

## Chapter 3

### Wave Properties of Particles

#### Overview of Chapter 3

Einstein introduced us to the particle properties of waves in 1905 (photoelectric effect). Compton scattering of x-rays by electrons (which we skipped in Chapter 2) confirmed Einstein's theories.

You ought to ask "Is there a converse?" Do particles have wave properties?

De Broglie postulated wave properties of particles in his thesis in 1924, based partly on the idea that if waves can behave like particles, then particles should be able to behave like waves.

Werner Heisenberg and a little later Erwin Schrödinger developed theories based on the wave properties of particles.

In 1927, Davisson and Germer confirmed the wave properties of particles by diffracting electrons from a nickel single crystal.

#### 3.1 de Broglie Waves

Recall that a photon has energy  $E=hf$ , momentum  $p=hf/c=h/\lambda$ , and a wavelength  $\lambda=h/p$ .

De Broglie postulated that these equations also apply to particles. In particular, a particle of mass  $m$  moving with velocity  $v$  has a de Broglie wavelength of

$$\lambda = \frac{h}{mv}.$$

where  $m$  is the relativistic mass

$$m = \frac{m_0}{\sqrt{1 - v^2/c^2}}.$$

In other words, it may be necessary to use the relativistic momentum in  $\lambda=h/mv=h/p$ .

In order for us to observe a particle's wave properties, the de Broglie wavelength must be comparable to something the particle interacts with; e.g. the spacing of a slit or a double slit, or the spacing between periodic arrays of atoms in crystals.

The example on page 92 shows how it is "appropriate" to describe an electron in an atom by its wavelength, but not a golf ball in flight.

A 46 gram golf ball moving at 30 m/s has a de Broglie wavelength of  $\lambda=h/mv=4.8 \times 10^{-34}$  m, which we will never be able to observe, so it makes no sense talking about the wave properties of a golf ball.

On the other hand, an electron moving with a (nonrelativistic) velocity of  $10^7$  m/s has a de Broglie wavelength of  $\lambda=h/mv=7.3 \times 10^{-11}$  m, which is quite small, but roughly comparable to

atomic dimensions, so we need to consider the wave nature of electrons when they are moving through solids.

Some things to think about. Particles are really "there" and the "wave" associated with a particle isn't the particle "spread out." We know this because collisions seem to be instantaneous.

Also, in a later section, we will see how a particle's wave has a phase velocity greater than the speed of light,  $c$ . Thus, the phase velocity cannot have a physical interpretation.

Some equations you need to know.

$$E = hf$$

$$p = \frac{h}{\lambda}$$

$$\omega = 2\pi f$$

$$k = \frac{2\pi}{\lambda}$$

$$\hbar = \frac{h}{2\pi}$$

$$E = \hbar\omega$$

$$p = \hbar k$$

### 3.2 Waves of What?

Sound waves consist of pressure differences in a medium. Water waves consist of different heights in water. What about matter waves?

The "thing" whose variations makes up matter waves is the wave function,  $\Psi$  ("psi", usually pronounced "si").

The wave function of a matter wave is not something we can see or sense. It has no direct physical significance.

$\Psi$  is the solution to Schrödinger's equation.

Remember I mentioned Schrödinger above, and said he developed a theory for the wave properties of particles. We'll learn about his equation before long.

$\Psi$  is, in general, complex. It cannot be directly measured. The time and/or space average of  $\Psi$  is zero. (That shouldn't bother you--the time/space average of a sine wave is zero but you measured sine waves in your Physics 24 labs.)

However,  $\Psi$  can tell us something about the matter it represents.

$\Psi^*\Psi$  tells us the probability of finding the body represented by  $Y$ .

In general,  $\Psi$  is a function of position  $(x,y,z)$  and time.

***The probability of finding the object described by  $\Psi$  at the position  $(xyz)$  at time  $t$  is proportional to the value of  $\Psi^*\Psi$  there.***

A value for  $\Psi^*\Psi$  of zero means the object is not there. A value of 1 for  $\Psi^*\Psi$  means the object is there.

In general, the value of  $\Psi^*\Psi$  is between zero and one. A small value means a small probability of finding the object there; a large value means a large probability of finding the object there.

Does this way of doing things bother anybody? It has bothered a lot of physicists. It's a radically different way of thinking.

Note the difference between the probability of an event and the event itself.

If we detect an electron, it was "there." It was not 50% "there."

If the probability of finding an electron at  $(xyz,t)$  is 50%, it doesn't mean that the electron is 50% "there." It means that half of our measurements would find the whole electron "there," and the other half would find no electron at all.

Let's apply these ideas to a collection of particles.

We may describe experiments which involve a large number of identical particles. In that case, it makes sense to talk about a density of particles. If each particle is described by the same wave function, we talk about a probability density

$$|\Psi|^2.$$

For a particle or system of particles described by the wavefunction  $\Psi$ ,

$$|\Psi|^2 dV = \Psi^* \Psi dV$$

is the probability of finding a particle (or the system) in an infinitesimal volume element  $dV$ .

To find the probability of finding the particle somewhere in space, we integrate the infinitesimal probability over all space.

We assume that the probability of finding a particle *somewhere* in space is 1 (otherwise, no particle, and nothing worth doing), so that

$$\int \Psi^* \Psi dV = 1.$$

Such a wavefunction is said to be ***normalized***.

Remember, the wavefunction tells us the probability of finding the particle at a particular point in space and time, but the particle is not "spread out" in some wave.

Actually determining  $\Psi$  is usually a difficult problem. We will often assume an appropriate wavefunction without going into the details of where it came from.

Example from Chapter 6.

In chapter 6, we will study the wave functions for electrons in hydrogen atoms.

We will find that the spatial part of  $\Psi$  is given by

$$\psi = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0},$$

where  $a_0$  is what we usually think of as the electron's orbital radius, and  $r$  is the radial distance of the electron from the nucleus.

To find the probability of finding the electron at a radial position between  $0.4a_0$  and  $0.6a_0$ , we will calculate

$$\int_{0.4a_0}^{0.6a_0} \psi^* \psi r^2 dr.$$

While deriving expressions for most  $\psi$ 's may be beyond this course, all of you should be able to do the integrals we will encounter.

### 3.3 Describing a Wave -- Part 1: The de Broglie Wave Velocity

We can easily calculate a velocity for de Broglie waves. Beiser calls it " $v_p$ ," and later shows that  $v_p$  is the phase velocity of the waves.

A wave velocity is given by  $v_p = f\lambda$ . De Broglie postulated that  $\lambda = h/mv$  for particles as well as waves.

De Broglie also postulated that a particle's energy should be given by  $E = hf$ , which, as Einstein showed us, is also  $E = mc^2$ . We can solve these two equations to give  $f = mc^2/h$ .

Combining our usual formula  $v_p = f\lambda$  for waves, with de Broglie's postulated equation for  $\lambda$  and our value for  $f$  which we just obtained gives for the velocity of the de Broglie waves

$$v_p = f\lambda = c^2/v$$

This equation gives us no problems when we think about photons as particles. Photons travel with a speed  $v=c$ , so that the "wave velocity" is  $v_p=c$ .

But particles with mass travel at velocities less than the speed of light, so that  $c^2/v$  must be **greater** than the speed of light. The de Broglie wave "velocity" of a particle with mass is greater than  $c$ !

De Broglie's postulated wave-like properties of particles lead us to conclude that the de Broglie wave "velocity" for a particle with mass is greater than  $c$ .

What does this mean? Right now, it means we must re-think what we mean by wave "velocity." Here is the program:

- (1) review the wave equation
- (2) see just what this "wave velocity" is
- (3) see that there are two kinds of velocities associated with waves.

The "wave velocity" we have been talking about so far is the phase velocity, which we have already encountered. The second kind of velocity is the "group velocity," which we will see is the particle velocity.

So, now we continue with the second half of the wave equation section...

### 3.3 Describing a Wave -- Part 2: Derivation of the Wave Equation

Most of you have seen the following in your Physics 23/24 or equivalent sequence.

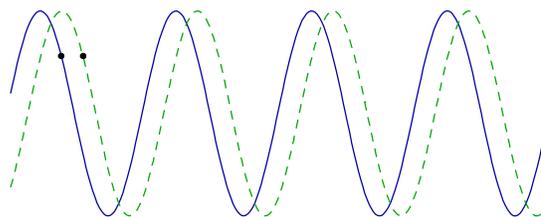
Consider a string stretched along the  $x$ -axis and vibrating in the  $y$ -direction. Beiser shows how to obtain the displacement  $y$  of any point on the string (i.e., at any position  $x$ ) at any time. The result is the *wave equation*

$$y = A \cos \left[ 2\pi f \left( t - \frac{x}{v_p} \right) \right],$$

where  $f$  is the frequency and  $v_p$  is the "wave speed."

Let's think about this " $v_p$ " for a minute.

It is the speed with which a wave travels down the string. But what do we mean by that? Pick some  $y$ -displacement. As the wave travels, that  $y$ -displacement travels to the left or right.



This is like riding on the crest of a wave. The phase velocity represents the movement of individual peaks.

Notice that no particle actually moves left or right. The particles in the string move up or down.

The *phase* of the wave is what is traveling to the left or right, hence the term "phase velocity." No particle actually moves with the phase velocity.

Furthermore, in matter waves, there isn't any matter vibrating in the  $y$ -direction.

If we get a phase velocity greater than  $c$ , we haven't moved any matter at a speed greater than  $c$ .

Beiser goes on to give two alternate forms of the wave equation.

$$y = A \cos \left[ 2\pi \left( ft - \frac{x}{\lambda} \right) \right],$$

and

$$y = A \cos(kx - \omega t).$$

In this latter equation, we have used the definitions of the *angular frequency* ( $\omega=2\pi f$ ) and *wave number* ( $k=2\pi/\lambda$ ).

In three dimensions, the wave equation becomes

$$y = A \cos(\vec{k} \cdot \vec{r} - \omega t).$$

What we just did: we derived the wave equation. We find that waves travel with a "phase velocity," which does not represent the actual velocity of any particle with mass. In the next section we will define the physically meaningful "group velocity."

Some things to note: we have done nothing more than "derive" the equation for a propagating wave.

The - sign corresponds to a wave moving ("propagating") to the right (in the +x direction).

A + sign corresponds to a wave moving ("propagating") to the left (in the -x direction).

These are "transverse" waves. They are "polarized" in the y direction.

In Chapter 2 we derived the phase velocity in a slightly different, but completely equivalent way.

Important: in the above equation for  $y(x,t)$ , the wave is infinitely extended in space. The wavelength (and therefore the momentum) of the wave is well defined.

But where is the particle represented by the wave? We can't find it. It could be anywhere along the x-axis.

To make a wave into a particle, we have to modulate it by summing multiple waves of different wavelengths and/or frequencies. Then the wave function will have both an obvious wavelength and spatial "length."

### 3.4 Phase and Group Velocities

Wave groups, which we hinted at above, are a superposition of different individual waves.

The waves interfere to produce some shape for the group.

The individual waves may move with a different velocity than the groups (in fact, because the de Broglie wave velocity varies with wavelength, the individual waves must move with different velocities).

Beiser gives an example of calculating the velocity,  $v_g$ , with which a wave group travels.

Consider two waves

$$y_1 = A \cos(\omega t - kx)$$

$$y_2 = A \cos[(\omega + d\omega)t - (k + dk)x].$$

Two waves are the minimal set out of which we can build a wave "packet" or "group".

With a little trigonometry, and using the fact that  $d\omega$  and  $dk$  are small compared to  $\omega$  and  $k$ , Beiser shows that

$$y_1 + y_2 = 2A \left[ \cos(\omega t - kx) \right] \left[ \cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right) \right].$$

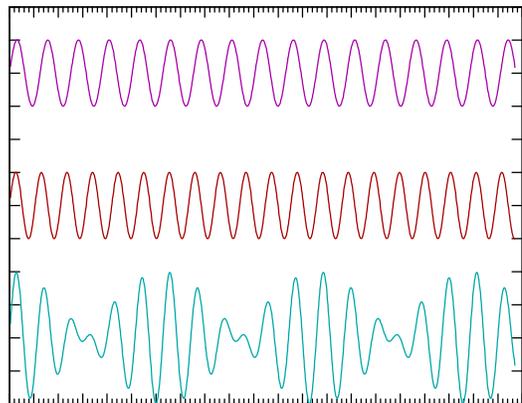
Notice that the wave represented by  $y_1 + y_2$  is built upon a wave of angular frequency  $\omega$  and wave number  $k$ , and is has superposed on it a modulation of frequency  $d\omega/2$  and wave number  $dk/2$ . The wave is sketched in figure 3.4.

The phase velocity of the wave groups is still  $v_p = \omega/k$ , while the groups (the modulation) move with a velocity  $v_g = (d\omega/2)/(dk/2) = d\omega/dk$ .

Here is a picture of two waves superposed to give a wave much like that in figure 3.4. The waves are  $y = \sin(t)$  and  $y = \sin(1.2t)$ .

Notice the wave "groups."

Summarizing: we learned that the phase velocity of wave groups is  $v_p = \omega/k$ , while the groups (the modulation) move with a group velocity  $v_g = (d\omega/2)/(dk/2) = d\omega/dk$ .



In general, the group velocity may be either greater or less than the phase velocity.

If the phase velocity  $v_p$  is the same for all wavelengths, as it is for light in a vacuum, then the phase and group velocities are the same.

Tell me some things about light moving through a medium other than a vacuum....

Finally, in this section Beiser shows how the group velocity of the de Broglie waves is what we would call the particle velocity. He does this by finding the angular frequency and wave number of de Broglie waves.

Angular frequency:

$$\omega = 2\pi f = \frac{2\pi m c^2}{h} = \frac{2\pi m_0 c^2}{h\sqrt{1-v^2/c^2}}.$$

Wave number:

$$k = \frac{2\pi}{\lambda} = \frac{2\pi m v}{h} = \frac{2\pi m_0 v}{h\sqrt{1-v^2/c^2}}.$$

I will often call  $k$  the wave vector--that's what it is in three dimensions.

Now to find phase and group velocities, all you have to do is take  $v_p = \omega/k$  and  $v_g = d\omega/dk$ , using the above expressions for  $\omega$  and  $k$ .

The results are  $v_p = c^2/v$  (we already knew that) and  $v_g = v$  (the particle velocity, we probably suspected that).

The de Broglie **wave group** associated with a moving particle travels with the same velocity as the particle. The phase velocity has no simple physical interpretation.

Here's a question for you: we have shown that a wave's phase velocity can be greater than  $c$ . Does this imply we can find a way to transmit information faster than the speed of light?

You already know or suspect the answer. The information in the wave is carried by the **modulation**. The modulation moves with the group velocity, which is less than (or at most equal to)  $c$ .

Summary of waves:

1. Waves oscillate in both space and time.
2. They may have amplitude modulations, phase modulations, or both.
3. They have phase and group velocities, as discussed above.
4. We wrote the wave equation in the form  $y = A \cos(kx - \omega t)$ . The  $-$  sign means propagating in the  $+x$  direction. What if I write  $y = A \cos(\omega t - kx)$ ? Any difference?
5. Another equivalent way to write the wave is  $y = A e^{j(kx - \omega t)}$ . Remember that Euler's relation says that  $e^{j\theta}$  is made up of sines and cosines. (Do you know/remember what Euler's relation says?)

Here are some things you ought to try with MathCad which are related to the last two lectures.

Consider this wave:

$$\Psi(x) = \exp(-x^2/0.2) \exp(10j\pi x)$$

Tell me something about it. (It is made up of a sinusoidal part and a Gaussian part. The sinusoidal part has no time in it, so it is non-propagating--it varies through space but doesn't move with time. The Gaussian part modulates the sinusoidal part.)

Try this to get some intuition going. Run Mathcad and plot the above wave for  $-1 \leq x \leq 1$  along with its complex conjugate and absolute value.

Because the probability of finding the "system" represented by this function in a "state"  $x$  is the absolute value squared, you get an idea of how a wave function describes where we might find a particle.

Also plot the real part of  $F$  (type  $\text{Re}(\text{ALT-h}(x))$  to get the real part) and the absolute value of  $F$  on the same plot. Also do it for the imaginary part of  $F$  (type  $\text{Im}(\text{ALT-h etc...})$ ).

### 3.5 Particle Diffraction

Davisson-Germer experiment (1927).

They scattered electrons from a nickel sample. Classical physics predicts only a weak angular variation of scattered intensity, and weak dependence on the incident electron energy.

This held true for the original nickel sample.

When the nickel was heated and then cooled, the scattering was found to depend on both angle and incident electron energy.

This is an example of a frequent occurrence in science: an "accident" in the lab reveals new science, *if only you are prepared to see the new science*.

The Davisson-Germer result would be no big deal for x-rays (in fact, x-ray diffraction was established long before their experiment), but the difference here is that electrons are particles. This experiment demonstrated the wave-like properties of electrons.

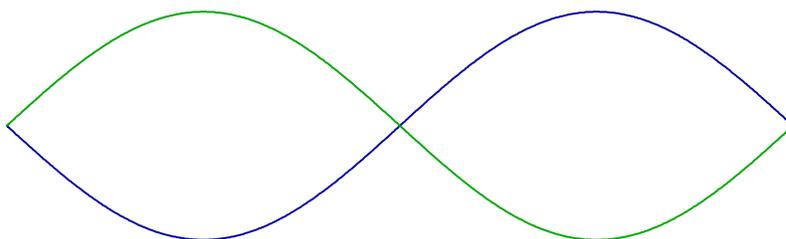
Figure 3.6, showing experimental results, is (perhaps) somewhat difficult to follow, but the equations in the text are sufficient to solve the problems.

That's all I'm going to lecture about this experiment. Read the text and be able to identify the experiment in a multiple choice question, and be able to work the problems.

### 3.6 Particle in a Box

Remember your Physics 23 vibrating string experiment. You couldn't set up arbitrary vibrations of the string. You always saw patterns like this:

You get standing waves because the wave pulses traveling down the string reflect (and change phase by  $180^\circ$ ) when they reach the ends.



The standing wave consists of a series of pulses moving up and down the string. These pulses superpose, and when they are in phase, you see maxima.

When they are out of phase, you see nodes.

You only see the minima and maxima when the pulse speeds are just right so that constructive interference can take place at certain locations. In other words, you only see the maxima for certain wavelengths of the vibration.

What does this have to do with a particle in a box?

Imagine we place a particle, represented by a wave, in a box. The particle wave will reflect when it hits the wall of the box, and then again when it hits the other end of the box.

Now, if the box is small enough (small compared to the particle wavelength), the particle wave "folds up" over and over again every time it reflects off a wall.

The segments of the wave bouncing back and forth interfere. If they interfere constructively, our particle can fit in the box. Otherwise -- no particle.

The folding of the particle wave packet to add in phase works when the length of the box is an integral number of half wavelengths of the particle wave, hence equation 3.17 in Beiser for the de Broglie wavelengths of a trapped particle:

$$\lambda_n = \frac{2L}{n}, \quad n = 1, 2, 3, \dots$$

The restrictions on the allowed wavelength also restrict the allowed energies of the particle in the box:

$$E_n = \frac{n^2 h^2}{8mL^2}, \quad n = 1, 2, 3, \dots$$

The permitted energies are called "energy levels" and the number n is called a "quantum number."

Think of the box as a potential well, inside which a particle is placed.

A free particle, outside the box, can have any energy, and any wavelength.

When you put the particle in the box, only certain wavelengths and energies are allowed (and note that zero is not one of the allowed energies). You most likely will have to add or remove energy to put a free particle into a box.

All of us in this room have discrete energy levels and quantum states, but as the example on page 106 shows, there are enough of them to form, for all practical purposes, the continuum that Newtonian mechanics supposes.

Electron in a box 0.1 nm ( $10^{-10}$  m) wide:

$$E_n = \frac{n^2 (6.626 \times 10^{-34})^2}{8(9.1 \times 10^{-31})(10^{-10})^2} = 6.0 \times 10^{-18} n^2 \text{ J} = 38 n^2 \text{ eV}.$$

The minimum energy is 38 eV, a significant amount, and the energy levels are far enough apart to be measurable.

10 gram marble in a box 10 cm wide:

$$E_n = \frac{n^2 (6.626 \times 10^{-34})^2}{8(1 \times 10^{-2})(10^{-1})^2} = 5.5 \times 10^{-64} n^2 \text{ J}.$$

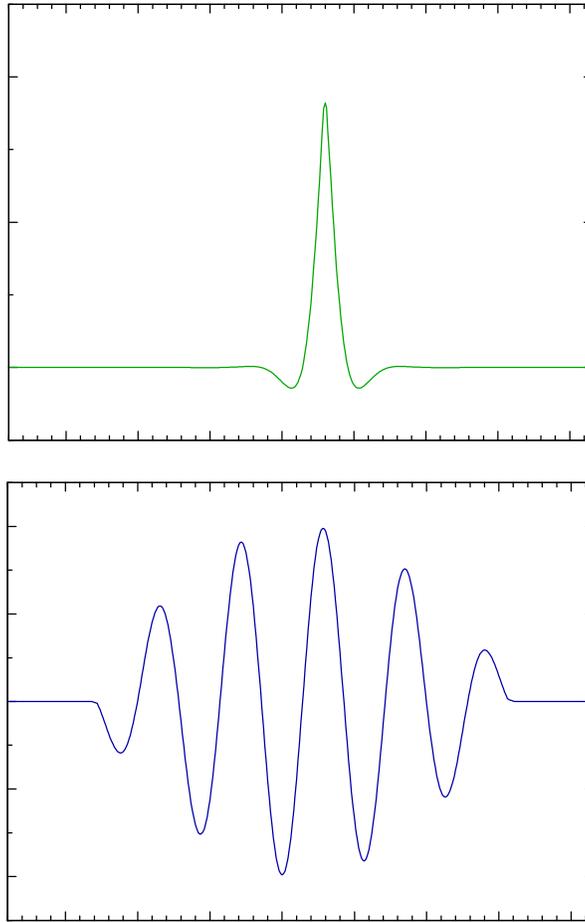
Minimum energy and speed is indistinguishable from zero, and a marble of reasonable speed has a quantum number on the order of  $10^{30}$ . In other words, we can't perceive the quantum features of the marble in the box.

### 3.7 Uncertainty Principle I -- derivation based on the wave properties of particles

Consider the particles represented by the wave groups shown in figure 3.12 (the picture is below in my notes).

The one in part (a) has a well-defined position, but a poorly defined wavelength, and therefore a large uncertainty in its momentum (remember--wavelength and momentum are related).

The one in part (b) has a relatively well-defined wavelength (and therefore momentum), but who knows where the particle is.



To quantify the uncertainties in the wave group's position and momentum, we need to go into much more detail about representing wave groups by summations of individual waves.

We may investigate some of those details later. For now, let's consider how to minimize the uncertainties in the wave group's position and momentum.

The wave number  $k$  and momentum are directly proportional (remember  $\lambda=h/p$  and  $k=2\pi/\lambda$ ), so we'll try to minimize  $\Delta x \Delta k$ .

We'll take Beiser's word for it that the minimum of the product  $\Delta x \Delta k$  occurs when the envelope representing the wave group is a Gaussian function. In this case,  $\Delta x \Delta k=1/2$ , and, in general,  $\Delta x \Delta k \geq 1/2$ .

The use of the wave number isn't very helpful to most of us, but we can use  $\lambda=h/p$  and  $k=2\pi/\lambda$  to relate  $\Delta k$  to  $\Delta p$ . After we do that, we find

$$\Delta x \Delta p \geq \frac{h}{4\pi}.$$

In other words, there are fundamental limits on how precisely we can simultaneously measure a particle's position and momentum.

These limits have nothing to do with our measurement techniques; they are built into nature.

We usually use the symbol  $\hbar$  for  $h/2\pi$ .

Planck's constant is so small that we never encounter the uncertainty principle in Newtonian mechanics.

Heisenberg discovered the uncertainty principle, so it is often called "Heisenberg's uncertainty principle."

A rigorous proof requires the wave group analysis I alluded to above.

### **3.8 Uncertainty Principle II -- derivation based on the particle properties of waves**

Imagine trying to measure an electron's position by detecting a photon colliding with it.

We need a short wavelength to accurately determine the electron's position (because the electron is so small).

But a short wavelength photon has lots of energy and momentum, and gives the electron a big kick, so we can't say much about how the initial momentum of the electron.

The better we try to measure the electron's position, the bigger the kick, and the less we know about the electron's momentum.

On the other hand, we can use a longer wavelength photon, but then we have a poorer idea of the position of the electron.

This kind of argument leads to something like  $\Delta x \Delta p \gg \hbar$ .

The above isn't a rigorous mathematical derivation (hence we are not worried about the "missing"  $4\pi$ ), but it is an easily understood illustration.

Don't be mis-led into thinking the uncertainty principle is simply some kind of measurement problem we haven't yet resolved, which the above kind of argument implies it might be.

### **3.9 Applying the Uncertainty Principle**

Since frequency and time are related, and since velocity and energy are related, we can come up with an alternate expression of the uncertainty principle:

$$\Delta E \Delta t \geq \frac{h}{4\pi}.$$

This means we can't simultaneously measure with arbitrary precision both a time for an event and the energy associated with that event.