Quantum Mechanics and Atomic Physics

Lecture 2:

Rutherford-Bohr Atom

and deBroglie Matter-Waves

http://www.physics.rutgers.edu/ugrad/361

Prof. Sean Oh

HW schedule changed!!

- ***First homework due on Wednesday Sept 14 and the second HW will be due on Monday Sept 19!***
- HW1 Will be posted today

Review from last time

- Planck's blackbody radiation formula
- Explained phenomena such as blackbody radiation and the photoelectric effect.
- Light regarded as stream of particles, photons

$$E = \sqrt{(pc)^2 + (mc^2)^2} = pc \quad \text{because } m=0$$

Also, E=hf (f: frequency), so pc=hf

➔ **p**=hf/c= **h/λ**, because λ=c/f

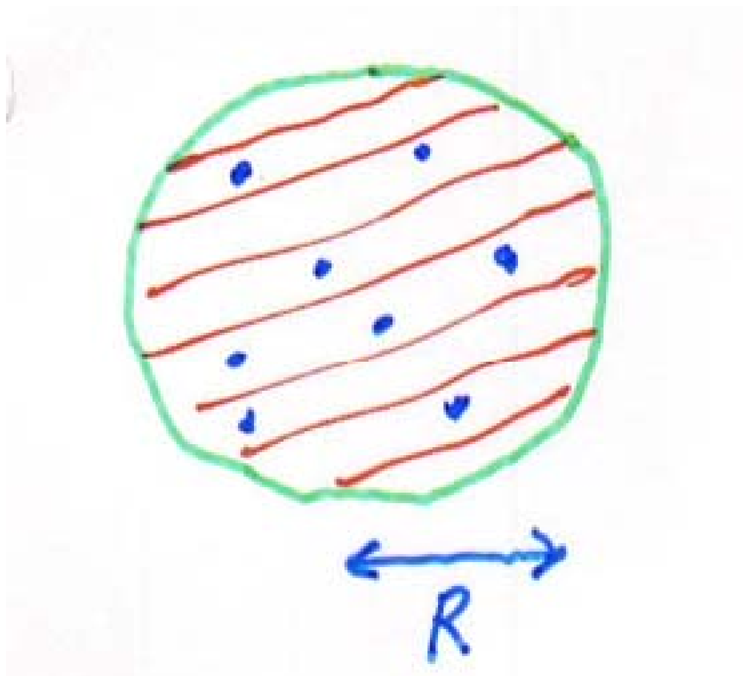
(λ: wave length, c: speed of light)

Composition of Atoms

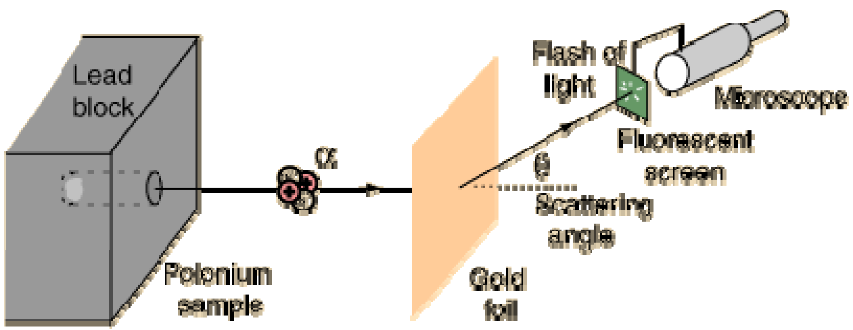
- ***If matter is primarily composed of atoms, what are atoms composed of?*** ↑
  - J.J. Thomson (1897): Identification of cathode rays as electrons and measurement of ratio (e/m) of these particles
    - Electron is a constituent of all matter!
    - Humankind's first glimpse into subatomic world!
  - Robert Millikan (1909): Precise measurement of electric charge
    - Showed that particles ~1000 times less massive than the hydrogen atom exist
  - Rutherford, with Geiger & Marsden (1910): Established the nuclear model of the atom
    - Atom = compact positively charged nucleus surrounded by an orbiting electron cloud

Thomson Model of Atoms (1898)

- Uniform, massive positive charge
- Much less massive point electrons embedded inside.
- Radius R.



Rutherford's α -scattering apparatus



http://hyperphysics.phy-astr.gsu.edu/Hbase/hframe.html

- Ernest Rutherford, with Hans Geiger and Ernest Marsden scattered alpha particles from a radioactive source off of a thin gold foil. (1911)
- Alpha deflection off of an electron
  - $\theta \sim m_e/m_\alpha \sim 10^{-4}$ rad $< 0.01^o$
- But what about deflection off a positive charge?

Experiment was set up to see if any alpha particles can be scattered through a large angle.

They didn't expect they would be, but it made a good research project for young Marsden (a graduate student).

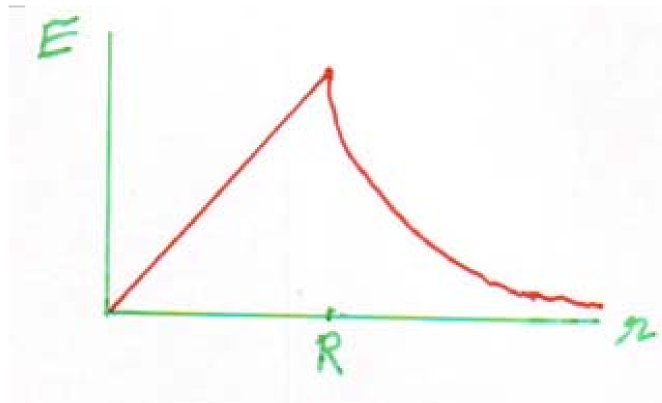
(Alpha-particle = 2 protons + 2 neutrons)

Deflection off positive charge

From Gauss's law we know:

For r < R, $\oint \vec{E} \cdot d\vec{s} = \frac{1}{\varepsilon_0} Q_{encl}$

$$E \cdot 4\pi r^2 = \frac{1}{\varepsilon_0}\rho\frac{4}{3}\pi r^3, \text{ where } \rho = \frac{Q}{\frac{4}{3}\pi R^3}$$



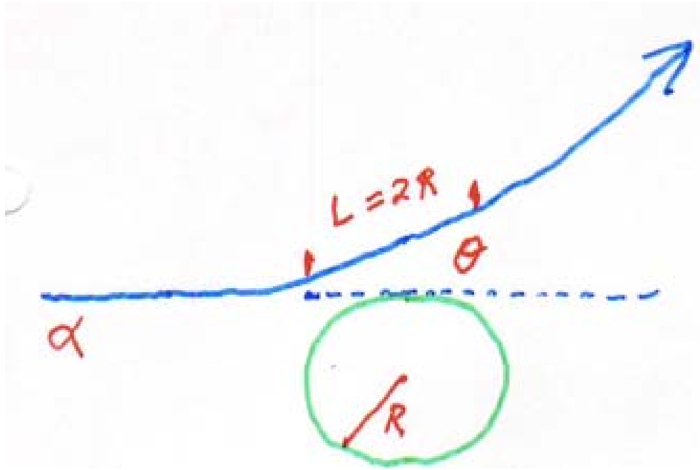
$$E = \frac{1}{4\pi\varepsilon_0}\frac{Qr}{R^3} \text{ for r < R}$$

and obviously...

$$E = \frac{1}{4\pi\varepsilon_0}\frac{Q}{r^2} \text{ for r > R}$$

Since the electric field E is maximum at r=R, expect maximum deflection for alpha particles just grazing the atom

What did they expect?



Consider only the region of length L or 2R.

$$F = q_\alpha E = \frac{1}{4\pi\varepsilon_0}\frac{2eQ}{R^2}$$

$v =$ speed of α

Traversal time is $\Delta t = \frac{L}{v} = \frac{2R}{v}$

Momentum change $\Delta p = F\Delta t$ (Impulse)

So...

$$\Delta p = \frac{1}{4\pi\varepsilon_0}\frac{4eQ}{Rv}$$

Also use $p = mv$

then $\theta_{\text{Thomson}} = \frac{\Delta p}{p} = \frac{1}{4\pi\varepsilon_0}\frac{4eQ}{Rv^2 m}$

For $R = 10^{-10}$ m, $v = 2\times10^7\, m/s, m = m_\alpha, Q = 79e$

$\Rightarrow \theta_{\text{Thomson}} \approx 0.02^o$, Very tiny.

- Much larger deflections observed! About one in 7500 alphas scattered through more than 90°
  - Impossible in Thomson model!

What they observed

- No deflection at all for most α particles
- Once every $\sim 10^4$ particles, they observed more than 90° deflections
- Inconsistent with the Thomson model
- Can be explained only if all the positive charge is concentrated to a radius of $\sim 10^4$ times smaller than the size of the atom itself

Rutherford Model

- "It was quite the most incredible event that has ever happened to me in my life. It was almost as incredible as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you. On consideration, I realized that this scattering backwards must be the result of a single collision, and when I made calculations I saw that it was impossible to get anything of that magnitude unless you took a system in which the greater part of the mass of the atom was concentrated in a minute nucleus. *It was then that I had the idea of an atom with a minute massive center carrying a charge.*"
  - Lord Rutherford, 1936

Rutherford Model

- Atom is composed of a nucleus carrying all the positive charge, and electrons orbiting around the small (~10^4 times smaller than the atom) nucleus in different orbits like planets orbiting around the sun.
- Problems: Orbiting electrons are accelerating charges and then they should emit electromagnetic radiation, eventually losing their energy and collapsing toward the nucleus.

The Bohr Atom

- The idea of the nuclear atom (Rutherford's planetary model) raised many questions at the next deeper level.
  - How do the the electrons move around the nucleus and how does their motion account for the observed spectral lines?
- In 1913, Niels Bohr published a revolutionary three-part paper.

First, Recall the Line Spectrum of Hydrogen

- In addition to (continuous) thermal spectrum, all atoms emit a discrete set of wavelengths specific to each type of atom
  - "Line spectrum"
- Rydberg formula (1913) for hydrogen:

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

$$\text{Rydberg constant } R_H = 1.09678 \times 10^{-3} \overset{o}{A}^{-1}$$

$$n_f = 1, 2, 3....$$

$$n_i = (n_f + 1), (n_f + 2), (n_f + 3), ...$$

$$\text{Balmer series, for } n_f = 2, n_i = 3 \Rightarrow \lambda = 6565\,\text{Å}$$

  - Why does Rydberg formula work?
  - Why is absorption spectrum = emission spectrum?

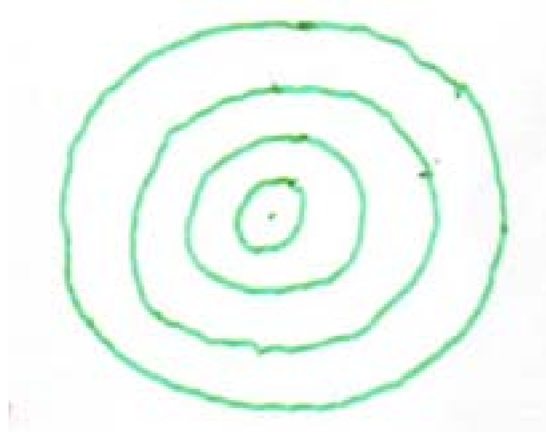
Hydrogen Wavelengths in Angstrom

		n_i					
SERIES	n_f	2	3	4	5	...	∞
LYMAN	1	1216	1026	973	950	...	914
BALMER	2		6565	4863	4342	...	3650
PASCHEN	3			18761	12824	...	8220
BRACKETT	4				40520	...	14590
PFUND	5					...	22790
	⋮						

SERIES LIMIT

Bohr Model of Hydrogen Atom

- Assumptions



1. Electron can only be in circular orbits that have orbital angular momenta:

   $$L \equiv mvr = n\hbar, \text{ where n} = 1, 2, 3, \ldots$$

2. Atom does not radiate while in such states
3. Atom radiates when electron jumps from one allowed orbit to another. Emitted photon carries off difference in energy between the orbits.

For fun see:
http://www.visionlearning.com/library/flash_viewer.php?oid=1347&mid=51

Bohr Atom

- Bohr began by assuming that the energies of the electron's orbit are dictated by Newtonian dynamics of circular orbit:

Z = charge of nucleus (1 for hydrogen)

$$\vec{F} = m\vec{a} \quad \left(\text{circular motion } a = \frac{v^2}{r}\right)$$

$$\uparrow$$

$$\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r^2} = m\frac{v^2}{r} \Rightarrow \underbrace{mv^2 = \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}}_{} \quad (1)$$

E=total energy
K=Kinetic energy
V=Potential energy

$$K = \frac{1}{2}mv^2 = \frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r}$$

$$E = K+U = \frac{1}{2}mv^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}$$

$$= \frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r} - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r} = -\frac{1}{8\pi\epsilon_0}\frac{Ze^2}{r}$$

"–" sign implies that energy must be added to atom to remove electron to infinity

Bohr Atom, con't

From (1) $\Rightarrow$ $r = \dfrac{1}{4\pi\epsilon_0}\dfrac{Ze^2}{mv^2}$ (2)

$L = mvr = n\hbar$ Bohr's key assumption

$\hbar \equiv \dfrac{h}{2\pi}$

$\Rightarrow v = \dfrac{n\hbar}{mr}$

(2) $\Rightarrow$ $r = \dfrac{1}{4\pi\epsilon_0}\dfrac{Ze^2}{m}\cdot\left(\dfrac{mr}{n\hbar}\right)^2 = \dfrac{Ze^2 m}{4\pi\epsilon_0\hbar^2}\dfrac{r^2}{n^2}$

$\Rightarrow r = \left(\dfrac{4\pi\epsilon_0\hbar^2}{Ze^2 m}\right)n^2 = 0.528\,n^2\,\text{Å}$

with $Z=1$ for hydrogen

So $r_1 = 0.528\,\text{Å}$, $r_2 = 2.112\,\text{Å}$, $r_3 = 4.752\,\text{Å}\ldots$

Called Bohr radius

Example

- Let's do problem 1-5 in your book.

Problem 1-5

Derive an expression for the speed of an electron in Bohr orbit n in terms of the speed of light. Is it justifiable to neglect relativistic effects in the development of the Bohr model?

Put $r = \dfrac{4\pi\varepsilon_0 \hbar^2 n^2}{m Z e^2}$

into $v = \dfrac{n\hbar}{mr}$

$\Rightarrow v = \dfrac{1}{4\pi\varepsilon_0} \dfrac{Ze^2}{\hbar n}$

As a fraction of c:

$\dfrac{v}{c} = \dfrac{1}{4\pi\varepsilon_0} \dfrac{Ze^2}{\hbar c n}$

use: $e = 1.602 \times 10^{-19}\ C$

$Z = 1$

$\varepsilon_0 = 8.854 \times 10^{-12}\ \dfrac{C^2}{Nm^2}$

$\hbar = 1.055 \times 10^{-34}\ J \cdot s$

$c = 3 \times 10^8\ m/s$.

$\Rightarrow \dfrac{v}{c} = 7.296 \times 10^{-3} \cdot \dfrac{1}{n} \simeq \underline{\underline{\dfrac{1}{137} \dfrac{1}{n}}}$

$n = 1, 2, 3, \ldots$

For all values of n, $v/c < 0.01 \Rightarrow$ Non-relativistic treatment is ok!

Fine Structure Constant:

$\alpha = \dfrac{1}{4\pi\varepsilon_0} \dfrac{Ze^2}{\hbar c} = \underline{\dfrac{1}{137}}$!

Energy Levels of Hydrogen

Finally,

$$E = K + V = \frac{1}{2}mv^2 - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}$$

$$\Rightarrow \boxed{E = -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2\, 2\hbar^2 n^2} = -\frac{1}{2}mc^2\frac{\alpha^2}{n^2}}$$

- For n=1, E_1=-2.17x10^{-18}J=-13.6eV
- Bohr model explains ionization energy of hydrogen in terms of fundamental constants!

  E_n=-13.6eV/n^2=-13.6eV, -3.4eV, -1.51 eV, etc.
- Lowest (n=1) orbit: *"Ground state"*
- n>1 orbits: *"Excited states"*
  - Atom radiates when electron in an excited state spontaneously jumps to a lower state: *"Quantum leap" or "Quantum jump"*

Energy level diagram for Hydrogen

n	E (eV)	r (Å)	v/c
∞	0	∞	0
4	−0.85	8.448	$\frac{1}{4}\cdot\frac{1}{137}$
3	−1.51	4.752	$\frac{1}{3}\cdot\frac{1}{137}$
2	−3.40	2.112	$\frac{1}{2}\cdot\frac{1}{137}$
1	−13.6	0.528	$\frac{1}{137}$

When electron jumps down, radiated photon energy:

$$\frac{hc}{\lambda} = E_i - E_f = -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2\, 2\hbar^2}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$\Rightarrow \frac{1}{\lambda} = \frac{mZ^2e^4}{(4\pi\varepsilon_0)^2\, 4\pi\hbar^3 c}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

- So Bohr model explains Rydberg formula and constant in terms of fundamental constants!

$$R_{Bohr} = 1.09737\times 10^{-3}\,\overset{o}{A}^{-1},\; R_{True} = 1.09678\times 10^{-3}\,\overset{o}{A}^{-1}$$

Bohr's Atomic model explained ..

- Explained the limited number of lines seen in the absorptions spectrum of Hydrogen compared to emission spectrum
- Emission of x-rays from atoms
- Chemical properties of atoms in terms of electron-shell model
- How atoms associate to form molecules

Deficiencies of Bohr Theory

- Many of the energy levels in hydrogen are actually doublets, i.e. two levels closely spaced in energy. Bohr theory cannot account for this.
- Quantization of angular momentum is just assumed, not explained or derived.
- Cannot explain spectra of complex atoms.
- Bohr theory is non-relativistic.
  - Not too bad since $v/c=1/137$, but it means theory can't be exactly right.

De Broglie Waves

- In 1924, Louis de Broglie proposed:
  - Since photons have wave and particle characteristics, perhaps all forms of matter have wave as well as particle properties
  - All particles have wavelike characteristics, with wavelength $\lambda=h/p$ (remember that this was the case only for light at that time)
  - Revolutionary idea with no experimental confirmation at the time!

Example

- An electron has K=0.2MeV. Find it's de Broglie wavelength.

$$E = mc^2 + K = 0.511 + 0.2 = \underline{0.711\ \text{MeV}}$$

$$p = \frac{1}{c}\sqrt{E^2 - (mc^2)^2} = \sqrt{(0.711)^2 - (0.511)^2} = 0.494\ \frac{\text{MeV}}{c}$$

$$h = 12400\ \text{Å}\ \frac{\text{eV}}{c} = 0.0124\ \text{Å}\ \frac{\text{MeV}}{c}$$

so $\lambda = \dfrac{0.0124\ \text{Å}\ \frac{\text{MeV}}{c}}{0.494\ \frac{\text{MeV}}{c}} = \underline{0.025\ \text{Å}}$

since $\lambda = h/p$

- wrong to use $K = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mK}$
- also wrong to use $E = pc \Rightarrow p = \frac{E}{c}$

Example

- Why didn't bullets show interference? Take the bullet mass to be 1.0 gram, speed=500m/s. Find wavelength.

Non-relativistic, so,

$p = mv = (0.001\,kg)(500\,m/s) = 0.5\ \frac{J\cdot s}{m}$

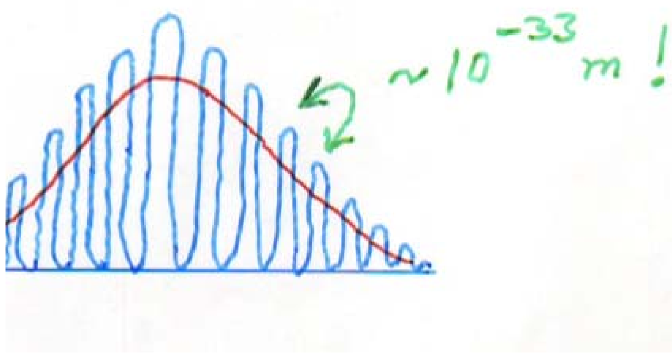
$\lambda = \frac{h}{p} = \frac{6.63\times10^{-34}\ J\cdot s}{0.5\ \frac{J\cdot s}{m}} = \underline{1.3\times10^{-33}\ m}$

Let's put into perspective:

Atomic sizes are of order 10^{-10} m.

Nuclear sizes are of order 10^{-15} m

For a bullet, λ is <u>infinitesimal</u>!



Summary

- Thomson →Rutherford →Bohr model of the atom
- deBroglie waves and the wave-particle duality
- Next time:
  - Introduction to Schrodinger's Equation

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