Physics 228, Lecture 11
Monday, February 28, 2005

Bohr Model; Wave-Particle Duality. Ch 38:5,8; 39:1

1 Bohr Model

Last time we began discussing some of the paradoxes and wrong consequences of classical mechanics when applied to the interactions of light with individual electrons. We mentioned some of the early quantum assumptions to explain these quantum effects. The early quantum mechanics was a struggle to find modifications to classical mechanics to explain these difficulties, and it was only after 25 years of somewhat ad-hoc models (starting with the Planck blackbody explanation) that a coherent theory of quantum mechanics developed. And as that theory is somewhat difficult to understand, many effects are still most easily discussed in terms of the old quantum models.

One of the most important of these models was the Bohr model of the atom, and most particularly of the hydrogen atom. The hydrogen atom is particularly simple because it consists of a single electron moving around the positively charged nucleus, which is usually just a single proton. The force which holds the electron in the atom is just the Coulomb attraction. The Rutherford atom would have the electron moving in orbits around the nucleus just as planets revolve around the sun. The classical mechanics of these situations are the same, but Bohr added some quantum mechanical rules.

Bohr asserted that of all the infinitely many orbits that classical mechanics would say were possible, only certain ones are allowed. In those orbits, the electron's motion can be considered classically, but without considering the classical electromagnetic radiation that the accelerating electron ought to be producing. The allowed orbits are those for which the angular momentum is an integral multiple of Planck's constant divided by 2π.

Let us assume the allowed orbits are all circular. If the electron is moving in a circle of radius r and velocity v, its angular momentum is

$$L = r \times p = m_e r v = n\hbar, \quad \text{with } \hbar = \frac{h}{2\pi},$$

and n a positive integer. The centripetal force is

$$F = k_e \frac{e^2}{r^2} = m_e \frac{v^2}{r}.$$

Plugging in $v = n\hbar/m_e r$ in this equation and then solving for r,

$$k_e \frac{e^2}{r^2} = m_e \frac{1}{r} \frac{n^2\hbar^2}{m_e^2 r^2} \longrightarrow r = \frac{n^2\hbar^2}{k_e m_e e^2}, \quad v = \frac{n\hbar}{m_e} \frac{k_e m_e e^2}{\hbar^2 n^2} = \frac{k_e e^2}{n\hbar}.$$

What is the energy of the electron in the n'th orbital, as it is called?

$$\begin{aligned} E &= T + U = \frac{1}{2} m_e v^2 - k_e \frac{e^2}{r} \\ &= \frac{1}{2} m_e \left(\frac{k_e e^2}{n\hbar} \right)^2 - k_e e^2 \frac{k_e m_e e^2}{n^2\hbar^2} \\ &= \frac{1}{2} m_e \frac{k_e^2 e^4}{n^2\hbar^2} - \frac{k_e^2 m_e e^4}{n^2\hbar^2} \\ &= -\frac{1}{2} \frac{k_e^2 m_e e^4}{\hbar^2} \frac{1}{n^2}. \end{aligned}$$

Notice that the allowed values for the energy are now only a discrete set of **"energy levels"** all given by a constant

$$E_1 = -\frac{1}{2} \frac{k_e^2 m_e e^4}{\hbar^2},$$

divided by the square of an integer. Also note that all these energies are negative — we are measuring energies relative to the energy the atom would have if the electron were infinitely far away, so all states of the atom which have the electron bound to the nucleus are states with negative energy.

Now lets ask how such atoms can radiate, that is, give off light and lose some energy in the process. We will assume that it does so by giving off a single photon of light with energy

$$E_\gamma = hf = \frac{hc}{\lambda} = E_i - E_f,$$

where E_i is the initial energy of the atom, $E_i = E_1/n_i^2$, and $E_f = E_1/n_f^2$ is the final energy of the atom. Thus

Repeat
Fig. 40.17
2 3/4" × 4"

$$\frac{1}{\lambda} = \frac{1}{hc}(-E_1) \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

Note

$$\begin{aligned}
\frac{-E_1}{hc} &= \frac{1}{hc} \times \frac{1}{2}\frac{k_e^2 m_e e^4}{\hbar^2} \\
&= \frac{k_e^2 m_e e^4}{4\pi\hbar^3 c} \\
&= \frac{(8.9875518 \times 10^9)^2 \cdot (9.1093897 \times 10^{-31}) \cdot (1.60217733 \times 10^{-19})^4}{4\pi(1.05457266 \times 10^{-34})^3 \cdot (2.99792458 \times 10^8)} \mathrm{m}^{-1} \\
&= 1.09737315 \times 10^7 \mathrm{m}^{-1} = \mathrm{R_H}\,!
\end{aligned}$$

So Bohr's model explains the hydrogen spectrum completely, including calculating the Rydberg constant in terms of fundamental constants!

When the hydrogen atom is in its lowest energy state, it is stable and cannot radiate simply because there is no lower state for it to go into after losing energy. That is the quantum mechanical explanation for why the electron does not radiate even though it is accelerating.

This lowest state is the $n = 1$ state, and when the electron is in this state, the Bohr model predicts the electron is orbiting in a circle of radius which is called the **Bohr radius** a_0:

$$a_0 = r(n{=}1) = \frac{\hbar^2}{k_e m_e e^2} = 5.29 \times 10^{-11}\mathrm{m}.$$

The higher energy states have radii n^2 times as big. Note a_0 sets an approximate scale for atomic physics, and all atoms in their ground states are approximately 10^{-10} m in diameter.

The Bohr model gives us the full set of possible bound energy states for a hydrogen atom. There can be transitions between these states, with the emission (or absorption) of a photon with

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right).$$

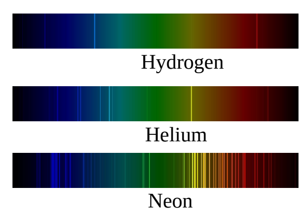
Our formula for the wavelengths gives

n_i	n_f	λ (nm)	color
4	3	1874.6	infrared
∞	3	820.1	infrared
6	2	410.0	violet
5	2	433.9	blue
4	2	486.0	green
3	2	656.1	red
2	1	121.5	ultraviolet

More complicated atoms also have a discrete set of states, although it is not possible to calculate the energies exactly for complex atoms the way it is for hydrogen. But the states play the same role, in particular for the emission and absorption of photons. As we saw, the atom can emit light if it is in a higher energy state by going to a lower energy state, placing the energy lost in the atom into a photon with energy $E = hc/\lambda$.

Last time we observed the spectra of three gases with hand-held diffraction gratings. Let's look again at the Hydrogen spectrum Can we make out the four lines which should be visible? here it is on the overhead, and we can just barely make out the $6 \to 2$ transition.

Now let's look at the look at the spectra of a more complex gas atom. Note that there are more individual frequencies emitted, but we do not have a continuous spectrum the way we did with the white incandescent bulb. These emission lines are due to atoms dropping from an excited state to a lower energy state, giving off a photon in the process.



Here is another spectrum, with dark lines instead of bright ones! What is that do to?

The reverse of emission can also happen — if light of the right frequency hits an atom in its ground state, the atom can absorb a photon and make a transition to an excited state, one with a larger value of n. This is true even for complicated atoms, although the energy levels are not given by such a simple formula as for Hydrogen. Notice that only photons of the right wavelengths can be absorbed this way, which explains why a gas in front of a continuum source produces an absorption spectrum with discrete black lines. As I mentioned, helium was first discovered by observing dark absorption lines in the spectrum of the sun, caused by absorption in the upper solar atmosphere. If the photon has enough energy to overcome the binding energy of the electron in the atom, it can remove it completely, that is, let the electron go out infinitely far way, thereby **ionizing** the atom.

The lowest energy state is called the **ground state**, with $n = 1$. The next state, with $n = 2$, is called the **first excited state**, and all other states are also called excited states, having more energy than the minimum the atom must have.

1.1 The Correspondence Principle

How can it be that we are now claiming that all the classical physics we learned in the last three semesters is wrong, and the true story is based on quantum mechanical principles? Didn't we have good evidence to support what we learned about Newtonian mechanics and Maxwell's theory of electromagnetism?

The same issue came up with spectial relativity, where we "threw out" the fundamental understanding of how coordinate systems were related, challenging Newtonian mechanics. But in that case it was pretty clear what was happening — the relativistic expressions, for example for momentum, reduced to the Newtonian expressions if we considered the formal limit $c \to \infty$, or more practically, differed quantitatively from the Newtonian expressions only by negligible amounts as long as the velocities of particles were much less than the speed of light.

In our treatment of quantum mechanical effects, it is less clear in what approximation quantum mechanical effects should be negligible, but we must have that the true physics is well approximated by classical physics when the situation is classical. Do the planets travel in Bohr orbits around the Sun?

Bohr answered this kind of question with his **correspondence principle**, which stated that the quantum mechanical predictions must agree with classical predictions when the quantization is negligible. In particular, consider the electron in a very highly excited state, say $n = 10000$. If the atom emits one photon while dropping into the $n = 9999$ state, the emitted photon will have an energy

$$\begin{aligned} E_\gamma &= hf = 2\pi\hbar f = E_{10000} - E_{9999} = \frac{1}{2}\frac{k_e^2 m_e e^4}{\hbar^2}\left(\frac{1}{9999^2} - \frac{1}{10000^2}\right) \\ &= 1.00015 \times 10^{-12}\frac{k_e^2 m_e e^4}{\hbar^2}, \end{aligned}$$

so $f = 1.00015 \times 10^{-12} \frac{k_e^2 m_e e^4}{2\pi\hbar^3}$. In the $n = 10000$ state, the radius is

$$r = \frac{n^2\hbar^2}{k_e m_e e^2} = 10^8 \frac{\hbar^2}{k_e m_e e^2},$$

and the velocity is

$$v = \frac{k_e e^2}{n\hbar} = 10^{-4} \frac{k_e e^2}{\hbar},$$

so the frequency with which the electron circles the nucleus is

$$f_c = \frac{v}{2\pi r} = 10^{-12} \left. \frac{k_e e^2}{2\pi\hbar} \middle/ \frac{\hbar^2}{k_e m_e e^2} \right. = 10^{-12} \frac{k_e^2 m_e e^4}{2\pi\hbar^3}.$$

Note that classical electrodynamics says the radiated wave should have the same frequency as the frequency at which the electron circles the nucleus, and we find that that agrees with the quantum mechanical prediction to about 1 part in 10^4.

2 Wave-Particle Duality

So, is light a wave, as interference and diffraction proved, overthrowing Newton's particle theory in the early nineteenth century, or does it consist of particles of light, called photons, as Einstein proposed and Compton scattering and atomic spectra seem to say. Clearly the answer is that neither of these classical ways of viewing light is complete, and that in some contexts light behaves as we would expect of a wave, and in others it behaves like a particle. A deeper understanding is necessary to include all these aspects in one coherent theoretical understanding.

But if each of the pictures, particle and wave, are necessary to describe various aspects of how light behaves, might this also be true of objects we have previously considered only to be particles? Might an electron also be a wave? This idea was put forth in 1923 by Louis de Broglie in his Ph. D. thesis. He noted that for light, a photon has energy $E = hf = hc/\lambda$ and momentum given by $p = E/c = h/\lambda$, so he suggested that all particles have an associated frequency and wavelength related to their energy and momentum by

$$E = hf, \quad p = \frac{h}{\lambda}.$$

Now just what this "wave" consisted of was completely unclear — what is oscillating when a particle is moving in a straight line? Can an electron undergo interference? The answer was found by an experiment by Davisson and Germer in 1927 when they scattered electrons off nickel and found the same kind of Bragg scattering that is observed for X-rays.

3 Quantization of L

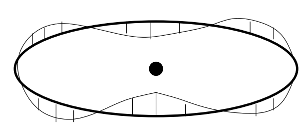
We saw that Bohr imposed, *ad hoc*, a quantization condition on the angular momentum of the electron,

$$L = n\hbar.$$

De Broglie's idea that a momentum is associated with a wavelength gives us a way of understanding this requirement. Consider an electron in a circular orbit of radius r and momentum p, and thus

$$L = n\hbar = |\vec{r} \times \vec{p}| = rp = r\frac{h}{\lambda} = \hbar\frac{2\pi r}{\lambda},$$

so the quantization condition can be interpreted as requiring an integer number of wavelengths to fit around the orbit. That is, whatever the de Broglie wave is, it needs to interfere constructively with itself as it circles the nucleus.



We will return to this after we have described the full quantum mechanical description of the hydrogen atom.

4 Summary

- In the Bohr model, electrons can travel in circular orbits around the nucleus obeying classical laws except that only orbits with angular momentum $L = n\hbar$ are allowed, and radiation is not considered in the classical motion.
- This predicts discrete orbits with

$$r = a_0 n^2, \quad v = \frac{k_e e^2}{n\hbar}, \quad E = \frac{E_0}{n^2},$$

where

$$a_0 = \frac{\hbar^2}{k_e m_e e^2} = 5.29 \times 10^{-11}\text{m}, \qquad \mathrm{E}_0 = -\frac{1}{2}\frac{\mathrm{k_e^2 m_e e^4}}{\hbar^2} = -13.606\text{eV}.$$

- Light is emitted or absorbed by atoms as they make a transition from one energy level to another, emitting or absorbing a photon with the energy required by energy conservation.

- For hydrogen, the Bohr model thus explains the Rydberg formula for the spectrum, including explaining the Rydberg constant R_H in terms of fundamental physical constants

- Bohr's correspondence principle says that for large excitation levels, the quantum mechanical results should agree with classical expectations.

- According to de Broglie, particles also have associated frequencies and wavelengths given by
$$E = hf, \quad p = \frac{h}{\lambda}.$$
Whatever these represent, it is possible for a particle to interfere with itself, as demonstrated by electron scattering off a crystal by Davisson and Germer.