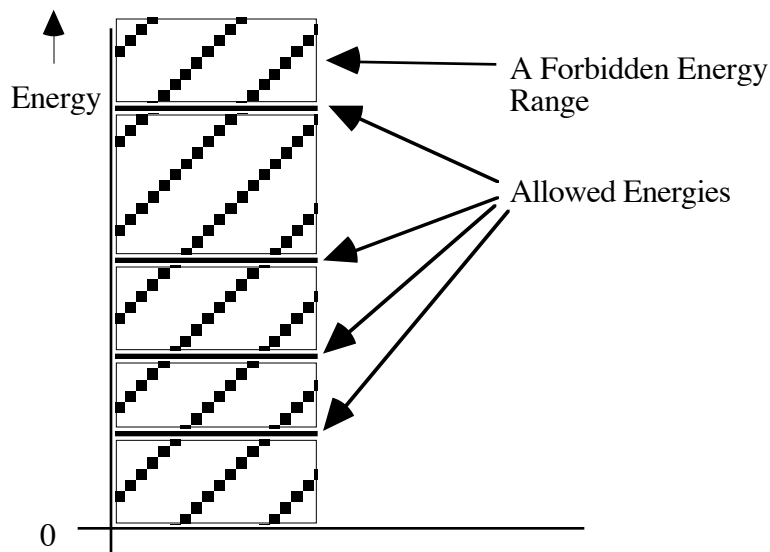
The wavelength for a quantum wave is the distance between consecutive appearances of the same color (e.g. from red to the next red). Look back at the predictions you made for your standing wave from the last session (*Guidebook Entry 11.3*) and answer the same question: what is the spacing between nodes in terms of the wavelength for a quantum standing wave?

Let's now imagine the case in which a particle is confined to a one-dimensional region of length  $L$ . If we impose the requirement that there is a node at each end of this region, find a mathematical relationship between the wavelength and the length  $L$ . [Hint: in this case, you will need to introduce a number that relates to the number of nodes between each end.]

Now, use the expression you derived in *Guidebook Entry 11.5* relating the wavelength to the energy to produce an expression for the kinetic energy in terms of the length  $L$ , the mass, Planck's constant  $h$ , and your number you defined just above.

Run the program 1dQBox from the folder Quantum Programs 11.2. Do they look like the standing waves you predicted? Describe what you see, and what the quantum numbers (related to the number of nodes) are for these three waves.

What you have just found is an expression that gives all the allowed energies for the so-called "particle in a one-dimensional box." The remarkable result is that measurement of energy in a confined quantum system has only certain allowed values. This is shown schematically in the figure below.



If these are the only allowed energies, then for a system to change from one energy to another is dramatically different than for a classical system. One common way for these transitions to occur is through the emission or absorption of light. But quantum mechanics has its will in this case again. To be specific, just as the objects we consider to be particles (electrons, protons, even whole atoms) the light itself is in discrete quantities--the photons we discussed in the last unit. In general, each transition from one energy level to another is accompanied by the emission or absorption of a photon. The energy of a photon is related to the frequency of the wave by the relation first stated by Planck

$$E = hf,$$

where  $f$  is the frequency of the photon and  $h$  is once again Planck's constant. In fact, this was the very first introduction of this constant, and the notion of quantization.

As a result, quantum mechanics restricts the frequencies, and hence colors, of light that are emitted or absorbed in a particular system. The next exercise allows you to investigate this quantitatively for the particle in a box, and observe this qualitatively with a discharge tube and a diffraction grating.

*Guidebook Entry 11.7: Transition Energies*

You should have found earlier that the energy of a quantum mechanical particle in a box is given by the expression

$$E = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{n^2 h^2}{8mL^2}.$$

Imagine that a particle in a state given by the quantum number  $n$  drops down to the next lowest level with quantum number  $n-1$ . What is the energy of the light emitted?

If this particle is an electron ( $m = 9.1 \times 10^{-31}$  kg) confined to a region of about 5 atomic widths (about  $1 \text{ nm} = 10^{-9}$  m), what are these transition energies? [You may wish to recall  $h = 6.6 \times 10^{-34}$  J sec.]

What are the wavelengths of the  $2 \rightarrow 1$  (i.e a transition from the  $n=2$  level to the  $n=1$  level) and  $3 \rightarrow 2$  transitions? You will need to use the Planck relation from above,  $E = hf$ , and the fact that light travels at the speed of light  $c = 3 \times 10^8$  m/sec.

Visible light has wavelengths from about 400 nm to 700 nm. How do these wavelengths you calculated above compare with visible light?

Many of the light sources we deal with use compound and/or solid sources, where there is not a consistent atomic system which is emitting the light. It is not surprising then that the emitted light will have a large variety of emitted wavelengths. Look at some of the white light sources with a diffraction grating (which we learned earlier has wavelength dependent diffraction), and describe what you see.

Now look through your grating at a hydrogen discharge tube source. Describe what you see here.

Let's return to the question of what the wave function really means. This is a rather subtle question, as evidenced by the fact that people were using quantum mechanics to do a great number of calculations for roughly a decade before there was an accepted explanation for the significance of the wave function itself! Even this explanation, which still represents our understanding of the wave function, is not entirely satisfying.

We suspected that the nodes in the wave function represents where the particle *isn't*. We also implicitly used this assumption when we created wave packets and said that they represented localized particles. Where the wave function is large (very bright in our color analogy), there is a great probability of finding the particle. Where the wave function is small, or dark, there is a much smaller probability of finding the particle. Although we will not do actual calculations with this fact, the probability is proportional to the *square* of the brightness of the wave function. Just as squaring a real number loses track of the  $\pm$  sign, squaring a complex number (technically, it is the number times its complex conjugate) loses the information about angle on the complex plane, what we represent by the hue. Only brightness information remains.

I keep referring to the probability of finding the particle. You might wonder, what do I mean by finding the particle? In a practical sense, we have a variety of pieces of equipment that can detect a particle, and they have a limited spatial extent of operation. In other words, if the detector spans the distance range from 1 to 3, then if it detects the particle, it must have been in the region from 1 to 3. If I have *two* detectors, say one from -2 to 0 and one from 1 to 3, then only *one* of them will detect the particle at any given time. This is not surprising if we think of particles as particles, but strange to think of for waves. Even though the particle is described by a spread-out wave function, it can only be detected at a single place at a single time. In that sense, it still is a particle.

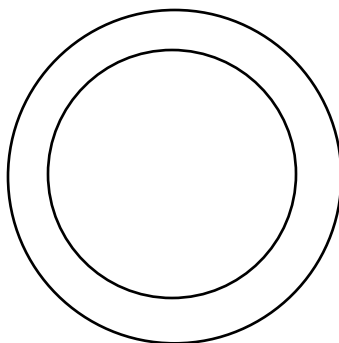
Two other details. First, why must there be nodes at the ends of a particle-in-a-box wave function? Why can't the wave function just suddenly go to zero? Just as we found with a rope, it was impossible to shake the end of the rope in a way to make a

corner propagate down the rope. Sharper turns are associated with shorter wavelengths and higher frequencies, and hence greater energies. A corner implies infinite frequency components, which simply are not allowed. Second, what does the color mean? The answer to this is simple: we just don't know. All that can be said is that it contains the wave interference information, so only the relative colors are important, since they are what determine whether the interference is constructive or destructive.

There is one more problem that is really a two-dimensional problem, but can be solved using one-dimensional arguments. This is for a quantum particle confined to a circular path. This is usually referred to as a quantized bead on a hoop. It is a reasonable approximation for electrons confined to a circular molecule such as benzene (well, physicists think of it as circular). Even more important, however, is the result of quantized angular momentum, which is a general result for systems with rotational symmetry.

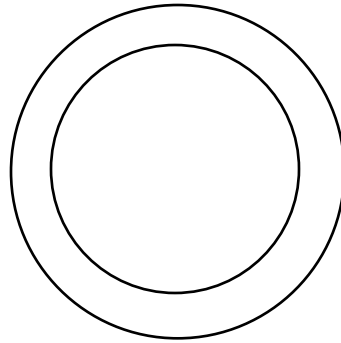
*Guidebook Entry 11.8: Quantum Particle on a Hoop*

Imagine that we have a quantum wave that is confined to a circular path. We no longer have any ends from which we can imagine getting reflections of a wave, or equivalently from which we have the requirement of a zero in the wave function. However, we still want the wave function to have only a single value at each point in space. With this in mind, arrange a full set of color letters around the ring shaped path below such that the colors are in phase again after a full transit around the loop.



If the hoop has a radius of  $R$ , how does the wavelength you drew above relate to that radius? Give your answer as a mathematical expression.

Is this the only possible arrangement you can think of? Draw a second one below.



Compare the simulations qHoopWaveA and qHoopWaveB. Describe the difference between the two.

Compare the simulations qHoopWaveA and qHoopWaveC. Describe the difference between the two.

What are the allowed wavelengths in terms of the circle radius  $R$ ?

Write a general expression for the wavelength in terms of a number (you can call it 'n' again) that gives the number of wavelengths you are fitting into the circle.

Can you translate this wavelength expression into an energy expression like you did for the particle in a box?

Recall that the angular momentum of an object is given by the momentum times the perpendicular distance from the center of the rotation. Find an expression for the angular momentum in this case too.

Are all possible angular momentum values allowed, or is angular momentum quantized? Explain.