Fundamentals of Quantum Mechanics for Materials Scientists

INTRODUCTION

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FQM

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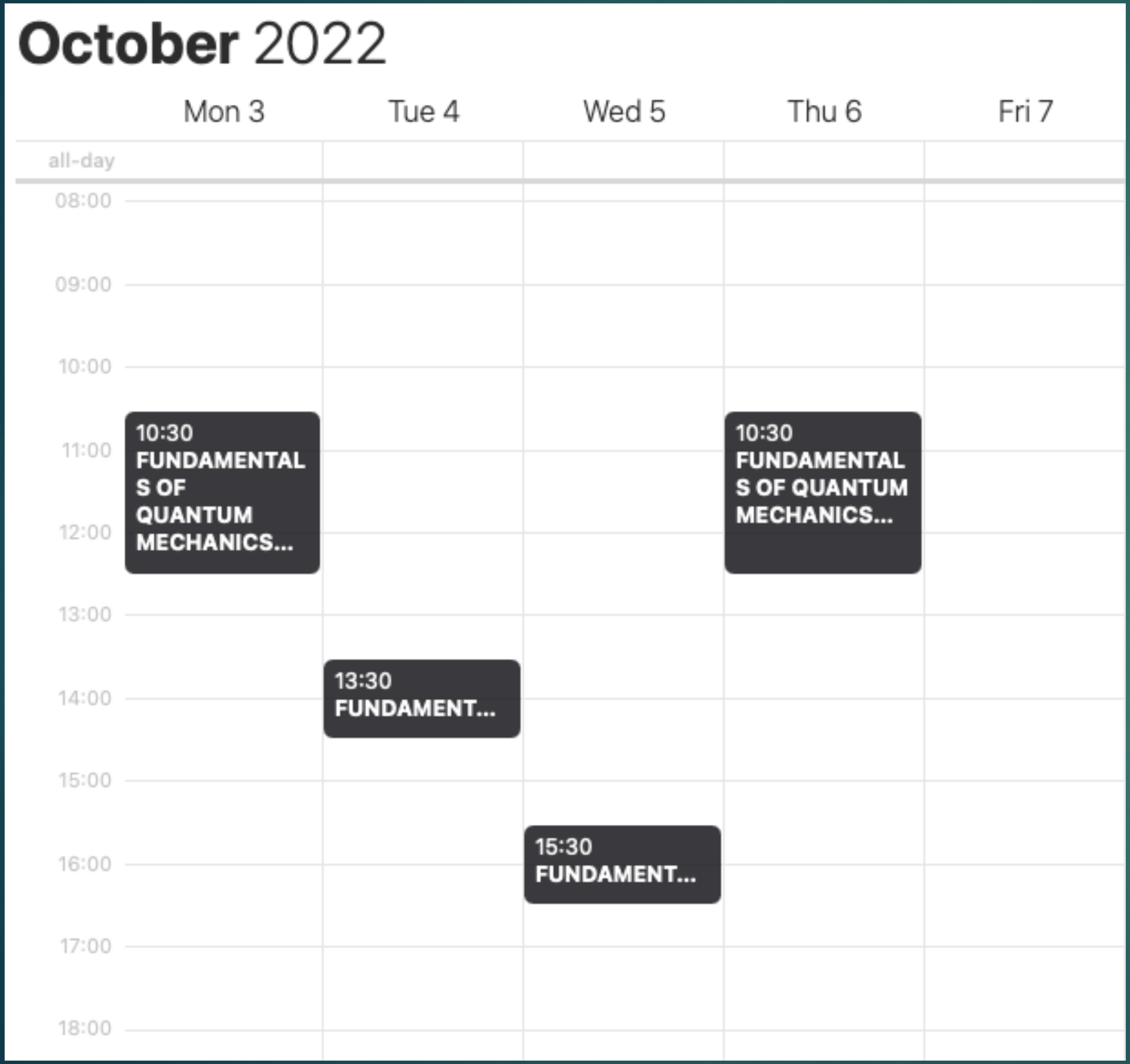
- contact me by email: emilio.scalise@unimib.it, if necessary we can plan a meeting
- You can ask question during/after lectures or by e-mail/e-learning

Lectures: class-room (and still live-streeming for a few weeks).

FQM



Lectures will be held in the class-room, but also in live-streaming.

I’ll upload the presentation after the lectures on the e-learning page

FQM

Lectures: live-streeming (and in the class-room), presentations uploaded on the e-learning page

Teaching break: 14-18 November

Assessment method

Students are evaluated through a discussion prepared by the students on a topic not treated during the course, and related to the **quantum information technology**. Students should prepare a short presentation and discuss an application of the basic concept of quantum mechanics, discussed during the course, particularly in the field of **quantum information technology**. The dcussion should evidence the understing of the main concepts of the course and to have gained basic knowledge of quantum mechanics.

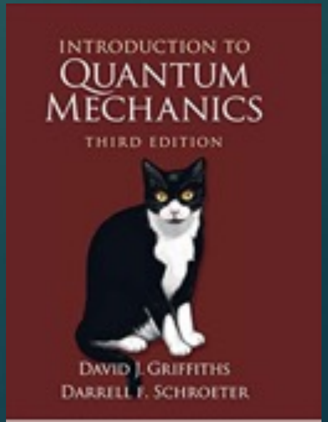
FQM

The main goal of this course is to provide a fundamental knowledge of quantum mechanics and the formal tools needed to fully understand the subsequent advances physics courses of the Master.

- **Textbooks:**

David A.B. Miller, Quantum Mechanics for Scientists and Engineers

L.I. Deych, Advanced Undergraduate Quantum Mechanics.



David J. Griffiths, Introduction to Quantum Mechanics.

Introduction

HISTORICAL AND EXPERIMENTAL FOUNDATION

Quantum mechanics around us

QUANTUM MECHANICS IS EVERYWHERE.

WE WILL SEE FEW EXAMPLES, STARTING WITH COLORS AND LIGHT, MOVING TO TRANSISTORS…

SO QM IS NECESSARY NOT ONLY TO UNDERSTAND THE WORLD AROUND US, BUT WE USE IT ROUTINELY IN MATERIALS SCIENCE AND ENGINEERING

QUANTUM TECHNOLOGY QUANTUM COMPUTER QUANTUM CRYPTOGRAPHY

QUANTUM ELECTRONICS QUANTUM OPTICS

QUANTUM WELL QUANTUM DOT QUANTUM SENSOR

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Quantum mechanics for MS and engineering

Quantum mechanics is essential for:

electronics for processing information

It supports all of solid state physics

Enables us to make transistors and integrated circuits

Most of the processes in small electronic devices can only be understood through quantum mechanics, and not just transistors:

***optics for sending information, …h*eavily quantum mechanical**

e.g., photons

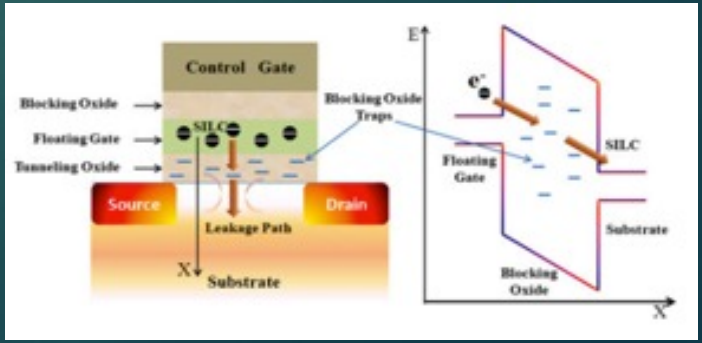
optoelectronic devices: *modern light-emitting diodes, semiconductor lasers, and modulators are quantum mechanically engineered*

storing information

magnetism of materials is a quantum mechanical phenomenon

optical storage relies also on quantum-mechanical optoelectronic devices

SSD are based on QM tunnelling through an oxide



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Quantum mechanics around us

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THERE ARE SOME BASIC PHILOSOPHICAL PROBLEMS AND PARADOX IN QUANTUM MECHANICS, AND IT HAS ALSO SOME BIZARRE, BUT TRUE CONSEQUENCES:

- ***"tunneling" allows particles to penetrate barriers that are "too high"***
- ***we cannot know simultaneously both the position and the momentum of a particle***
- **Heisenberg's uncertainty principle**

  a particle may exist in a superposition state, **e.g., it is neither definitely in a "state" up, or down**
- ***when we measure it, we always find it to have a definite value,*** *known as "collapse of the wavefunction"*, **e.g., to be definitely up or down.**

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QM…work in progress

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- **Theory of elementary particles** ***and its impact on on the understanding the nature of the universe***

- **Exploiting special features of quantum mechanics for technology:** ***e.g., cryptography*** or for ***quantum computing***

Naturally dealing with so-called "entangled states" , *may handle problems more efficiently than classical computers*

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QM as a practical tool

THERE ARE SOME BASIC PHILOSOPHICAL PROBLEMS AND PARADOX IN QUANTUM MECHANICS:

(E.G. MEASUREMENT PROBLEM…SCHRÖDINGER CAT PARADOX)

BUT ALTHOUGHT IT IS NOT EASY TO UNDERSTAND EVERYTHING IN QM,

IT IS MUCH EASER TO USE QM AND **IT WORKS EXTREMELY WELL**!

We would need to work with integrals and matrices, and perform some linear transform.

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Colors and light

Looking everyday objects we see different colors.
Why are these things are the color that they are?

Actually, it was a related problem of color that got us started in quantum mechanics.

It was known and evident that hot objects give off light. In the latter two decades of the 19th century, electric lighting was becoming increasingly popular, especially after the successful invention of incandescent light bulbs

However, a key problem with such filament light bulbs is that they're not very efficient at conducting the electric power into light power.

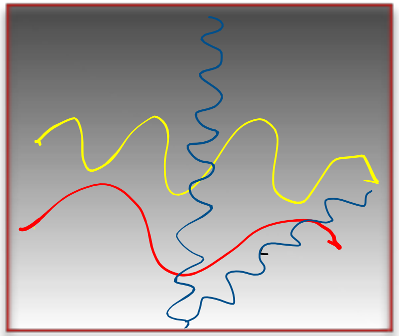
Understanding efficiency of light bulbs, is something that involved both science and engineering in the latter years of the 19th century.

Black-body radiation

Goal: understanding the light emission from hot bodies

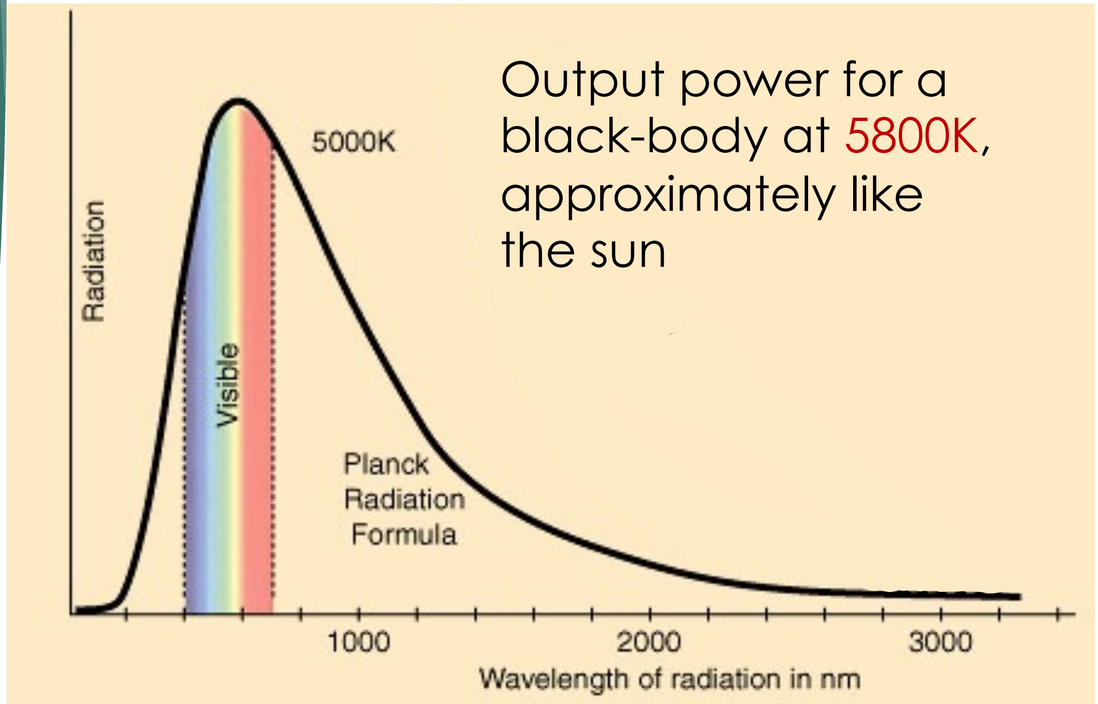
Black-body: idealized object which absorbs all frequencies, thus the best possible emitter of thermal radiation.

Black-body



Black-body spectrum: by the late 1890's, accurate measurements could be made of the output power for different colors (wavelength) that came off as you heated bodies up to different temperatures

Problem: explaining why the black-body spectrum had this shape. (why is it this color when you heat something up?)



Black-body radiation

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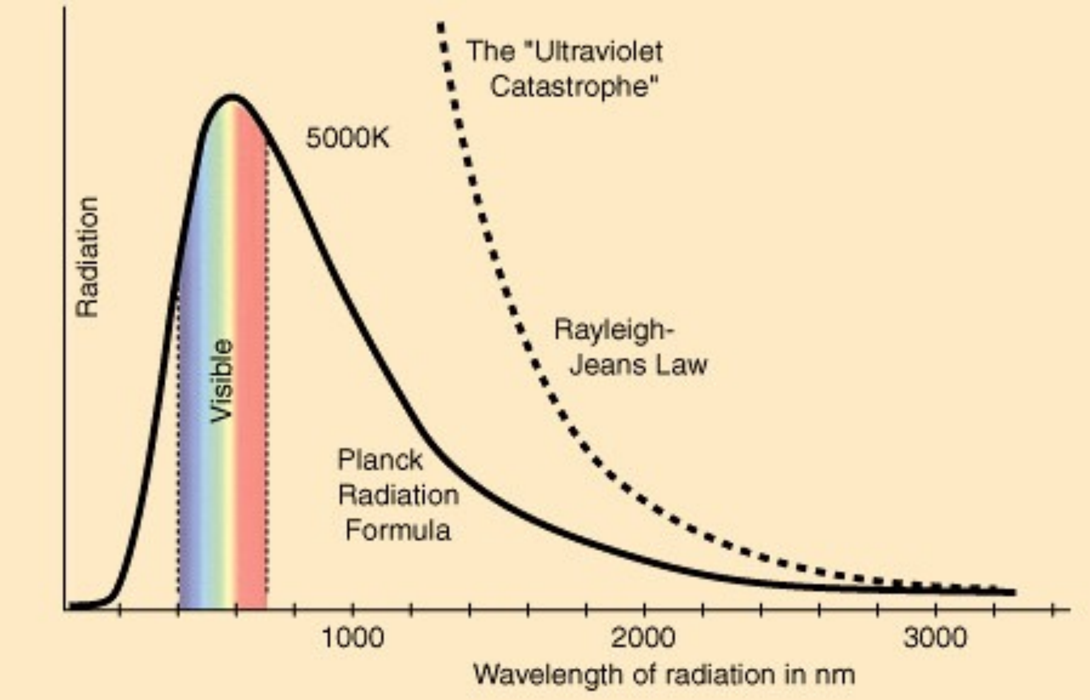
Classical physics can be used to derive an equation which describes the intensity of blackbody radiation as a function of frequency for a fixed temperature, the result is known as the **Rayleigh-Jeans law**:

$$\mu(\omega) = \frac{k_B T}{\pi^2 c^3}\omega^2$$

$\mu(\omega)$=energy per unit volume and freq.

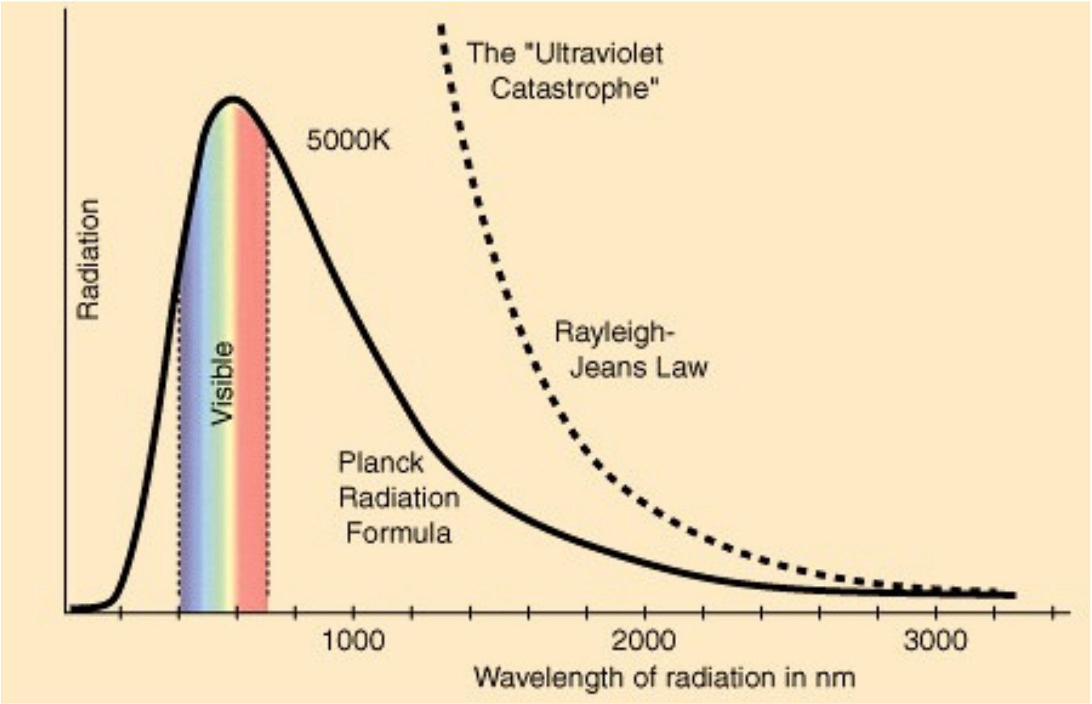


Black-body radiation

This divergence for high frequencies is called the ultraviolet catastrophe:

(P. Ehrenfest definition)

$$\int_0^\infty \mu(\omega)\mathrm{d}\omega = \infty$$



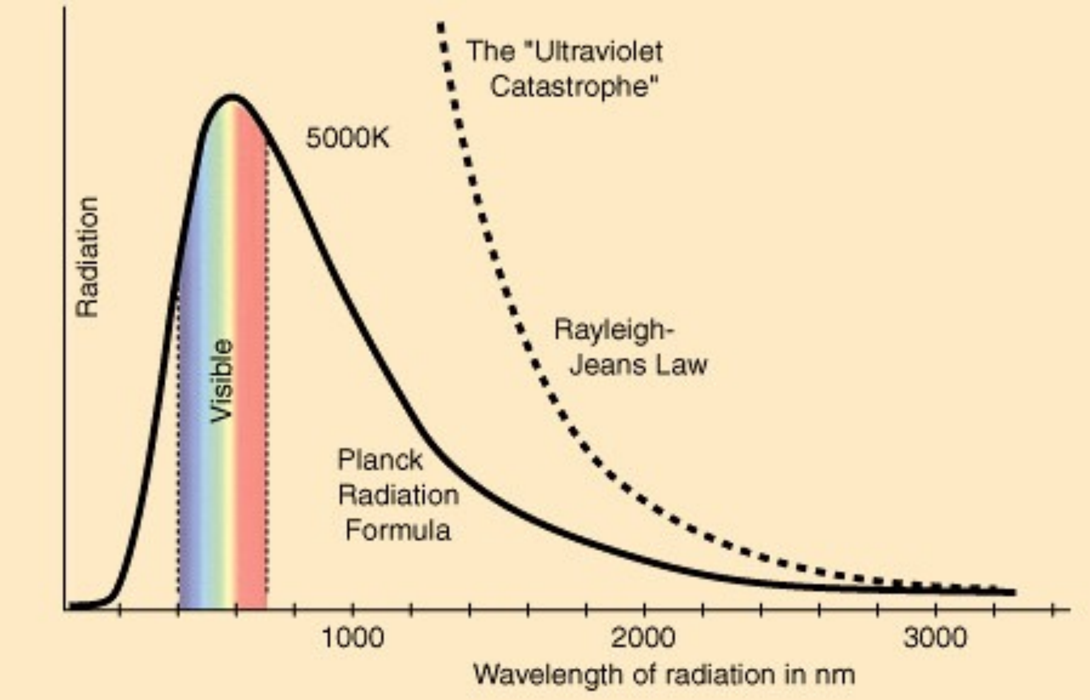
Black-body radiation

- 1900: **Max Planck** explained (based on empirical observation) the black-body radiation by assuming that the energies of the oscillations of atoms (actually particles at that time) which gave rise to the radiation must be proportional to integer multiples of the frequency, called quanta:

$$E = h\nu$$

$$h = 6.62606957 \times 10^{-34}\ J\ s$$

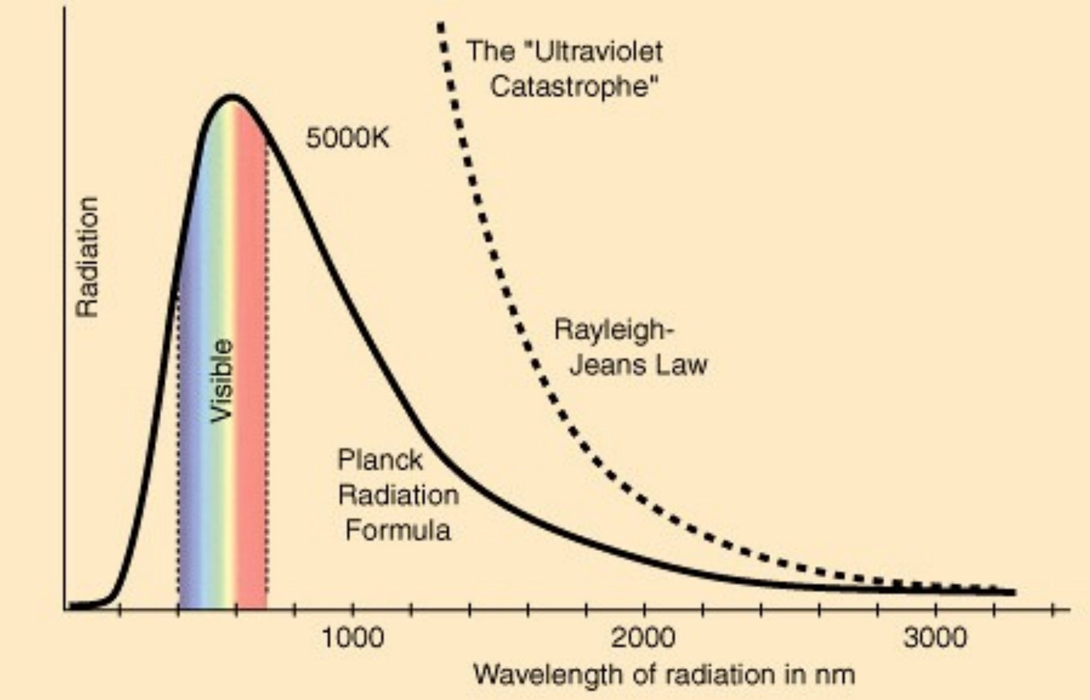
This proposal is now regarded as a start of quantum mechanics.



Black-body radiation

- Using statistical mechanics, Planck derived an equation similar to the Rayleigh-Jeans equation, but with the adjustable parameter h (ħ):

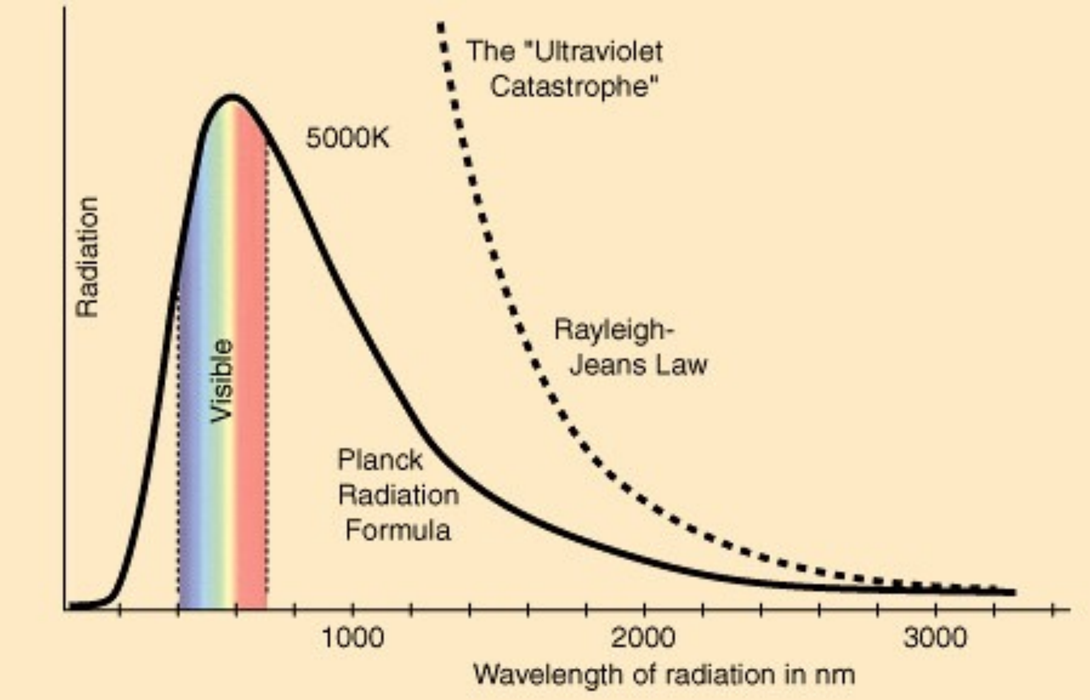
$$\mu(\omega) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\hbar\omega/k_B T} - 1}$$



Black-body radiation

- **Planck** was proposing these **quanta of emission**, he was not actually proposing that light existed only in such quanta, because at that time we had this extremely successful theory of electromagnetism (Maxwell eq.), and that theory had light as **waves**, not **particles**

$$E = h\nu$$



Black-body radiation

- Planck's explanation introduced unusual entities, those **oscillators** whose <u>energy cannot be changed continuously</u>, but must be a multiple of an elementary energy quantum.

- This idea of energy quantization was very revolutionary but not accept immediately by physicist, until **Einstein's theory of photoelectric effect** (1905), where Einstein also postulated quanta of energy.

- In 1911 Planck finally declared that his initial speculation was reflecting the physical reality.

- But let's go back to 1905…

Photoelectric effect

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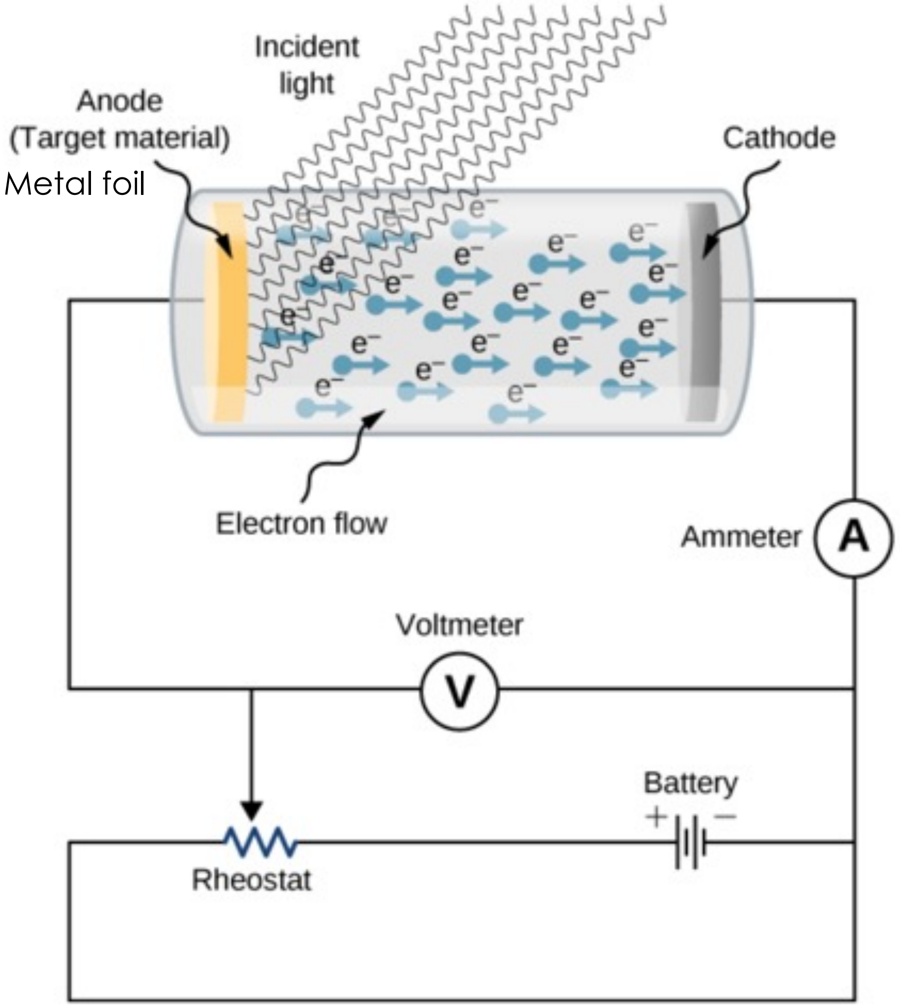
- Classically, if **(continuous) light waves shines** upon a metal foil, electrons should be emitted with **kinetic energy depending on the intensity of light**.

- **The experiments disagree this prediction**: when we shine the light, yeah we get more electrons off, but the stopping voltage remains the same. That is, the electrons always seem to be emitted with the same kinetic energy. And furthermore, if we change to a shorter wavelength, say moving from blue or ultraviolet further into the ultraviolet, then we have to increase the stopping voltage to stop the flow of current.



Derived from University Physics by OpenStax University Physics

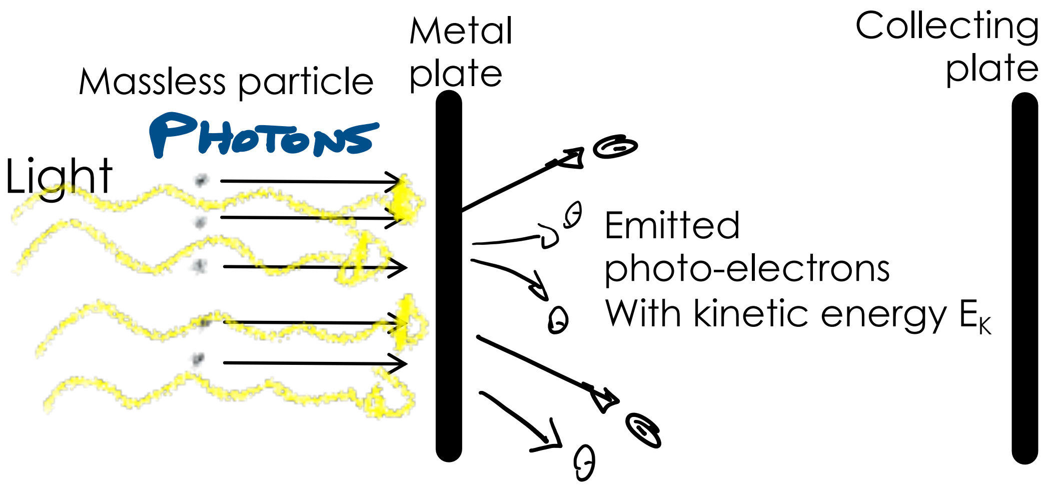
Photoelectric effect

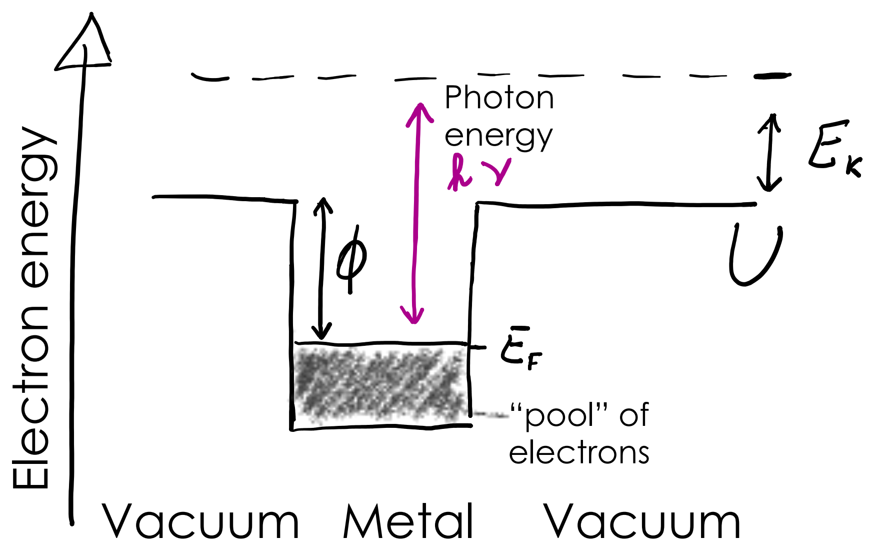
- In 1905 **Albert Einstein** hypothesized that light consists of photons, quanta of energy

$$E = h\nu$$

- According to this hypothesis, an electron that is bound in the metal can only be dislodged by an incident photon if its energy exceeds the energy **of the barrier, so called work function ∅**
The kinetic energy of the emitted electrons is:

$$E_k = \frac{mv_e^2}{2} = h\nu - \emptyset$$





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Photoelectric effect

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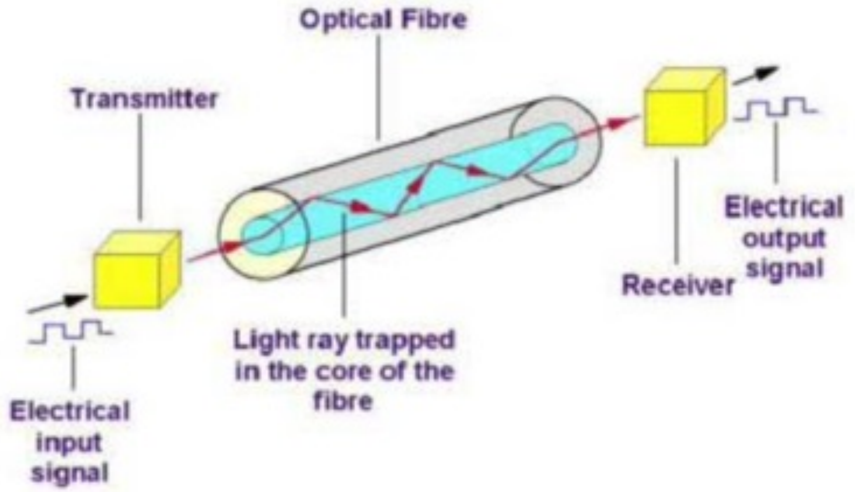
- It was this proposal, explaining the photoelectric effect, that led to Einstein's Nobel Prize.
- The key concept proved by Einstein is that light light is actually made up out of particles, but still keeping its wave nature.
- And so we come to something we call **wave-particle duality**. We are saying here that light is displaying both wave character, and is also made of particles.
- Although this seems very bizarre, we are verifying every day and moment the wave-particle duality, by optical fibre communications.



Matter, atomic structure

- Our **understanding of matter was very poor** in the classical physics world of the 19th century, as compared to electromagnetism theory for light.
  E.g., we really had no good idea of what atoms really were and where something like the periodic table of the elements actually comes from.

- Let's start from the simplest element, the **H atom**.
  When we heat up hydrogen, a gas under normal conditions, it emits light.
  But it does so only at a very specific set of wavelengths. Why?

H-δ: 410.2 nm   H-γ: 434.1 nm   H-β: 486.1 nm   H-α: 656.3 nm

Bohr model of H atom

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- Electrons orbit around the proton.

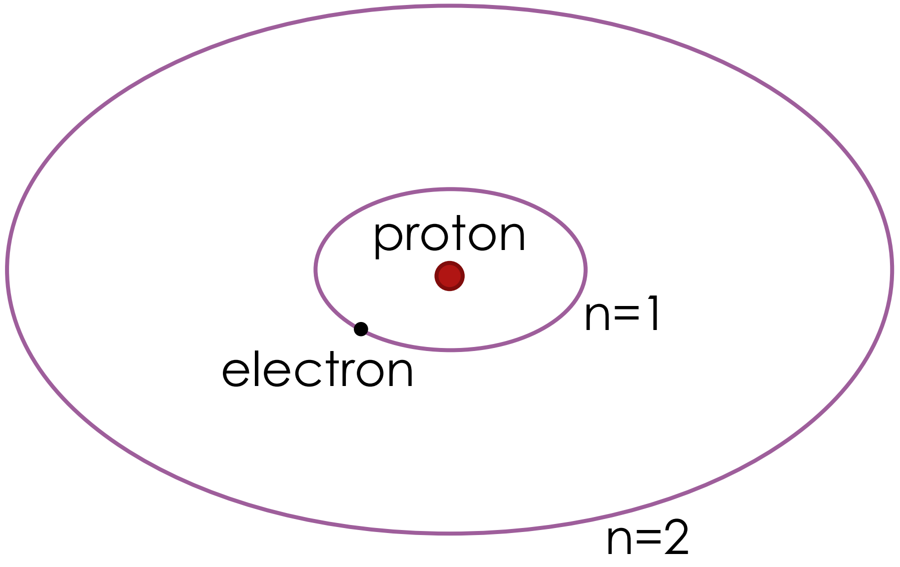
- Bohr's assumption: angular momentum of the electron can only exist in units of Planck's constant (divided by 2π).

$$\hbar = \frac{\mathbf{h}}{2\pi}$$

h-bar Reduced Planck's constant

$$\omega = 2\pi\nu \qquad (ang. freq.)$$

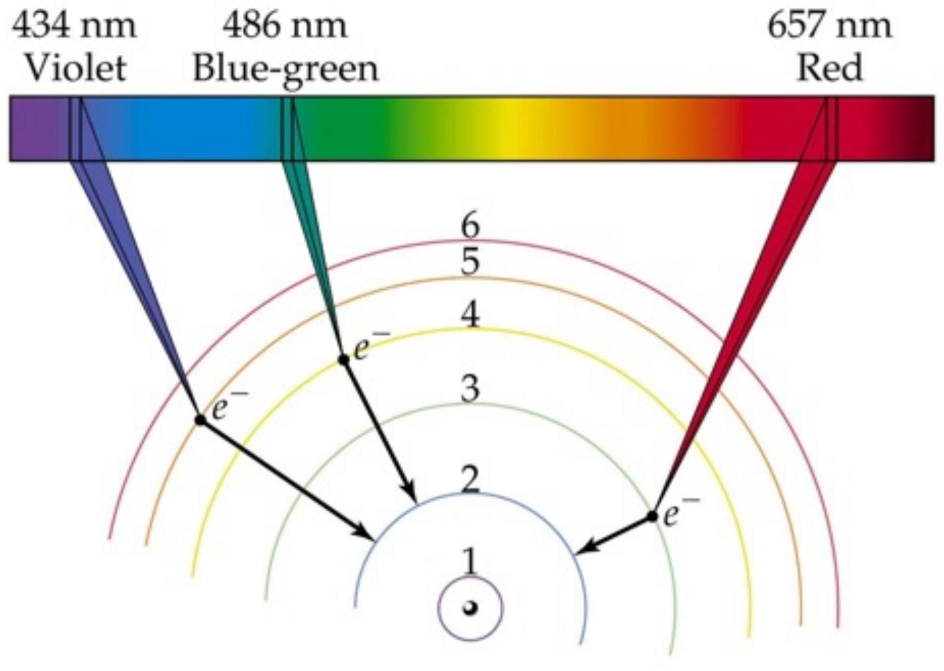
$$thus \quad E_n = n\hbar\,\omega$$



Bohr model of H atom

- The photon energies of the spectral lines come from the separation of the energies of the different orbits, which are attained at distances for which the angular momentum of the revolving electron is an integer multiple of $\hbar$
- This model successfully incorporates Planck's constant into the theory of matter.
- It also gets the approximate size of the hydrogen atom correct.
  That size is roughly 1/10 of a nanometer in diameter, or 1 ångström (Å). More precisely its radius is

  1 Bohr = 0.5291777721092 Å



Bohr model of H atom

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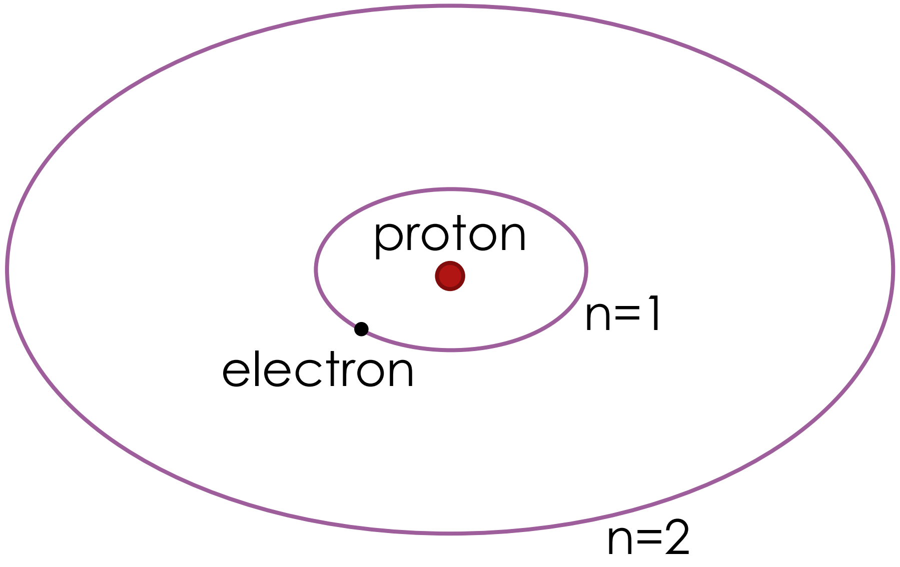
Bohr model **is actually wrong** for several aspects:

- It does not quite get this angular momentum right, especially for small n.
- the atom would be radiating electromagnetic radiation all the time, because the spinning electron will lose energy.

- The key point is that the **electron is not some small classical particle in an orbit**.



de Broglie model

- **In 1923, de Broglie** (1923) suggested that not only light, normally considered as a wave, can have particle-like character, but also **regular particles** (i.e. electrons, neutrons, atoms, etc.) can manifest **wavelike properties**.

$$\lambda = \frac{h}{p}$$

where p is the particle's moment

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Wave-particle duality, waves and matrix formulation

A few years later and during same period (1925-1926), two other physicist were crucial for the development of quantum physics:
Schrödinger and **Heisenberg**.

- The former got quickly famous in the scientific community for the Schrödinger equation, his idea was closer to the de Broglie **matter wave idea**
- **Heisenberg** developed a **matrix formulation** of quantum mechanics.