Engineering Physics

Course Code: BPHY101L; Course Type: Theory Only (TH)

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Module-3: Elements of quantum Mechanics

Syllabus

Need for Quantum Mechanics: Idea of Quantization (Planck and Einstein) - Compton effect (Qualitative)– de Broglie hypothesis - justification of Bohr postulate-Davisson-Germer experiment - Wave function and probability interpretation - Heisenberg uncertainty principle - Gedanken experiment (Heisenberg's microscope) - Schrödinger wave equation (time-dependent and time-independent).

Reference Books:

1. H. D. Young and R. A. Freedman, University Physics with Modern Physics, 2020, 15th Edition, Pearson, USA., Section 40.1 to 40.6, Page No: 1321-1350
2. Concepts of Modern Physics; Sixth Edition; Arthur Beiser
3. Raymond A. Serway, Clement J. Mosses, Curt A. Moyer Modern Physics, 2010, 3rd Indian Edition Cengage learning.

What we will learn in this Modulo

What is **physics**?

What is **modern physics**? What is **classical physics**?

Why modern physics is so important?

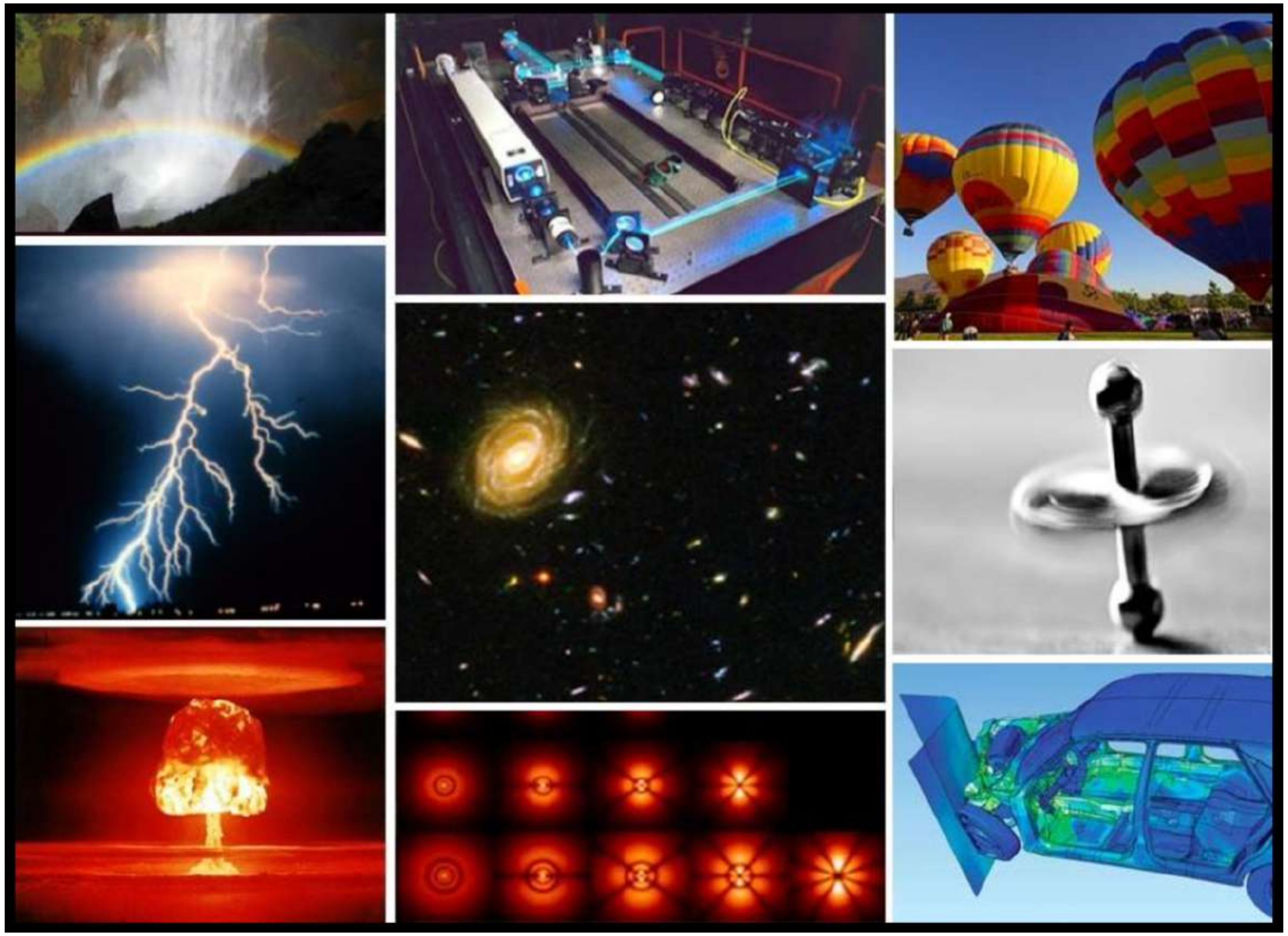
How did it emerge?

Origin of Quantum Mechanics and its Applications

Physics

Physics means "knowledge of nature"

- Physics is the study of nature
- It is the most fundamental of the natural sciences (what are other natural sciences?)
- Goal of physics: to understand how the universe works



Classical Mechanics(16th-19th Century)

Movement of bodies due to forces

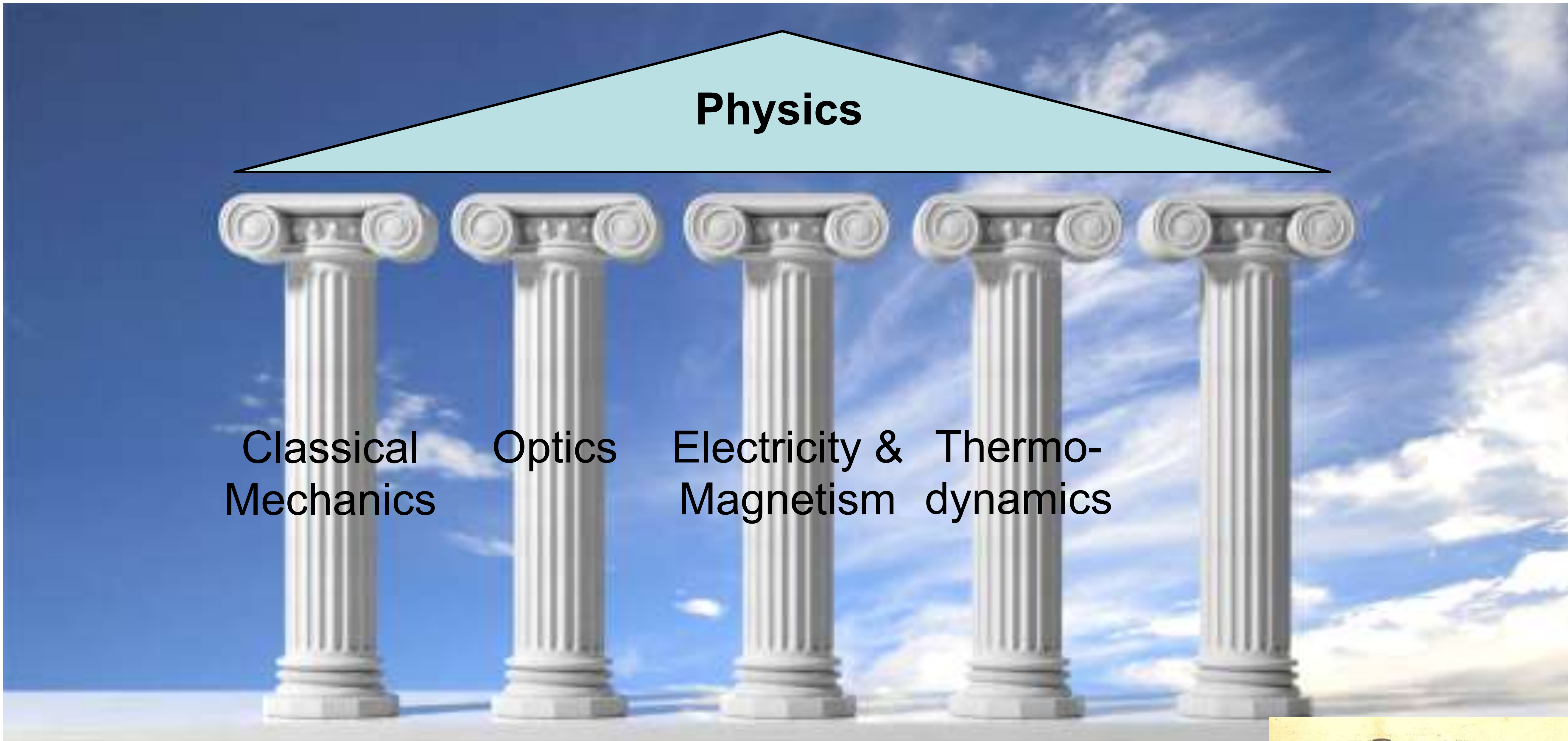
Which forces and examples do you know that have to do with mechanics?

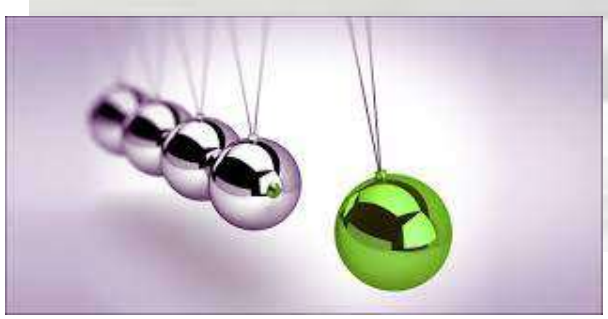
Collision of billiard balls

Aerodynamics of an airplane

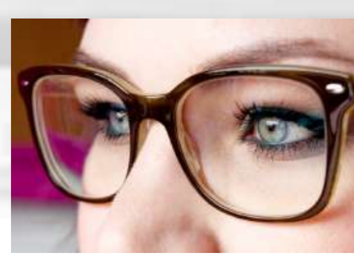
Movement of planets around the sun

Classical Mechanics(16th-19th Century)





Classical Mechanics

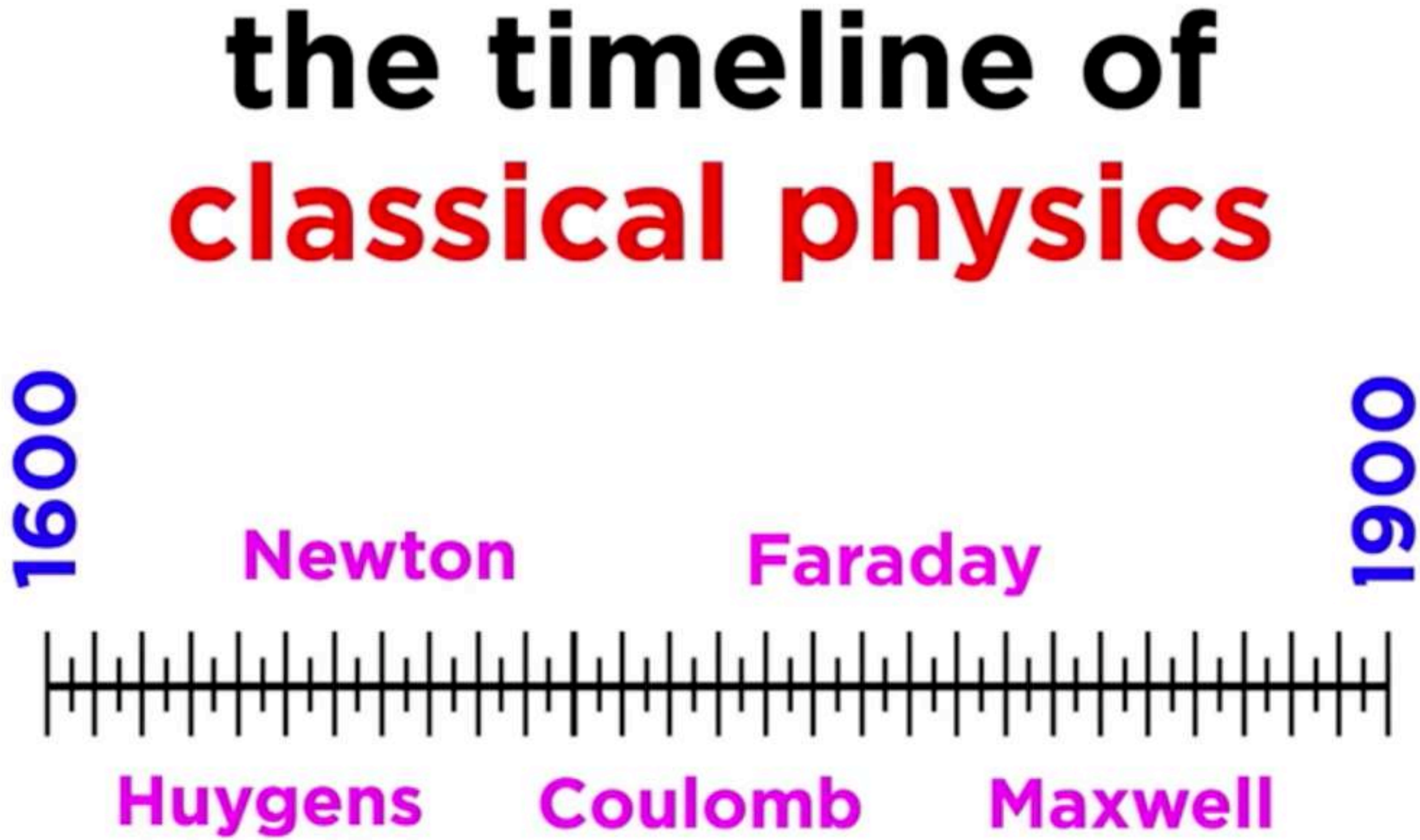


Optics

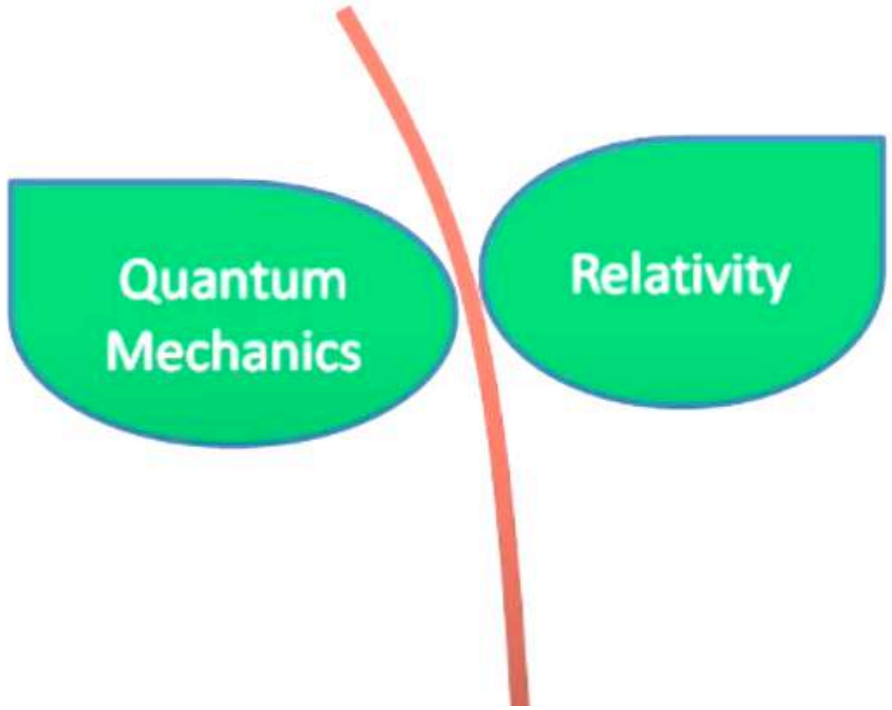
Electricity and Magnetism

Thermodynamics

Classical Mechanics (16th-19th Century)

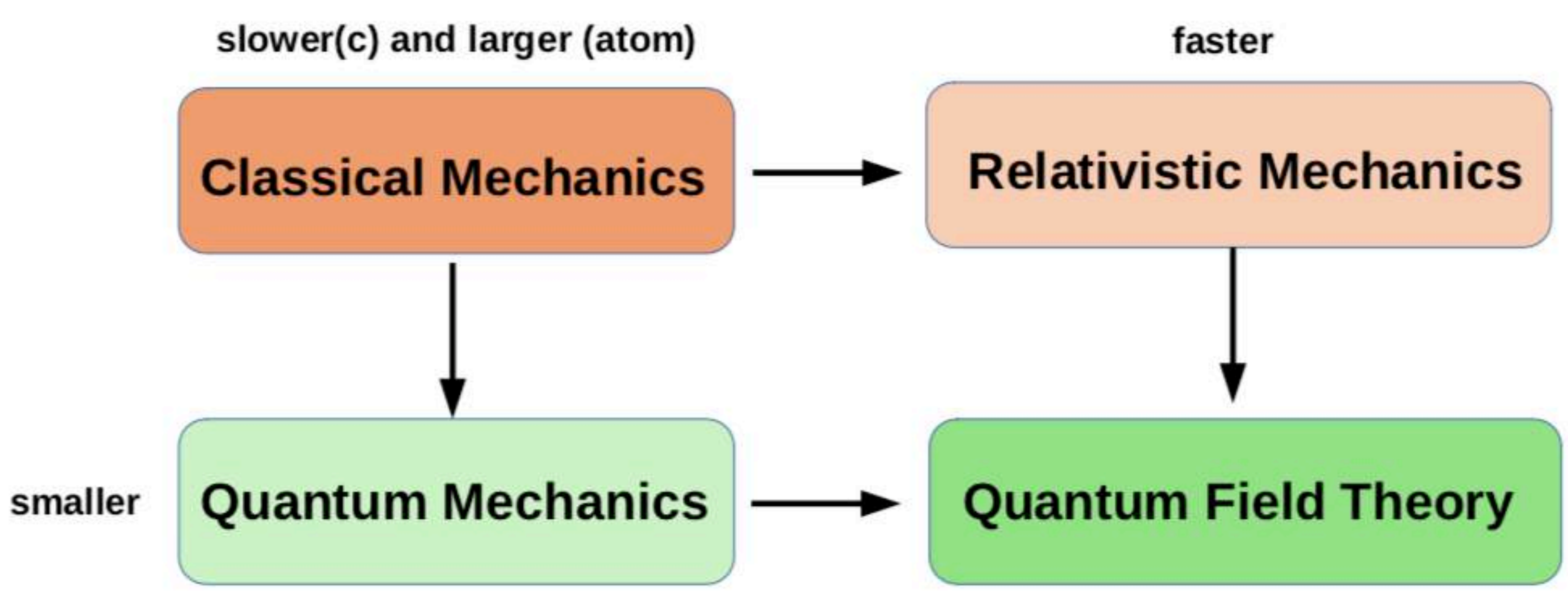


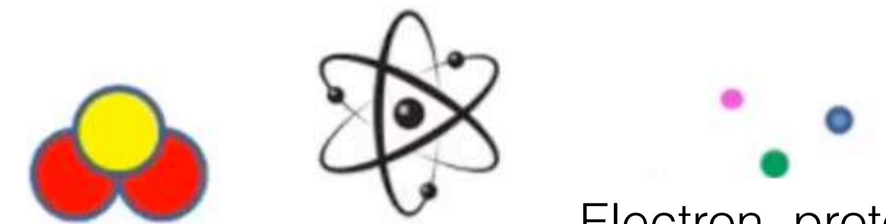
Born of Quantum Mechanics



Relativity works when speed of object is almost equal to speed of light

Quantum mechanics works well when size of objects is very small ,nearly size of atom, electron & proton



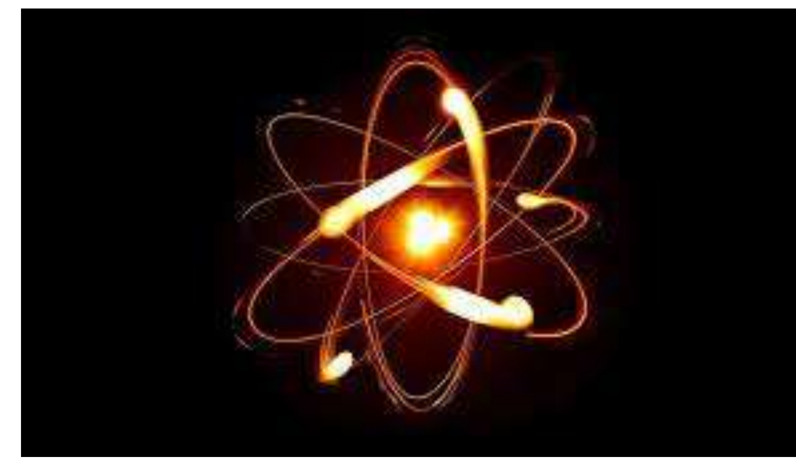


Molecules Atom Electron, proton, neutron, α-particle,

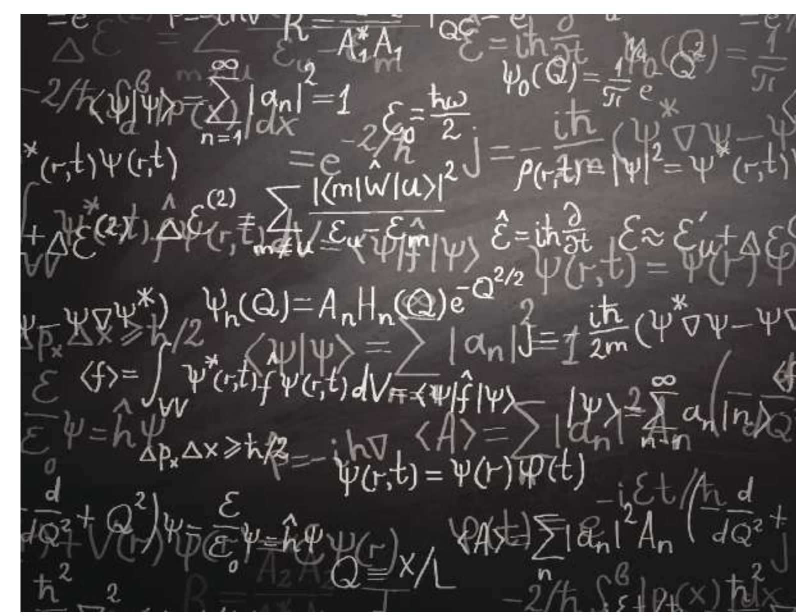
Quantum Mechanics

What is QM ?

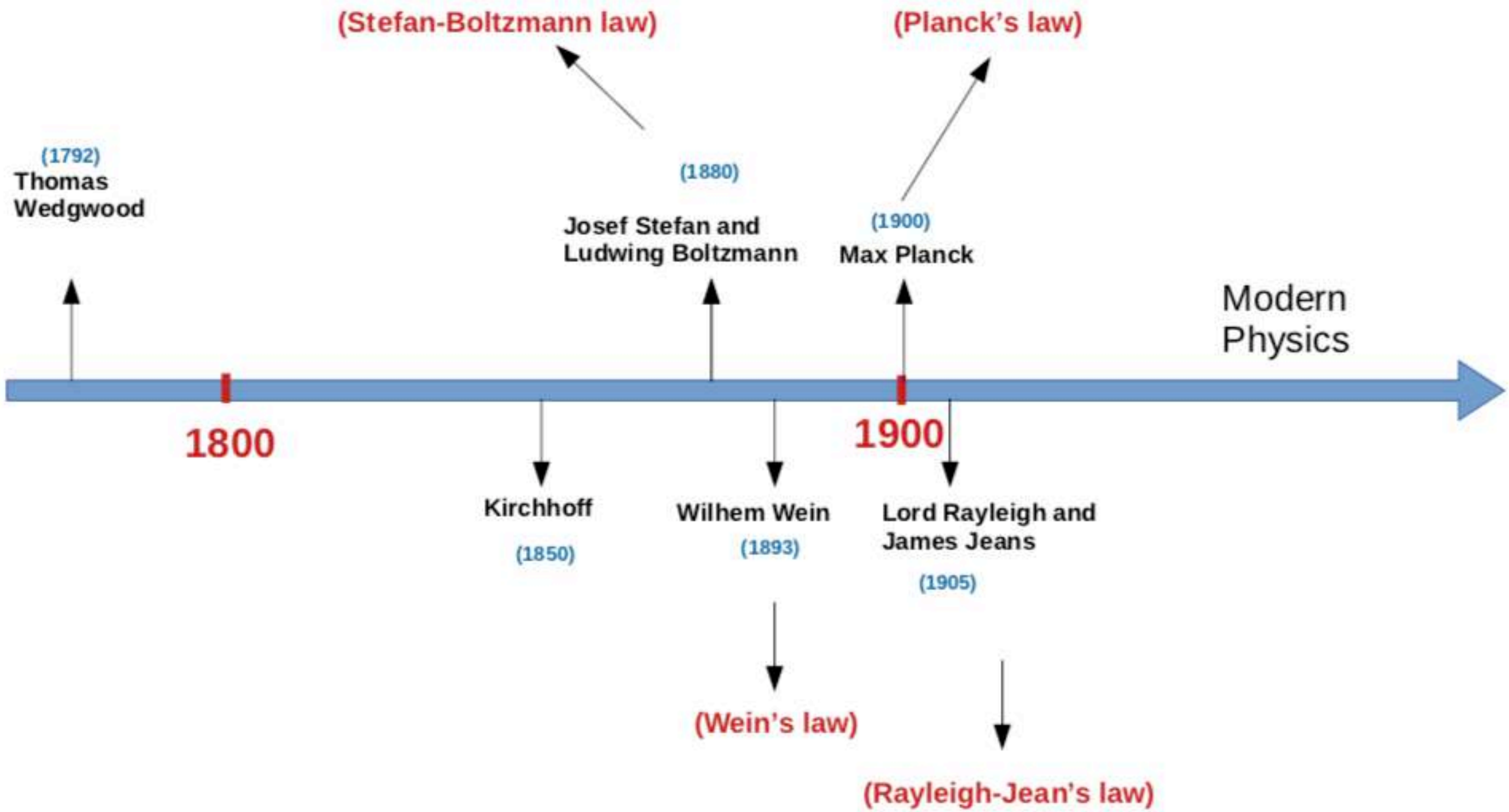
Quantum mechanics is a fundamental theory in physics that provides a description of the physical properties of nature at the scale of atoms and subatomic particles. It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology, and quantum information science.



The branch of mechanics that deals with the mathematical description of the motion and interaction of subatomic particles, incorporating the concepts of quantisation of energy, wave–particle duality, the uncertainty principle, and the correspondence principle.



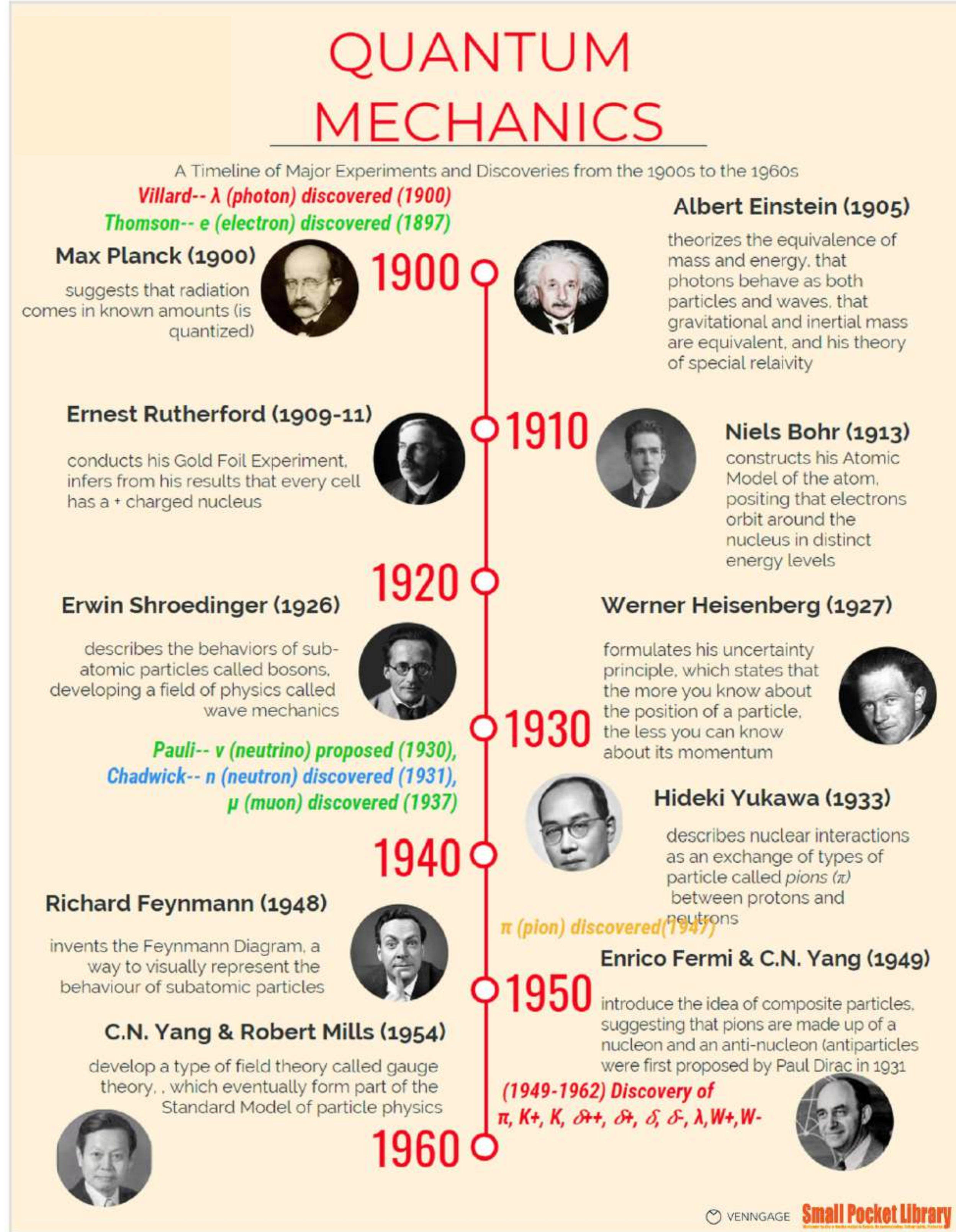
Development of Quantum Mechanics



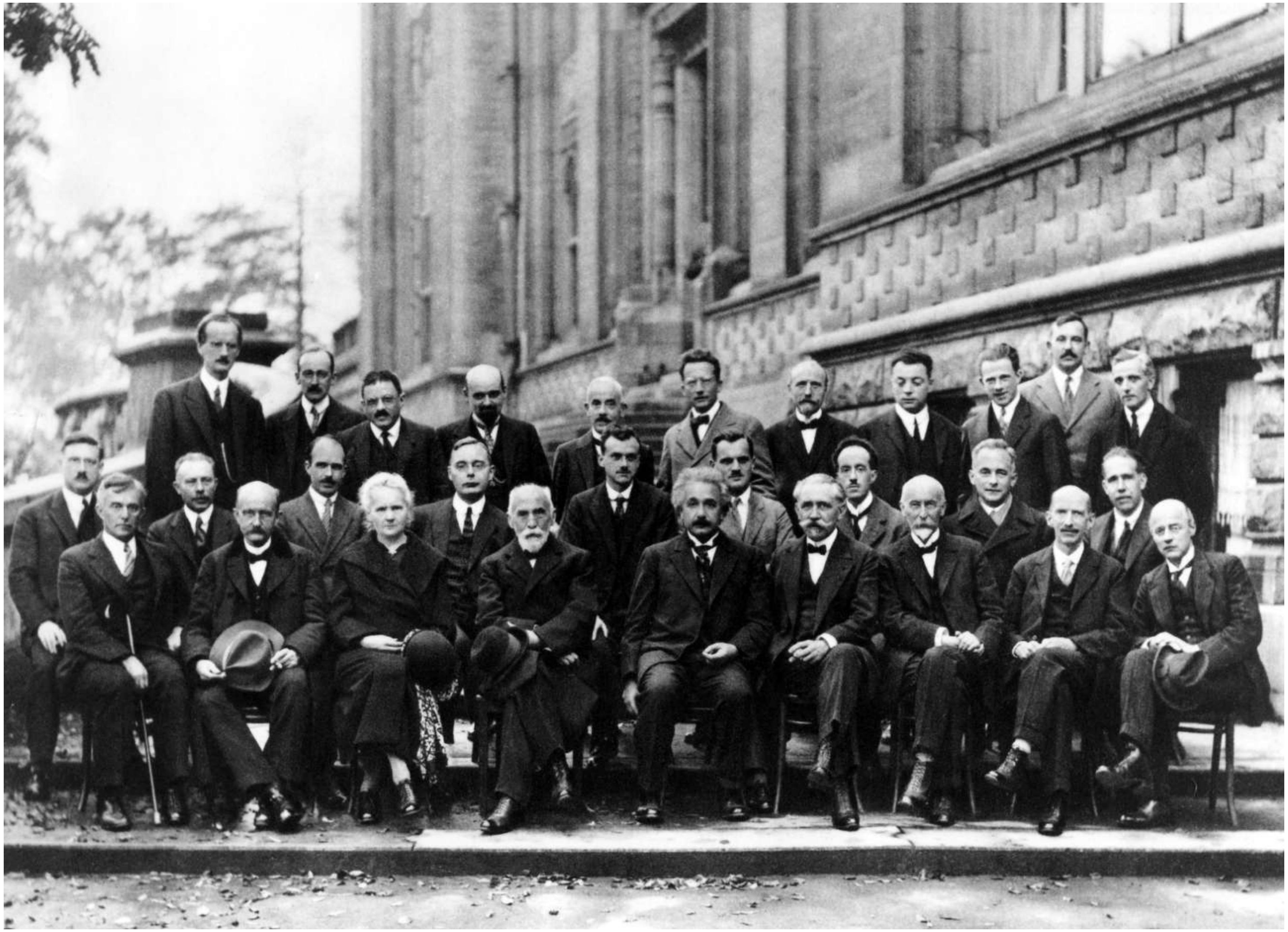
Development of Quantum Mechanics

Development of QM

- No one Had a aim to build quantum mechanics It built by itself
- Historical period of 1897 to 1940 where the ideas of quantum mechanics evolved and settled
- Niels Bohr, de Broglie, Werner Heisenberg, Erwin Schrödinger, Max Born, Wolfgang Pauli, Paul Dirac
- Quantum mechanics plays a decisive role when technology becomes delicate



Development of Quantum Mechanics



The Solvay Conference in 1927 in Brussels, 5th council of physics

Back row L-R: A. Piccard, E. Henriot, P. Ehrenfest, E. Herzen, Th. de Donder, E. Schrödinger, E. Verschaffelt, W. Pauli, W. Heisenberg, R. Fowler, L. Brillouin
Middle row L-R: P. Debye, M. Knudsen, W.L. Bragg, H.A. Kramers, P.A.M Dirac, A. Compton, L. de Broglie, M. Born, N. Bohr
Front row L-R: I. Langmuir, M. Planck, M. Curie, H. Lorentz, A. Einstein, P. Langevin, C. E. Guye, C.T.R Wilson, O.W. Richardson

Role of QM in Technology

Quantum mechanics plays a decisive role when technology becomes delicate, i.e. devices become exceedingly small

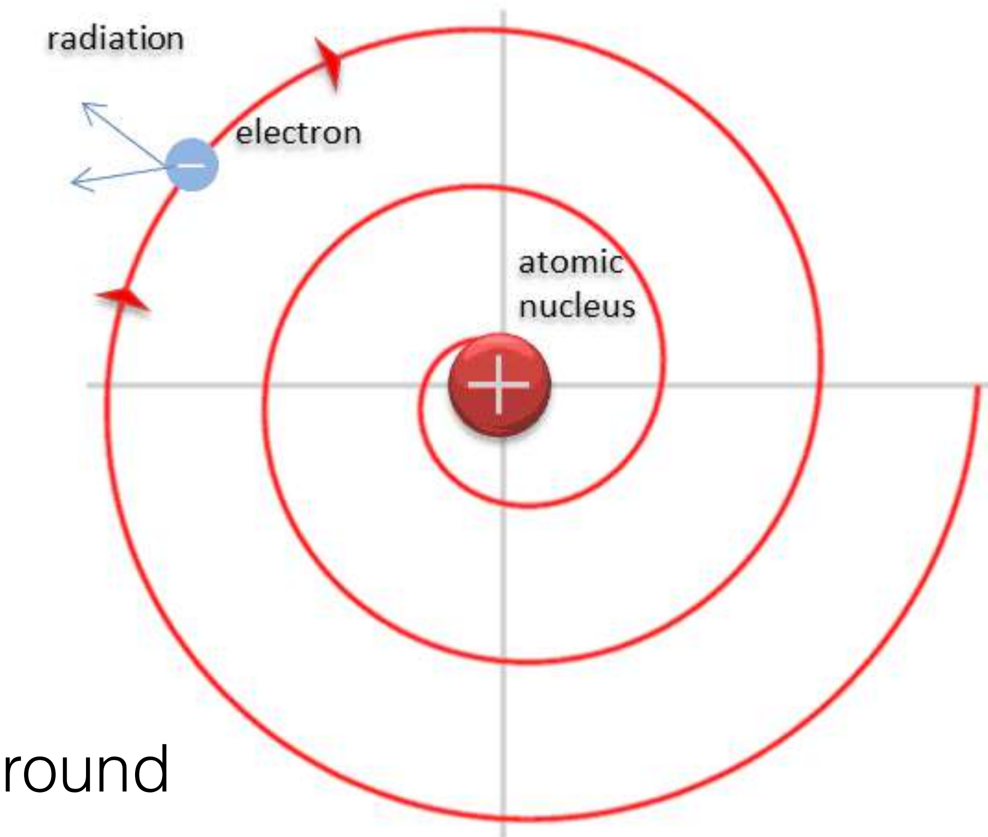
- Invention of Transistor – Reduced size, cost, and power consumption of an electronic gadget
- High precession microscopes -SEM, TEM, STEM, AFM
- LASER
- SQUID
- Single electron transistor
- Photonics- Photon based electronics
  Spintronics-electron spin based electronics
- (Quantum Computers)
- Nanotechnology
- Molecular electronics

Failure of Classical Mechanics (16th-19th Century)

Newtonian classical theorems failed to explain behaviour of atoms, molecules or electronics, or an object when moving with a very high speed.

In an atom:

- Negatively charged electrons revolving around positively charged nucleus
- According to classical picture, there should be electrostatic force of attraction between them.thus they should come close to each other and collapse.



- In an atom negatively charged electrons revolving around positively charged nucleus
- According to classical picture, there should be electrostatic force of attraction between them.thus they should come close to each other and collapse.

Quantum Mechanics

Development of QM to explain three important Experiments:

(Classical, Newtonian mechanics fails to explain)

1. **Black Body Radiation**
2. **Photoelectric Effect**
3. **Compton Effect**

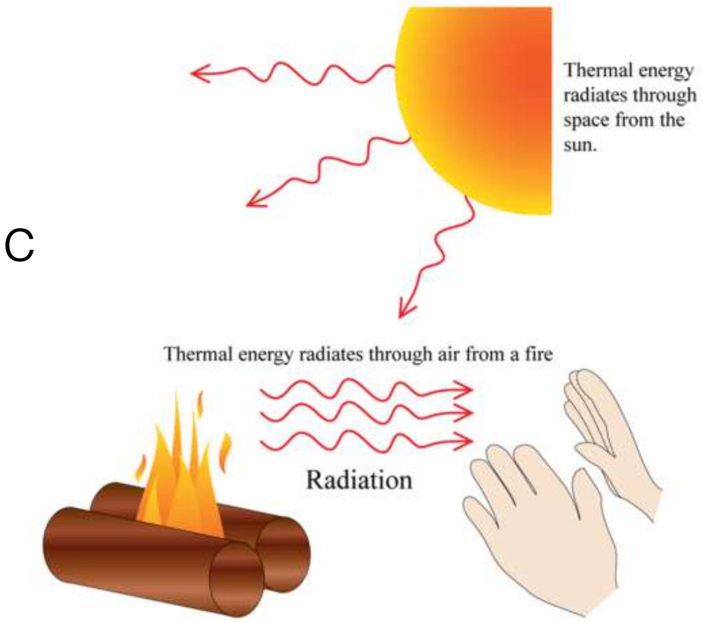
Radiation

Radiation:The mode of energy transfer which need no medium is called radiation

Experimental Observations

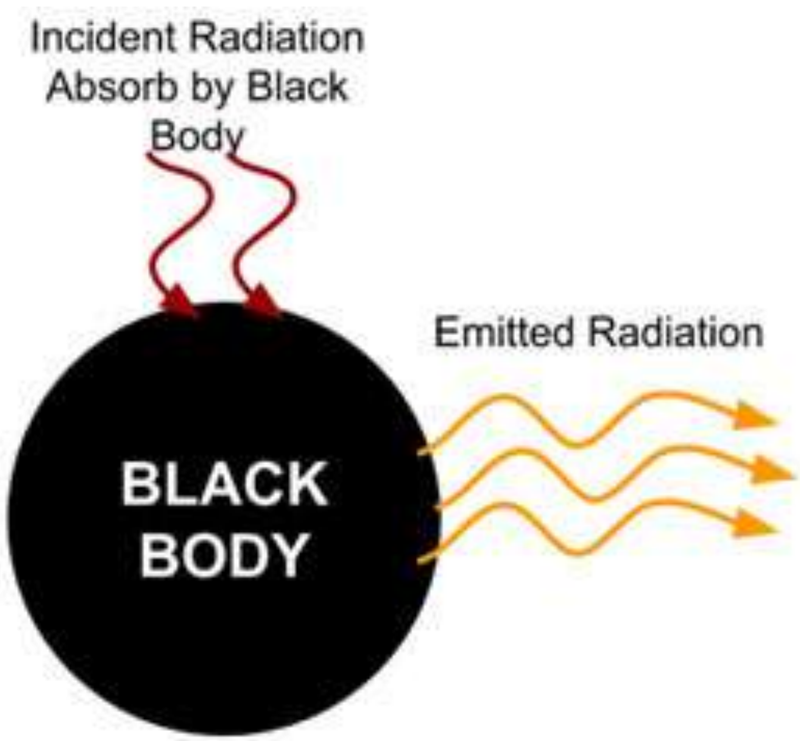
- All bodies emit and absorb electromagnetic radiation (thermal/optical) over various wavelengths.
- All body which temp > 0K, emits radiation

- According to classical mechanics, thy radiate EMW
- As the temperature of anybody rises, the body glows with the colors corresponding to the higher frequency (smaller wavelength) of the electromagnetic spectrum.



- For a body in thermal equilibrium, the power of emitted radiation is proportional to the power absorbed.
- All object emits all kind of wavelengths

Black-Body



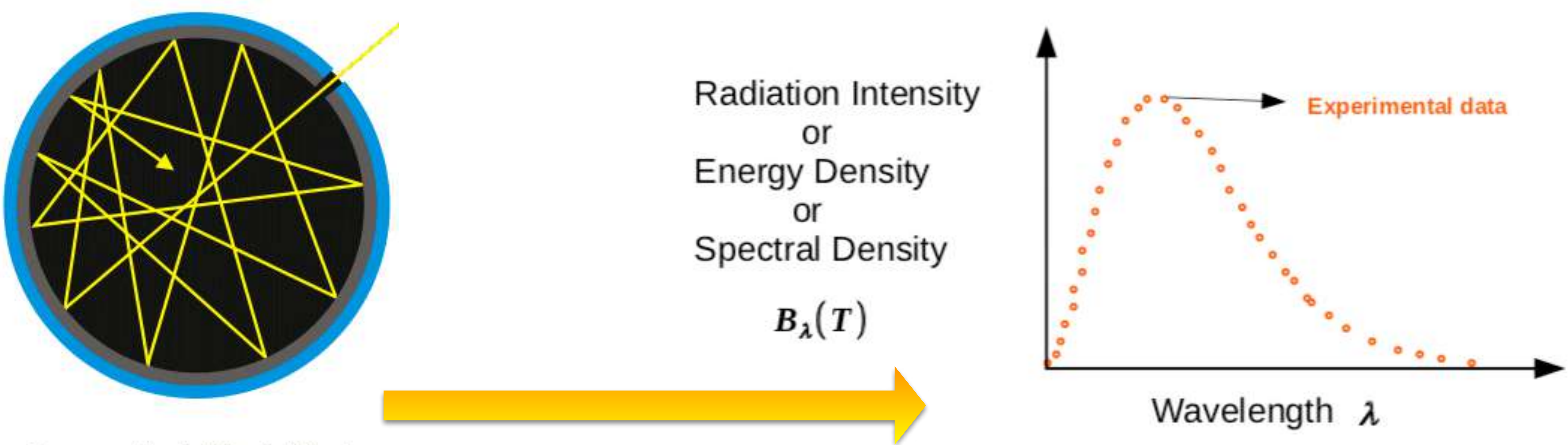
- The non-reflective, opaque object which absorbs all the radiation that falls upon it is called a blackbody.
- At room temperature, it appears black as no visible light is emitted
- At a particular temperature the black body would emit the maximum amount of energy possible for that temperature

It is one that absorbs all the EM radiation (light…) that strikes it. It must emit radiation at the same rate as it absorbs it so a black body also radiates well.

Blackbody radiation: When a black body is at a uniform temperature, its emission has a characteristic frequency distribution that depends on the temperature. Its mission is called black-body radiation. The wavelength (i.e. color) of radiant energy emitted by such a body depends on only its temperature, not its surface or composition

Realisation of blackbody

A black body is an idealization in physics that pictures a body that absorbs all electromagnetic radiation incident on it irrespective of its frequency or angle. A blackbody is a conceptual thing and can b realised like this figures as Ferry's Blackbody

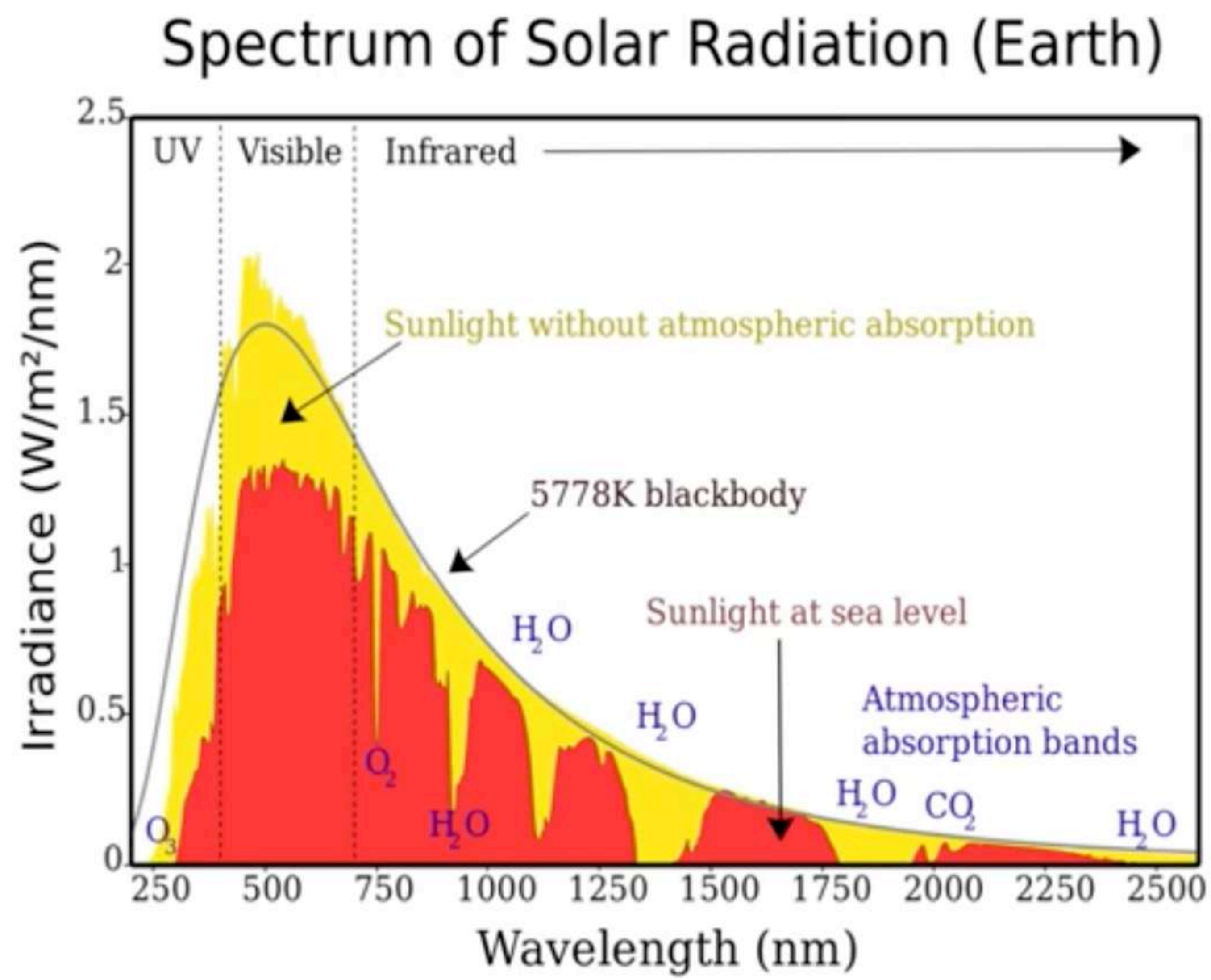


Conceptual Black Body

The **intensity of radiation emitted by such an object per unit volume per time** at different wavelength is called the **black body radiation spectrum (energy density or spectral density).** Let us call it as $B\lambda(T)$.

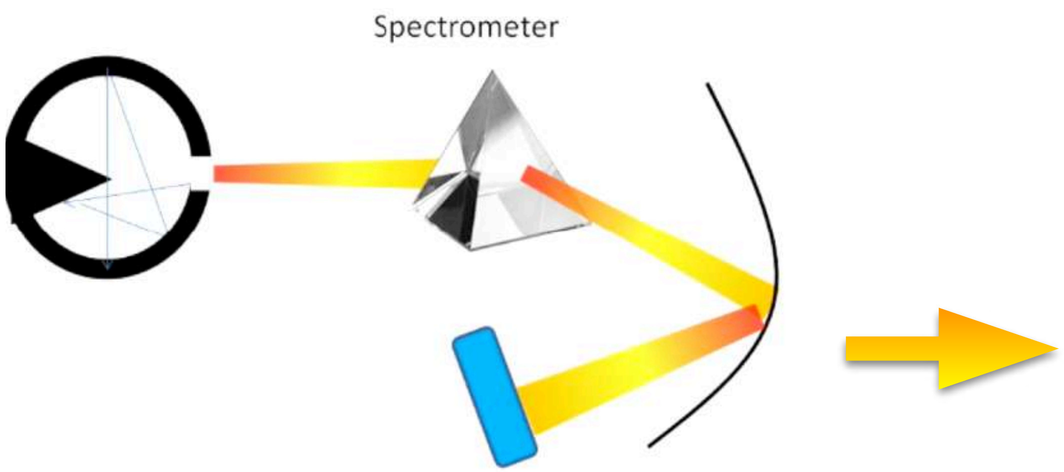
Black Body Radiation: SUN as an examples

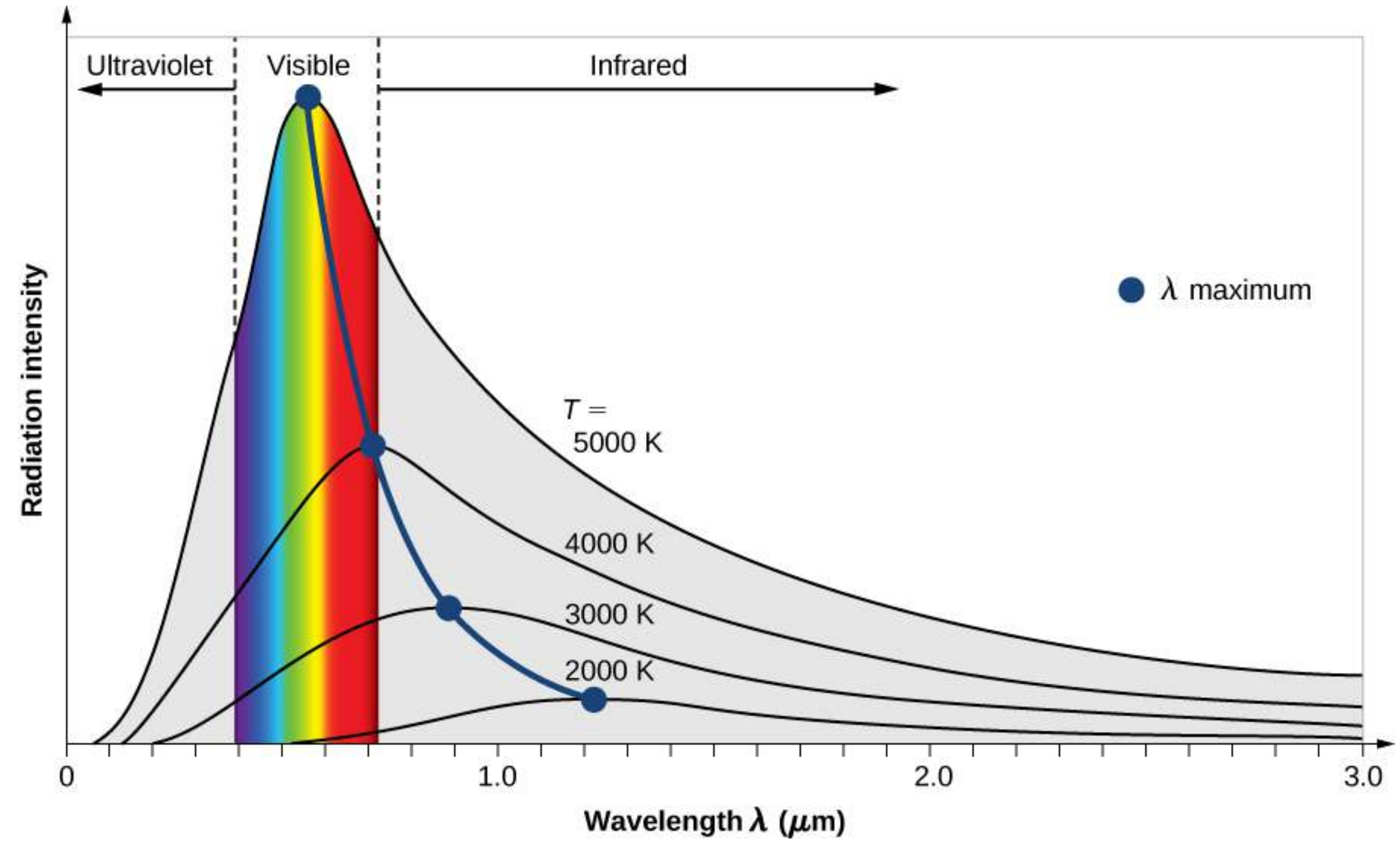
the sun is a blackbody



the light emitted by the sun (in yellow) matches the blackbody spectrum for 5778 K

Blackbody Radiation

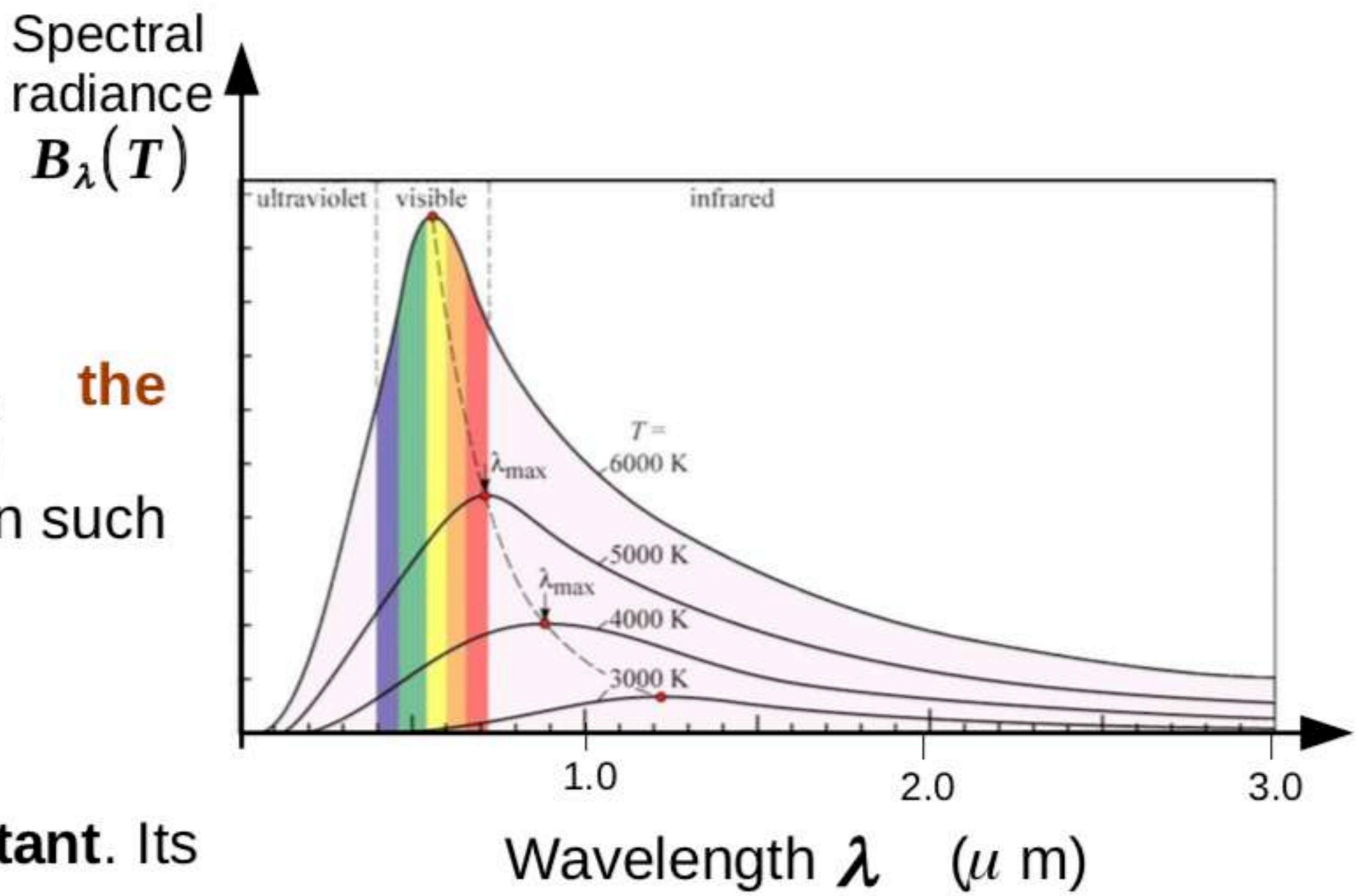




Experimental Observations:

- The energy distribution curve is continuous: all wavelengths of EMW are emitted
- The curve is a bell-shaped curve, i.e. non-monotonic function of the wavelength
- At a specific wavelength, the emitted power is maximum and inversely proportional to the temperature of the blackbody
- Total spectral radiance is directly proportional to the fourth power of the temperature

Wein's displacement law



Wein's displacement law

In the blackbody radiation spectrum, **the wavelength at maximum intensity** (λ_{max}) increases with decrease in **temperature (T)** in such a way that

$$\lambda_{max}\, T = b$$

where **b** is the **Wien's displacement constant**. Its value is

$$b = 2.898 \times 10^{-3}\ m\ K$$

Stefan-Boltzmann law

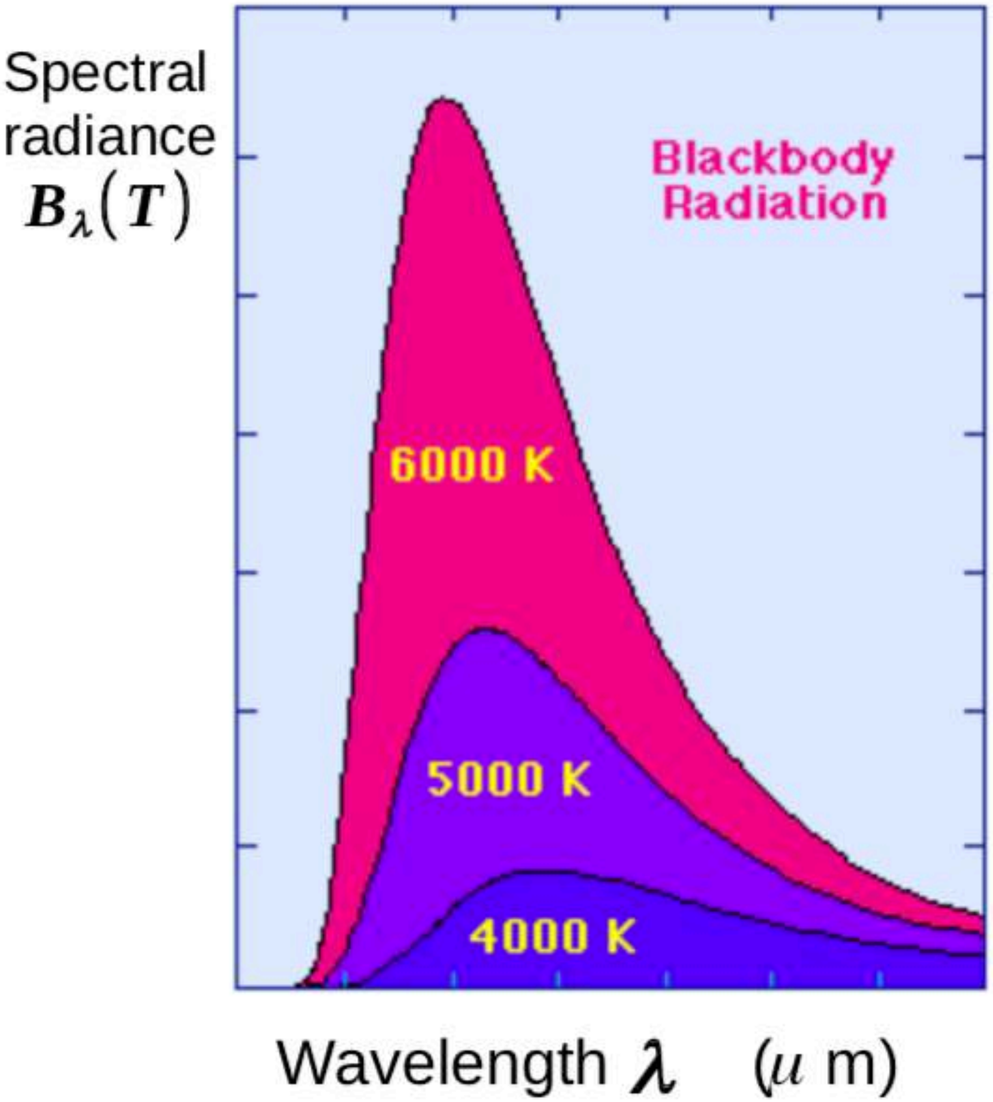
Stefan-Boltzmann law

The **power emitted per unit area** at the surface of the blackbody at all frequencies (**area under the curve**) is directly proportional to the fourth power of the temperature

$$P = \sigma T^4$$

σ is called **Stefan-Boltzmann constant. Its value is,**

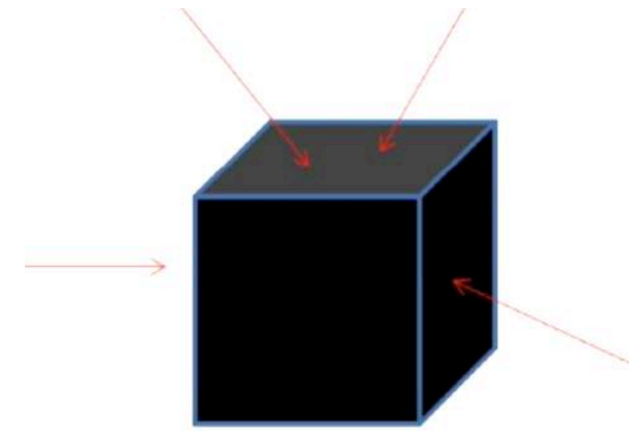
$$\sigma = 5.67 \times 10^{-8}\ J\ s^{-1}\ m^{-2}\ K^{-4}$$

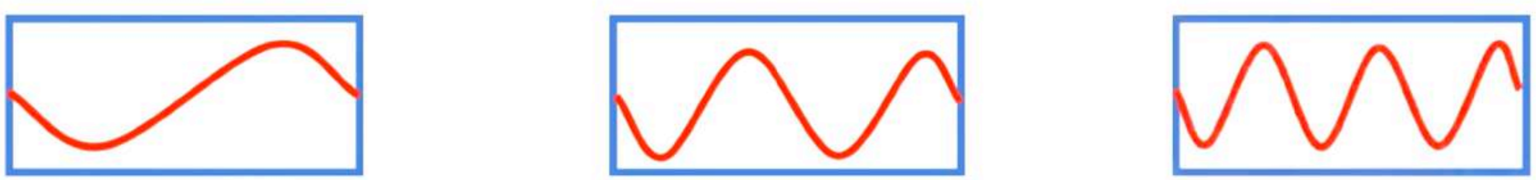


But how does the radiation spectrum itself depend on wavelength?

Rayleigh-Jeans Law: Classical Approach

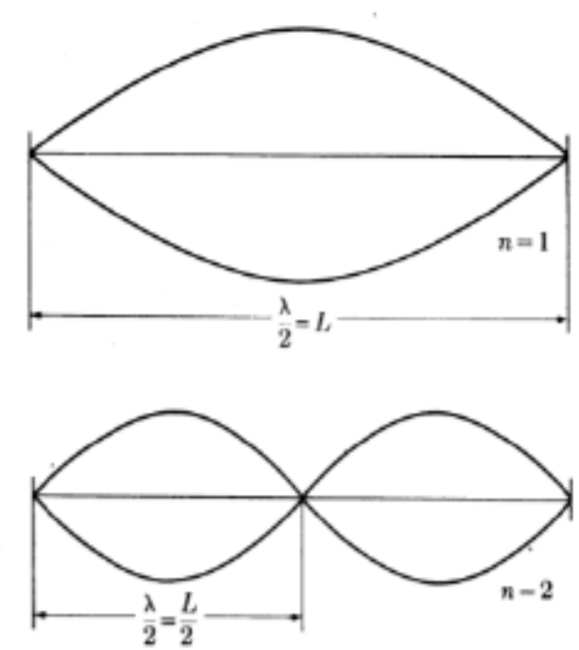
- A cavity is at absolute temperature T.
- The walls of the cavity are perfect reflectors and radiation consist of standing electromagnetic waves.
- The condition for standing waves in such a cavity is that the path length from wall to wall must be whole number of half-wavelengths. So that the node occurs at each reflecting surface.
- The average energy per standing wave; $\bar{\epsilon} = k_B T$





1 mode	2 mode	3 mode
$\frac{1}{2}kT$	$\frac{2}{2}kT$	$\frac{3}{2}kT$

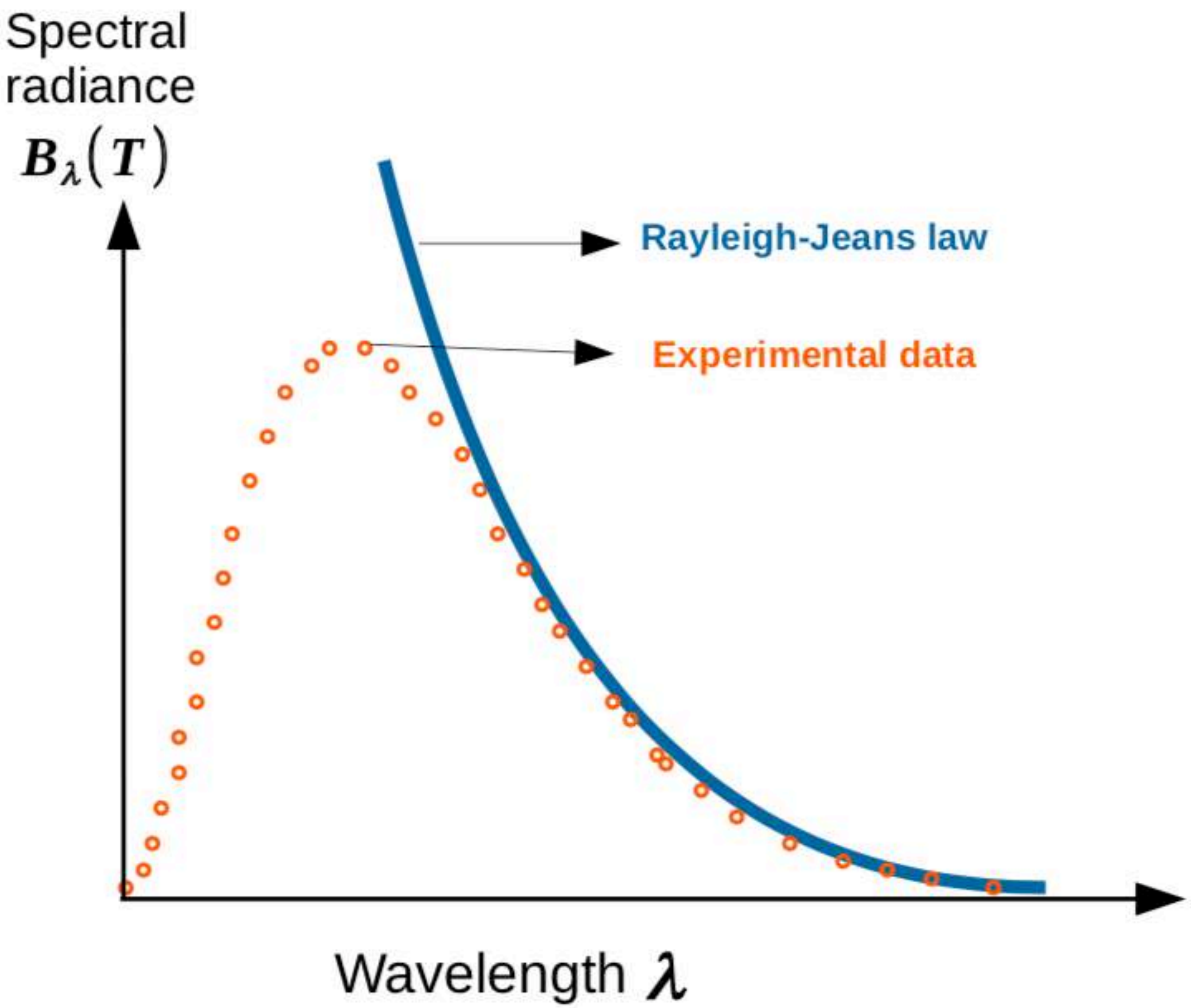
$$B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}$$



Standing waves which can be fitted between two perfectly reflecting walls forms a standing wave.

Rayleigh-Jeans Law: Classical Approach

$$B_\lambda(T) = \frac{8\pi k_B T}{\lambda^4}$$



k_B : Boltzmann constant = 1.38 x 10^{-23}

Failure

- based classical physics arguments

- it works only for large wavelengths

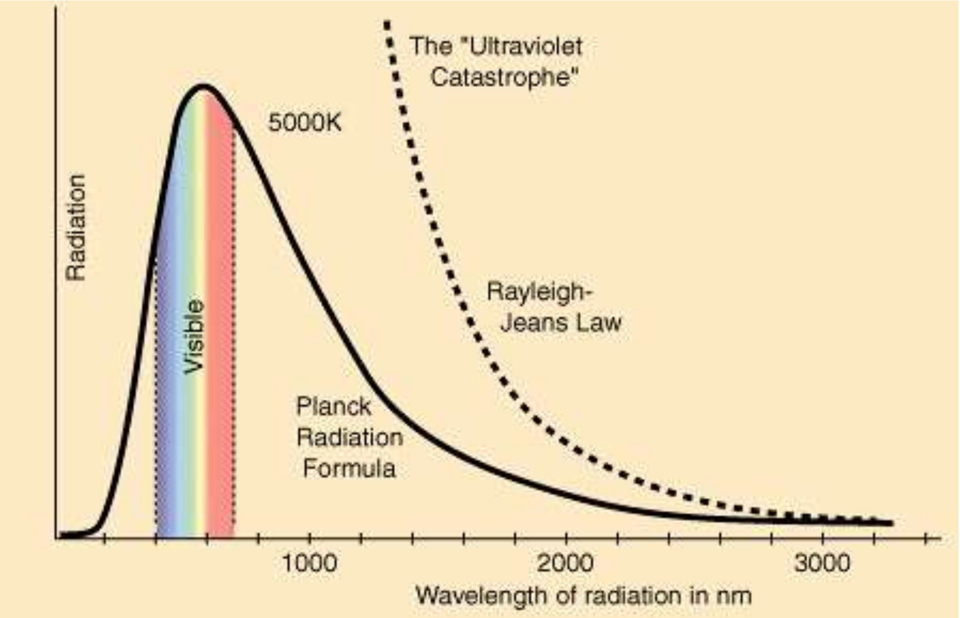
- does not reproduce Wein's displacement law and Stefan-Boltzmann law

ultra-violet catastrophe!

Ultraviolet means low wavelength!

Rayleigh-Jeans Law: Ultraviolet catastrophe

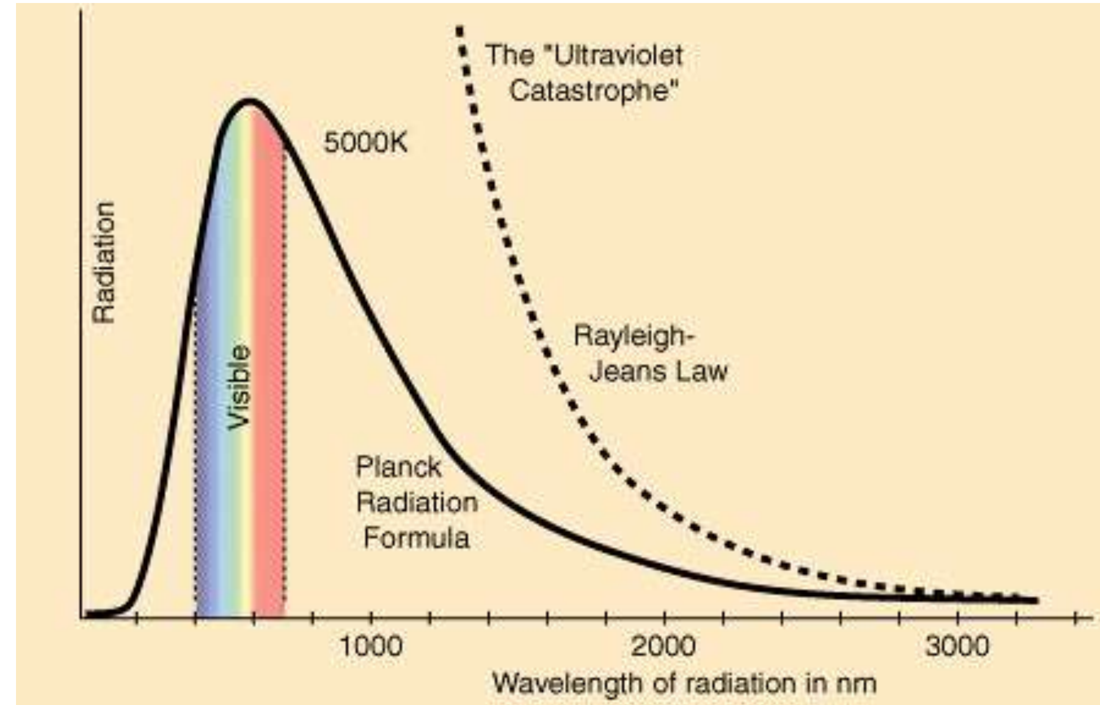
- Rayleigh-Jeans law gives an approximate spectral radiance for blackbody radiation.
- Rayleigh-Jeans law based on classical physics arguments in which the energy is assumed to be continuous.
- It predicts an energy output that diverges towards infinity as wavelength decreases.
- This equation agrees with experimental measurements for long wavelengths (low frequencies) and failure at short wavelengths.
- The law fails to explain the behaviour of the spectral radiance for low wavelengths.
- **The failure of Rayleigh-Jeans law to match with experiment for low wavelengths (high frequencies) is called the ultra-violet catastrophe!**



$$B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}$$

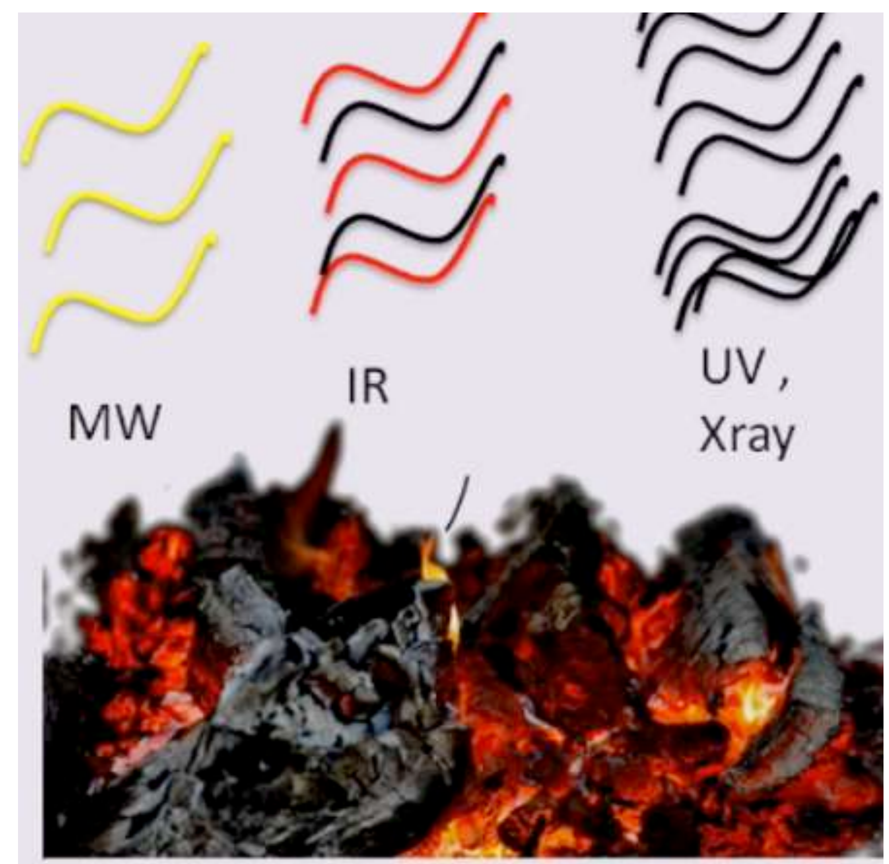
Rayleigh-Jeans Law: Ultraviolet Catastrophe

$$B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}$$



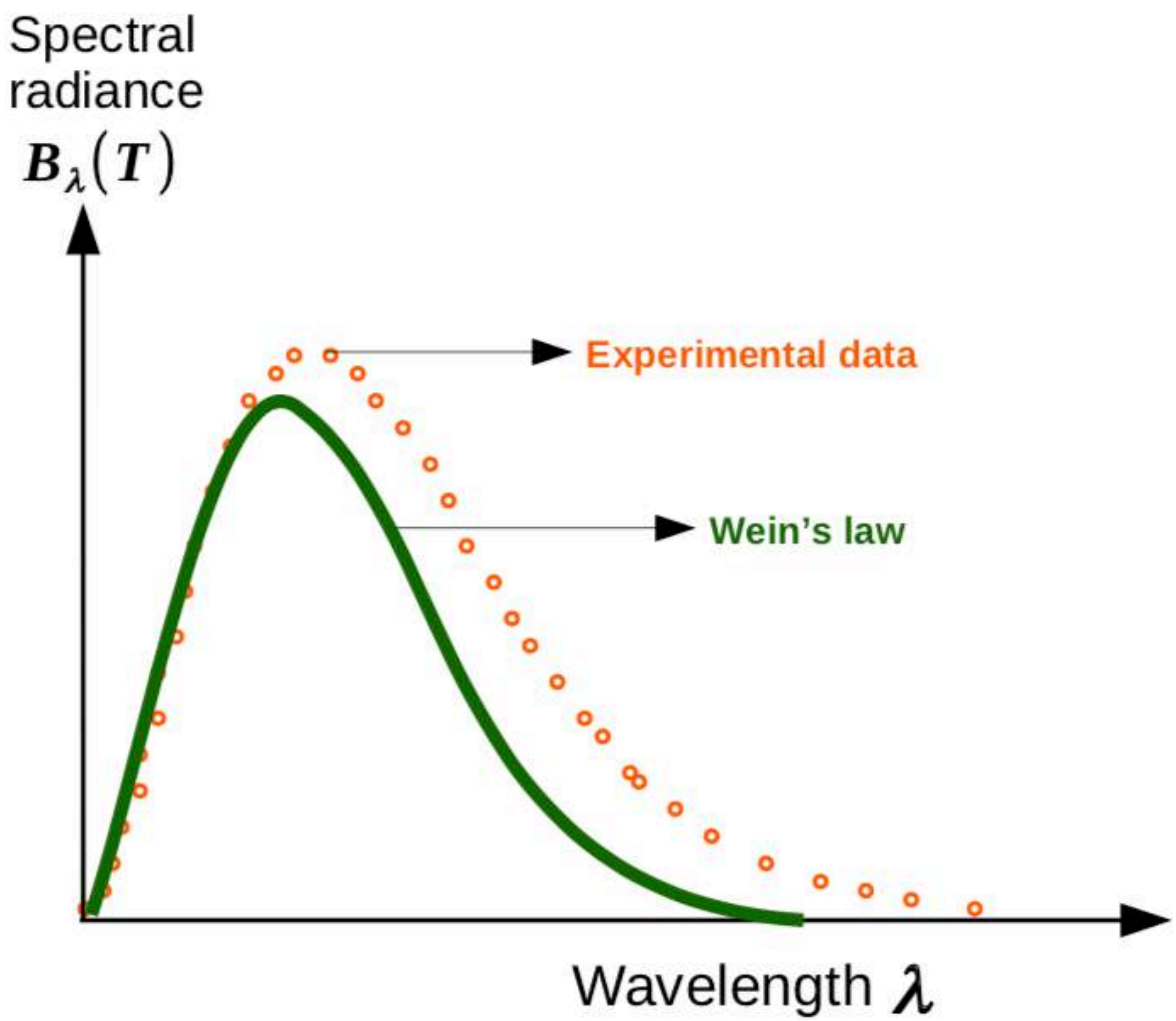
Discrepancy between theory and experiments at higher frequencies (shorter wavelength) Ultra-violet Catastrophe

Low-frequency radiations-radio waves, Microwave, IR, and visible



High-frequency radiations: X-ray, gamma ray and Ultraviolet

Wein's Law

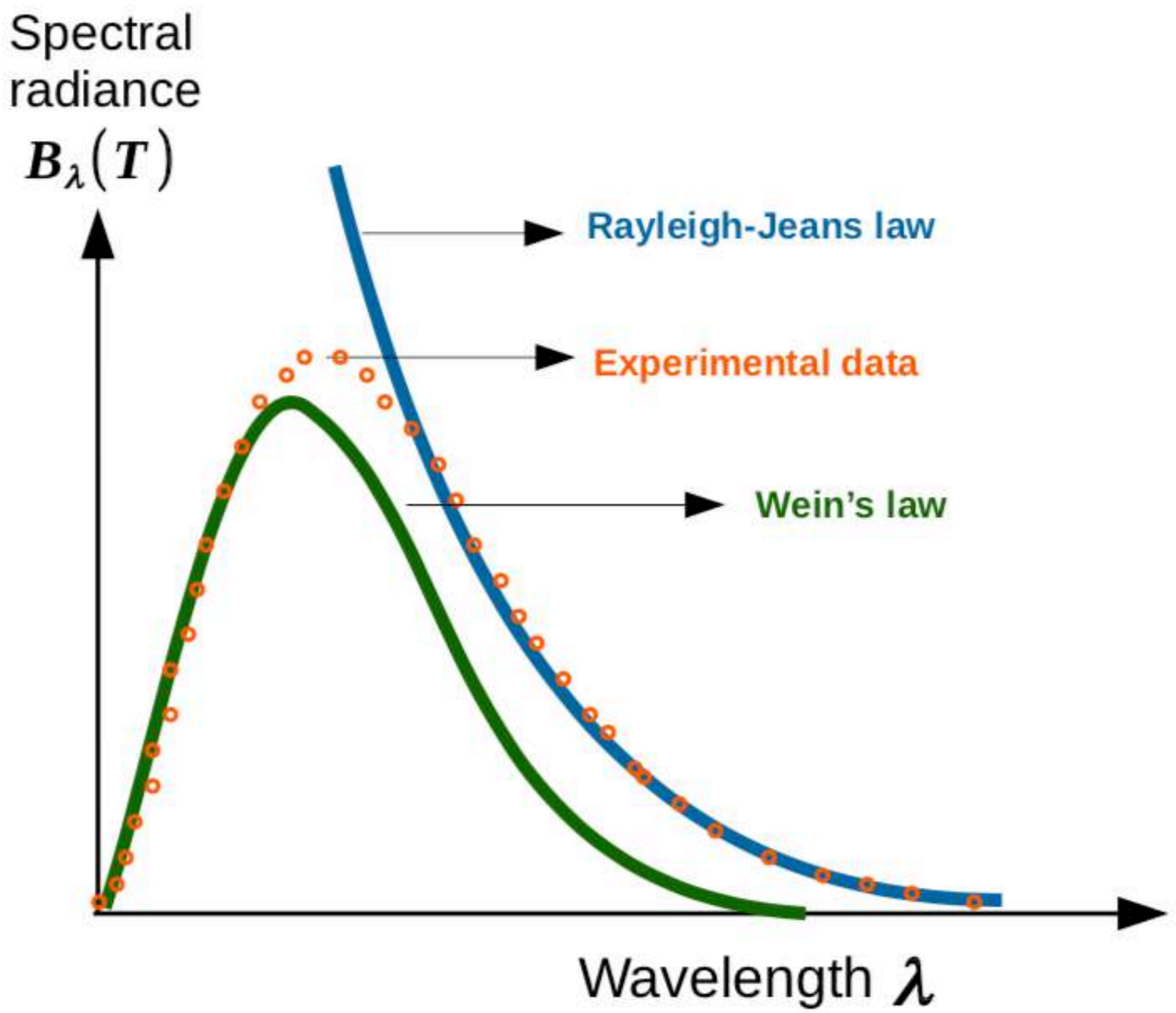


This law can be derived using standard classical physics tools.

$$B_\lambda(T) = \frac{8\ \pi\ h\ c}{\lambda^5}\ e^{\frac{-h\ c}{\lambda\ k_B\ T}}$$

Works only for small wavelengths

Failures of classical approach

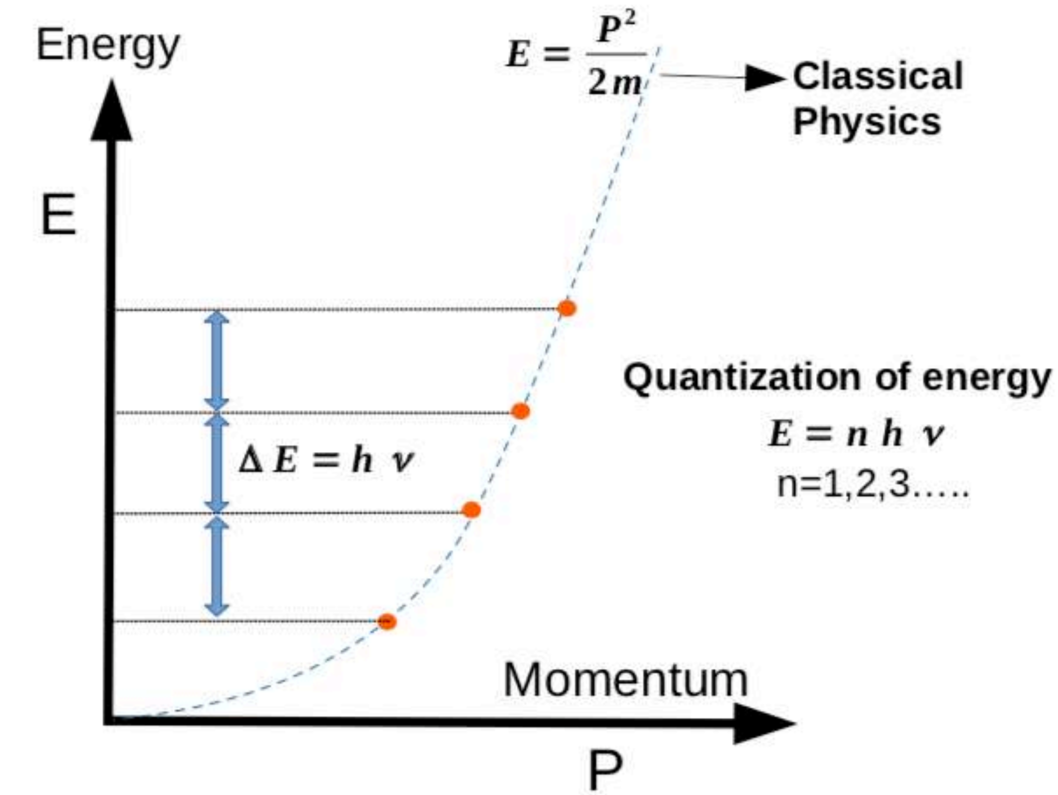


Classical theory fails to find a mathematical description of blackbody radiation intensity!

Max-Planck's Theory of Blackbody Radiation

Hypothesis:

- A black body contains a **large number of oscillating particles**:
- Each particle is vibrating with a characteristic frequency.
- The frequency of radiation emitted by the oscillator is the same as the oscillator **frequency.**
- **Sources of radiations are atoms in a state of oscillations**
- The oscillator can absorb energy in multiples of small unit called quanta.
- This **quantum of radiation** is **photon.**



Electromagnetic radiation from heated bodies is not emitted continuously in the form of waves. But the energy is emitted in the form of discrete packets of energy called photon.

$$E = nh\nu$$

where **n = 1,2,3,….**, h = **6.63×10^{-34}** Js is the Planck's constant and ν is the frequency

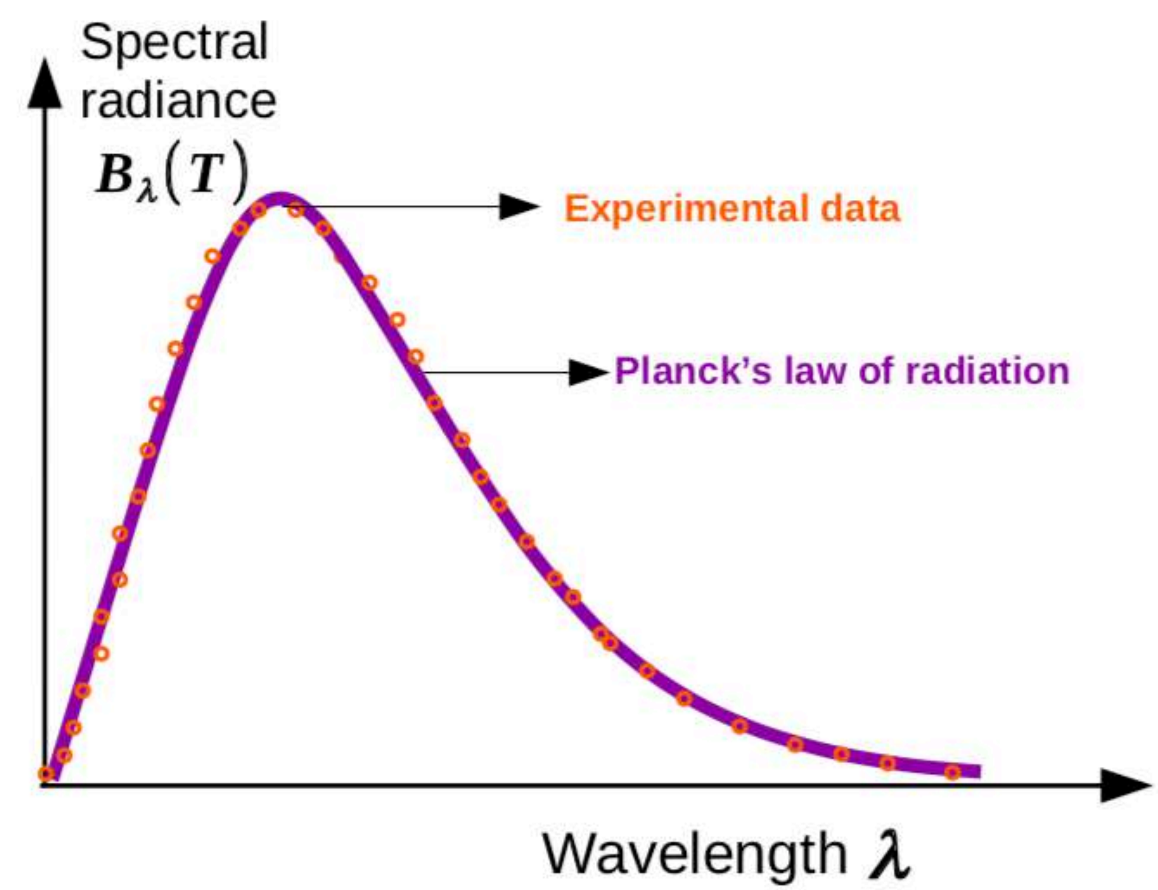
Planck's Theory of Blackbody Radiation

Electromagnetic radiation from heated bodies is not emitted continuously in the form of waves. But the energy is emitted in the form of discrete packets of energy called photon. By using the concept of quantisation, i.e. $E = nh\nu$, he derived the mathematical description as:

Spectral radiance

$$B_\lambda(T) = \frac{8\pi h c}{\lambda^5}\frac{1}{e^{\left(\frac{hc}{\lambda k_B T}\right)}-1}$$

Derivation (not in the syllabus)



Planck's law of radiation **matches perfectly with the experiment**.

Planck's Theory of Blackbody Radiation

How Planck derived radiation spectrum? (continued..)

$B_\lambda(T)$ = density of photons of wavelength λ X energy of each photon Of wavelength λ

$$B_\lambda(T) = \frac{8\pi}{\lambda^4} \times \frac{hc/\lambda}{e^{\left(\frac{hc}{\lambda k_B T}\right)} - 1}$$

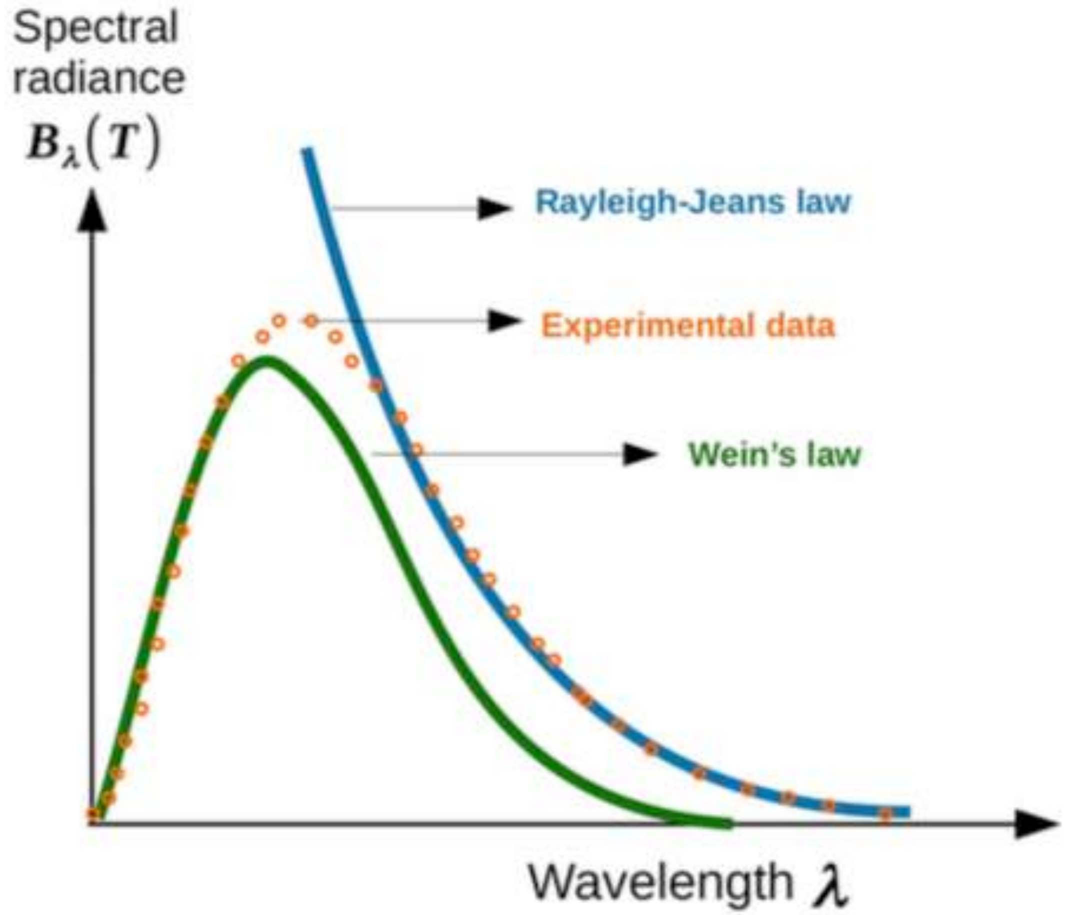
Planck's formula for spectral radiance

$$B_\lambda(T) = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{\left(\frac{hc}{\lambda k_B T}\right)} - 1}$$

Classical Vs Quantum approach for BlackBody

Classical Physics

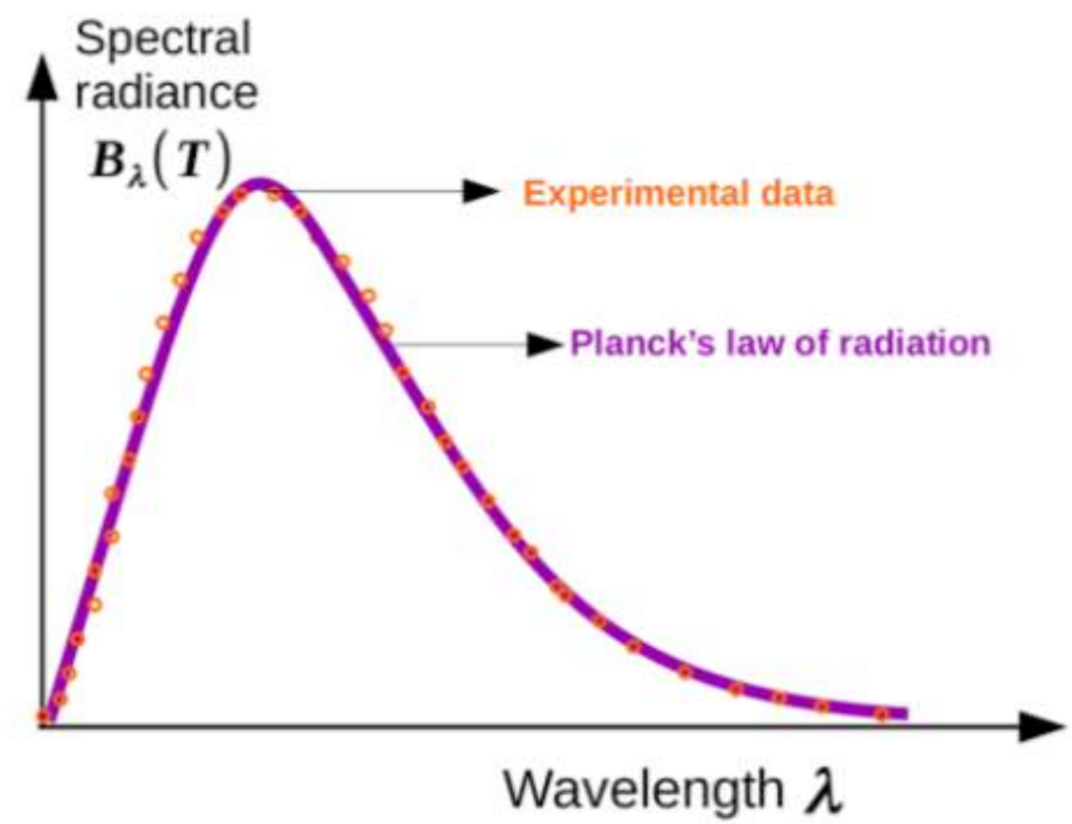
Rayleigh-Jeans law $B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}$



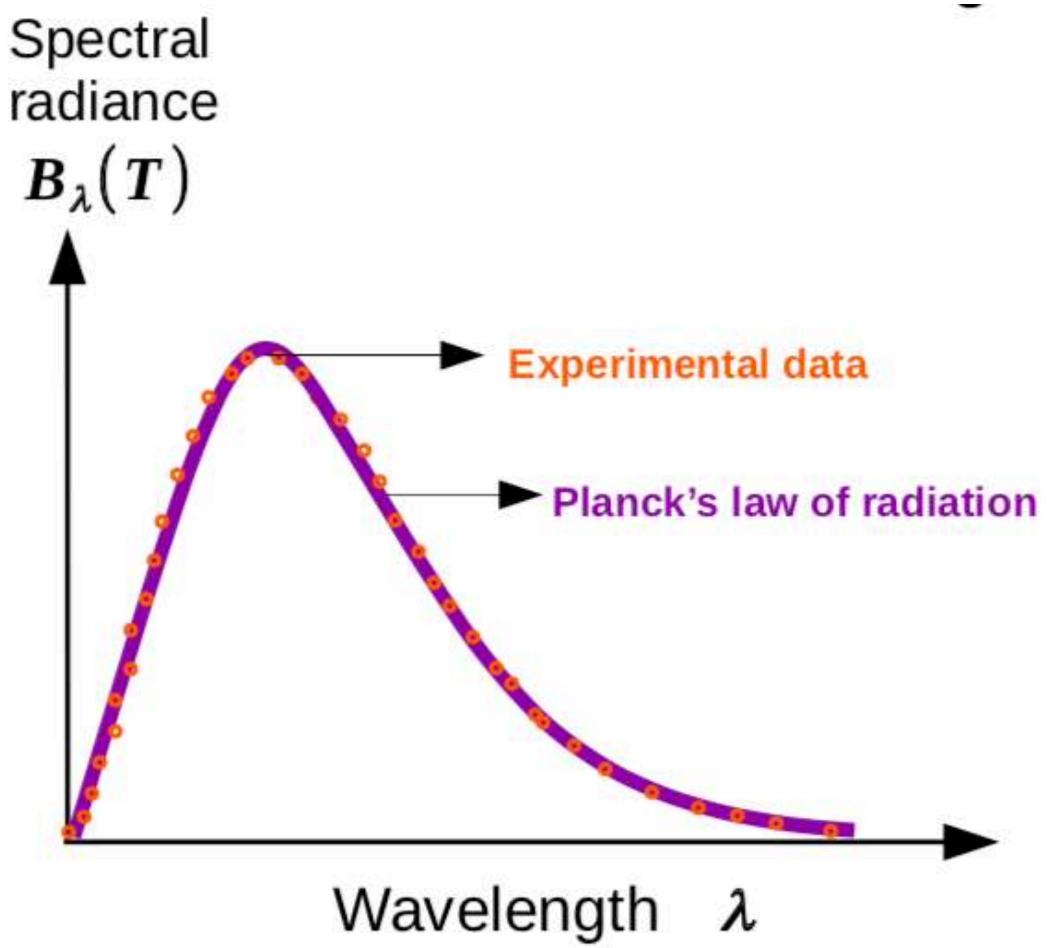
Quantum Physics

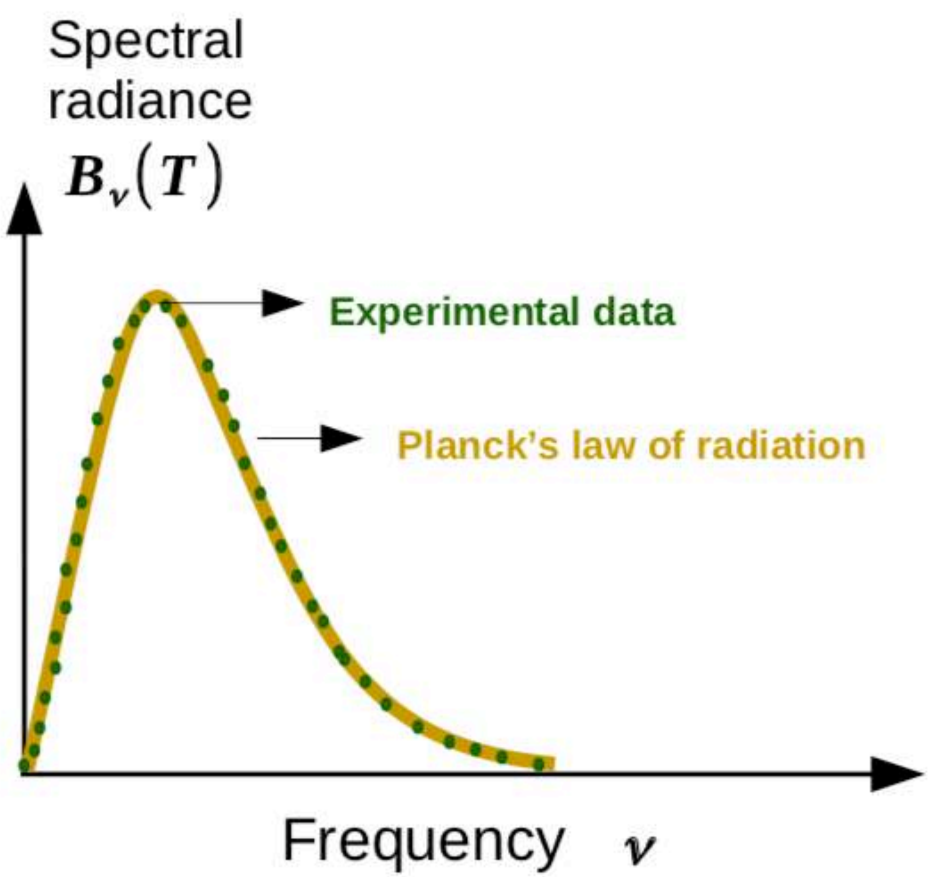
Planck's law

$$B_\lambda(T) = \frac{8\,\pi\,h\,c}{\lambda^5}\,\frac{1}{e^{\left(\frac{h\,c}{\lambda\,k_B\,T}\right)}-1}$$



Max-Planck's Theory: Frequency





$$B_\lambda(T) = \frac{8\pi h c}{\lambda^5} \frac{1}{e^{\left(\frac{hc}{\lambda k_B T}\right)} - 1}$$

$$B_\nu(T) = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{\left(\frac{h\nu}{k_B T}\right)} - 1}$$

Max-Planck's Theory of Blackbody Radiation

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Spectral radiance

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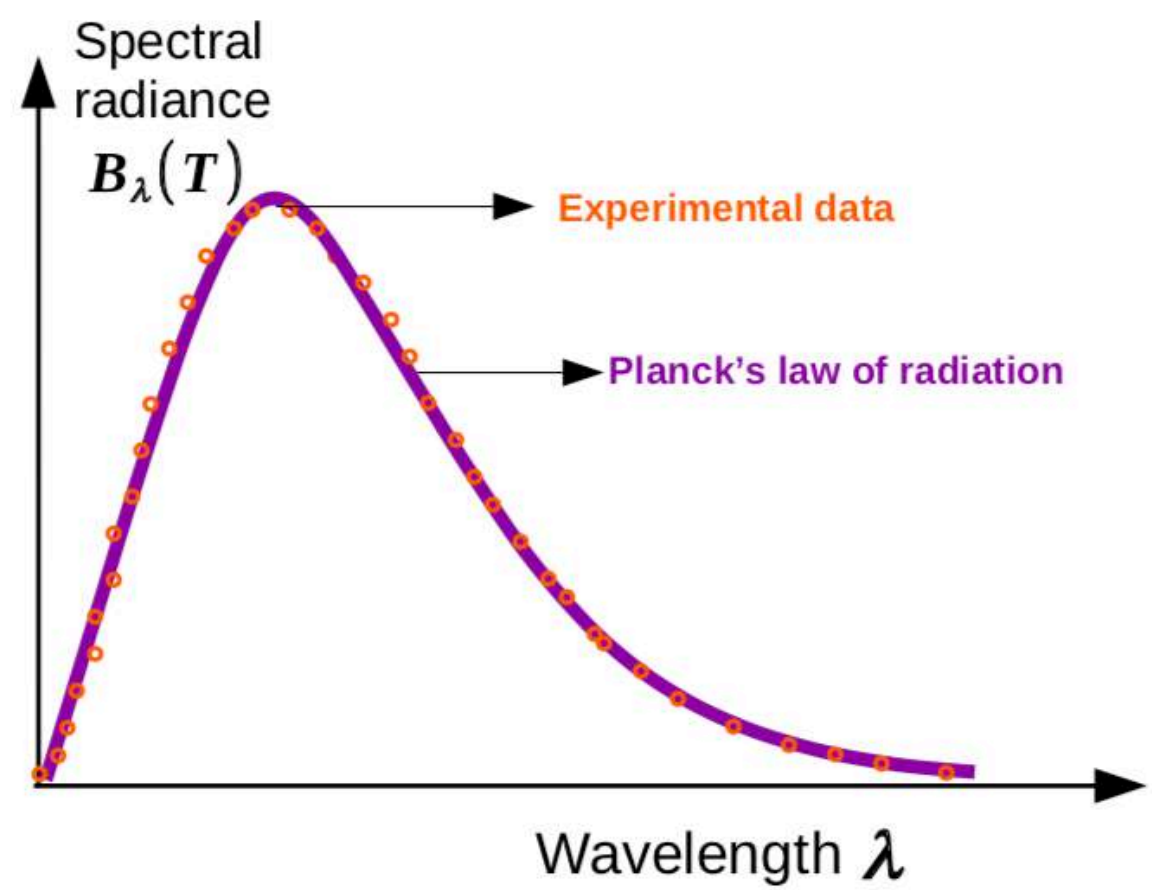
Derivation (not in the syllabus)



Planck's law of radiation **matches perfectly with the experiment**.

Max-Planck's Theory of Blackbody Radiation

$$B_\lambda(T) = \frac{8\pi h c}{\lambda^5}\frac{1}{e^{\left(\frac{hc}{\lambda k_B T}\right)} - 1}$$

Wavelength = λ is large

$e^{(\frac{hc}{\lambda k_\beta T})}$ **is small**

$e^x \approx 1 + x$

$$B_\lambda(T) \approx \frac{8\pi h c}{\lambda^5}\frac{1}{1+\left(\frac{hc}{\lambda k_B T}\right) - 1} = \frac{8\pi k_B T}{\lambda^4}$$

Rayleigh-Jeans Law

Wavelength = λ is small

$e^{(\frac{hc}{\lambda k_\beta T})}$ **is large**

$e^x - 1 \approx e^x$

$$B_\lambda(T) \approx \frac{8\pi h c}{\lambda^5}\frac{1}{e^{\left(\frac{hc}{\lambda k_B T}\right)}} = \frac{8\pi h c}{\lambda^5} e^{\frac{-hc}{\lambda k_B T}}$$

Wein's Law

Possible Questions in Exam

1. What is ultraviolet catastrophe? How Planck's law rectified it?

2. Explain how classical Physics failed to explain black body radiation spectrum. How could Planck's hypothesis elucidate the black body spectrum?

3. Describe blackbody radiation and draw Blackbody radiation spectrum for three Temperatures.

4. Show that Rayleigh-Jeans law and Wein's law can be derived from Planck's law of black body radiation.

Compton Effect

Development of QM to explain three important Experiments:

(Classical, Newtonian mechanics fails to explain)

1. **Black Body Radiation**
2. **Photoelectric Effect**
3. **Compton Effect / Compton Scattering**

Compton Effect/Scattering

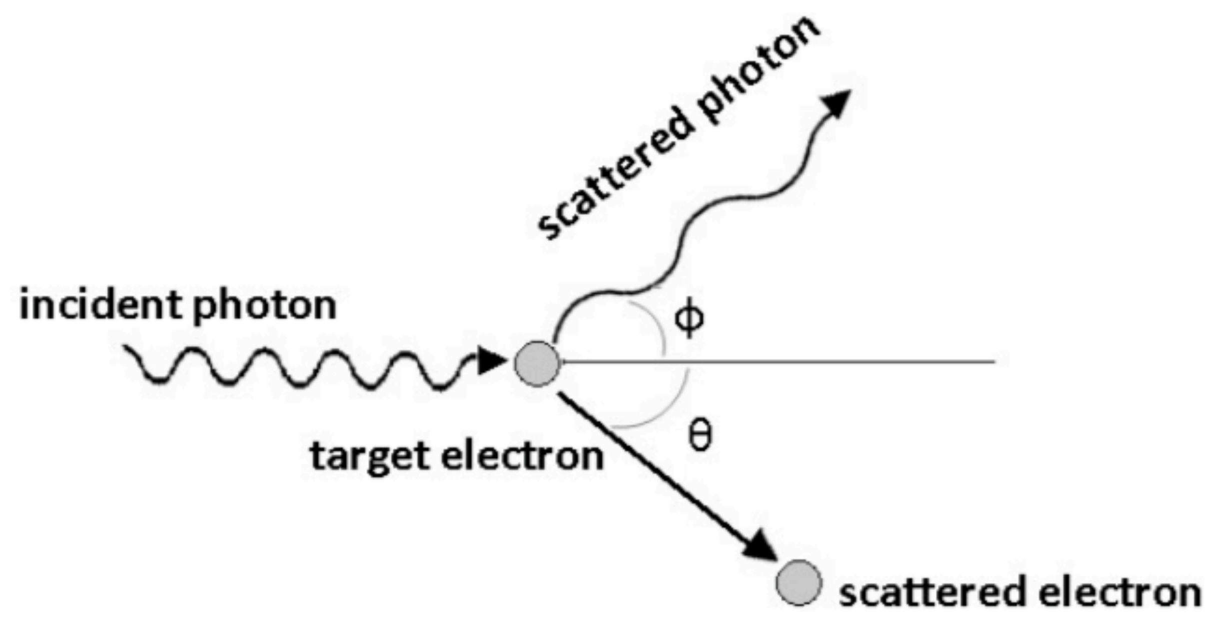
- It is another important development that led to **birth of modern physics**

- It questions wave nature of light and gives an evidence for the **failure of classical wave theory** of light

- It was thought that the electric field of the incident wave accelerates the charged electron and results in **emission of radiation at the same frequency** as the incident wave.

- **Compton showed** experimentally and theoretically that the **wavelength of the light get shifted** depending on the scattering angle.

Compton Effect/Scattering



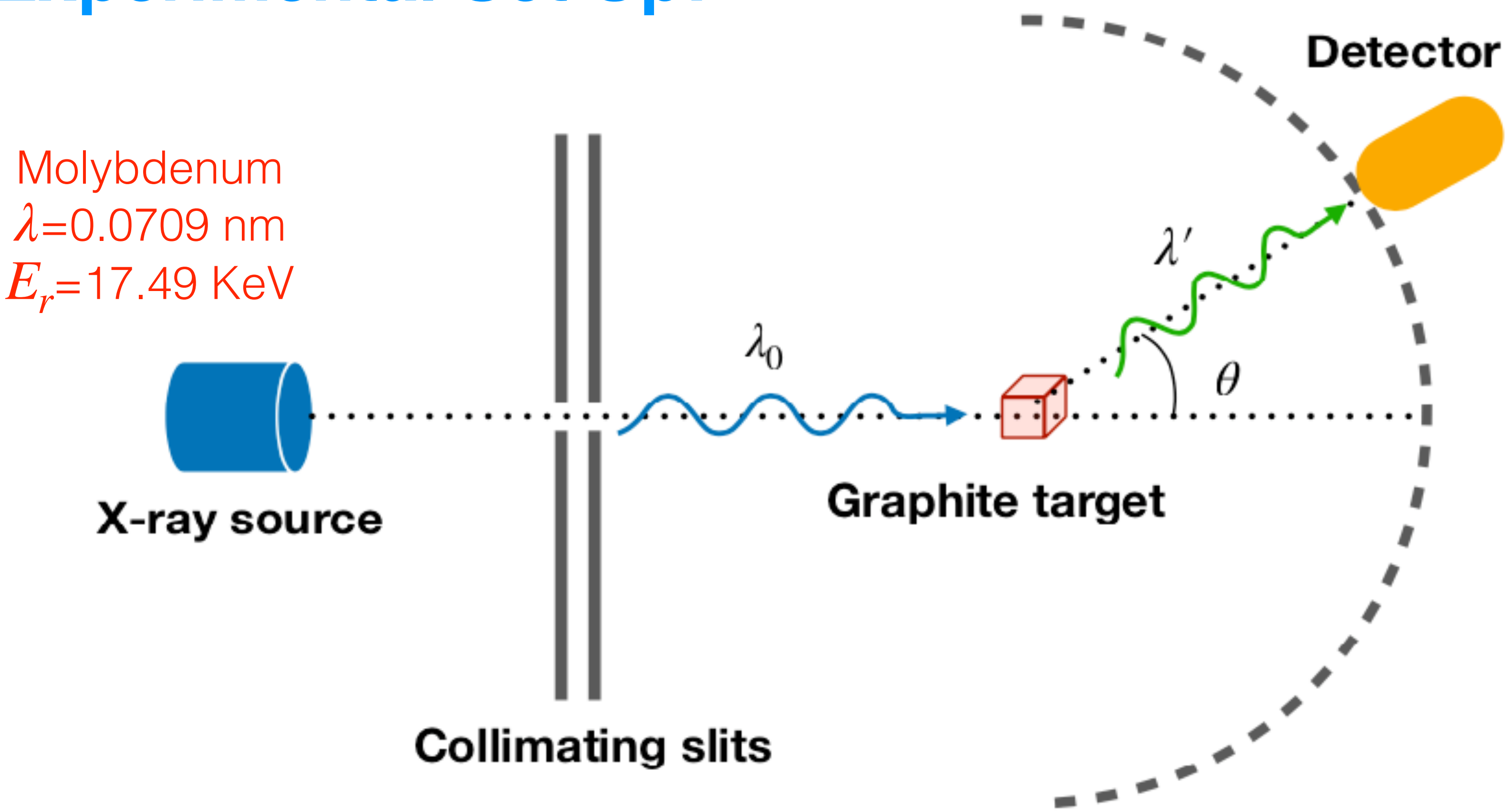
A phenomenon in which a **collision between a photon and an electron** results in an **increase in the kinetic energy of the electron** and a corresponding **increase in the wavelength of the photon.**

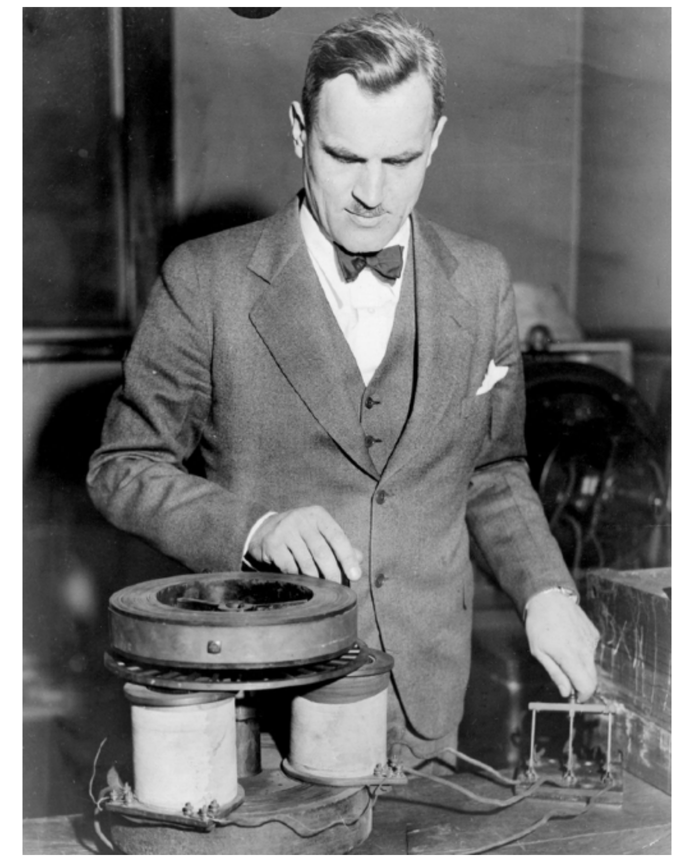
Holly Compton predicted the shift in wavelength **theoretically** and **measured the shift experimentally.** This discovery gave an **evidence for the particle nature of light!**

Compton Effect/Scattering Experiment

Aim: The Compton Effect was an experiment conducted by Arthur H. Compton in 1923 that further confirmed the quantum theory of light.

Experimental Set Up:

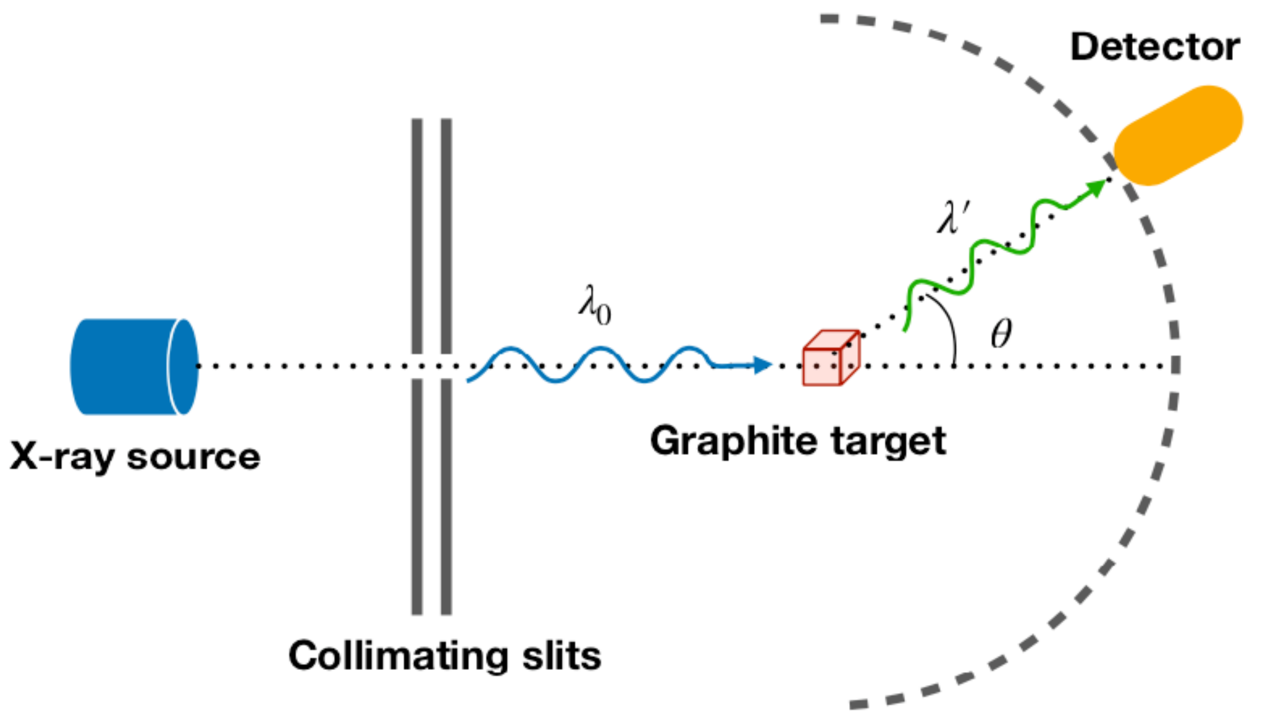




Nobel Prize for Physics in 1927

Holly Compton directed EMW (x-rays) at electrons and observed the phenomenon of collision of photons originating from x-rays and electrons. He predicted the shift in wavelength theoretically and measured the shift experimentally. This discovery gave an evidence for the particle nature of light!

Compton Effect: Observations & Results



He found that the incident waves had slightly shorter wavelengths than the waves produced after collision (scattered waves)

Wavelength of the scattered x-ray

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta)$$

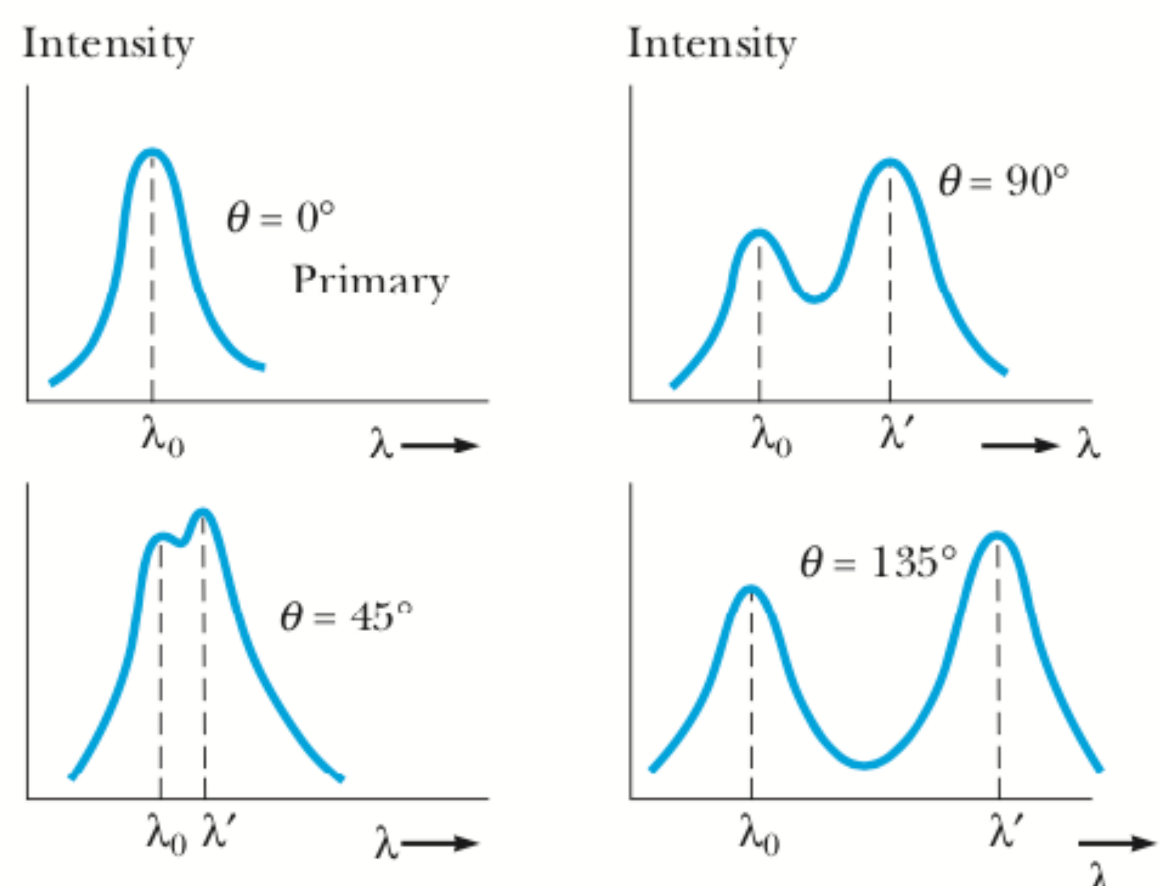
Compton wavelength

$$\lambda_C = \frac{h}{m_e c} = 0.0243\,\text{Å}$$

Case-1: $\theta = 0^\circ$
$\lambda' = \lambda_0$

Case-2: $\theta = 90^\circ$
$\lambda' = \lambda_0 + \lambda_C$

Case-3: $\theta = 180^\circ$
$\lambda' = \lambda_0 + 2\lambda_C$



Compton Effect: Conclusions

What wave theory predicts: (Classical view)

- The wave theory predicts that **no wavelength change should take place**.
- The Incoming EM wave causes the electron to oscillate with the same frequency as the wave.
- Therefore, the oscillating electron should reemit the EM waves with the same frequency (Thomson scattering)

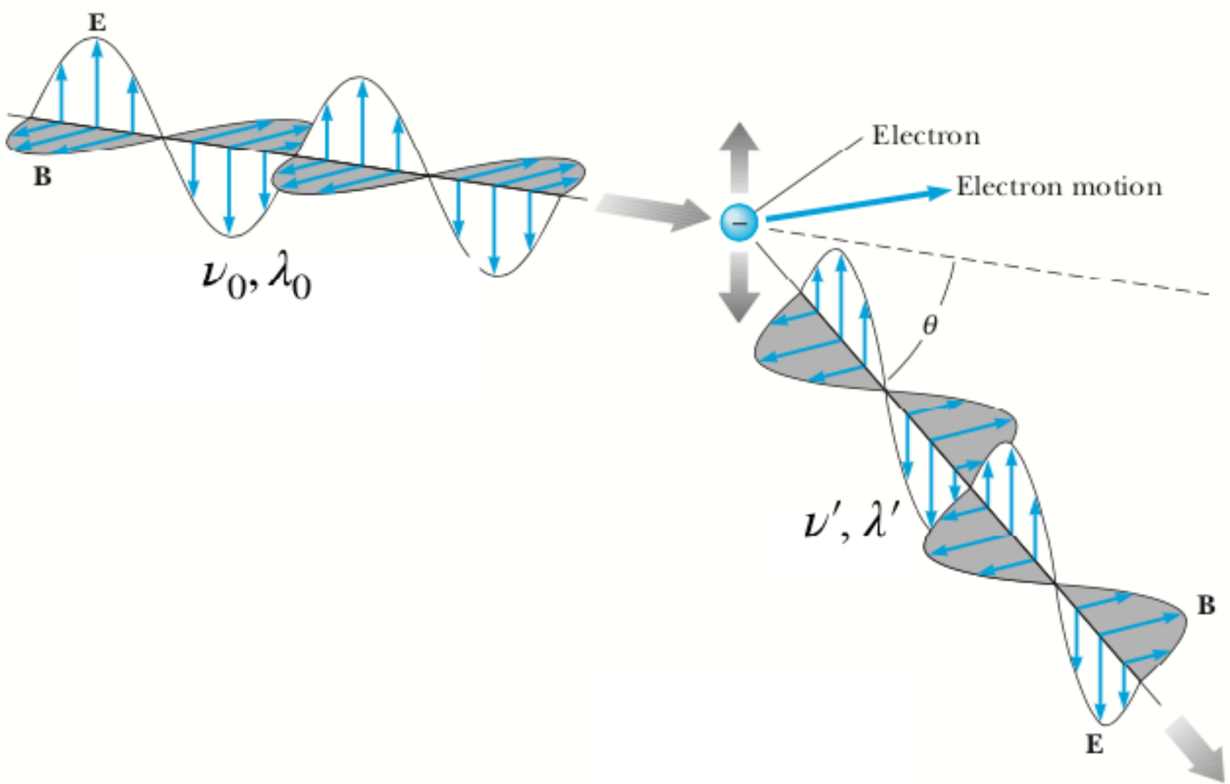
Confirmation of quantum theory:

- Incoming photon collides with the electron and transfers some of the energy to the electron.
- The scattered photons now have less energy than before and so decrease in frequency by Δv and an increase wavelength by $\Delta\lambda$
- This violates classical Thomson scattering
- This transfer of energy during collisions tells about the particle nature of photons

Compton Effect: Conclusions

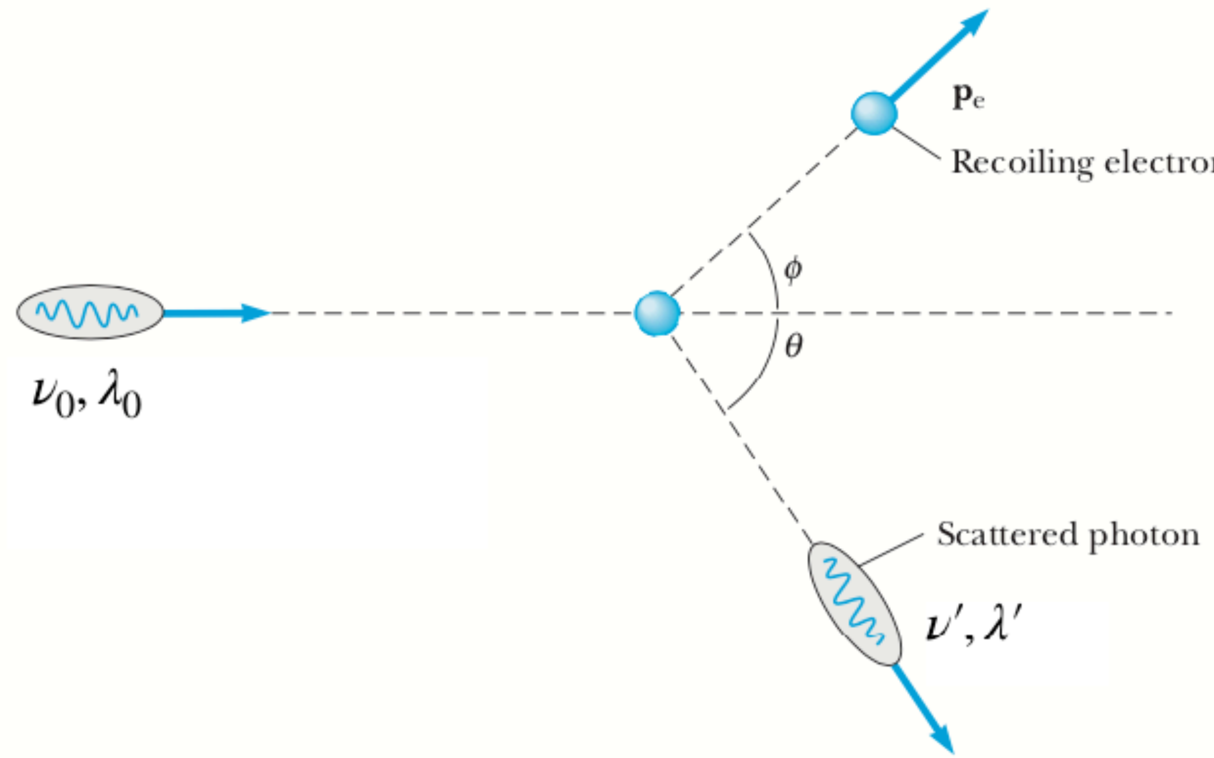
Classical Picture	Quantum Picture

Classical Picture



- Electron should accelerate in the direction of x-ray propagation.
- It should cause forced oscillations of the electron and re-radiation at frequency $\nu' < \nu_0$.
- Frequency of scattered x-ray should depend on incident x ray intensity and exposure length.

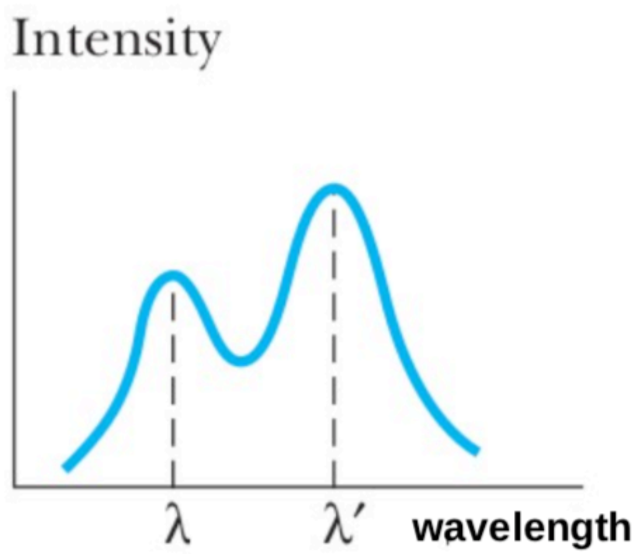
Quantum Picture



- Scattered frequency ν' independent of incident field amplitude and length of exposure. It only depend upon angle θ.
- Photon as massless **particle** collides with electron, imparting momentum to it, and thus scatters with lower frequency $\nu' < \nu_0$.

Compton Effect: Conclusions

The unshifted peak at λ is caused by **x-rays scattered from electrons tightly bound to carbon atoms**. This unshifted peak is actually predicted by Compton shift equation the electron mass is replaced by the mass of a carbon atom, which is about 23,000 times the mass of an electron.



These observations gives an **evidence for the particle nature of light!**

Dual nature of light!

Wavelength of the scattered x-ray

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta)$$

Compton wavelength

$$\lambda_C = \frac{h}{m_e c} = 0.0243\text{Å}$$

Possible Questions

1. What is Compton effect? At what condition the Compton wavelength shift can be maximum? Plot the Compton spectra for three different scattering angles.

Possible Questions

X-rays of wavelength $\lambda = 0.2\ nm$ are aimed at a block of carbon. The scattered x-rays are observed at an angle of $\theta = 45^o$ to the incident beam. Calculate (i) the increased wavelength of the scattered x-rays at this angle (ii) the kinetic energy imparted to the recoiling electron.

Wavelength of incident x-ray $\lambda = 0.2\ nm$

Angle $\theta = 45^o$

Planck's constant $h = 6.63 \times 10^{-34}\ J\ s$

Mass of electron $m_e = 9.1 \times 10^{-31}\ kg$

Velocity of light $c = 3 \times 10^8\ m\ s^{-1}$

Compton shift $$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta) = \frac{6.63 \times 10^{-34}}{(9.1 \times 10^{-31})(3 \times 10^8)}(1 - \cos 45) \approx 0.711 \times 10^{-12}\ m$$

(i) Wavelength of scattered x-ray $$\lambda' = \lambda + \frac{h}{m_e c}(1 - \cos\theta)$$

$$= 0.2 \times 10^{-9} + 0.711 \times 10^{-12}$$

$$= 0.2007 \times 10^{-9}\ \text{m} = 0.2007\ \text{nm}$$

Information so far in QM

From the electromagnetic theory (till 1905) we know light are the EM wave (interference, diffraction etc)

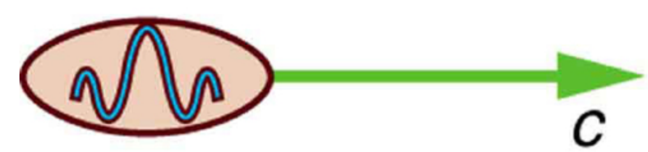
After 1905, In QM, a few examples change the concept and show that the light (EM wave) behaves like a particle:

- Photoelectric effect and Blackbody radiation show that light can be interpreted as a bunch of massless-energy-bundles called **photons**.
- Then, Compton scattering established that these photons in fact are particles.

Information so far in QM

Wave	**Particle**
Laser grating	**Photo electric effect**
Newton's rings	**Compton effect**
Maxwell's equation	**Black body radiation**

Wave



Particle

Light acts like both particle and wave!

de Broglie Hypothesis

in 1924, de Broglie's hypothesis stated that for any moving particle/ object is associated with wave properties. These waves are known as matter waves

Nobel Prize for Physics in 1929

If an object having momentum p, then, the wavelength (λ) of the matter wave associated with that object is given as:

wavelength
(wave property)

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

Momentum
(particle property)

$h = 6.623 \times 10^{-34}$ **Js**

(Planck's constant)

de Broglie Hypothesis

Calculate the De Broglie wavelength of the (a) electron moving at 2×10^6 m/s and a cricket ball of mass 200gm moving at 20 m/s. Which of this entity particle behaves more like a wave and which of the entity behaves more like a particle?

$$\lambda_B = \frac{h}{p} = \frac{h}{mv}$$

Electron

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

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

$$\lambda = \frac{6.63\times10^{-34}}{9.1\times10^{-32}\times2\times10^{6}}$$

$$\lambda = 3.64\times10^{-10}m$$

$$\lambda = 3.64A^{o}$$

Cricket ball

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

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

$$\lambda = \frac{6.63\times10^{-34}}{200\times10^{-3}\times20}$$

$$\lambda = 1.6575\times10^{-10}m$$

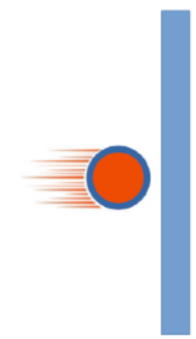
$$\lambda = 1.6575\times10^{-34}m$$

de-Broglie's relationship is not significant to the macroscopic objects

de Broglie Waves in other Parameter

If a charged particle of charge, **q** and mass **m** is accelerated with a potential difference (applied voltage), **V**, then the de Broglie's wave associated with the charge particle is :

Initial Scenario
Potential energy= qV
Kinetic energy = 0



Final Scenario
Potential energy= 0
Kinetic energy = qV

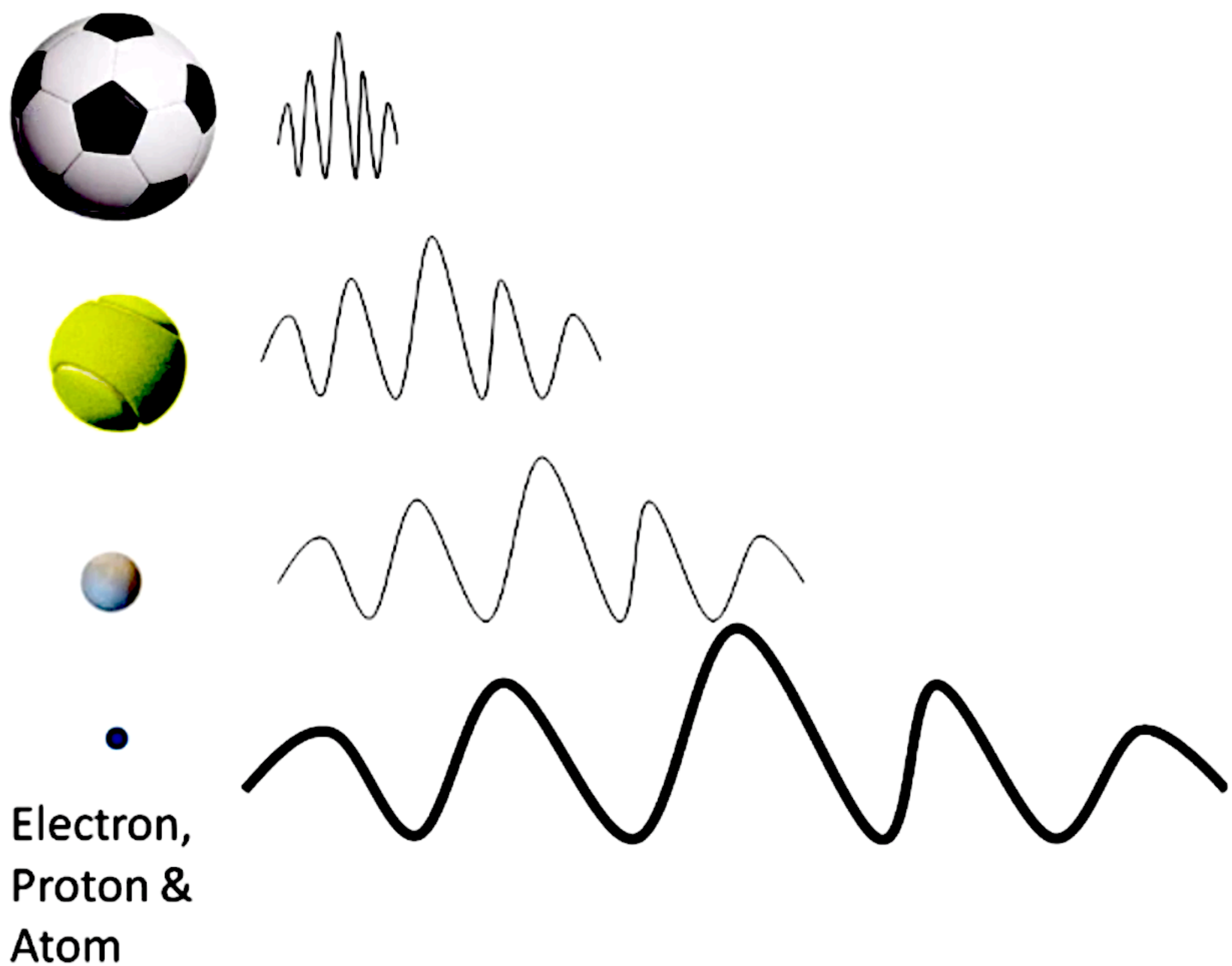
we know that, if the charge particle is accelerated, then the electrostatic work done on the charge parcel is converted into its kinetic energy:

$$\frac{1}{2}mv^2 = \frac{p^2}{2m} = qV = E \quad \Rightarrow \quad \lambda_B = \frac{h}{\sqrt{2mqV}}$$

$$p = \sqrt{2mqV}$$

de Broglie Hypothesis

$$\lambda_B = \frac{h}{p} = \frac{h}{mv}$$



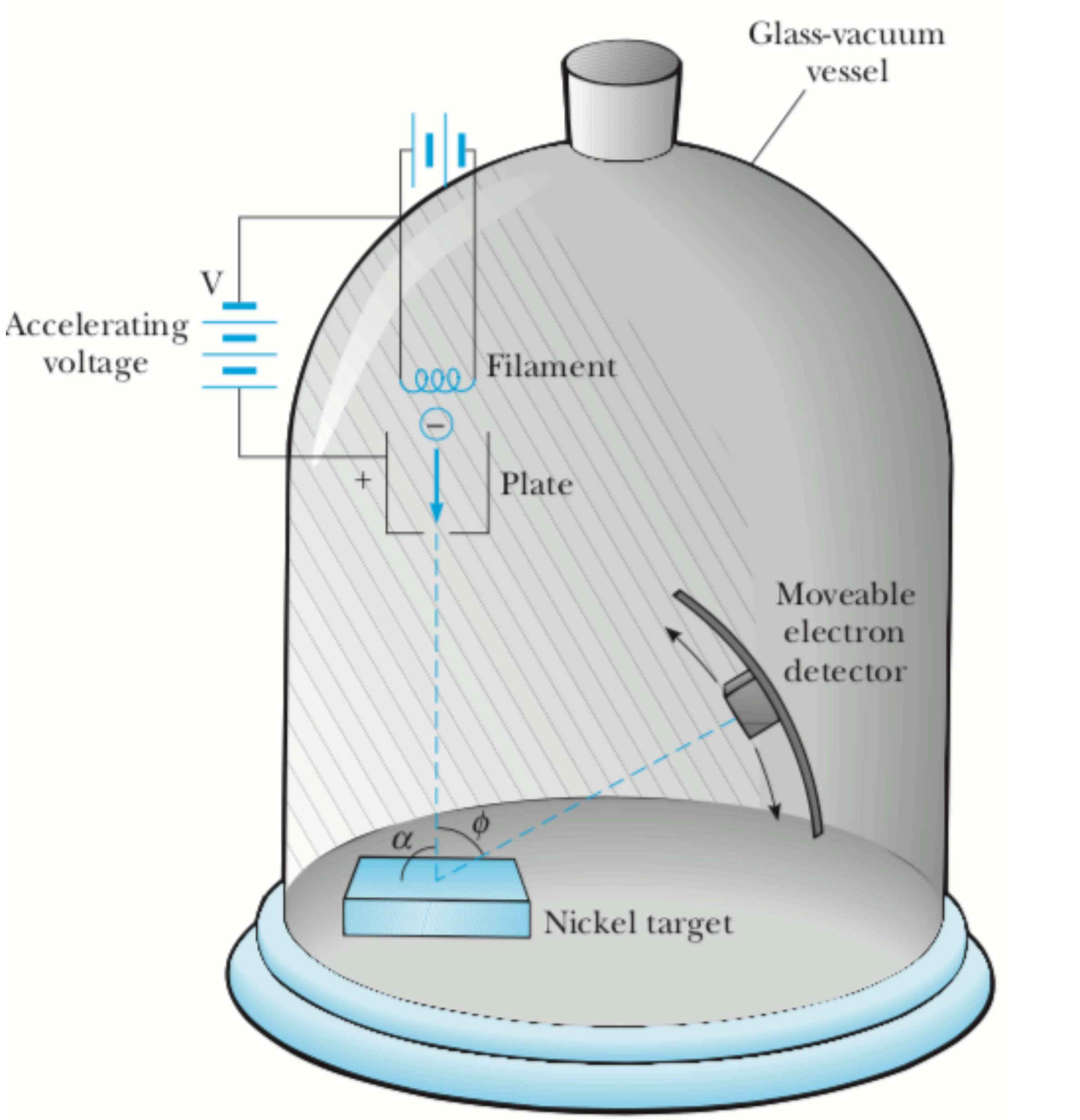
de-Broglie's relationship is not significant to the macroscopic objects

Davisson-Germer Experiment (Proof of Matter Wave)

The Davisson–Germer experiment gives the first-ever evidence for the wave nature of matter. Direct experimental proof that electrons possess a wavelength $\lambda = \dfrac{h}{p}$ was provided by the diffraction experiments of American physicists Clinton J. Davisson and Lester H. Germer at the Bell Laboratories in New York City in 1927

Nobel Prize for Physics in 1937

Davisson-Germer Experiment (Proof of Matter Wave)



Schematic of the Davisson-Germer experiments

Aim of the experiment is to demonstrate the wave nature of electrons.

The **experimental set-up** consists of following parts

(i) evacuated chamber

(ii) a battery connected to filament

(iii) a high tension battery

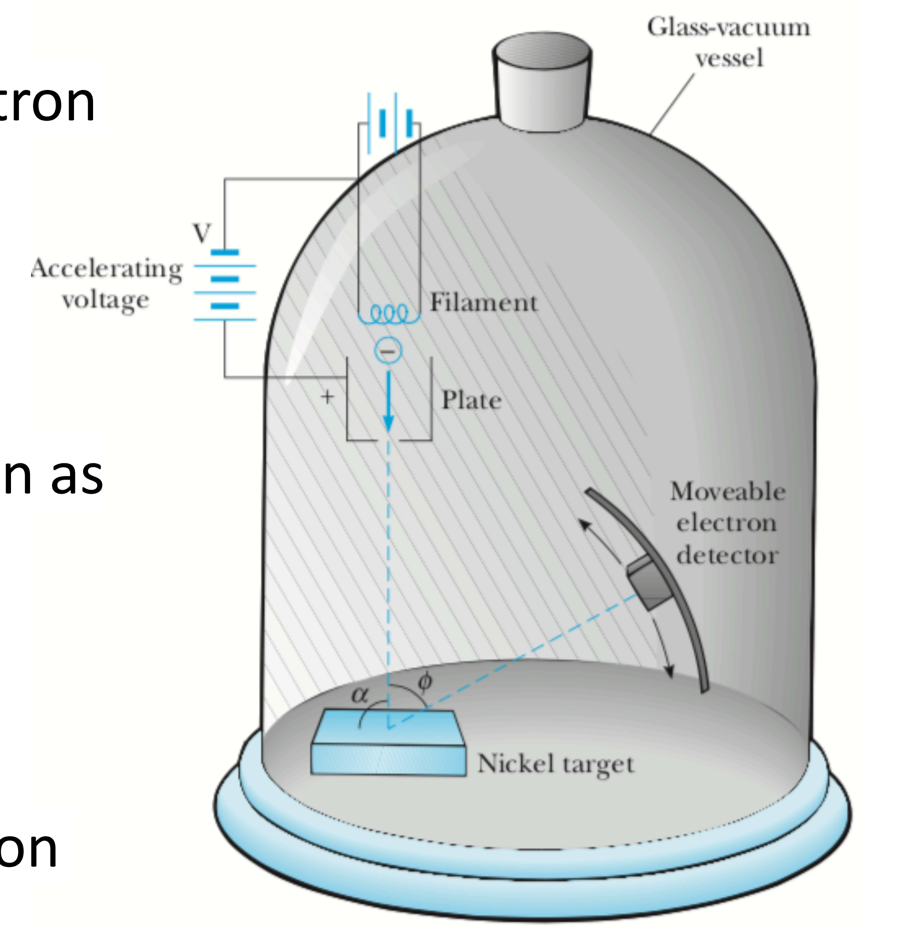
(iv) Nickel target

(v) movable detector

Davisson-Germer Experiment: Procedure

Experiment:

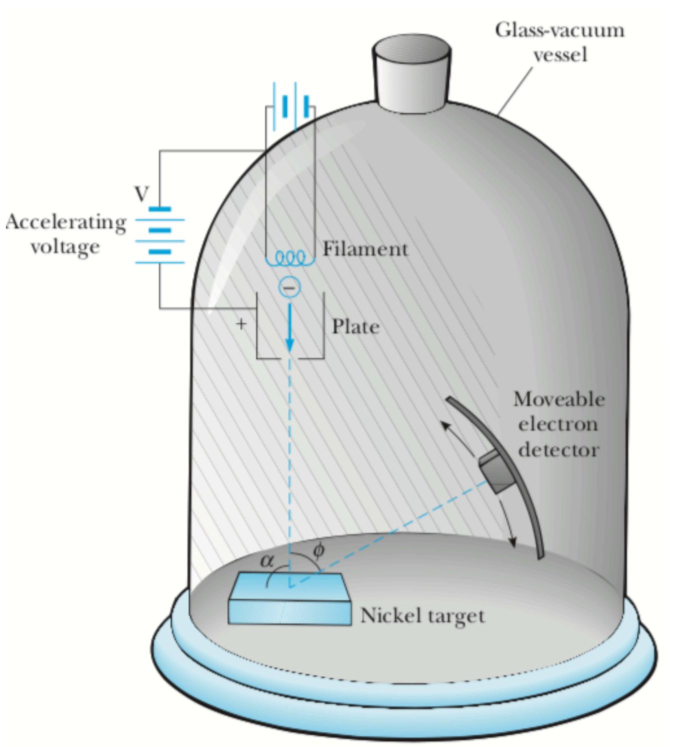
- **Evacuated chamber** is used to avoid any hindrance to the electron motion.
- **A filament connected to battery** heats when the battery is switched on.
- The heated filament starts emitting electron in a process known as "thermionic emission".
- Electrons emitted by the filament are accelerated to get the desired velocity by applying a suitable voltage.
- **A high tension battery** is used to accelerate the emitted electron towards nickel target.
- In the experiment, the **voltage applied was 54 volts.** **Nickel target** is a highly crystalline (single crystal) substance.



Schematic of the Davisson-Germer experiments

- Upon striking the target, electron shows diffraction pattern.The electrons are scattered in all directions from the nickel crystal.
- **Movable detector** is used to measure the intensity of electrons at different angles.
- The intensity of the scattered electron beam is measured for different values of scattered angle, ϕ, and for different voltages

Davisson-Germer Experiment: Results



Schematic of the Davisson-Germer experiments

A beam of **electrons is accelerated through a potential difference V= 54 volts.**

After passing through a small aperture, the **beam strikes a single crystal of nickel.**

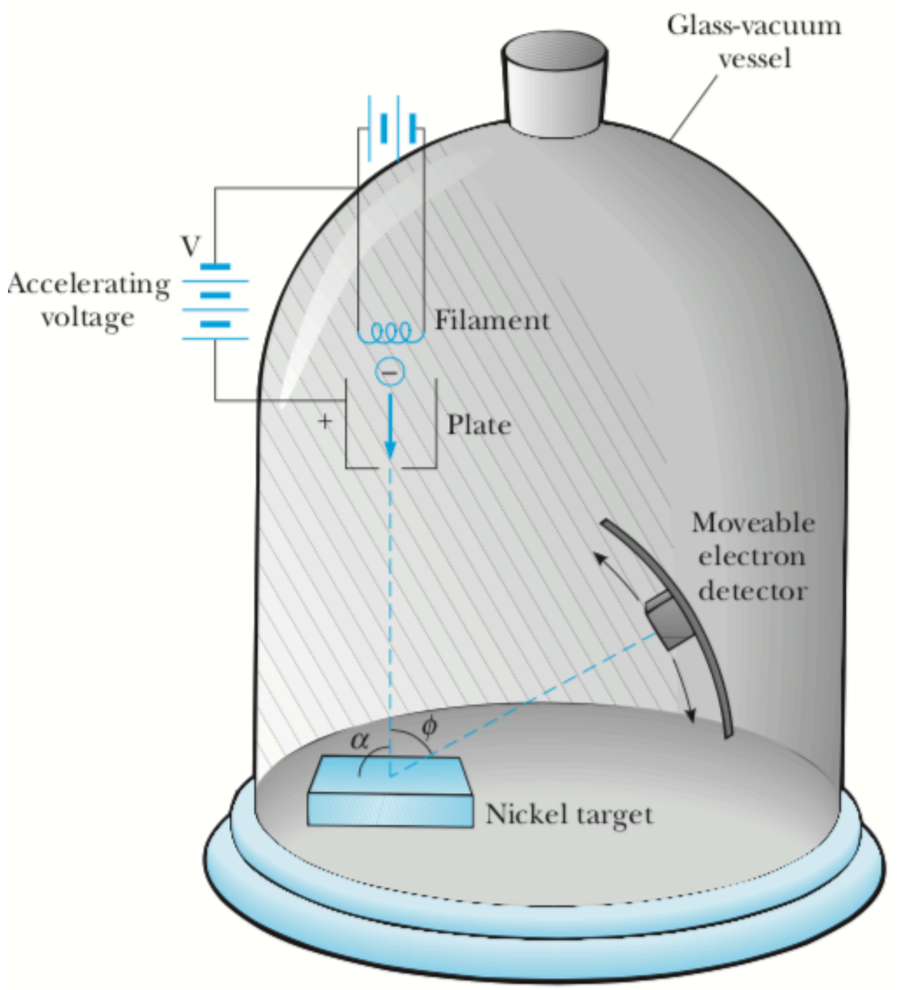
Electrons are scattered in all directions by the atoms of the crystal.

Scattered **electrons were detected by the movable detector.**

When the accelerating voltage is set at 54 V, there is an **intense reflection of the beam at the angle ϕ = 50° .**

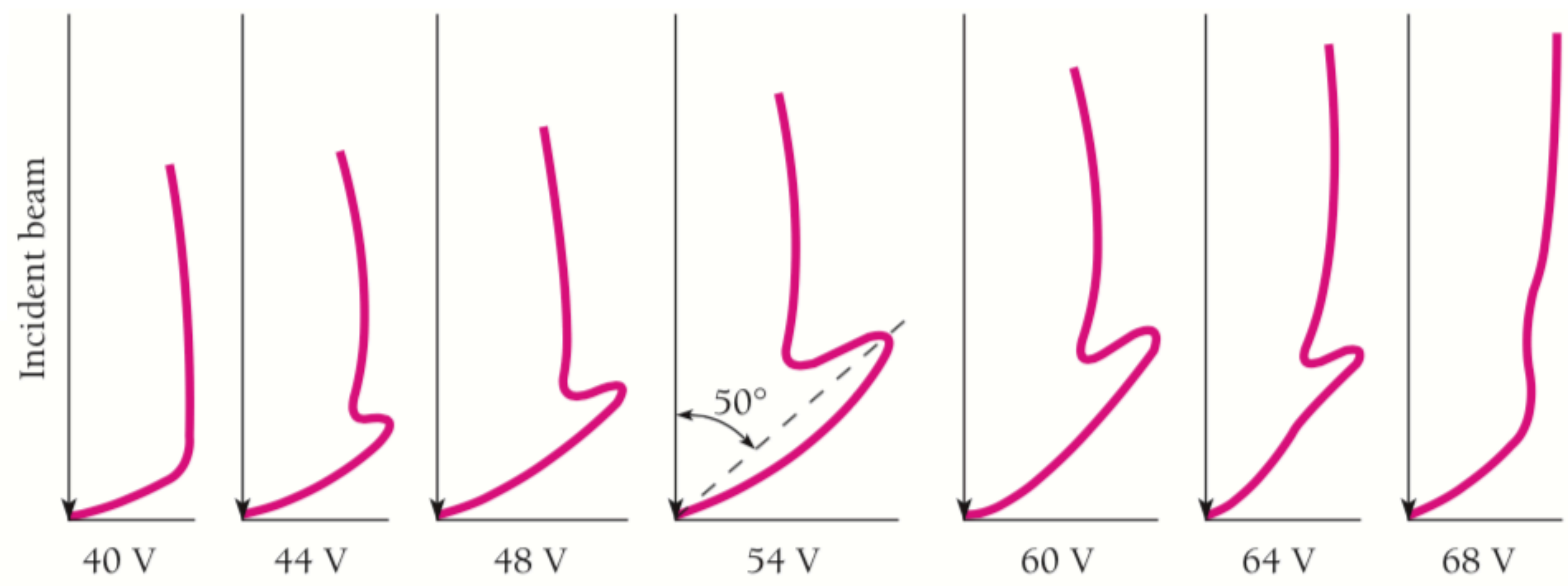
At the angle at maximum intensity, wavelength of electrons can be calculated in two ways: **(i) de Broglie's formula** and **(ii) Bragg's condition for constructive interference**

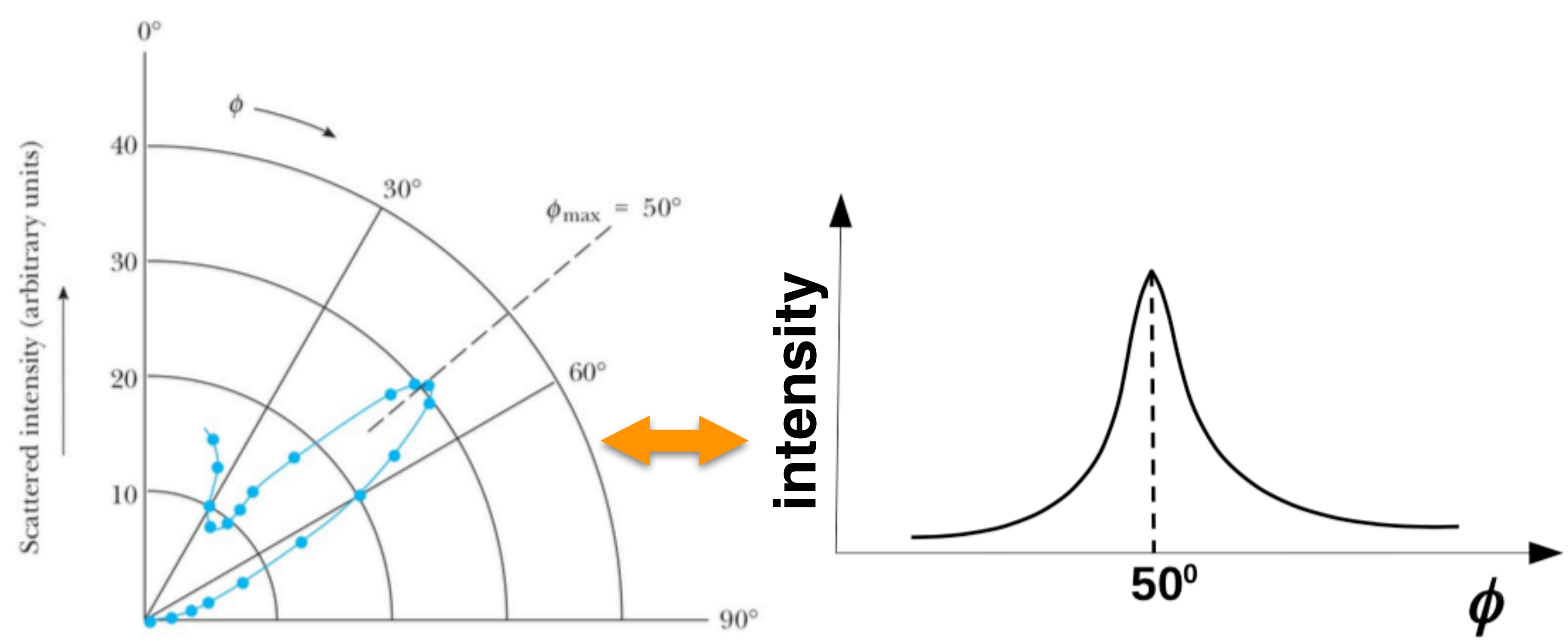
Davisson-Germer Experiment: Results



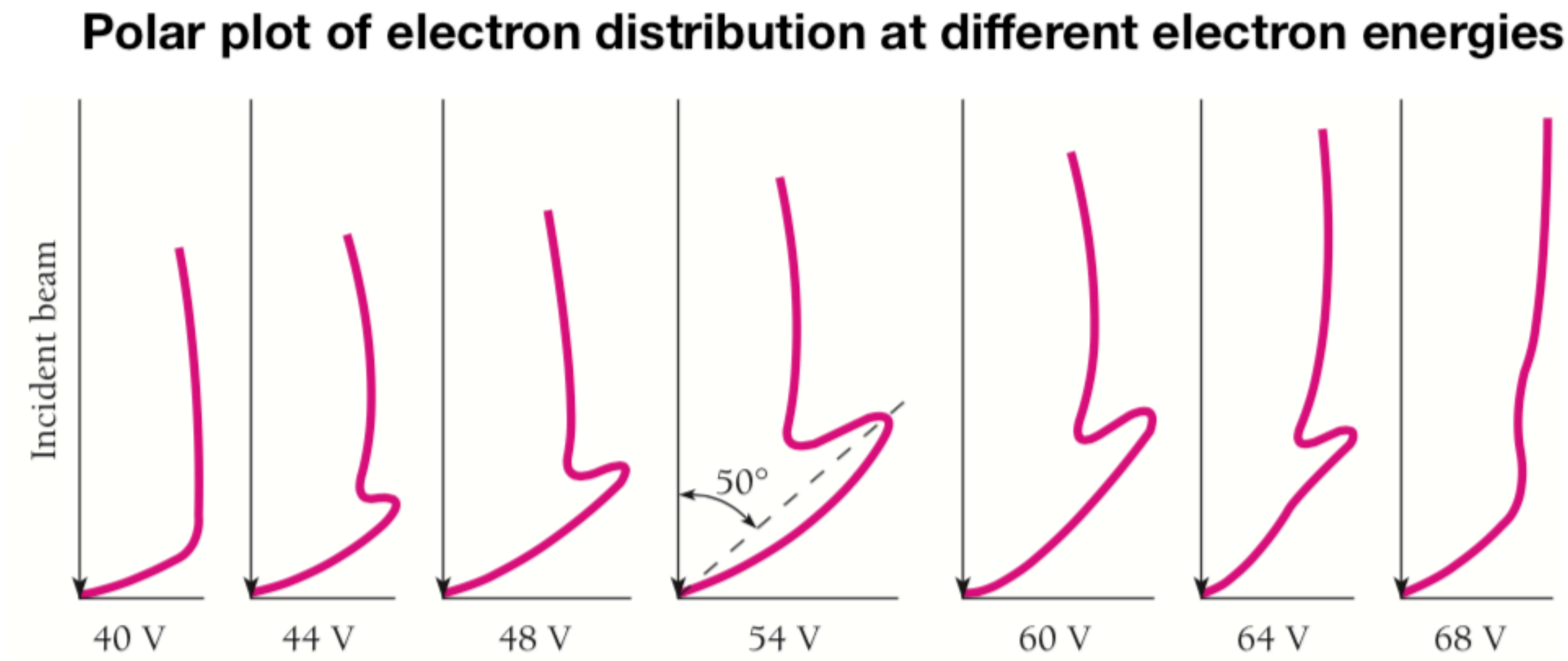
Schematic of the Davisson-Germer experiments

Polar plot of electron distribution at different electron energies





Davisson-Germer Experiment: Results



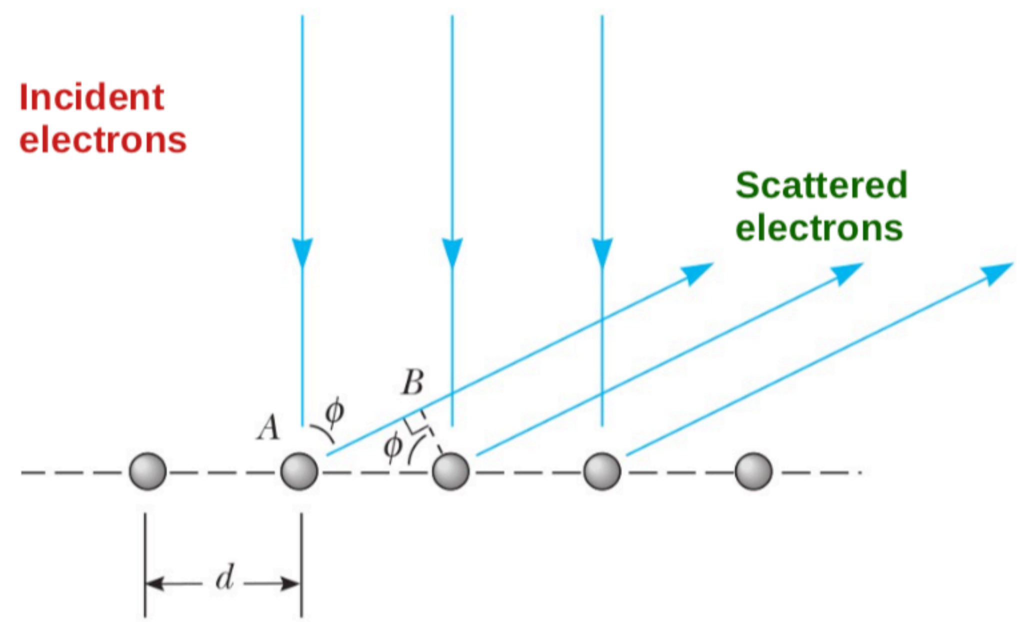
From these experimental curves, the following inferences can be drawn :

- The intensity of scattered electrons depends upon the angle of scattering φ.
- Always a 'bump' or a kink occurs in the curve at φ = 50°, the angle which the scattered beam makes with the incident beam.
- The size of the bump goes on increasing as the accelerating voltage is increased.
- The size of the bump becomes maximum when the accelerating voltage is 54 volts.
- The size of the bump starts decreasing with a further increase in the accelerating voltage.

Davisson-Germer Experiment: Results Analysis

What is Bragg's condition?

Because the electrons were of low energy, they did not penetrate very far into the crystal, and it is sufficient to consider the diffraction to take place in the plane of atoms on the surface.



Bragg's condition is the condition for constructive interference:

$$AB = d\sin(\phi) = n\lambda$$

Davisson-Germer Experiment: Results Analysis

For n=1 $\quad d\sin(\phi)=\lambda \quad$ is the condition for constructive interference

For Nickel: d=2.15 A^0 and angle $\phi = 50^0$. Therefore, we expect that the wavelength of incident electron must be:

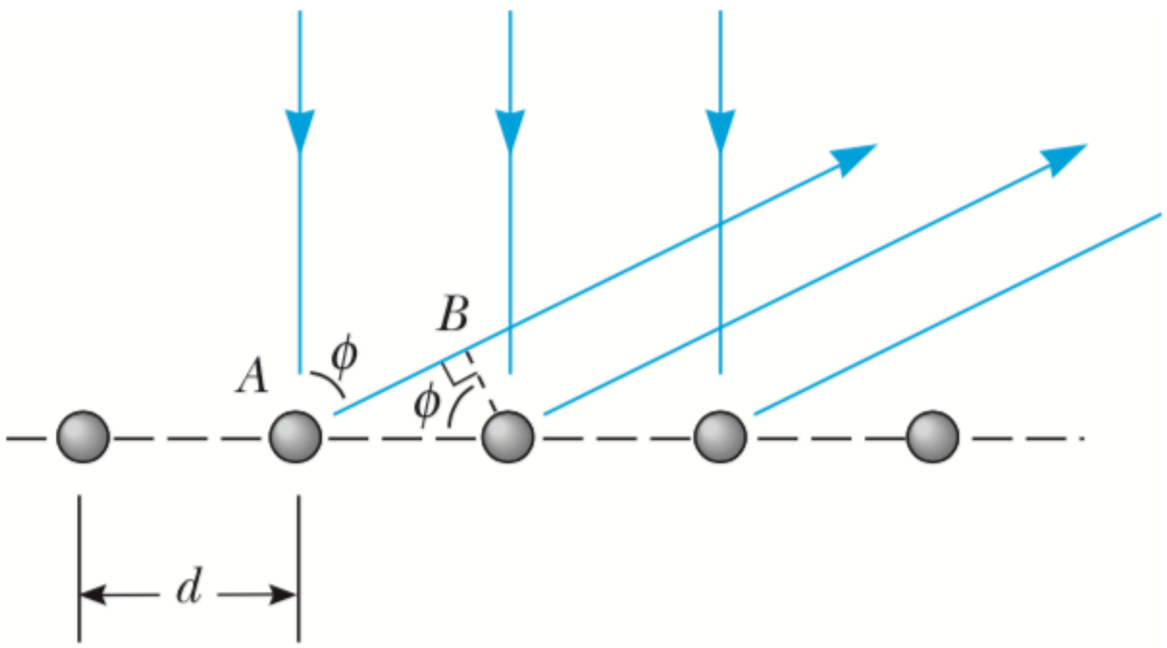
$$\lambda = d\sin(\phi) = 2.15\ \sin(50^0) \approx 1.65\, A^0$$

For electrons, mass m=9.11 x 10^{-31} kg, charge q=1.6 x 10^{-19}C. Potential used by the Devisson and Germer in their experiment is V=54 volts. Therefore, de Broglie Wavelength is:

$$\lambda = \frac{h}{\sqrt{2mqV}} = \frac{6.6\, x\, 10^{-34}}{\sqrt{2\, x\, 9.11\, x\, 10^{-31}\, x\, 1.6\, x\, 10^{-19}\, x\, 54}} \approx 1.67\ A^o$$

Therefore, electrons must have wave properties.

Davisson-Germer Experiment: Results Analysis



$$AB = d\sin\phi = n\lambda$$

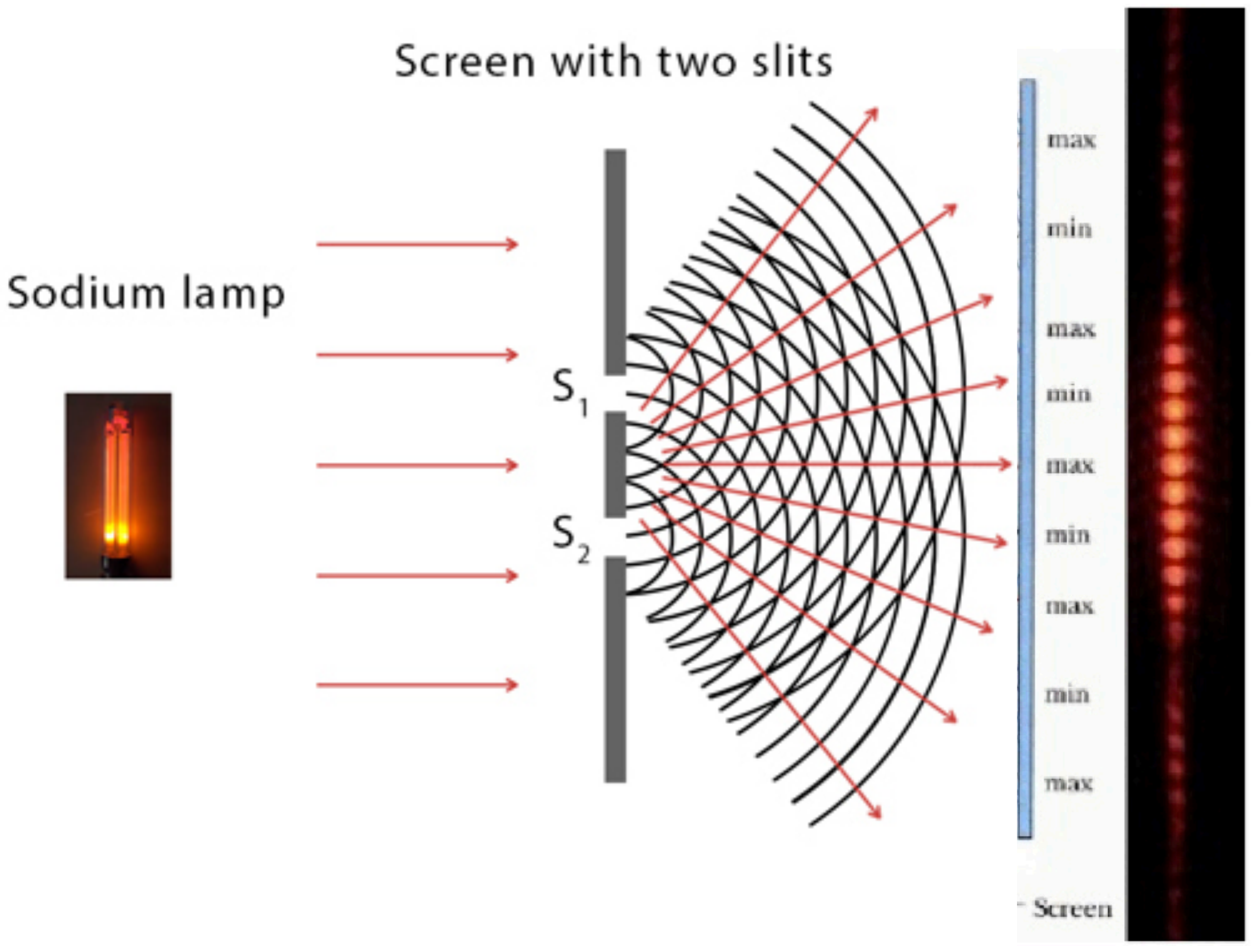
- According to classical physics, there should be very little variation in the intensity of the electron beam with the angle of scattering voltages
- The appearance of the bump in a particular direction is due to constructive interference of electrons scattered from different layers of regularly spaced atoms of the Nickel crystal.
- This establishes the wave nature of electron.
- The selective reflection of the 54-volt electrons at an angle of 50° between the incident and the scattered beam can be termed the diffraction of electrons from the regularly spaced electrons of nickel crystal by virtue of their wave nature.

$$\lambda_B = \frac{h}{\sqrt{2m_e eV}}$$

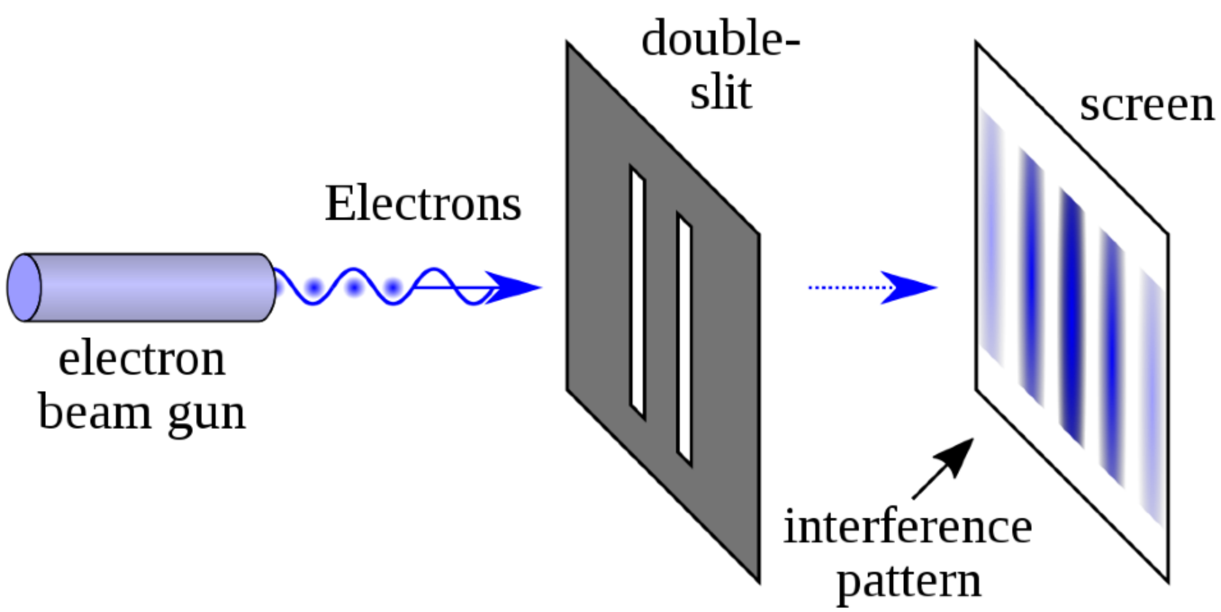
$$\lambda_{Experiment} = \lambda_{DeBroglie} = \frac{h}{\sqrt{2m_e eV}} = 0.165nm$$

Wave Nature of Electron by Double Slit Experiment

Wave



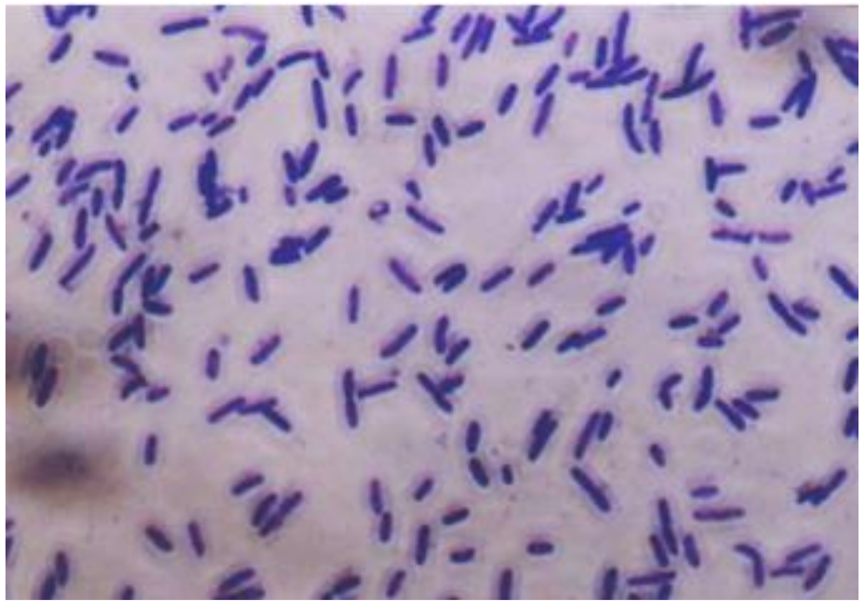
Particle



Wave Nature of Electron: Invention of Electron Microscope

With a visible light microscope, we are limited to being able to resolve objects which are at least about $\underline{0.5*10^{-6}\ m} = \underline{0.5\ \mu m} = \underline{500\ nm}$ in size.

This is because visible light, with a wavelength of ~500 nm cannot resolve objects whose size is smaller than it's wavelength.



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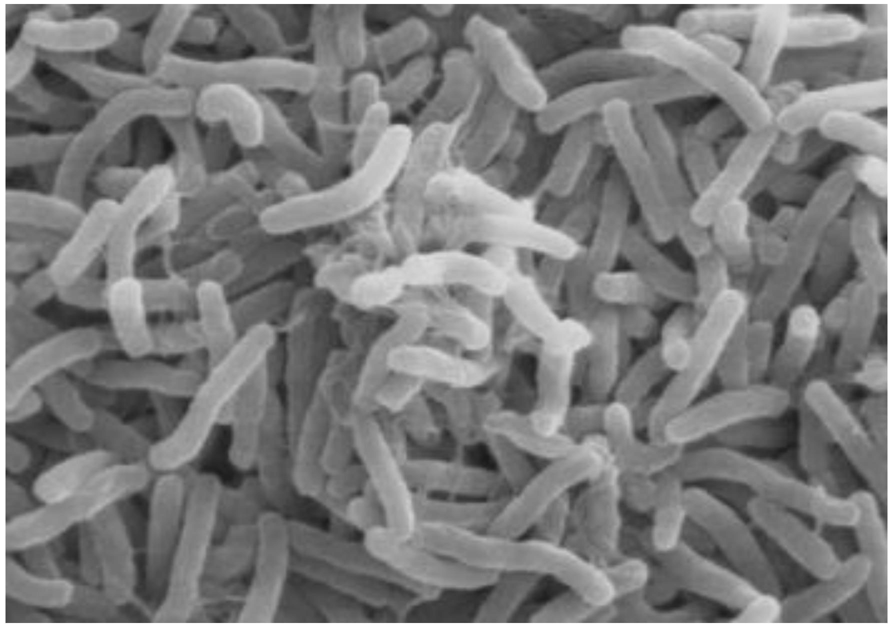
Bacteria, as viewed using visible light



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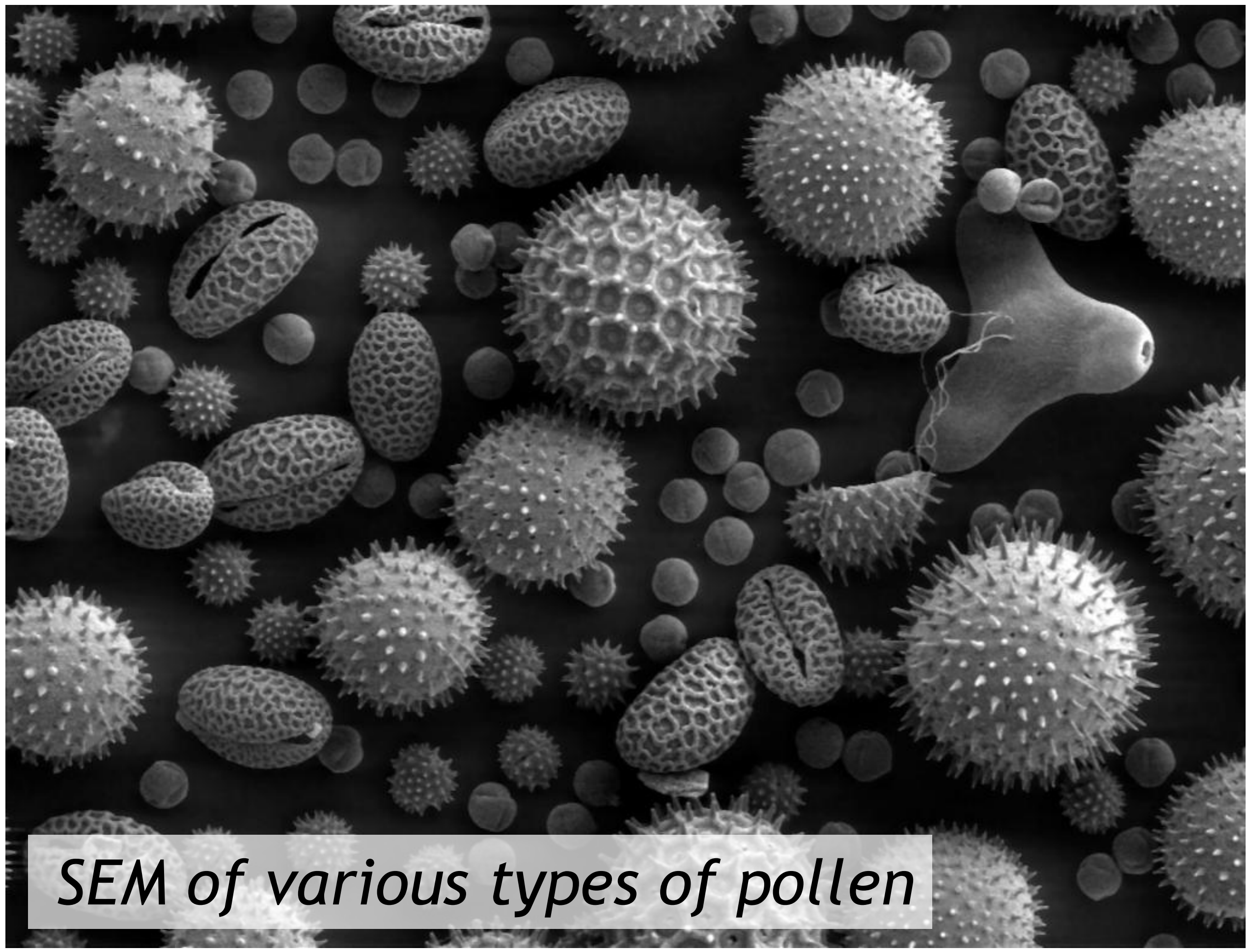
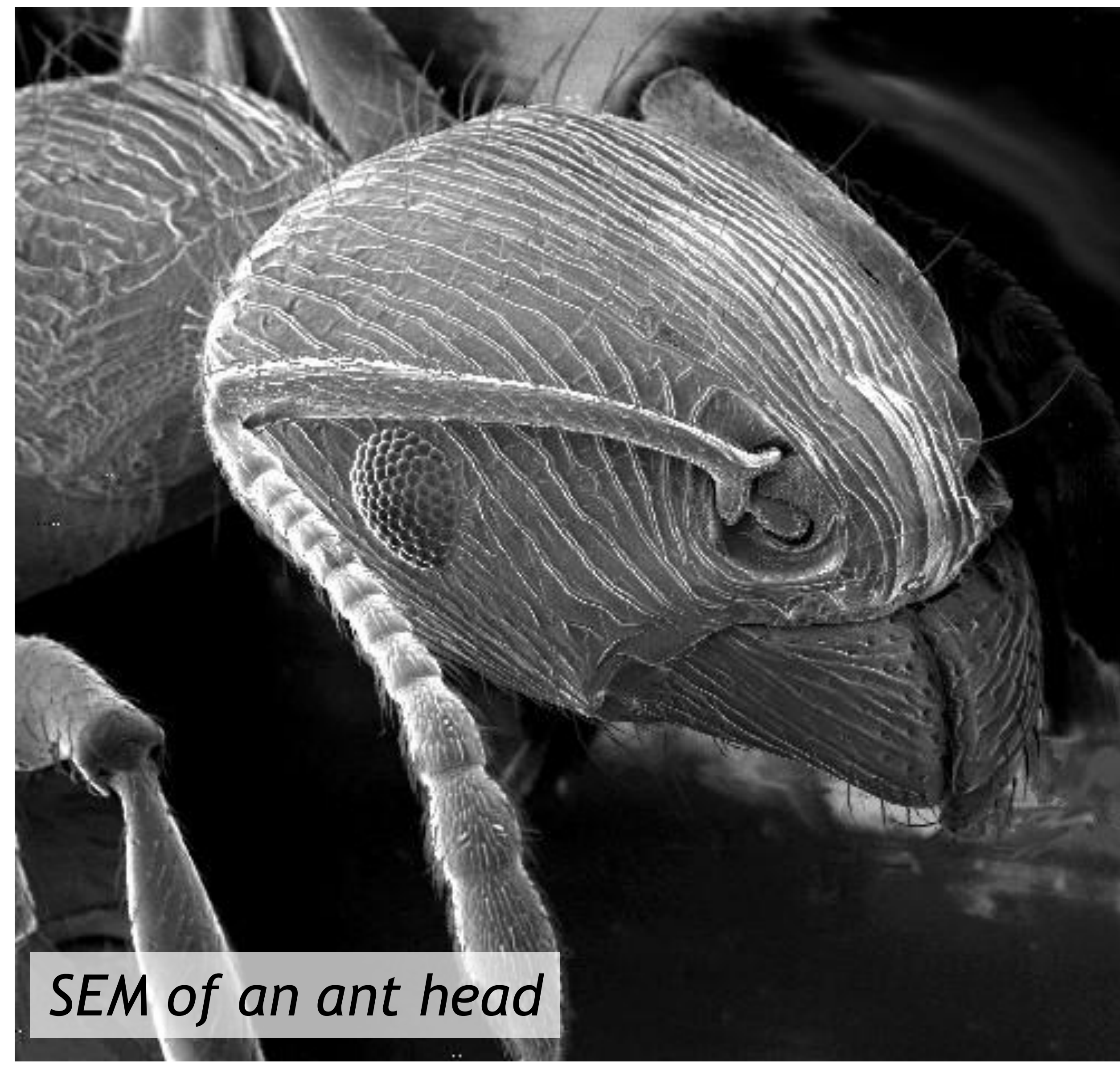
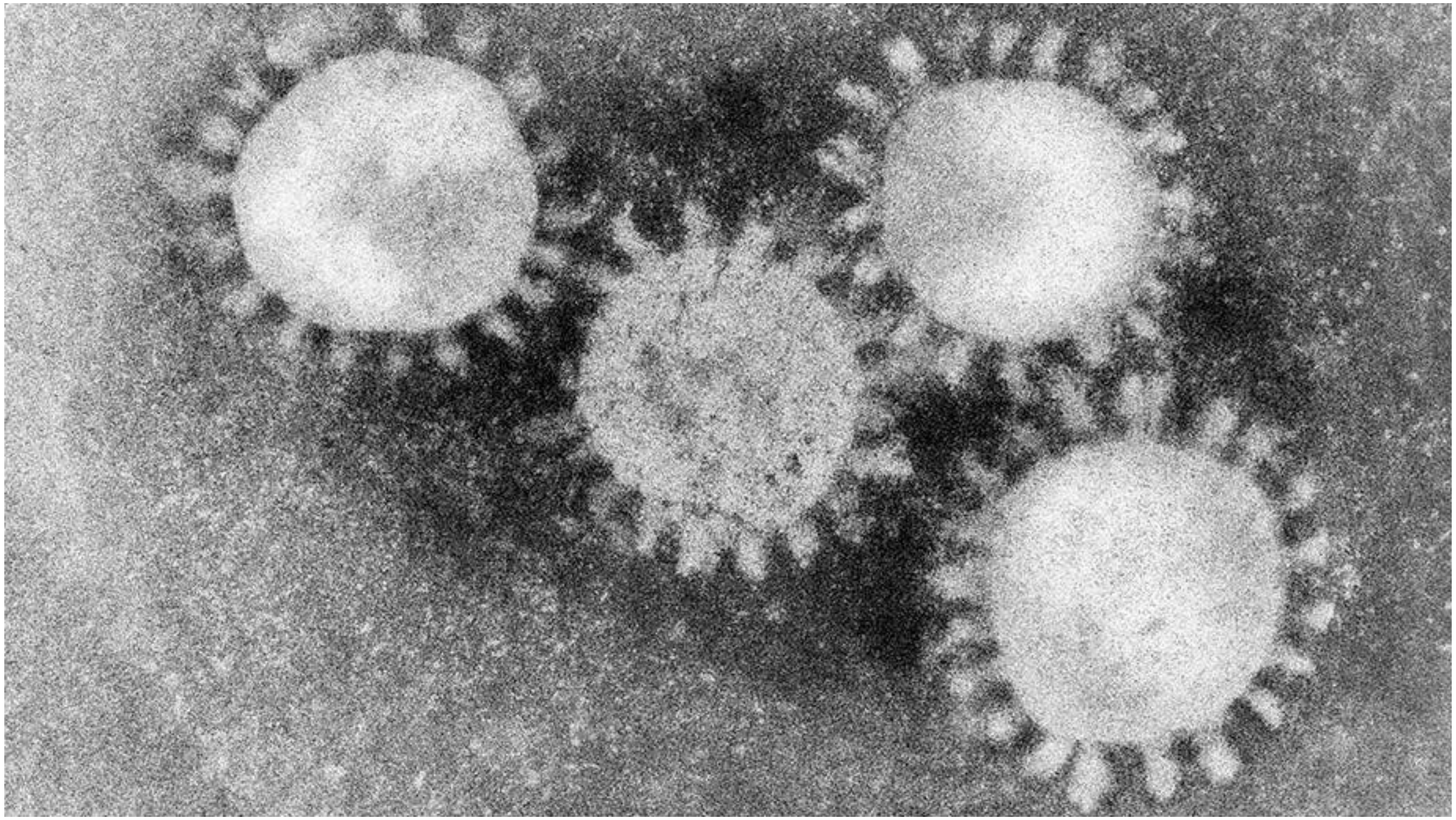
Bacteria, as viewed using electrons!

Wave Nature of Electron: Invention of Electron Microscope

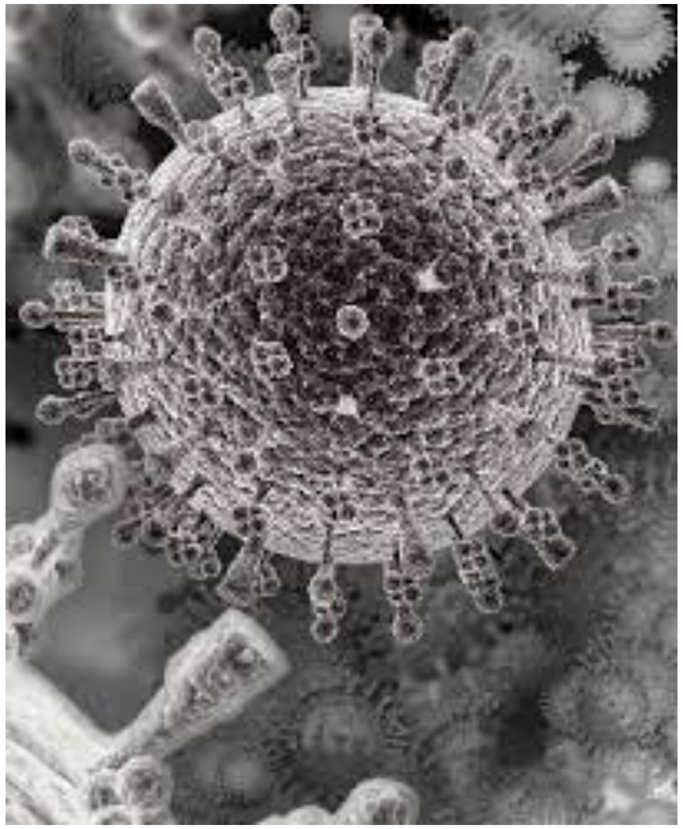




Wave Nature of Electron: Invention of Electron Microscope



Corona Virus-SARS-COVID-19



Possible Questions

1. **What is matter wave and explain how demission-german experiment prove the existence of matter wave**
2. **Briefly describe the experiment which show that the matter wave is exist in nature**
3. **Numerical on De Broglie formula for microscopic and macroscopic object**

So far in Quantum Mechanics

From the electromagnetic theory (till 1905) we know light are the EM wave (interference, diffraction etc)

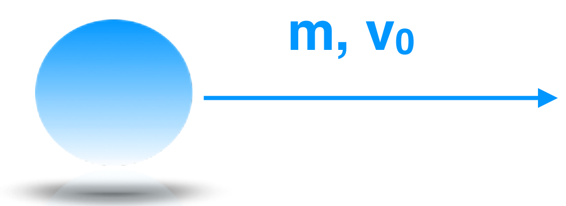
After 1905, In QM, a few examples change the concept and show that the light (EM wave) behaves like a particle:

- Photoelectric effect and Blackbody radiation show that light can be interpreted as a bunch of massless-energy-bundles called **photons.**
- Then, Compton scattering established that these photons in fact are particles.
- De Broglie's hypothesis stated that matter too will have both the particle and wave nature, $\lambda = \frac{h}{p}$ (every moving particle – microscopic or macroscopic –has its own wavelength).
- Davisson-Germer experiment proved the wave nature of matter by diffracting electrons through a crystal

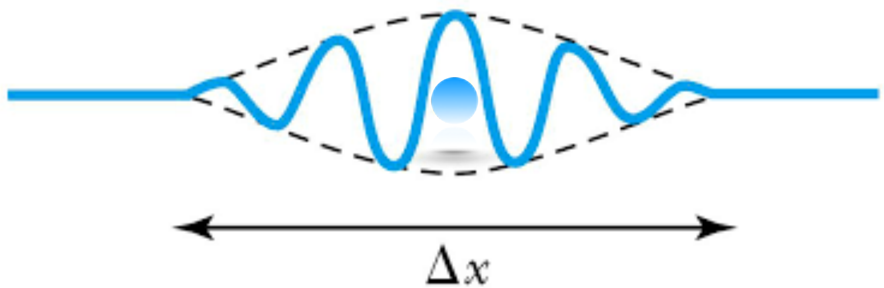
Uncertainty for Position for a Matter Wave

According to De Broglie, for matter wave of definite momentum, the wavelength can be defined as:

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



Classical particle



Quantum particle as wave packet

Heisenberg Uncertainty Principle

If a measurement of position is made with precision Δx and a simultaneous measurement of momentum in the x direction is made with precision Δp, then the product of the two uncertainties can never be smaller than $\frac{h}{4\pi}$. That is,

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

It asserts that the **position and momentum of a particle cannot be simultaneously measured with arbitrarily high precision**

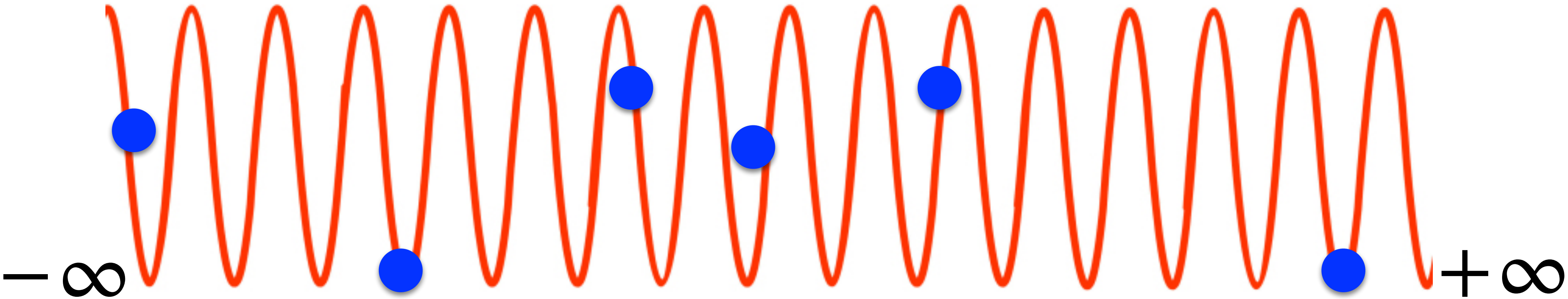
or

It is impossible to determine simultaneously with unlimited precision the position and momentum of a particle

Heisenberg Realised that…

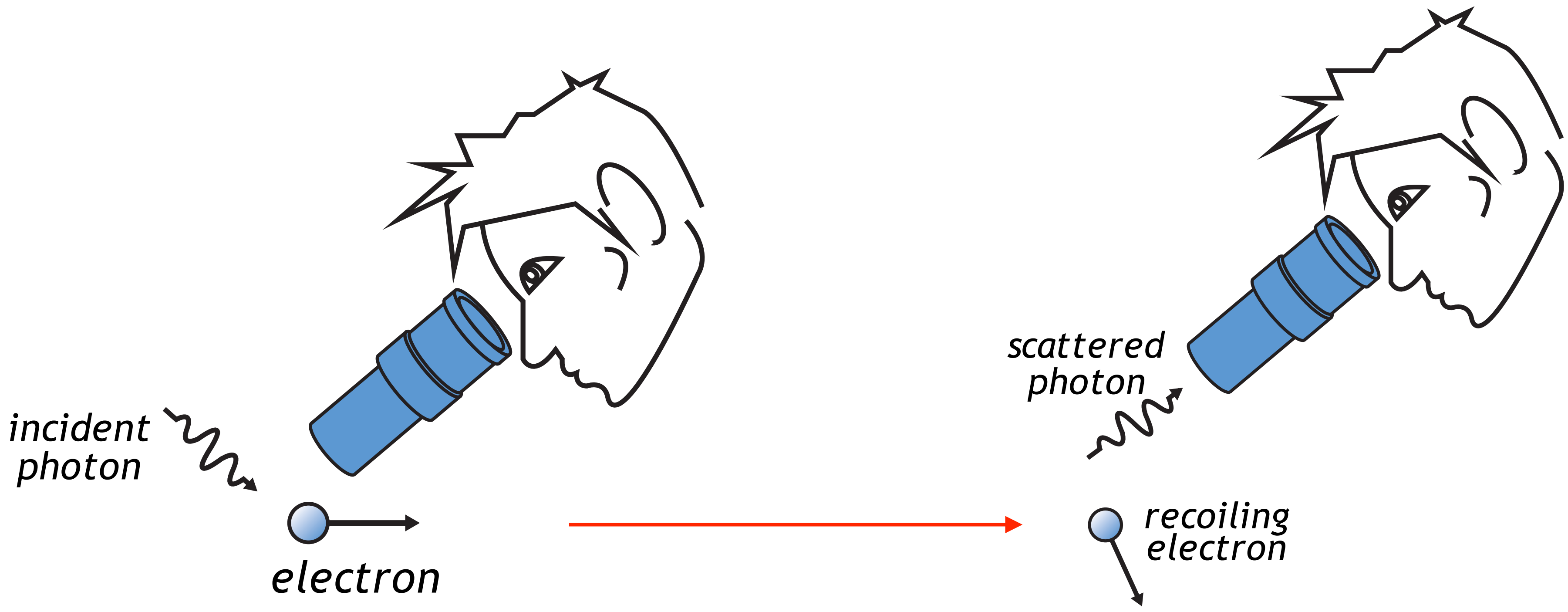
According to De Broglie, for matter wave of definite momentum, the wavelength can be defined as:

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



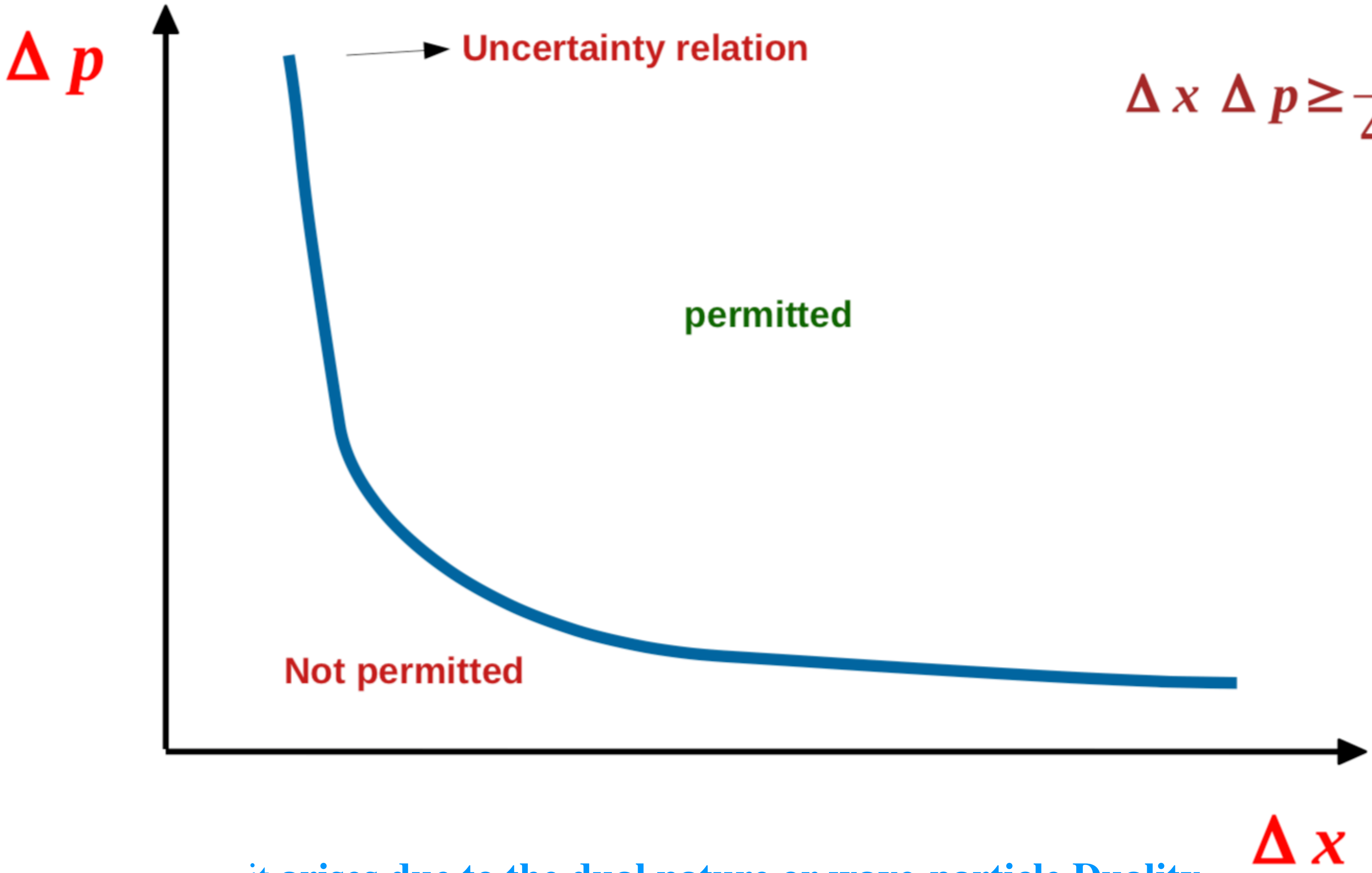
A pure **wave has a well defined momentum**, but not the position. **A pure particle has a well defined position** but not momentum

Position-Momentum of an electron Measurement



- ➡ A photon with a short wavelength has a large energy
- ➡ Thus, it would impart a large 'kick' to the electron
- ➡ But to determine its momentum accurately, electron must only be given a small kick
- ➡ This means using light of long wavelength !

Heisenberg Uncertainty Principle



$$\Delta x \, \Delta p \geq \frac{h}{4\pi}$$

it arises due to the dual nature or wave-particle Duality

Heisenberg Uncertainty Principle: Examples

Cricket ball
Macroscopic Object

- A pitcher throws a 0.1-kg baseball at 40 m/s
- So momentum is 0.1 x 40 = 4 kg m/s
- Suppose the momentum is measured to an accuracy of 1 %, i.e.,

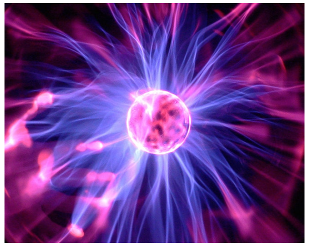
$$\Delta p = 0.01\, p = 4 \times 10^{-2} \text{ kg m/s}$$

- The uncertainty in position is then

$$\Delta x \geq \frac{h}{4\pi \Delta p} = 1.3 \times 10^{-33} \mathrm{m}$$

- No wonder one does not observe the effects of the uncertainty principle in everyday life!

Heisenberg Uncertainty Principle: Examples



Electron (microscopic object)

Same situation, but baseball replaced by an electron which has mass 9.11×10^{-31} kg traveling at 40 m/s

So momentum = 3.6×10^{-29} kg m/s
and its uncertainty = 3.6×10^{-31} kg m/s

$\Delta p = 0.01\,p = 4 \times 10^{-2}$ kg m/s

The uncertainty in position is then

$$\Delta x \geq \frac{h}{4\pi\Delta p} = 1.4 \times 10^{-4}\mathrm{m}$$

Numericals: Heisenberg Uncertainty Principle

Consider a 100-g tennis ball confined to a room 15 m on a side. Assume the ball is moving at 10.0 m/s along the x axis. Compute the uncertainty in velocity.

Mass of the tennis ball $m = 100\,g = 0.1\,kg$

Maximum uncertainty in position $\Delta x = 15\,m$

Uncertainty in momentum $\Delta p = m \Delta v$

$$\Delta v \geq \frac{h}{4\pi m \Delta x} = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 0.1 \times 15} \approx 0.35 \times 10^{-34}\ ms^{-1}$$

$$\frac{\Delta v}{v} \geq \frac{0.35 \times 10^{-34}}{10} = 0.35 \times 10^{-35}$$

this is insignificant for practical purposes!

Numericals: Heisenberg Uncertainty Principle

A measurement establishes the position of a proton with an accuracy of 10pm. Find the uncertainty in the proton's velocity. Mass of proton is m=1.67x10^{-27} kg.

Mass of proton $m = 1.67 \times 10^{-27}\, kg$

Maximum uncertainty in the position of proton $\Delta x = 10\, pm = 10^{-11} m$

Uncertainty in momentum $\Delta p = m \Delta v$

$$\Delta v \geq \frac{h}{4\pi m \Delta x} = \frac{6.63 \times 10^{-34}}{4 \times 3.142 \times 1.6 \times 10^{-27} \times 10^{-11}} \approx 3.2 \times 10^{3}\ ms^{-1}$$

This is significant for practical purposes!

Implications

- It is impossible to know *both* the position and momentum exactly, i.e., $\Delta x=0$ and $\Delta p=0$
- These uncertainties are inherent in the physical world and have nothing to do with the skill of the observer
- Because *h* is so small, these uncertainties are not observable in normal everyday situations

$$\Delta x \Delta p \geq \frac{h}{4\pi}$$

Possible Questions

1. Explain Heisenberg uncertainty principle. Why it is insignificant for macroscopic objects?

2. State Heisenberg uncertainty principle. How is it related to wave-particle duality?

Classical …to…Quantum

- In **classical physics, there is no restriction on the measurement on the position and momentum.**
- In fact, we can solve **Newton's equation** of motion and determine the position and momentum accurately at arbitrary time.

- However, **this does not seem to be the case for microscopic particles.**
- Microscopic particles must obey **(i) wave-particle duality and (ii) Heisenberg uncertainty principle.**
- **There is no distinction between wave and particle.**

How to understand the motion of such microscopic particle and determine time evolution of such systems ?

Wavefunctions

Wavefunction

A wavefunction is a mathematical description of the state of a system.

Ψ (x,t), Psi

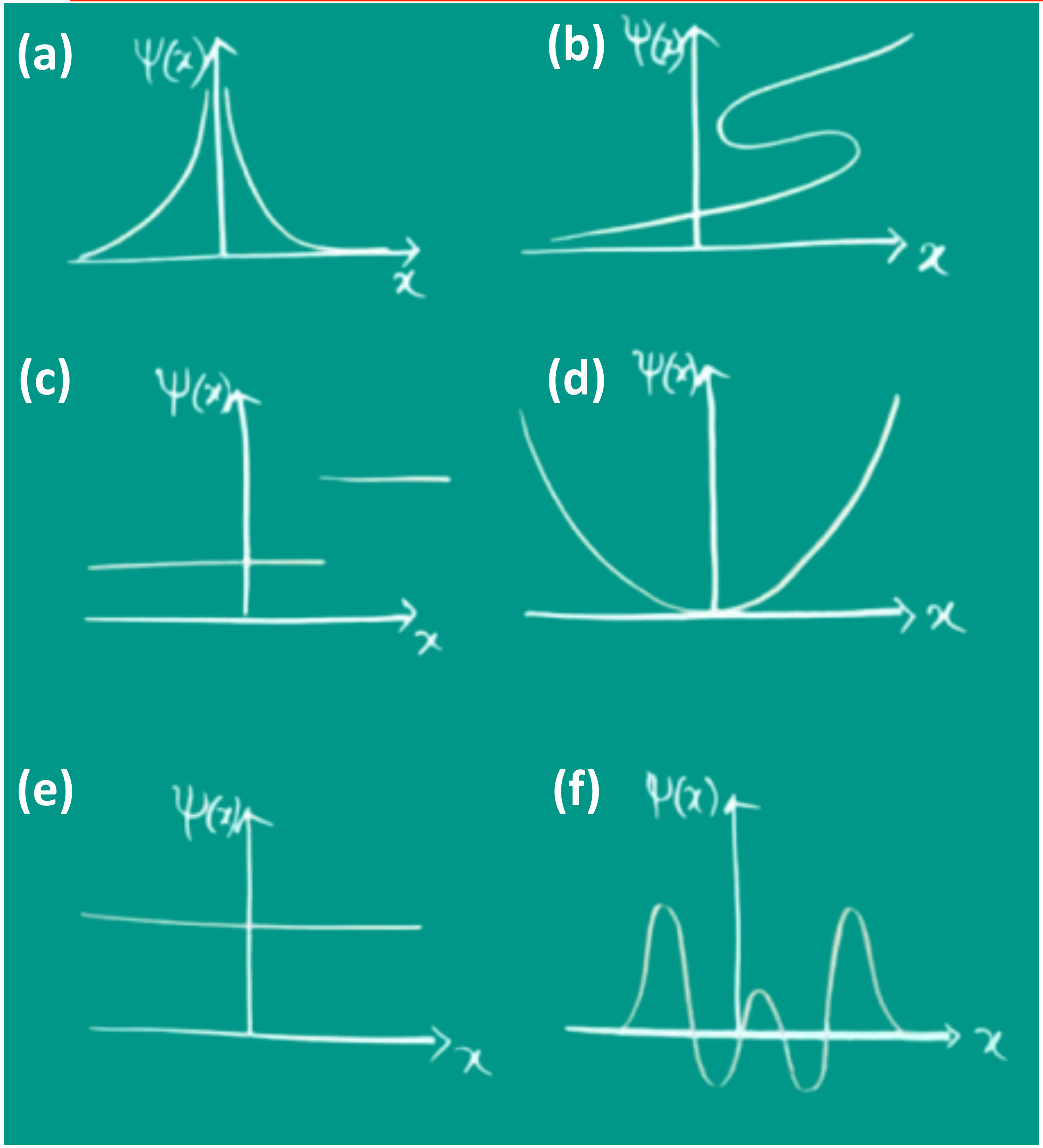
It is generally represented as $\Psi(x, t)$ where x is the position and t is the time

- **Complex Valued Function**
- **Does not have any physical meaning or not associated with any physical quantities**
- **But the square of the wave function, $|\psi|^2$ is real and has physical meaning, it tell us the probability/likelihood of finding the particle in that define region**

Properties of Wave Function

- **A wave function is a mathematical description of the state of a system.**
  - All measurable quantities, such as energy, momentum, position, etc of the system can be deduced from the wave function.
- **It is a complex function**
  - Generally represented as $\psi(x, y, z, t) = A + iB$.
- **Wave function ψ is finite, single-valued , and continuous everywhere.**
- **Its derivatives $\partial\psi/\partial \mathrm{x}$, $\partial\psi/\partial \mathrm{y}$, $\partial\psi/\partial \mathrm{z}$ is also finite, single-valued, and continuous everywhere.**
- **Wavefunction must be Normalizable**
  - $$\int_{-\infty}^{\infty} |\psi|^2 \mathrm{dx} = 1$$
- **It follows the principle of superposition.**
  - $\psi = \psi_1 + \psi_2$ also represent wave function

Well Behaved Wavefunction



(a). NO- Not Finite

(b). NO- Not Single Valued

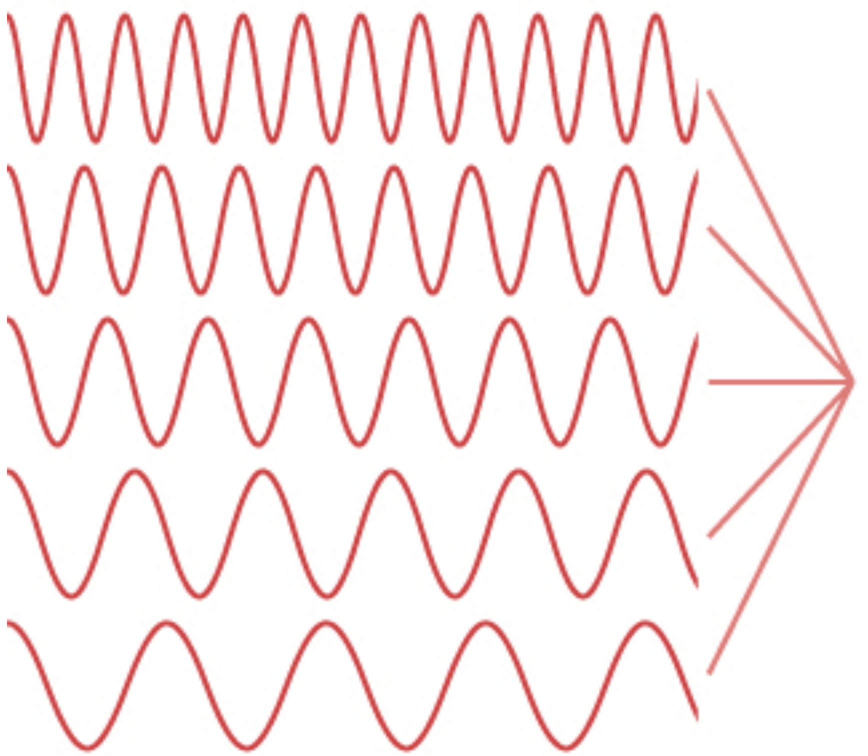
(c). NO- Not Continuous

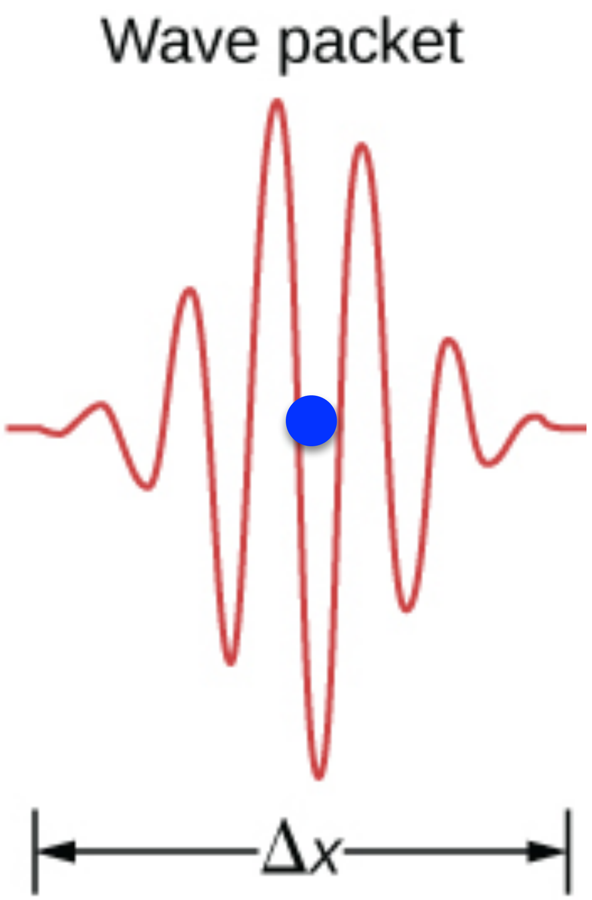
(d). NO- Not Finite

(e). NO- Probability is not Finite

(f). YES- a well behaved wavefunction

Wave - - - Wavefunction





Longer wavelength
Less information about position
Δx is large

Shorter wavelength
More information about position
Δx is small

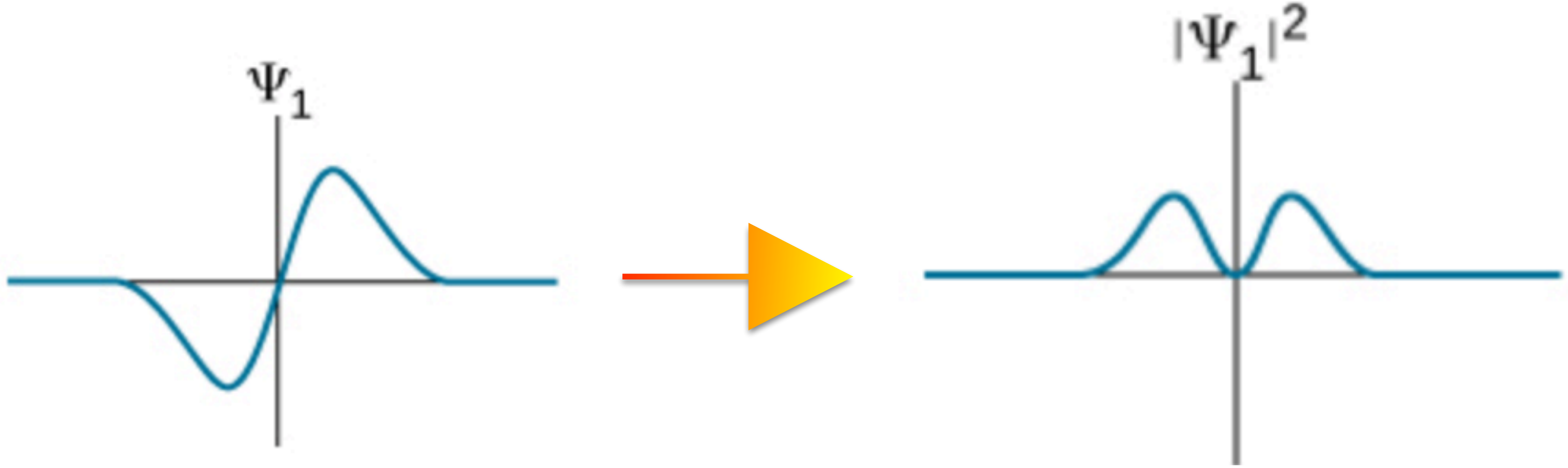
The mathematical expression that satisfy all the condition, which represent the wave packet corresponds to a quantum particle is a wave function

Concept of Probability

The wave function is not an observable quantity and it does not have any direct physical meaning. In fact, it is a **complex-valued function.**

But square of the wave function, $|\Psi|^2$ is physical (observable).

$|\Psi|^2$ gives the probability (density) of finding the system described by the wave function at the point in space at time t: $|\Psi|^2 = \Psi\,\Psi^*$



Normalisation of Wave Function ψ

$$\int_{-\infty}^{\infty} \psi^* \psi \, dV = \int_{-\infty}^{\infty} |\psi|^2 dV = 1$$

If $$\int_{-\infty}^{\infty} \psi^* \psi \, dV = N \Rightarrow \psi' = \frac{1}{\sqrt{N}} \psi$$

$$\Rightarrow \int_{-\infty}^{\infty} \psi'^* \psi' \, dV = \int_{-\infty}^{\infty} |\psi'|^2 dV = 1$$

⇩

Normalisation of a wave function

Normalisation of Wave Function ψ

Example: Normalize the given wave function and calculate the constant " A"

$$\Psi(x) = Ae^{-\lambda(x-a)^2}$$

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = \int_{-\infty}^{\infty} A^2 e^{-2\lambda(x-a)^2} \, dx = 1$$

$$\therefore x - a = u; \ dx = du$$

$$\Rightarrow \int_{-\infty}^{\infty} A^2 e^{-2\lambda u^2} \, du = A^2 \sqrt{\frac{\pi}{2\lambda}} = 1$$

$$\Rightarrow A^2 = \sqrt{\frac{2\lambda}{\pi}}$$

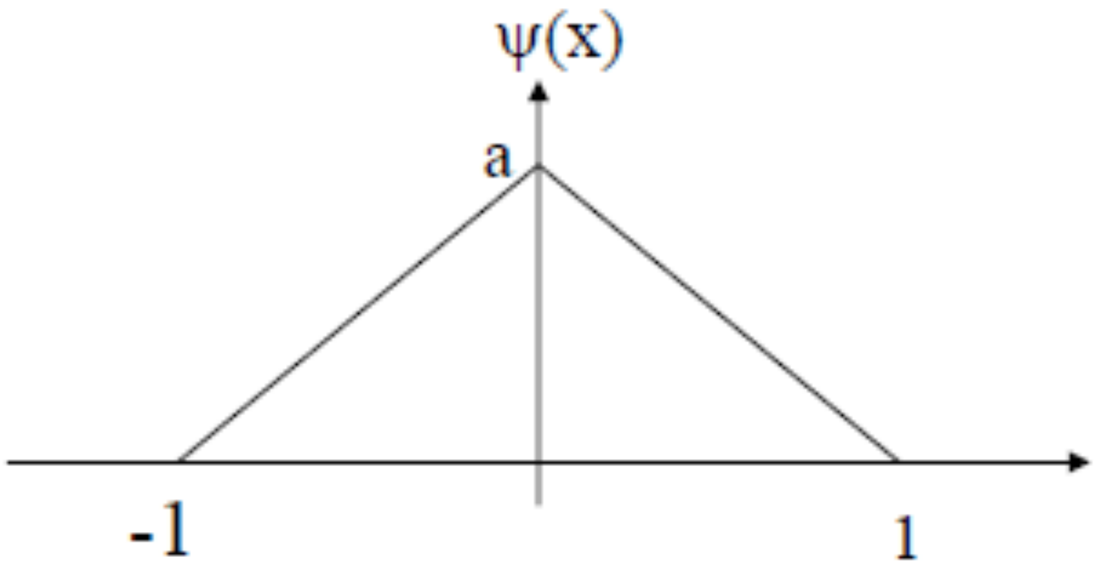
$$\Rightarrow A = \left(\frac{2\lambda}{\pi}\right)^{1/4}$$

$$\Rightarrow \Psi'(x) = \left(\frac{2\lambda}{\pi}\right)^{1/4} e^{-\lambda(x-a)^2}$$

Normalisation of Wave Function ψ

If $\int_{-\infty}^{\infty} \psi^* \psi \, dV = N \Rightarrow \psi' = \frac{1}{\sqrt{N}} \psi \Rightarrow \int_{-\infty}^{\infty} \psi'^* \psi' \, dV = \int_{-\infty}^{\infty} |\psi'|^2 dV = 1$

Example: If a wavefunction is not normalized, we can make it so by dividing it with a normalization constant. E.g.



$$f(x) = \begin{cases} a(1-x) & x \geq 0 \\ a(1+x) & x < 0 \end{cases}$$

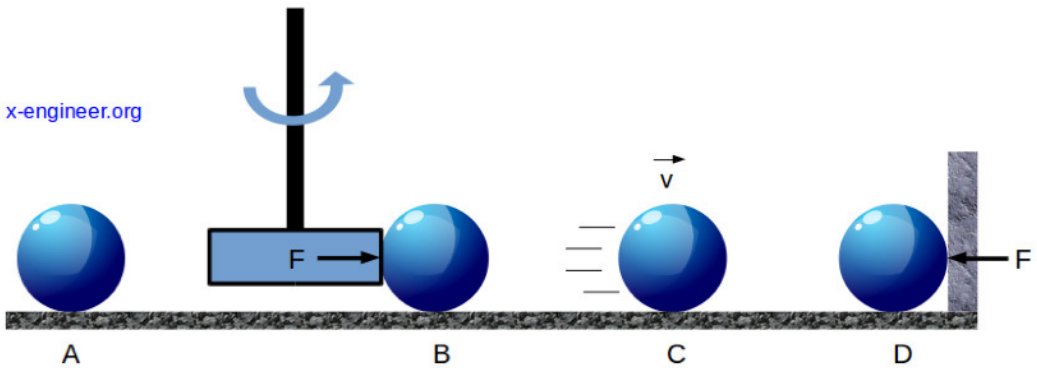
$$\therefore \int_{-\infty}^{\infty} |f(x)|^2 \, dx = 2\int_0^1 [a(1-x)]^2 dx$$

$$= 2a^2 \left[-\frac{(1-x)^3}{3} \right]_0^1$$

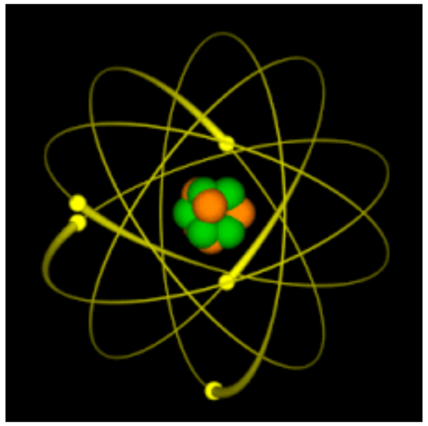
$$= \frac{2}{3} a^2 \neq 1$$

$\therefore$ f(x) is not normalixed, but $\psi(x) = \frac{f(x)}{\sqrt{\frac{2}{3}a}}$ is!

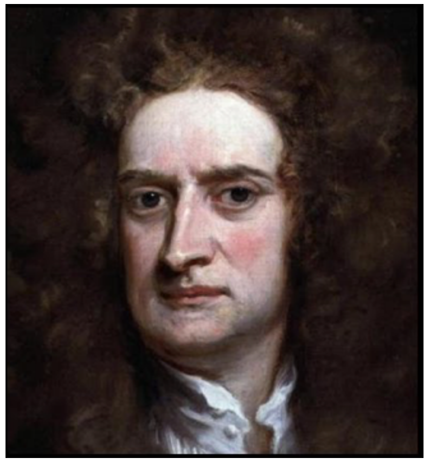
Understanding the Microscopic System



Macroscopic system



Microscopic system



- Governed by **classical physics**
- **Newtons Laws of motions and conservation of momentum to describe the motion and behaviour of system**

- Governed by **Quantum physics**
- **Obey duality nature**
- **Heisenberg uncertainty**
- **Behave as wave**
- **Express by Wave function** ψ
- **Newtons Laws of motions can not apply directly to describe the motion and behaviour of such system**

Schrödinger Wave Equation

Schrödinger Wave Equation

Schrödinger Equation is a mathematical expression that describes the change of a physical quantity over time in which the quantum effects like wave-particle duality are significant…

- In other words, we can say that …..It is a differential equation for the de Broglie waves associated with particles and describes the motion of particles.
- The Schrodinger equation is the fundamental equation of wave mechanics in the same sense as Newton's second law of motion of classical mechanics

The Schrödinger Equation has two forms:

- Time-dependent Schrödinger Equation
- Time-independent Schrödinger Equation

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = H\psi(r,t)$$

$$Where,\ H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V \qquad \frac{\partial^2}{\partial r^2} \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$$

$V = time\ dependant\ Potential\ energy$

Derivation: Time-dependent Schrödinger Wave Equation

Consider a particle of having mass **m**, moving in the **x**-direction; having total energy **E** and momentum, **p**

⇒Then, according to classical mechanics, the total energy associated with the particle is:

$$\Rightarrow E = KE + PE$$

$$\Rightarrow E = \frac{p^2}{2m} + V$$

⇒If the particle is associated with a matter wave, then it can be represented as a wave function, ψ:

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

k, is the propagation vector and ω, angular frequency

Derivation: Time-dependent Schrödinger Wave Equation

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

we know that,

$$\Rightarrow E = h\nu$$

$$\Rightarrow E = h\frac{\omega}{2\pi} = \hbar\omega$$

$$\Rightarrow \omega = \frac{E}{\hbar} \ldots\ldots\ldots (a)$$

Also, we know that,

$$\lambda = \frac{h}{p} \Rightarrow p = \frac{h}{\lambda}; \quad k = \frac{2\pi}{\lambda}$$

$$\Rightarrow p = \frac{hk}{2\pi} = \hbar k \quad \Rightarrow k = \frac{p}{\hbar} \ldots\ldots (b)$$

on substituting the eq. "a & b" in wave function $\psi(x,t)$

$$\psi(x,t) = Ae^{i(\frac{p}{\hbar}x-\frac{E}{\hbar}t)}$$

$$\Rightarrow = Ae^{\frac{i}{\hbar}(px-Et)} \ldots\ldots\ldots (1)$$

Taking the partial derivative w.r.t. to position of the wave function $\psi(x,t)$:

$$\Rightarrow \frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{x}} = = Ae^{\frac{i}{\hbar}(px-Et)}\left(\frac{ip}{\hbar}\right)$$

$$\Rightarrow \frac{\partial^2\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{x}^2} = Ae^{\frac{i}{\hbar}(px-Et)}\left(\frac{ip}{\hbar}\right)^2$$

$$\Rightarrow \frac{\partial^2\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{x}^2} = \left(\frac{ip}{\hbar}\right)^2\psi(x,t)$$

$$\Rightarrow p^2\psi(x,t) = -\hbar^2\frac{\partial^2\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{x}^2} \ldots\ldots (2)$$

Derivation: Time-dependent Schrödinger Wave Equation

$$\psi(x,t) = Ae^{i(\frac{p}{\hbar}x - \frac{E}{\hbar}t)}$$

$$= Ae^{\frac{i}{\hbar}(px - Et)} \ldots\ldots\ldots (1)$$

Let's take the partial derivative w.r.t. to time of the wave function $\psi(x,t)$:

$$\Rightarrow \frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{t}} = Ae^{\frac{i}{\hbar}(px-Et)}\left(\frac{-iE}{\hbar}\right)$$

$$\Rightarrow \frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{t}} = \left(\frac{-iE}{\hbar}\right)\psi(x,t)$$

$$\Rightarrow E\psi(x,t) = \left(\frac{\hbar}{-i}\right)\frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{t}}$$

$$\Rightarrow E\psi(x,t) = i\hbar\frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{t}} \ldots\ldots\ldots (3)$$

$$E = \frac{\mathrm{p}^2}{2\mathrm{m}} + \mathrm{V}$$

operating over the wave function $\psi(x,t)$:

$$E\psi(x,t) = \frac{\mathrm{p}^2}{2\mathrm{m}}\psi(\mathrm{x},\mathrm{t}) + \mathrm{V}\psi(\mathrm{x},\mathrm{t})$$

using the equation 2 and 3, the above equation can be changes to

$$i\hbar\frac{\partial\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{t}} = -\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2\psi(\mathrm{x},\mathrm{t})}{\partial \mathrm{x}^2} + \mathrm{V}\psi(\mathrm{x},\mathrm{t})$$

⇩

Time-dependent Schrödinger Wave Equation in 1D

Derivation: Time-dependent Schrödinger Wave Equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t)$$

1D

$$\Rightarrow i\hbar\frac{\partial\psi(x,y,z,t)}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi(x,y,z,t)}{\partial x^2} + \frac{\partial^2\psi(x,y,z,t)}{\partial y^2} + \frac{\partial^2\psi(x,y,z,t)}{\partial z^2}\right] + V\psi(x,y,z,t)$$

3D

$$\Rightarrow i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(r,t)}{\partial r^2} + V\psi(r,t)$$

$$\Rightarrow i\hbar\frac{\partial\psi(r,t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(r,t) + V\psi(r,t)$$

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = H\psi(r,t)$$

$$H \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V$$

Time-dependent Schrödinger Wave Equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t)$$

$$H \equiv -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + V$$

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = H\psi(r,t) = E\psi(r,t)$$

This is called the **time-dependent Schrodinger equation**. One has to solve this equation with appropriate boundary conditions to find the **wavefunction ψ(x) and energy eigenvalues E**. Any condition imposed on the motion of a particle will affect the potential energy U, which is a function of x & t. By knowing the exact form of U, the equation may be solved for Ψ. The time-dependent Schrodinger equation is used to explain non-stationary phenomena, such as the electronic transition between two states of atom.

Time-independent Schrödinger Wave Equation

The Schrödinger Equation has two forms:

- Time-dependent Schrödinger Equation
- Time-independent Schrödinger Equation

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t)$$

$$i\hbar\frac{\partial\psi(r,t)}{\partial t} = H\psi(r,t)$$

Time-independent Schrödinger Wave Equation

In many atomic phenomena, the **potential energy** of the particle is **independent of time and depends only on the position** of the particle. In such situations, the differential equation for de-Broglie waves associated with particles is called the time-independent (**stationary/steady state**) Schrodinger wave equation.

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

$$\Rightarrow \psi(x,t) = Ae^{i(\frac{p}{\hbar}x-\frac{E}{\hbar}t)}$$

$$\Rightarrow = Ae^{i(\frac{p}{\hbar}x)}e^{(-i\frac{E}{\hbar}t)} \qquad (\therefore \; e^{m+n} = e^m + e^n)$$

$$\Rightarrow = \psi(x)\ \phi(t)$$

$$\boxed{\psi(x,t) = \psi(x)\ \phi(t)}$$

separation of variables

Time-independent Schrödinger Wave Equation

we know that, the time dependent scrounger wave equation for particle moving in x direction is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V\psi(x,t)$$

$$\psi(x,t) = \psi(x)\,\phi(t)$$

$$\Rightarrow\ i\hbar\frac{\partial\psi(x)\phi(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)\phi(t)}{\partial x^2} + V\psi(x)\phi(t)$$

$$\Rightarrow\ \psi(x)\left[i\hbar\frac{\partial\phi(t)}{\partial t}\right] = \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\right]\phi(t)$$

$$\Rightarrow\ \frac{1}{\phi(t)}\left[i\hbar\frac{\partial\phi(t)}{\partial t}\right] = \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\right]\frac{1}{\psi(x)}$$

Function of time — Function of position

Time-independent Schrödinger Wave Equation

$$\frac{1}{\phi(t)}\left[i\hbar\frac{\partial\phi(t)}{\partial t}\right] = \left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\right]\frac{1}{\psi(x)}$$

Function of time — Function of position

$$\psi(x,t) = \psi(x)\,\phi(t)$$
$$\psi(x) = Ae^{i(\frac{p}{\hbar}x)}$$
$$\phi(t) = e^{(-i\frac{E}{\hbar}t)}$$

$\Rightarrow$ LHS= RHS = S (Separation variable constant)

Lets find that constant, by calculating the LHS, as we know that:

$$LHS = \frac{1}{\phi(t)}\left[i\hbar\frac{\partial\phi(t)}{\partial t}\right] \quad \text{and} \quad \phi(t) = e^{(-i\frac{E}{\hbar}t)}$$

upon substitution, we will have

$$\frac{1}{\phi(t)}\left[i\hbar\frac{\partial}{\partial t}e^{(-i\frac{E}{\hbar}t)}\right] \Rightarrow \frac{1}{\phi(t)}\left[i\hbar e^{(-i\frac{E}{\hbar}t)}\left(\frac{-iE}{\hbar}\right)\right] \Rightarrow \frac{1}{\phi(t)}\left[i\hbar\,\phi(t)\left(\frac{-iE}{\hbar}\right)\right] \Rightarrow E$$

$\Longrightarrow$ LHS= RHS = E (total energy of the system)

Time-independent Schrödinger Wave Equation

$$E = \Big[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\Big]\frac{1}{\psi(x)}$$

$$\Rightarrow \frac{1}{\psi(x)}\Big[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\Big] = E$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x) = E\psi(x)$$

The is differential equation in position only and can be easily solved to get energy of the system

$$\Big[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\Big]\psi(x) = E\psi(x)$$

$$H\psi(x) = E\psi(x)$$

where the above equation is Eigen value equation and H is the hamiltonian, and E is the solution

Time-independent Schrödinger Wave Equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x) = E\psi(x)$$

we can also rearrange the above equation as:

$$\Rightarrow \; -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x) - E\psi(x) = 0$$

$$\Rightarrow \; \frac{\partial^2\psi(x)}{\partial x^2} - \frac{2m}{\hbar^2}\left(V - E\right)\psi(x) = 0$$

$$\boxed{\frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V\right)\psi(x) = 0}$$

Free particle: Time-independent Schrödinger Wave Equation

For a free particle, $V(x) = 0$

$$\Rightarrow \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V\right)\,\psi(x) = 0$$

$$\Rightarrow \frac{\partial^2 \psi(x)}{\partial x^2} = -\frac{2mE}{\hbar^2}\,\psi(x)$$

$$\Rightarrow \frac{\partial^2 \psi(x)}{\partial x^2} = -k^2\,\psi(x) \qquad \therefore k = \sqrt{\frac{2mE}{\hbar^2}}$$

So, The solution to time independent Schrodinger Equation is: $\psi(x) = Ae^{ikx}$

and we know that, $\phi(t) = e^{(-i\frac{E}{\hbar}t)}$

So, The final solution is: $\psi(x,t) = \psi(x)\,\phi(t) = Ae^{-i(kx - \frac{E}{\hbar}t)}$

Possible Questions

1. **Outline the concepts of Wave function ?**
2. **Write down the characteristics and its physical significance of wave function?**
3. **Write down the time dependent Schrodinger wave equation and explain its each term?**
4. **For a matter wave, derive the time-dependent Schrodinger wave equation?**
5. **Derive the time-independent Schrodinger equation from the time dependent Schrodinger equation or Using the separation variable method, derive the time independent Schrodinger wave equation?**

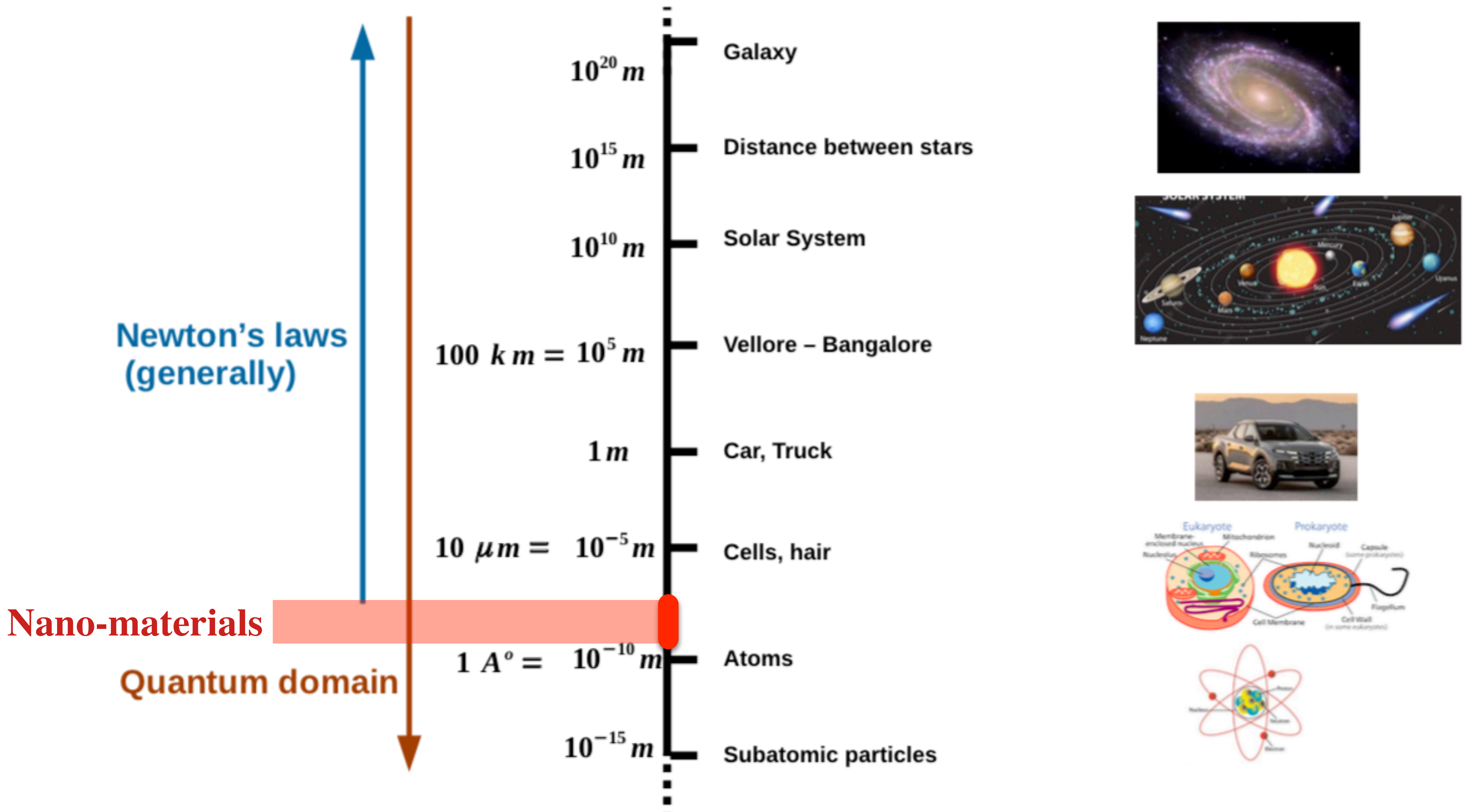
Basics of Nanophysics

It is a branch of nanoscience in which the **physics of structures and artefacts with dimensions in the nanometer** ($10^{-9}\ nm$) **range or of phenomena occurring in nanoseconds.**

- Nano Science:
- Nano Technology
- Nanoparticle
- Nano Materials

What is this "Nano" or "Nanoscale" ?

Concept of Nanoscale



The Nano-scale involves the range from approximately 1 nm to 100 nm

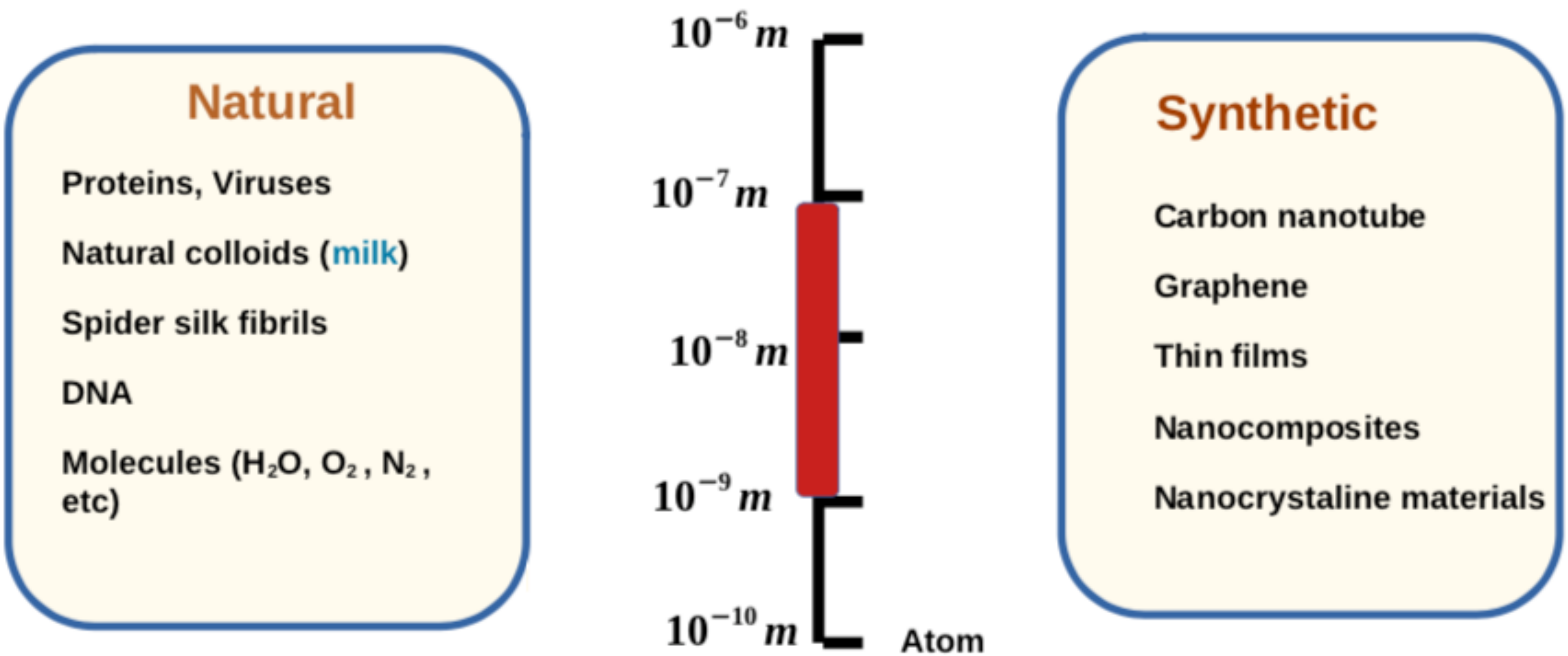
Materials based on their Sizes

Materials

Bulk Materials	Nano Materials
Size above 100nm	Size range 1nm - 100nm
Seen in simple microscope or eye	Cannot be seen in simple microscope or eye
Low reactivity	High reactivity
Properties cannot be tuned easily	Properties can be tuned easily
Examples: Sand, Cement, allumina, Salt and much more.	Examples: Gold nanoparticles, Carbon nanotubes, Proteins

Nano-materials

Nano Materials are the materials containing nano crystals i.e their grain size is in the 100nm range. The nano materials may be metals, alloys, ceramics..



Classification of Nano-Structures: Geometry

According to their dimensions, they are classified into the following:

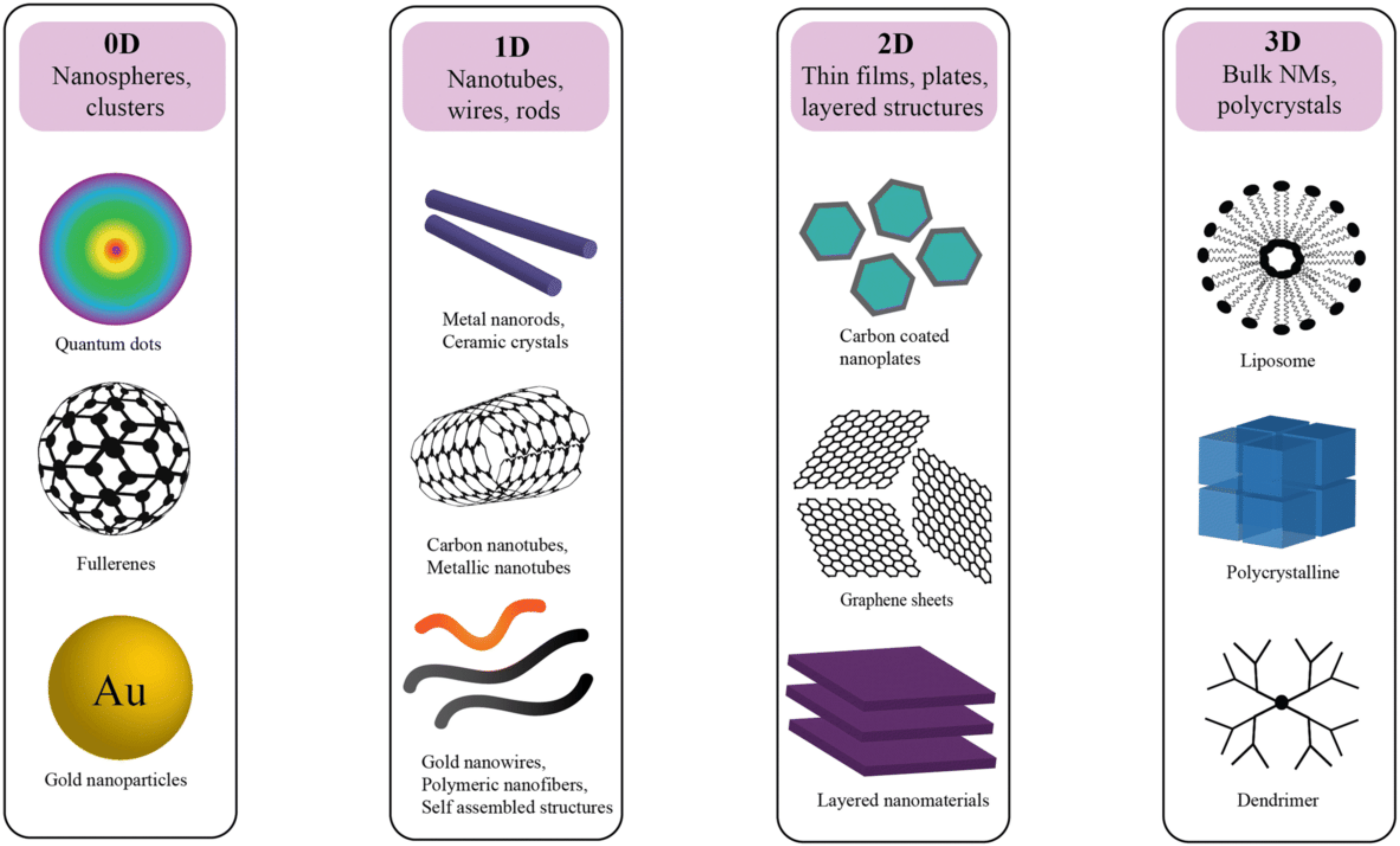
- Zero-dimensional (0D) nanostructures: In this, all three dimensions are in the nanometric range.
- **Ex. Nanoparticles or well-separated nano-powders.**

- One- dimensional (1D) nanostructure: In this, two dimensions are in the nanometric range and third dimension remain large. These structures have a shape like rods.
- **Ex. Nanotubes, Nanorods, etc.**

- Two- dimensional (2D) nanostructure: In this, only one dimension is in the nanometric range while the other two dimensions remain large. These display plane-like structures.
- **Ex. Nano thin films, Nano coating, Nano layers, etc..**

- Three-dimensional (3D) nanostructure :
- In this, all three dimensions are outside the nanometric size range.
- It may consist of a **group of** nanowires, nanotubes, or different distributions of nanoparticles.

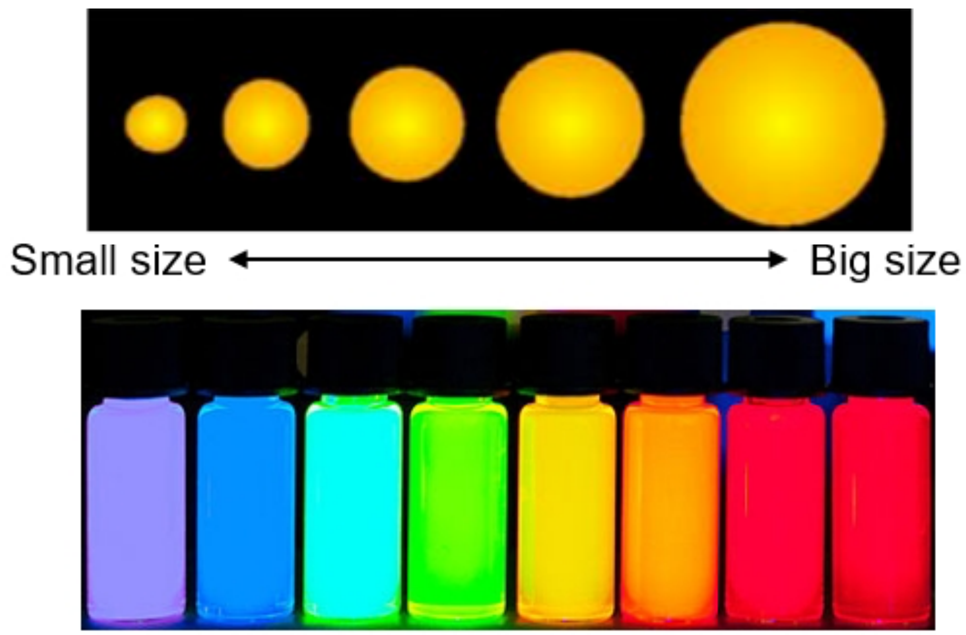
Classification of Nano-Structures: Geometry



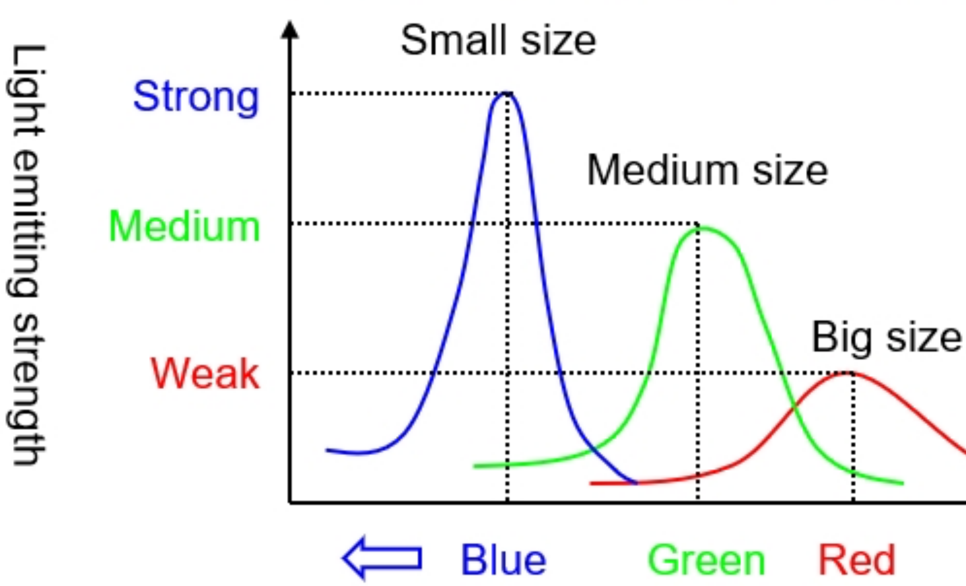
Based on their size they have applications in the different areas of science and technology.

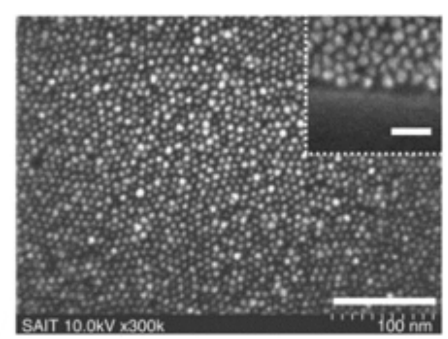
Importance of Nanostructure: Size Effect

Gold does not glitter at nanoscale



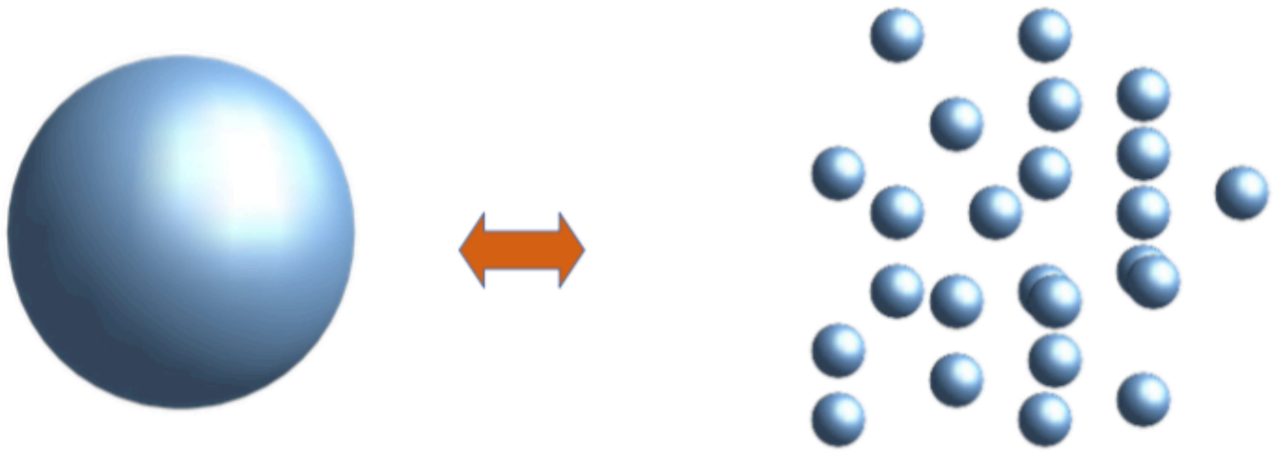
	Macroscale	Nanoscale
Copper	Opaque	Transparent
Platinum	Inert	Catalytic
Aluminuim	Stable	Combustible
Gold	Solid at room temperature	Liquid at room temperature
Silicon	Insulator	Conductor





They show size-dependent physical properties. The Optical, electrical, Mechanical, Melting point, Electrical conductivity, Chemical reactivity, and magnetic permeability changes significantly etc..)

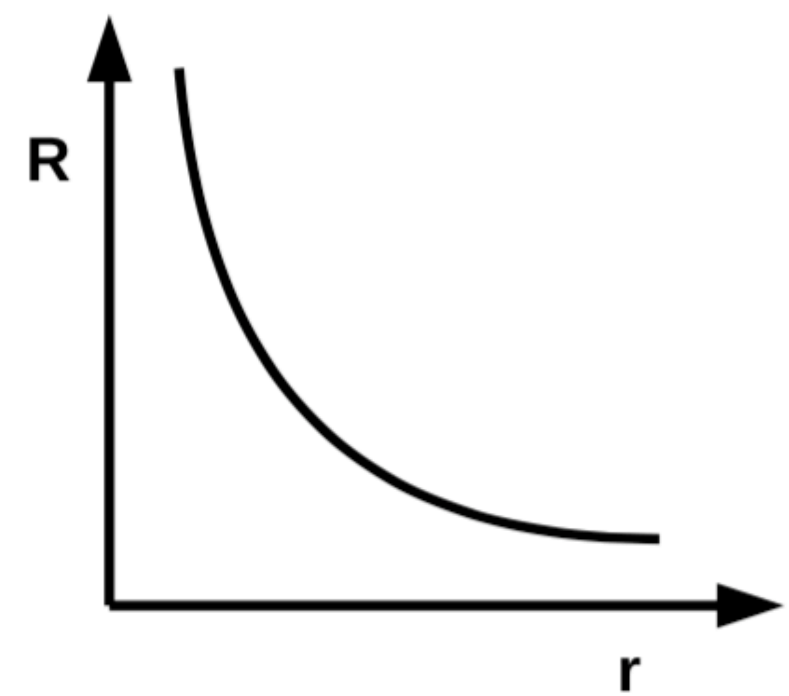
Importance of Nanostructure: Size Effect



$$V = \frac{4}{3}\pi r^3$$

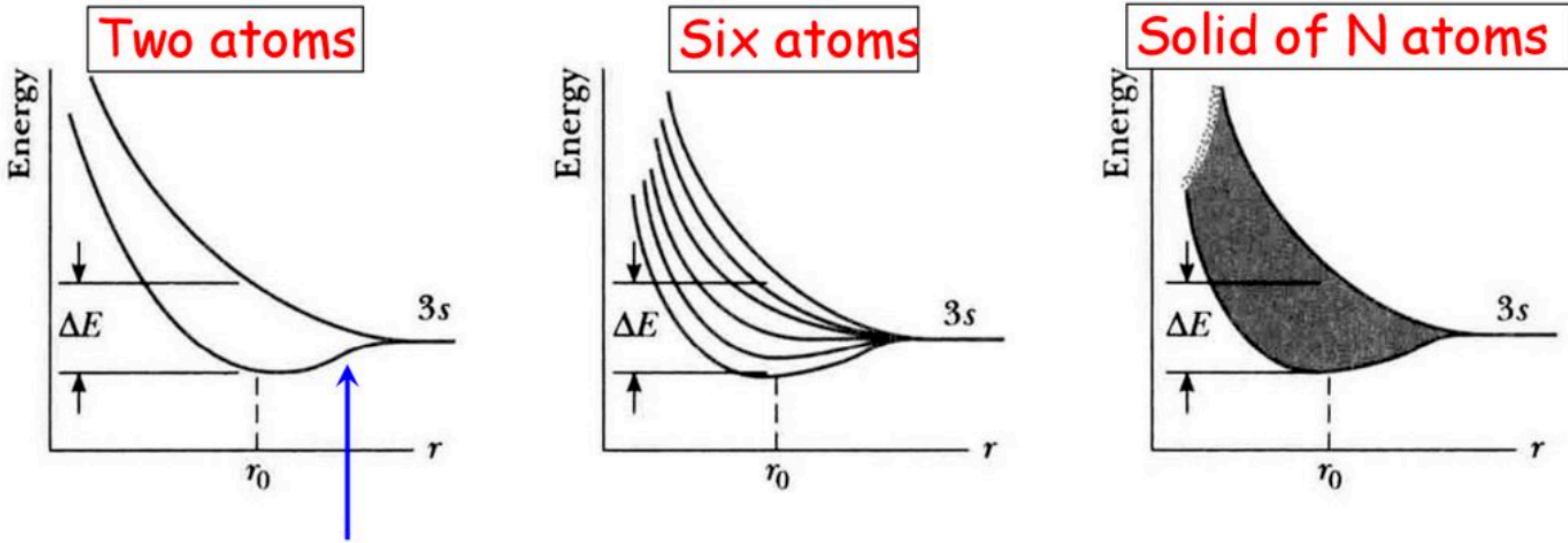
$$A = 4\pi r^2$$

$$R = \frac{A}{V} = \frac{3}{r}$$



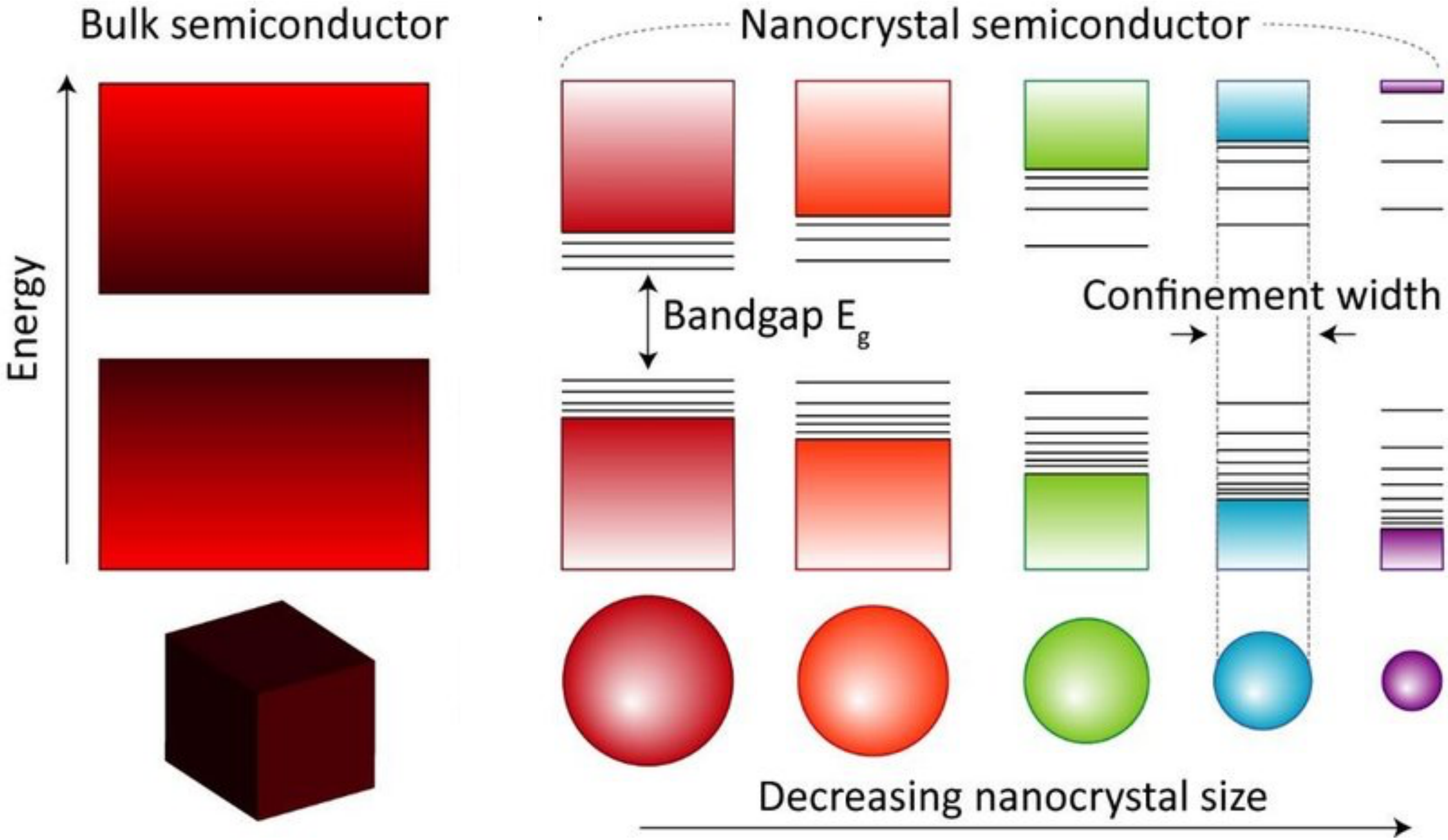
Surface to volume ratio increases: Chemical properties

Band Energy in Solids



Electrons must occupy different energies due to Pauli Exclusion principle.

Nanostructure: Size Effect-Band Energy



Quantum Confinement

Quantum confinement effect is observed when the **electron/hole is confined in small-size** particles whose **dimensions are comparable to the De Broglie wavelength** of an electron. It means we trap the particle and restrict its motion. As a result of **geometrical constraints**, electrons feel the presence of the particle boundaries and change their **physical properties drastically.**

Quantum confinement is only observed at dimensions below 2-4 nm

- ✓ Nano material (size <100 nm)
- ✓ Quantum material (size 1-3 nm)

Quantum confinement is more prominent in semiconductors because they have an energy gap in their electronic band structure. Metals do not have a bandgap, so quantum size effects are less prevalent.

Quantum Confinement Types

1D confinement: Quantum Wells

Particles are confined in one direction and are free to move in two directions.

only one dimension is in the nanometer range

1-dimension confinement and two degrees of freedom

2D confinement: Quantum Wire

Particles are confined in two directions and are free to move in one direction.

only two dimensions are in the nanometer range

2-dimensions confinement and one degree of freedom

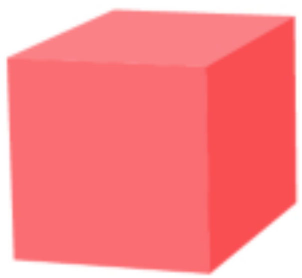
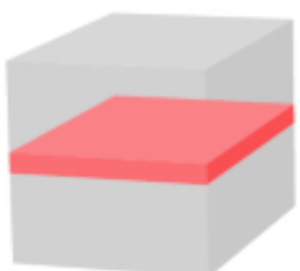
3D confinement: Quantum Dot

Particles are confined in all three directions and can not move freely in any spatial direction.

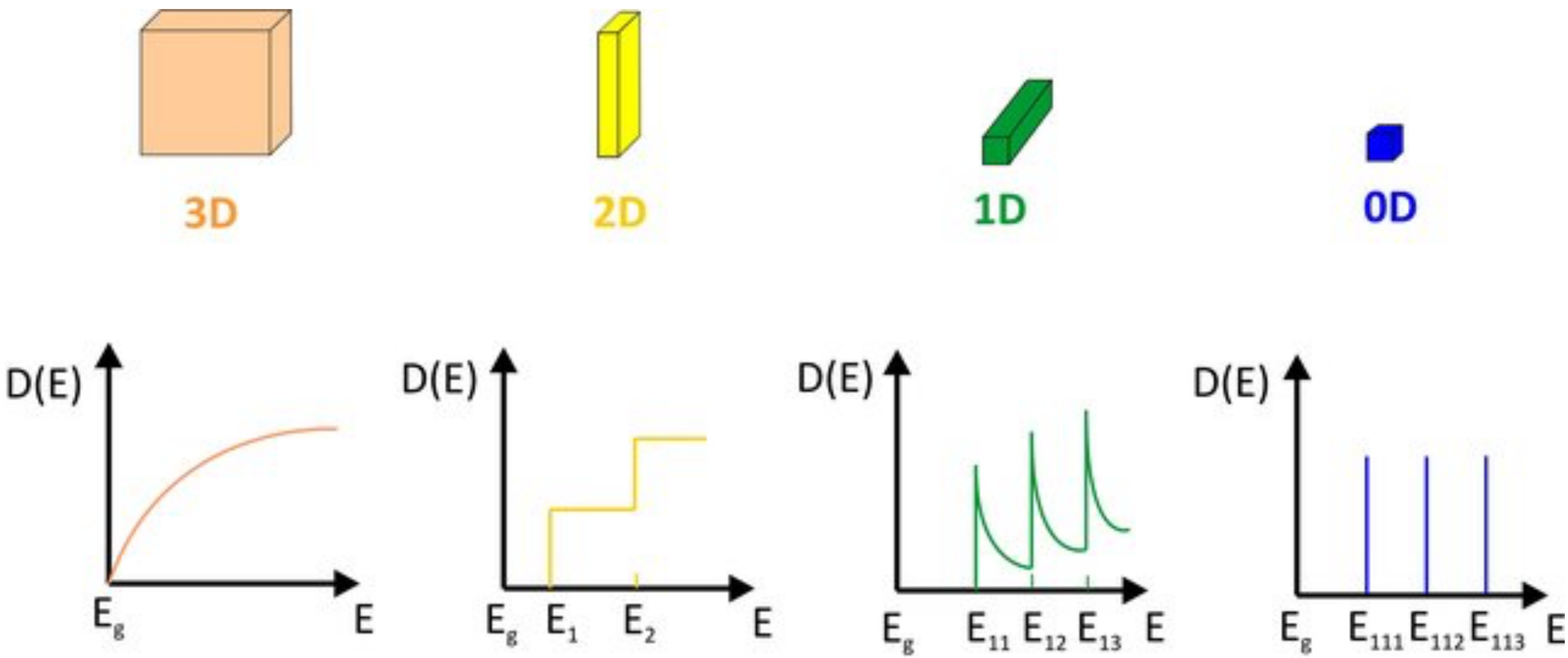
all three dimensions are in the nanometer range

3-dimensions confinement and zero degree of freedom

Quantum Confinement Types

Size		D_f	D_c	$D_f + D_c$
	Bulk	3	0	3
	Quantum Well	2	1	3
	Quantum Wire	1	2	3
	Quantum Dot	0	3	3

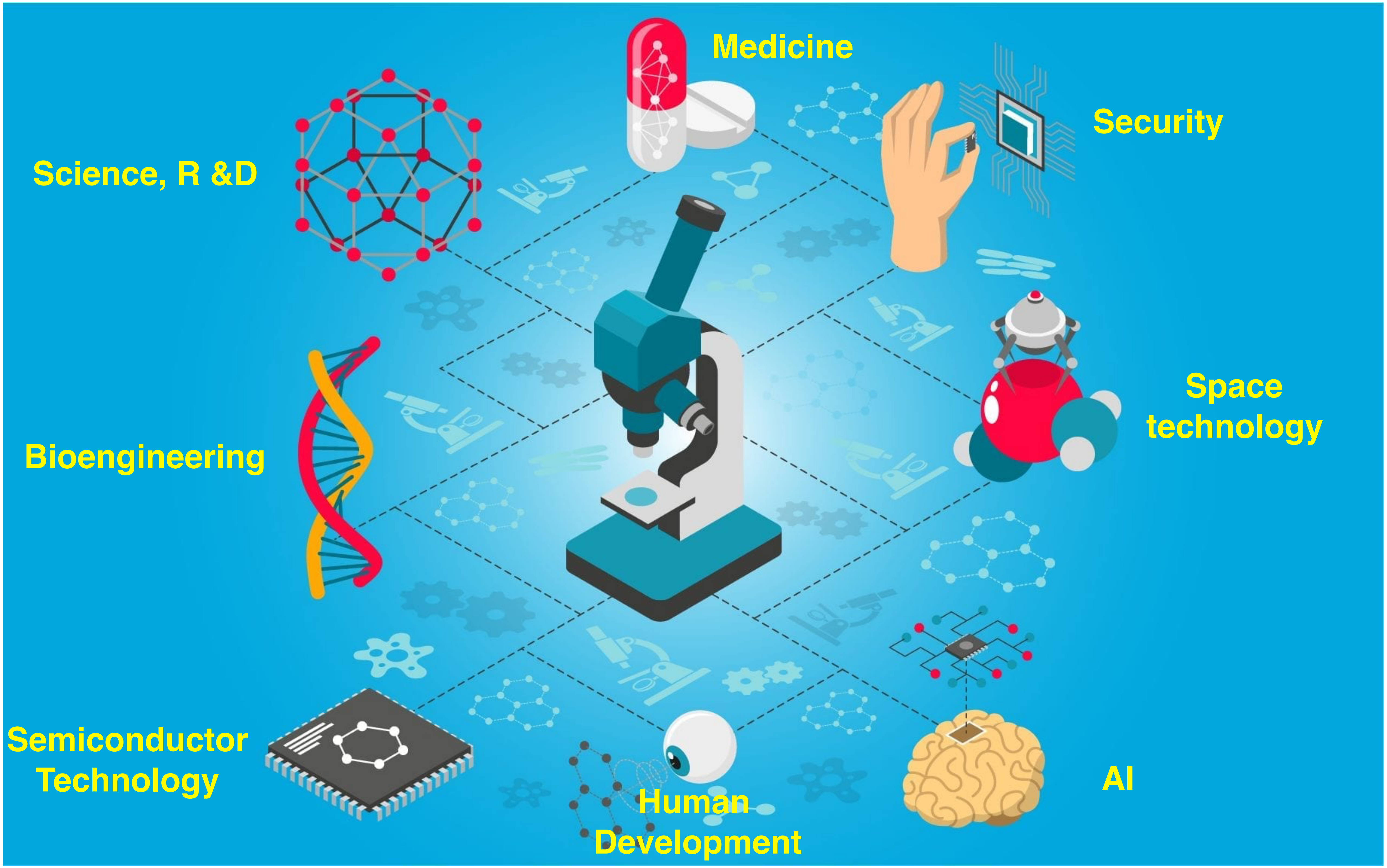
Quantum Confinement



$D(E) \propto E^{\frac{1}{2}}$ $D(E) \propto E^{0}$ $D(E) \propto E^{-\frac{1}{2}}$ $D(E) \propto \delta(E)$

Density of states: quantifies the number of different states at a particular energy level that electrons are allowed to occupy

Applications



Numerical on Quantum Mechanics (**Try by urself**)

1. Electrons with energy of 2eV are incident on a barrier of 3eV height and 0.2nm wide. Find the tunneling probability through this potential barrier.
2. An electron is in a box 0.1nm across. Find its permitted energies. Compute the difference between energies of ground and the first exited state.
3. Electrons with energies of 0.4eV are incident on a barrier 1 eV high and 0.1nm wide. Find the approximate probability for these electrons to penetrate the barrier.
4. Electrons with energies of 1.0 eV and 2.0 eV are incident on a barrier 10.0 eV high and 0.50 nm wide. (a) Find their respective transmission probabilities. (b) How are these affected if the barrier is doubled in width?
5. A black body is maintained at two temperatures 27^{O}C and 927^{O}C. Find the ratio of power emitted.
6. Calculate the De Broglie wavelength of an electron having a kinetic energy of 1keV.

Numerical on Quantum Mechanics (**Try by urself**)

7. An electron has a de Broglie wavelength of 2 pm. Find its kinetic energy. Ignore relativistic effects in the computation.

8. A beam of x-rays is scattered by a carbon target. At 45^{o} from the beam direction the scattered x-rays have a wavelength of 2.2 pm. What is the wavelength of the x-rays in the direct beam?

9. An x-ray photon whose initial frequency was 1.5×10^{19} Hz emerges from a collision with an electron with a frequency of 1.2×10^{19} Hz. How much kinetic energy was imparted to the electron?

10. At what scattering angle will incident 100-keV x-rays leave a target with an energy of 90keV?

11. The wavefunction of a free particle is : $\Psi(x,t) = A\, e^{i(k x - \omega t)}$. Show that the wavefunction satisfies the Schrodinger equation ? calculate the potential V

Numerical on Quantum Mechanics (**Try by urself**)

12. **Use the uncertainty principle to show that lowest energy of a particle confined in a box cannot be zero.**

13. **Draw the wave function/probability density/Energy corresponding to first three energy levels for particle confined between two rigid wall. Also write the corresponding formula for wave functions, probability density and energies.**