A little quantum mechanics.

These notes are not a substitute for reading the book and working problems.

What is light?

1) Maxwell showed that light (visible, x-rays, radio, gamma, etc.) obeyed the wave equation; $\frac{\partial^2 E(x,t)}{\partial x^2} = \frac{1}{\sqrt{\mu\varepsilon}} \frac{\partial^2 E(x,t)}{\partial t^2}$ where *E(x,t)* represents the electric (or magnetic) field.

- Experimentally we know light is a wave because it demonstrates diffraction, dispersion, interference, resolution which depends on wavelength; all the stuff that waves do.

2) However Einstein showed that, in order to explain the photo-electric effect, light has to sometimes behave like a particle, called the photon, with energy $E = hf$ where is the frequency and is Planck's constant. The photoelectric effect says photons can knock electrons loose and cause a current flow $hf = KE_{\max} + \phi$ where ϕ is the energy needed to free the electron.

- The Compton effect and the ultraviolet catastrophe (problems from trying to calculate blackbody radiation using classical physics) are further experimental evidence that light is a particle (see text for details).

3) So light is not classical: It behaves like a wave (diffraction, etc.) but arrives in lumps (as photons). Which effect you measure depends on the experiment.

What are electrons?

1) Some of the time electrons behave like particles. For example in a CRT (old style television tube) the electrons act like particle- they are accelerated by a potential and hit the screen like a particle.
2) Davidson and Germer, however, showed that electrons reflecting off a crystal act as if they are waves. Electron diffraction is now used as a research tool in chemistry and physics (see text for details).
3) de Broglie postulated a wavelength for the electron: $\lambda = h/p$where $p = mv$ is momentum. Schrodinger came up with a wave equation for electrons. It is not the same as the wave equations for photons because electrons have mass, do not travel at $3\times10^8 m/s$ and interact with electric and magnetic fields (photons do not have mass, do travel at the speed of light and do not interact with other electric or magnetic fields).

Wave equation for electrons (Schrodinger's equation).

The one dimensional version (meaning the electron can only move along the x-axis) of Schrodinger's equation is

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

where $\hbar = h/2\pi$, is the electron mass, $i = \sqrt{-1}$, and $V(x)$ is the electric potential that the electron feels (for the three dimensional case of an electron trapped in a hydrogen atom $V(x)$ is the coulomb potential of the nucleus $V(x) = \frac{-kq}{r}$).

- The equation for electrons is different than for electromagnetic waves because electrons have mass and react to electrical potentials (photons do not).
- Generic solutions are $\Psi(x,t) = Ae^{i(kx-\omega t)}$. Since the solutions are imaginary they can be written as $\Psi(x,t) = \Psi_{\mathrm{Re}}(x,t) + i\Psi_{\mathrm{Im}}(x,t)$ or $\Psi(x,t) = A(x,t)e^{i\theta(x,t)}$ where $\theta(x,t) = \tan^{-1}\frac{\Psi_{\mathrm{Im}}}{\Psi_{\mathrm{Re}}}$ is called the phase.
- Direct substitution of the generic solution into Schrodinger's equation shows that $E = \frac{p^2}{2m} + V$ where is momentum. This shows energy of the electron equals kinetic energy plus potential energy which we already know classically. To get this we have to have $E = hf$ for the energy of the electron, just as it was for the photon.
- For 'static' cases where the electron is going to basically stay put (analogous to static mechanics or static electricity where nothing moves) the time independent Schrodinger's equation becomes $\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2} + V(x)\Psi(x) = E\Psi(x)$

What does the electron wave function, $\Psi(x,t)$ tell us?

Everything! Everything that can be known about the electron. But first note that $\Psi(x,t)$ is imaginary so we always have to multiply by the complex conjugate to get a real number (we can only measure real quantities). For example for an imaginary number $\kappa = A + Bi$ we have $\kappa^* = A - Bi$ and $\kappa^*\kappa = A^2 + B^2$ which is real.

- $\Psi^*(x,t)\Psi(x,t)dx$ is the probability of finding the electron in the region dx. (This is kind of like the diffraction pattern for light- for light the pattern tells us where photons will land, for electrons it tells us where the most likely place to find the electron is).
- $\int_{-\infty}^{\infty}\Psi^*(x,t)\Psi(x,t)dx = 1$, in other words, there is a 100% chance of finding the electron somewhere.
- The expected value of any quantity can be found by integrating. So the expected location (kind of like the average location) is $<x> = \int_{-\infty}^{\infty}\Psi^*(x,t)x\Psi(x,t)dx$. There are expectation values for momentum, energy, etc.

How about a simple example?

Imagine we throw an electron into a one dimensional box that is infinitely strong and let it settle down (time independent or so called stationary states). (Yes this is a 'toy' model- it doesn't exist in nature but you have to start somewhere.)

- So we want to solve Schrodinger's time independent equation for zero potential between the locations $x = 0$ and $x = L$ which is $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$. (Note: Stationary states are analogous to standing waves on a string; the equation for a standing wave is $A\sin(kx)\cos(\omega t)$ where the shape is given by the sine function but the shape changes over time; a point which is often ignored at looking at the first few modes of a guitar string.)
- Outside of $x = 0$ and $x = L$ the wave function doesn't exist (the electron can't go there).
- Generic solutions look like $\psi(x) = A\sin kx + B\cos kx$ (or exponentials or …. But don't worry about those for now).
- But there are conditions (boundary conditions): We must have $\psi(x = 0) = 0$ and $\psi(x = L) = 0$. Why? So the probability drops off to zero smoothly at the boundaries (probabilities are 'fuzzy' they can't end abruptly as a point). The first condition means $B = 0$ and the second means we have to have $kx = n\pi$ where $n = 1,2,3,...$ so that $\psi(x = L) = A\sin n\pi L = 0$.
- Substitute $\psi(x) = A\sin kx$ into Schrodinger's equation (take two derivatives with respect to x and use $V = 0$ from $0 \le x \le L$and we find out that, to be a solution, we have to have $k = \frac{\sqrt{2mE}}{\hbar}$ (try it yourself- see if you get this).
- Combining the boundary condition $kx = n\pi$ with $k = \frac{\sqrt{2mE}}{\hbar}$ we find that $E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}$. Energy is quantized (depends on the whole numbers =1, 2, 3…)!!!!
- Moral of the story: forcing the wave to fit into a box forces the energy to become quantized. Free electrons don't have this problem and can have any energy. Bound electrons will always have quantized energies.
- Where is the electron? We don't know exactly. All we have is the probability of finding it in certain places (but not in others). For this problem $\psi^*(x)\psi(x) = A^2\sin^2 kx$ and $k = n\pi / L$. These are the 'orbitals' or 'electron clouds' that chemistry books draw for the hydrogen atom but in this case they are 'orbitals' for the one dimensional electron box problem.
- What about the amplitude, *A*? This can be determined using the normalization condition $\int_{-\infty}^{\infty}\psi^*(x)\psi(x)dx = 1 = \int_0^L A^2\sin^2(kx)dx$ where we only integrate from $x = 0$ to $x = L$. When you do this you find out $A = \sqrt{\frac{2}{L}}$. (Try it!).
- The 'recipe' for solving a quantum problem:
    - Write the appropriate Schrodinger equation.
    - Write the generic solutions.
    - Apply boundary conditions.
    - Substitute solution into equation to determine other constants.
    - Normalize to get coefficients.

What about the uncertainty principle?

We have to describe electrons as waves, right? Right, experiments say so!

- For a free electron Schrodinger's equation has the solution $\psi(x) = A\sin kx$ but now there are no restrictions on *k*, no boundaries so no quantized energy.
- But where is the electron? Any where! (Well, anywhere in one dimension- we are still talking about a one dimensional case.)
- What if we want to localize the electron? Well, Fourier said we can get any wave shape we want by adding together sine waves. So let's add a bunch of sine waves together to get a *wave packet*: a shape that is localize in one place.
- Wait! Let's do a simple case first. Add $A\sin(k_1 x - \omega_1 t)$ to $A\sin(k_2 x - \omega_2 t)$. Go on, do it!
- You should have gotten $2A\cos(\frac{1}{2}\Delta kx - \frac{1}{2}\Delta\omega t)\sin(k_{ave}x - \omega_{ave}t)$ where $\Delta k = k_1 - k_2$, $\Delta\omega = \omega_1 - \omega_2$and $k_{ave} = (k_1 + k_2)/2$, $\omega_{ave} = (\omega_1 + \omega_2)/2$. Sketch a picture of this. It is an envelope of a slowly changing cosine with a more rapidly changing sine wave inside. One way to look at it is a series of packets of waves.
- At $t = 0$ the cosine part is zero if $\frac{1}{2}\Delta kx = n\pi$. So two successive locations where cosine is zero is $\frac{1}{2}\Delta kx_1 = \pi$ and $\frac{1}{2}\Delta kx_2 = 2\pi$. Subtracting these gives $\frac{1}{2}\Delta k\Delta x = \pi$. But wait, de Broglie said $k = 2\pi/\lambda$ and $p = h/\lambda$ for electrons. So $\frac{1}{2}\Delta k\Delta x = \Delta p\Delta x = h$, which is basically the uncertainty principle (don't worry about the missing factors of π we'll eat that pie later).
- But what does the uncertainty principle mean? If one of the packets represents the electron we see that the range of possible locations of that electron is between x_1 and x_2; in other words the uncertainty of location of the electron is Δx. Because a wave packet is of finite length we have a range of possible locations of the electron.
- What if we tried to add more waves to get the packet smaller? This is going to require adding more different values of *k* so the Δk will have to get larger. Since *k* is related to momentum then the uncertainty in moment, Δp has to get larger.
- When we add an infinite number of waves we find that $\Delta x\Delta p \geq \hbar/2$.
- If we go back and set $x = 0$ and do with frequency what we did with *k* we get $\Delta E\Delta t \geq \hbar/2$ since frequency is related to energy.
- The uncertainty principle is a direct consequence of describing the electron as a wave: you can't locate a wave at single point.

Is any of this stuff 'real'? YES!!!! Computer circuitry, electron microscopes, tunneling microscopes, nuclear fission, etc. cannot be explained without using quantum mechanics.