Quantum Mechanics and Atomic Physics

Lecture 2:
Rutherford-Bohr Atom
and deBroglie Matter-Waves

http://www.physics.rutgers.edu/ugrad/361
Prof. Eva Halkiadakis
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.
Example

Light of $\lambda = 2500$ Angstroms shines on Potassium ($\omega_0=2.20\text{eV}$).

a) Find the maximum kinetic energy of the photoelectrons.

b) Find the stopping potential.

c) If the recoiling ion moves along the photon direction, find its momentum and kinetic energy.
a) Max kinetic energy

\[ E_\gamma = h \nu = \frac{hc}{\lambda} = \frac{(12400 \text{ Å} \cdot \frac{eV}{c})}{2500 \text{ Å}} \cdot c = 4.96eV \]

Photoelectric equation: \[ E_\gamma = \omega_0 + K_{\text{max}} \]

\[ \Rightarrow K_{\text{max}} = 4.96 - 2.20 = 2.76eV \]

b) \[ K_{\text{max}} = eV_0 \Rightarrow V_0 = 2.76 \text{ Volts} \]
c) $m_e = 0.511 \text{MeV}/c^2$, $K_e = 2.76 \text{eV}$, therefore non-relativistic

\[
K = \frac{1}{2} m v^2 \Rightarrow v = \sqrt{\frac{2K}{m}} \Rightarrow p = m v = \sqrt{2Km}
\]

\[
|p_e| = \sqrt{2 \cdot 2.76 \text{eV} \cdot 0.511 \times 10^6 \frac{\text{eV}}{c^2}} = 1661 \frac{\text{eV}}{c}
\]

\[
p_\gamma = \frac{E_\gamma}{c} = \frac{4.96 \text{eV}}{c} = 4.96 \frac{\text{eV}}{c}
\]

Momentum conservation: $p_\gamma = p_{\text{ion}} - p_e$

\[
\Rightarrow p_{\text{ion}} = p_\gamma + p_e = 4.96 + 1661 \approx 1665 \frac{\text{eV}}{c}
\]
Potassium has $A = 39$, so its mass is about

$$m = 39 \cdot 939 \, \frac{MeV}{c^2} = 3.66 \times 10^4 \, \frac{MeV}{c^2} = 3.66 \times 10^{10} \, \frac{eV}{c^2}$$

$$K = \frac{p^2}{2m} = \frac{(1665 \, \frac{eV}{c})^2}{2 \cdot 3.66 \times 10^{10} \, \frac{eV}{c^2}} = 3.8 \times 10^{-5} \, eV$$

So the ion has substantial momentum (much more than that of the photon) but negligible kinetic energy. So the true energy eqn. is:

$$E_\gamma + m_e c^2 + m_{\text{ion}} c^2 = \omega_0 + m_e c^2 + K_e + m_{\text{ion}} c^2 + K_{\text{ion}}$$

$$\Rightarrow E_\gamma = \omega_0 + K_e + K_{\text{ion}}$$

$$\approx \omega_0 + K_e \text{ because } K_{\text{ion}} \approx 0.$$
Composition of Atoms

If matter is primarily composed of atoms, what are atoms composed of?

- Michael Faraday (1833): Discover of the law of electrolysis
  - Mass $\propto (q)(\text{atomic weight})/(\text{valence } #)$
- 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 $\alpha$-scattering apparatus

- 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
  - $\theta \sim \frac{m_e}{m_\alpha} \sim 10^{-4}$ rad $< 0.01^\circ$
- 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 $r < R$, $\oint \vec{E} \cdot \, d\vec{s} = \frac{1}{\varepsilon_0} Q_{encl}$

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

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

and obviously...

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

Since the electric field $E$ is maximum at $r=\text{R}$, expect maximum deflection for alpha particles just grazing the atom
What did they expect?

Consider only the region of length L or 2R.

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

\[ v = \text{speed of } \alpha \]

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

For \( R = 10^{-10} \text{ m}, \ v = 2 \times 10^7 \text{ m/s}, \ m = m_\alpha, Q = 79e \)

\[ \Rightarrow \theta_{\text{Thomson}} \approx 0.02^\circ, \ \text{Very tiny.} \]

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

- A positive charge in a small but massive nucleus with electrons orbiting it.
- Alpha heading directly at nucleus has a distance of closest approach $D$.

\[ \nu = \text{Initial speed of } \alpha \]
\[ z = 2, \ Z = 79 \]
\[ \frac{1}{2} \frac{mv^2}{m} = \frac{1}{4\pi\varepsilon_0} \frac{zZe^2}{D} \implies D = \frac{1}{4\pi\varepsilon_0} \frac{2zZe^2}{mv^2} \]

- If not head-on, impact parameter $b$ is perpendicular distance from alphas initial line of flight to nucleus.

\[ \text{Classical Mechanics: } \cot \frac{\theta}{2} = \frac{2b}{D} \]
Rutherford Model, con’t

- Alphas coming within circles of radius $b$ around the gold nuclei will scatter through $\theta$ or more. $S =$ area of gold foil

- #Gold nuclei = $nSt$, where $n =$ #atoms/volume
- Cross-sectional area for scattering through $\theta$ or more is $\sigma = \pi b^2$ around each nucleus.
- Total area for such scattering is $= \sigma nSt$
- So fraction of alphas scattering through $\theta$ or more is

$$\frac{N_s}{N_i} = \frac{\sigma nSt}{S} = \sigma nt$$
Example

- Geiger-Marsden used 3MeV alphas on gold (Z=79, A=197) with density=19.3g/cm³, thickness t=5000 Angstrom.

- How many scatter through more than 90°?
Evidently, atoms are mostly empty space!

\[ D = \frac{1}{4\pi e_0} \frac{23 e^2}{mv^2} = 7.58 \times 10^{-19} \text{ m} \]

\[ b = \frac{D}{\alpha \cot \theta/2} = 3.79 \times 10^{-14} \text{ m} \]

\[ \sigma = 7\pi b^2 = 4.51 \times 10^{-23} \text{ cm}^2 \]

\[ t = 5000 \text{ Å} = 5 \times 10^{-5} \text{ cm} \]

\[ h = \frac{\text{# Atoms}}{\text{Volume}} = \frac{N_0 \left( \frac{\text{atoms}}{\text{mole}} \right) \rho \left( \frac{\text{grams}}{\text{cm}^3} \right)}{A \left( \frac{\text{grams}}{\text{mole}} \right)} \]

\[ = 5.90 \times 10^{22} \text{ atoms} \frac{\text{cm}^{-3}}{\text{cm}^3} \]

(used Avogadro’s number \( N_0 = 6.022 \times 10^{23} \text{ atoms/mole} \))

So, \( \frac{N_s}{N_i} = \sigma nt = 1.33 \times 10^{-4} \)

\[ \Rightarrow \text{about} \frac{1}{7500} \text{ } \]
The Bohr Atom

- The idea of the nuclear atom (Rutherford’s planetary model) raised many questions at the next deeper level.
  - How do 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:

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

Rydberg constant \( R_H = 1.09678 \times 10^{-3} \text{ Å}^{-1} \)

\( n_f = 1, 2, 3 \ldots \)

\( n_i = (n_f + 1), (n_f + 2), (n_f + 3), \ldots \)

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

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<th>SERIES</th>
<th>( n_f )</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>...</th>
<th>( \infty )</th>
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<tr>
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<td></td>
<td></td>
<td>...</td>
<td>22790</td>
<td></td>
</tr>
</tbody>
</table>

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.

\[ \hbar = \frac{\hbar}{2\pi} \]
Bohr Atom

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

\[
\frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{r^2} = \frac{mv^2}{r} \quad (1)
\]

\[K = \frac{1}{2} mv^2 = \frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{2r}\]

\[Z = \text{charge of nucleus} = 1 \text{ for hydrogen}\]

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

\[\Rightarrow E = -\frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{2r}\]

\[\text{negative sign} \Rightarrow \text{energy must be added to atom to remove electron and make total } E = \alpha.\]

E=total energy
K=Kinetic energy
V=Potential energy
Bohr Atom, con’t

From (1) \[ r = \frac{L}{\frac{2e^2}{4\pi\varepsilon_0 \frac{mv^2}{r}}} \]

\[ L = mvr = n\hbar \Rightarrow v = \frac{n\hbar}{mr} \]

\[ r = \frac{4\pi\varepsilon_0 \hbar^2 n^2}{m^2 e^2} \]

Numerically allowed radii are

\[ r = 0.528 n^2 \text{Å} \]

\[ a_0 = 0.528 \text{Å} \text{ (in your book)} \]

\[ r_1 = 0.528 \text{Å}, r_2 = 2.112 \text{Å}, r_3 = 4.752 \text{Å}, \ldots \]
Example

Let’s do problem 1-5 in your book.

Put $r = \frac{4\pi\varepsilon_0}{mze^2} \frac{k^2 n^2}{n^2}$

Into $v = \frac{nh}{mr}$

$\Rightarrow v = \frac{1}{4\pi\varepsilon_0} \frac{z e^2}{hn}$

As a fraction of $c$,

$v = \frac{1}{4\pi\varepsilon_0} \frac{z e^2}{hc n}$

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?

\[
\begin{align*}
\text{We:} & \quad e = 1.602 \times 10^{-19} \text{C} \\
\text{z} & \quad = 1 \\
\varepsilon_0 & \quad = 8.854 \times 10^{-12} \frac{\text{C}^2}{\text{Nm}^2} \\
k & \quad = 1.055 \times 10^{-34} \text{J.s} \\
c & \quad = 3 \times 10^8 \text{m/s} \\
\Rightarrow v & = \frac{7.296 \times 10^{-3}}{h} \frac{1}{n} \approx \frac{1}{137} \frac{1}{n} \\
\text{For all values of } n, \frac{v}{c} < 0.01 \Rightarrow \text{Non-relativistic treatment is ok!} \\
\text{Fine Structure Constant:} \\
\alpha & = \frac{1}{4\pi\varepsilon_0} \frac{z e^2}{hc} = \frac{1}{137} \frac{1}{n}
\end{align*}
\]
Energy Levels of Hydrogen

For \( n=1 \), \( E_1 = -2.17 \times 10^{-18} \text{J} = -13.6 \text{eV} \)

Bohr model explains ionization energy of hydrogen in terms of fundamental constants!

\[
E_n = -\frac{mZ^2e^4}{(4\pi\varepsilon_0)^2 \frac{1}{2} \frac{\alpha^2}{n^2}} = -\frac{\frac{1}{2} mc^2 \alpha^2}{n^2}
\]

- 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

<table>
<thead>
<tr>
<th>n</th>
<th>E (eV)</th>
<th>r (Å)</th>
<th>v/c</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>∞</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>-0.85</td>
<td>8.448</td>
<td>(\frac{1}{4} \cdot \frac{1}{137})</td>
</tr>
<tr>
<td>3</td>
<td>-1.51</td>
<td>4.752</td>
<td>(\frac{1}{3} \cdot \frac{1}{137})</td>
</tr>
<tr>
<td>2</td>
<td>-3.40</td>
<td>2.112</td>
<td>(\frac{1}{2} \cdot \frac{1}{137})</td>
</tr>
<tr>
<td>1</td>
<td>-13.6</td>
<td>0.528</td>
<td>(\frac{1}{137})</td>
</tr>
</tbody>
</table>

When electron jumps down, radiated photon energy:

\[
\frac{\hbar c}{\lambda} = E_i - E_f = -\frac{m^2 e^4}{(4\pi \varepsilon_0)^2} \frac{1}{2 \hbar^2} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)
\]

\[
\Rightarrow \frac{1}{\lambda} = \frac{m^2 e^4}{(4\pi \varepsilon_0)^2} \frac{1}{9 \pi \hbar^3 c} \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)
\]

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

\[
R_{Bohr} = 1.09737 \times 10^{-3} \, \text{Å}^{-1}, \quad R_{True} = 1.09678 \times 10^{-3} \, \text{Å}^{-1}
\]
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
- Nuclear origin of beta-particles
- 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.
- Notions of fixed radii and speeds are inconsistent with uncertainty principle (more on this in a moment...)
- 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 $\lambda = \frac{h}{p}$.
  - Revolutionary idea with no experimental confirmation at the time!
Example

- An electron has $K=0.2\text{MeV}$. Find its de Broglie wavelength.

\[
E = mc^2 + K = 0.511 + 0.2 = 0.711 \text{ MeV}
\]

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

\[
\hbar = 12400 \text{ Å eV} = 0.0124 \text{ Å MeV} \frac{\hbar}{c}
\]

So \[
\lambda = \frac{0.0124 \text{ Å MeV}}{0.494 \text{ MeV}} = 0.025 \text{ Å}
\]

Since \[
\lambda = \frac{\hbar}{p}
\]

- Wrong to use \[
K = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mK}
\]

- Also wrong to use \[
E = pc \Rightarrow p = \frac{E}{c}
\]
Wave-Particle Duality

- Emission and absorption: behave as particles
- Propagation: behave as waves

http://www.feynmanlectures.caltech.edu/
Wave-Particle Duality
(From Feynman Lectures on Physics)

- How a bullet behaves in a double-slit experiment:

- The bullet’s behavior is particle-like.
Wave-Particle Duality
(From Feynman Lectures on Physics)

- How a wave behaves in a double-slit experiment:

- A wave will pass through both slits simultaneously, resulting in an interference pattern. Light is wavelike.
Wave-Particle Duality
(From Feynman Lectures on Physics)

- What happens if you “shine” electrons?

- But this seems wavelike, too...
Summary

- Thomson → Rutherford → Bohr model of the atom
- deBroglie waves and the wave-particle duality

Next time:
- Heisenberg uncertainty principle
- Introduction to Schrodinger’s Equation

First homework due on Monday Sept 18!