8.3 Atomic Physics

Atomic Spectra
Bohr Model
Particle in a Box

Atomic spectra and atomic structure.

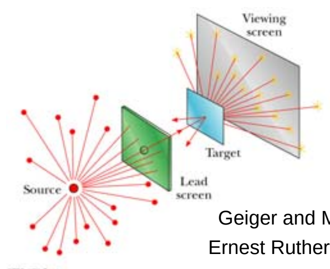
The spectra of atoms provide information about the energies of the electron in the atom.

Sharp peaks at discrete wavelengths indicate that only specified energies are allowed in the atom.

For the Hydrogen atom the Bohr theory explains the energies in a simple manner based on a quantization of angular momentum.

The quantization is explained by the de Broglie theory in terms of standing waves for the electron.

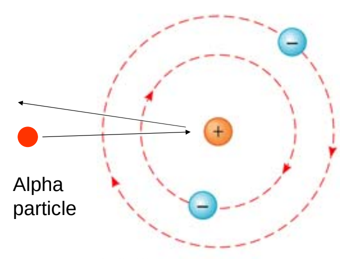
Atomic structure



Geiger and Marsden
Ernest Rutherford 1911

The scattering of alpha particles (He^{2+}) nuclei from a thin gold foil. The back scattering of a few alpha particles showed that the nucleus is a small compact object.

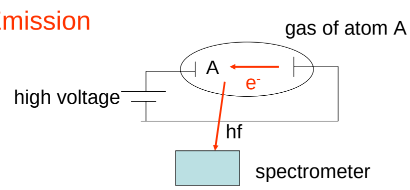
Planetary model of the atom



Scattering from a small compact nucleus

Atomic spectra

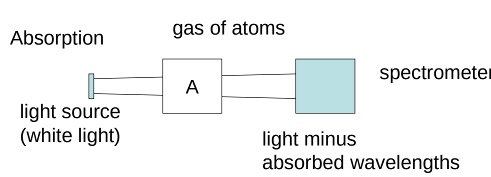
Emission



Excitation e^- (fast) + A -> e^- (slow) + A^*

Emission A^* -> A + hf

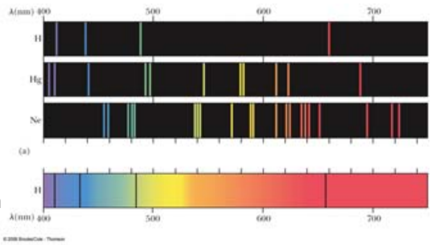
Atomic Spectra



Atomic Spectra

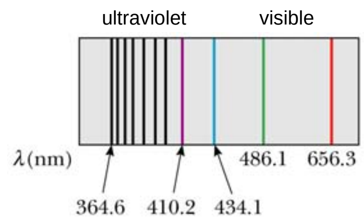
Emission

Absorption
(dark lines)



Discrete spectral lines are observed.

Balmer series for Hydrogen



Lowest λ

Highest λ

A series of peaks closer together (continuum) at low λ

Rydberg Constant

The Balmer series could be analyzed mathematically in terms of an empirical equation.

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

Rydberg Constant $R_H = 1.0973732 \times 10^7\ m^{-1}$

n = 3,4, 5 .... Integers larger than 2.

Disagreement with classical theory

Classical physics predicts that the energy of the electron can have any value- not discrete values observe.

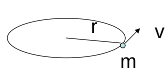
The classical theory could not explain why the electron did not fall into the nucleus. Like a satellite falling into the earth.

Bohr Theory

1. Electrons move in circular orbits.
2. Only specified atomic energy levels are allowed.
3. Energy is emitted when electron go from one energy level to another.
4. The orbital angular momentum of the electron is "quantized" in units of h/2π = $\hbar$ (called h bar)

L = mvr = n$\hbar$

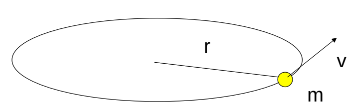
n=1, 2, 3 ....



Angular momentum of a tennis ball

$L = n\hbar$ is quantized. What is n?

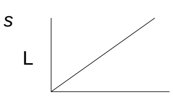
r= 0.5 m
m = 0.1 kg
v= 2 m/s



L =mvr $= (0.1kg)(2m/s)(0.5m) = 0.1\frac{kgm^2}{s} = 0.1J \cdot s$

$$\hbar = \frac{h}{2\pi} = \frac{6.6x10^{-34} J \cdot s}{2\pi} = 1.05x10^{-34} J \cdot s$$

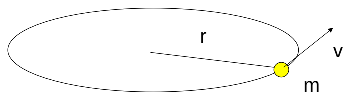
$$L = \frac{0.1J \cdot s}{1.0x10^{-34} J \cdot s / \hbar} = 10^{33}\hbar$$



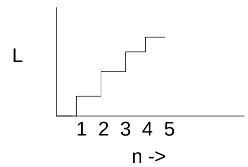
n=10^{33} n is so large that quantization is not apparent

Angular momentum of an electron

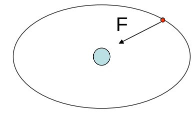
m=9.1x10^{-31}kg
r =0.1 x10^{-9} m



L is much smaller.
Quantization is apparent



Classical dynamics For central force (hydrogen atom)



Relation between v and r

$$F = ma = \frac{mv^2}{r} = \frac{k_e e^2}{r^2}$$

$$mv^2 = \frac{k_e e^2}{r}$$

v and r are not independent variables

Total energy E=KE+PE

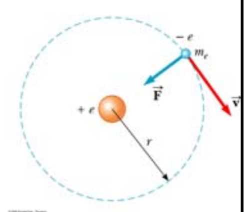
$$E = \frac{1}{2}mv^2 - \frac{k_e q_1 q_2}{r} = -\frac{k_e e^2}{2r}$$

Bohr theory for hydrogen atom

Classical energies

$$E = -\frac{k_e e^2}{2r}$$

any value of r is allowed



Quantum condition

Bohr restricted the values of r

$mvr = n\hbar$ angular momentum is quantized

n= 1, 2, 3, ... integers

$mv = \frac{nh}{2\pi r}$ momentum increases as 1/r

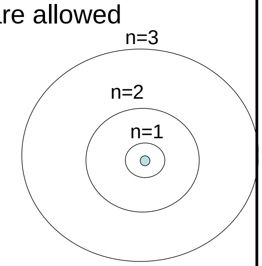
Results from Bohr theory

Only specific values of r are allowed

$$r_n = \frac{n^2\hbar^2}{m_e k_e e^2}$$

n=1, 2, 3, ... integers

radius increases as n^2



For n=1

$$r_1 = \frac{(1)^2(1.05x10^{-34}Js)}{(9.1x10^{-31}kg)(8.9x10^9 NmC^{-2})(1.6x10^{-19}C)^2} = 5.3x10^{-11}m$$

Size of the Hydrogen atom in the ground state 0.053 nm

Excited state energy levels

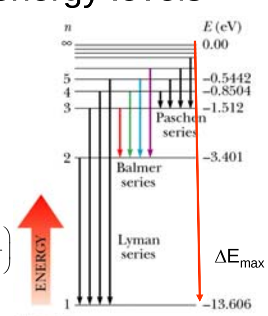
Energy levels are quantized
(proportional to 1/n^2)

$$E_n = -\frac{m_e k_e^2 e^4}{2\hbar^2}\left(\frac{1}{n^2}\right) = -\frac{13.6}{n^2}eV$$

Emission energies

$$\Delta E = E_{initial} - E_{final} = 13.6\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

hf$_{max}$ =13.6 eV



ΔE_{max}

Predicts spectral lines in the ultraviolet (Lyman series) and infrared (Paschen series), maximum energies, continuum.

Agreement with Rydberg equation

$$\frac{1}{\lambda} = \frac{\Delta E}{hc} = \frac{m_e k_e^2 e^4}{4\pi c\hbar^3}\left(\frac{1}{n_{final}^2} - \frac{1}{n_{initial}^2}\right)$$

$$R = \frac{m_e k_e^2 e^4}{4\pi c\hbar^3}$$

$$R = \frac{9.109x10^{-31}(8.987x10^9)^2(1.602x10^{-19})^4}{4\pi(2.997x10^8)(1.054x10^{-34})^3} = 1.099x10^7 m^{-1}$$

In excellent agreement with the experimental value 1.097x10^7 m^{-1}

Example

Find the wavelength of the transition from n=3 to n=2.

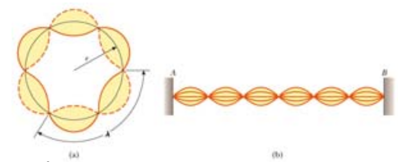
$$\frac{1}{\lambda} = R\left(\frac{1}{n^2_{final}} - \frac{1}{n^2_{initial}}\right) = (1.097x10^7 m^{-1})\left(\frac{1}{2^2} - \frac{1}{3^2}\right)$$

$$= 1.097x10^7\left(\frac{1}{4} - \frac{1}{9}\right) = 1.52x10^6 m^{-1}$$

$$\lambda = 6.56x10^{-7} m = 656 nm$$

red line in Balmer series

de Broglie wavelength picture of Bohr theory



$$mvr = n\frac{h}{2\pi}$$ quantization of angular momentum

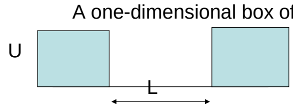
$$2\pi r = n\left(\frac{h}{mv}\right) = n\lambda$$ circumference = $n\lambda$

Quantization of angular momentum is equivalent to forming circular standing waves.
minimum circumference = one wavelength

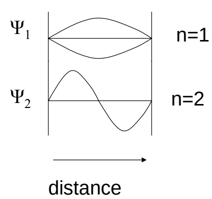
Particle in a Box (prob. 32)

A simple quantum model for a confined particle.

A one-dimensional box of length L



potential energy
U =0 inside the box,
U=∞ outside the box



A particle in a box has wave properties of a standing wave on a string fixed at both ends.

Particle in a box

Find the kinetic energy of the particle in the box

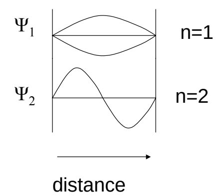
The wavelength is

$$\lambda_n = \frac{2L}{n} = \frac{h}{p_n}$$

The energy is

$$E_n = \frac{p_n^2}{2m} = \left(\frac{n^2h^2}{4L^2}\right)\frac{1}{2m} = \frac{n^2h^2}{8L^2m}$$

$$E_1 = \frac{h^2}{8L^2m}$$



The lowest energy state is not zero but gets lower for larger boxes

Bohr theory

Shows that the energy levels in the hydrogen atom are quantized.

Correctly predicts the energies of the hydrogen atom (and hydrogen like atoms.)

The Bohr theory is incorrect in that it does not obey the uncertainty principle. It shows electrons in well defined orbits.

Quantum mechanical theories are used to calculate the energies of electrons in atoms. (i.e. Shrödinger equation)

Extension of the Bohr Theory

Bohr theory can only be used to predict energies of Hydrogen-like atoms. (i.e. atoms with only one electron) This includes H, He^+, Li^{2+} ....

For example He^+ (singly ionized helium has 1 electron and a nucleus with a charge of Z = +2)

For this case the energy for each state is multiplied by Z^2 =4

$$E_n = -\frac{m_e k_e^2 z^2 e^4}{2\hbar^2}\left(\frac{1}{n^2}\right)$$

$$E_n = -13.6(Z^2)\frac{1}{n^2} = -13.6(2^2)\left(\frac{1}{n^2}\right) = -54.4\left(\frac{1}{n^2}\right)eV$$

for He^+