Waves

Waves diffract and waves interfere. We care about the wavelike properties of something when it is interacting with something that is on the same length scale of the wavelength. Like an array of atoms. Or two waves interacting.

There are consequences of this.

One of them can be found looking at the Bohr model for the atom. If the electron is in an orbit of fixed radius (note: it is in the Bohr model but isn't in the real world), then only certain values of the wavelength are allowed. This is to prevent the wave from interfering with itself. The wavelength must be related to the circumference of the orbit such that

$$2\pi r = n\lambda$$

r is the radius and 2pi x r = circumference. The wavelength must be an integral fraction of the circumference. Thus n=1 the wavelength is the circumference, or n=5 there are 5 waves as you go around the orbit. This is instructive to two reasons even though it is not reality.

1. You can see that imposing wavelike solution on the problem with a boundary condition (that they don't interfere with themselves) gives rise to quantized solutions.

2. If you combine this with Bohr's idea of quantize angular momentum you arrive at a relationship between wavelength and linear momentum.

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

This is the DeBroglie wavelength. The idea is that everything has a wavelength that depends on it momentum (p). As you will see on the HW the wavelength for large (classical) objects are ridiculously small. The wavelengths for things like electrons can be small, but are in the range of "atomic things"

The Heisenberg Uncertainty Principle

Simply stated we need to realize that if we are going to "think" about particles as waves there will be odd consequences. One is indeterminancy.

Let's look at the classical world. If I know exactly where a particle is and exactly where it is going, then I know everything. That is with the initial conditions I can solve Newton's equation and I know the position, velocity, momentum, energy…. for every particle in the system until the end of time.

In the quantum world this is not the case. It is not that is hidden from us, it is simply that we cannot actually ask the question in the first place. That is it is not possible to know exactly the position and momentum of a QM particle to begin with. Not because we aren't clever enough, but because they it is not possible to ever know.

The Heisenberg uncertainty principle states that uncertainty in position time the uncertainty in momentum is always greater than h-bar divided by 2.   That is to say we can always be less certain (feel free to have no information), but we can never pin things down beyond this point. Don't despair Planck's constant is a very small number (and you get to divide it by 4 pi). Thus the total uncertainty is very very small. Unless the positions and momenta are very small. Then it matters. For you and me it doesn't. For the electron it does.

QUANTUM MECHANICS

Let us begin by stating that there are certain things which we must simply accept and there is no way to prove them. They are the things that we postulate must be true. They cannot be proven but if they are accepted then what follows bears out in the real world. As such QM offers a tool to predict things in chemistry (ionization energy, bond lengths, dipole moments, bond strengths,…) that can be measured in the lab. When these prediction turn out to be accurate we accept that the machinery is correct.   We leave the philosophy to others.

Step one.   In Quantum Mechanics all the information about the system is contained in the wavefunction. It is from this that we would calculated any property of the system (like the energy, or the angular momentum). The name of the game is to find the wavefuction. You may have already encountered this under different names such a "the orbital for the electron". There is one useful interpretation of the wavefunction (as we can't simply leave it as a tool. We want to know what it is). That is that the square of the wavefunction is the probability of finding the particle at a given location. As such we would like our wavefunctions to be normalized. That is we would like the integral over all space of the functions squared to be equal to 1.(This I didn't explicitly talk about in class today, but I will go over again next time) What is the probability of finding the particle somewhere in the universe? One. It must be somewhere. Therefore if I intergrate the wavefunction squared over the entire universe I should get one.

In one dimension, x, we write the wavefunction as

$\psi(x) = $ some function

Then the wavefucntion will such that

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = 1$$

What else do we know about the wavefunction. It should be a "normal function". It should be continuous (and have a continuous first derivative).

How do we find the wavefunction? It is the solution to the Schrödinger equation

The Schrödinger equation

There is not derivation of the Schrödinger equation. If you had more physics classes (particularly in wave mechanics) then this might seem like a reasonable equation. However, for us it is what it is. The simple version of the equation is that the Hamiltonian operating on the wavefuction yields the energy times the wavefunction.

$$\hat{H}\psi(x) = E\psi(x)$$

What is an operator? An operator is a mathematical operation that does something to the wavefunction. Takes it derivative, Multiplies it by 5., ….

The Hamiltonian operator in QM is a specific operator that is the total energy operator. The potential energy part of it is simple, it simply multiplies the wavefunction by the potential energy. The kinetic energy part is "unusual". The kinetic energy is related to the second derivative of the wavefunction. As such the Schrödinger equation in one dimension (labeled here as a coordinate x) is

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

Where V(x) is the potential energy as a function of position x. We now have an equation that we can solve to find the wavefunction or wavefunctions. We'll see that there will be more than one solution. Each solution will have its own energy. This is the equation for all time independent QM problems (although here we have a simple version that has only one coordinate).

We need to find a function that when we take its second derivative with respect to x, multiply by hbar square, and divide by negative 2m, and then add the potentially energy times that function is equal to a constant (the energy) time the same function. Simple! Actually it is for many forms of the potential. In addition, if we have a big computer we could do it numerically for anything.