Quantum Mechanics

References:

1. S. Gasiorowicz, Quantum Physics

2. The Feynman Lectures on Physics, Vol III

3. D. J. Griffiths, Introduction to Quantum Mechanics

4. R. S. Saraswat and G. P. Sastry, Lecture Notes and Problems Bank

5. S. Bharadwaj and S. P. Khastgir, Physics I: Oscillations and Waves

Why quantum mechanics ?

- At the current stage, quantum mechanics may be regarded as the fundamental description of atomic phenomena (small length scales). However, why should one at all need to invoke a new description, which departs radically from classical physics?

- Universally accepted notions, before the advent of QM:

  i) Motions of bodies could be explained by Newton's laws on perceptible scales (terrestrial and celestial);

  ii) Light is an electromagnetic wave (Young's interference experiments in 1803 and Maxwell in 1864);

  iii) Elementary particles (e.g. electrons discovered by Thomson in 1897) behave like point particles.

- However, the classical framework was unable to provide a satisfactory explanation for a few observations like

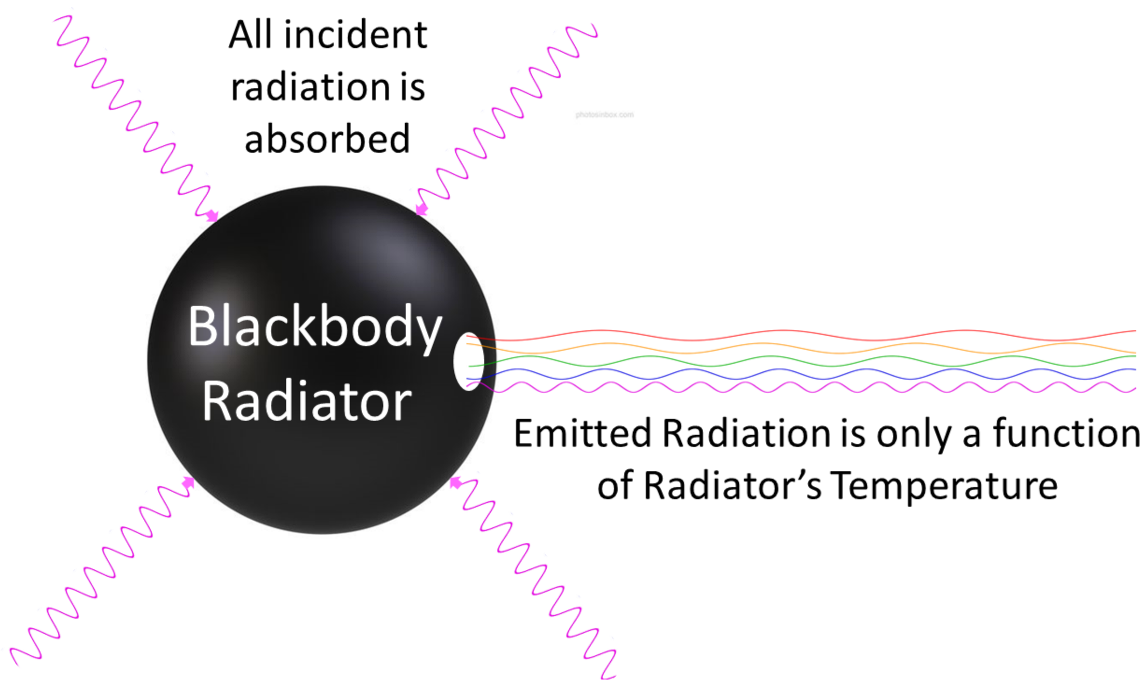
  1. Spectral distribution of blackbody radiation (Planck 1900)
  2. Photoelectric effect (Becquerel 1839, Hertz 1887, Einstein 1905)
  3. Stability and discreet spectrum of the atom
     (Balmer, Rydberg 1885-88, Bohr 1913)
  4. Compton effect (Compton 1920)

- A fresh perspective into the mechanical laws was necessary.

- Later on there were other experiments which led to further verification of the emerging new paradigm of QM

  1. Franck-Hertz experiment (1914)
  2. Davisson-Germer experiment (1923-27)
  3. Stern-Gerlach experiment (1922)

Blackbody radiation



Blackbody radiation

- When a body is heated, it radiates.

- In equilibrium, the energy emitted per unit area per unit time, also known as emissive power E, depends on the frequency and the temperature in general.

- Another relevant quantity is the absorptivity, defined as the fraction of incident radiation of wavelength λ that is absorbed.

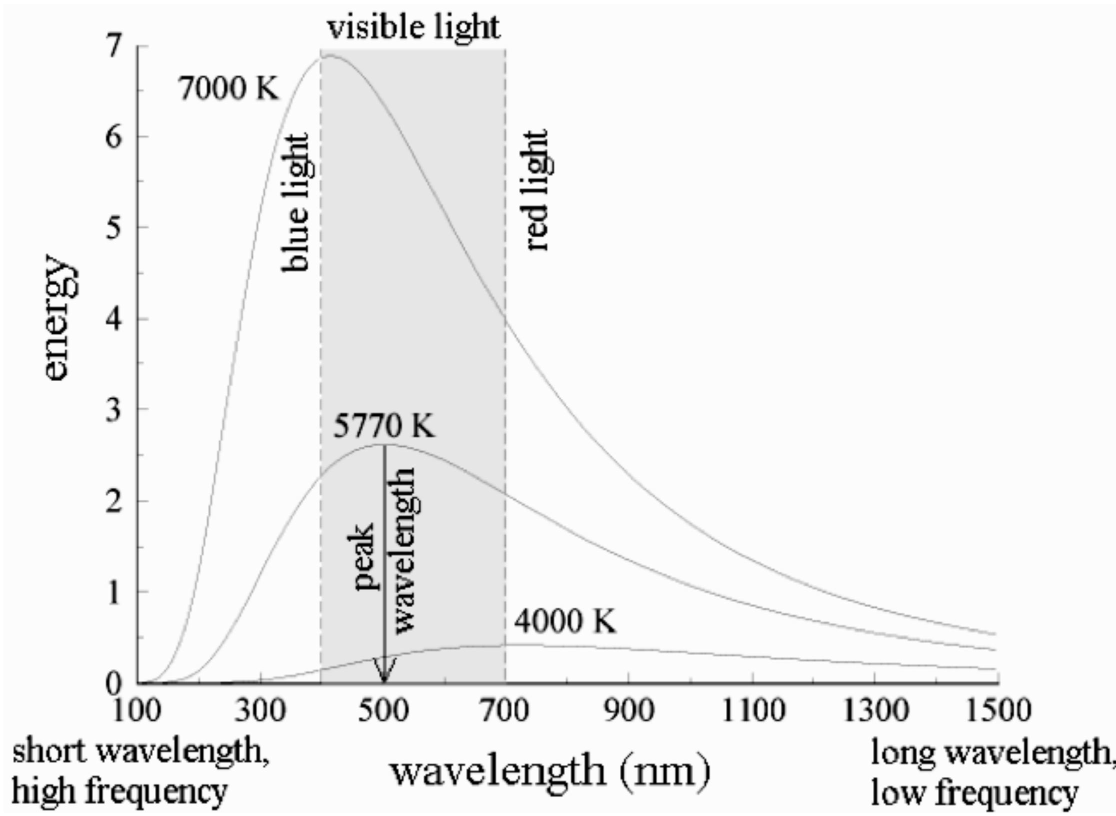
- Kirchoff's work on thermal radiation showed that for a given λ, the ratio of emissive power and absorptivity is the same for all bodies.

- In other words, it says that a body emits radiation at a given temp T and a given frequency ω exactly as well as it absorbs it (the same radiation).

- A special case in the black body, which is a perfect absorber (absorptivity is 1). When light shines on it, it absorbs all the radiation which is converted into heat stored within it.

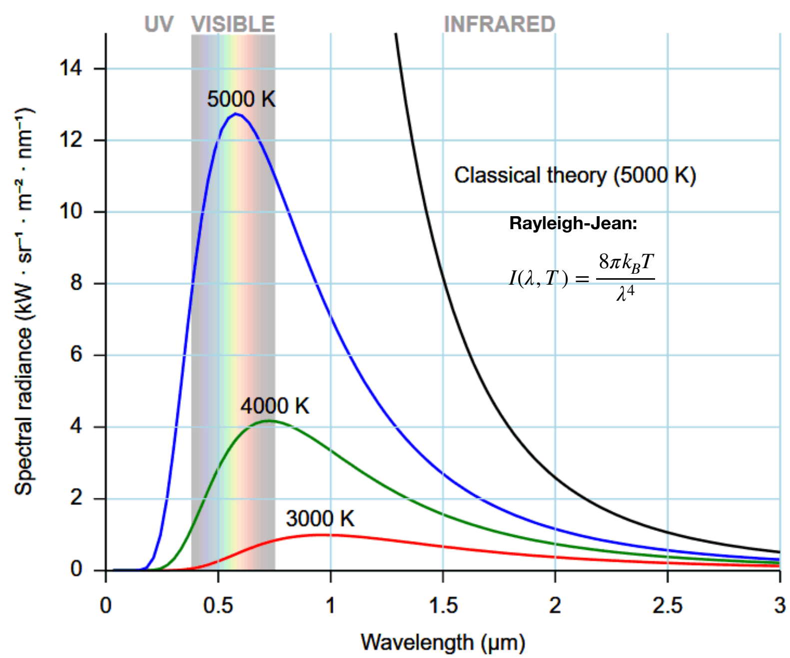
- This implies that a blackbody is also a perfect emitter of EM radiation. Thus, $E(\lambda, T)$ becomes a universal function in this case. What is the profile of this radiation?

Experimental spectra of blackbody radiation



Note: λ_{max} decreases with increase in temperature.

Explaining the observed blackbody spectrum



The Rayleigh-Jean law, uses the classical principles of electromagnetism and thermodynamics to explain the blackbody spectrum.

Fails to reproduce the observed behaviour at short wavelengths.

Planck's law of black body radiation (1900)

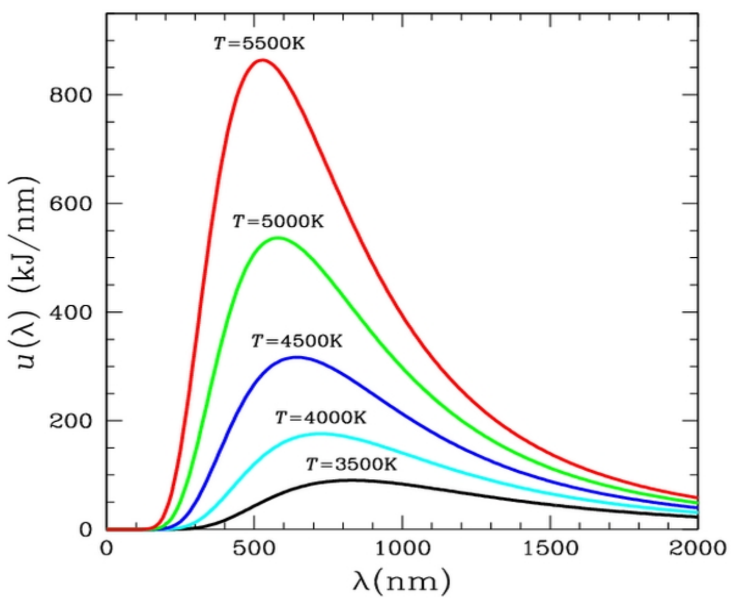
Planck's assumption (1900):

Radiation of a given frequency *ν* could only be emitted and absorbed in "quanta" (discrete bundles) of energy

$$E = h\nu$$

h =6.626x10^{-34} J-sec (Planck's constant)

ν: frequency of radiation



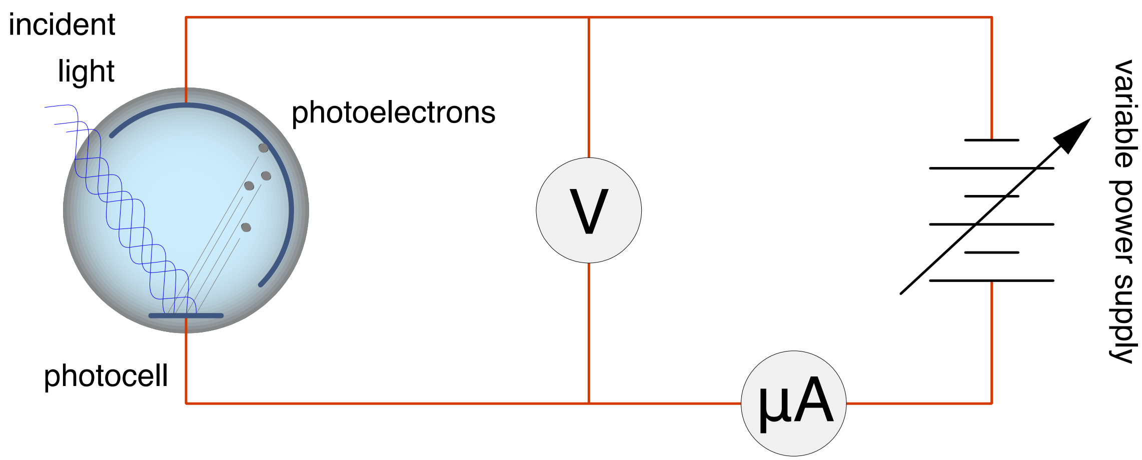
$$u_\nu d\nu = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/K_BT}-1}d\nu$$

Lessons from Planck's explanation

- In some scenarios it may be essential to consider a particulate character of EM radiation (in contrast to a wavelike character);

- For some reason, observable quantities like energy may be allowed to take only discrete set of values.

Photoelectric effect



Under the right conditions light can be used to push electrons, freeing them from the surface of a solid. This process is called the photoelectric effect (or photoelectric emission or photoemission)

Main experimental observations

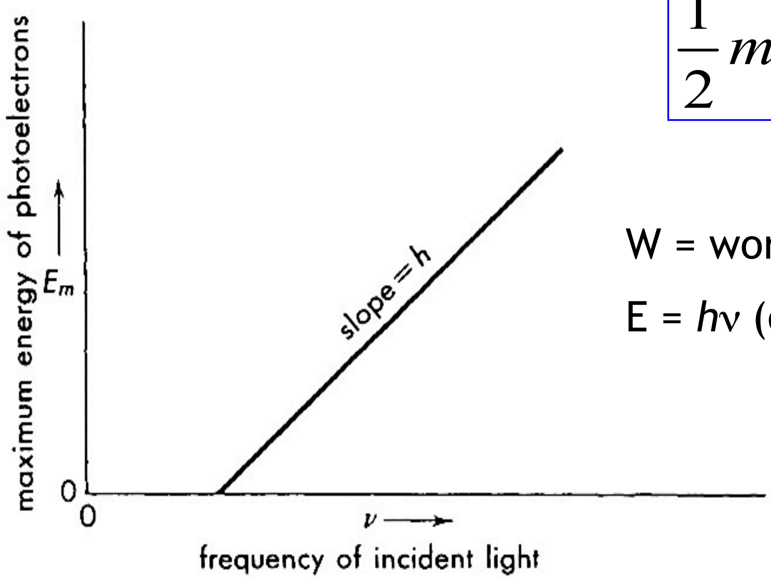
(Alexandre Edmond Becquerel 1839, Heinrich Hertz 1887, Nikola Tesla 1901, Philipp von Lenard 1902)

- When polished metal surfaces are irradiated, they emit electrons;
- This emission depends on the wavelength of light. Only when the freq. of the light falling on the surface exceeds a critical frequency, the emission takes place. This critical frequency varies from metal to metal;
- The magnitude of the current is proportional to the intensity of the radiation;
- The energy of each photoelectron is independent of the intensity, but varies linearly with frequency of light.

As it turns out, there is no way to explain all these features based on the wavelike property of light!

Einstein's explanation of the photoelectric effect

In 1905, *Albert Einstein* proposed the well-known equation explaining the photoelectric effect.



$$\boxed{\frac{1}{2} m_e v_k^2 = E_k = h\nu - W}$$

W = work function (threshold energy)

E = $h\nu$ (quantized energy of light)

In 1916, *Robert Andrews Millikan* confirms Einstein's explanation and formula.

Key elements of Einstein's explanation

- Einstein's explanation assumes that light is composed of packets of definite energy (photons).
- These, when colliding with electrons, transfer energy to them. The more is the energy of these quanta, the more is the energy gained by the electrons (for a fixed amount that may be wasted as heat in each collision).
- Energy of a photon was given in terms of the frequency of light by $h\nu$, so the kinetic energy of emitted electrons varied linearly with frequncy ν

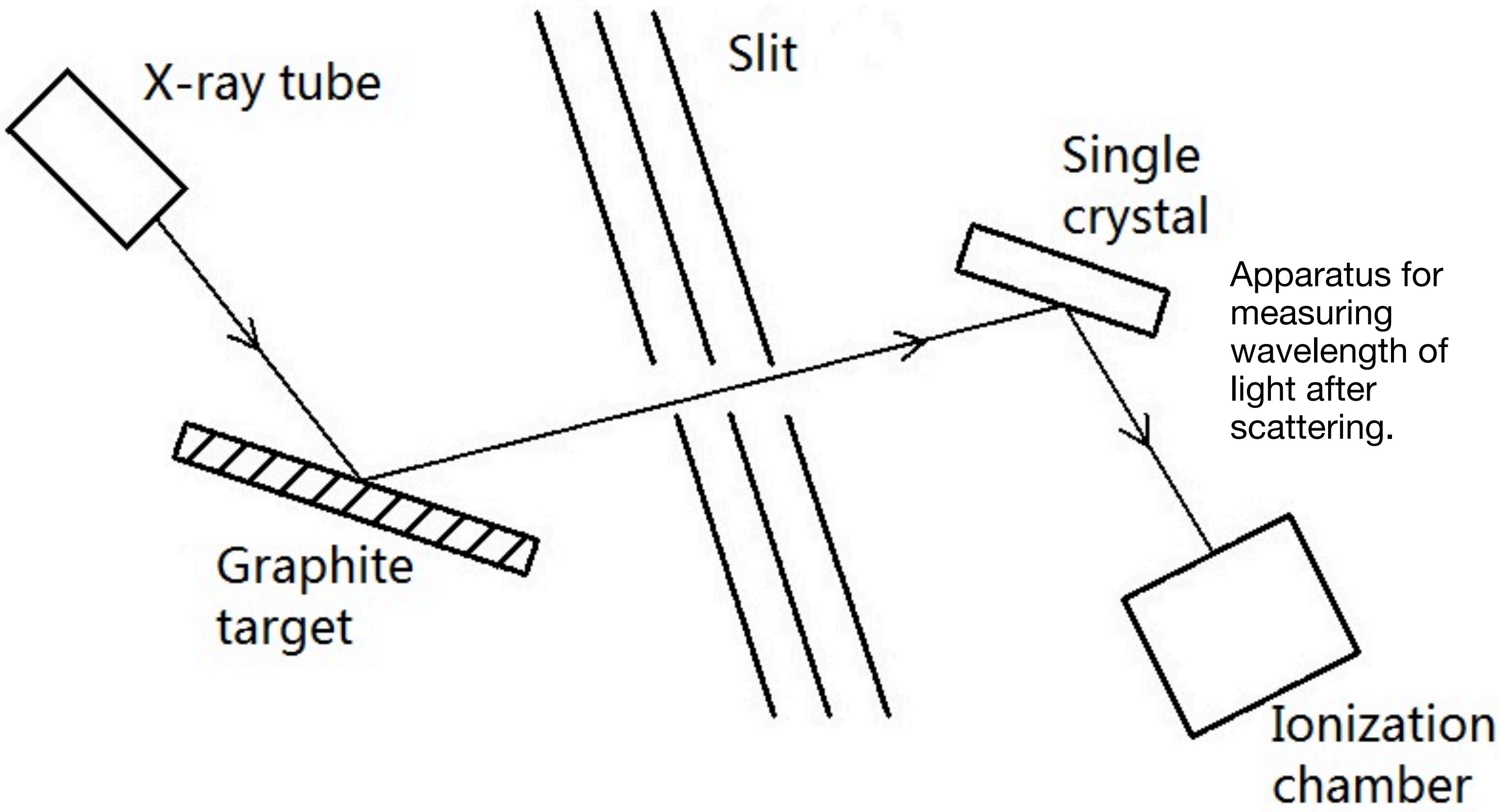
  $$E_k = \frac{1}{2} m_e v_k^2 = h\nu - W$$

  W is the threshold energy required to separate the electron from the metal.

Lesson: Light could (at times) behave as a single quanta (photon), and can interact with other particles (electrons) as a single particle.

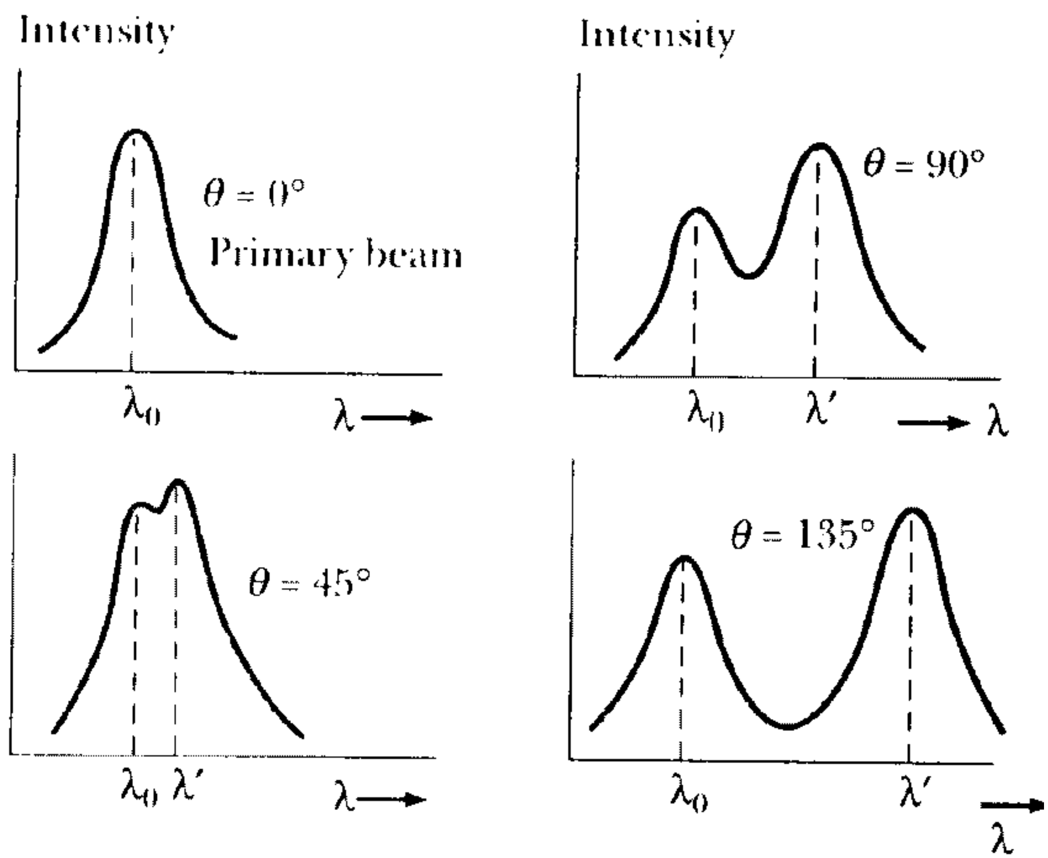
The Compton effect (1923)

Experimental set-up

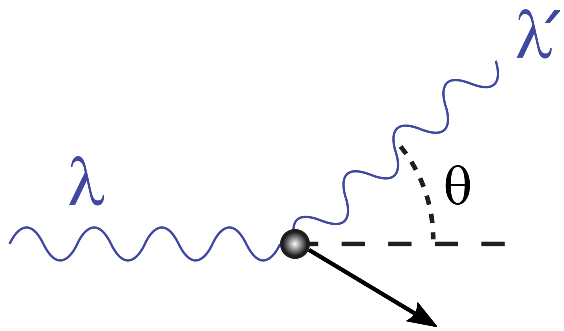


The Compton effect

Experimental results



The Compton effect



$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

- λ : Initial wavelength of scattering photon
- λ' : wavelength after scattering
- m_e : mass of electron
- θ : scattering angle
- h : Planck's constant
- c : speed of light in vacuum

- Inelastic scattering of light by an electron, where the wavelength of scattered light is different from that of incident radiation: *Compton shift*.

- The observed Compton shift formula can only be explained by considering appropriate energy conservation and *momentum conservation* between the light quanta and the recoiling electron.

Photons : light particles with definite energy and momentum.

Explaining the Compton effect

- The energy of a relativistic free particle is related to the magnitude of its momentum by

$$E^2 = p^2c^2 + m^2c^4, \text{ where } m = \text{rest mass.}$$

- The rest mass of the proposed photon is zero, so for photon

$$E = pc, \;\; E = h\nu = \frac{hc}{\lambda}, \;\; p = \frac{h\nu}{c} = \frac{h}{\lambda}.$$

- Let $E_e^{(i)} = m_e c^2$ is the initial energy of the electron at rest (zero momentum), and $E_e^{(f)} = \sqrt{(p_e^2c^2 + m_e^2c^4)}$ is the finial energy of the electron (which recoils with momentum p_e). Also let (E_λ, p_λ) and $(E_{\lambda'}, p_{\lambda'})$ be the energy and momentum of the incident and scattered photon respectively. Then, Energy conservation implies

$$\begin{aligned} & E_e^{(i)} + E_\lambda = E_e^{(f)} + E_{\lambda'} \\ \Rightarrow \quad & p_e^2c^2 = (E_\lambda - E_{\lambda'} - m_e c^2)^2 - m_e^2c^4 \end{aligned}$$

- The conservation of momentum implies

$$\vec{p}_\lambda = \vec{p}_e + \vec{p}_{\lambda'}$$

$$\Rightarrow \quad p_e^2 = (\vec{p}_\lambda - \vec{p}_{\lambda'}) \cdot (\vec{p}_\lambda - \vec{p}_{\lambda'}), \quad \text{squaring}$$

$$\Rightarrow \quad p_e^2 c^2 = (p_\lambda^2 + p_{\lambda'}^2 - 2 p_\lambda p_{\lambda'} \cos\theta) c^2, \qquad \text{where } \theta \text{ is scattering angle}$$

Use the result from conservation of energy

$$\Rightarrow \quad ((E_\lambda - E_{\lambda'} - m_e c^2)^2 - m_e^2 c^4) = p_\lambda^2 c^2 + p_{\lambda'}^2 c^2 - 2 p_\lambda p_{\lambda'} c^2 \cos\theta,$$

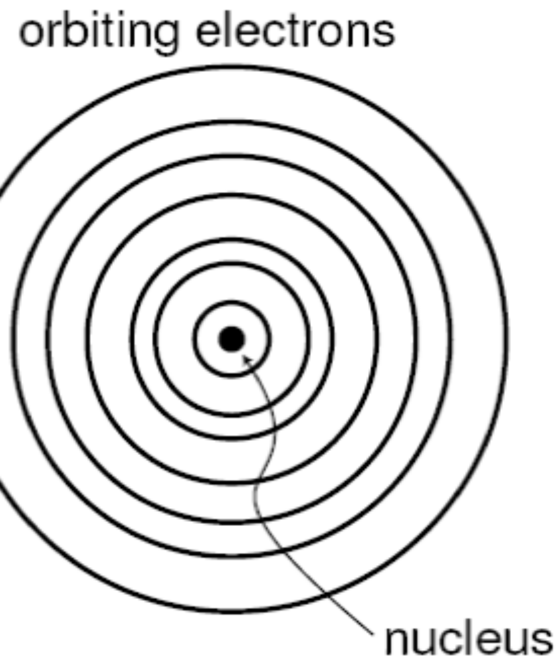
$$\Rightarrow \quad \left(\left(\frac{hc}{\lambda} - \frac{hc}{\lambda'} - m_e c^2 \right)^2 - m_e^2 c^4 \right) = \left(\frac{h}{\lambda} \right)^2 c^2 + \left(\frac{h}{\lambda'} \right)^2 c^2 - 2 \left(\frac{h}{\lambda} \right) \left(\frac{h}{\lambda'} \right) c^2 \cos\theta,$$

Simplify to obtain

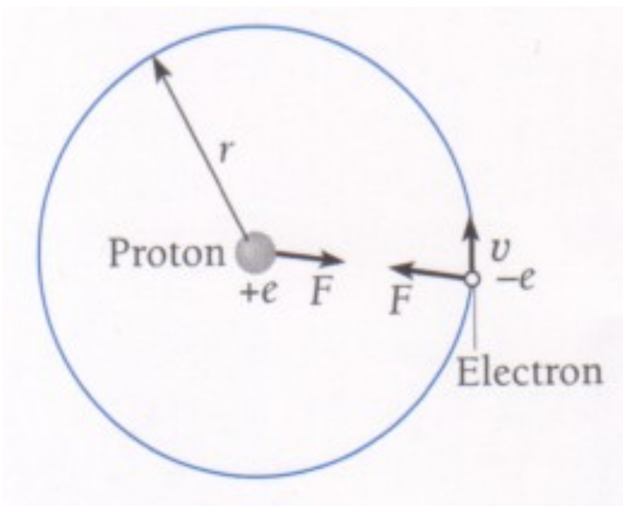
$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

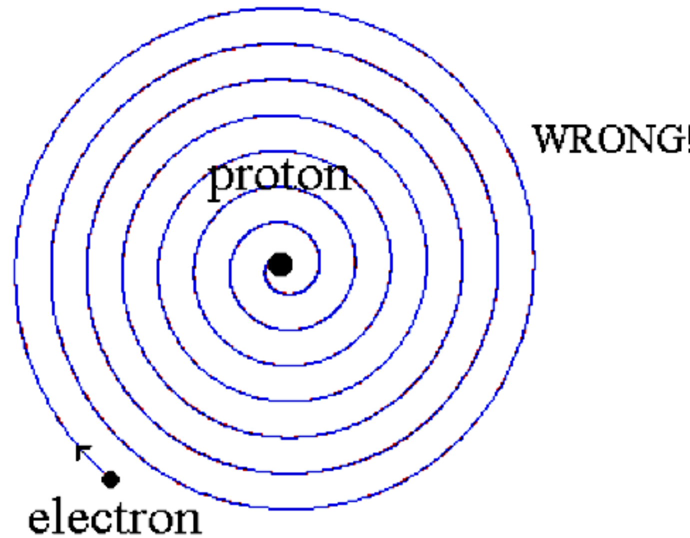
Structure of the atom

Rutherford (Geiger-Marsden) gold-foil experiments (1908-13)



Stability of the atom





<u>**Classical Electrodynamics:**</u> **charged particles radiate EM energy (photons) when their velocity vector changes (e.g. they accelerate).**

The electron should lose all of its energy and spiral down into the proton, *i.e.* lifetime of an atom is a mere 10^{-12} seconds! WRONG!!!

How is the atom stable?

Hydrogen spectrum

Balmer series (1885) : Discrete spectra of the hydrogen atom

Rydberg formula (1888)

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right), \; n_1 = 2, \; n_2 = 3, 4, 5 \ldots$$

Classical theory neither explain stable atom nor discrete atomic spectra

A more sophisticated model of the atom is necessary.

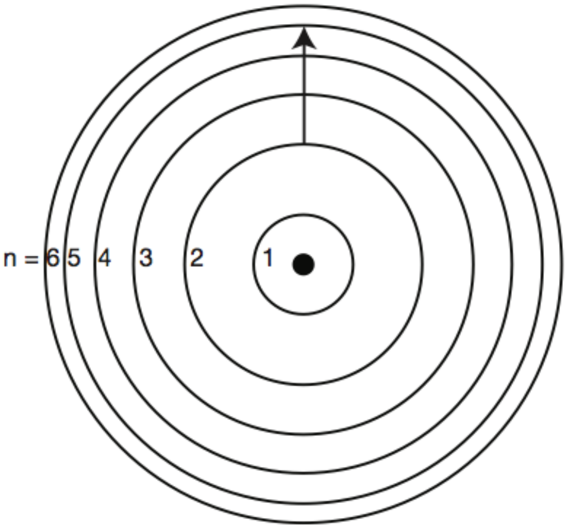
The model of the atom (Rutherford, Bohr, Sommerfeld,..)

The main idea

- Electrons move in stationary orbits, the angular momentum being an integral multiple of $\hbar$. The electrons in these orbits do not radiate inspite of their acceleration.

- Transitions between these orbits correspond to gain or loss of energy (e.g. transition to a lower energy state results in an emission of em radiation). $E = E_n - E_{n-1} = h\nu = \hbar\omega$ is the energy of the quanta emitted due to a transition from the nth to n-1 th (allowed) orbit.

Bohr's model of the atom



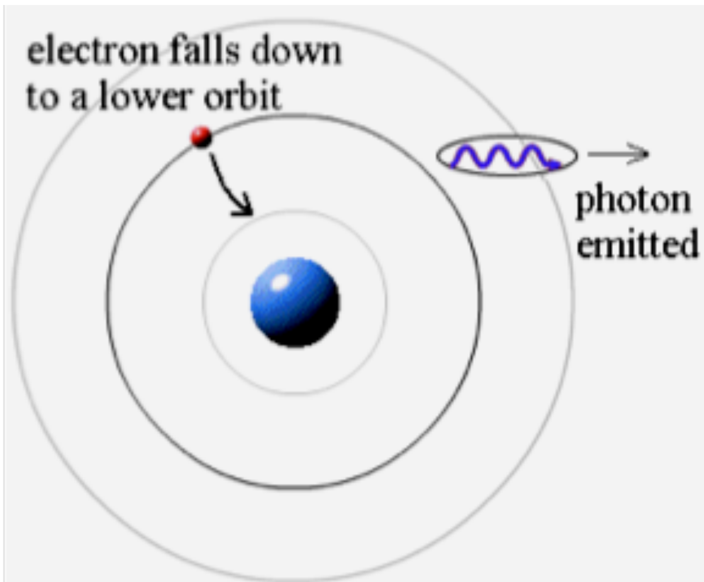
Bohr's hypothesis:

1) Electrons stay in 'fixed orbits' around nucleus
2) Angular momentum is quantized in those fixed orbit
3) No radiation loss in fixed orbits

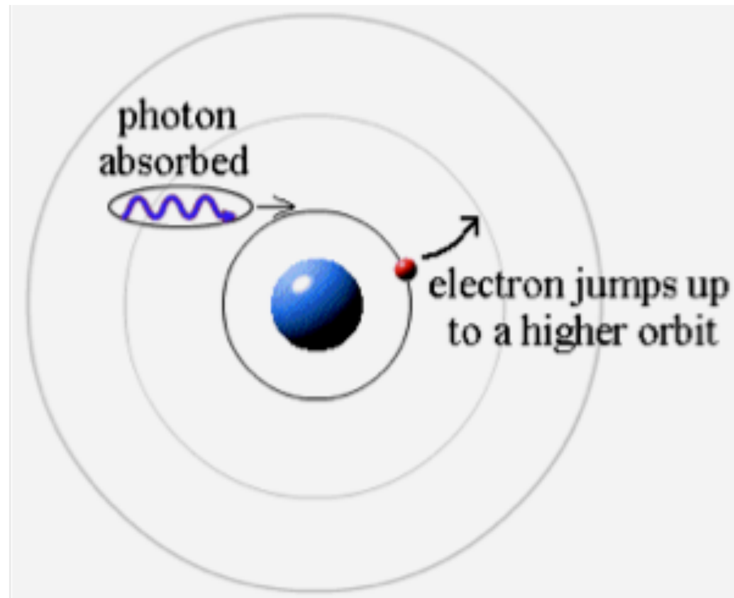
$$L = mvr = \frac{nh}{2\pi} = n\hbar$$

Drawbacks: Postulates were ad-hoc and could not be easily extended to atoms with multi-electrons.

Explanation of hydrogen spectra



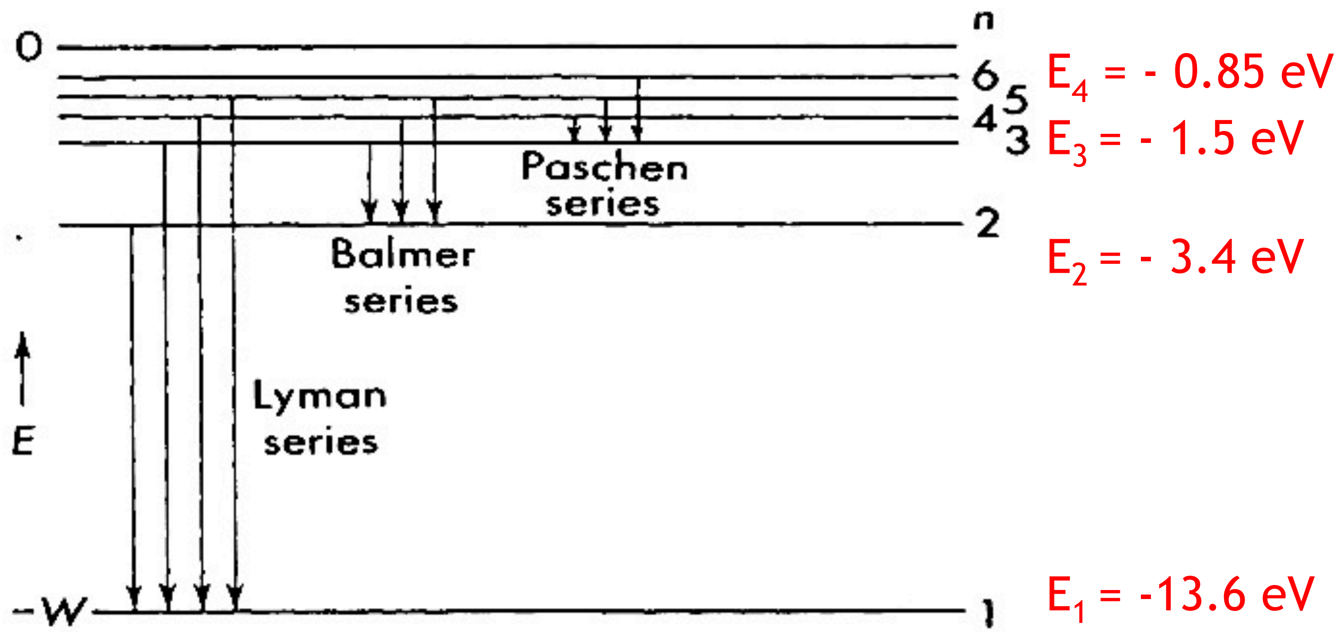
The electron falls down to a lower orbit and the atom loses energy. A photon carries away the energy lost by the atom.



A photon is absorbed by the atom, which gains the photon's energy. The electron uses this energy to jump up to a higher orbit.

These transitions produce discrete spectra of emitted light from hydrogen atoms

Energy levels of the hydrogen atom



$E_3 - E_2 = 1.9$ eV ➔ $\lambda = 652.6$ nm

$E_4 - E_2 = 2.55$ eV ➔ $\lambda = 486$ nm

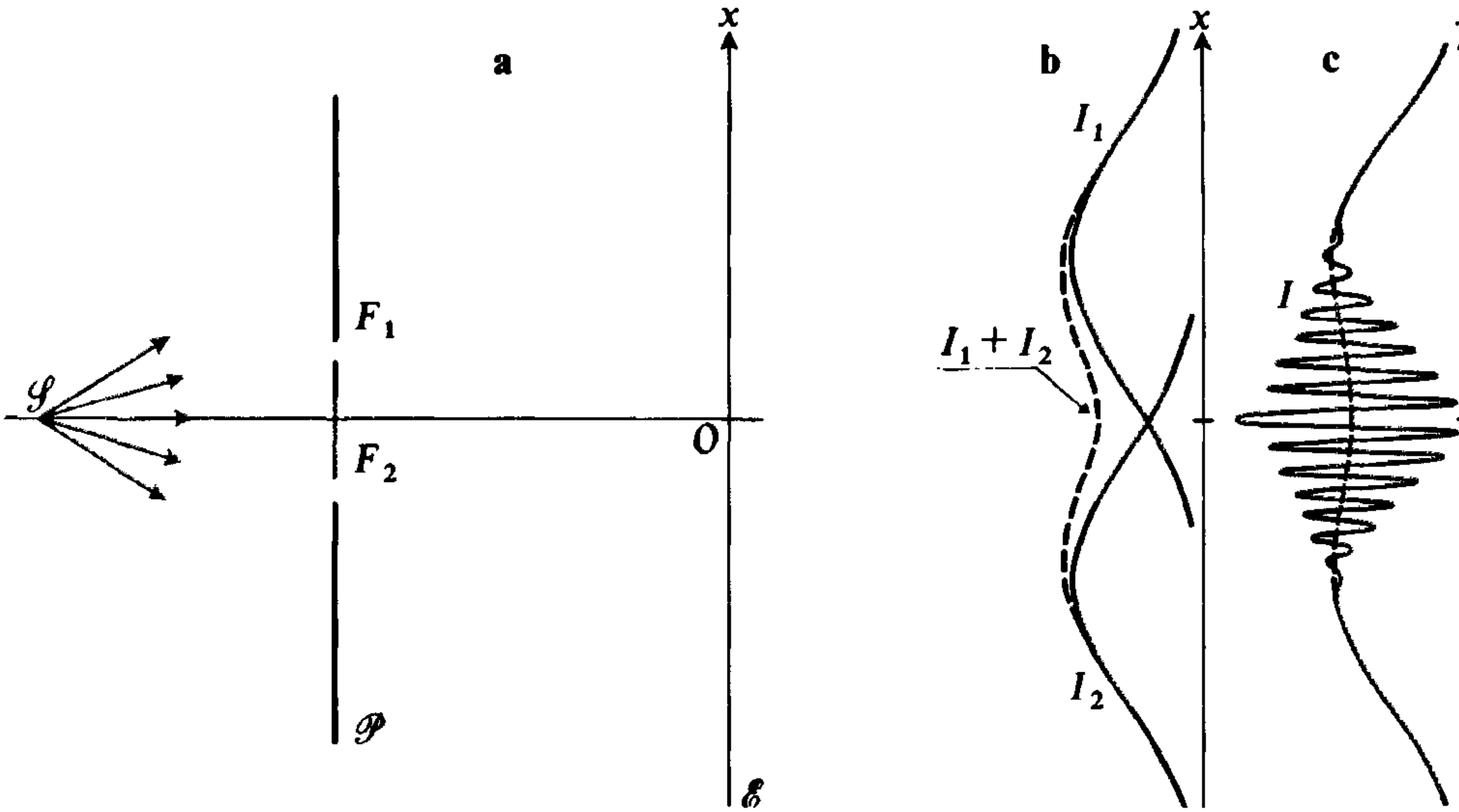
Balmer series

The most important conclusion so far

Several experimental observations suggest EM radiation should considered to be a flux of discrete particles with definite energy and momentum.

Then what about the interference and diffraction experiments demonstrating the wave nature of light?

Looking back at the YDS experiment



YDS experiment with low intensity

- In the particle picture of light the intensity of a light source is proportional to the number of photons emitted per second.

- Let us diminish the intensity of the source until the photons strike the screen one by one. What happens to the interference pattern ?

- Let us put a photographic plate instead of the screen and find out. We make the following observations

  – Large exposure time (many photons strike the plate one by one) $\rightarrow$ the fringes are observed on the screen (wave-like behaviour).

  – Small exposure time (few photons strike the plate) $\rightarrow$ a few localized impact on the screen, no weak interference pattern (particle like behaviour).

- We need a new way to accommodate both the dual picture of a wave and a particle simultaneously.

The de Broglie hypothesis (1923)

Material particles, just like photons, have a wave like nature.

- With a free material particle of energy E and momentum $\mathbf{p}$, we can associate a wave whose angular frequency $\omega = 2\pi\nu$ and a wave vector given by (the same relation as the photon)

$$E = h\nu = \hbar\omega, \mathbf{p} = \hbar\mathbf{k}$$

- The corresponding wavelength is (de Broglie relation)

$$\lambda = \frac{2\pi}{|\mathbf{k}|} = \frac{h}{|\mathbf{p}|}$$

- The small value of Planck's constant in SI units is the reason why such matter waves are hard to observe at the scale of a meter or centimeter.

Then what about interference and diffraction with matter waves?