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**?

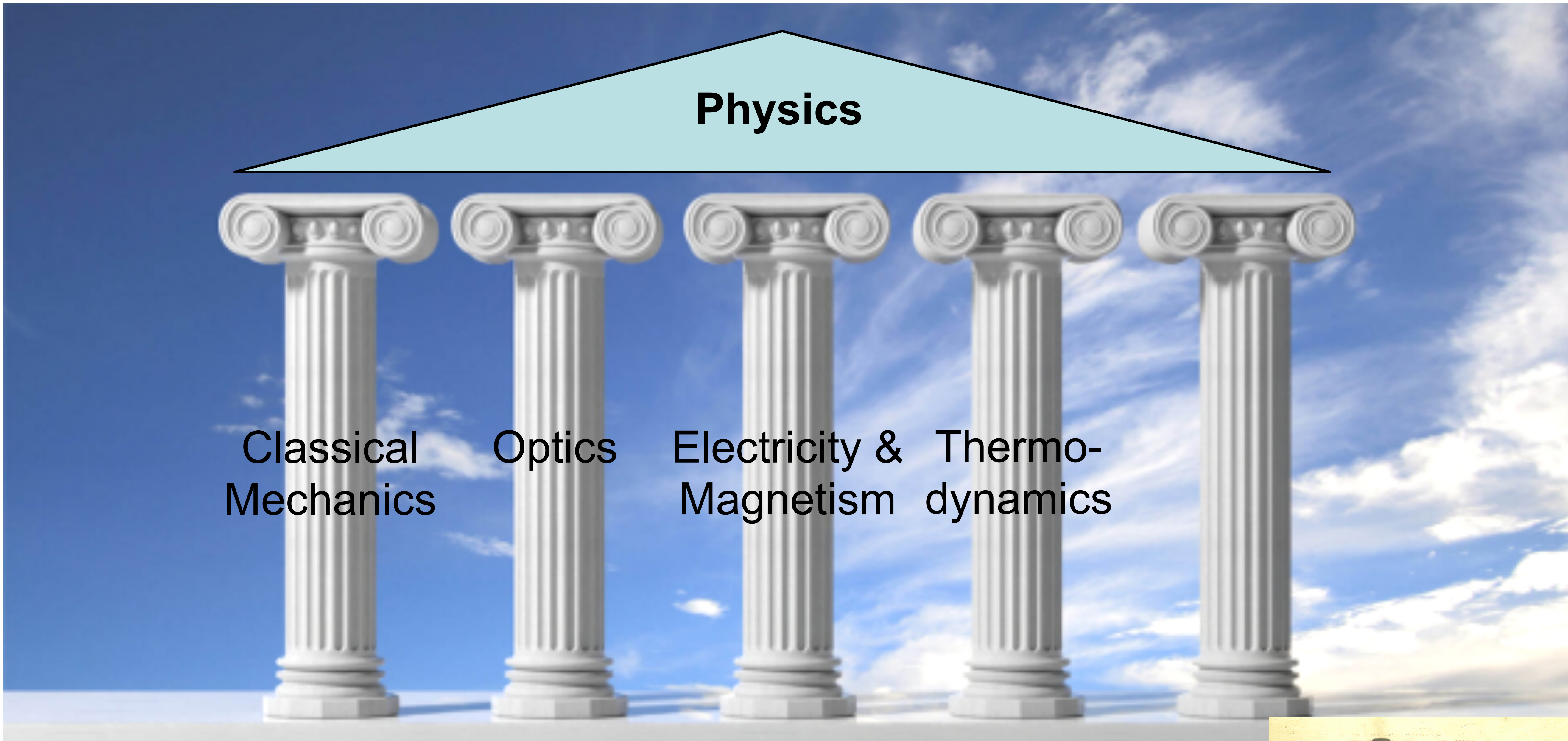
What is **modern physics**? What is **classical physics**?

Why modern physics is so important?

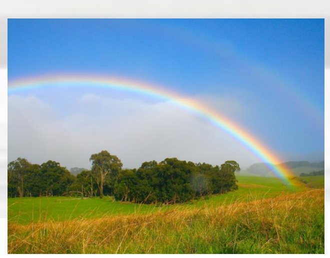
How did it emerge?

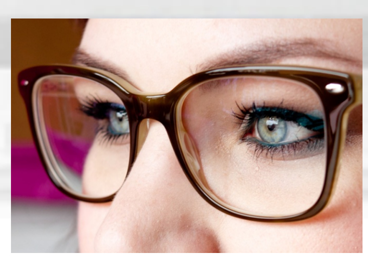
Origin of Quantum Mechanics and its Applications

Classical Mechanics(16^{th}-19^{th} Century)



Classical Mechanics



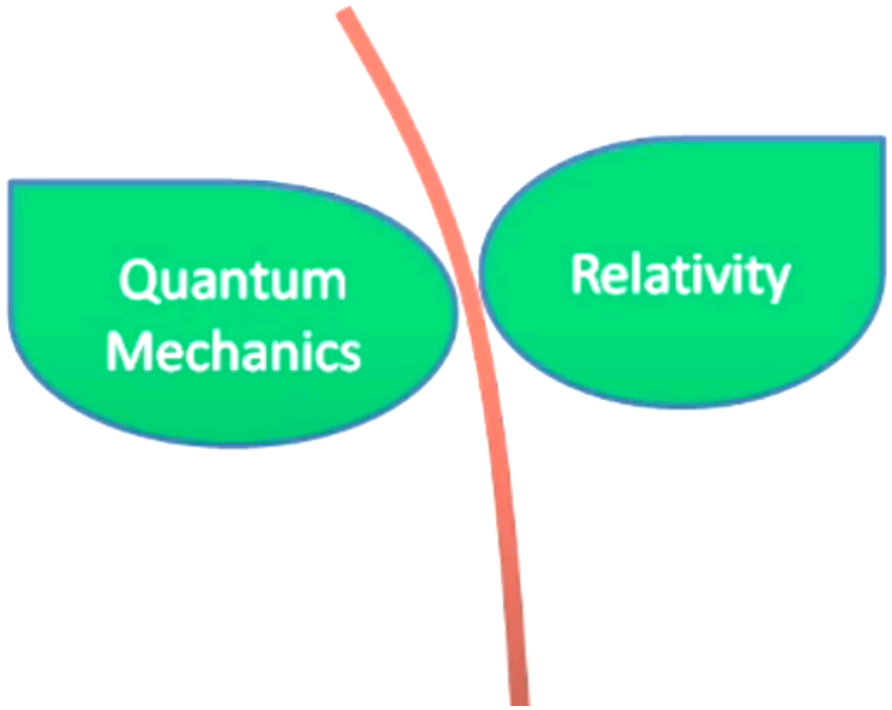


Optics

Electricity and Magnetism

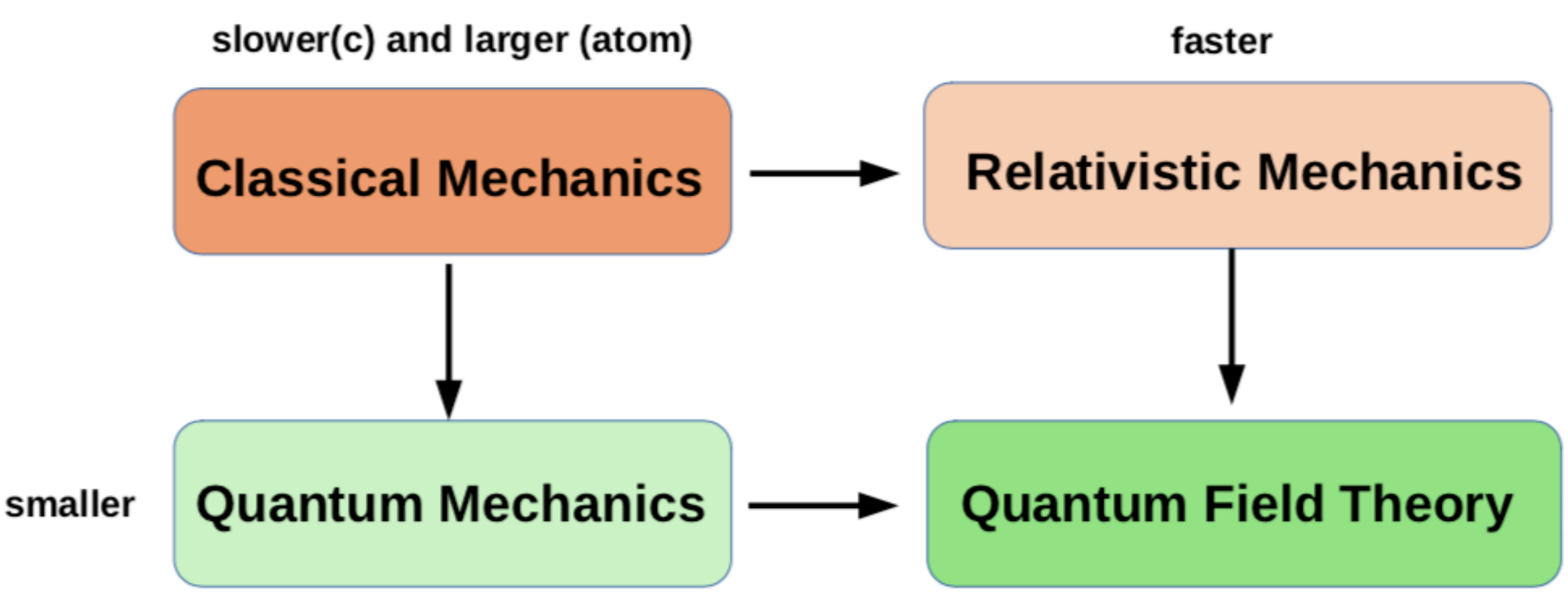
Thermodynamics

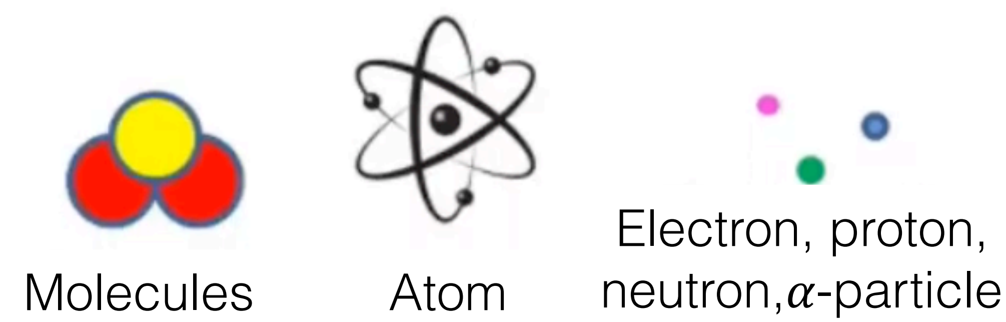
Born of Quantum Mechanics



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

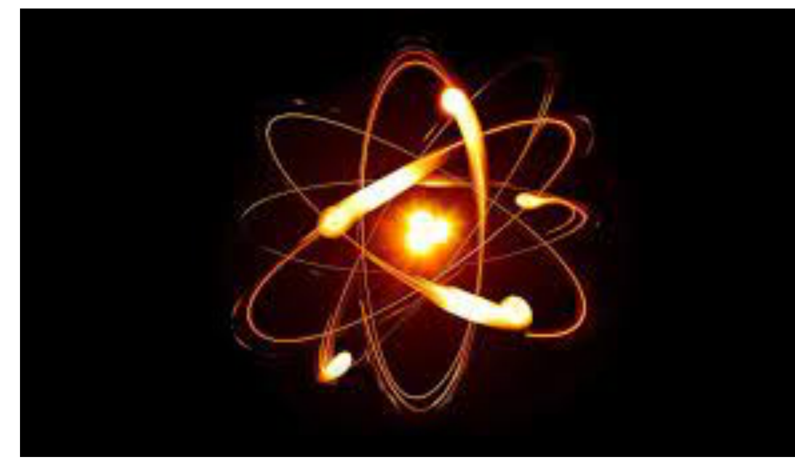




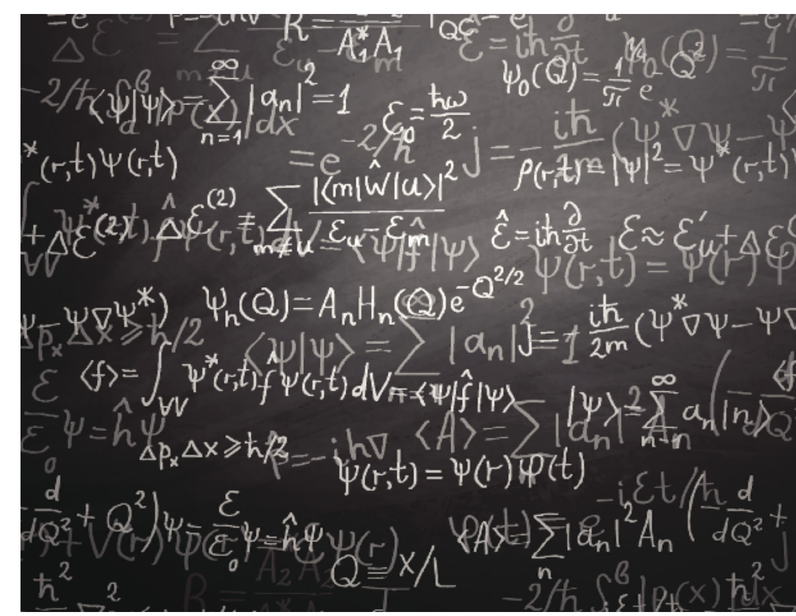
Quantum Mechanics

What is QM ?

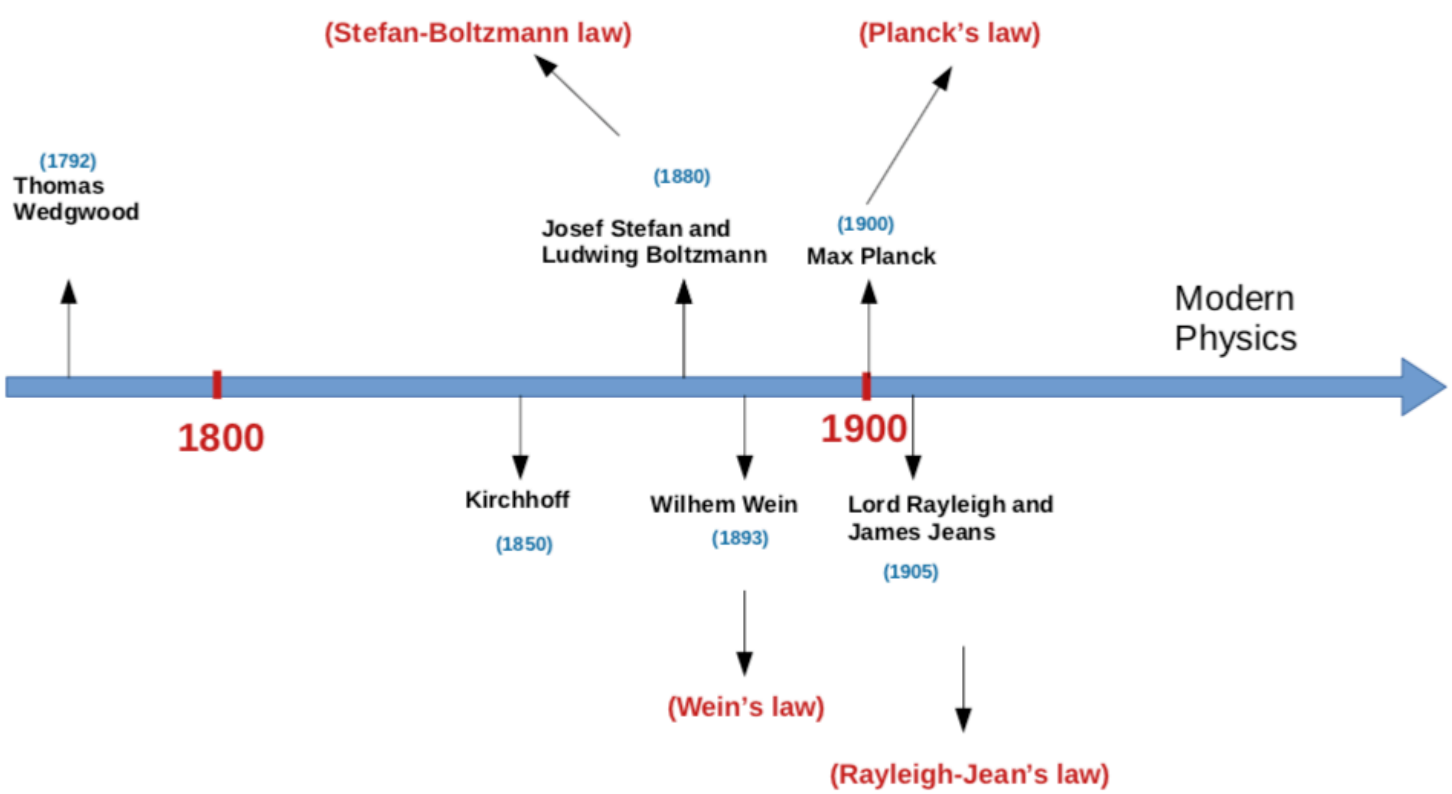
Quantum mechanics is a fundamental theory in physics that provides a description of the physical properties of nature at the scale of atoms and subatomic particles. It is the foundation of all quantum physics including quantum chemistry, quantum field theory, quantum technology, and quantum information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

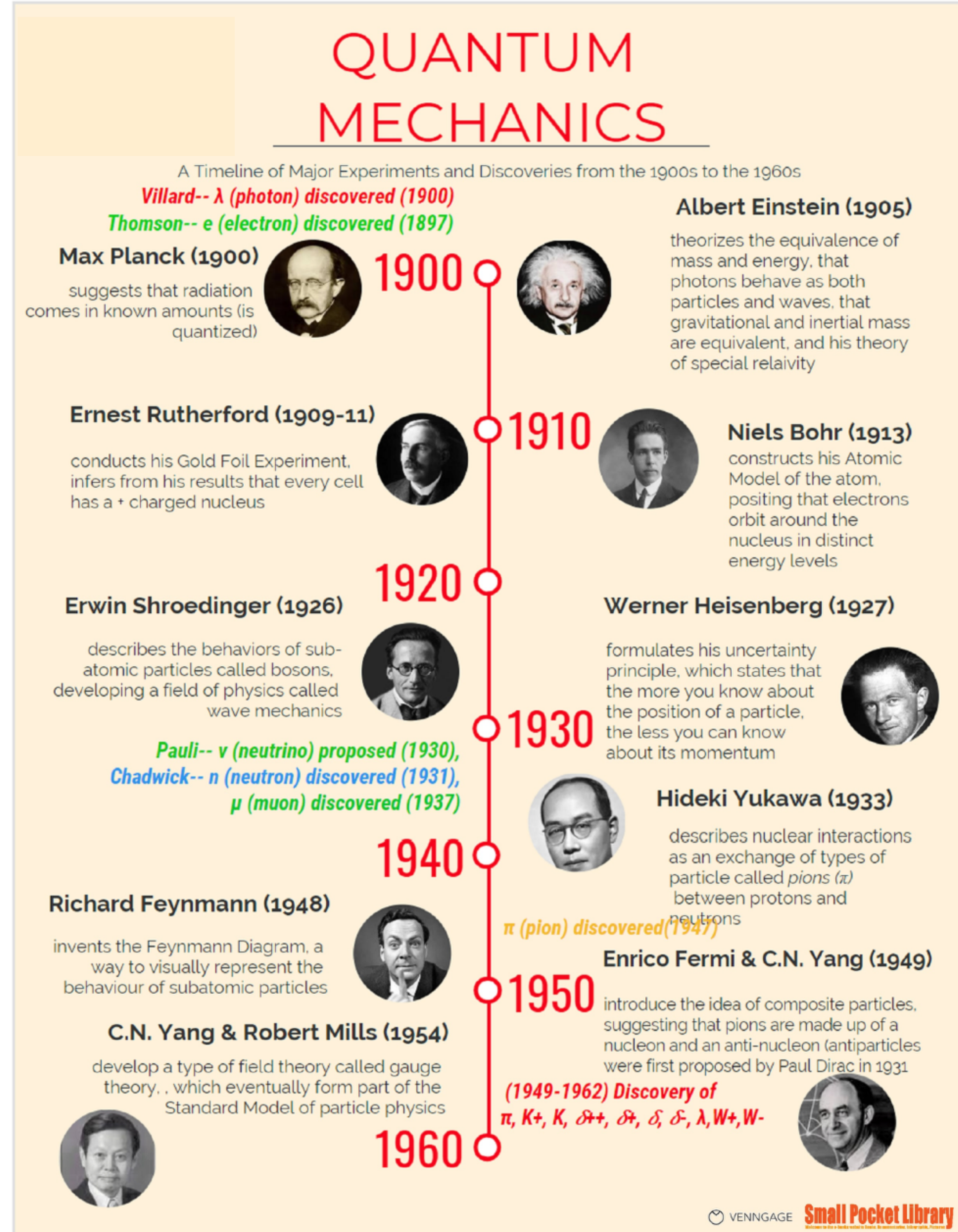


The branch of mechanics that deals with the mathematical description of the motion and interaction of subatomic particles, incorporating the concepts of quantisation of energy, wave–particle duality, the uncertainty principle, and the correspondence principle.



Development of Quantum Mechanics





Role of QM in Technology

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

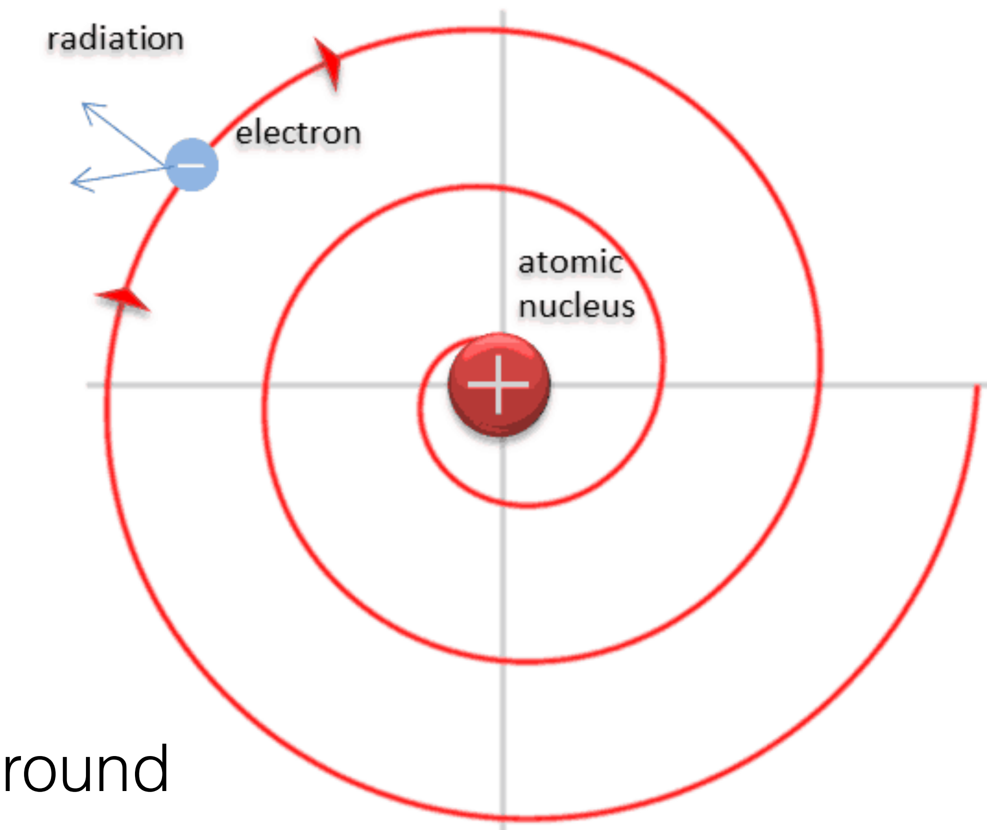
- Invention of Transistor – Reduced size, cost, and power consumption of an electronic gadget
- High precession microscopes -SEM, TEM, STEM, AFM
- LASER
- SQUID
- Single electron transistor
- Photonics- Photon based electronics
  Spintronics-electron spin based electronics
- (Quantum Computers)
- Nanotechnology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

Failure of Classical Mechanics (16^{th}-19^{th} 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**

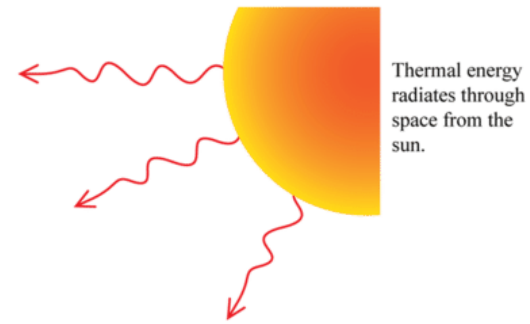
Radiation

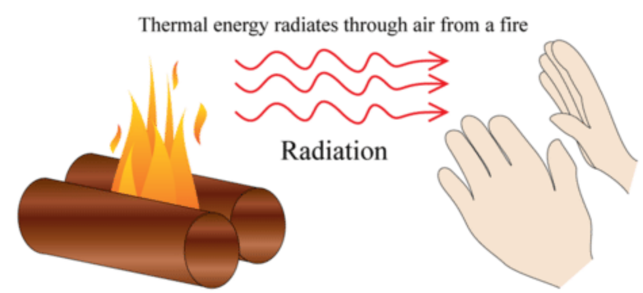
Radiation:The mode of energy transfer which need no medium is called radiation

Experimental Observations

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

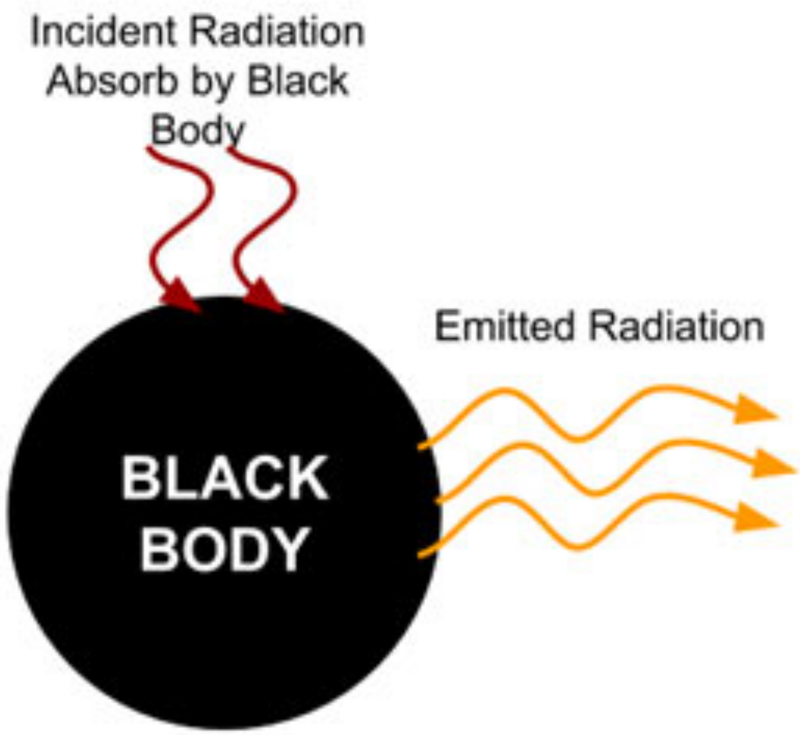
- According to classical mechanics, thy radiate EMW
- As the temperature of anybody rises, the body glows with the colors corresponding to the higher frequency (smaller wavelength) of the electromagnetic spectrum.





- 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



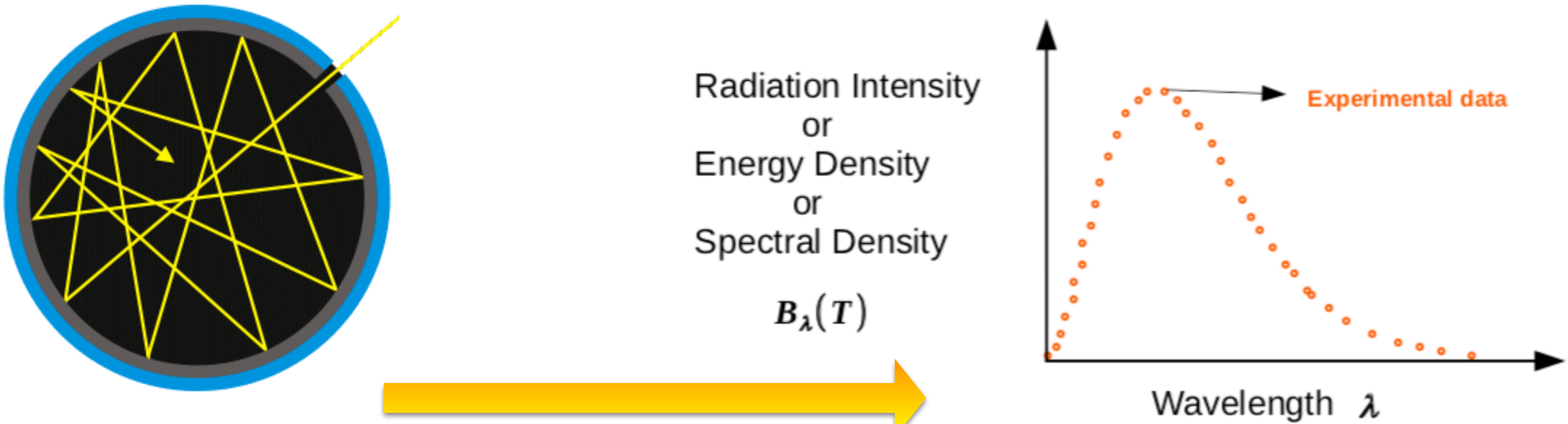
- The non-reflective, opaque object which absorbs all the radiation that falls upon it is called a blackbody.
- At room temperature, it appears black as no visible light is emitted
- At a particular temperature the black body would emit the maximum amount of energy possible for that temperature

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

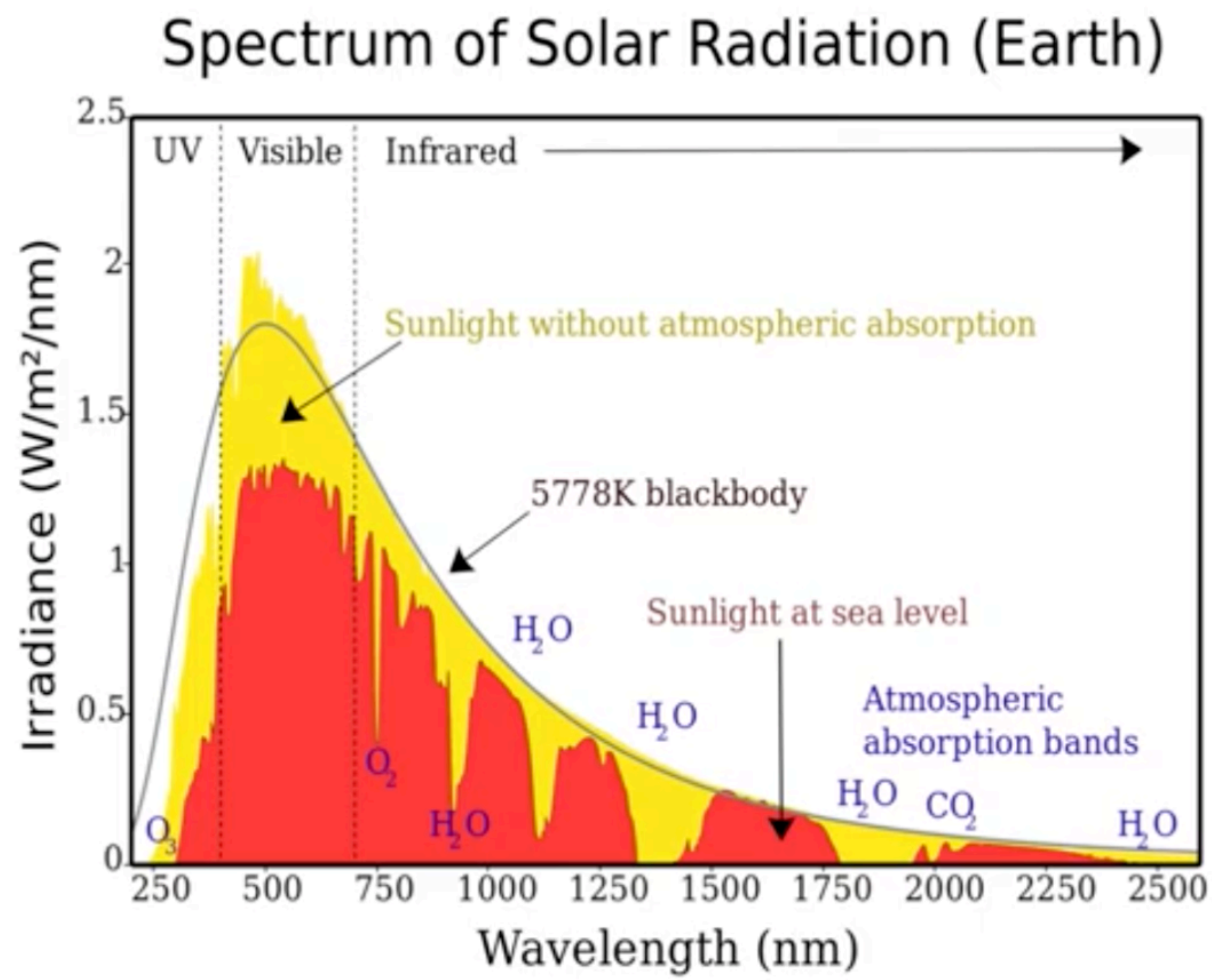


Conceptual Black Body

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 $B_\lambda(T)$.

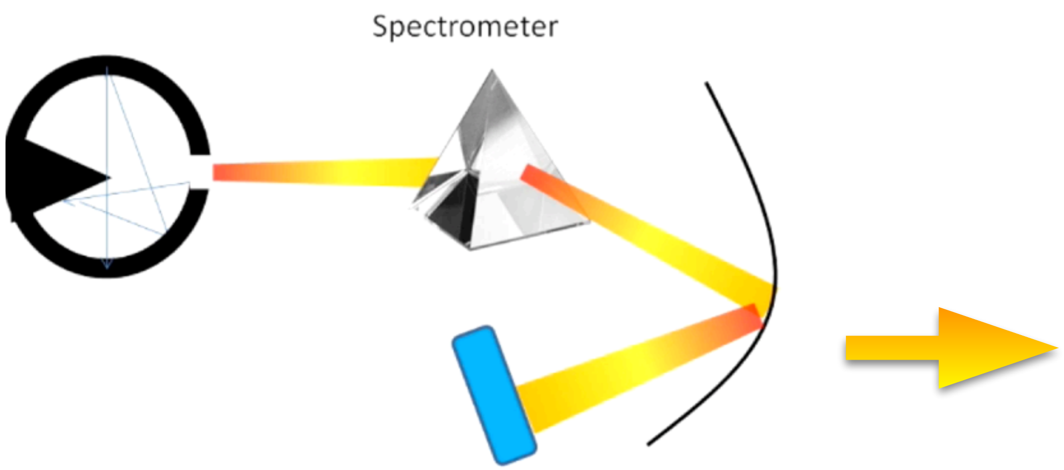
Black Body Radiation: SUN as an examples

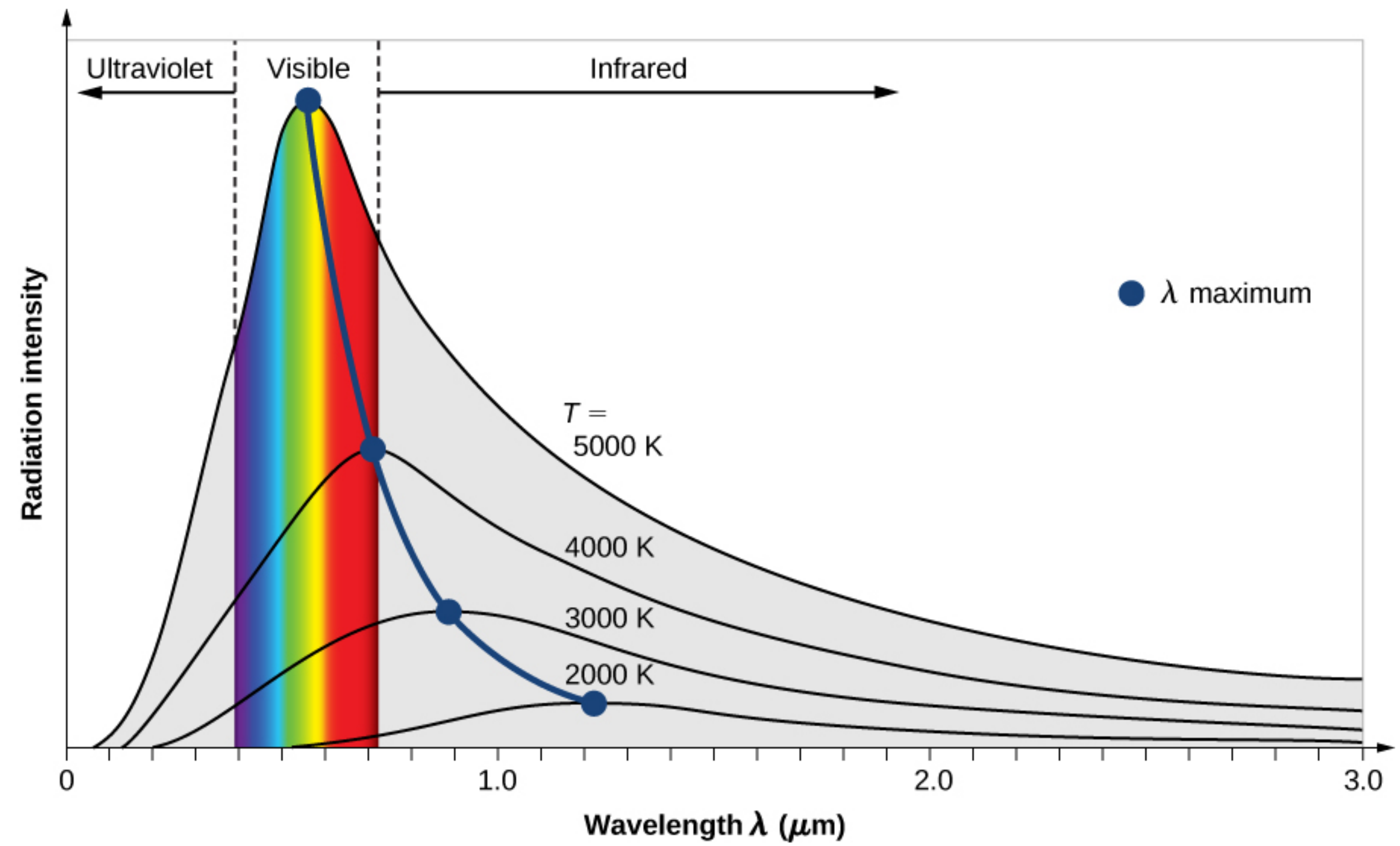
the sun is a blackbody



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

Blackbody Radiation

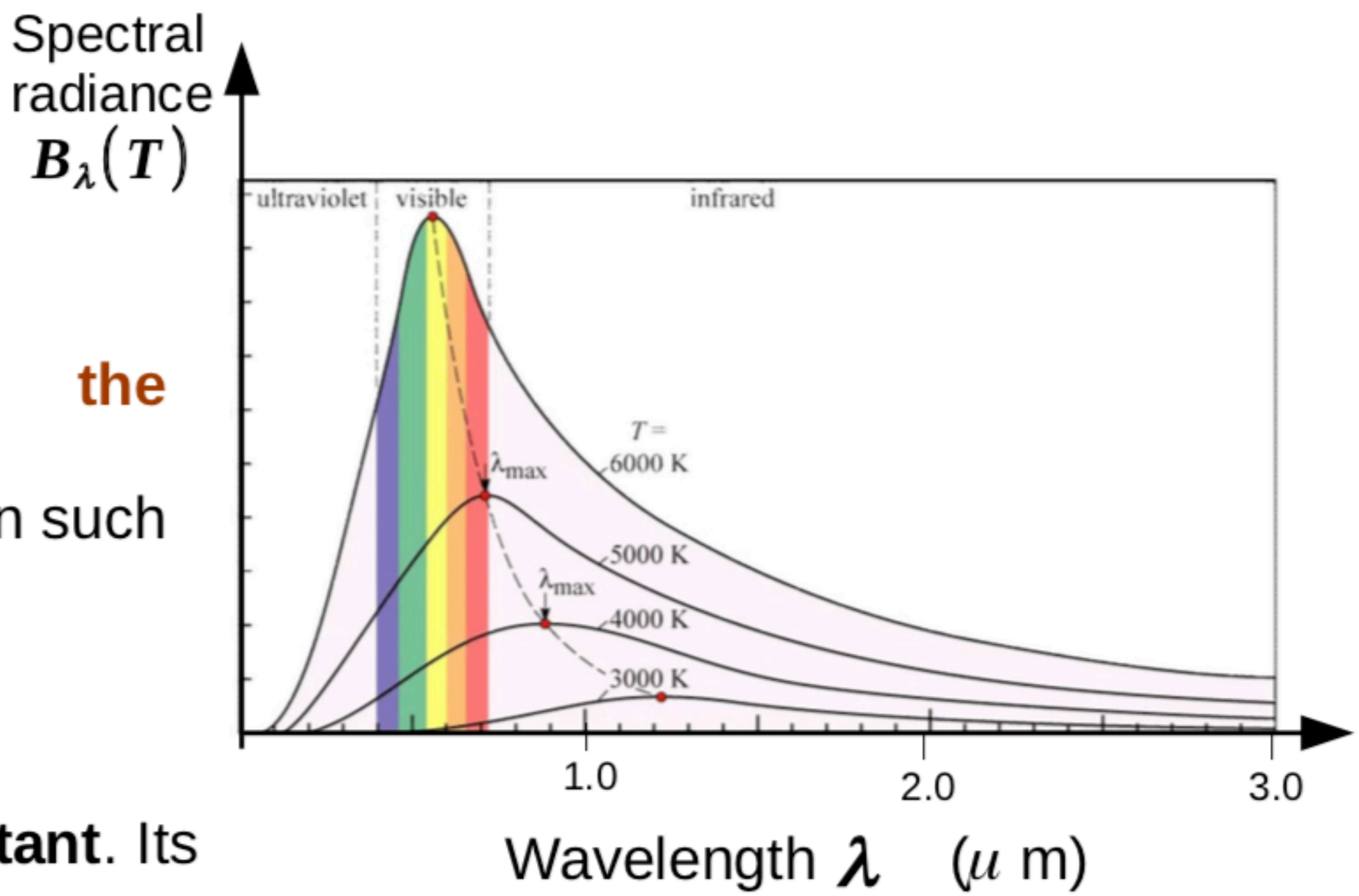




Experimental Observations:

- 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

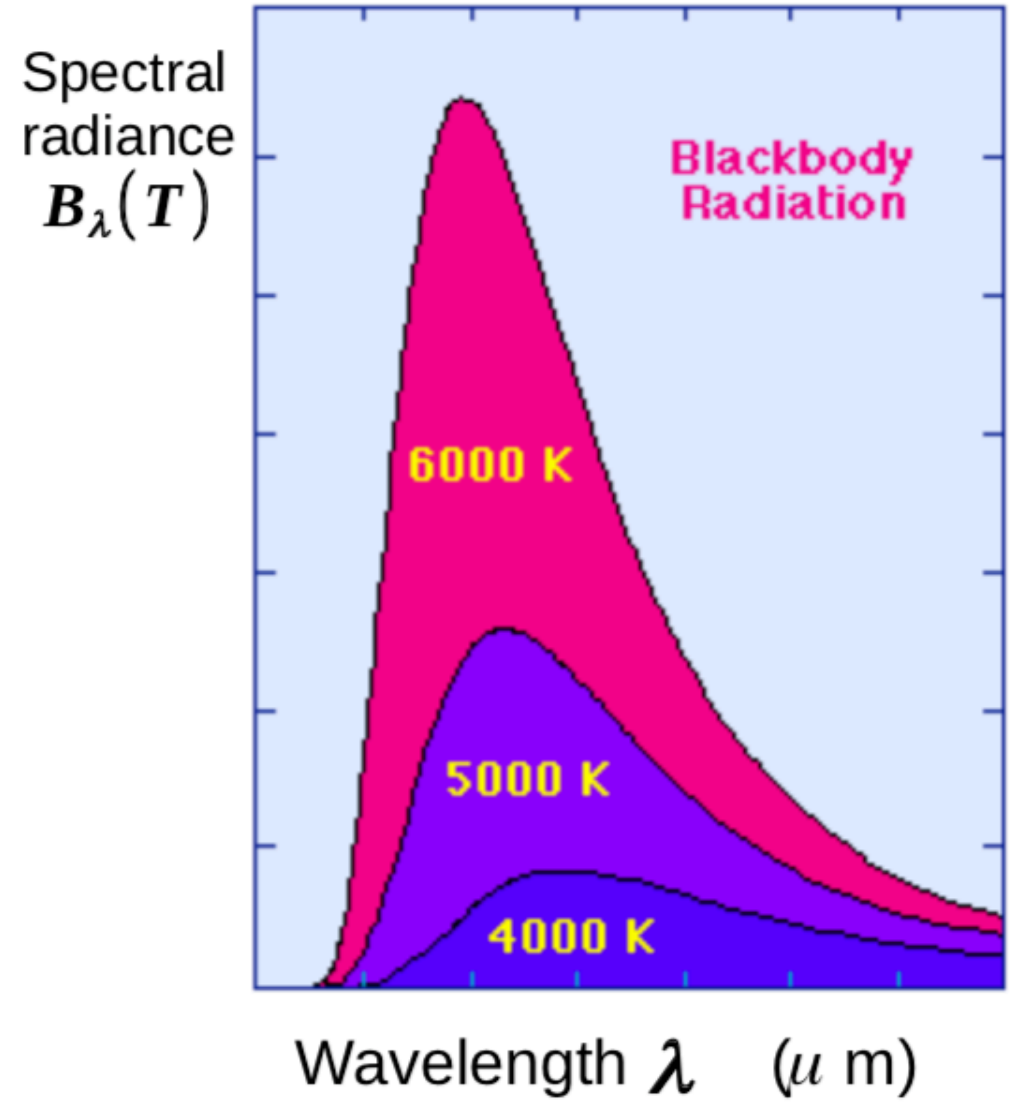
Stefan-Boltzmann law

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,**

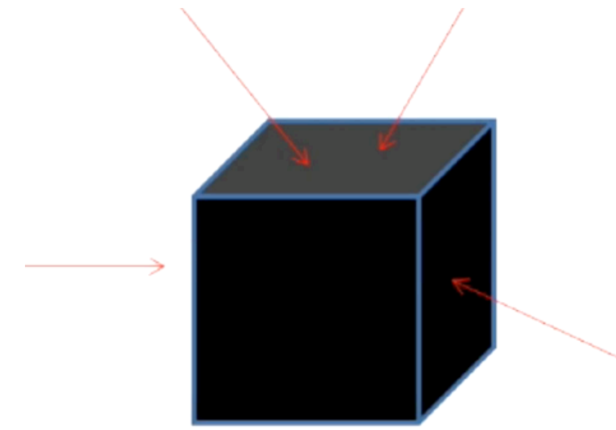
$$\sigma = 5.67 \times 10^{-8}\ J\ s^{-1}\ m^{-2}\ K^{-4}$$

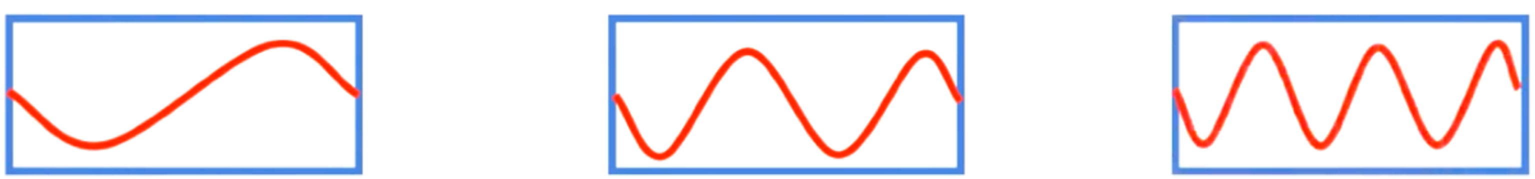


But how does the radiation spectrum itself depend on wavelength?

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; $\bar{\epsilon} = k_B T$



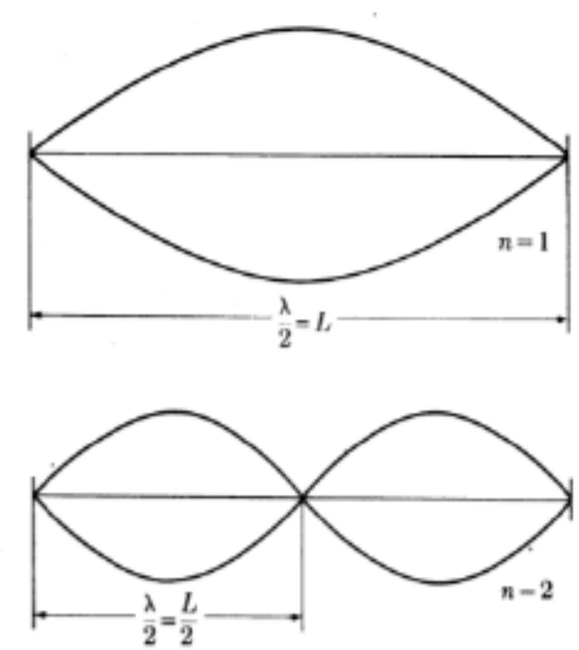


1 mode $\frac{1}{2}kT$

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

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

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

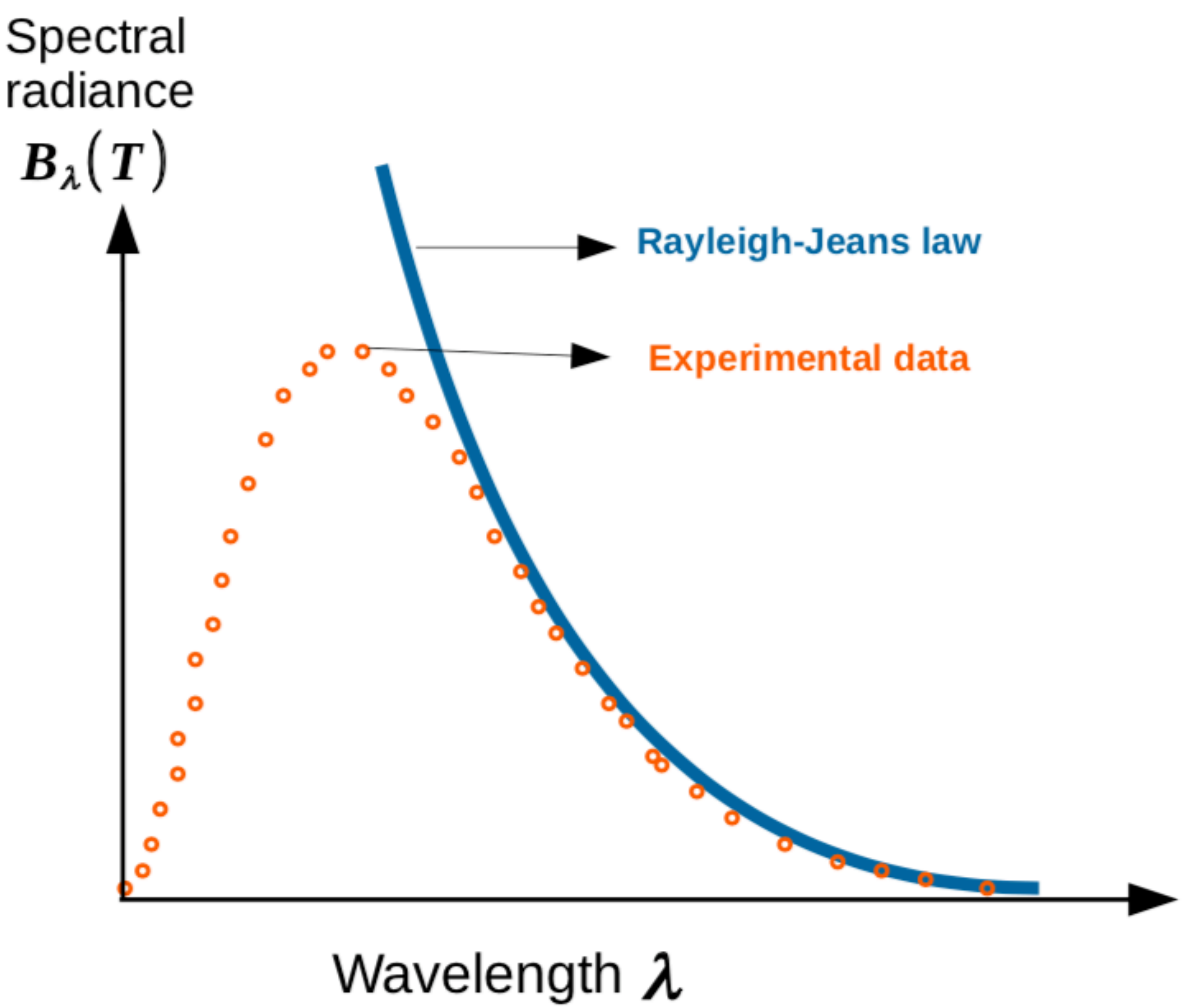


Standing waves which can be fitted between two perfectly reflecting walls forms a standing wave.

Rayleigh-Jeans Law: Classical Approach

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

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



Failure

- based classical physics arguments

- it works only for large wavelengths

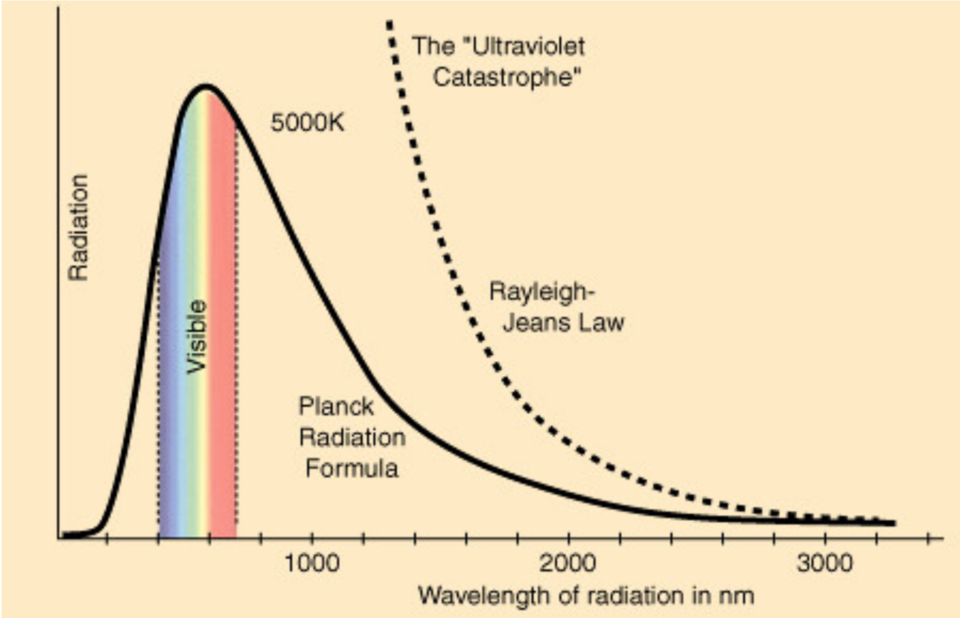
- does not reproduce Wein's displacement law and Stefan-Boltzmann law

ultra-violet catastrophe!

Ultraviolet means low wavelength!

Rayleigh-Jeans Law: Ultraviolet catastrophe

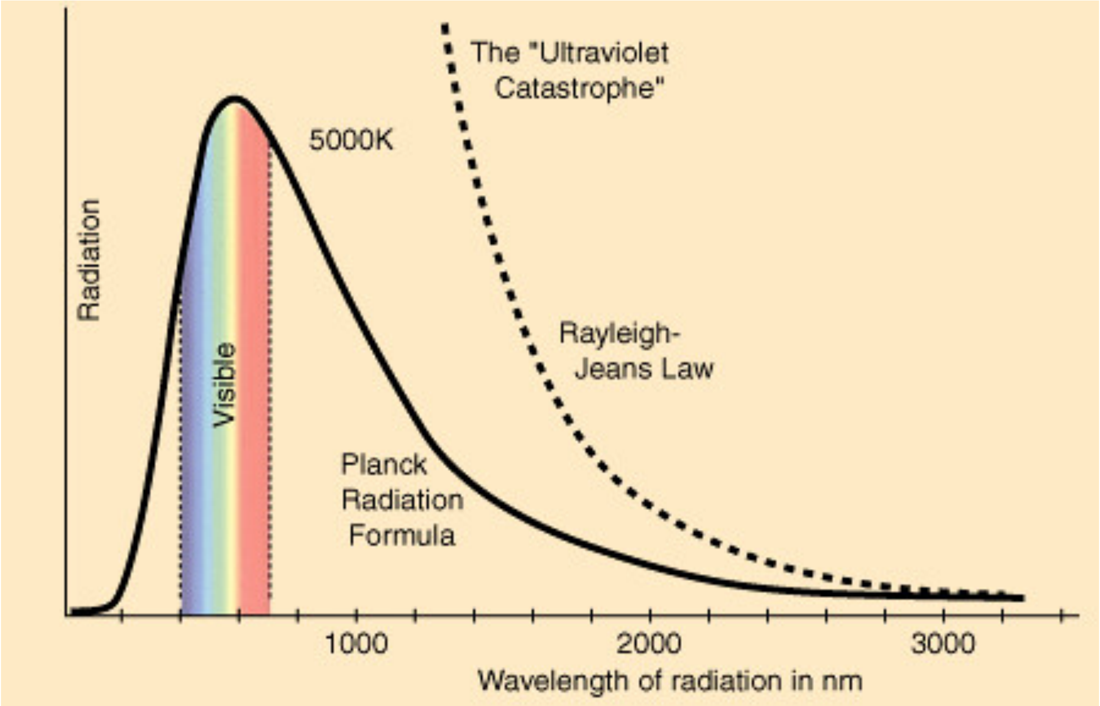
- Rayleigh-Jeans law gives an approximate spectral radiance for blackbody radiation.
- Rayleigh-Jeans law based on classical physics arguments in which the energy is assumed to be continuous.
- It predicts an energy output that diverges towards infinity as wavelength decreases.
- This equation agrees 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!**



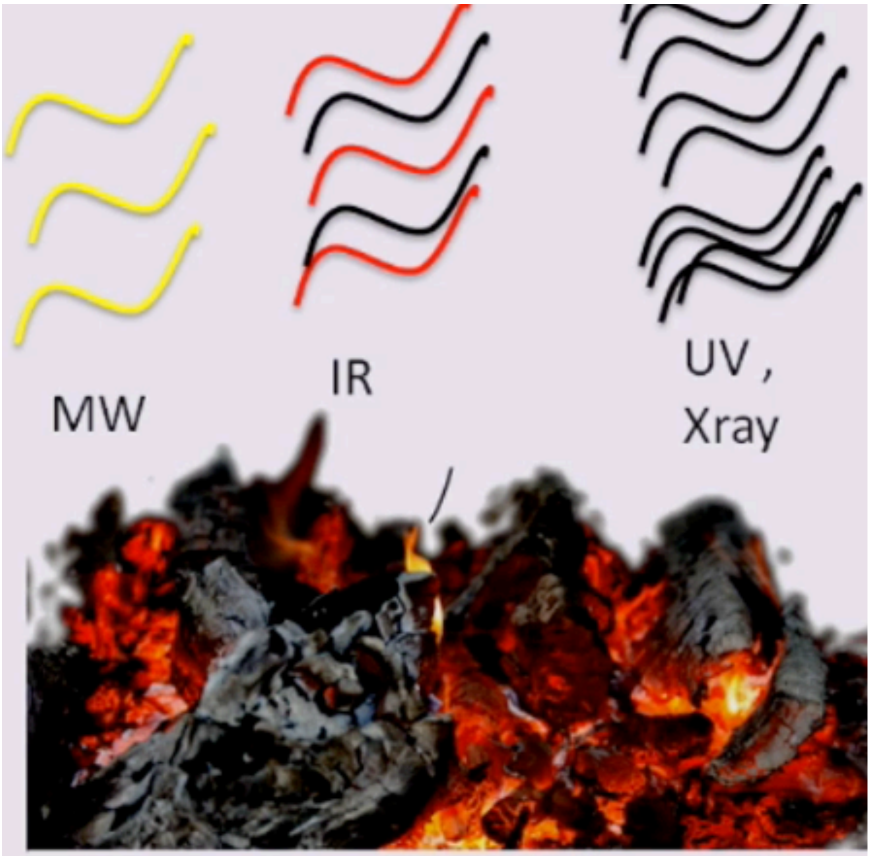
$$\boxed{B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}}$$

Rayleigh-Jeans Law: Ultraviolet Catastrophe

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



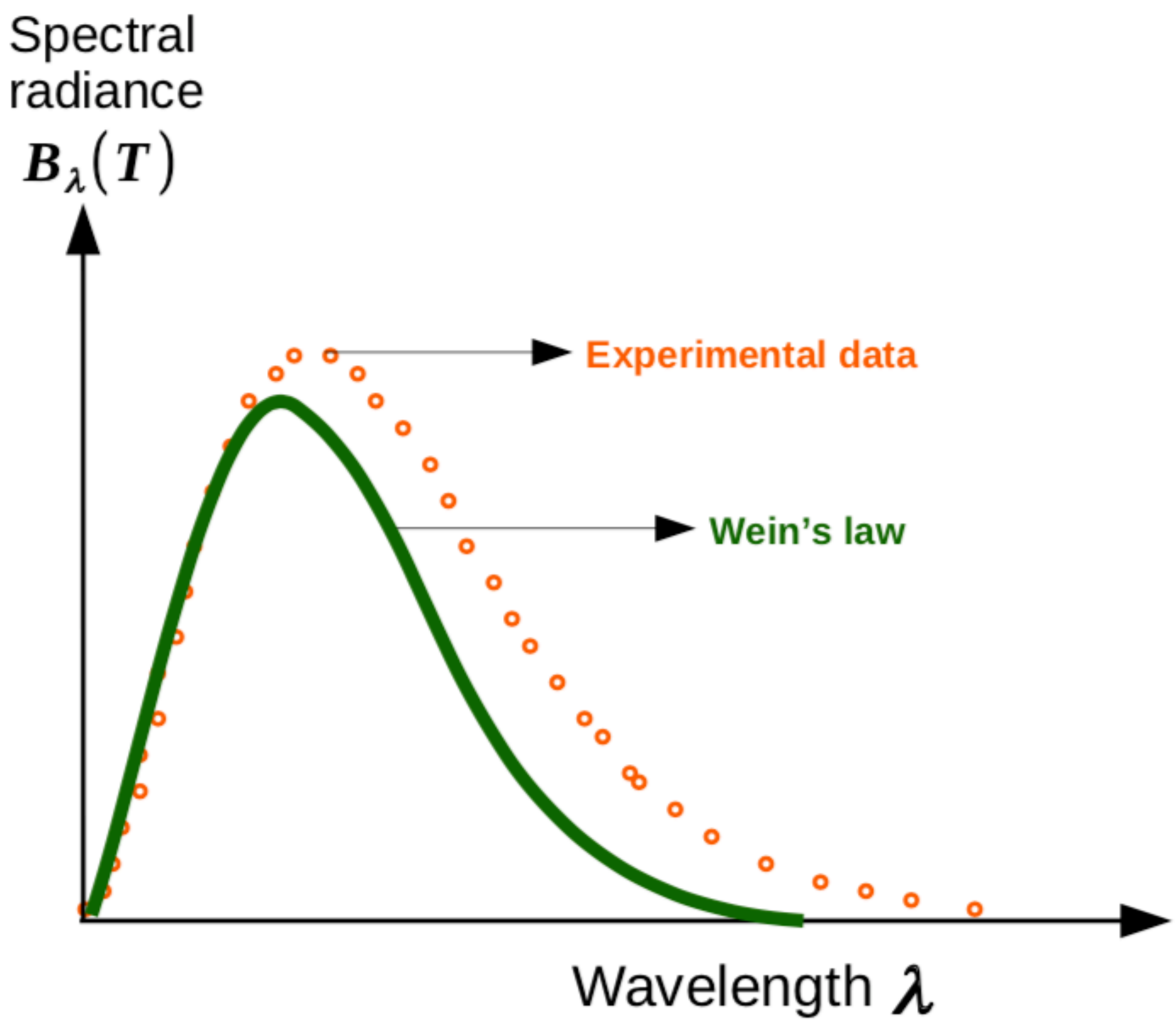
Discrepancy between theory and experiments at higher frequencies (shorter wavelength) Ultra-violet Catastrophe



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

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

Wein's Law

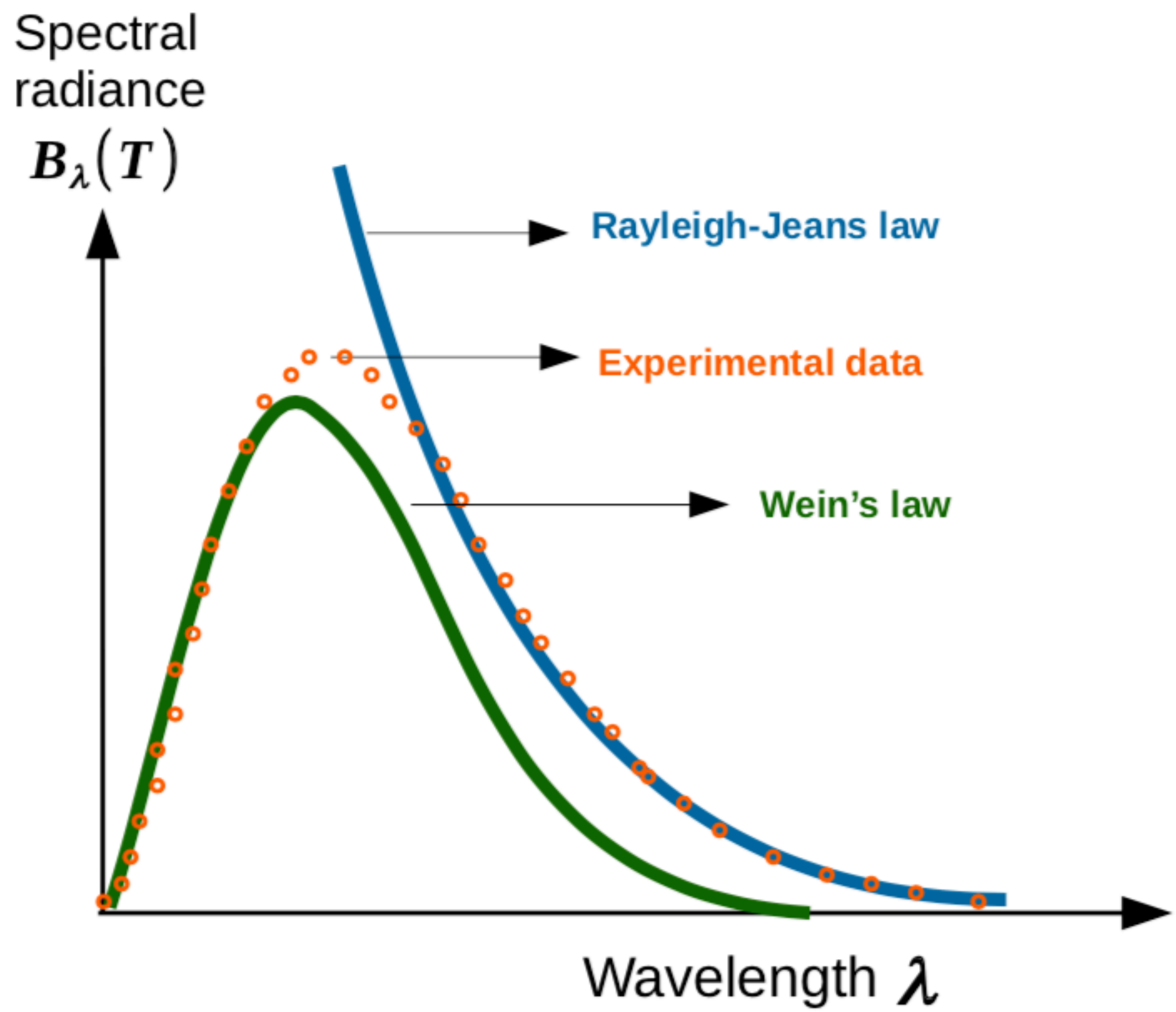


This law can be derived using standard classical physics tools.

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

Works only for small wavelengths

Failures of classical approach

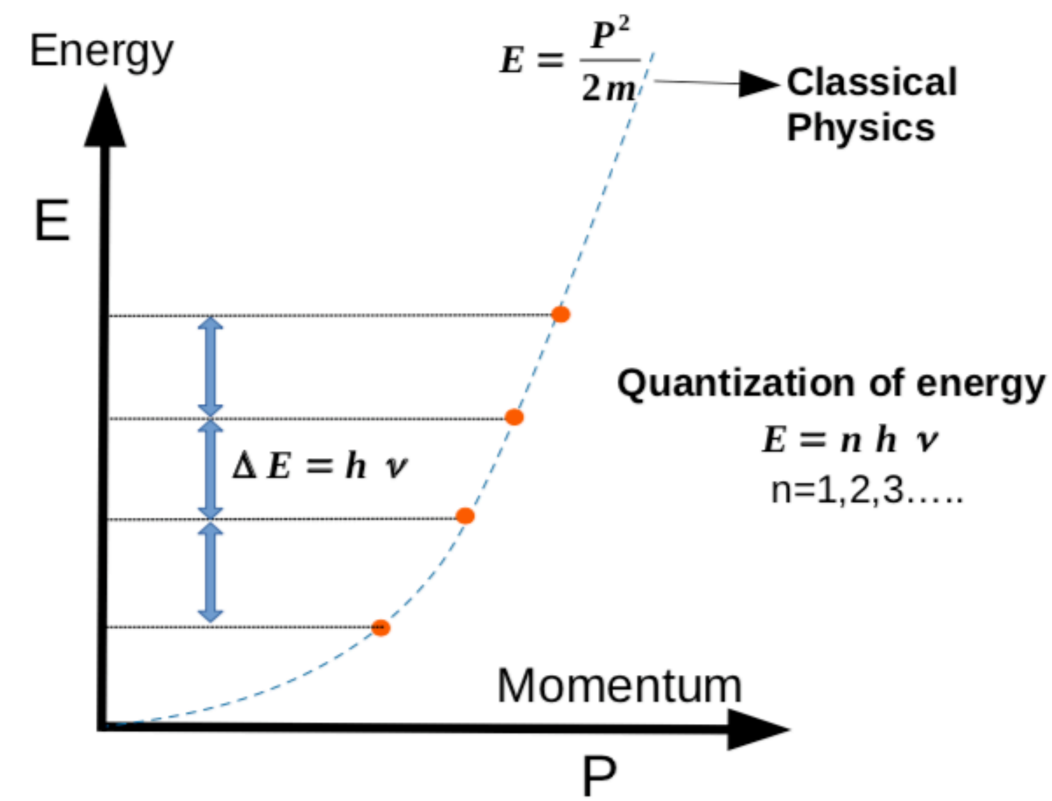


Classical theory fails to find a mathematical description of blackbody radiation intensity!

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

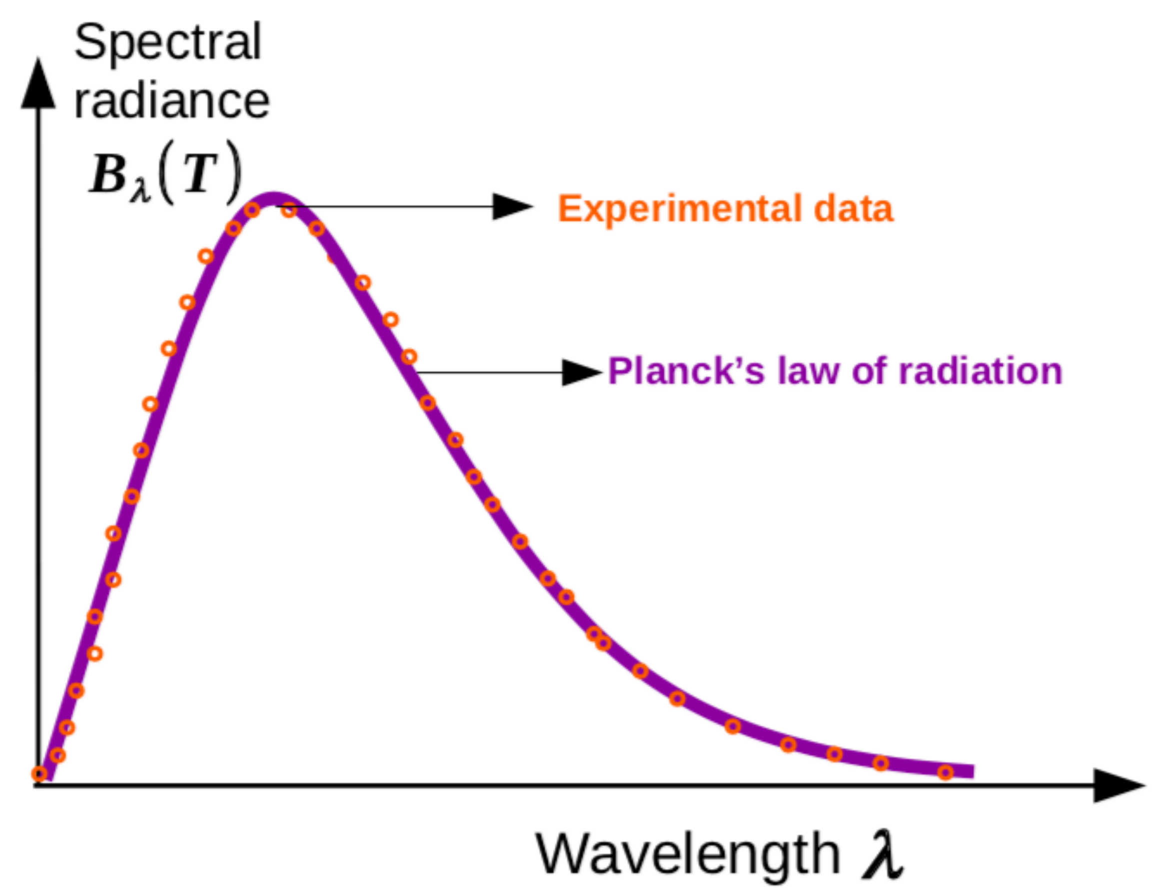
Planck's Theory of Blackbody Radiation

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

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

Derivation (not in the syllabus)

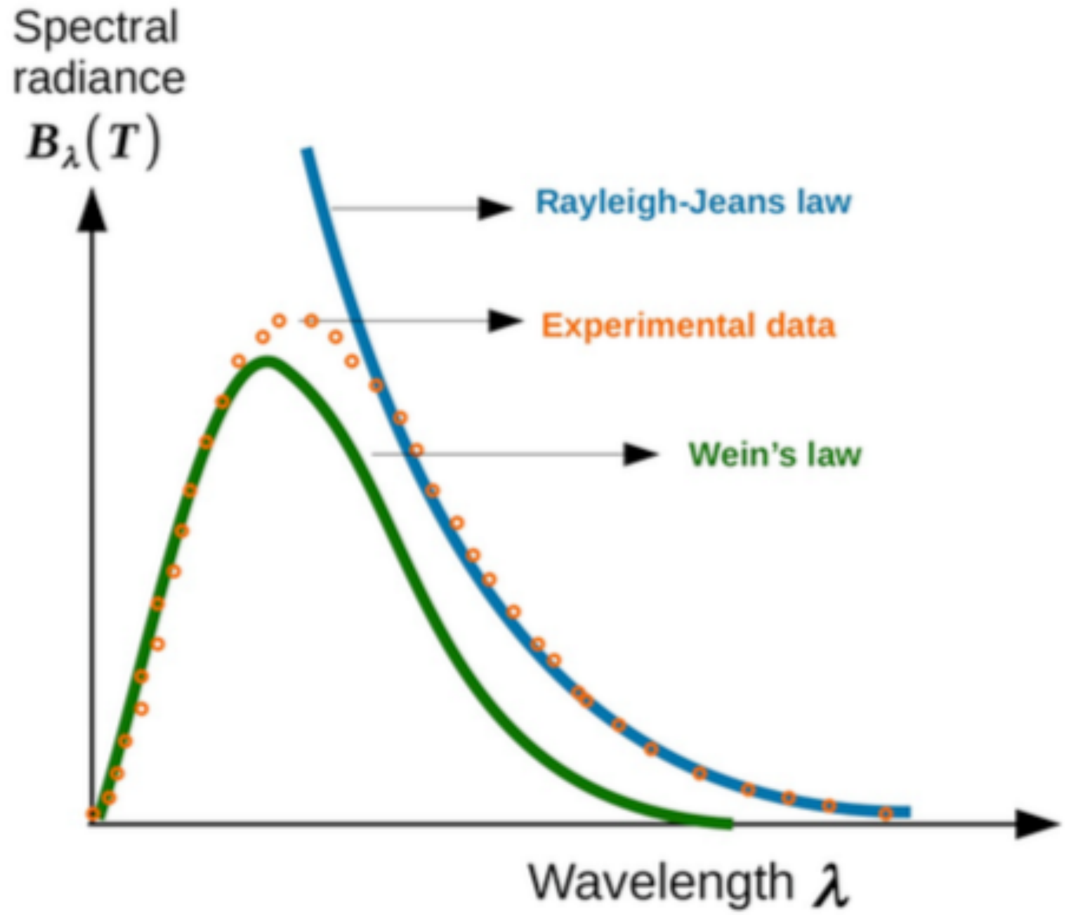


Planck's law of radiation **matches perfectly with the experiment**.

Classical Vs Quantum approach for BlackBody

Classical Physics

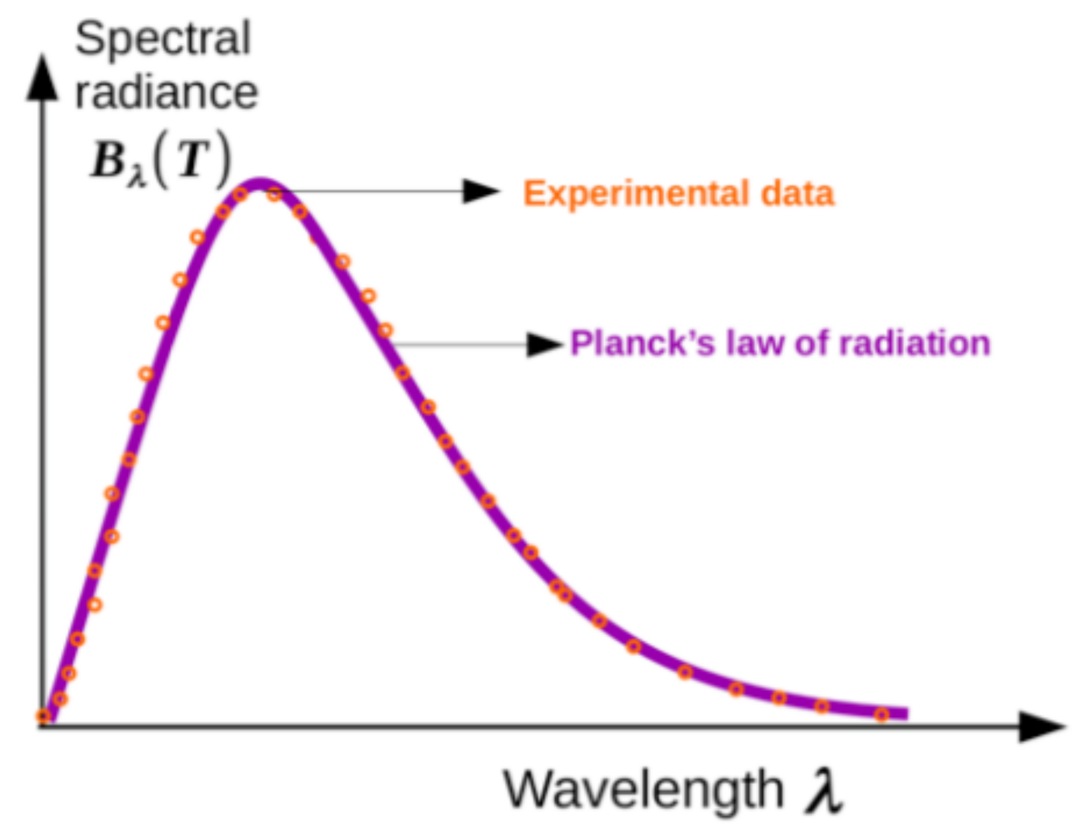
Rayleigh-Jeans law $$B_\lambda(T) = \frac{8\,\pi\,k_B\,T}{\lambda^4}$$



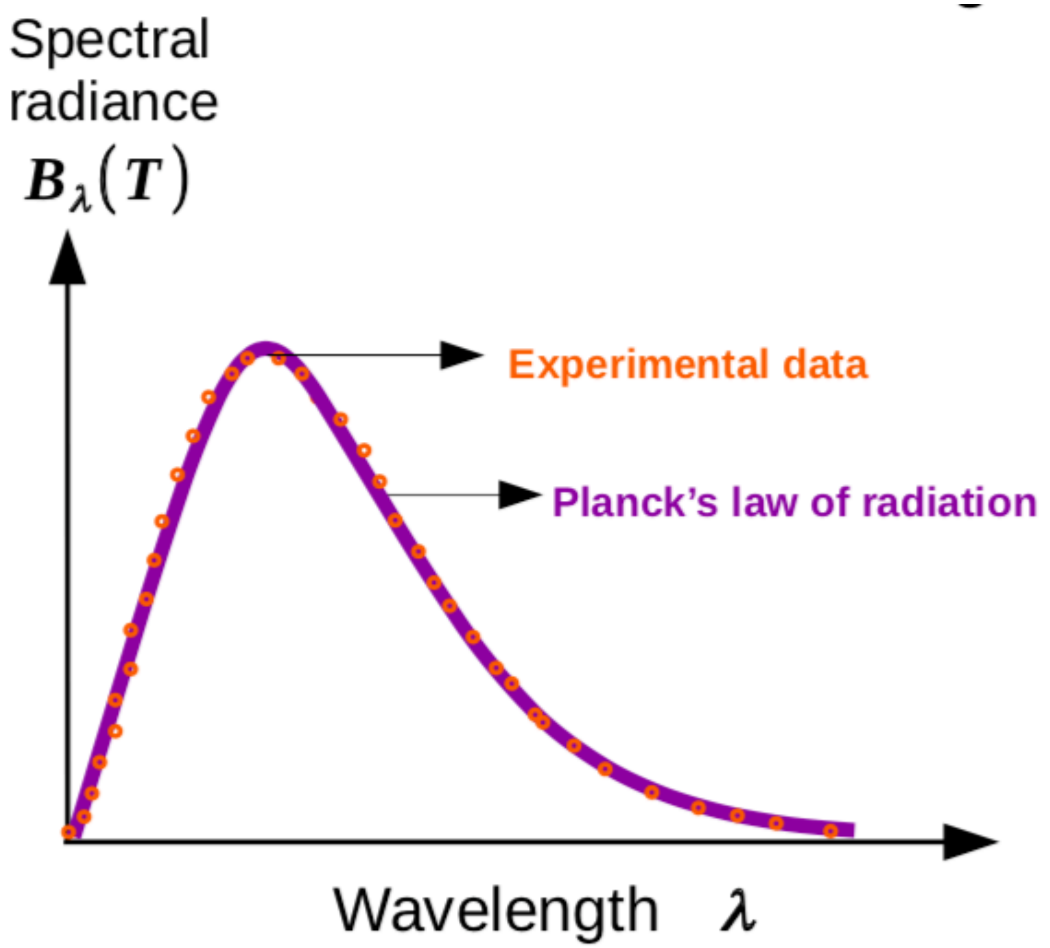
Quantum Physics

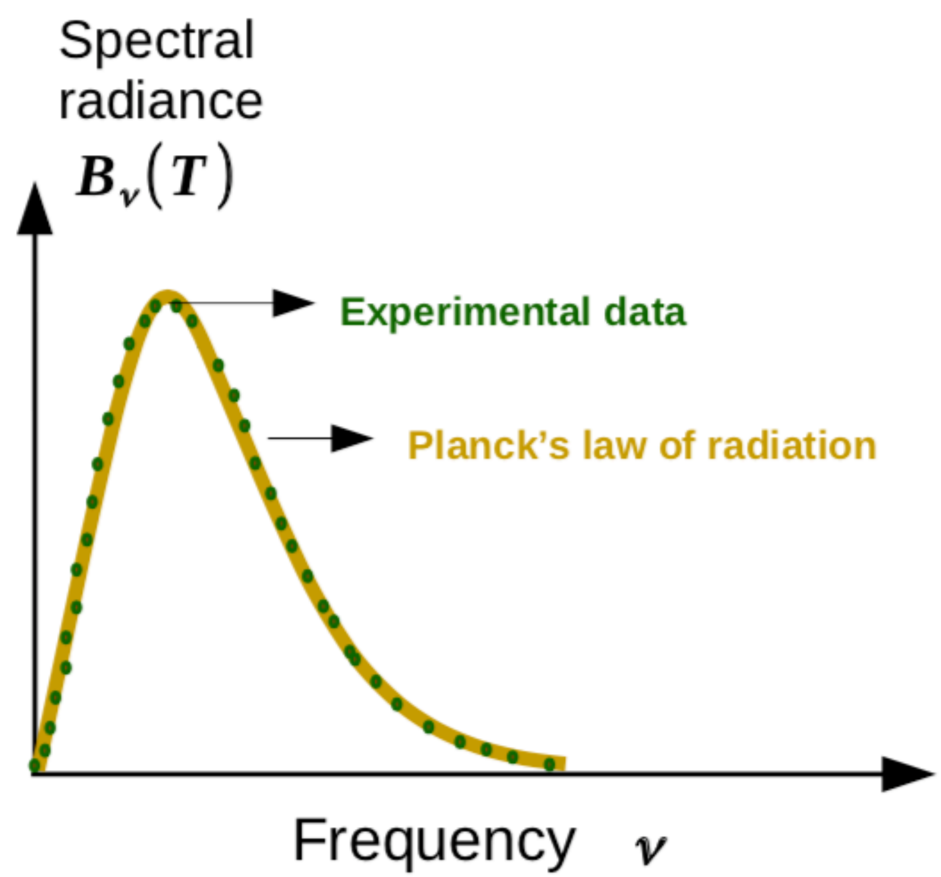
Planck's law

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



Max-Planck's Theory: Frequency





$$B_\lambda(T) = \frac{8\,\pi\,h\,c}{\lambda^5}\,\frac{1}{e^{\left(\frac{h\,c}{\lambda\,k_B\,T}\right)}-1} \quad \Longleftrightarrow \quad B_\nu(T) = \frac{8\,\pi\,h\,\nu^3}{c^3}\,\frac{1}{e^{\left(\frac{h\,\nu}{k_B\,T}\right)}-1}$$

Max-Planck's Theory of Blackbody Radiation

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:

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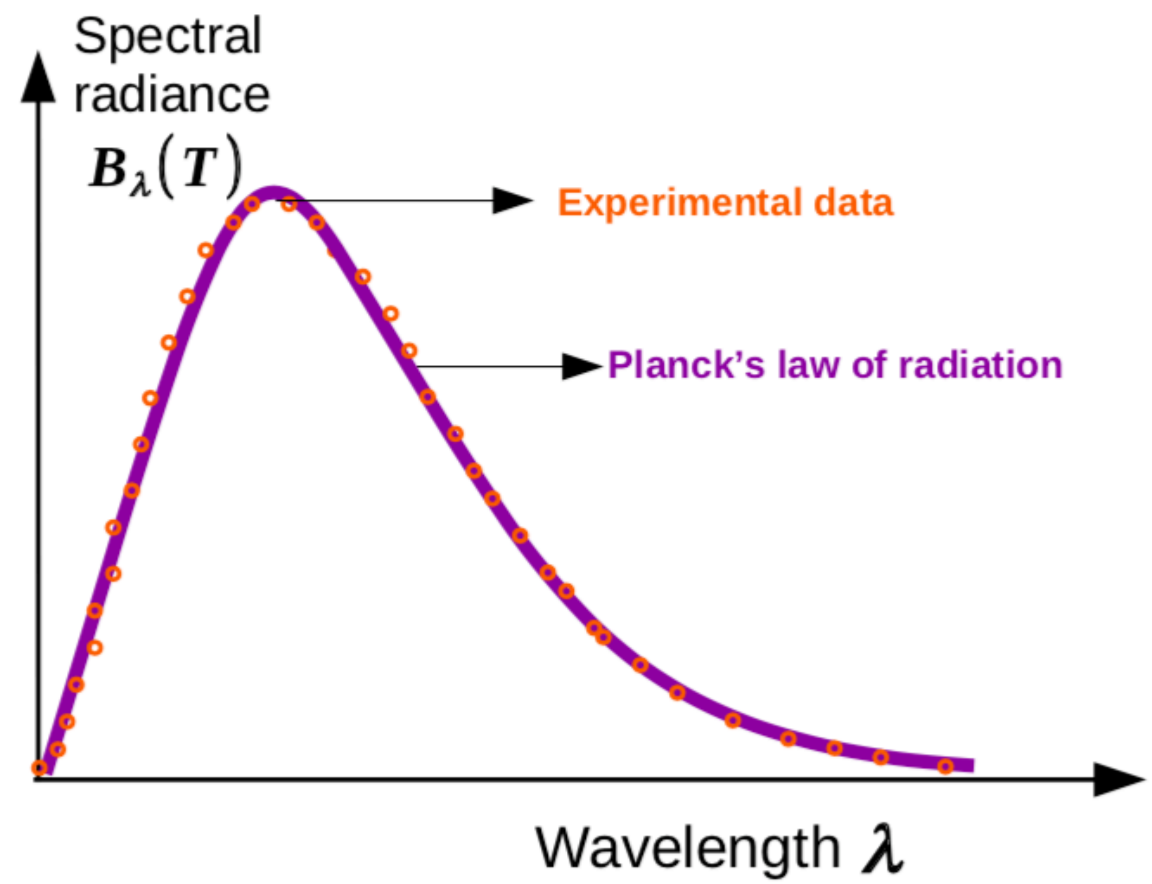
Derivation (not in the syllabus)



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

$e^{\left(\frac{hc}{\lambda k_\beta T}\right)}$ **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

$e^{\left(\frac{hc}{\lambda k_\beta T}\right)}$ **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.

should be frequently repolished" to ensure reliable operation of the spark.[2] Apparently this result was initially quite mysterious to Hertz. In an effort to resolve the mystery, he later investigated this side effect and concluded that it was the ultraviolet light from the initial spark acting on a clean metal surface that caused current to flow more freely between the poles of the spark gap. In the process of verifying the electromagnetic wave theory of light, Hertz had discovered the photoelectric effect, a phenomenon that would undermine the priority of the wave theory of light and establish the particle theory of light on an equal footing.

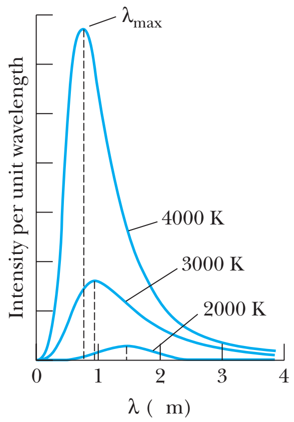


Figure 3.3 Emission from a glowing solid. Note that the amount of radiation emitted (the area under the curve) increases rapidly with increasing temperature.

3.2 BLACKBODY RADIATION

The tremendous success of Maxwell's theory of light emission immediately led to attempts to apply it to a long-standing puzzle about radiation—the so-called "blackbody" problem. The problem is to predict the radiation intensity at a given wavelength emitted by a hot glowing solid at a specific temperature. Instead of launching immediately into Planck's solution of this problem, let us develop a feeling for its importance to classical physics by a quick review of its history.

Thomas Wedgwood, Charles Darwin's relative and a renowned maker of china, seems to have been the first to note the universal character of all heated objects. In 1792, he observed that all the objects in his ovens, regardless of their chemical nature, size, or shape, became red at the same temperature. This crude observation was sharpened considerably by the advancing state of spectroscopy, so that by the mid-1800s it was known that glowing solids emit continuous spectra rather than the bands or lines emitted by heated gases. (See Fig. 3.3.) In 1859, Gustav Kirchhoff proved a theorem as important as his circuit loop theorem when he showed by arguments based on thermodynamics that for any body in thermal equilibrium with radiation[3] the emitted power is proportional to the power absorbed. More specifically,

$$e_f = J(f, T)A_f \tag{3.1}$$

where e_f is the power emitted per unit area per unit frequency by a particular heated object, A_f is the absorption power (fraction of the incident power absorbed per unit area per unit frequency by the heated object), and $J(f, T)$ is a universal function (the same for all bodies) that depends only on f, the light frequency, and T, the absolute temperature of the body. A *blackbody* is defined as an object that absorbs all the electromagnetic radiation falling on it and consequently appears black. It has $A_f = 1$ for all frequencies and so Kirchhoff's theorem for a blackbody becomes

Blackbody

$$e_f = J(f, T) \tag{3.2}$$

[2] H. Hertz, *Ann. Physik* (Leipzig), 33:983, 1887.

[3] An example of a body in equilibrium with radiation would be an oven with closed walls at a fixed temperature and the radiation within the oven cavity. To say that radiation is in thermal equilibrium with the oven walls means that the radiation has exchanged energy with the walls many times and is homogeneous, isotropic, and unpolarized. In fact, thermal equilibrium of radiation within a cavity can be considered to be quite similar to the thermal equilibrium of a fluid within a container held at constant temperature—both will cause a thermometer in the center of the cavity to achieve a final stationary temperature equal to that of the container.

Equation 3.2 shows that the power emitted per unit area per unit frequency by a blackbody depends only on temperature and light frequency and not on the physical and chemical makeup of the blackbody, in agreement with Wedgwood's early observation.

Because absorption and emission are connected by Kirchhoff's theorem, we see that a blackbody or perfect absorber is also an ideal radiator. In practice, a small opening in any heated cavity, such as a port in an oven, behaves like a blackbody because such an opening traps all incident radiation (Fig. 3.4). If the direction of the radiation is reversed in Figure 3.4, the light emitted by a small opening is in thermal equilibrium with the walls, because it has been absorbed and re-emitted many times.

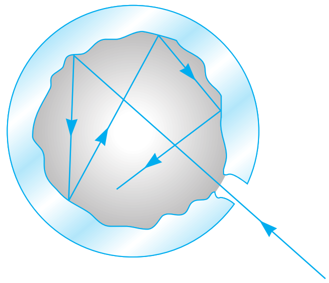


Figure 3.4 The opening to the cavity inside a body is a good approximation of a blackbody. Light entering the small opening strikes the far wall, where some of it is absorbed but some is reflected at a random angle. The light continues to be reflected, and at each reflection a portion of the light is absorbed by the cavity walls. After many reflections essentially all of the incident energy is absorbed.

The next important development in the quest to understand the universal character of the radiation emitted by glowing solids came from the Austrian physicist Josef Stefan (1835–1893) in 1879. He found experimentally that the total power per unit area emitted at all frequencies by a hot solid, e_{total}, was proportional to the fourth power of its absolute temperature. Therefore, Stefan's law may be written as

$$e_{\text{total}} = \int_0^{\infty} e_f \, df = \sigma T^4 \tag{3.3}$$

where e_{total} is the power per unit area emitted at the surface of the blackbody at all frequencies, e_f is the power per unit area per unit frequency emitted by the blackbody, T is the absolute temperature of the body, and σ is the Stefan–Boltzmann constant, given by $\sigma = 5.67 \times 10^{-8}\ \text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-4}$. A body that is not an ideal radiator will obey the same general law but with a coefficient, a, less than 1:

Stefan's law

$$e_{\text{total}} = a\sigma T^4 \tag{3.4}$$

Only 5 years later another impressive confirmation of Maxwell's electromagnetic theory of light occurred when Boltzmann derived Stefan's law from a combination of thermodynamics and Maxwell's equations.

EXAMPLE 3.1 Stefan's Law Applied to the Sun

Estimate the surface temperature of the Sun from the following information. The Sun's radius is given by $R_s = 7.0 \times 10^8$ m. The average Earth–Sun distance is $R = 1.5 \times 10^{11}$ m. The power per unit area (at all frequencies) from the Sun is measured at the Earth to be $1400\ \text{W/m}^2$. Assume that the Sun is a blackbody.

Solution For a black body, we take $a = 1$, so Equation 3.4 gives

$$e_{\text{total}}(R_s) = \sigma T^4 \tag{3.5}$$

where the notation $e_{\text{total}}(R_s)$ stands for the total power per unit area at the surface of the Sun. Because the problem gives the total power per unit area at the Earth, $e_{\text{total}}(R)$, we need the connection between $e_{\text{total}}(R)$ and $e_{\text{total}}(R_s)$. This comes from the conservation of energy:

$$e_{\text{total}}(R_s)\cdot 4\pi R_s^2 = e_{\text{total}}(R)\cdot 4\pi R^2$$

or

$$e_{\text{total}}(R_s) = e_{\text{total}}(R)\cdot \frac{R^2}{R_s^2}$$

Using Equation 3.5, we have

$$T = \left[\frac{e_{\text{total}}(R)\cdot R^2}{\sigma R_s^2}\right]^{1/4}$$

or

$$T = \left[\frac{(1400\ \text{W/m}^2)(1.5\times 10^{11}\ \text{m})^2}{(5.6\times 10^{-8}\ \text{W/m}^2\cdot\text{K}^4)(7.0\times 10^8\ \text{m})^2}\right]^{1/4}$$
$$= 5800\ \text{K}$$

As can be seen in Figure 3.3, *the wavelength marking the maximum power emission of a blackbody*, λ_{max}, shifts toward shorter wavelengths as the blackbody gets hotter. This agrees with Wedgwood's general observation that objects in his kiln progressed from dull red to orange to white in color as the temperature was raised. This simple effect of $\lambda_{max} \propto T^{-1}$ was not definitely established, however, until about 20 years after Kirchhoff's seminal paper had started the search to find the form of the universal function $J(f, T)$. In 1893, Wilhelm Wien proposed a general form for the blackbody distribution law $J(f, T)$ that gave the correct experimental behavior of λ_{max} with temperature. This law is called *Wien's displacement law* and may be written

$$\lambda_{max} T = 2.898 \times 10^{-3}\ \text{m} \cdot \text{K} \tag{3.6}$$

where λ_{max} is the wavelength in meters corresponding to the blackbody's maximum intensity and T is the absolute temperature of the surface of the object emitting the radiation. Assuming that the peak sensitivity of the human eye (which occurs at about 500 nm—blue-green light) coincides with λ_{max} for the Sun (a blackbody), we can check the consistency of Wien's displacement law with Stefan's law by recalculating the Sun's surface temperature:

$$T = \frac{2.898 \times 10^{-3}\ \text{m} \cdot \text{K}}{500 \times 10^{-9}\ \text{m}} = 5800\ \text{K}$$

Thus we have good agreement between measurements made at all wavelengths (Example 3.1) and at the maximum-intensity wavelength.

Exercise 1 How convenient that the Sun's emission peak is at the same wavelength as our eyes' sensitivity peak! Can you account for this?

Spectral energy density of a blackbody

So far, the power radiated per unit area per unit frequency by the blackbody, $J(f, T)$ has been discussed. However, it is more convenient to consider the spectral energy density, or *energy per unit volume per unit frequency of the radiation within the blackbody cavity,* $u(f, T)$. For light in equilibrium with the walls, the power emitted per square centimeter of opening is simply proportional to the energy density of the light in the cavity. Because the cavity radiation is isotropic and unpolarized, one can average over direction to show that the constant of proportionality between $J(f, T)$ and $u(f, T)$ is $c/4$, where c is the speed of light. Therefore,

$$J(f, T) = u(f, T)c/4 \tag{3.7}$$

An important guess as to the form of the universal function $u(f, T)$ was made in 1893 by Wien and had the form

$$u(f, T) = Af^3 e^{-\beta f/T} \tag{3.8}$$

where A and β are constants. This result was known as Wien's exponential law; it resembles and was loosely based on Maxwell's velocity distribution for gas molecules. Within a year the great German spectroscopist Friedrich Paschen

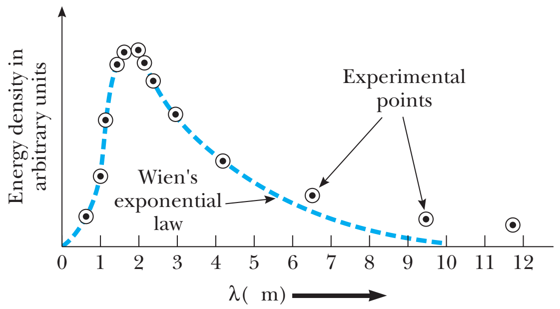


Figure 3.5 Discrepancy between Wien's law and experimental data for a blackbody at 1500 K.

had confirmed Wien's guess by working in the then difficult infrared range of 1 to 4 μm and at temperatures of 400 to 1600 K.[4]

As can be seen in Figure 3.5, Paschen had made most of his measurements in the maximum energy region of a body heated to 1500 K and had found good agreement with Wien's exponential law. In 1900, however, Lummer and Pringsheim extended the measurements to 18 μm, and Rubens and Kurlbaum went even farther—to 60 μm. Both teams concluded that Wien's law failed in this region (see Fig. 3.5). The experimental setup used by Rubens and Kurlbaum is shown in Figure 3.6. It is interesting to note that these historic

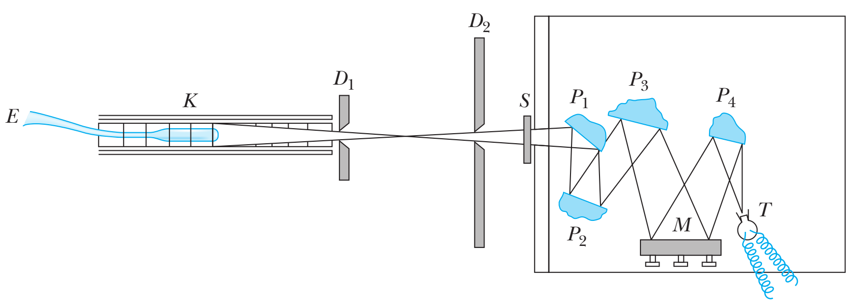


Figure 3.6 Apparatus for measuring blackbody radiation at a single wavelength in the far infrared region. The experimental technique that disproved Wien's law and was so crucial to the discovery of the quantum theory was the method of residual rays (*Restrahlen*). In this technique, one isolates a narrow band of far infrared radiation by causing white light to undergo multiple reflections from alkalide halide crystals (P_1–P_4). Because each alkali halide has a maximum reflection at a characteristic wavelength, quite pure bands of far infrared radiation may be obtained with repeated reflections. These pure bands can then be directed onto a thermopile (T) to measure intensity. E is a thermocouple used to measure the temperature of the blackbody oven, K.

[4]We should point out the great difficulty in making blackbody radiation measurements and the singular advances made by German spectroscopists in the crucial areas of blackbody sources, sensitive detectors, and techniques for operating far into the infrared region. In fact, it is dubious whether Planck would have found the correct blackbody law as quickly without his close association with the experimentalists at the Physikalisch Technische Reichsanstalt of Berlin (a sort of German National Bureau of Standards)—Otto Lummer, Ernst Pringsheim, Heinrich Rubens, and Ferdinand Kurlbaum.

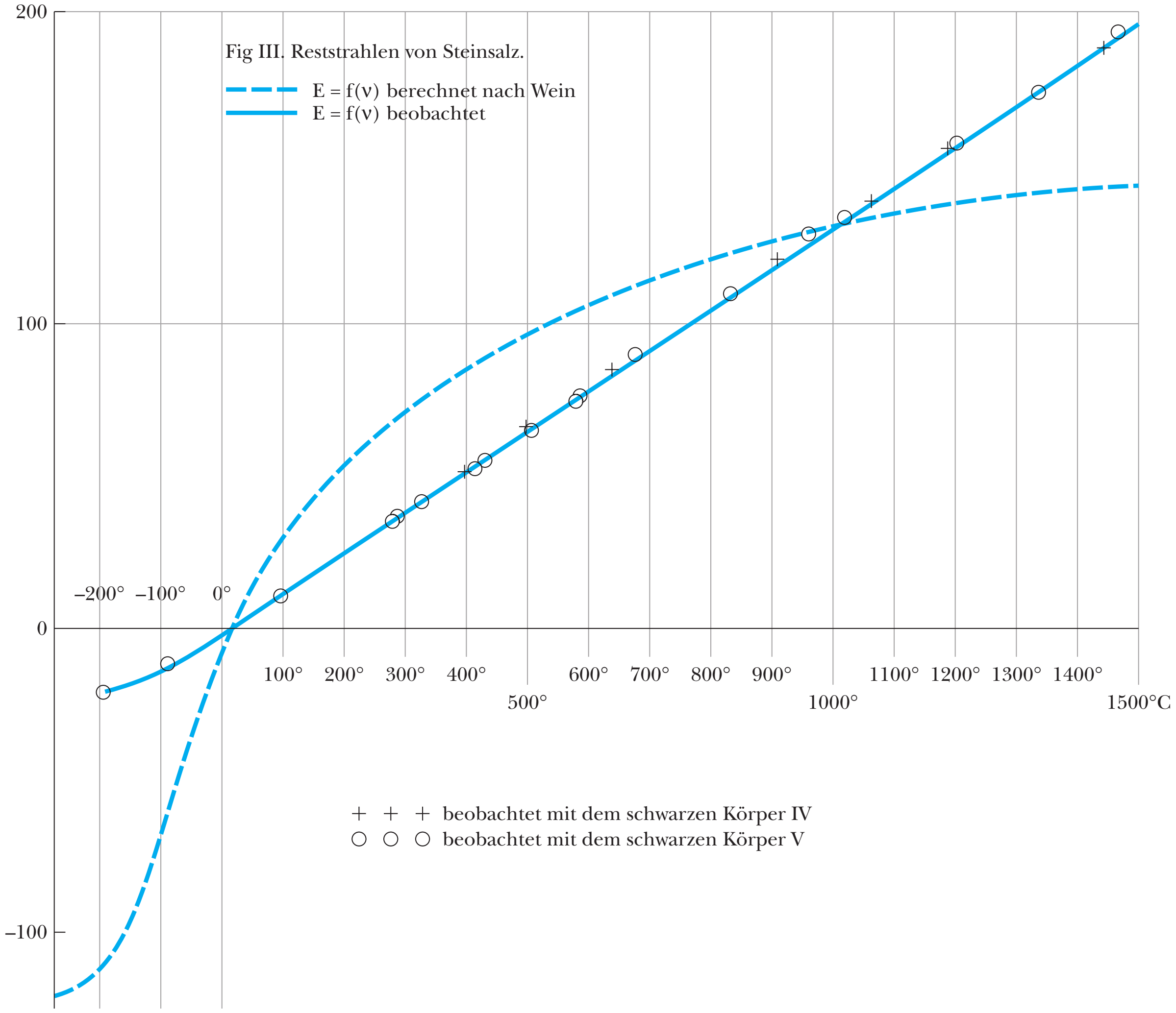


Figure 3.7 Comparison of theoretical and experimental blackbody emission curves at 51.2 μm and over the temperature range of $-188°$ to 1500°C. The title of this modified figure is "Residual Rays from Rocksalt." *Berechnet nach* means "calculated according to," and *beobachtet* means "observed." The vertical axis is emission intensity in arbitrary units. (*From H. Rubens and S. Kurlbaum,* Ann. Physik, *4:649, 1901.*)

experiments involved the measurement of blackbody radiation intensity at a fixed wavelength and variable temperature. Typical results measured at $\lambda = 51.2\ \mu$m and over the temperature range of $-200°$ to $+1500°$C are shown in Figure 3.7, from the paper by Rubens and Kurlbaum.

Enter Planck

On a Sunday evening early in October of 1900, Max Planck discovered the famous blackbody formula, which truly ushered in the quantum theory. Planck's proximity to the Reichsanstalt experimentalists was extremely important for his discovery—earlier in the day he had heard from Rubens that his latest measurements showed that $u(f, T)$, the spectral energy density, was proportional to T for long wavelengths or low frequency. Planck knew that Wien's law agreed well with the data at high frequency and indeed had been working hard for several years to derive Wien's exponential law from the principles of statistical mechanics and Maxwell's laws. Interpolating between the two limiting forms (Wien's exponential law and an energy density proportional to temperature), he immediately found a general formula, which he sent to Rubens, on a postcard, the same evening. His formula was[5]

$$u(f, T) = \frac{8\pi hf^3}{c^3}\left(\frac{1}{e^{hf/k_BT} - 1}\right) \tag{3.9}$$

where h is Planck's constant $= 6.626 \times 10^{-34}\ \mathrm{J \cdot s}$, and k_B is Boltzmann's constant $= 1.380 \times 10^{-23}\ \mathrm{J/K}$. We can see that Equation 3.9 has the correct limiting behavior at high and low frequencies with the help of a few approximations. At high frequencies, where $hf/k_BT \gg 1$,

$$\frac{1}{e^{hf/k_BT} - 1} \approx e^{-hf/k_BT}$$

so that

$$u(f, T) = \frac{8\pi hf^3}{c^3}\left(\frac{1}{e^{hf/k_BT} - 1}\right) \approx \frac{8\pi hf^3}{c^3}\, e^{-hf/k_BT}$$

and we recover Wien's exponential law, Equation 3.8. At low frequencies, where $hf/k_BT \ll 1$,

$$\frac{1}{e^{hf/k_BT} - 1} = \frac{1}{1 + \dfrac{hf}{k_BT} + \cdots - 1} \approx \frac{k_BT}{hf}$$

and

$$u(f, T) = \frac{8\pi hf^3}{c^3}\left(\frac{1}{e^{hf/k_BT} - 1}\right) \approx \frac{8\pi f^2}{c^3}\, k_BT$$

This result shows that the spectral energy density is proportional to T in the low-frequency or so-called classical region, as Rubens had found.

We should emphasize that Planck's work entailed much more than clever mathematical manipulation. For more than six years Planck (Fig. 3.8) labored to find a rigorous derivation of the blackbody distribution curve. He was driven, in his own words, by the fact that the emission problem "represents something absolute, and since I had always regarded the search for the absolute as the loftiest goal of all scientific activity, I eagerly set to work." This work was to occupy most of his life as he strove to give his formula an ever deeper physical interpretation and to reconcile discrete quantum energies with classical theory.

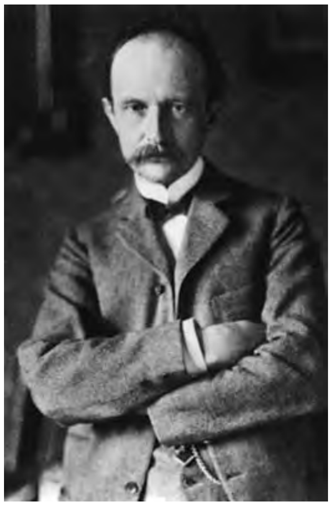


Figure 3.8 Max Planck (1858–1947). The work leading to the "lucky" blackbody radiation formula was described by Planck in his Nobel prize acceptance speech (1920): "But even if the radiation formula proved to be perfectly correct, it would after all have been only an interpolation formula found by lucky guess-work and thus, would have left us rather unsatisfied. I therefore strived from the day of its discovery, to give it a real physical interpretation and this led me to consider the relations between entropy and probability according to Boltzmann's ideas. After some weeks of the most intense work of my life, light began to appear to me and unexpected views revealed themselves in the distance." (*AIP Niels Bohr Library, W. F. Meggers Collection*)

[5]Planck originally published his formula as $u(\lambda, T) = \dfrac{C_1}{\lambda^5}\left(\dfrac{1}{e^{C_2/\lambda T} - 1}\right)$, where $C_1 = 8\pi ch$ and $C_2 = hc/k_B$. He then found best-fit values to the experimental data for C_1 and C_2 and evaluated $h = 6.55 \times 10^{-34}\ \mathrm{J \cdot s}$ and $k_B = N_A/R = 1.345 \times 10^{-23}\ \mathrm{J/K}$. As R, the universal gas constant, was fairly well known at the time, this technique also resulted in another method for finding N_A, Avogadro's number.

The Quantum of Energy

Planck's original theoretical justification of Equation 3.9 is rather abstract because it involves arguments based on entropy, statistical mechanics, and several theorems proved earlier by Planck concerning matter and radiation in equilibrium.[6] We shall give arguments that are easier to visualize physically yet attempt to convey the spirit and revolutionary impact of Planck's original work.

Planck was convinced that blackbody radiation was produced by vibrating submicroscopic electric charges, which he called resonators. He assumed that the walls of a glowing cavity were composed of literally billions of these resonators (whose exact nature was unknown at the time), all vibrating at different frequencies. Hence, according to Maxwell, each oscillator should emit radiation with a frequency corresponding to its vibration frequency. **Also according to classical Maxwellian theory, an oscillator of frequency f could have any value of energy and could change its amplitude continuously as it radiated any fraction of its energy.** This is where Planck made his revolutionary proposal. To secure agreement with experiment, **Planck had to assume that the total energy of a resonator with mechanical frequency f could only be an integral multiple of hf or**

$$E_{\text{resonator}} = nhf \qquad n = 1, 2, 3, \ldots \tag{3.10}$$

where h is a fundamental constant of quantum physics, $h = 6.626 \times 10^{-34}\ \text{J}\cdot\text{s}$, known as Planck's constant. In addition, he concluded that emission of radiation of frequency f occurred when a resonator dropped to the next lowest energy state. *Thus the resonator can change its energy only by the difference* ΔE *according to*

$$\Delta E = hf \tag{3.11}$$

That is, it cannot lose just any amount of its total energy, but only a finite amount, hf, the so-called quantum of energy. Figure 3.9 shows the quantized energy levels and allowed transitions proposed by Planck.

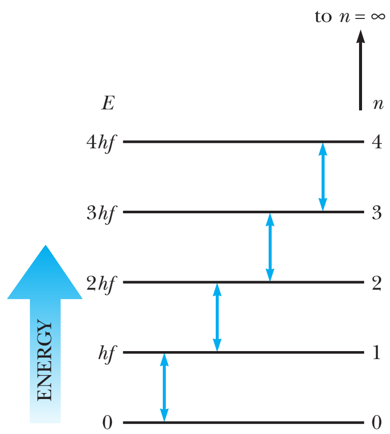


Figure 3.9 Allowed energy levels according to Planck's original hypothesis for an oscillator with frequency f. Allowed transitions are indicated by the double-headed arrows.

[6]M. Planck, *Ann. Physik*, 4:553, 1901.

EXAMPLE 3.2 A Quantum Oscillator versus a Classical Oscillator

Consider the implications of Planck's conjecture that *all* oscillating systems of natural frequency f have discrete allowed energies $E = nhf$ and that the smallest change in energy of the system is given by $\Delta E = hf$.

(a) First compare an atomic oscillator sending out 540-nm light (green) to one sending out 700-nm light (red) by calculating the minimum energy change of each. For the green quantum,

$$\begin{aligned}\Delta E_{\text{green}} &= hf = \frac{hc}{\lambda}\\ &= \frac{(6.63 \times 10^{-34}\,\text{J}\cdot\text{s})(3.00 \times 10^{8}\,\text{m/s})}{540 \times 10^{-9}\,\text{m}}\\ &= 3.68 \times 10^{-9}\,\text{J}\end{aligned}$$

Actually, the joule is much too large a unit of energy for describing atomic processes; a more appropriate unit of energy is the electron volt (eV). The electron volt takes the charge on the electron as its unit of charge. By definition, an electron accelerated through a potential difference of 1 volt has an energy of 1 eV. An electron volt may be converted to joules by noting that

$$\begin{aligned}E &= V\cdot q = 1\text{ eV} = (1.602 \times 10^{-19}\,\text{C})(1\,\text{J/C})\\ &= 1.602 \times 10^{-19}\,\text{J}\end{aligned}$$

It is also useful to have expressions for h and hc in terms of electron volts. These are

$$h = 4.136 \times 10^{-15}\,\text{eV}\cdot\text{s}$$

$$hc = 1.240 \times 10^{-6}\,\text{eV}\cdot\text{m} = 1240\,\text{eV}\cdot\text{nm}$$

Returning to our example, we see that the minimum energy change of an atomic oscillator sending out green light is

$$\Delta E_{\text{green}} = \frac{3.68 \times 10^{-19}\,\text{J}}{1.602 \times 10^{-19}\,\text{J/eV}} = 2.30\text{ eV}$$

For the red quantum the minimum energy change is

$$\begin{aligned}\Delta E_{\text{red}} &= \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34}\,\text{J}\cdot\text{s})(3.00 \times 10^{8}\,\text{m/s})}{700 \times 10^{-9}\,\text{m}}\\ &= 2.84 \times 10^{-19}\,\text{J} = 1.77\text{ eV}\end{aligned}$$

Note that the minimum allowed amount or "quantum" of energy is not uniform under all conditions as is the quantum of charge—the quantum of energy is proportional to the natural frequency of the oscillator. Note, too, that the high frequency of atomic oscillators produces a measurable quantum of energy of several electron volts.

(b) Now consider a pendulum undergoing small oscillations with length $\ell = 1$ m. According to classical theory, if air friction is present, the amplitude of swing and consequently the energy decrease *continuously* with time, as shown in Figure 3.10a. Actually, *all* systems vibrating with frequency f are quantized (according to Equation 3.10) and lose energy in discrete packets or quanta, hf. This would lead to a decrease of the pendulum's energy in a stepwise manner, as shown in Figure 3.10b. We shall show that there is no contradiction between quantum theory and the observed behavior of laboratory pendulums and springs.

An energy change of one quantum corresponds to

$$\Delta E = hf$$

where the pendulum frequency f is

$$f = \frac{1}{2\pi}\sqrt{\frac{g}{\ell}} = 0.50\text{ Hz}$$

Thus,

$$\begin{aligned}\Delta E &= (6.63 \times 10^{-34}\,\text{J}\cdot\text{s})(0.50\,\text{s}^{-1})\\ &= 3.3 \times 10^{-34}\,\text{J}\\ &= 2.1 \times 10^{-15}\,\text{eV}\end{aligned}$$

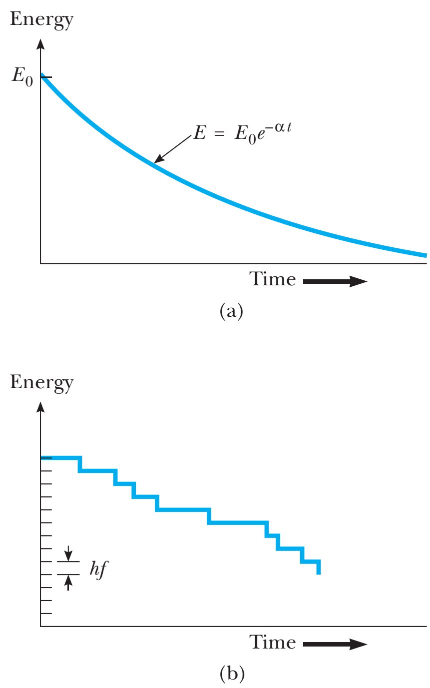


Figure 3.10 (Example 3.2) (a) Observed classical behavior of a pendulum. (b) Predicted quantum behavior of a pendulum.

Because the total energy of a pendulum of mass m and length ℓ displaced through an angle θ is

$$E = mg\ell(1 - \cos\theta)$$

we have for a typical pendulum with $m = 100$ g, $\ell = 1.0$ m, and $\theta = 10°$,

$$E = (0.10 \text{ kg})(9.8 \text{ m/s}^2)(1.0 \text{ m})(1 - \cos 10°) = 0.015 \text{ J}$$

Therefore, the fractional change in energy, $\Delta E/E$, is unobservably small:

$$\frac{\Delta E}{E} = \frac{3.3 \times 10^{-34} \text{ J}}{1.5 \times 10^{-2} \text{ J}} = 2.2 \times 10^{-32}$$

Note that the energy quantization of large vibrating systems is unobservable because of their low frequencies compared to the high frequencies of atomic oscillators. Hence there is no contradiction between Planck's quantum postulate and the behavior of macroscopic oscillators.

Exercise 2 Calculate the quantum number, n, for this pendulum with $E = 1.5 \times 10^{-2}$ J.

Answer 4.6×10^{31}

Exercise 3 An object of mass m on a spring of stiffness k oscillates with an amplitude A about its equilibrium position. Suppose that $m = 300$ g, $k = 10$ N/m, and $A = 10$ cm. (a) Find the total energy. (b) Find the mechanical frequency of vibration of the mass. (c) Calculate the change in amplitude when the system loses one quantum of energy.

Answer (a) $E_{\text{total}} = 0.050$ J; (b) $f = 0.92$ Hz; (c) $\Delta E_{\text{quantum}} = 6.1 \times 10^{-34}$ J, so

$$\Delta A \approx -\frac{\Delta E}{\sqrt{2Ek}} = -6.1 \times 10^{-34} \text{ m}$$

Until now we have been concentrating on the remarkable quantum properties of single oscillators of frequency f. Planck explained the continuous spectrum of the blackbody by assuming that the heated walls contained resonators vibrating at many different frequencies, each emitting light at the same frequency as its vibration frequency. By considering the conditions leading to equilibrium between the wall resonators and the radiation in the blackbody cavity, he was able to show that the spectral energy density $u(f, T)$ could be expressed as the product of the number of oscillators having frequency between f and $f + df$, denoted by $N(f)\,df$, and the average energy emitted per oscillator, $\overline{E}$. Thus we have the important result

$$u(f, T)\,df = \overline{E}N(f)\,df \tag{3.12}$$

Furthermore, Planck showed that the number of oscillators with frequency between f and $f + df$ was proportional to f^2 or

$$N(f)\,df = \frac{8\pi f^2}{c^3}\,df \tag{3.13}$$

(See Appendix 1 on our book Web site at http://info.brookscole.com/mp3e for details.)

Substituting Equation 3.13 into Equation 3.12 gives

$$u(f, T)\,df = \overline{E}\,\frac{8\pi f^2}{c^3}\,df \tag{3.14}$$

This result shows that the spectral energy density is proportional to the product of the frequency squared and the average oscillator energy. Also, since $u(f, T)$ approaches zero at high frequencies (see Fig. 3.5), $\overline{E}$ must tend to zero at high frequencies faster than $1/f^2$. The fact that the mean oscillator energy must become extremely small when the frequency becomes high guided Planck in the development of his theory. In the next section we shall see that the failure of $\overline{E}$ to become small at high frequencies in the classical Rayleigh–Jeans theory led to the "ultraviolet catastrophe"—the prediction of an infinite spectral energy density at high frequencies in the ultraviolet region.

3.3 THE RAYLEIGH–JEANS LAW AND PLANCK'S LAW

OPTIONAL

Rayleigh–Jeans Law

Both Planck's law and the Rayleigh–Jeans law (the classical theory of blackbody radiation formulated by Lord Rayleigh, John William Strutt, 1842–1919, English physicist, and James Jeans, 1887–1946, English astronomer and physicist) may be derived using the idea that the blackbody radiation energy per unit volume with frequency between f and $f + df$ can be expressed as the product of the number of oscillators per unit volume in this frequency range and the average energy per oscillator:

$$u(f, T)\,df = \overline{E}\,N(f)\,df \tag{3.12}$$

It is instructive to perform both the Rayleigh–Jeans and Planck calculations to see the effect on $u(f, T)$ of calculating $\overline{E}$ from a *continuous* distribution of classical oscillator energies (Rayleigh–Jeans) as opposed to a *discrete* set of quantum oscillator energies (Planck). We discuss Lord Rayleigh's derivation first because it is a more direct classical calculation.

While Planck concentrated on the thermal equilibrium of cavity radiation with oscillating electric charges in the cavity walls, Rayleigh concentrated directly on the electromagnetic waves in the cavity. Rayleigh and Jeans reasoned that the standing electromagnetic waves in the cavity could be considered to have a temperature T, because they constantly exchanged energy with the walls and caused a thermometer within the cavity to reach the same temperature as the walls. Further, they considered a standing polarized electromagnetic wave to be equivalent to a one-dimensional oscillator (Fig. 3.11). Using the same general idea as Planck, they expressed the energy density as a product of the number of standing waves (oscillators) and the average energy per oscillator. They found the average oscillator energy $\overline{E}$ to be independent of frequency and equal to $k_B T$ from the Maxwell-Boltzmann distribution law (see Chapter 10). According to this distribution law, the probability P of finding an individual system (such as a molecule or an atomic oscillator) with energy E above some minimum energy, E_0, in a large group of systems at temperature T is

$$P(E) = P_0 e^{-(E-E_0)/k_B T} \tag{3.15}$$

where P_0 is the probability that a system has the minimum energy. In the case of a *discrete* set of allowed energies, the average energy, $\overline{E}$, is given by

$$\overline{E} = \frac{\Sigma E \cdot P(E)}{\Sigma P(E)} \tag{3.16}$$

where division by the sum in the denominator serves to normalize the total probability to 1. *In the classical case considered by Rayleigh,* an oscillator could have any

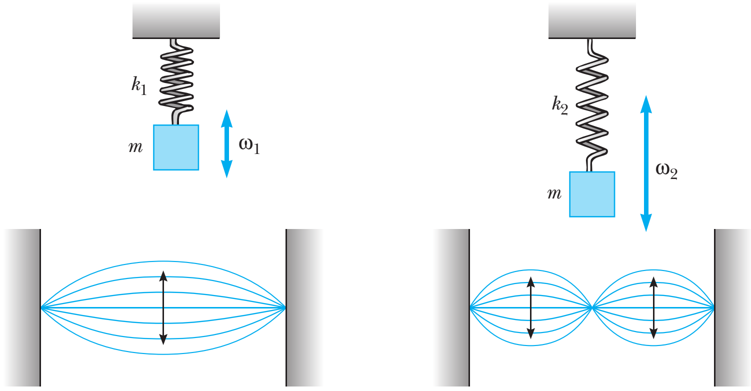


Figure 3.11 A one-dimensional harmonic oscillator is equivalent to a plane-polarized electromagnetic standing wave.

energy E in a continuous range from 0 to ∞. Thus the sums in Equation 3.16 must be replaced with integrals, and the expression for $\overline{E}$ becomes

$$\overline{E} = \frac{\displaystyle\int_0^\infty E e^{-E/k_B T} dE}{\displaystyle\int_0^\infty e^{-E/k_B T}\, dE} = k_B T$$

The calculation of $N(f)$ is a bit more complicated but is of importance here as well as in the free electron model of metals. Appendix 1 on our Web site gives the derivation of the density of modes, $N(f)\ df$. One finds

$$N(f)\, df = \frac{8\pi f^2}{c^3}\, df \tag{3.45}$$

or in terms of wavelength,

$$N(\lambda)\, d\lambda = \frac{8\pi}{\lambda^4}\, d\lambda \tag{3.46}$$

The spectral energy density is simply the density of modes multiplied by $k_B T$, or

Density of standing waves in a cavity

$$u(f, T)\, df = \frac{8\pi f^2}{c^3}\, k_B T\, df \tag{3.17}$$

In terms of wavelength,

Rayleigh–Jeans blackbody law

$$u(\lambda, T)\, d\lambda = \frac{8\pi}{\lambda^4}\, k_B T\, d\lambda \tag{3.18}$$

However, as one can see from Figure 3.12, this classical expression, known as the Rayleigh–Jeans law, does not agree with the experimental results in the short wavelength region. Equation 3.18 diverges as $\lambda \to 0$, predicting unlimited energy emission in the ultraviolet region, which was dubbed the "ultraviolet catastrophe." One is forced to conclude that classical theory fails miserably to explain blackbody radiation.

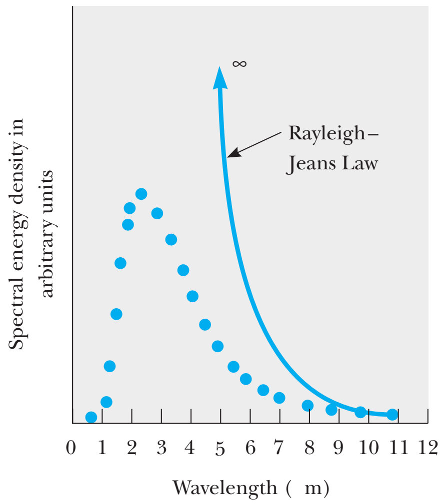


Figure 3.12 The failure of the classical Rayleigh–Jeans law (Equation 3.18) to fit the observed spectrum of a blackbody heated to 1000 K.

Planck's Law

As mentioned earlier, Planck concentrated on the energy states of resonators in the cavity walls and used the condition that the resonators and cavity radiation were in-equilibrium to determine the spectral quality of the radiation. By thermodynamic reasoning (and apparently unaware of Rayleigh's derivation), he arrived at the same expression for $N(f)$ as Rayleigh. However, Planck arrived at a different form for $\overline{E}$ by allowing only discrete values of energy for his resonators. He found, using the Maxwell-Boltzmann distribution law,

$$\overline{E} = \frac{hf}{e^{hf/k_BT} - 1} \tag{3.19}$$

(See the book Web site at http://info.brookscole.com/mp3e for Planck's derivation of $\overline{E}$.)

Multiplying $\overline{E}$ by $N(f)$ gives the Planck distribution formula:

Planck blackbody law

$$u(f, T)\,df = \frac{8\pi f^2}{c^3}\left(\frac{hf}{e^{hf/k_BT} - 1}\right) df \tag{3.9}$$

or in terms of wavelength, λ,

$$u(\lambda, T)\,d\lambda = \frac{8\pi hc\,d\lambda}{\lambda^5(e^{hc/\lambda k_BT} - 1)} \tag{3.20}$$

Equation 3.9 shows that the ultraviolet catastrophe is avoided because the $\overline{E}$ term dominates the f^2 term at high frequencies. One can qualitatively understand why $\overline{E}$ tends to zero at high frequencies by noting that the first allowed oscillator level (hf) is so large for large f compared to the average thermal energy available (k_BT) that Boltzmann's law predicts almost zero probability that the first excited state is occupied.

In summary, Planck arrived at his blackbody formula by making two startling assumptions: (1) the energy of a charged oscillator of frequency f is limited to discrete values nhf and (2) during emission or absorption of light, the change in energy of an oscillator is hf. But Planck was every bit the "unwilling revolutionary." From most of Planck's early correspondence one gets the impression that his concept of energy quantization was really a desperate calculational device, and moreover a device that applied only in the case of blackbody radiation. It remained for the great Albert Einstein, the popular icon of physics in the 20th century, to elevate quantization to the level of a universal phenomenon by showing that light itself was quantized.

EXAMPLE 3.3 Derivation of Stefan's Law from the Planck Distribution

In this example, we show that the Planck spectral distribution formula leads to the experimentally observed Stefan law for the total radiation emitted by a blackbody at all wavelengths,

$$e_{\text{total}} = 5.67 \times 10^{-8}\, T^4\ \text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-4}$$

Solution Since Stefan's law is an expression for the total power per unit area radiated at all wavelengths, we must integrate the expression for $u(\lambda, T)\, d\lambda$ given by Equation 3.20 over λ and use Equation 3.7 for the connection between the energy density inside the blackbody cavity and the power emitted per unit area of blackbody surface. We find

$$e_{\text{total}} = \frac{c}{4}\int_0^\infty u(\lambda, T)\, d\lambda = \int_0^\infty \frac{2\pi hc^2}{\lambda^5(e^{hc/\lambda k_B T} - 1)}\, d\lambda$$

If we make the change of variable $x = hc/\lambda k_B T$, the integral assumes a form commonly found in tables:

$$e_{\text{total}} = \frac{2\pi k_B^4 T^4}{c^2 h^3}\int_0^\infty \frac{x^3}{(e^x - 1)}\, dx$$

Using

$$\int_0^\infty \frac{x^3}{(e^x - 1)}\, dx = \frac{\pi^4}{15}$$

we find

$$e_{\text{total}} = \frac{2\pi^5 k_B^4}{15c^2h^3}\, T^4 = \sigma T^4$$

Finally, substituting for k_B, c, and h, we have

$$\sigma = \frac{(2)(3.141)^5(1.381 \times 10^{-23}\ \text{J/K})^4}{(15)\,(2.998 \times 10^8\ \text{m/s})^2\,(6.626 \times 10^{-34}\ \text{J}\cdot\text{s})^3}$$
$$= 5.67 \times 10^{-8}\ \text{W}\cdot\text{m}^{-2}\cdot\text{K}^{-4}$$

Exercise 4 Show that

$$\int_0^\infty \frac{2\pi hc^2}{\lambda^5(e^{hc/\lambda k_B T} - 1)}\, d\lambda = \frac{2\pi k_B^4 T^4}{h^3 c^2}\int_{x=0}^\infty \frac{x^3}{(e^x - 1)}\, dx$$

3.4 LIGHT QUANTIZATION AND THE PHOTOELECTRIC EFFECT

We now turn to the year 1905, in which the next major development in quantum theory took place. The year 1905 was an incredible one for the "willing revolutionary" Albert Einstein (Fig. 3.13). In this year Einstein produced three immortal papers on three different topics, each revolutionary and each worthy of a Nobel prize. All three papers contained balanced, symmetric, and unifying new results achieved by spare and clean logic and simple mathematics. The first work, entitled "A Heuristic[7] Point of View

[7]A heuristic argument is one that is plausible and enlightening but not rigorously justified.

Engineering Physics

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

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Tunneling Applications

- $\alpha - \beta$, Radio Active decay
- Nuclear Fusion and Fission Process
- Tunnel Diode
- SQUID
- Quantum Computing
- **Scanning Tunnelling Microscope**

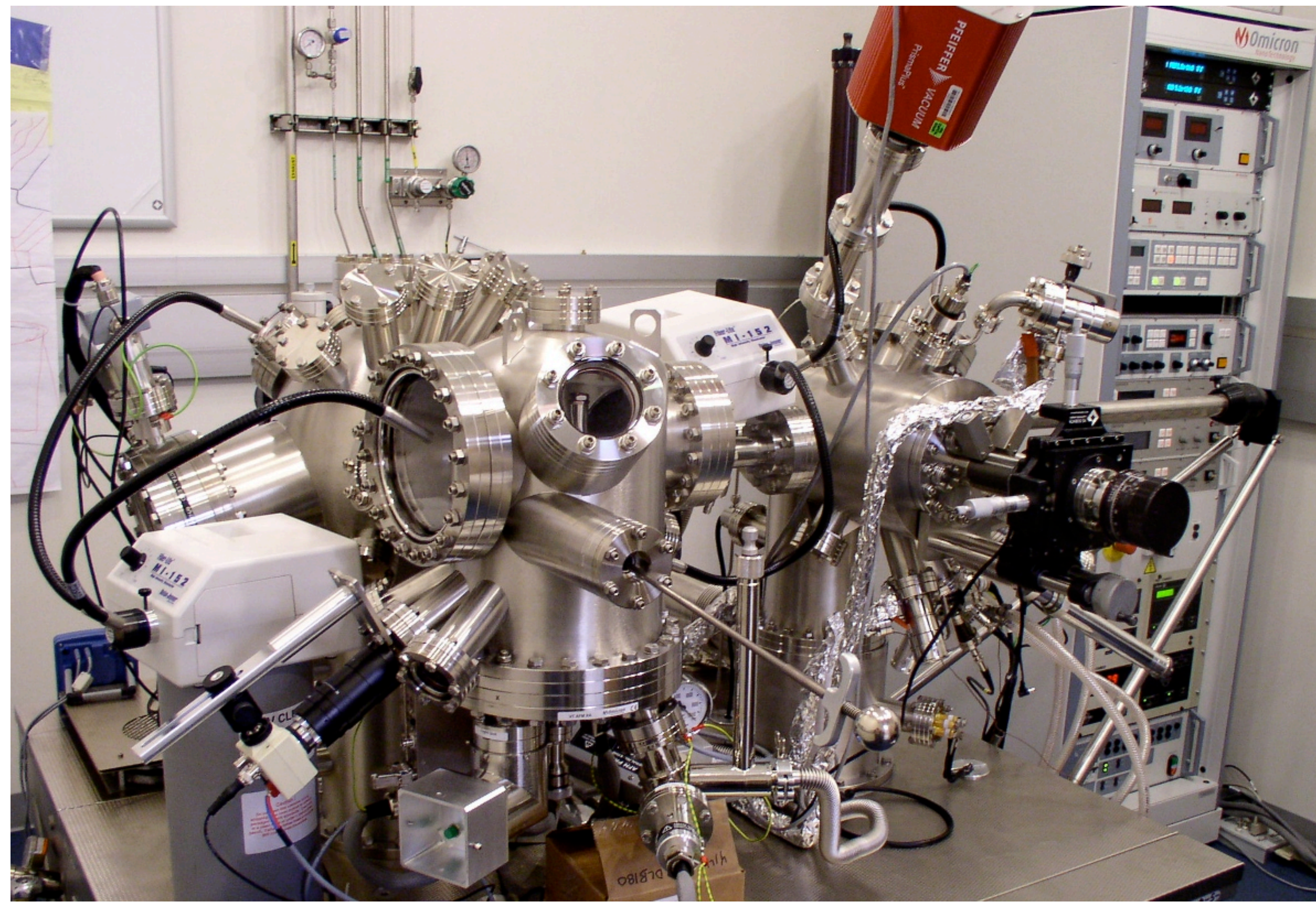
Scanning Tunnelling Microscope (STM)

Scanning Tunneling Microscopy (STM), is an imaging technique used to obtain ultra-high resolution images at the atomic scale, **without using light or electron** beam **by using** the concept of **quantum tunneling**.

1981
Gerd Binnig and
Heinrich Rohrer
@ IBM Zürich

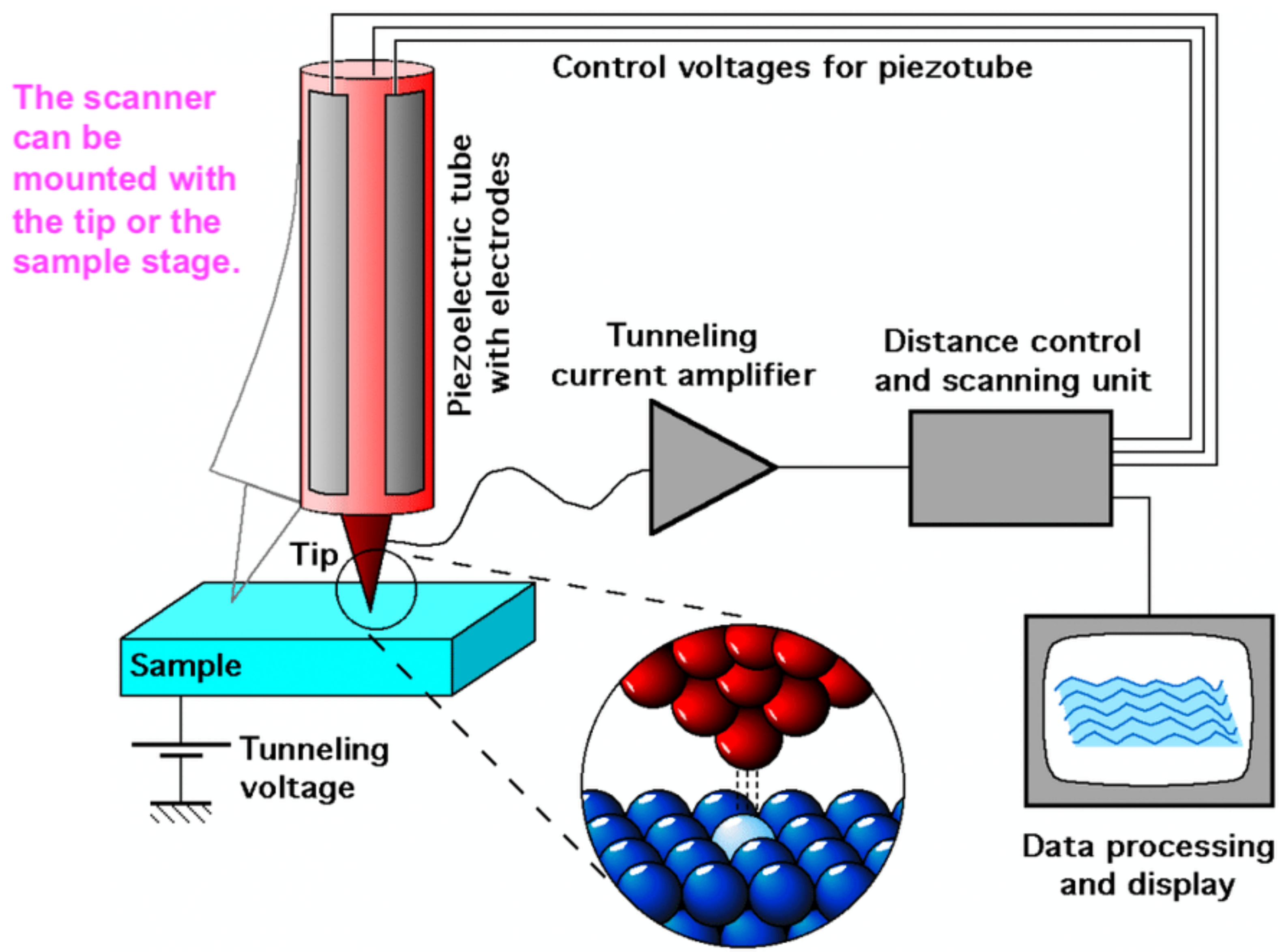
Nobel Prize in Physics in 1986

- Construction
- Working Principle
- Mode of Operation
- Applications



Ultra-high vacuum and low-temperature STM set-up. The system needs a clean environment such as the particle take 40 km distance travel for a single collision

STM: Construction



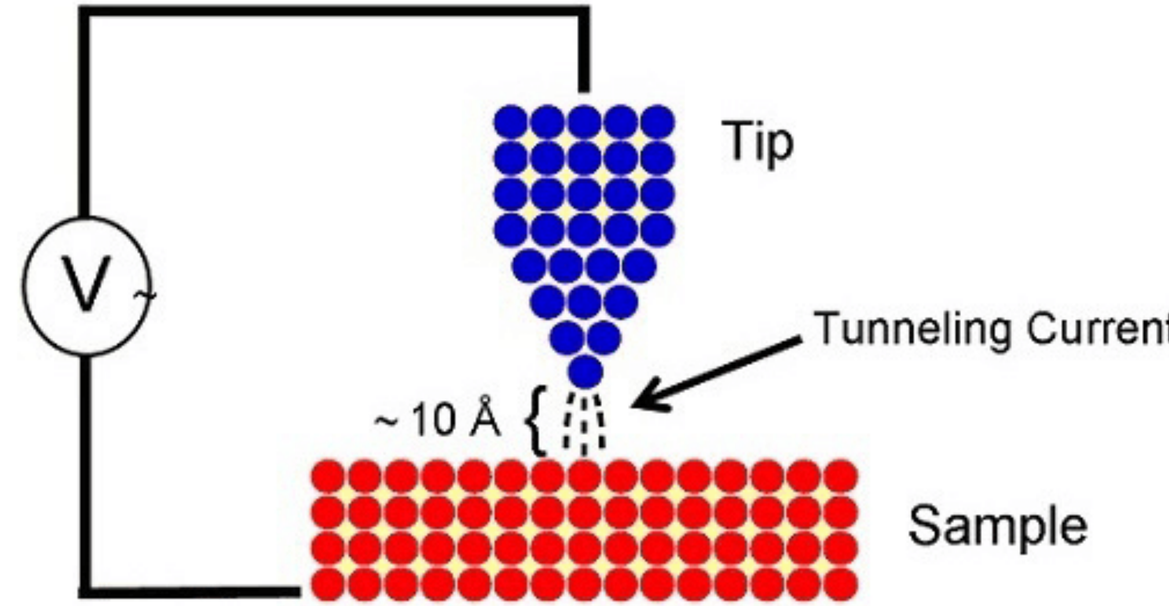
<u>Five basic components:</u>

1. Metal tip,
2. Piezoelectric scanner,
3. Current amplifier (nA),
4. Bipotentiostat (bias),
5. Feedback loop (current).

- Tunneling current from tip to sample or vice-versa depending on bias;
- Current is exponentially dependent on distance;
- Raster scanning gives 2D image;
- Feedback is normally based on constant current, thus measuring the height on surface.

STM: Working Principle

- STM is based on the concept of **quantum tunneling**
- An electrically conducting probe with a very sharp edge is brought near the surface to be studied
- The empty space between the tip and the surface represents the "barrier"
- The tip and the surface are two walls of the "potential well"electrons to tunnel through the vacuum separating the tip and the sample



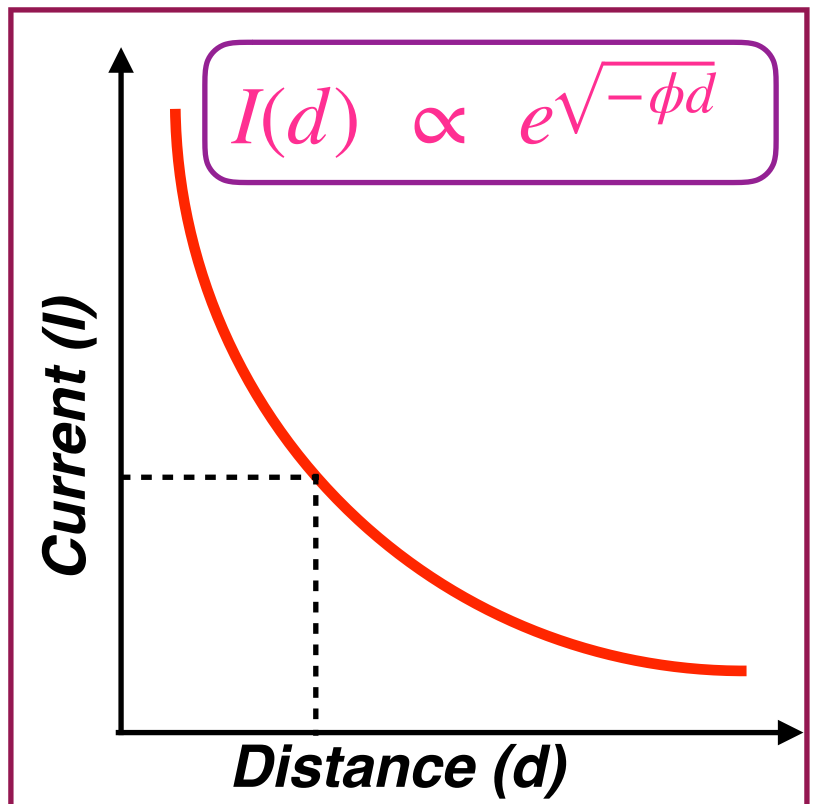
From the concept of tunneling from a potential barrier, we know that:

$$\boxed{T = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\kappa L}}$$

Tunneling current: $I \propto e^{-kd}$

$$\therefore k = \sqrt{\frac{2m\phi}{\hbar^2}}$$

ϕ: the work function (energy barrier)



- 0.1 nm change in separation produces n order of magnitude change in current
- Atomic scale resolution up to 0.1 nm
- Scan on the surface to give the 2D image of sample

STM: Working Principle

The **tip is brought close to the sample**.

A **bias voltage is applied** between the sample and the tip.

Fine control of the tip position is achieved by **piezoelectric scanner** tubes whose length can be altered by a control voltage. The scanner is gradually elongated until the **tip starts receiving the tunneling current**.

The **tip–sample separation** is then kept somewhere in the **4–7 A^o range.**

Once tunneling is established, the sample **bias and tip position with respect to the sample are varied according to the requirements** of the experiment.

STM: Working Principle

As the number of electrons that will actually tunnel is vary dependent upon the thickness of the barrier, the **tunneling current depends on the sample-tip separation.**

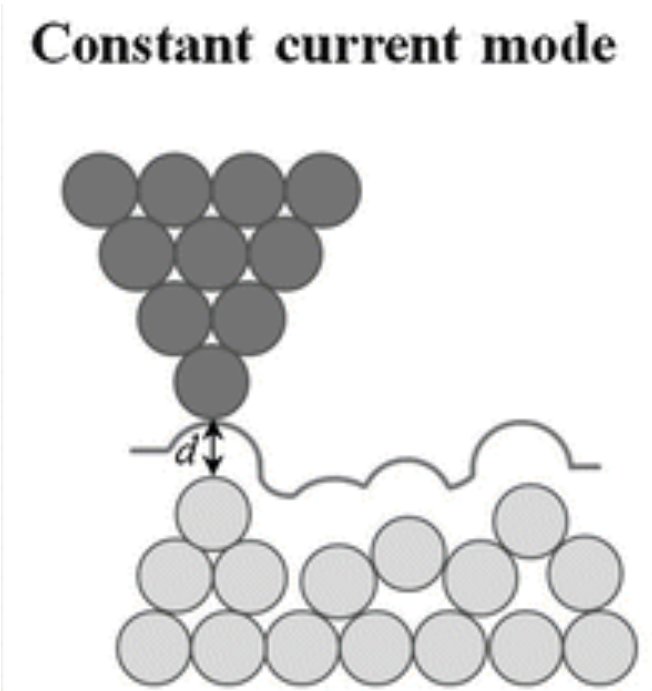
As the tip is moved across the surface, **the changes in surface height cause changes in the tunneling current.** Noting the tunneling current, surface height is estimated.

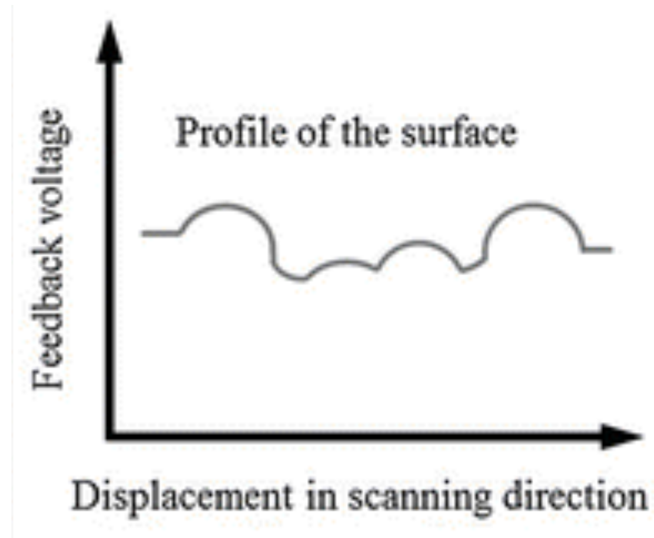
Digital images of the surface are formed in one of the two different modes:

(i) Constant-height mode: in this mode changes of the tunneling current are mapped directly.

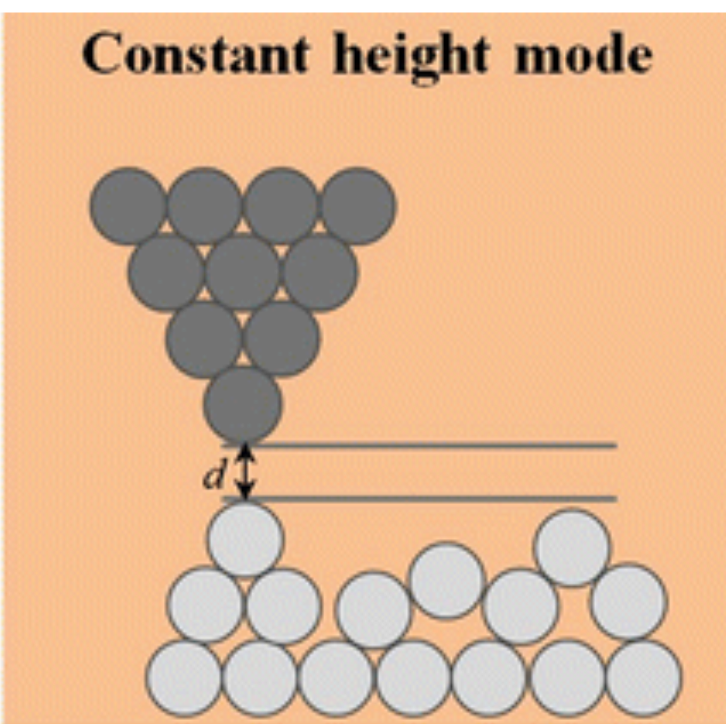
(ii) Constant-current mode: in this mode, the voltage that controls the height of the tip is recorded while the tunneling current is kept at a predetermined level. A feedback electronics adjust the height by a voltage to the piezoelectric height-control mechanism.

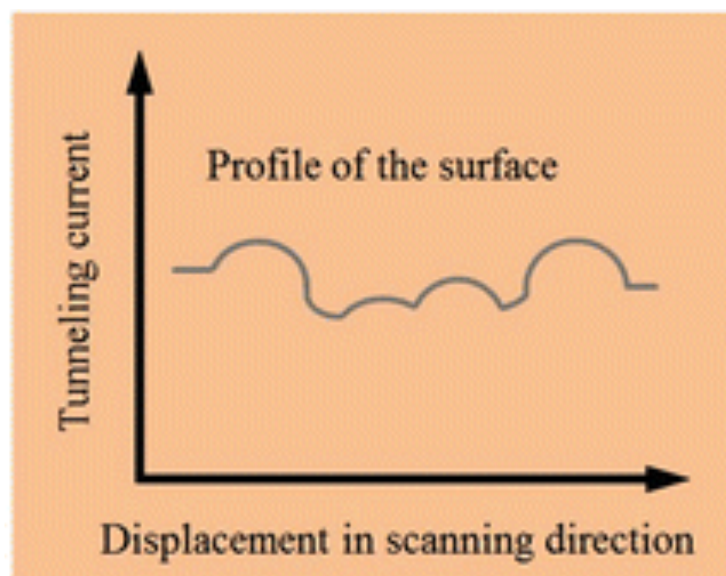
STM: Mode of Operation





- Image the surface with constant tunnel current and variable height
- Feed back loop help to maintain a constant current
- Surface (height) structure can detect





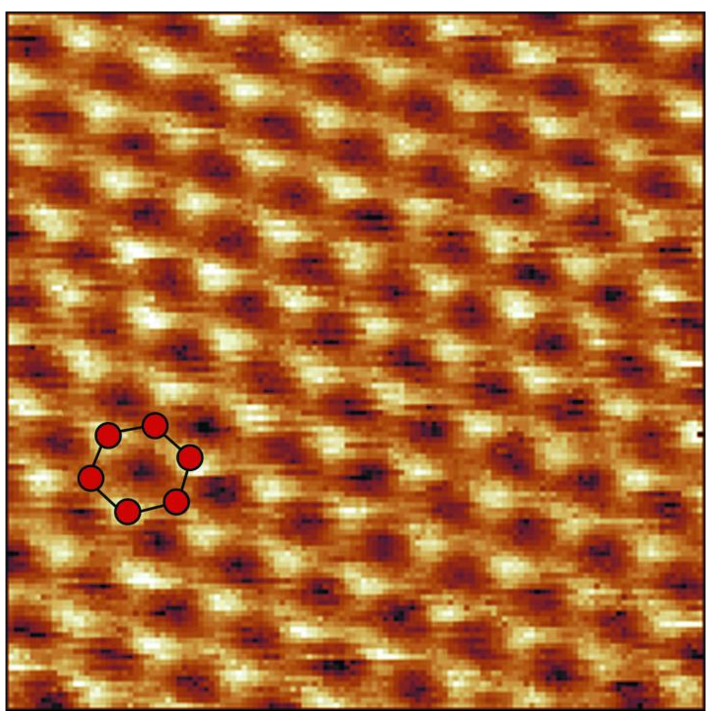
- Image the surface with constant height and variable tunnel current
- Electron density on the surface can detect

STM: Applications

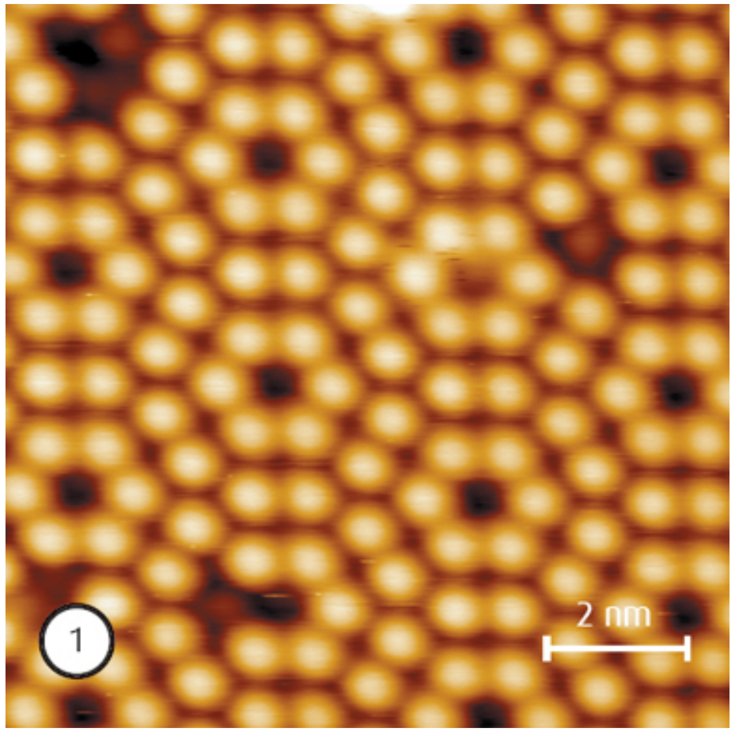
Widely used in nanotechnology:

- Image the surface structure
- Estimate surface roughness
- 3D images of the surface
- Locate the defect on the surface of the crystal
- Understand the electric structure of materials

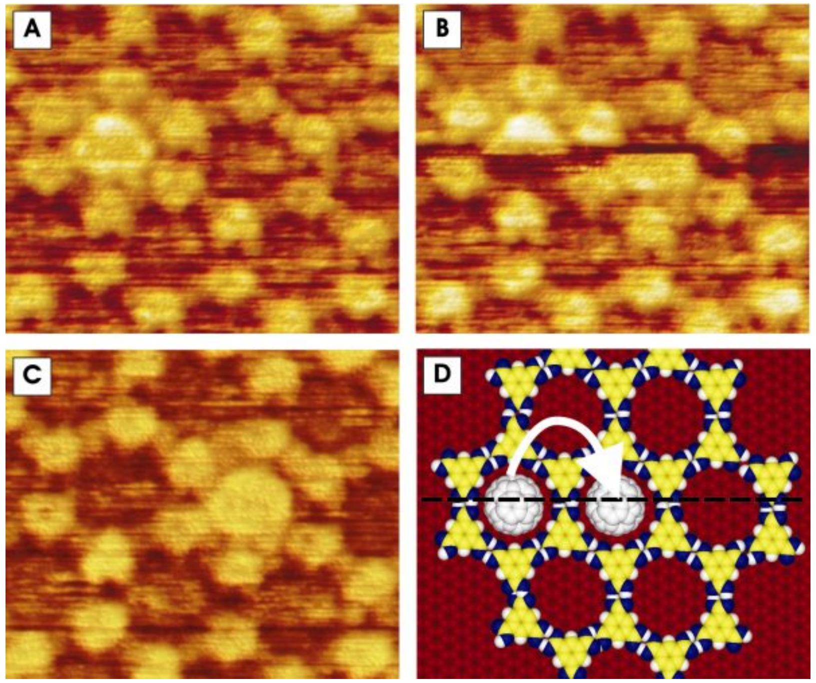
Graphite



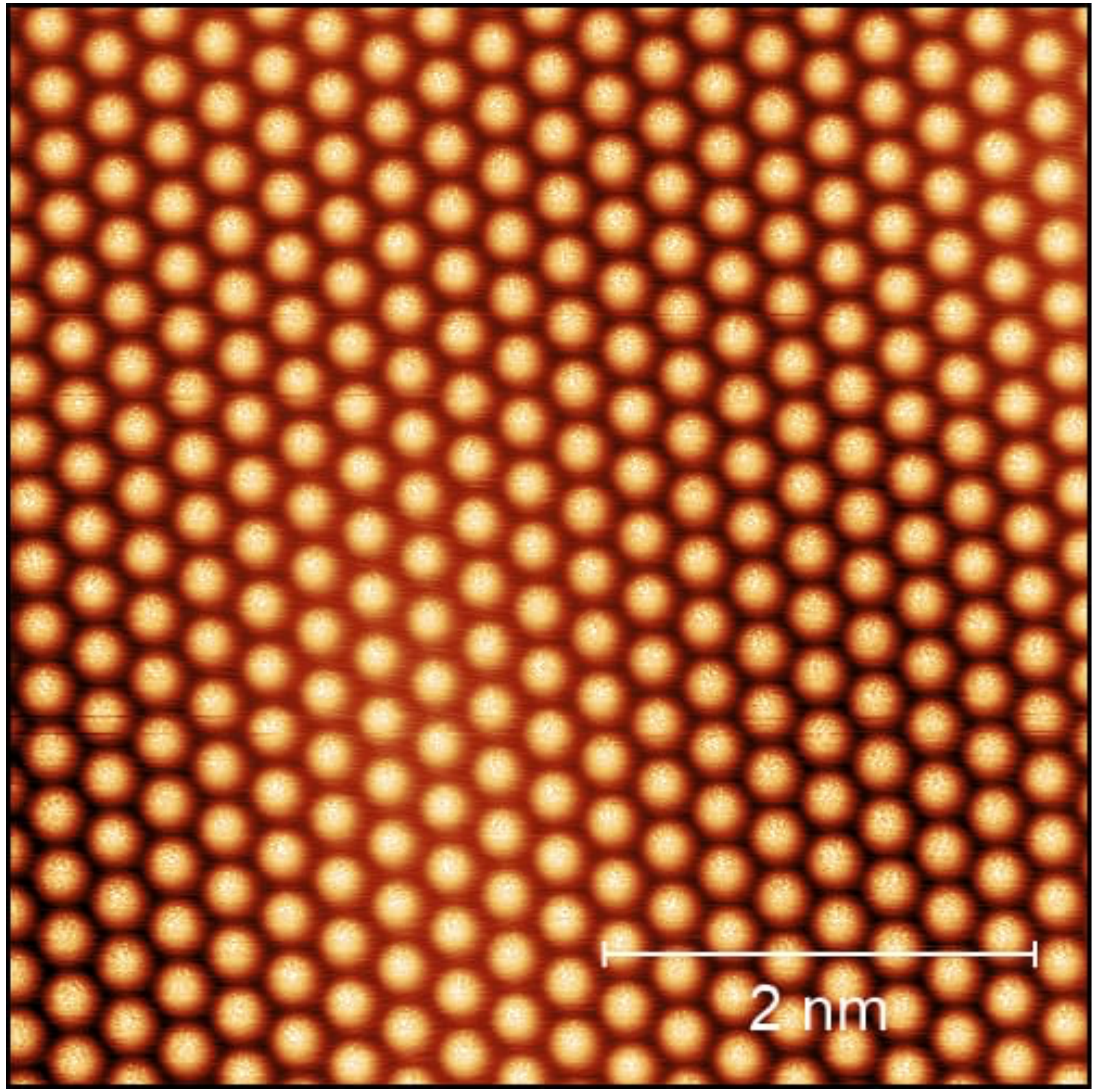
Silicon



C 60 Molecule



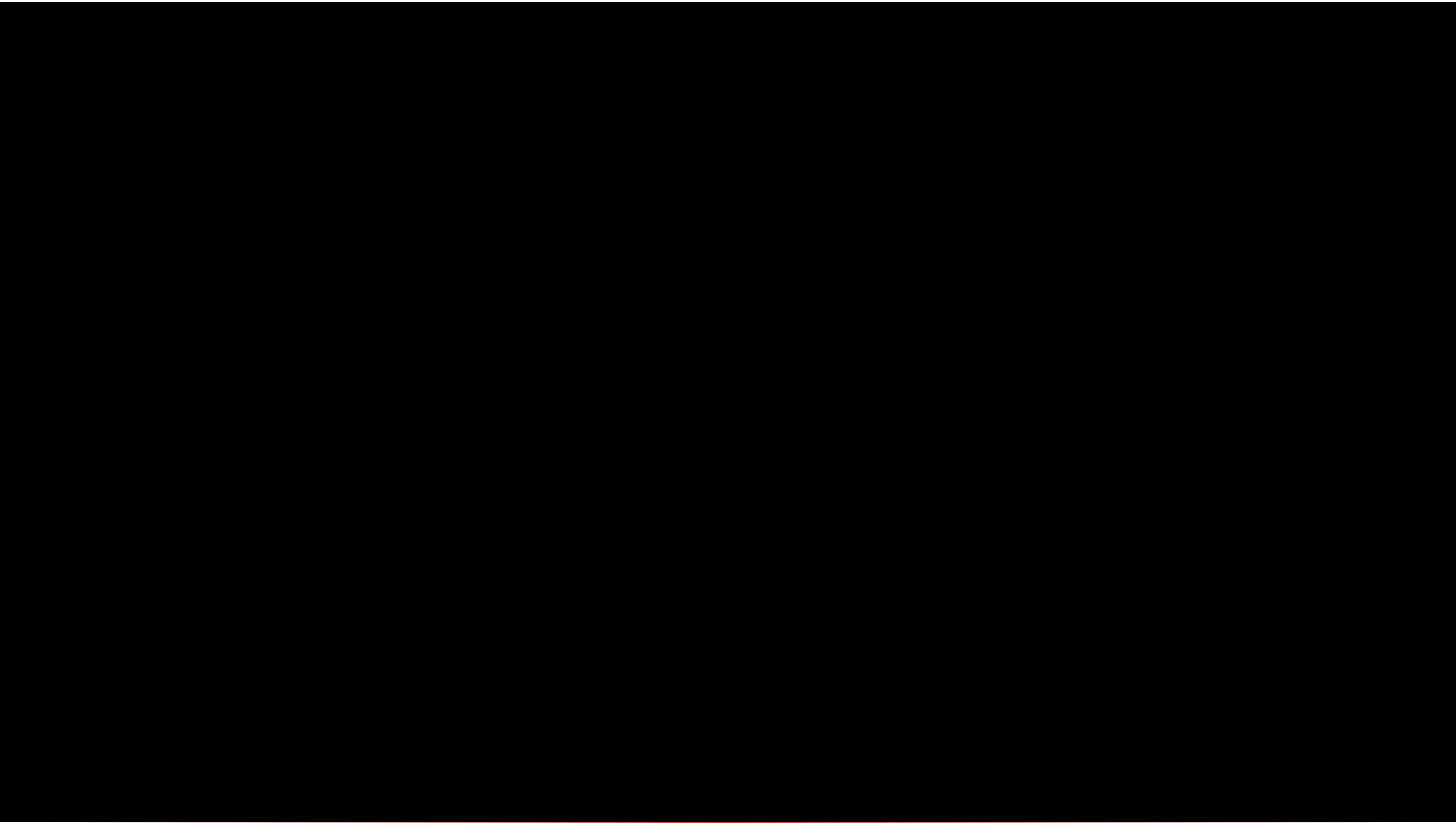
STM: Applications



Arrangement of atoms in Silver (Ag)

STM: Manipulating with atoms

Direct Measurement of *$|\psi|^2$* *using STM and to manipulate atoms*



Engineering Physics

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

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Module-4

Application of Quantum Physics

Syllabus

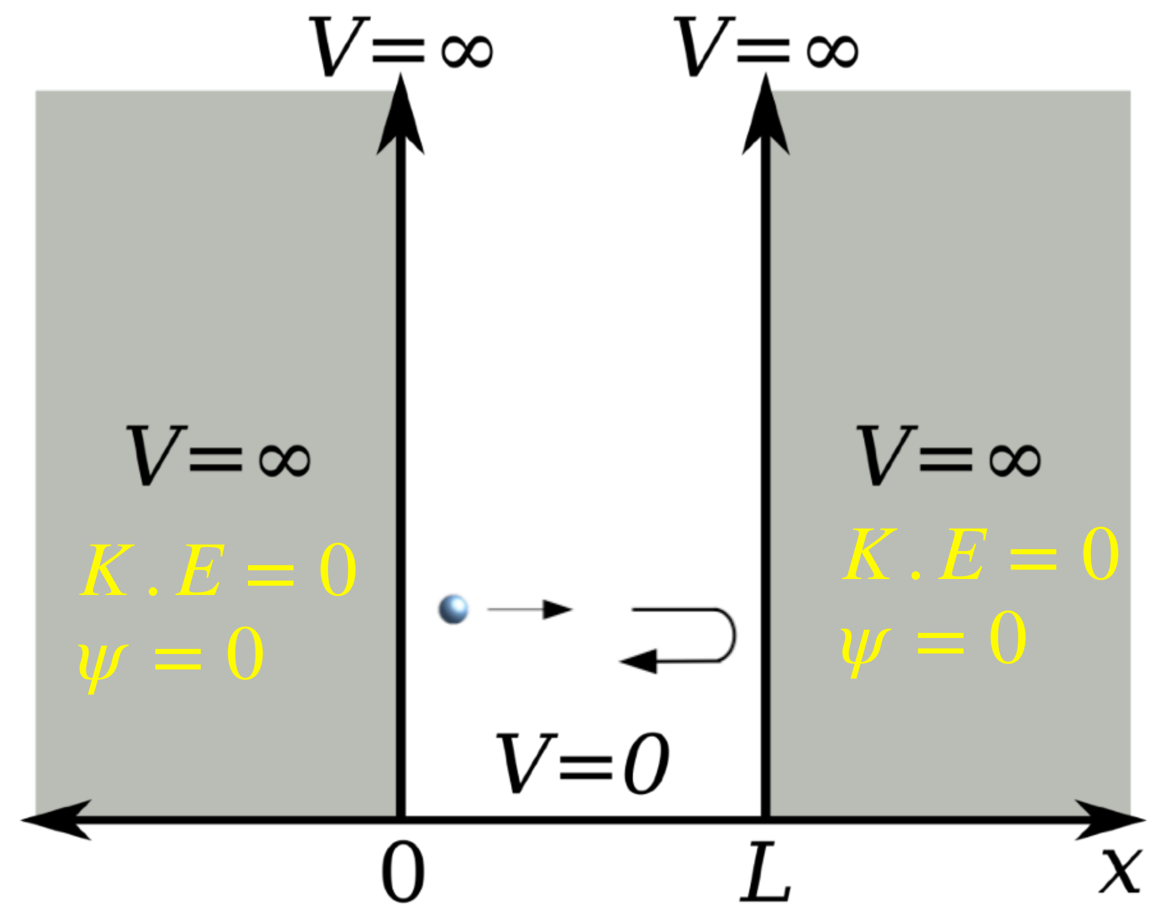
Eigenvalues and eigenfunction of a particle confined in a one-dimensional box - Basics of nanophysics - Quantum confinement and nanostructures - Tunnel effect (qualitative) and scanning tunneling microscope.

Reference Books:

1. H. D. Young and R. A. Freedman, University Physics with Modern Physics, 2020, 15th Edition, Pearson, USA., Section 41.1 to 41.3, Page No: 1360-1365
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.

Particle in a 1-Dimensional Potential Box

Lets consider a particle is trapped in a one dimensional infinite potential box of length L



Our aim is to understand the properties of the particle by using Schrödinger Wave Equation to describe its :

- **Energy**
- **Wavefunction**
- **Probability density**

As the potential is only position-dependent, so we can apply the time-independent Schrödinger Wave Equation, here, and we know that the equation is:

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

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

Boundary conditions

$$V(x) = \begin{cases} 0 & \text{if } 0 \leqslant x \leqslant L \\ \infty & \text{otherwise} \end{cases}$$

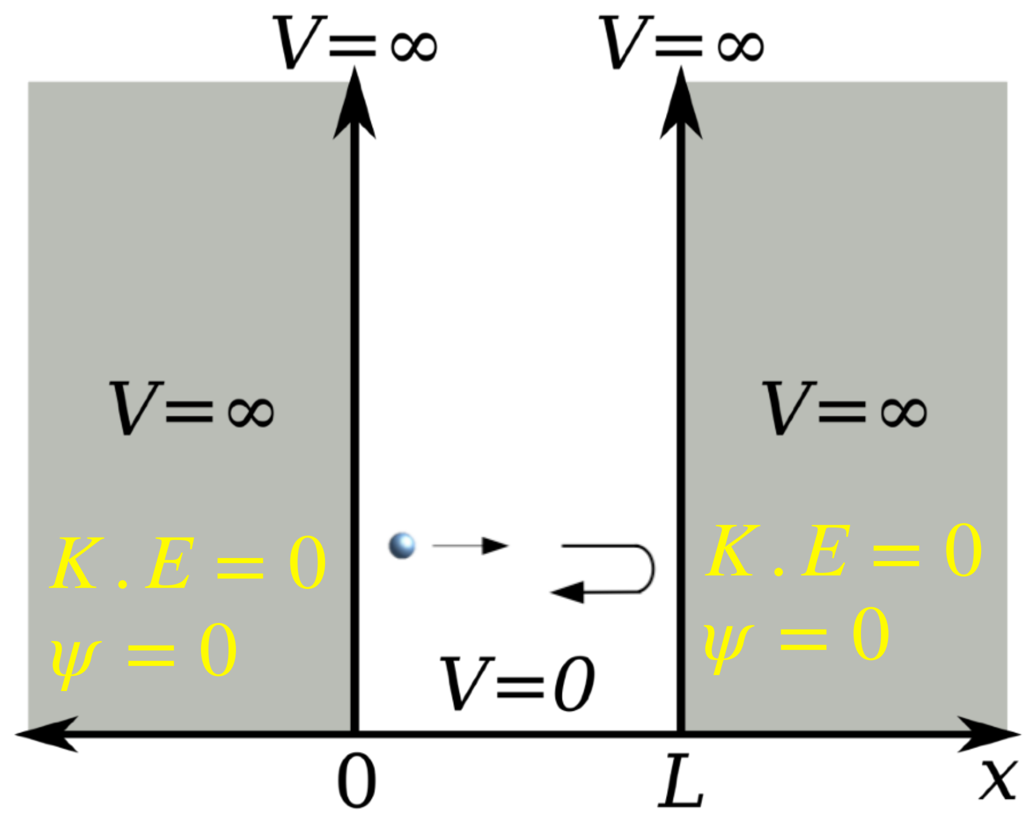
(i) at, $x=0, \psi=0$ **(ii) at,** $x=L, \psi=0$

Particle in a 1-Dimensional Potential Box

Boundary conditions

$$V(x) = \begin{cases} 0 & \text{if } 0 \leqslant x \leqslant L \\ \infty & \text{otherwise} \end{cases}$$

(i) at, $x = 0, \psi = 0$ **(ii) at,** $x = L, \psi = 0$



Three important steps

1. Solve time independent Schrodinger equation to get $\psi(x)$

2. Show that energy levels are quantized using boundary conditions

$$\psi(x=0) = \infty \qquad \text{and} \qquad \psi(x=L) = \infty$$

3. Find the complete wavefunctions using normalization $\int_0^L |\psi(x)|^2 dx = 1$

Particle in a 1-Dimensional Potential Box

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

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

For particle, $V(x)=0$

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

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

$$\Rightarrow \frac{\partial^2\psi(x)}{\partial x^2}+k^2\,\psi(x)=0$$

it is second order partial differential equation, and the possible solution for the equation is:

$$\psi(x)=A\sin(kx)+B\cos(kx)$$

where, A & B are constant

Boundary conditions:

- $V=\infty$ for $x\leq 0$ and $x\geq L$
- $V=0$ for $0<x<L$

(i) at, $x=0,\ \psi=0$ **(ii) at,** $x=L,\ \psi=0$

2. Let's apply the Boundary conditions (i):

(i) at, $x=0,\ \psi=0$

$$\Rightarrow \psi=A\ sin(kx)+B\ cos(kx)$$

$$\Rightarrow \psi=0+B\ cos(0) \quad \Rightarrow \quad 0=0+B$$

$$\Rightarrow B=0$$

So the wave function reduced to:

$$\psi=A\ sin(kx)$$

Let's apply the Boundary conditions (ii):

(ii) at, $x=L,\ \psi=0$

$$\Rightarrow \psi=A\ sin(kx)=A\ sin(kL)=0$$

$$\Rightarrow kL=n\pi\ldots\ldots n=1,\ 2,\ 3..$$

Particle in a 1-Dimensional Potential Box

so now we have:

$$\therefore k = \sqrt{\frac{2mE}{\hbar^2}} \qquad kL = n\pi$$

$$\Rightarrow \frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{n^2\pi^2}{L^2} = \frac{2mE}{\hbar^2}$$

$$\Rightarrow \frac{n^2\pi^2\hbar^2}{2mL^2} = E \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\Rightarrow E = \frac{n^2h^2}{8mL^2}$$

$$\boxed{E_n = \frac{n^2h^2}{8mL^2}}$$

We got energy of that trapped article, lets Let's find its wave function(i):

we know that: $\psi = A\ sin(kx)$ & $kL = n\pi$

3. Now apply the normalization to the wave function:

$$\Rightarrow \int_0^L \psi^* \psi\ dx = \int_0^L |\psi|^2 dx = 1$$

$$\Rightarrow \int_0^L \left(A\ \sin\left(\frac{n\pi x}{L}\right)\right)^2 dx = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$\Rightarrow \frac{A^2}{2} \int_0^L \left(1 - \cos 2(kx)\right) dx = 1$$

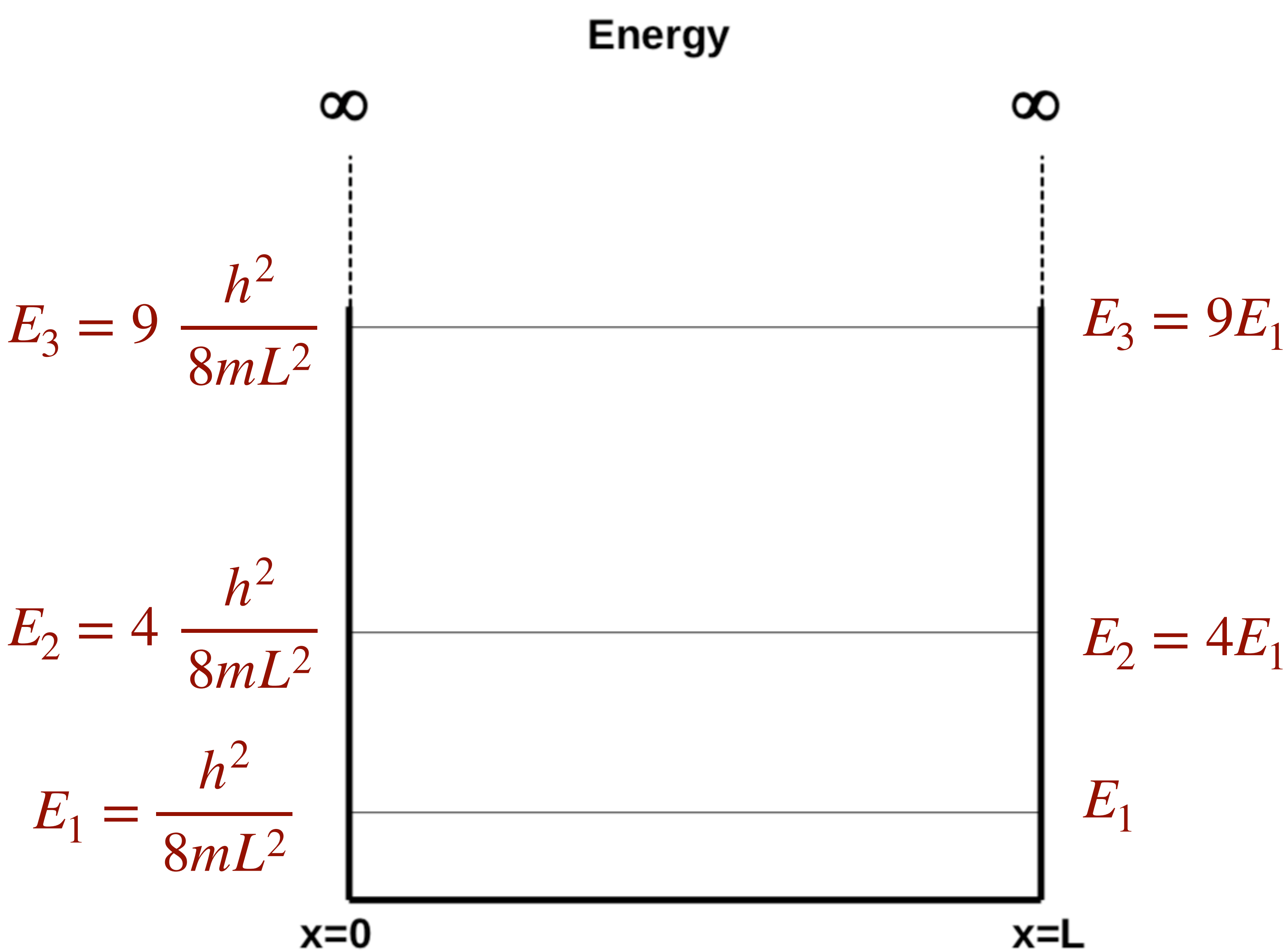
$$\Rightarrow \frac{A^2}{2}\left[[L]_L - [0]_0\right] = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\Rightarrow \boxed{\psi = \sqrt{\frac{2}{L}}\ sin\left(\frac{n\pi x}{L}\right)}$$

Particle in a 1-Dimensional Potential Box: Energy

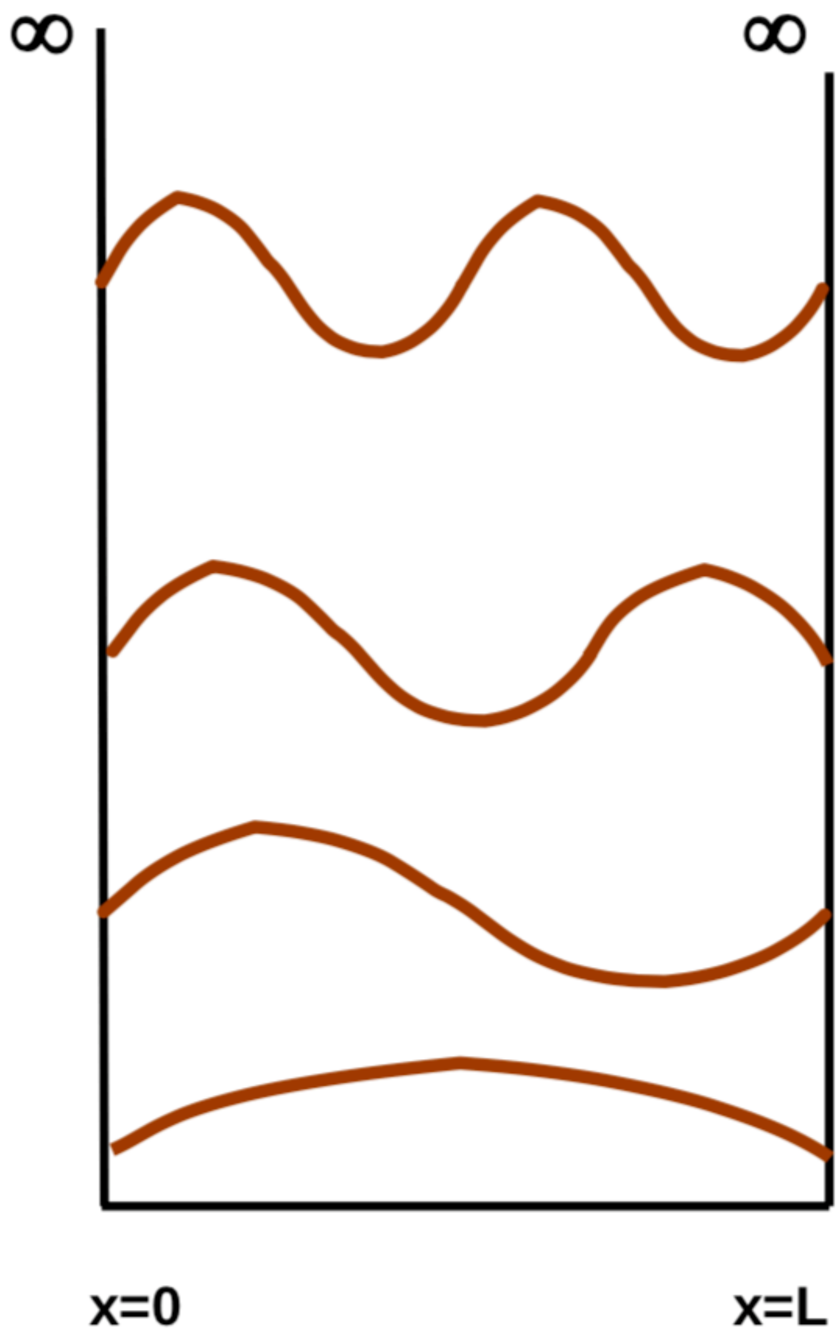
so now we have energy and the wave function as :

$$E_n = \frac{n^2h^2}{8mL^2} \qquad E_1 = \frac{h^2}{8mL^2} \qquad , E_2 = 4E_1,\ E_3 = 9E_1 \ldots.$$



Particle in a 1-Dimensional Potential Box: Wavefunction

so the wave function as : $\psi = \sqrt{\frac{2}{L}}\, sin(\frac{n\pi x}{L})$



n=4 $\psi_4(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{4\pi}{L}x\right)$

n=3 $\psi_3(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi}{L}x\right)$

n=2 $\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi}{L}x\right)$

n=1 $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$

Engineering Physics

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

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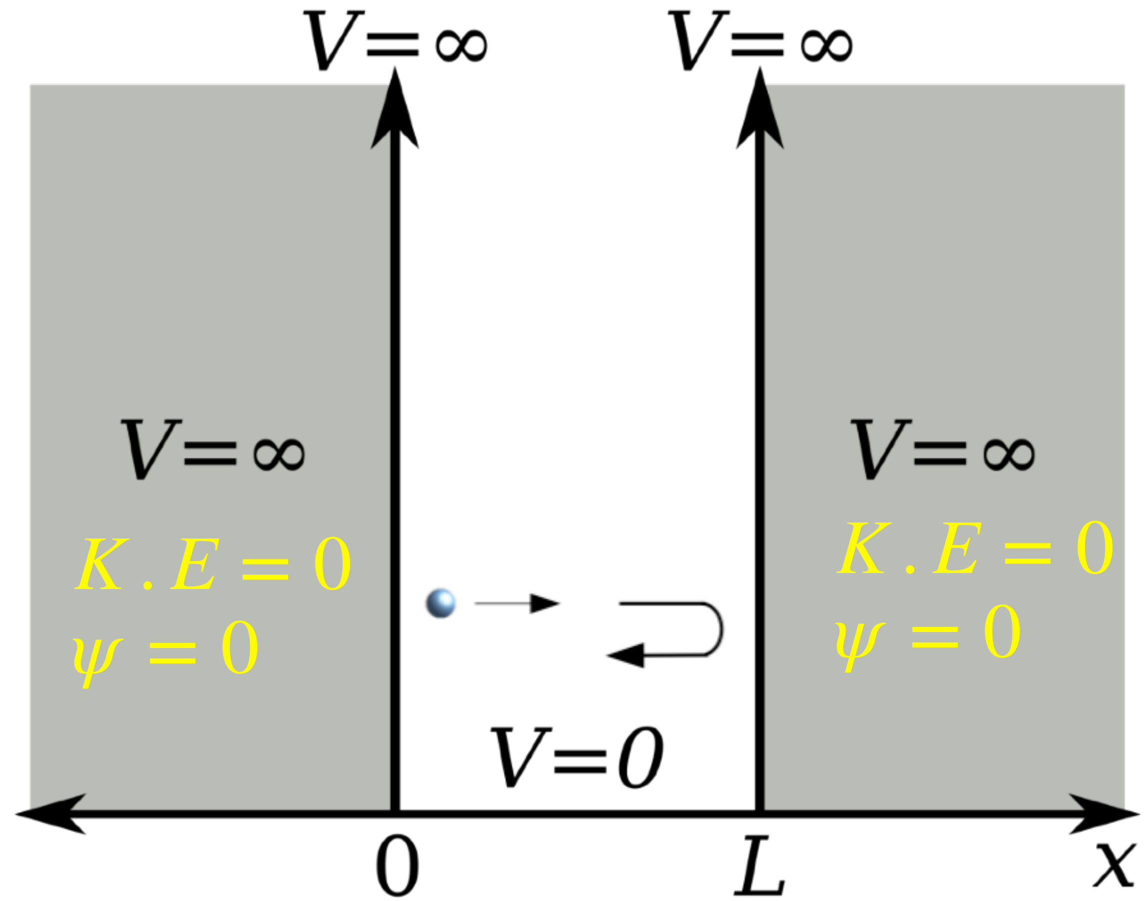
Particle in a 1-Dimensional infinite Potential Box

Energy:

$$E_n = \frac{n^2h^2}{8mL^2}$$



wave function as :

$$\psi = \sqrt{\frac{2}{L}}\, sin\left(\frac{n\pi x}{L}\right)$$

Boundary conditions

$$V(x) = \begin{cases} 0 & \text{if } 0 \leqslant x \leqslant L \\ \infty & \text{otherwise} \end{cases}$$

(i) at, $x=0, \psi=0$ **(ii) at,** $x=L, \psi=0$

The probability density is defined as : $P = |\psi|^2$

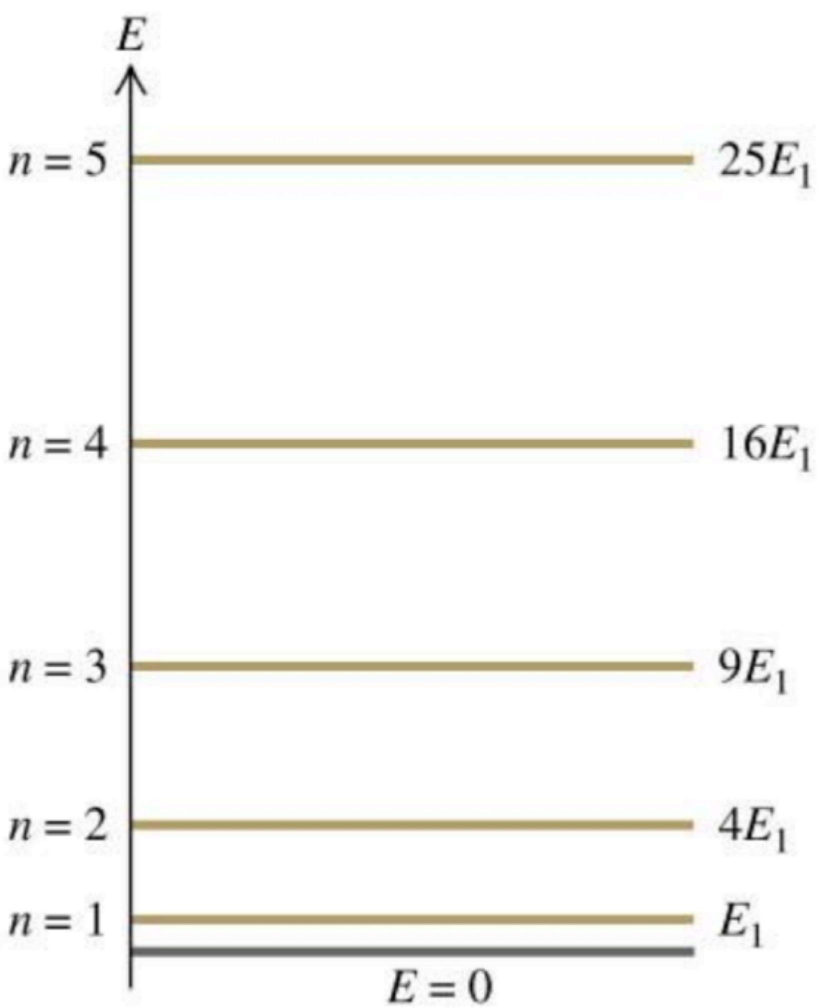
$$P = \frac{2}{L}\, sin^2\left(\frac{n\pi x}{L}\right)$$

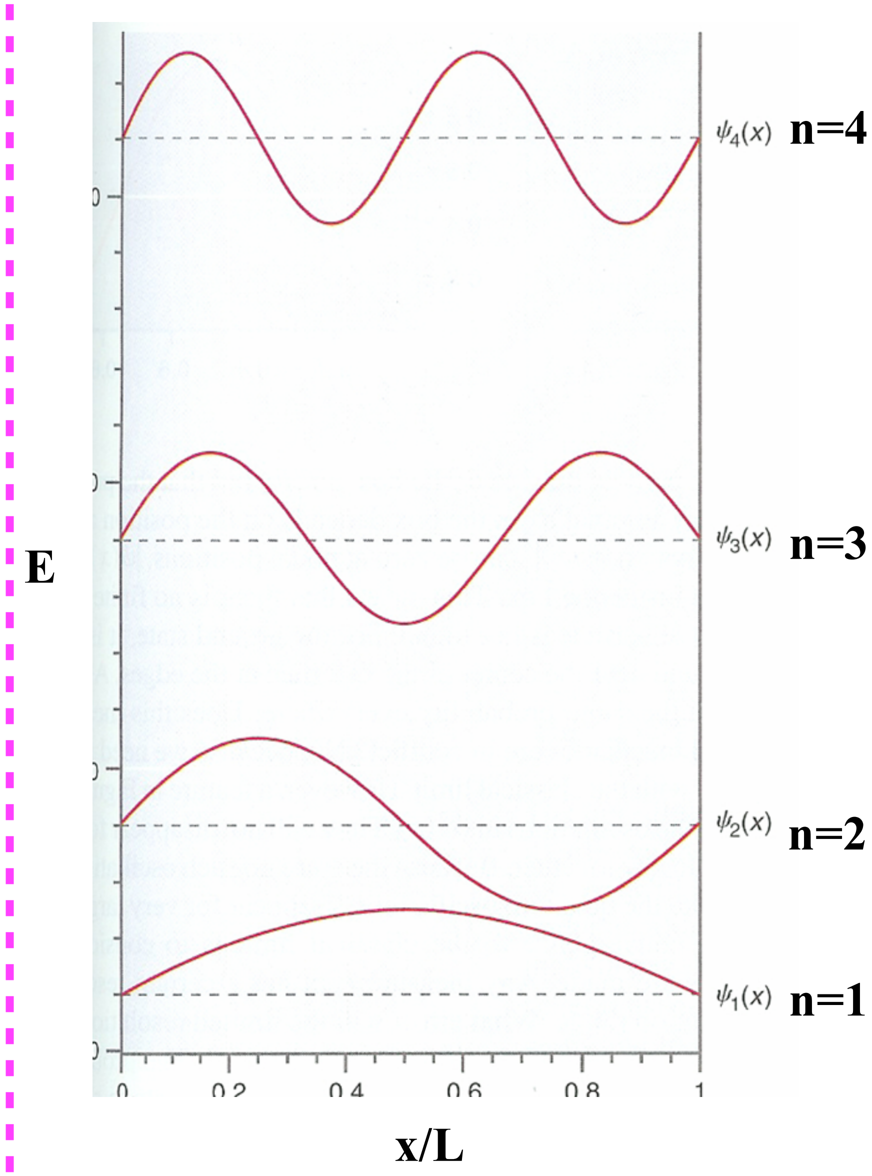
Graphical representation of E, ψ. and P

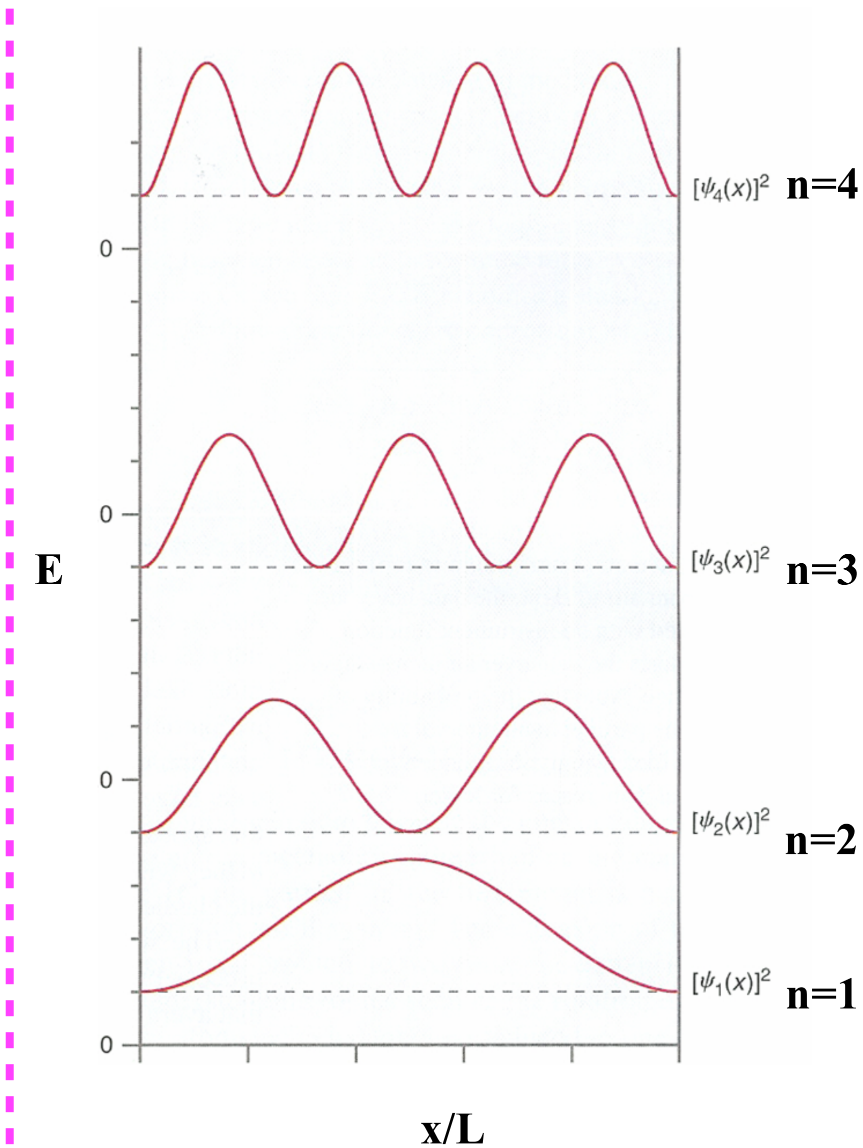
$$E_n = \frac{n^2h^2}{8mL^2}$$

$$\psi = \sqrt{\frac{2}{L}}\, sin(\frac{n\pi x}{L})$$

$$P = \frac{2}{L}\, sin^2(\frac{n\pi x}{L})$$







$$E_1 : E_2 : E_3 \ldots : E_n = 1 : 4 : 9 \ldots : n^2$$

Facts Learn from Particle in a 1-D Potential Box

Sr.	Particular	Classical Mechanics	Quantum Mechanics
1	Energy of particle	A particle enclosed in a rigid box can have <u>any value</u> of energy from 0 to ∞	Only certain <u>discrete values</u> of energy that are integral multiples of $\frac{h^2}{8mL^2}$ are permitted
2	Minimum value of energy	Minimum energy of the particle <u>can be zero</u>.	Minimum energy of the particle <u>cannot be zero</u>.

- The energy of a particle is quantized. This means it can only take on discrete energy values.
- The lowest possible energy for a particle is NOT zero (even at 0 K).
- This means the particle always has some kinetic energy.
- The square of the wavefunction is related to the probability of finding the particle in a specific position for a given energy level.
- In classical physics, the probability of finding the particle is independent of the energy and the same at all points in the box

Particle in a 3-Dimensional Potential Box

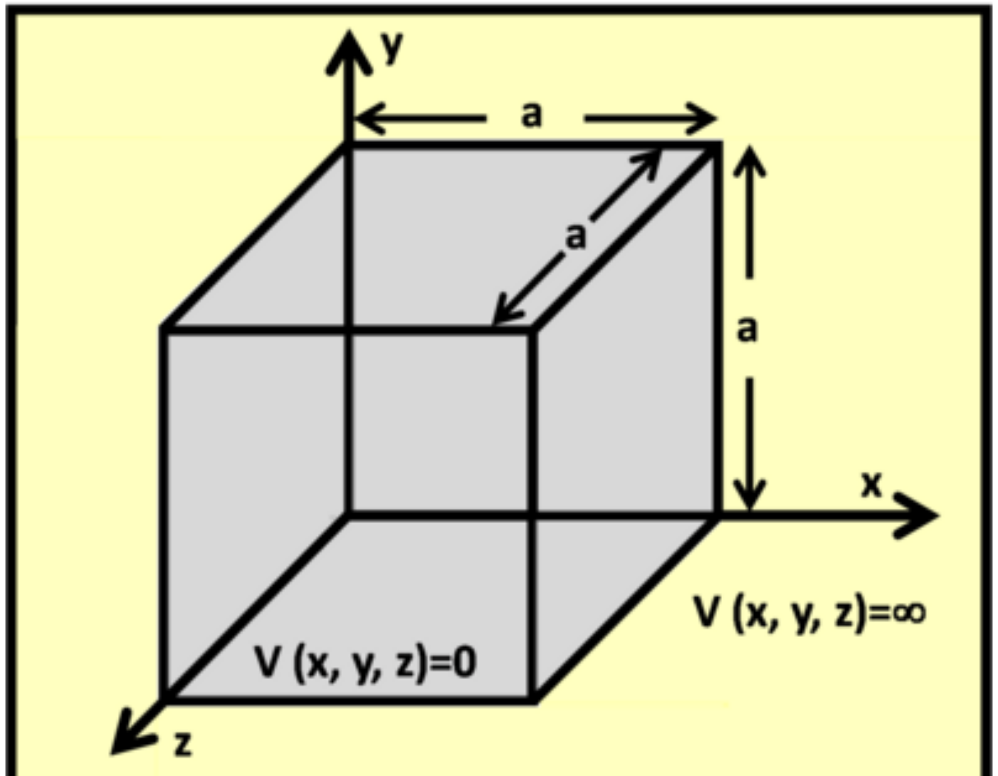


Fig. Particle in 3D Cubic Rigid Box

Wave functions and energies for particle in a 3D box:

$$\psi(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n_x \pi x}{a}\right) \qquad n_x = \{1,2,3,\ldots\}$$

$$\psi(y) = \sqrt{\frac{2}{b}}\,\sin\left(\frac{n_y \pi y}{b}\right) \qquad n_y = \{1,2,3,\ldots\}$$

$$\psi(z) = \sqrt{\frac{2}{c}}\,\sin\left(\frac{n_z \pi z}{c}\right) \qquad n_z = \{1,2,3,\ldots\}$$

eigenfunctions

$$E_x + E_y + E_z = E = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

eigenvalues

$$E = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

eigenvalues if $a = b = c = L$

Particle in a 1-D Potential Box: Numerical

Calculate the ground state and third excited energies of an electron trapped in one dimensional potential well of width L=2 nm.

Mass of electron, m= 9.1 x 10^{-31}kg

Size of the box, L=2 nm= 2 x 10^{-9} m

Eigen-energies, $$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} = \frac{n^2 h^2}{8mL^2} = n^2 \frac{(6.63\times 10^{-34})^2}{8\times(9.1\times 10^{-31})\times(2\times 10^{-9})^2} \quad J$$

$$= n^2 \frac{43.9569\times 10^{-68}}{291.2\times 10^{-49}} \quad J \quad \approx n^2 0.151\times 10^{-19}\, J$$

$$= n^2 \frac{0.151\times 10^{-19}}{1.6\times 10^{-19}} eV = 0.0943\, n^2\, eV$$

For the ground state, n=1 and $E_1 = 0.0943\, eV$

For the third excited state, n=4 therefore, $E_4 = 16\, E_1 = 1.5\, eV$

Particle in a 1-D Potential Box: Numerical

An object of mass 1mg is confined to move between two rigid walls separated by 1cm. Calculate the minimum speed of the object. If the speed of the object is 3cm/s, find the corresponding value of n.

Mass m=1mg = 10^{-3} g

Box size L = 1cm = 10^{-2} m

Lowest energy
$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = \frac{h^2}{8mL^2} = \frac{(6.63\times10^{-34})^2}{8\times10^{-3}\times(10^{-2})^2} = 5.49\times10^{-61} \quad J$$

$$v_1=\sqrt{2mE_1} = \sqrt{2\times10^{-3}\times(5.49\times10^{-61})} = 3.31\times10^{-32}\, ms^{-1}$$

Do the second part!

Particle in a finite Potential Box

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

Region-1, $V \neq 0$

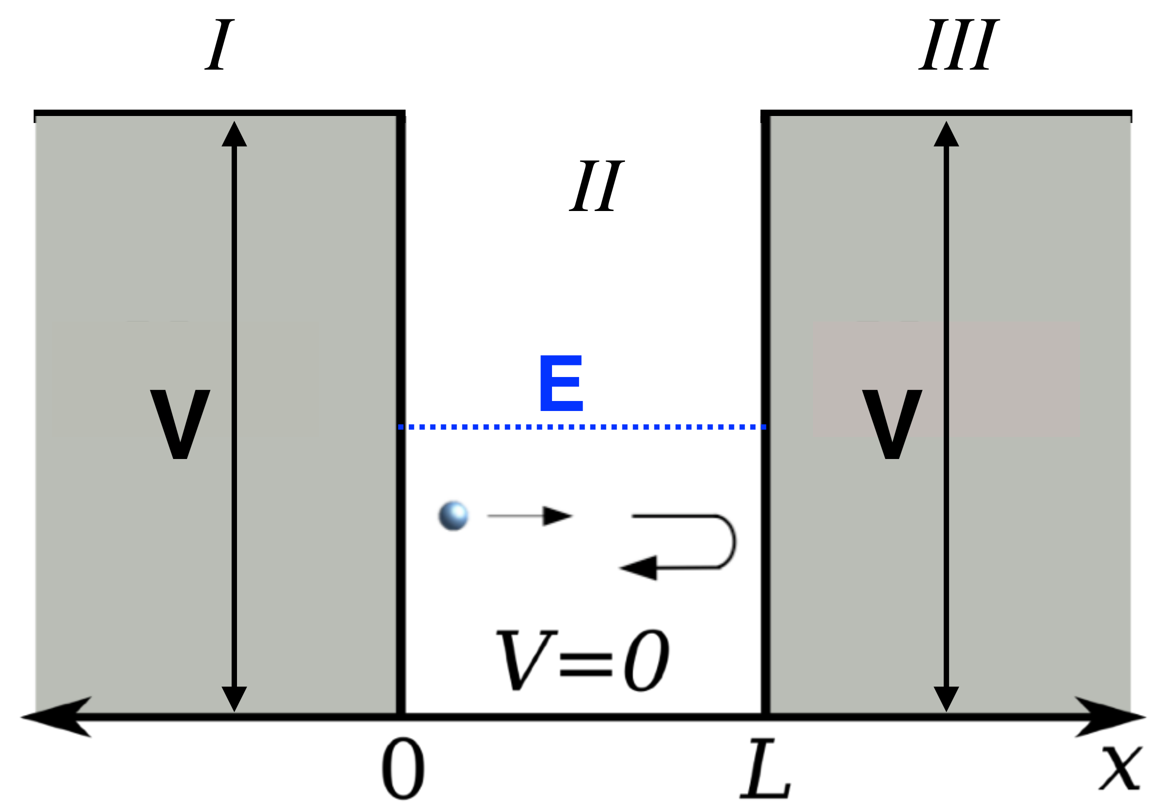
$$\Rightarrow \frac{\partial^2\psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\ \psi(x) = 0$$

Region-2, $V = 0$

$$\Rightarrow \frac{\partial^2\psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\ \psi(x) = 0$$

Region-2, $V = 0$

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



$$V(x) = \begin{cases} V & x \leq 0 & Region - I \\ 0 & x \leq 0 - to - x \geq L & Region - II \\ V & x \geq L & Region - III \end{cases}$$

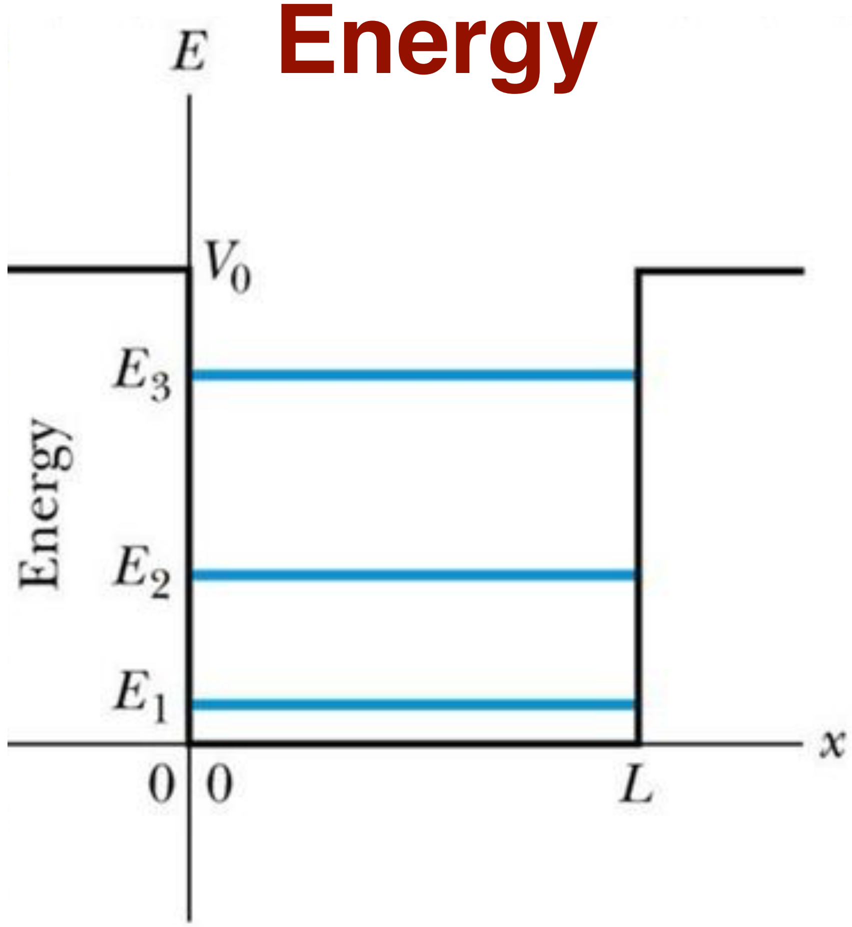
$$\psi_1(x) = Ae^{k_1 x}$$
$$\psi_2(x) = Ce^{k_2 x} + De^{-k_2 x}$$
$$\psi_3(x) = Be^{-k_1 x}$$

$$\therefore k_1 = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

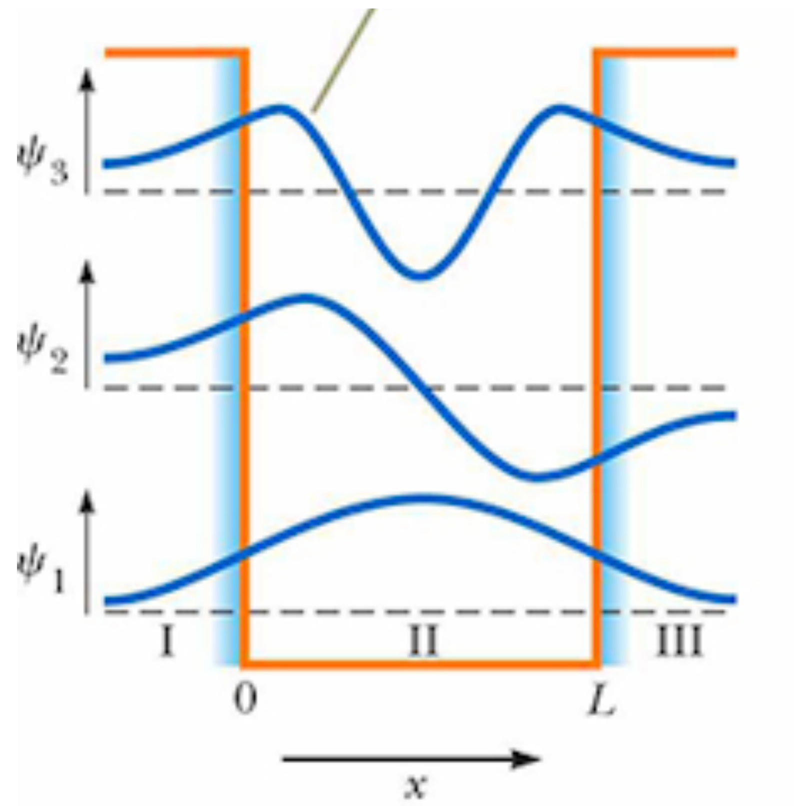
$$\therefore k_2 = \sqrt{\frac{2mE}{\hbar^2}}$$

Particle in a finite Potential Box

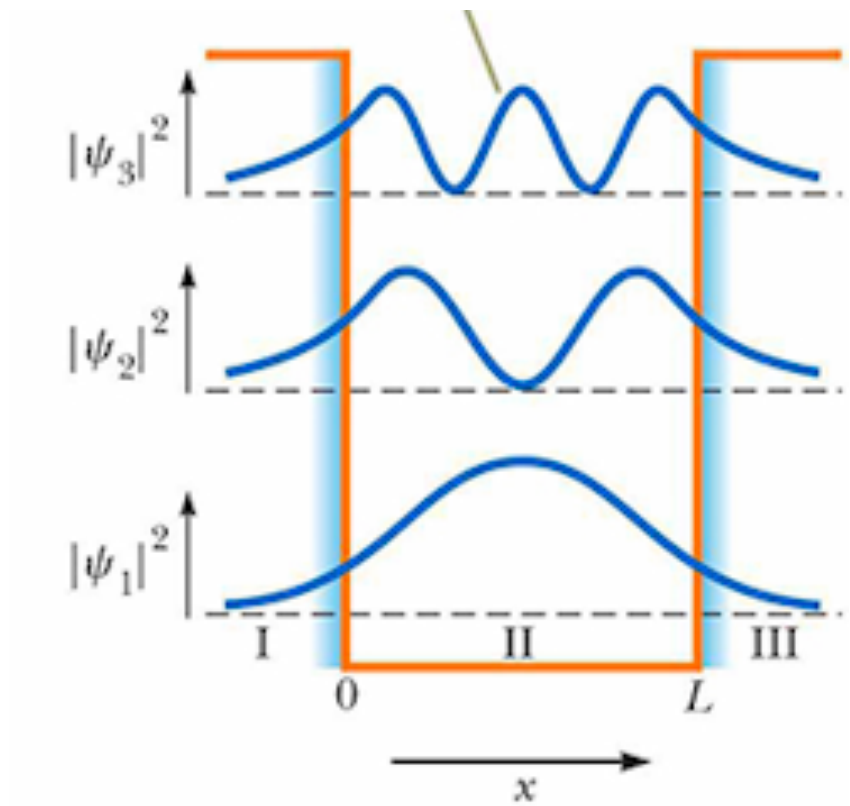
Energy



wave function



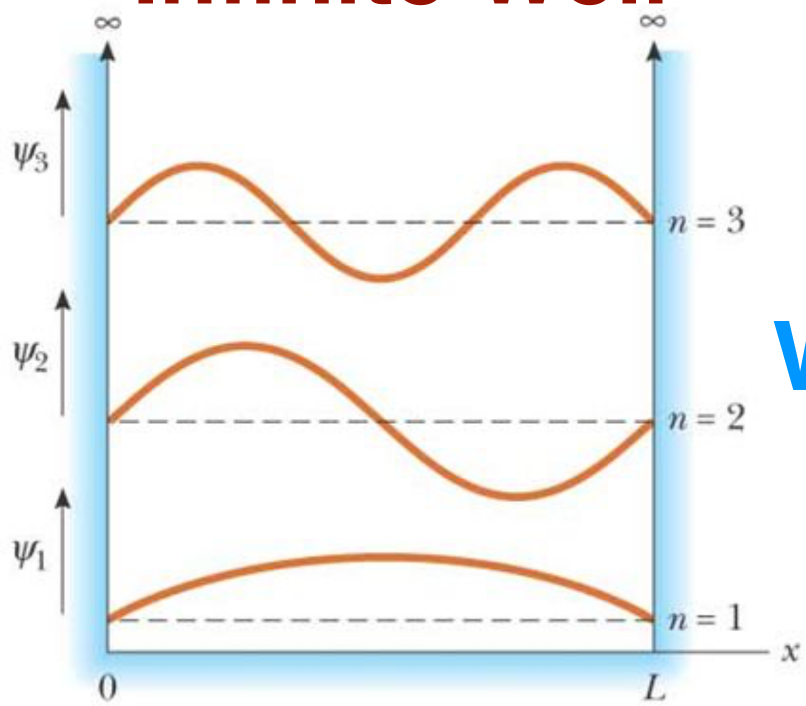
Probability



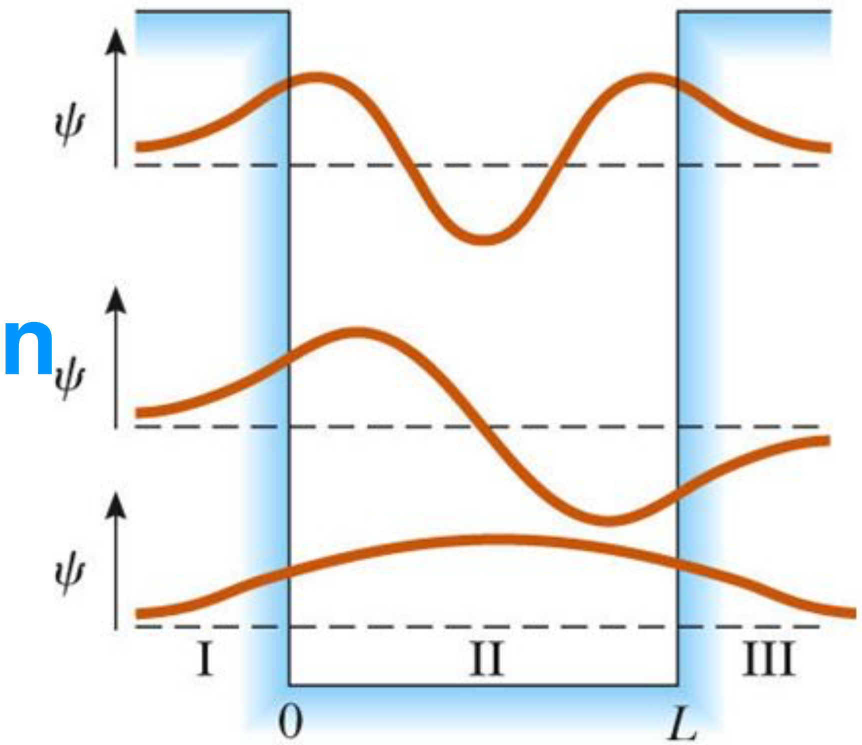
the wave function of the particle extends outside the well and the probability of the finding particle outside of the box increases

Infinite Vs Finite potential well

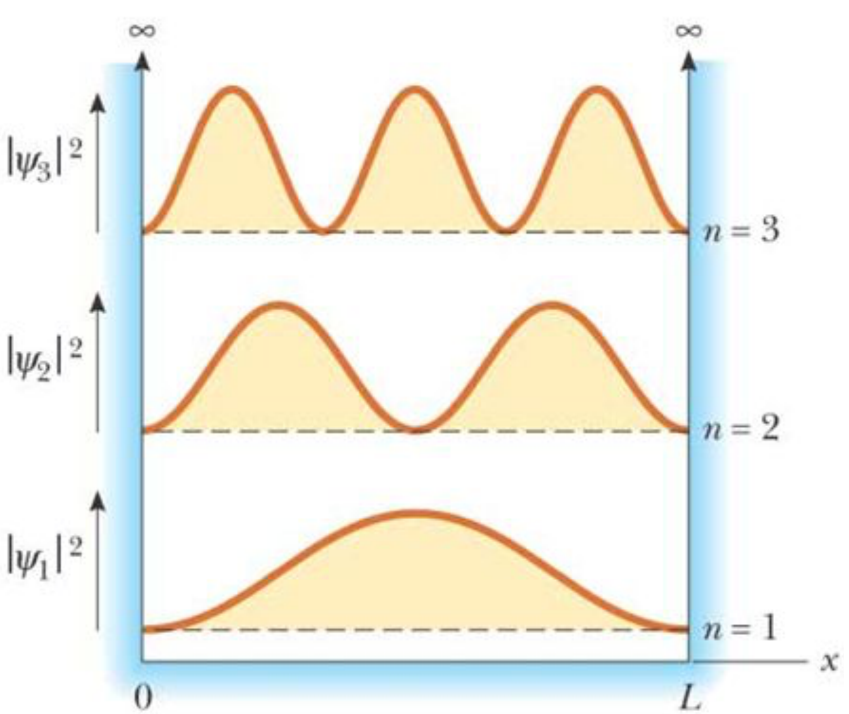
Infinite Well

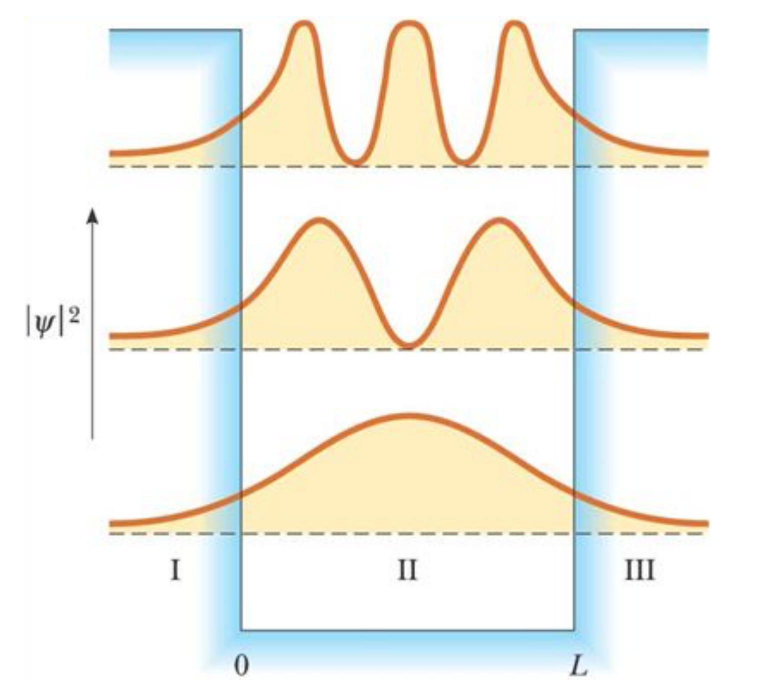


Finite Well



Wave function





Probability

Possible Question in Exam

1. Show that the energy of an electron in an infinite potential well varied as the square of the natural numbers.

2. Solve the Schrodinger wave equation for the motion of a free particle with mass 'm' and in a one-dimensional infinite potential well of width 'L'.

3. Calculate the minimum energy required to an electron to transit from the third energy level to the 4th energy level, if it is trapped within a one-dimension well of length 1.0 nm?

4. Derive the Eigen energy level of an particle trapped in a potential box. Plot the Energy, corresponding wave function and probability of the electron if it is in the 3rd excited state.

5. A particle is confined to one dimensional potential well of width 2 nm. It is found that when energy of the particle is 230 eV its Eigen functions have five antinodes. Find the mass of the particle in the lowest energy level.

6. An electron is bound in one-dimensional infinite well of width 5 nm. Find the energy values at 2nd excited states

Engineering Physics

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

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Information so far in QM

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

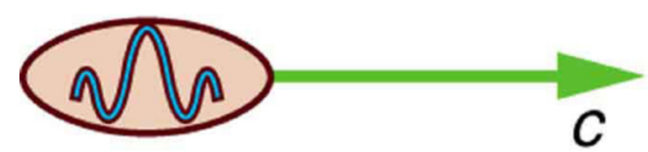
After 1905, In QM, a few examples change the concept and show that the light (EM wave) behaves like a particle:

- 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

<u>**Wave**</u>	<u>**Particle**</u>
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

Nobel Prize for Physics in 1929

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

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?

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

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

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

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

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

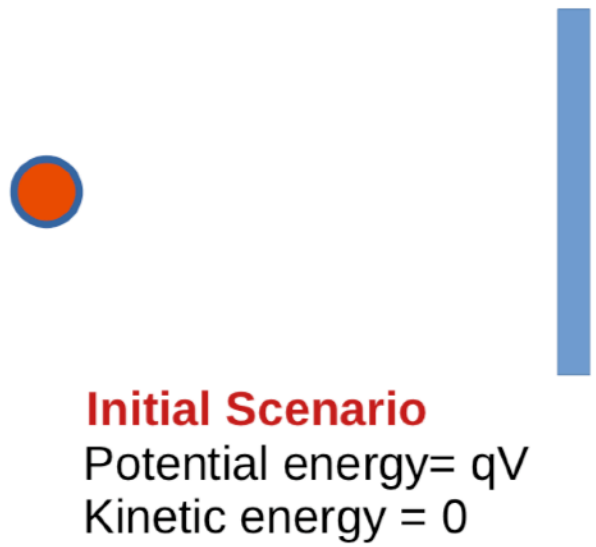
$$\lambda = 1.6575\times10^{-10}m$$

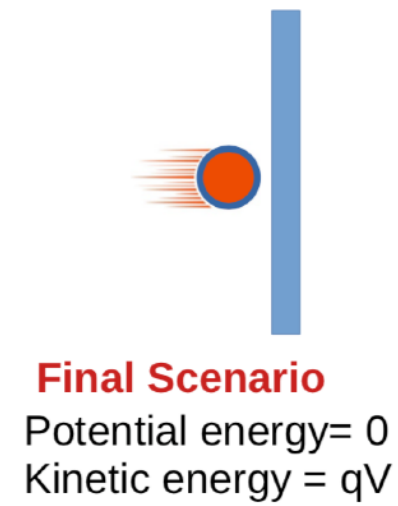
$$\lambda = 1.6575\times10^{-34}m$$

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 :





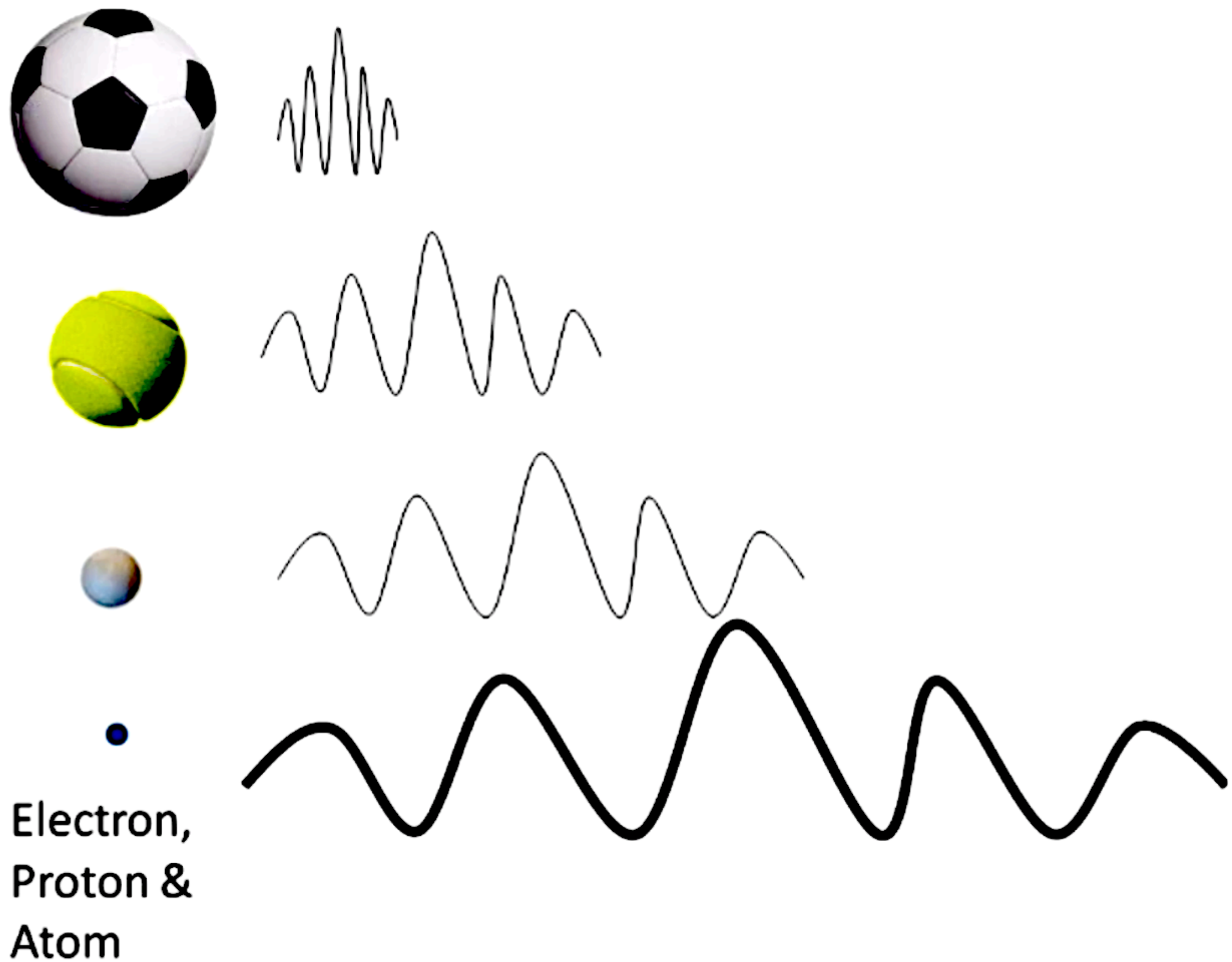
we know that, if the charge particle is accelerated, then the electrostatic work done on the charge parcel is converted into its kinetic energy:

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

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

de Broglie Hypothesis

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



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

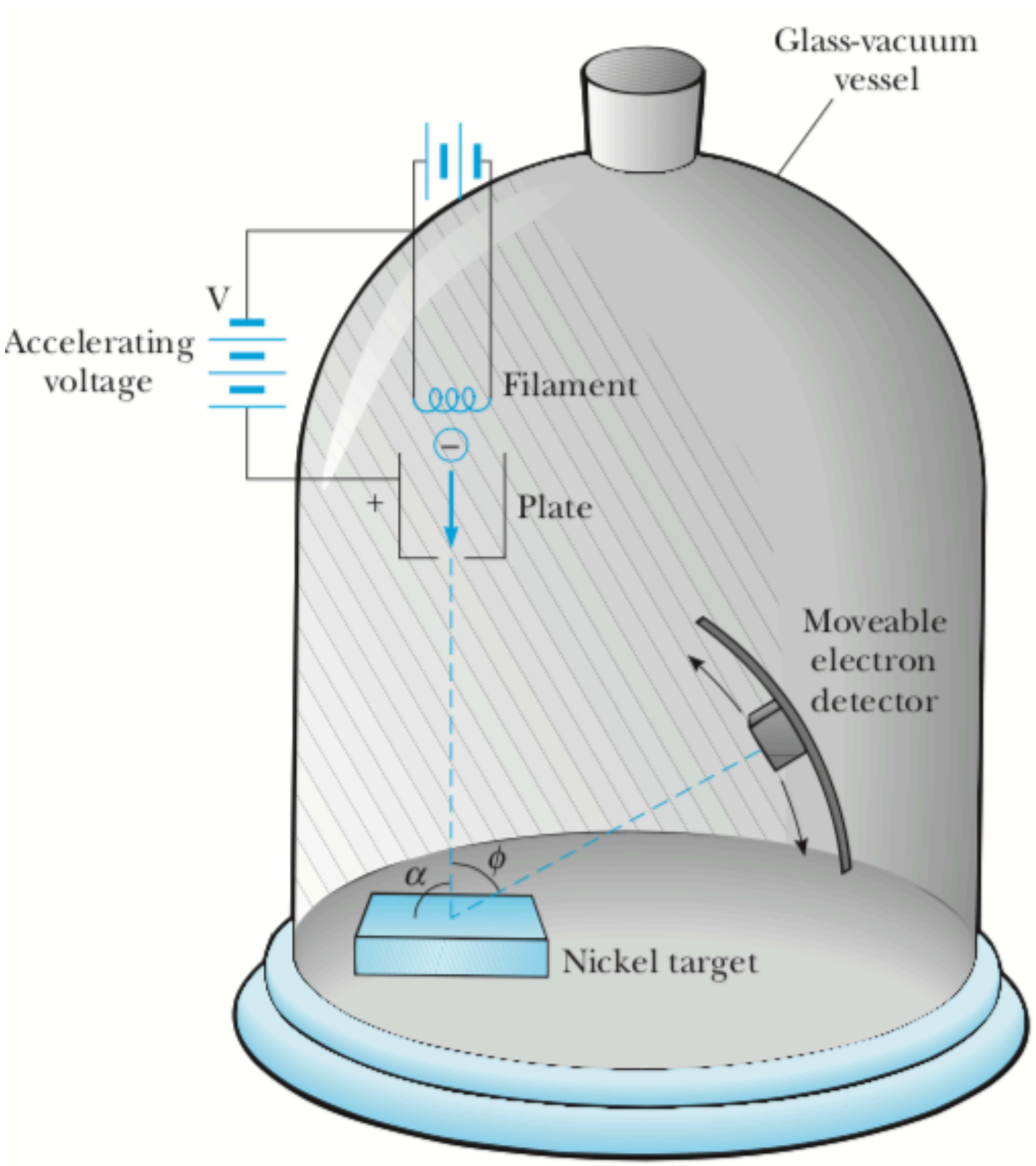
Davisson-Germer Experiment (Proof of Matter Wave)

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

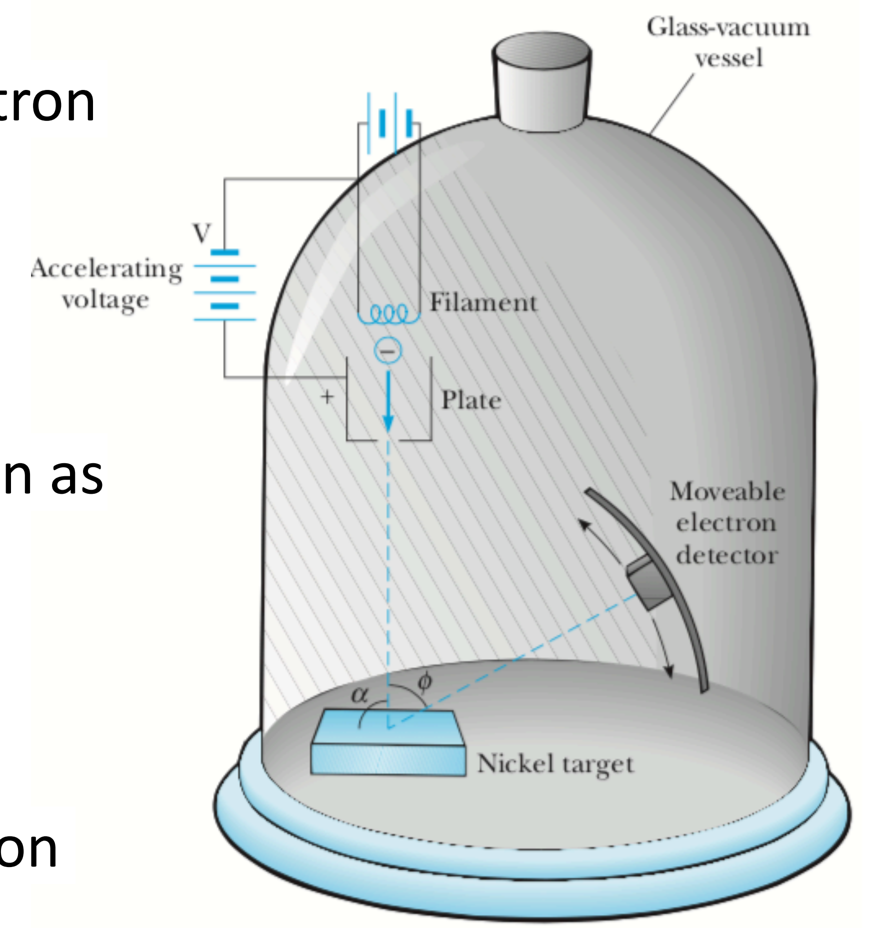
(iv) Nickel target

(v) movable detector

Davisson-Germer Experiment: Procedure

Experiment:

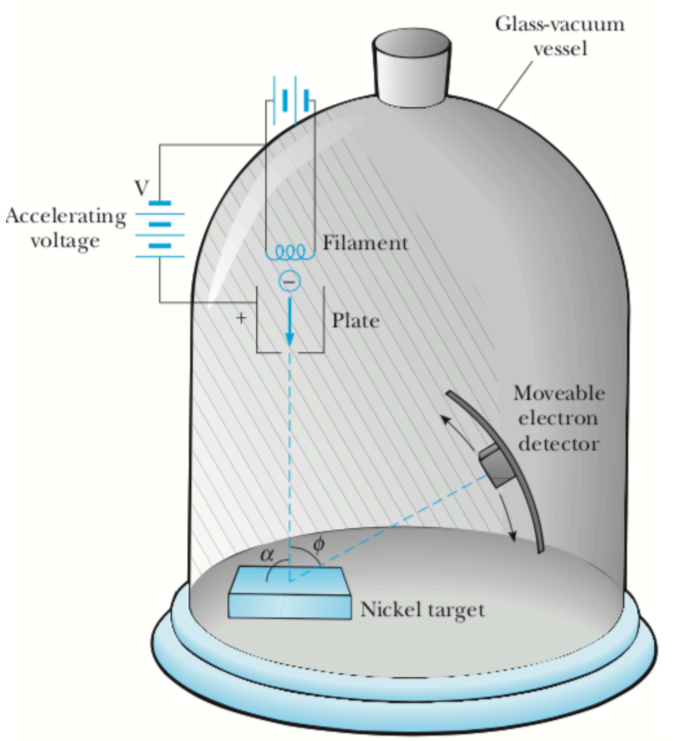
- **Evacuated chamber** is used to avoid any hindrance to the electron motion.
- **A filament connected to battery** heats when the battery is switched on.
- The heated filament starts emitting electron in a process known as "thermionic emission".
- Electrons emitted by the filament are accelerated to 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.**

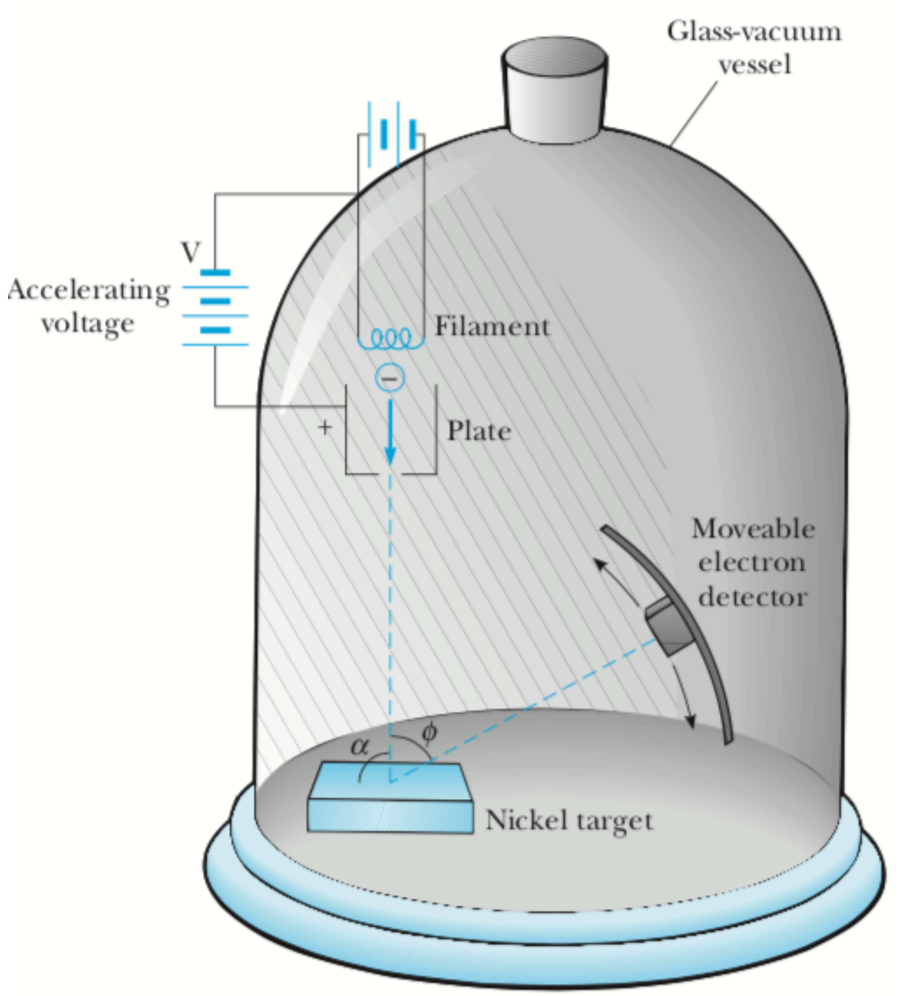
Electrons are scattered in all directions by the atoms of the crystal.

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° .**

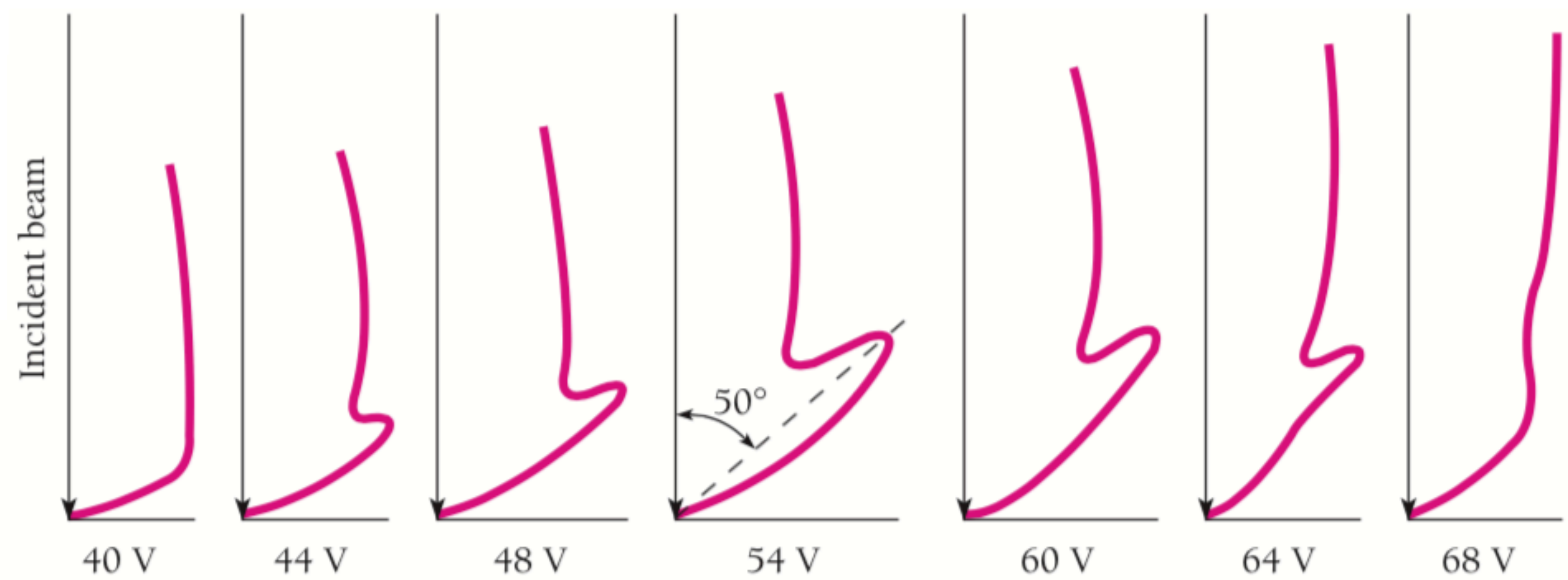
At the angle at maximum intensity, wavelength of electrons can be calculated in two ways: **(i) de Broglie's formula** and **(ii) Bragg's condition for constructive interference**

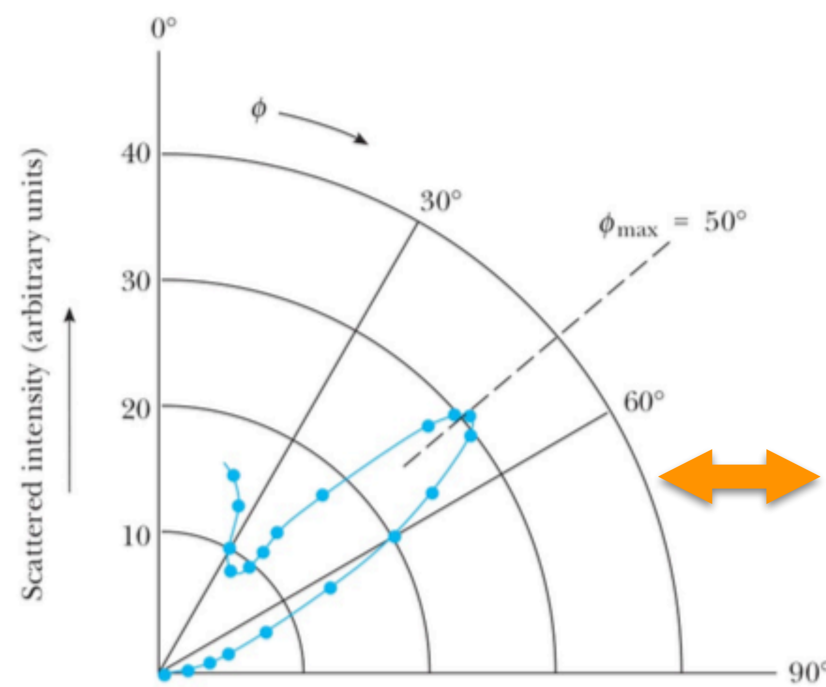
Davisson-Germer Experiment: Results

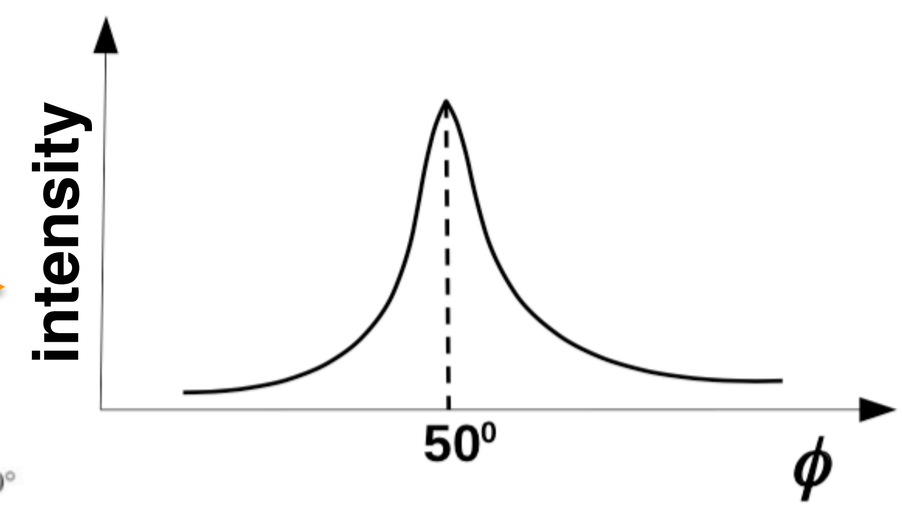


Schematic of the Davisson-Germer experiments

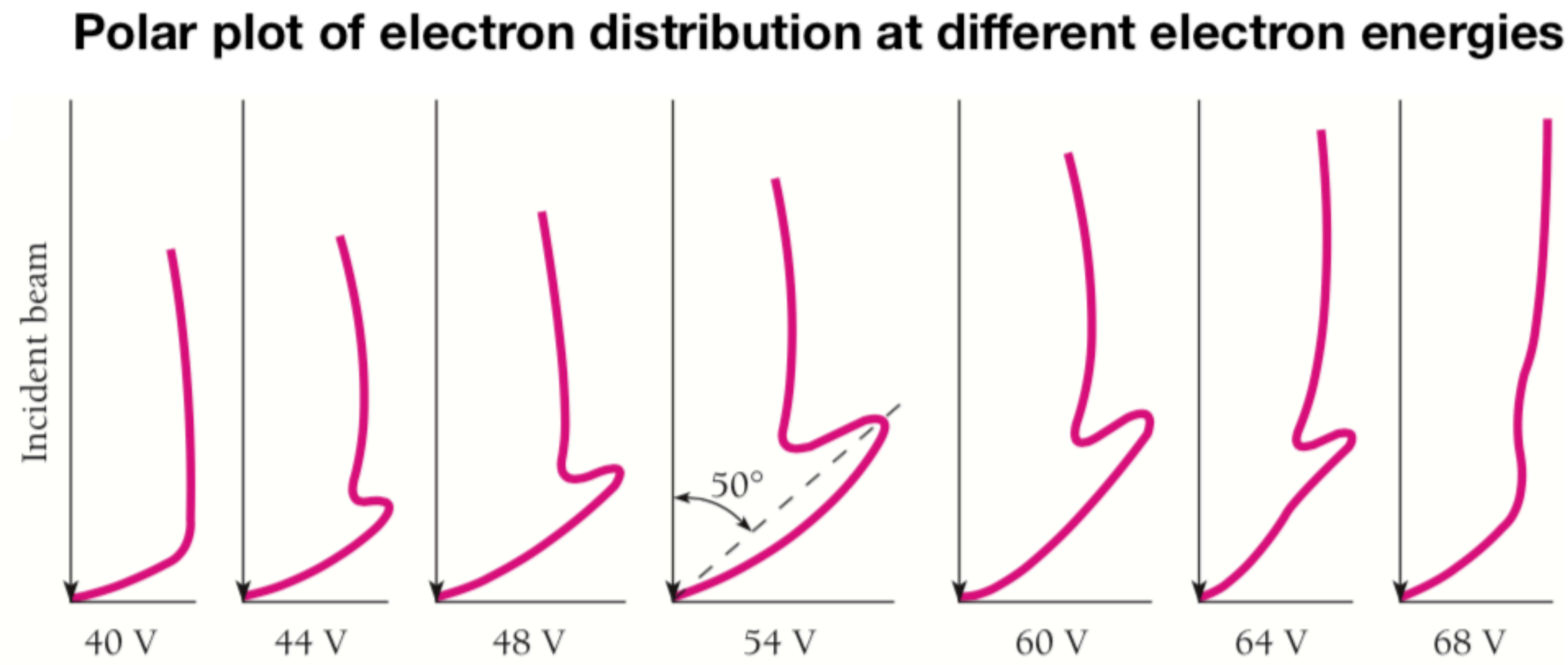
Polar plot of electron distribution at different electron energies







Davisson-Germer Experiment: Results



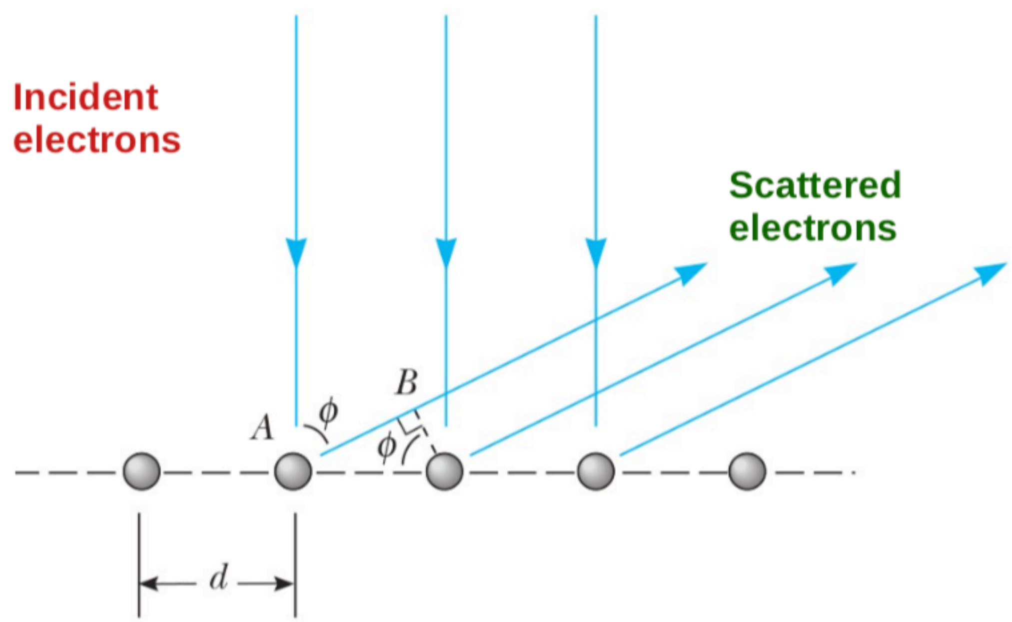
From these experimental curves, the following inferences can be drawn :

- 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 $$d\sin(\phi)=\lambda$$ 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:

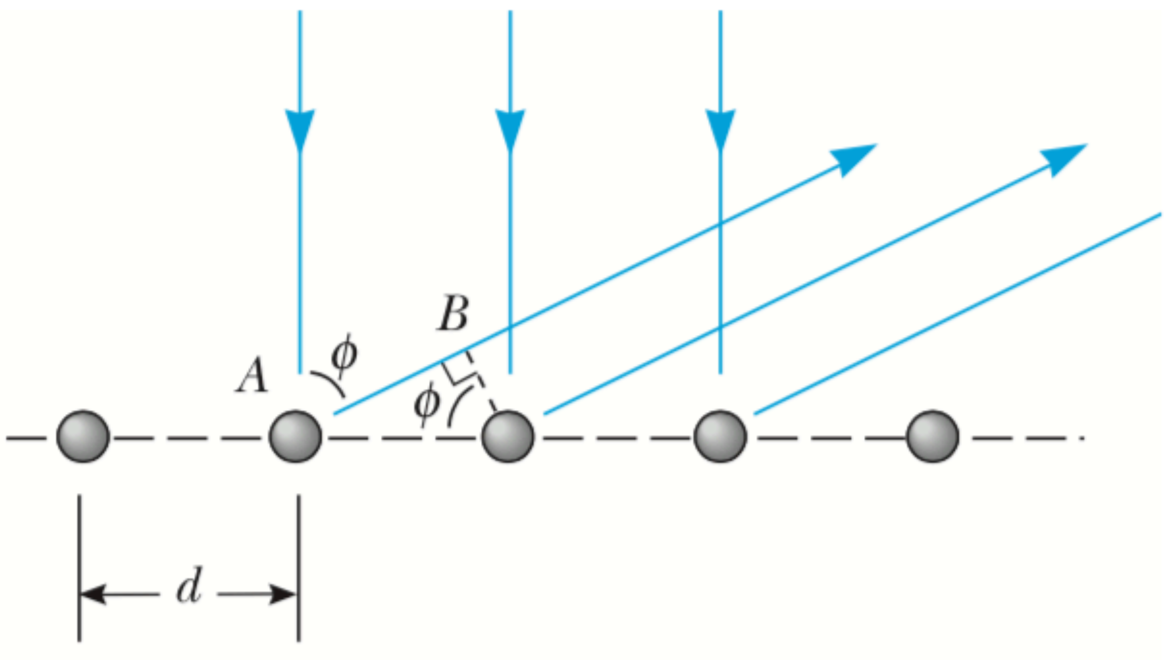
$$\boxed{\lambda = d\sin(\phi) = 2.15\ \sin(50^0) \approx 1.65\, A^0}$$

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:

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

Therefore, electrons must have wave properties.

Davisson-Germer Experiment: Results Analysis



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

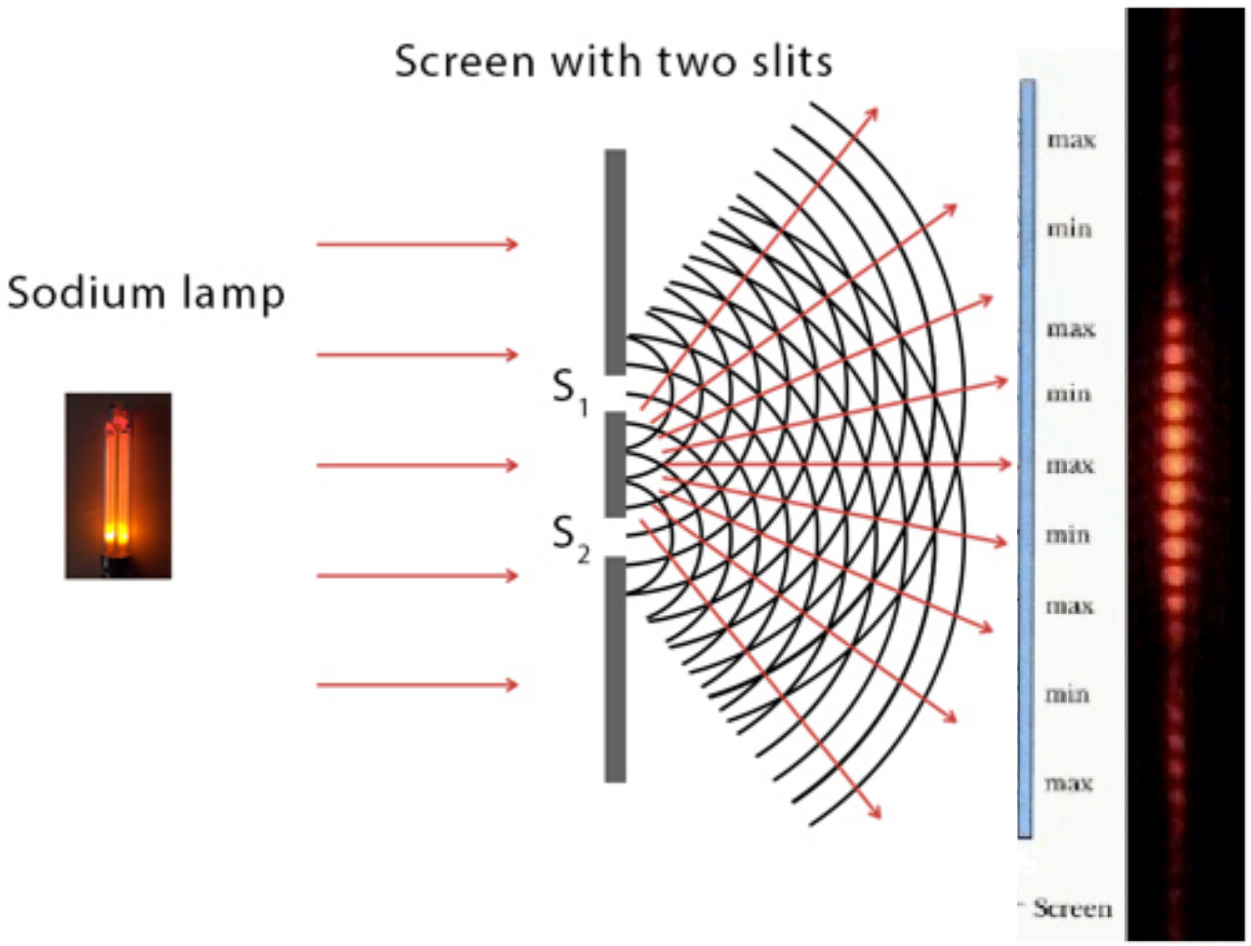
$$\lambda_B = \frac{h}{\sqrt{2m_e eV}}$$

- 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.

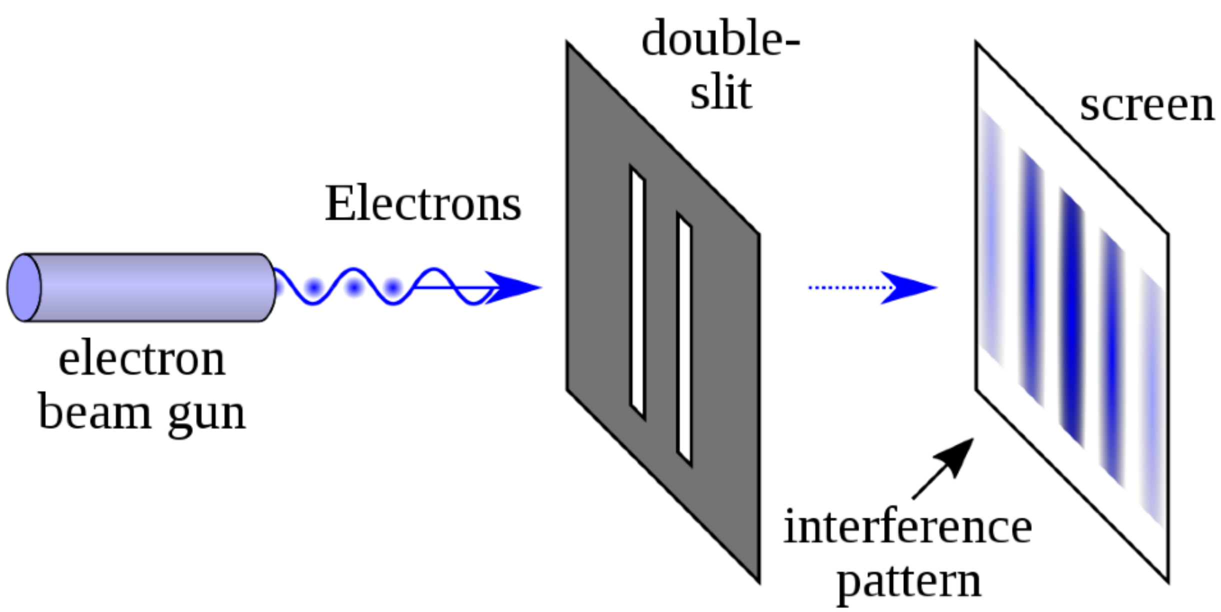
$$\lambda_{Experiment} = \lambda_{DeBroglie} = \frac{h}{\sqrt{2m_e eV}} = 0.165nm$$

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 <u>$0.5*10^{-6}$ m</u> = <u>0.5 μm</u> = <u>500 nm</u> in size.

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

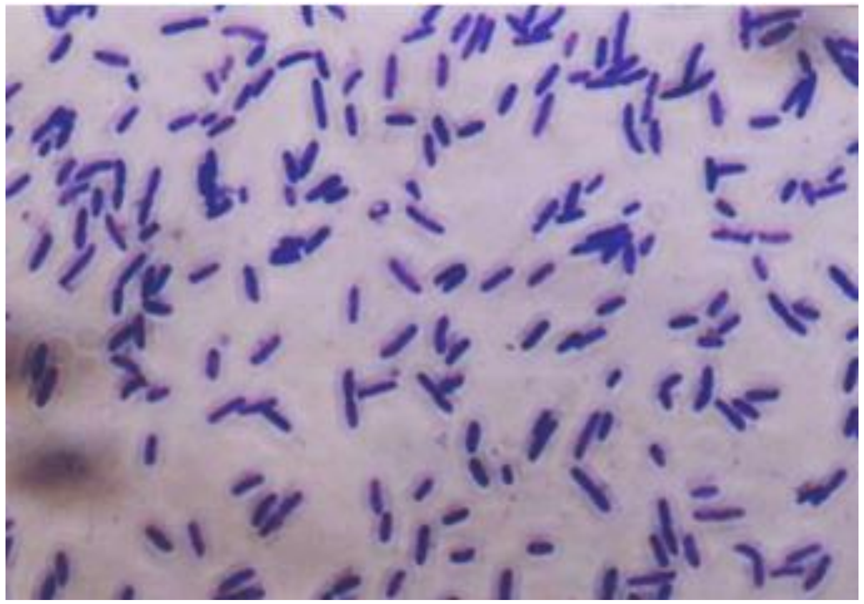
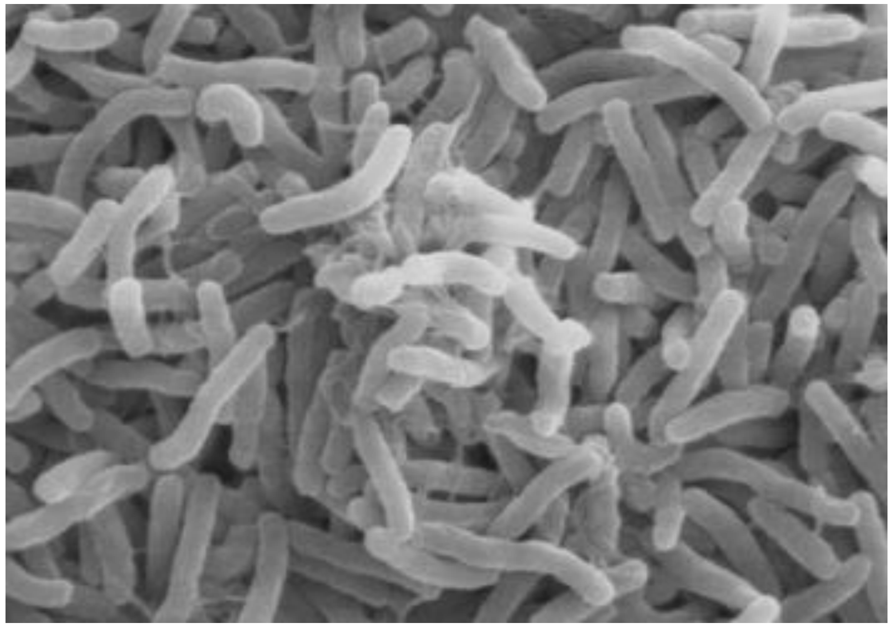


Image is in the public domain

Bacteria, as viewed using visible light



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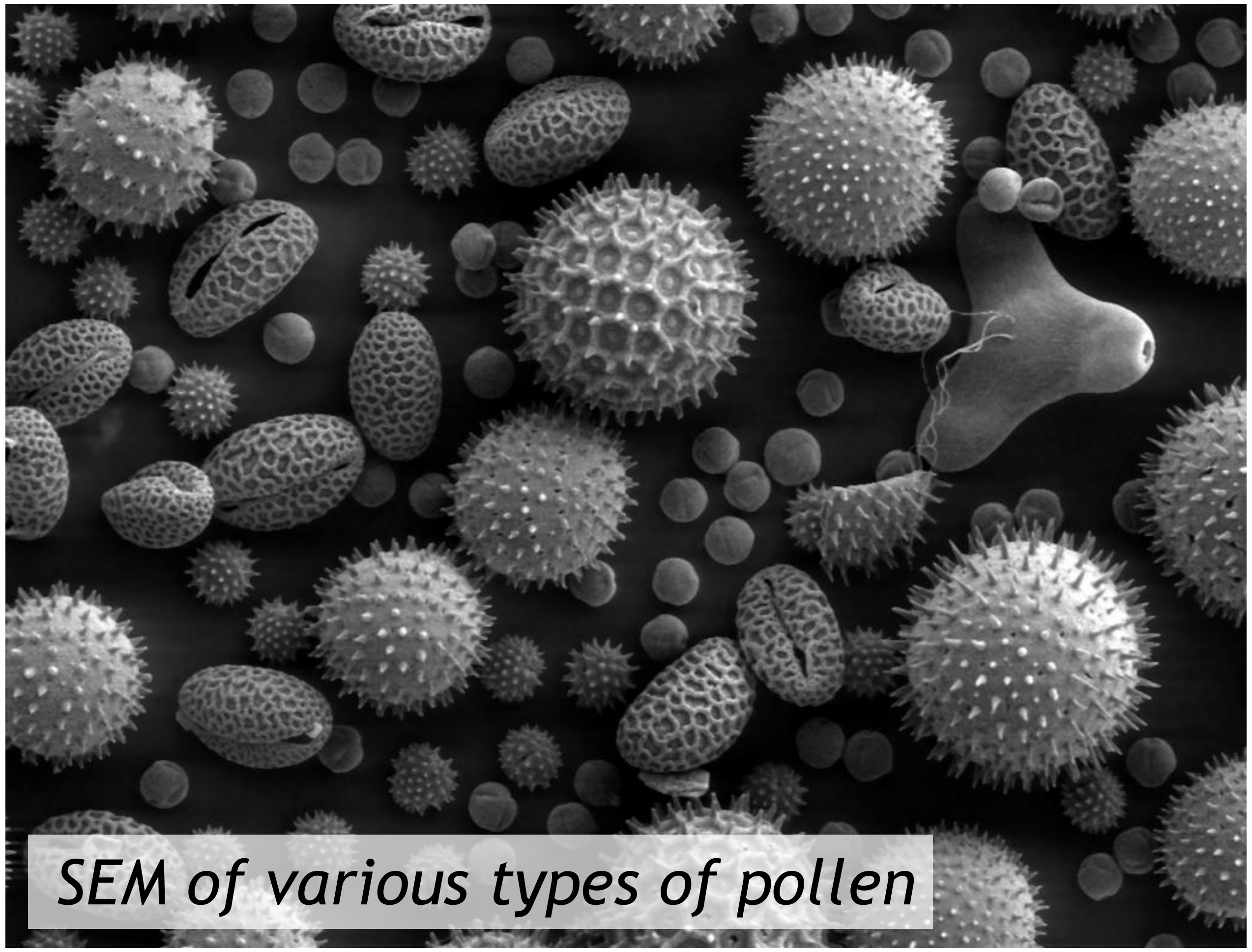
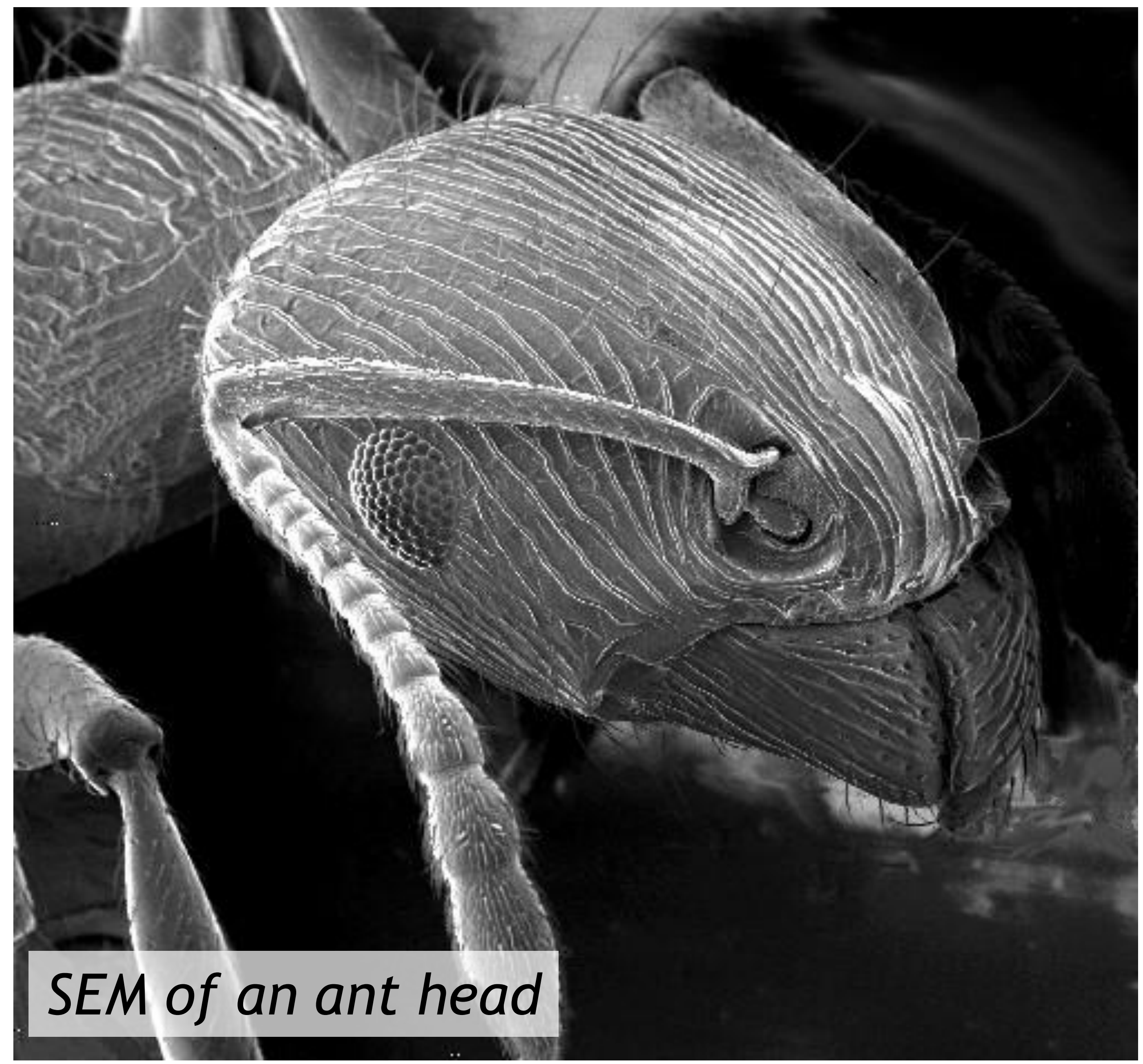
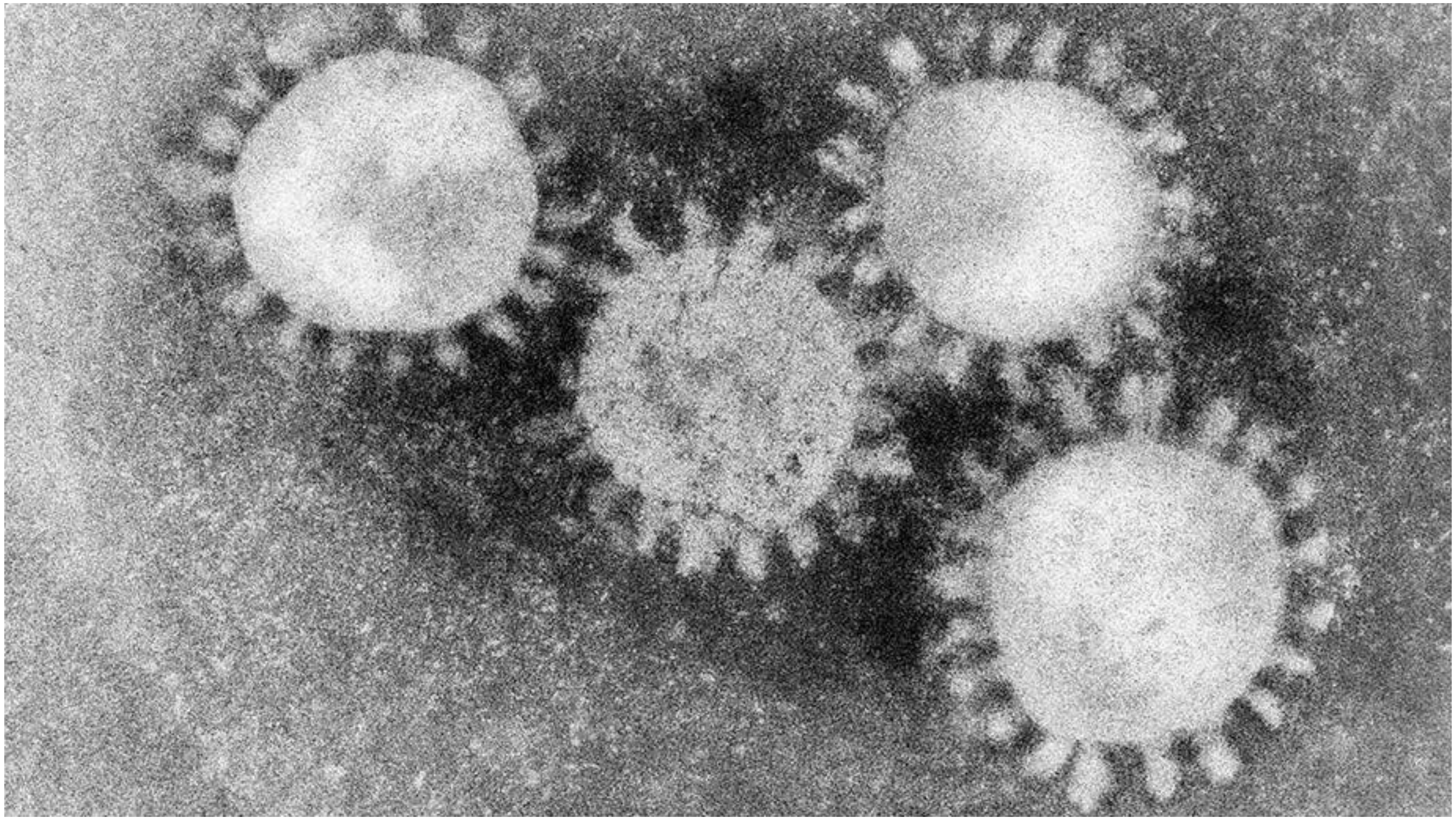
Bacteria, as viewed using electrons!

Wave Nature of Electron: Invention of Electron Microscope

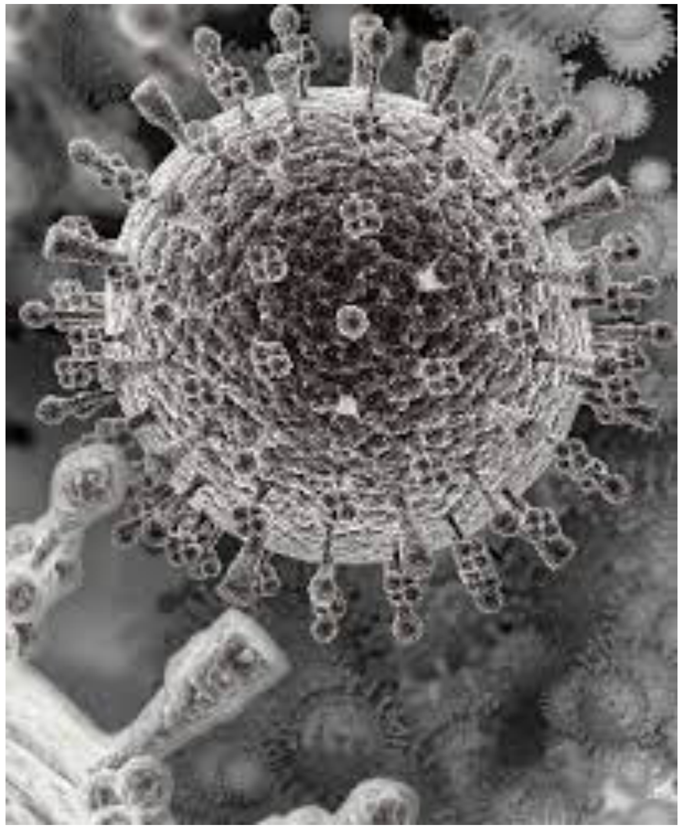




Wave Nature of Electron: Invention of Electron Microscope



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**

Engineering Physics

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

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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

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

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

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

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

$$\Rightarrow \underbrace{\frac{1}{\phi(t)}\ \left[i\hbar\frac{\partial\phi(t)}{\partial t}\right]}_{\text{Function of time}} = \underbrace{\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V\psi(x)\right]\frac{1}{\psi(x)}}_{\text{Function of position}}$$

Time-independent Schrödinger Wave Equation

$$\underbrace{\frac{1}{\phi(t)}\left[i\hbar\frac{\partial\phi(\mathrm{t})}{\partial\mathrm{t}}\right]}_{\text{Function of time}} = \underbrace{\left[-\frac{\hbar^2}{2\mathrm{m}}\frac{\partial^2\psi(\mathrm{x})}{\partial \mathrm{x}^2} + \mathrm{V}\psi(\mathrm{x})\right]\frac{1}{\psi(x)}}_{\text{Function of position}}$$

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

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

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

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

upon substitution, we will have

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

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

Time-independent Schrödinger Wave Equation

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

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

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

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

$$\Downarrow$$

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

$$\Downarrow$$

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

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?**

Engineering Physics

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

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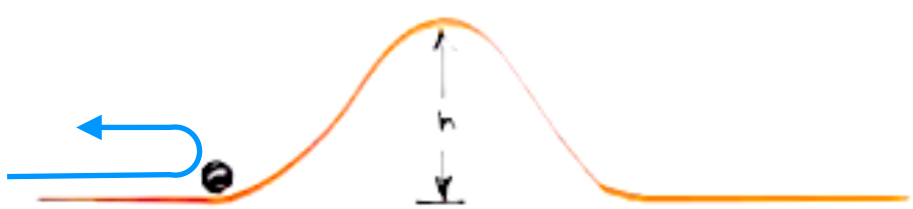
Tunneling

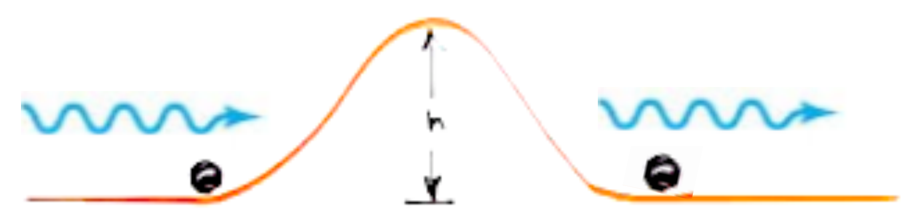
From our discussion of the finite potential well, the wave function of the particle **extends outside the well** and the probability of the finding particle outside of the box increases. So you can think that even if the **total energy, E of the particle is less than the V**, still, there is the probability we can find it outside, which is **forbidden in classical mechanics**. Here the concept of **tunneling** starts

Classical point of view



- **Macroscopic object**
- **The object having mass=m, K.E=E, PE=V=0**
- **if, E < V = mgh, it will not pass the Hill**

Quantum point of view



- **Microscopic object**
- **if, E<V, there is a finite probability the particle can found other side of the Hill**

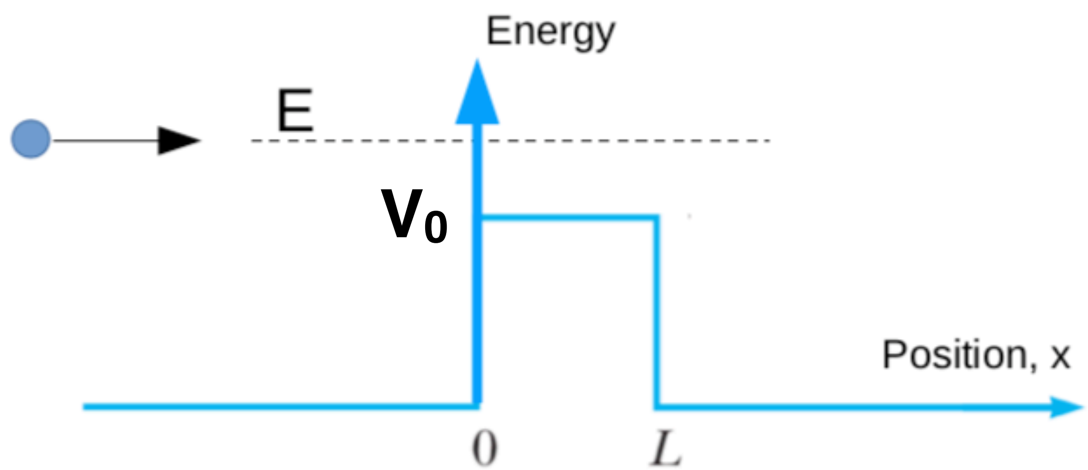
Barriers and Quantum Tunneling

Consider a particle of energy ***E* approaching a potential barrier of height V_0** and the potential everywhere else is zero. Now we consider the situation where classically the particle does not have enough energy to surmount the potential barrier, $E < V_0$

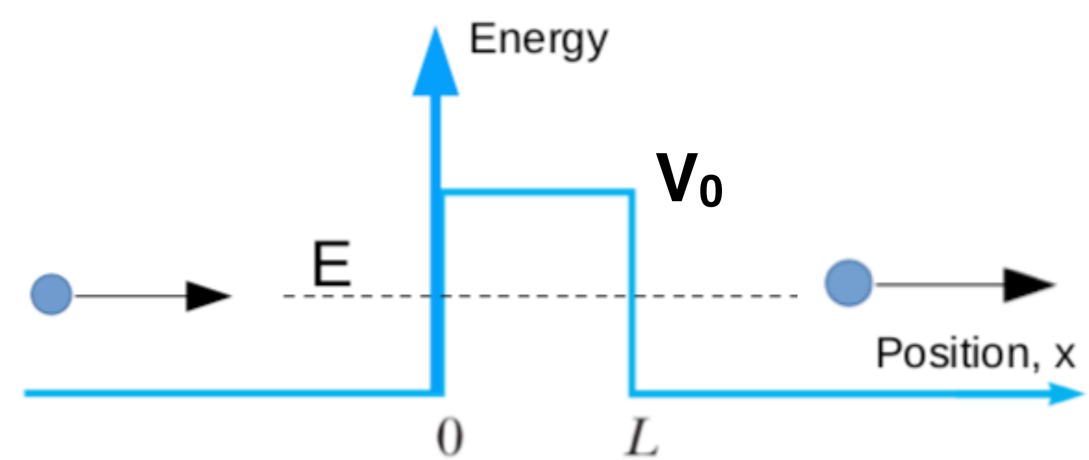
V_0—is height of the **potential barrier**

L—is the **width of the potential barrier**

E—is the **total energy of the incident particle**



(a) Particle crosses the barrier because **$E>V_0$**



(b) Particle does not cross the barrier because **$E<V_0$**

Quntum tunneling is a phenomenon in which an microscopic **object** such as an electron or atom **passes through a potential energy barrier** although that does not have sufficient energy to penetrate it.

Quantum Tunneling : Platform No 9 $\frac{3}{4}$

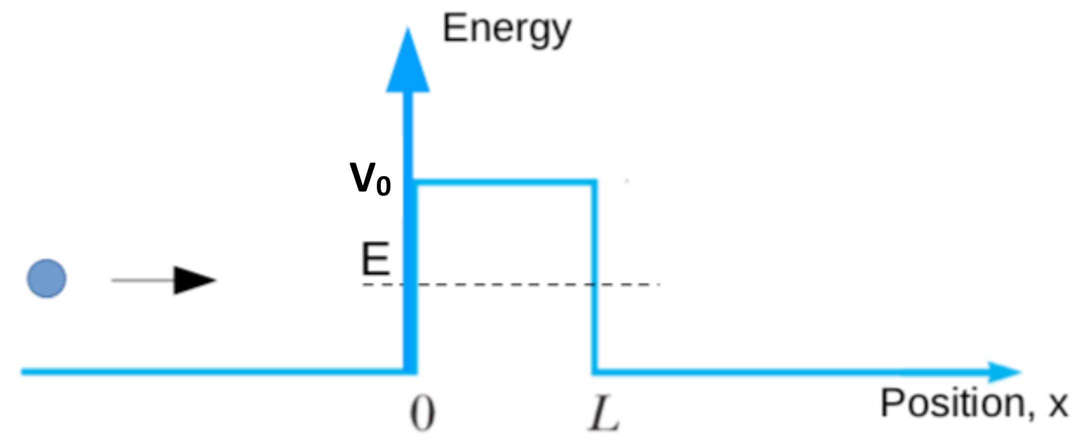
Quantum Tunneling : Platform No 9 $\frac{3}{4}$

Quantum Tunneling

Tunneling is purely a **quantum phenomena** and can understood by solving Schrodinger equation for a particle moving towards a potential barrier.

Time independent Schrodinger Equation is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{x^2} + V_0(x)\,\psi = E\,\psi$$



Where the potential is

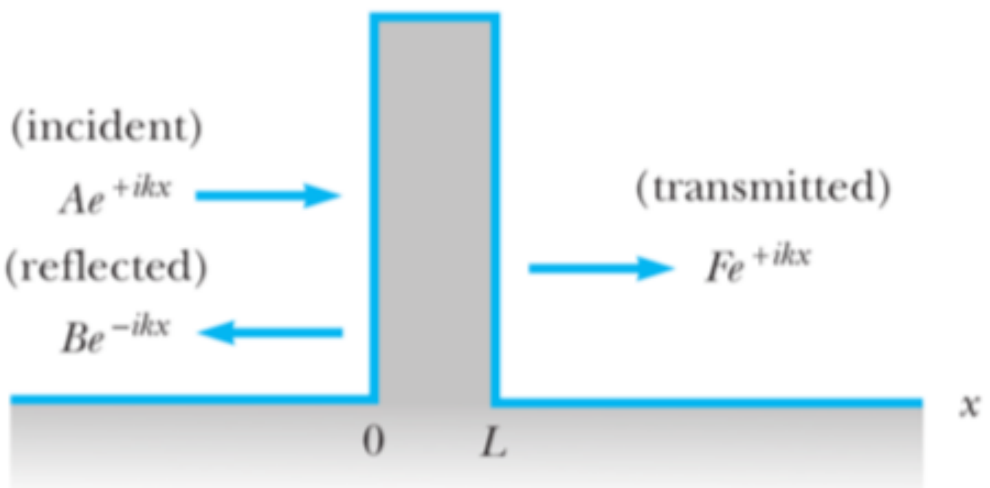
$$V_0(x) = \begin{cases} 0 & \text{if} \quad x < 0 \\ V_0 & \text{if} \quad 0 \leqslant x \leqslant L \\ 0 & \text{if} \quad x > L \end{cases}$$

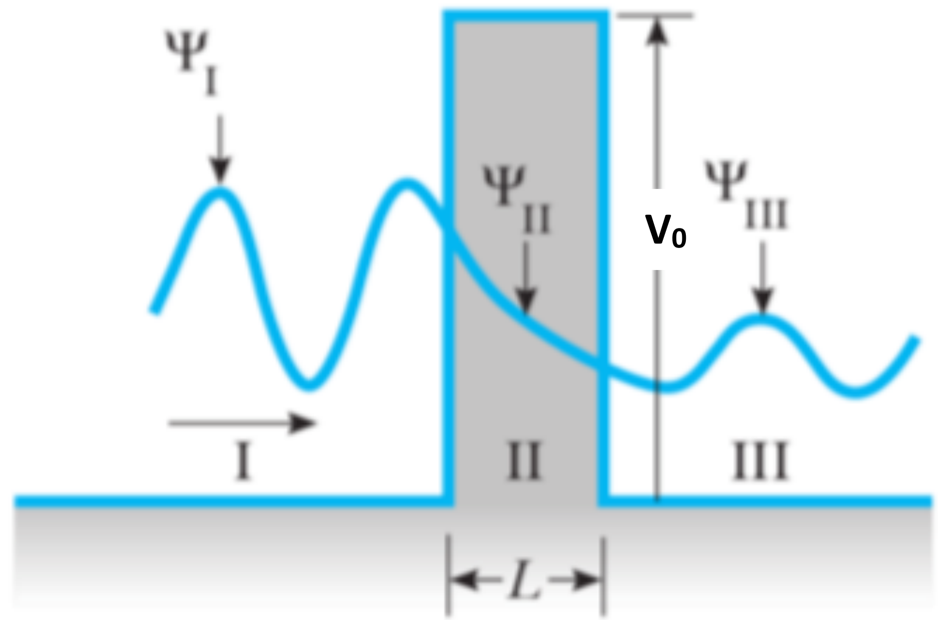
Quantum Tunneling

So quantum results that there is a non-zero probability

➔ the particle can penetrate the barrier and emerge on the other side

➔ **the incident particle can tunnel the barrier**





$\psi_1 =$ *Sinusoidal*

$\psi_2 =$ *Exponetntial Decay or Evanescent wave*

$\psi_3 =$ *Sinusoidal (lower amplitude)*

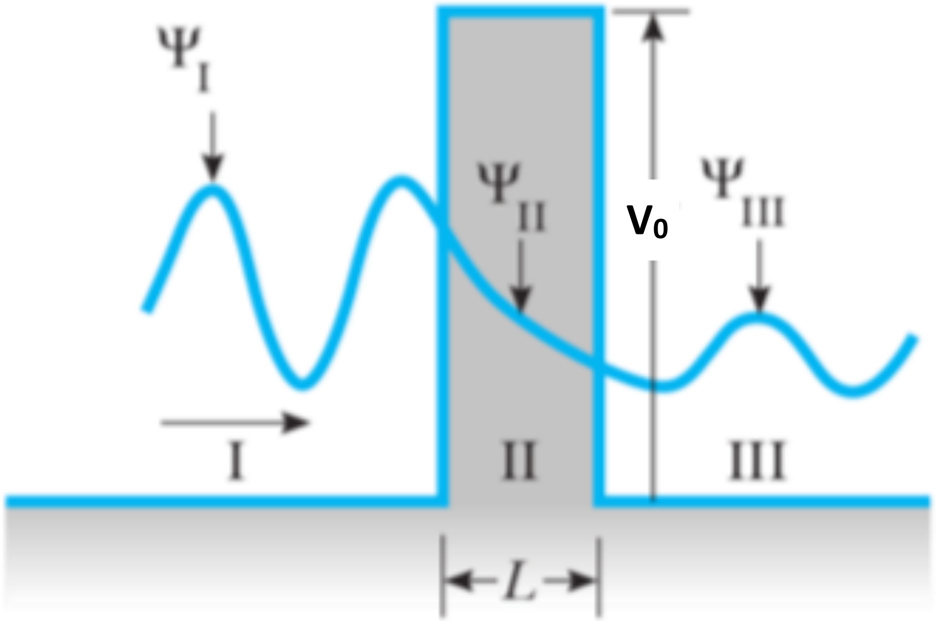
Reflection probability
$$R = \frac{(\Psi^*\Psi)_{\text{reflected}}}{(\Psi^*\Psi)_{\text{incident}}} = \frac{B^*B}{A^*A} = \frac{|B|^2}{|A|^2}$$

Transmission probability
$$T = \frac{(\Psi^*\Psi)_{\text{transmitted}}}{(\Psi^*\Psi)_{\text{incident}}} = \frac{F^*F}{A^*A} = \frac{|F|^2}{|A|^2}$$

$$R + T = 1$$

Remember, transmission probability is zero in classical physics!

Barriers and Tunneling



Region I $(x<0)$	$V=0$	$\dfrac{d^2\psi_I}{dx^2}+\dfrac{2m}{\hbar^2}E\psi_I=0$
Region II $(0<x<L)$	$V=V_0$	$\dfrac{d^2\psi_{II}}{dx^2}+\dfrac{2m}{\hbar^2}(E-V_0)\psi_{II}=0$
Region III $(x>L)$	$V=0$	$\dfrac{d^2\psi_{III}}{dx^2}+\dfrac{2m}{\hbar^2}E\psi_{III}=0$

The wave function in region II becomes:

$$\psi_{II}=Ce^{\kappa x}+De^{-\kappa x} \quad \text{where} \quad \kappa=\frac{\sqrt{2m(V_0-E)}}{\hbar}$$

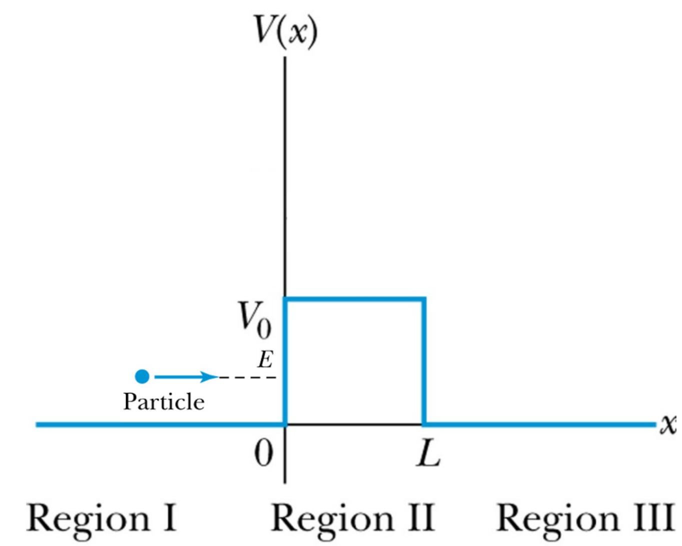
The transmission probability that describes the phenomenon of **tunneling** is:

$$T=\left[1+\frac{V_0{}^2\sinh^2(\kappa L)}{4E(V_0-E)}\right]^{-1}$$

$$T=\left[1+\frac{V_0{}^2\sinh^2(\kappa L)}{4E(V_0-E)}\right]^{-1} \xrightarrow{\sinh(kL)\xrightarrow{kL\to\infty}\frac{1}{2}e^{kL}} \boxed{T=16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\kappa L}}$$

Tunneling: Problem

In a particular semiconducting device, electrons that are accelerated through a potential difference of 5 V attempt to tunnel through a barrier of width 0.8 nm and height 10 V. **What fraction of electrons are able to tunnel through the barrier?**



Given:

$$L = 0.8 \text{ nm},\ E = 5\ eV,\ V_0 = 10\ V$$

$$T = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\kappa L}$$

$$\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar} = \frac{2\pi\sqrt{2mc^2(V_0-E)}}{hc} = \frac{2\pi\sqrt{2\left(0.511\times10^6 eV\right)(10eV-5eV)}}{1240eV\cdot nm} = 11.5\ nm^{-1}$$

$$\therefore \kappa L = \left(11.5\ nm^{-1}\right)0.8\ nm = 9.2$$

Approximately → $T = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\kappa L} = 16\left(\frac{5eV}{10eV}\right)\left(1-\frac{5eV}{10eV}\right)e^{-2(9.2)} = 4.1\times10^{-8}$

Tunneling Applications

- $\alpha - \beta$, Radio Active decay
- Nuclear Fusion and Fission Process
- Tunnel Diode
- SQUID
- Quantum Computing
- **Scanning Tunnelling Microscope**

Engineering Physics

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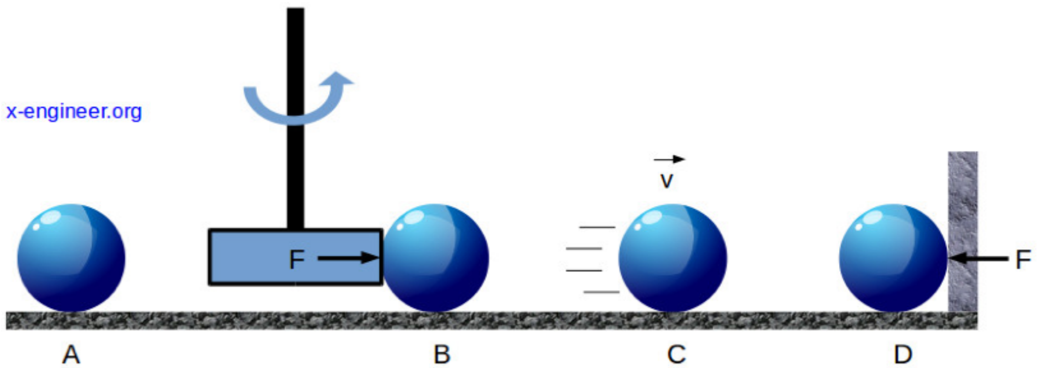
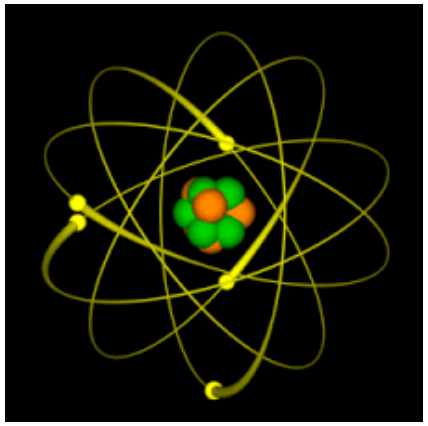
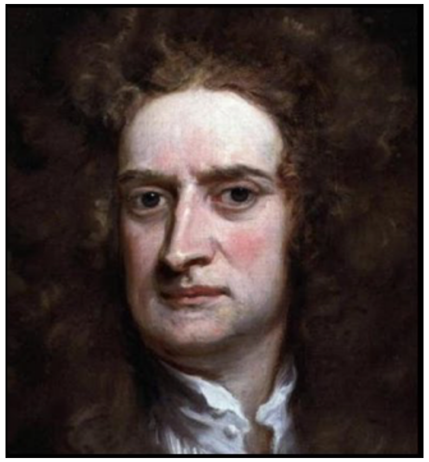
Understanding the Microscopic System



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

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

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

$V = time\ dependant\ Potential\ energy$

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 $\psi(x,t)$:

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

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

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

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

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 $\psi(x,t)$:

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

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

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

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

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

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

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

$$\Downarrow$$

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

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

$$\Downarrow$$

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

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

This is called the **time-dependent Schrodinger equation**. One has to solve this equation with appropriate boundary conditions to find the **wavefunction $\psi(x)$ 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.

Possible Questions

1. **Construct the one dimensional time dependent Schrodinger wave equation for microscopic particle in motion/for a matter wave?**

Engineering Physics

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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.

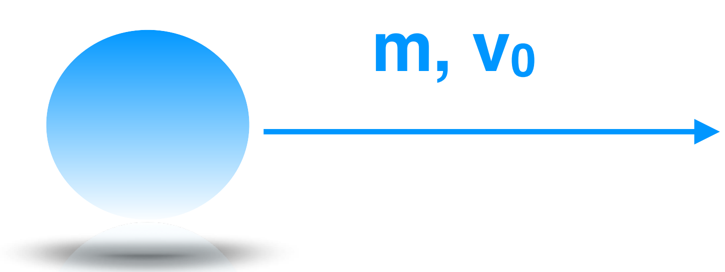
- De Broglie's hypothesis stated that matter too will have both the particle and wave nature, $\lambda = \frac{h}{p}$ (every moving particle – microscopic or macroscopic –has its own wavelength).

- Davisson-Germer experiment proved the wave nature of matter by diffracting electrons through a crystal

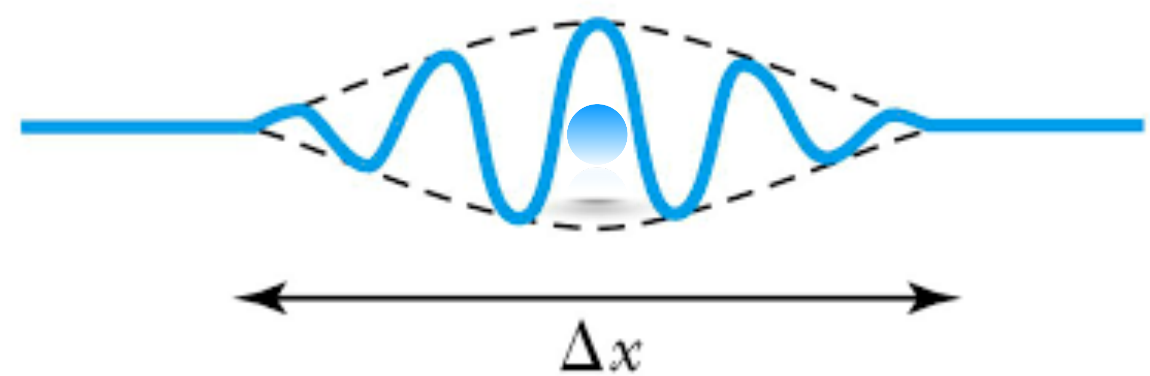
Uncertainty for Position for a Matter Wave

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

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



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,

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

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

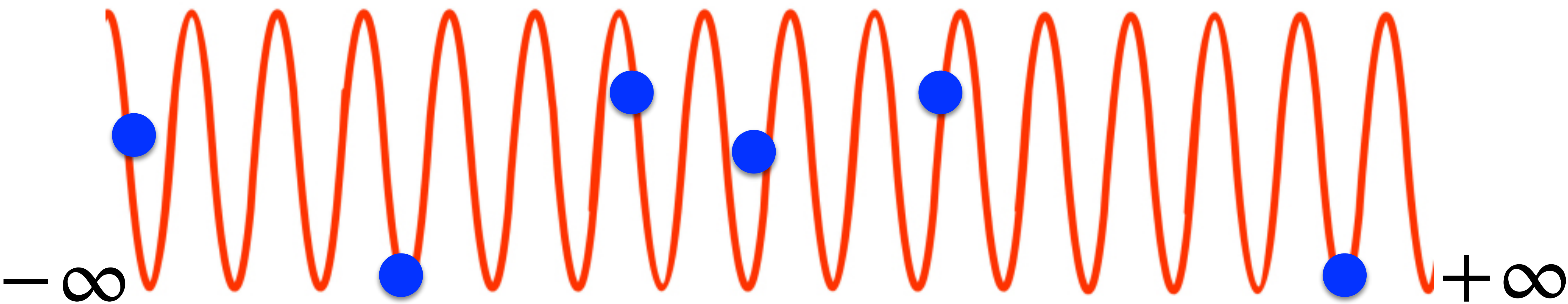
or

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

Heisenberg Realised that…

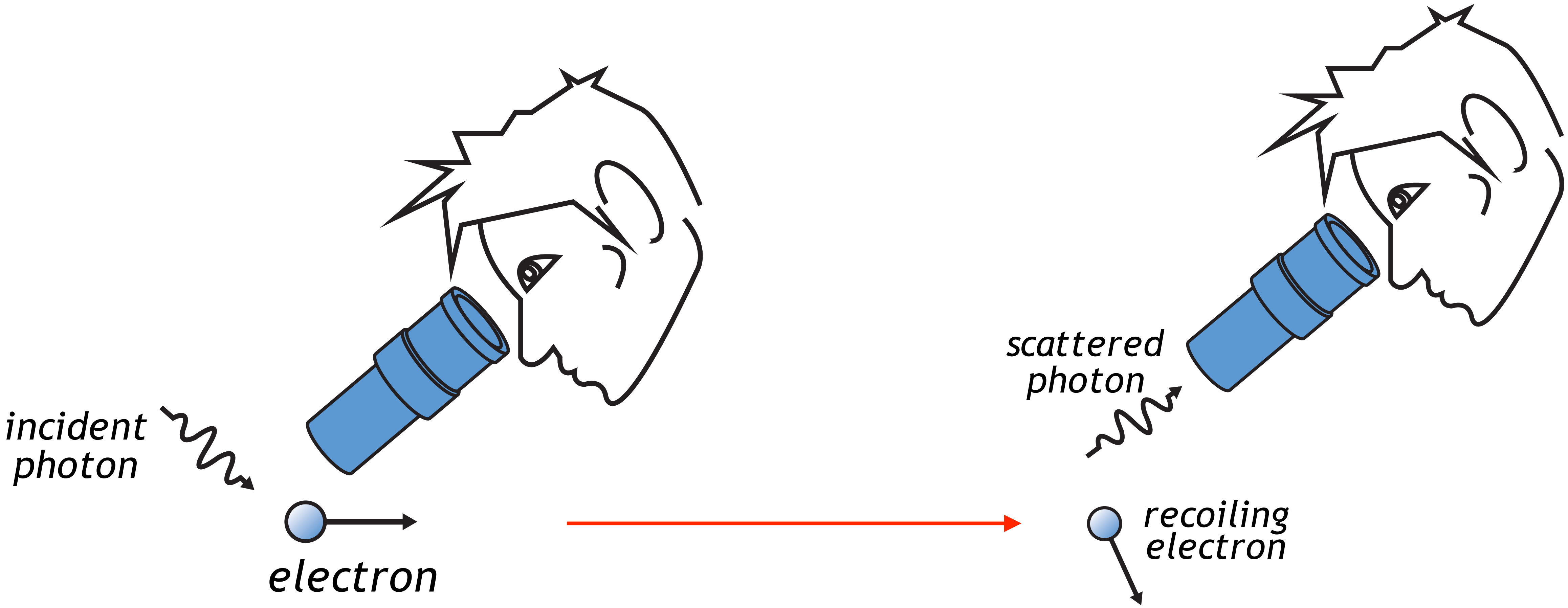
According to De Broglie, for matter wave of definite momentum, the wavelength can be defined as:

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



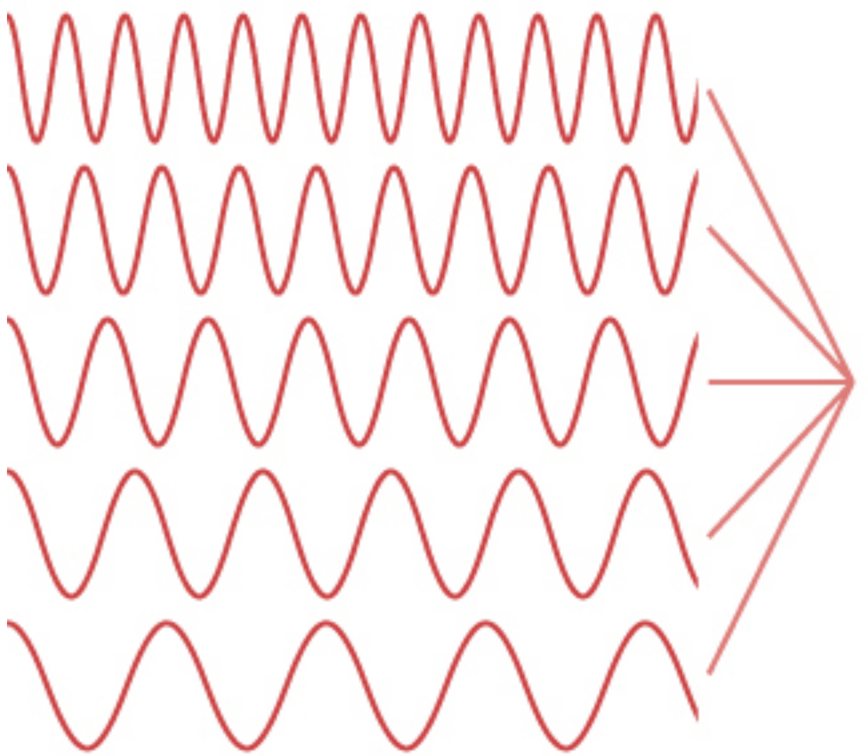
A pure **wave has a well defined momentum**, but not the position. **A pure particle has a well defined position** but not momentum

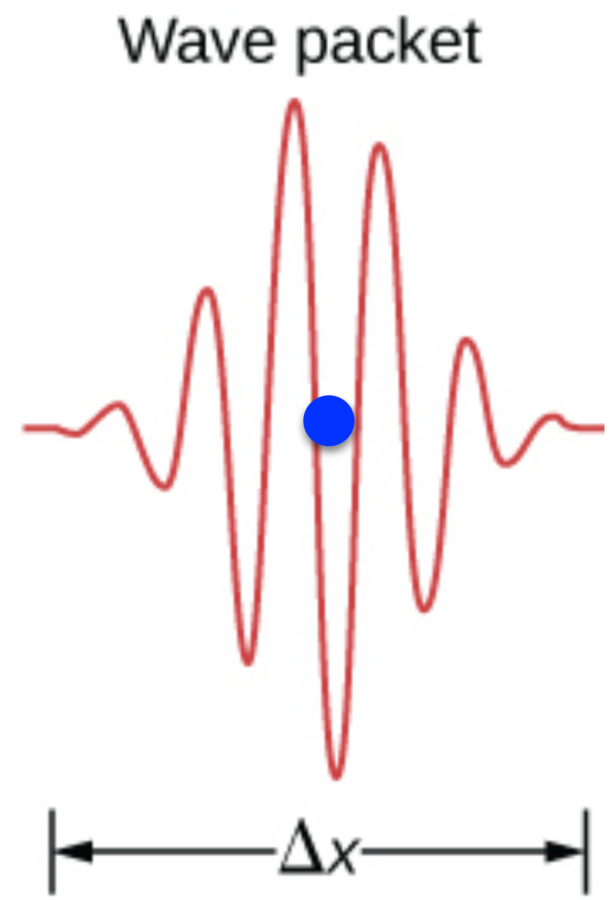
Position-Momentum of an electron Measurement



- ➡ 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 Realised that…

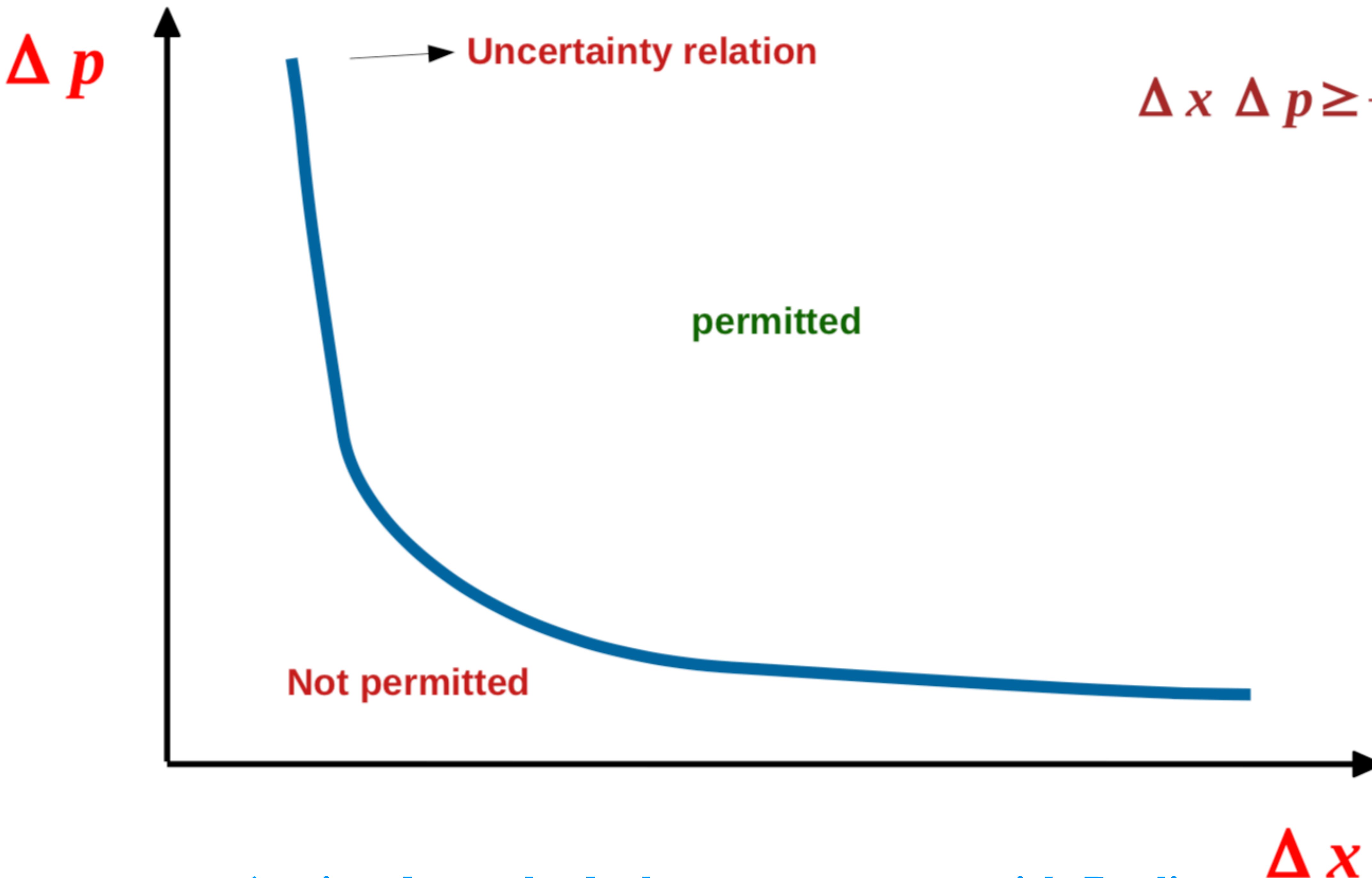




Longer wavelength
Less information about position
Δx is large

Shorter wavelength
More information about position
Δx is small

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 x 10^{-31} kg traveling at 40 m/s

So momentum = 3.6 x 10^{-29} kg m/s
and its uncertainty = 3.6 x 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 value, which is certainly not measurable and will have no consequences on practical measurement of velocities

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

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

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?**

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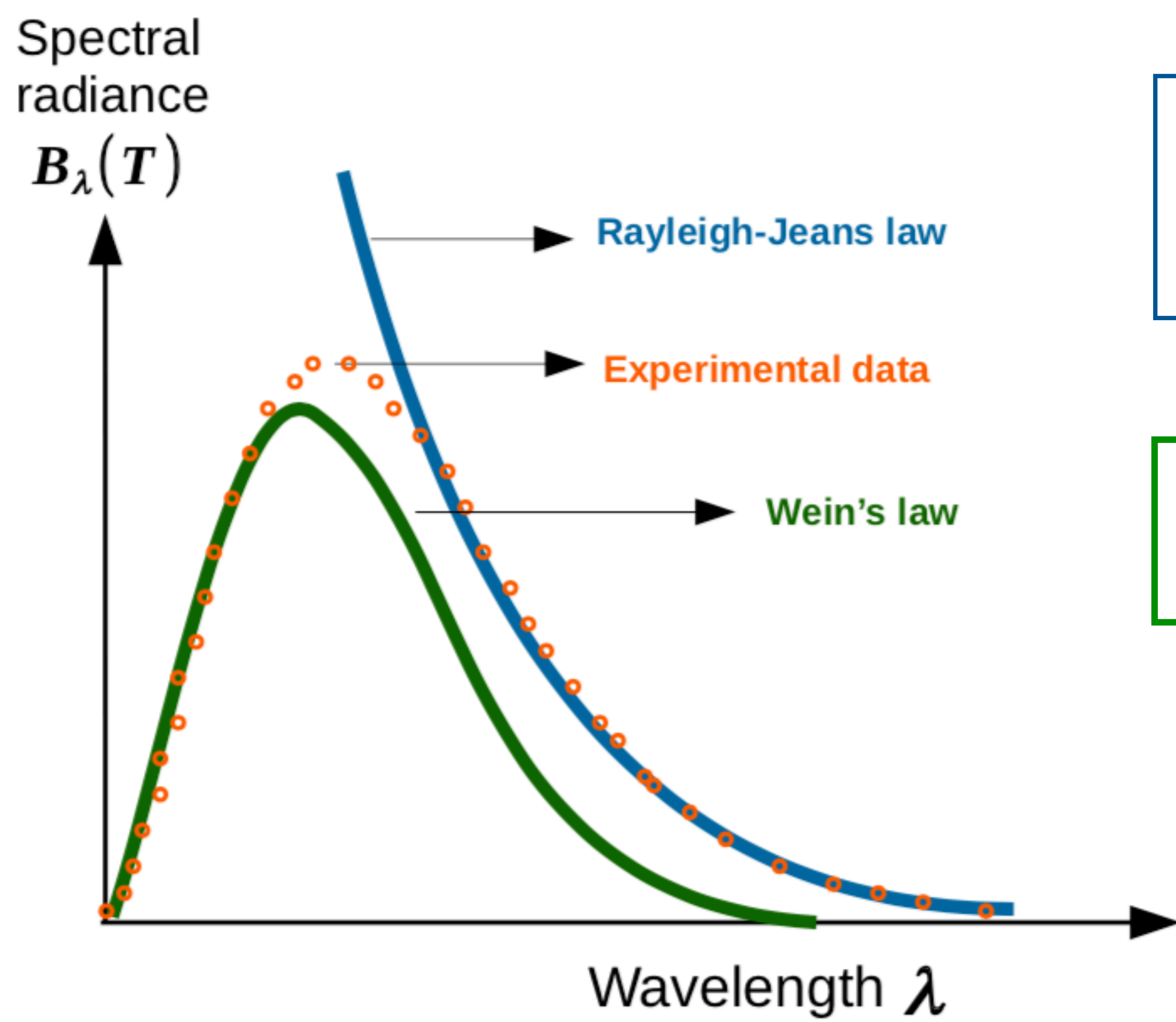
Failures of classical approach



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

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

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

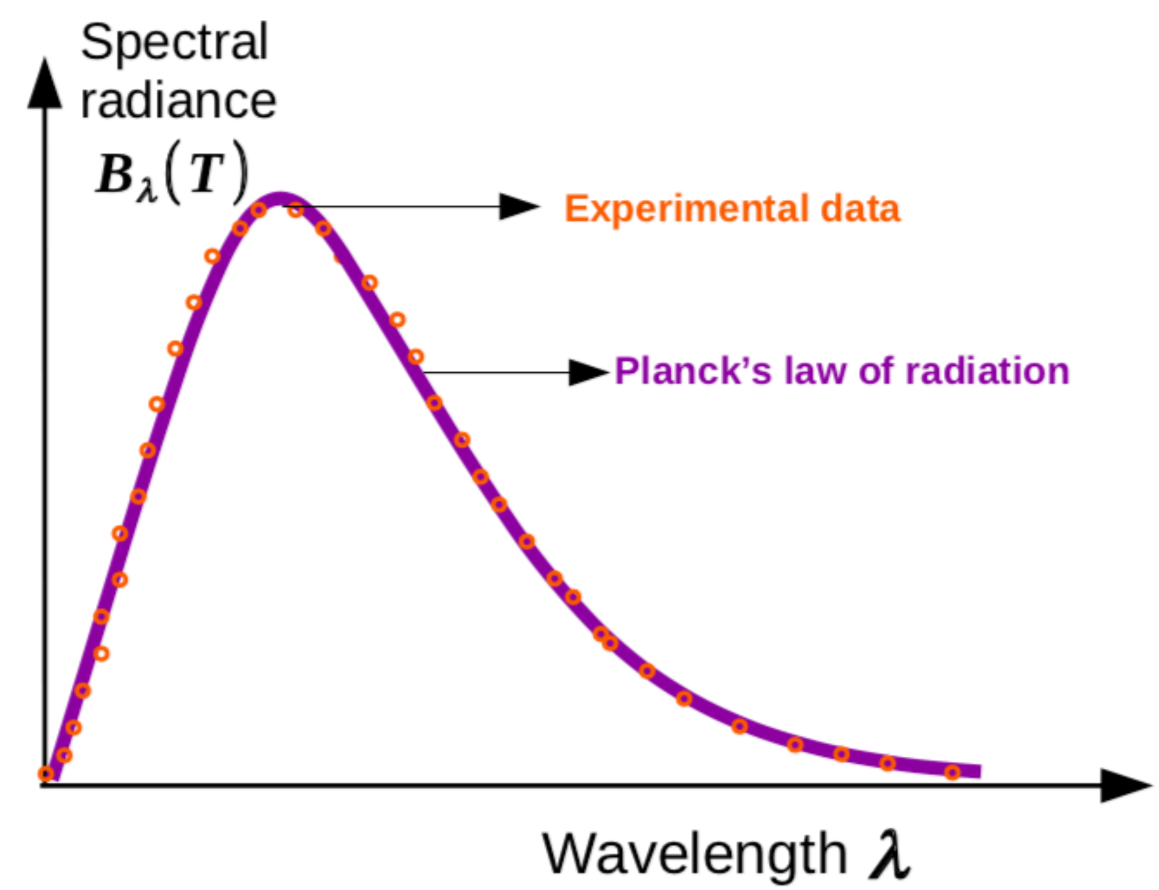
Max-Planck's Theory of Blackbody Radiation

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

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

Derivation (not in the syllabus)



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

Max-Planck's Theory of Blackbody Radiation

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

Wavelength = λ is large

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

$e^x \approx \; 1 + x$

Wavelength = λ is small

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

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

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

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

Rayleigh-Jeans Law

Wein's Law

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

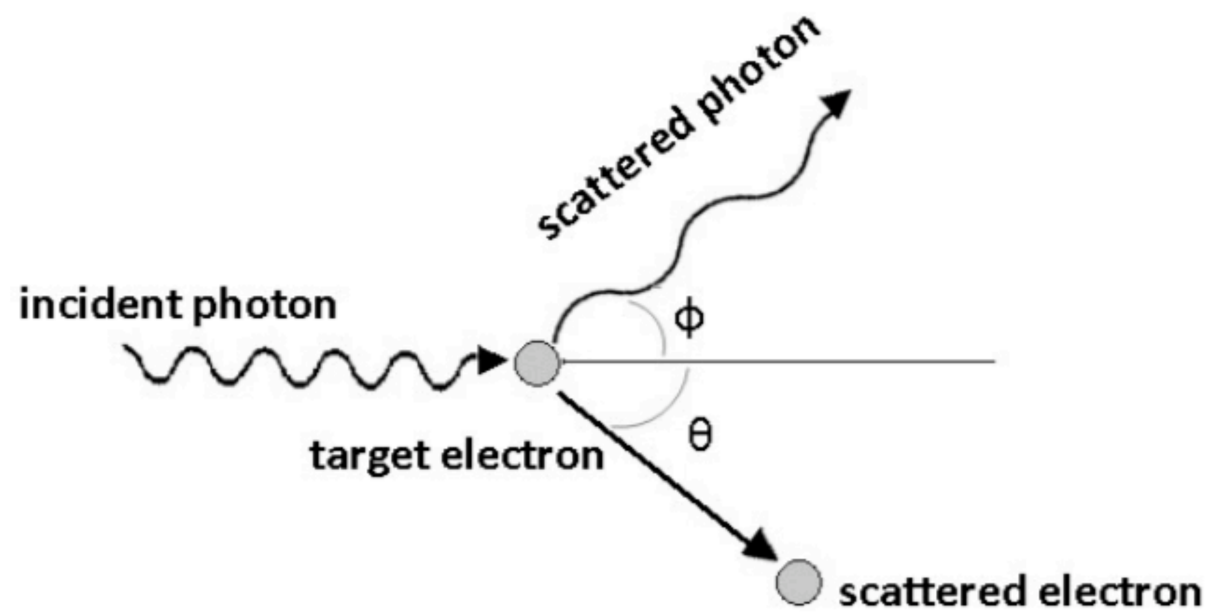
- It is another important development that led to **birth of modern physics**

- 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



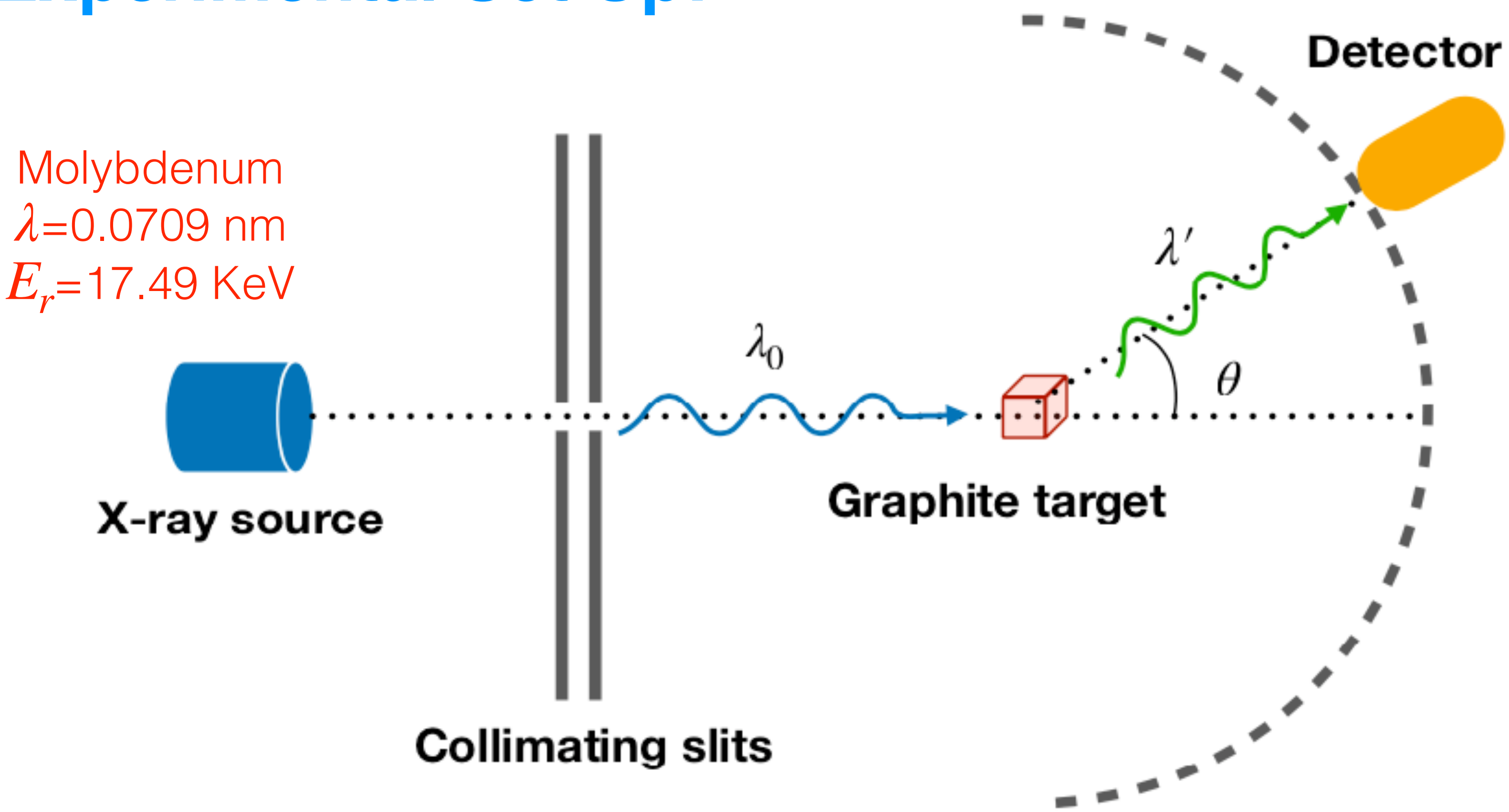
A phenomenon in which a **collision between a photon and an electron** results in an **increase in the kinetic energy of the electron** and a corresponding **increase in the wavelength of the photon.**

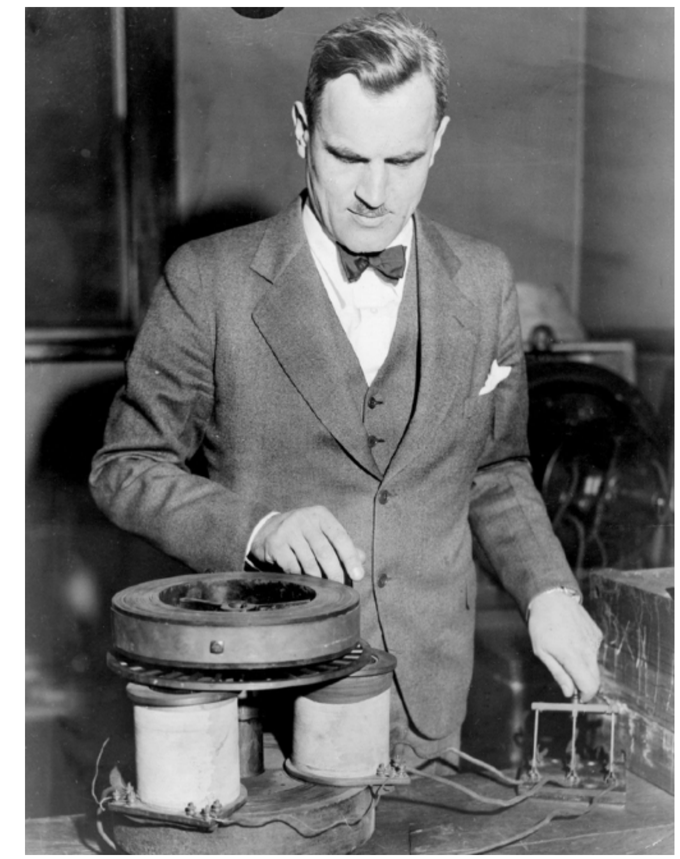
Holly Compton predicted the shift in wavelength **theoretically** and **measured the shift experimentally.** This discovery gave an **evidence for the particle nature of light!**

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

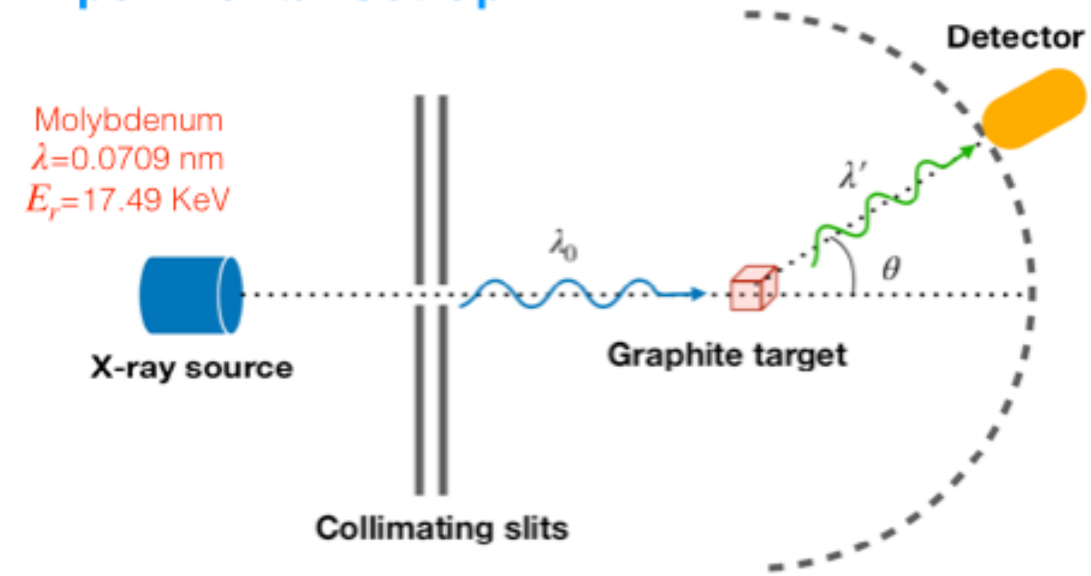
Holly Compton directed EMW (x-rays) at electrons and observed the phenomenon of collision of photons originating from x-rays and electrons. He predicted the shift in wavelength theoretically and measured the shift experimentally. This discovery gave an evidence for the particle nature of light!

Compton Effect/Scattering: Experiment

Components

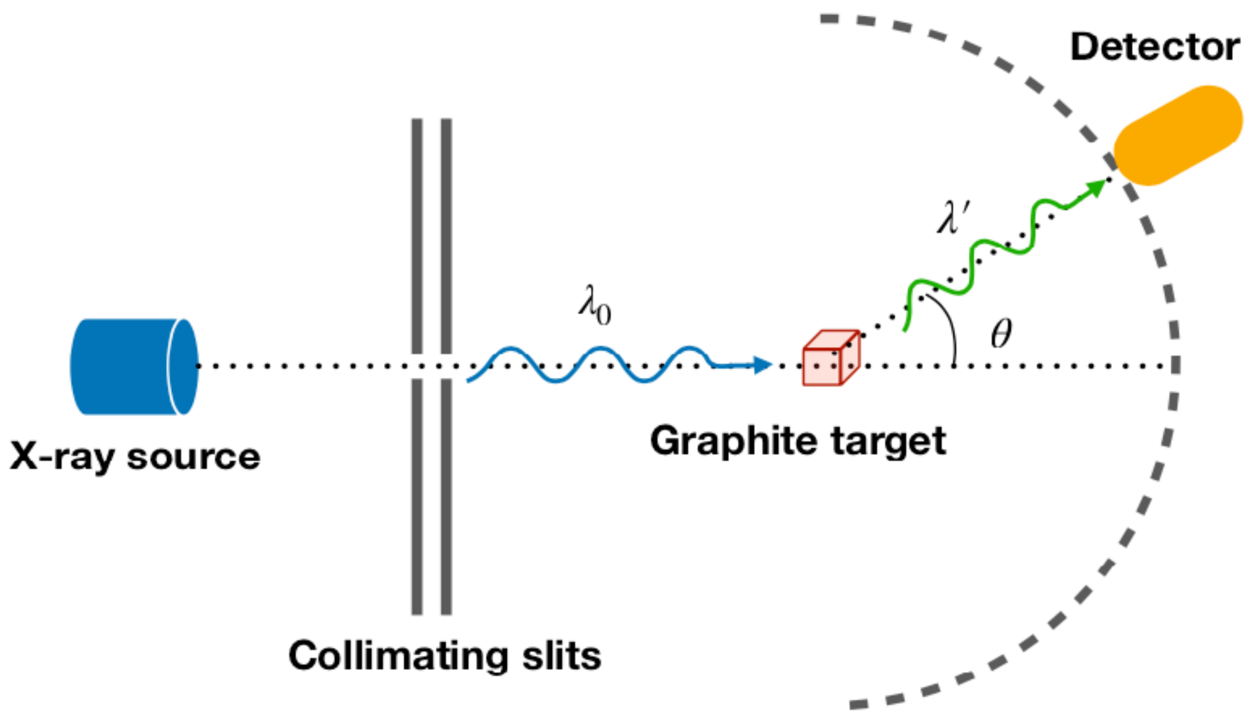
- X-ray source
- Collimator
- Graphite target
- Movable detector

Experimental Set Up:



- Apparatus consists of an **x-ray source** that emits a powerful radiation.
- A **collimator** is used to parallelise the beam from the point source.
- A **carbon target** with a low atomic number, Z=12, was used because atoms with small Z have a **higher percentage of loosely bound electrons**.
- The wavelength was measured with a **rotating crystal spectrometer**, and the intensity was determined by an **ionization chamber** that generated a current proportional to the x- ray intensity.
- Compton measured the dependence of scattered x-ray intensity on wavelength at **angles of 0^o, 45^o, 90^o, and 135^o**

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

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

Compton wavelength

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

Case-1: $\theta = 0°$

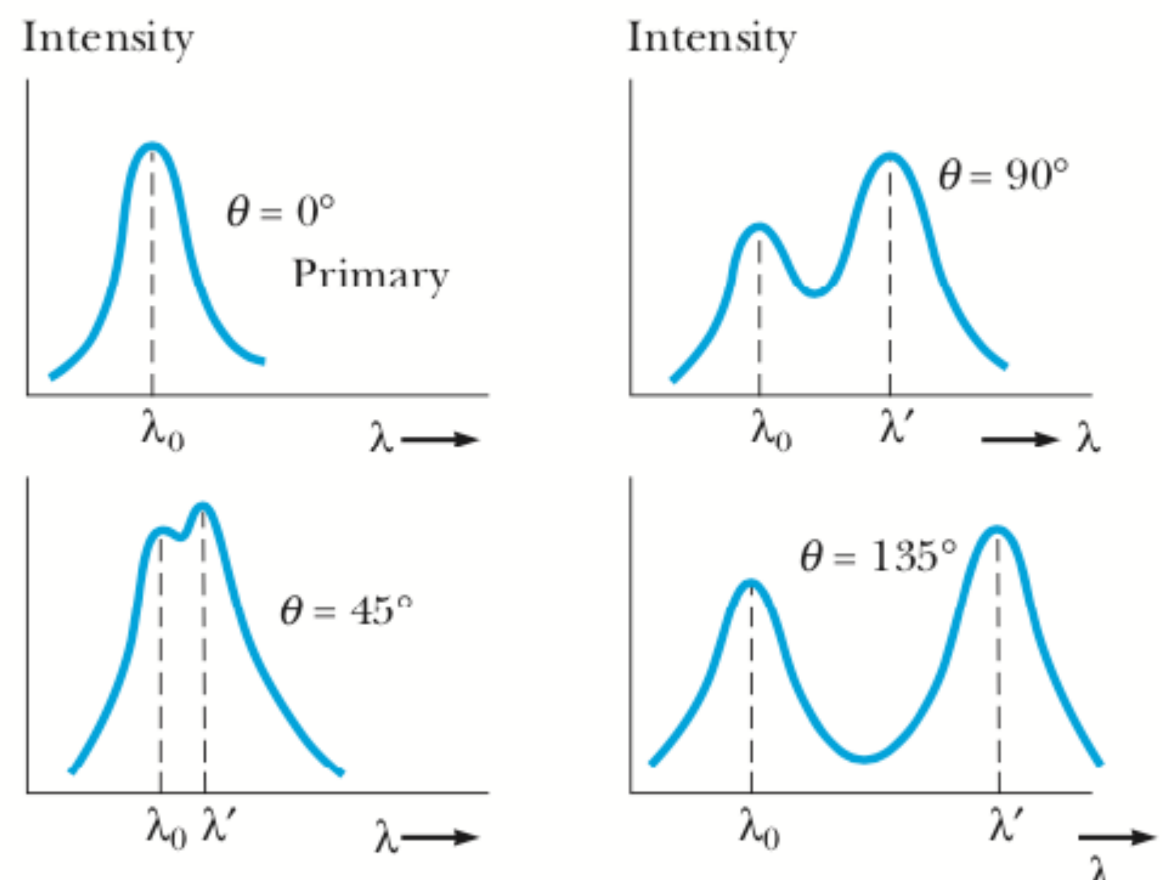
$\lambda' = \lambda_0$

Case-2: $\theta = 90°$

$\lambda' = \lambda_0 + \lambda_C$

Case-3: $\theta = 180°$

$\lambda' = \lambda_0 + 2\lambda_C$



Compton Effect: Conclusions

What wave theory predicts: (Classical view)

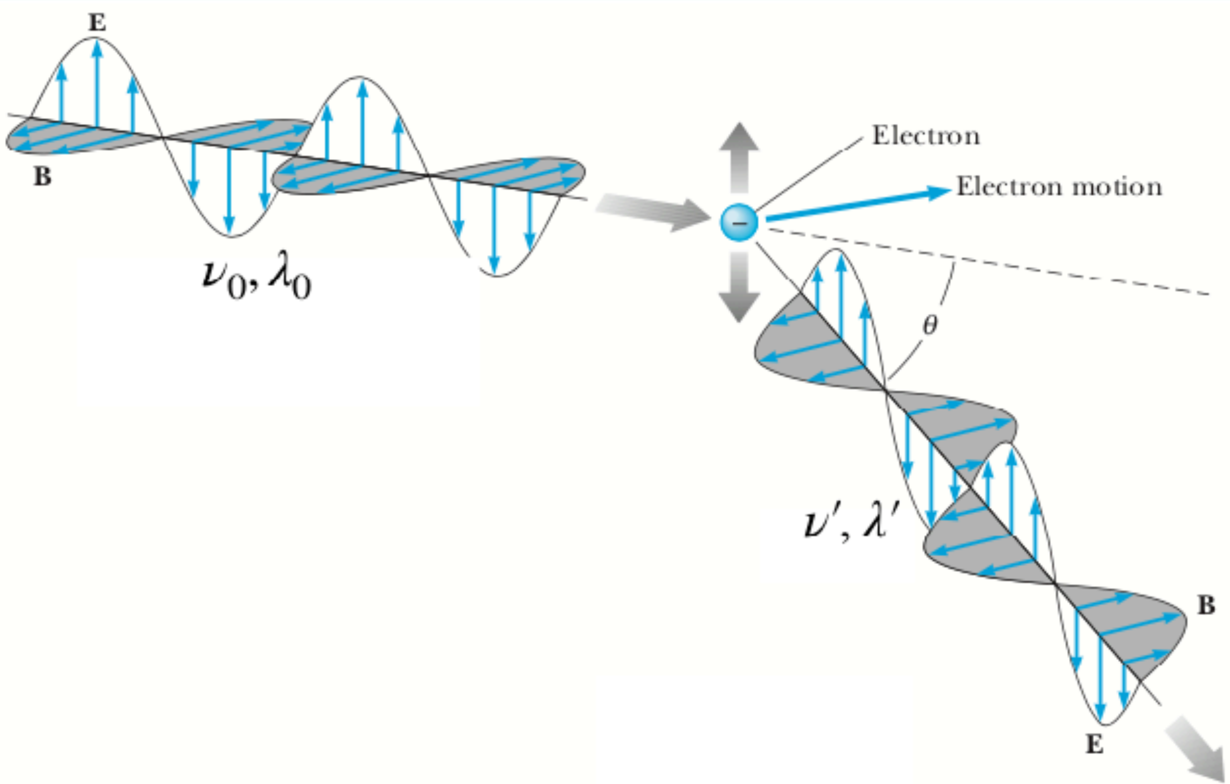
- The wave theory predicts that **no wavelength change should take place**.
- The Incoming EM wave causes the electron to oscillate with the same frequency as the wave.
- Therefore, the oscillating electron should reemit the EM waves with the same frequency (Thomson scattering)

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 $\Delta\nu$ 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

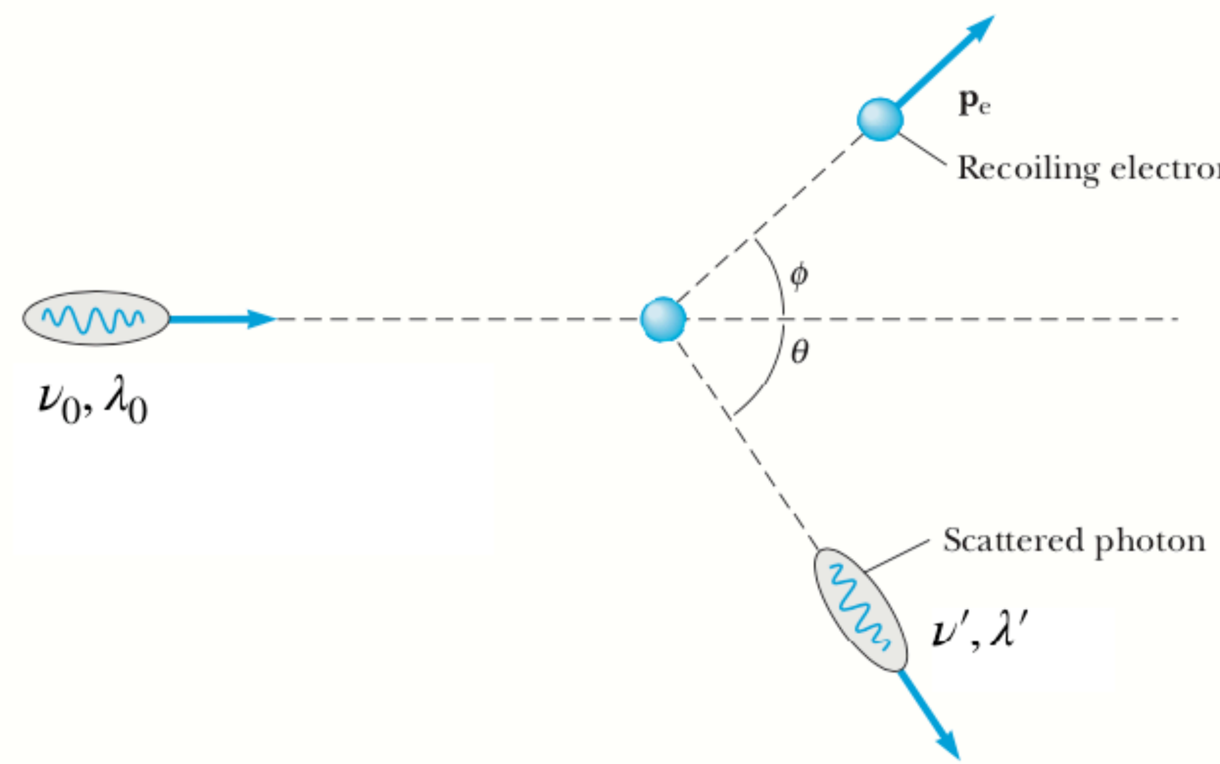
Compton Effect: Conclusions

Classical Picture



- 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.

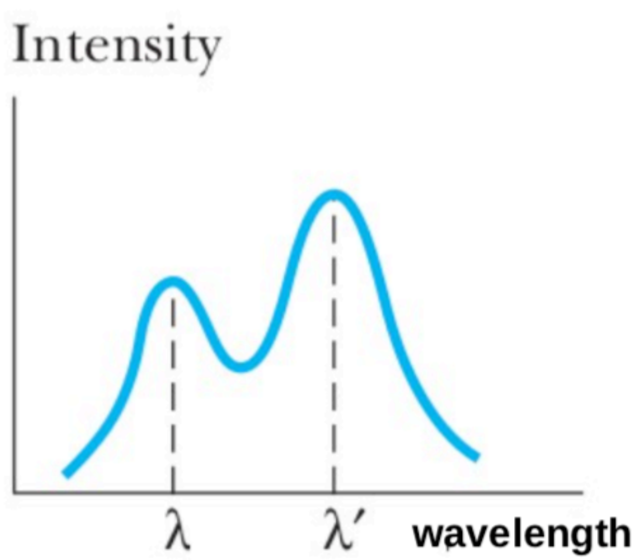
Quantum Picture



- 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

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

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 $h = 6.63\times10^{-34}\ J\ s$

Mass of electron $m_e = 9.1\times10^{-31}\ kg$

Velocity of light $c = 3\times10^{8}\ m\ s^{-1}$

Compton shift $\lambda' - \lambda = \frac{h}{m_e c}(1-\cos\theta) = \frac{6.63\times10^{-34}}{(9.1\times10^{-31})(3\times10^{8})}(1-\cos 45) \approx 0.711\times10^{-12}\, m$

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

$$= 0.2\times10^{-9} + 0.711\times10^{-12}$$

$$= 0.2007\times10^{-9}\ \text{m} = 0.2007\ \text{nm}$$

of motion $F = ma$, the basic principle of classical mechanics, can be derived from Schrödinger's equation provided the quantities it relates are understood to be averages rather than precise values. (Newton's laws of motion were also not derived from any other principles. Like Schrödinger's equation, these laws are considered valid in their range of applicability because of their agreement with experiment.)

5.4 LINEARITY AND SUPERPOSITION

Wave functions add, not probabilities

An important property of Schrödinger's equation is that it is linear in the wave function Ψ. By this is meant that the equation has terms that contain Ψ and its derivatives but no terms independent of Ψ or that involve higher powers of Ψ or its derivatives. As a result, a linear combination of solutions of Schrödinger's equation for a given system is also itself a solution. If Ψ_1 and Ψ_2 are two solutions (that is, two wave functions that satisfy the equation), then

$$\Psi = a_1\Psi_1 + a_2\Psi_2$$

is also a solution, where a_1 and a_2 are constants (see Exercise 8). Thus the wave functions Ψ_1 and Ψ_2 obey the superposition principle that other waves do (see Sec. 2.1) and we conclude that interference effects can occur for wave functions just as they can for light, sound, water, and electromagnetic waves. In fact, the discussions of Secs. 3.4 and 3.7 assumed that de Broglie waves are subject to the superposition principle.

Let us apply the superposition principle to the diffraction of an electron beam. Figure 5.2*a* shows a pair of slits through which a parallel beam of monoenergetic electrons pass on their way to a viewing screen. If slit 1 only is open, the result is the intensity variation shown in Fig. 5.2*b* that corresponds to the probability density

$$P_1 = |\Psi_1|^2 = \Psi_1^*\Psi_1$$

If slit 2 only is open, as in Fig. 5.2*c*, the corresponding probability density is

$$P_2 = |\Psi_2|^2 = \Psi_2^*\Psi_2$$

We might suppose that opening both slits would give an electron intensity variation described by $P_1 + P_2$, as in Fig. 5.2*d*. However, this is not the case because in quantum

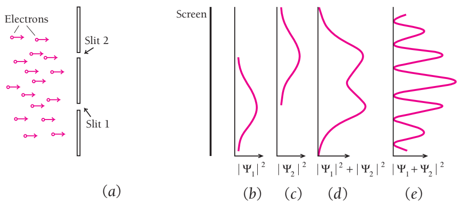


Figure 5.2 (*a*) Arrangement of double-slit experiment. (*b*) The electron intensity at the screen with only slit 1 open. (*c*) The electron intensity at the screen with only slit 2 open. (*d*) The sum of the intensities of (*b*) and (*c*). (*e*) The actual intensity at the screen with slits 1 and 2 both open. The wave functions Ψ_1 and Ψ_2 add to produce the intensity at the screen, not the probability densities $|\Psi_1|^2$ and $|\Psi_2|^2$.

mechanics wave functions add, *not* probabilities. Instead the result with both slits open is as shown in Fig. 5.2*e*, the same pattern of alternating maxima and minima that occurs when a beam of monochromatic light passes through the double slit of Fig. 2.4.

The diffraction pattern of Fig. 5.2*e* arises from the superposition Ψ of the wave functions Ψ_1 and Ψ_2 of the electrons that have passed through slits 1 and 2:

$$\Psi = \Psi_1 + \Psi_2$$

The probability density at the screen is therefore

$$\begin{aligned} P = |\Psi|^2 = |\Psi_1 + \Psi_2|^2 &= (\Psi_1^* + \Psi_2^*)(\Psi_1 + \Psi_2) \\ &= \Psi_1^*\Psi_1 + \Psi_2^*\Psi_2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1 \\ &= P_1 + P_2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1 \end{aligned}$$

The two terms at the right of this equation represent the difference between Fig. 5.2*d* and *e* and are responsible for the oscillations of the electron intensity at the screen. In Sec. 6.8 a similar calculation will be used to investigate why a hydrogen atom emits radiation when it undergoes a transition from one quantum state to another of lower energy.

5.5 EXPECTATION VALUES

How to extract information from a wave function

Once Schrödinger's equation has been solved for a particle in a given physical situation, the resulting wave function $\Psi(x, y, z, t)$ contains all the information about the particle that is permitted by the uncertainty principle. Except for those variables that are quantized this information is in the form of probabilities and not specific numbers.

As an example, let us calculate the **expectation value** $\langle x \rangle$ of the position of a particle confined to the x axis that is described by the wave function $\Psi(x, t)$. This is the value of x we would obtain if we measured the positions of a great many particles described by the same wave function at some instant t and then averaged the results.

To make the procedure clear, we first answer a slightly different question: What is the average position $\bar{x}$ of a number of identical particles distributed along the x axis in such a way that there are N_1 particles at x_1, N_2 particles at x_2, and so on? The average position in this case is the same as the center of mass of the distribution, and so

$$\bar{x} = \frac{N_1x_1 + N_2x_2 + N_3x_3 + \cdots}{N_1 + N_2 + N_3 + \cdots} = \frac{\sum N_i x_i}{\sum N_i} \tag{5.16}$$

When we are dealing with a single particle, we must replace the number N_i of particles at x_i by the probability P_i that the particle be found in an interval dx at x_i. This probability is

$$P_i = |\Psi_i|^2\, dx \tag{5.17}$$

where Ψ_i is the particle wave function evaluated at $x = x_i$. Making this substitution and changing the summations to integrals, we see that the expectation value of the

EXAMPLE 5.1 Why Don't We See the Wave Properties of a Baseball?

An object will appear "wavelike" if it exhibits interference or diffraction, both of which require scattering objects or apertures of about the same size as the wavelength. A baseball of mass 140 g traveling at a speed of 60 mi/h (27 m/s) has a de Broglie wavelength given by

$$\lambda = \frac{h}{p} = \frac{6.63 \times 10^{-34}\ \mathrm{J \cdot s}}{(0.14\ \mathrm{kg})(27\ \mathrm{m/s})} = 1.7 \times 10^{-34}\ \mathrm{m}$$

Even a nucleus (whose size is $\approx 10^{-15}$ m) is much too large to diffract this incredibly small wavelength! This explains why all macroscopic objects appear particle-like.

EXAMPLE 5.2 What Size "Particles" Do Exhibit Diffraction?

A particle of charge q and mass m is accelerated from rest through a small potential difference V. (a) Find its de Broglie wavelength, assuming that the particle is nonrelativistic.

Solution When a charge is accelerated from rest through a potential difference V, its gain in kinetic energy, $\frac{1}{2}mv^2$, must equal the loss in potential energy qV. That is,

$$\tfrac{1}{2}mv^2 = qV$$

Because $p = mv$, we can express this in the form

$$\frac{p^2}{2m} = qV \qquad \text{or} \qquad p = \sqrt{2mqV}$$

Substituting this expression for p into the de Broglie relation $\lambda = h/p$ gives

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mqV}}$$

(b) Calculate λ if the particle is an electron and $V = 50$ V.

Solution The de Broglie wavelength of an electron accelerated through 50 V is

$$\begin{aligned}\lambda &= \frac{h}{\sqrt{2m_e qV}} \\ &= \frac{6.63 \times 10^{-34}\ \mathrm{J \cdot s}}{\sqrt{2(9.11 \times 10^{-31}\ \mathrm{kg})(1.6 \times 10^{-19}\ \mathrm{C})(50\ \mathrm{V})}} \\ &= 1.7 \times 10^{-10}\ \mathrm{m} = 1.7\ \text{Å}\end{aligned}$$

This wavelength is of the order of atomic dimensions and the spacing between atoms in a solid. Such low-energy electrons are routinely used in electron diffraction experiments to determine atomic positions on a surface.

Exercise 1 (a) Show that the de Broglie wavelength for an electron accelerated from rest through a *large* potential difference, V, is

$$\lambda = \frac{12.27}{V^{1/2}}\left(\frac{Ve}{2m_e c^2} + 1\right)^{-1/2} \tag{5.7}$$

where λ is in angstroms (Å) and V is in volts. (b) Calculate the percent error introduced when $\lambda = 12.27/V^{1/2}$ is used instead of the correct relativistic expression for 10 MeV electrons.

Answer (b) 230%.

5.2 THE DAVISSON–GERMER EXPERIMENT

Direct experimental proof that electrons possess a wavelength $\lambda = h/p$ was furnished by the diffraction experiments of American physicists Clinton J. Davisson (1881–1958) and Lester H. Germer (1896–1971) at the Bell Laboratories in New York City in 1927 (Fig. 5.3).[1] In fact, de Broglie had already suggested in 1924 that a stream of electrons traversing a small aperture should exhibit diffraction phenomena. In 1925, Einstein was led to the necessity of postulating matter waves from an analysis of fluctuations of a molecular gas. In addition, he noted that a molecular beam should show small but measurable diffraction effects. In the same year, Walter Elsasser pointed out that the slow

[1] C. J. Davisson and L. H. Germer, *Phys. Rev.* 30:705, 1927.

Figure 5.3 Clinton J. Davisson (left) and Lester H. Germer (center) at Bell Laboratories in New York City. (*Bell Laboratories, courtesy AIP Emilio Segrè Visual Archives*)

electron scattering experiments of C. J. Davisson and C. H. Kunsman at the Bell Labs could be explained by electron diffraction.

Clear-cut proof of the wave nature of electrons was obtained in 1927 by the work of Davisson and Germer in the United States and George P. Thomson (British physicist, 1892–1975, the son of J. J. Thomson) in England. Both cases are intriguing not only for their physics but also for their human interest. The first case was an accidental discovery, and the second involved the discovery of the particle properties of the electron by the father and the wave properties by the son.

The crucial experiment of Davisson and Germer was an offshoot of an attempt to understand the arrangement of atoms on the surface of a nickel sample by elastically scattering a beam of low-speed electrons from a polycrystalline nickel target. A schematic drawing of their apparatus is shown in Figure 5.4. Their device allowed for the variation of three experimental parameters—electron energy; nickel target orientation, α; and scattering angle, ϕ. Before a fortunate accident occurred, the results seemed quite pedestrian. For constant electron energies of about 100 eV, the scattered intensity rapidly decreased as ϕ increased. But then someone dropped a flask of liquid air on the glass vacuum system, rupturing the vacuum and oxidizing the nickel target, which had been at high temperature. To remove the oxide, the sample was reduced by heating it cautiously[2] in a flowing stream of hydrogen. When the apparatus was reassembled, quite different results were found: Strong variations in the intensity of scattered electrons with angle were observed, as shown in Figure 5.5. The prolonged heating had evidently annealed the nickel target, causing large single-crystal regions to develop in the polycrystalline sample. These crystalline regions furnished the extended regular lattice needed to observe electron diffraction. Once Davisson and Germer realized that it was the elastic scattering from *single crystals* that produced such unusual results (1925), they initiated a thorough investigation of elastic scattering from large single crystals

[2]At present this can be done without the slightest fear of "stinks or bangs," because 5% hydrogen–95% argon safety mixtures are commercially available.

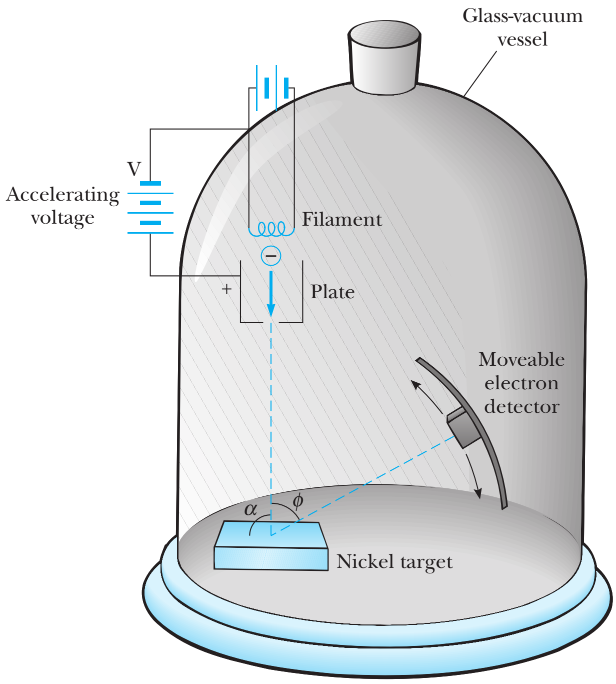


Figure 5.4 A schematic diagram of the Davisson–Germer apparatus.

with predetermined crystallographic orientation. Even these experiments were not conducted at first as a test of de Broglie's wave theory, however. Following discussions with Richardson, Born, and Franck, the experiments and their analysis finally culminated in 1927 in the proof that electrons experience diffraction with an electron wavelength that is given by $\lambda = h/p$.

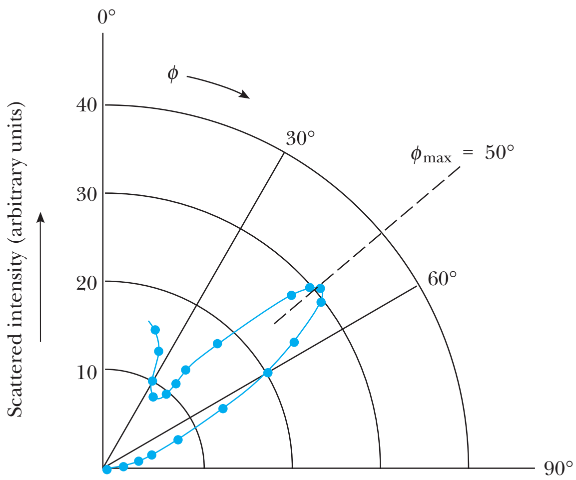


Figure 5.5 A polar plot of scattered intensity versus scattering angle for 54-eV electrons, based on the original work of Davisson and Germer. The scattered intensity is proportional to the distance of the point from the origin in this plot.

The idea that electrons behave like waves when interacting with the atoms of a crystal is so striking that Davisson and Germer's proof deserves closer scrutiny. In effect, they calculated the wavelength of electrons from a simple diffraction formula and compared this result with de Broglie's formula $\lambda = h/p$. Although they tested this result over a wide range of target orientations and electron energies, we consider in detail only the simple case shown in Figures 5.4 and 5.5 with $\alpha = 90.0°$, $V = 54.0$ V, and $\phi = 50.0°$, corresponding to the $n = 1$ diffraction maximum. In order to calculate the de Broglie wavelength for this case, we first obtain the velocity of a nonrelativistic electron accelerated through a potential difference V from the energy relation

$$\tfrac{1}{2} m_e v^2 = eV$$

Substituting $v = \sqrt{2Ve/m_e}$ into the de Broglie relation gives

$$\lambda = \frac{h}{m_e v} = \frac{h}{\sqrt{2Vem_e}} \tag{5.8}$$

Thus the wavelength of 54.0-V electrons is

$$\begin{aligned}\lambda &= \frac{6.63 \times 10^{-34}\ \mathrm{J\cdot s}}{\sqrt{2(54.0\ \mathrm{V})(1.60 \times 10^{-19}\ \mathrm{C})(9.11 \times 10^{-31}\ \mathrm{kg})}}\\ &= 1.67 \times 10^{-10}\ \mathrm{m} = 1.67\ \text{Å}\end{aligned}$$

The experimental wavelength may be obtained by considering the nickel atoms to be a reflection diffraction grating, as shown in Figure 5.6. Only the surface layer of atoms is considered because low-energy electrons, unlike x-rays, do not penetrate deeply into the crystal. Constructive interference occurs when the path length difference between two adjacent rays is an integral number of wavelengths or

$$d \sin \phi = n\lambda \tag{5.9}$$

As d was known to be 2.15 Å from x-ray diffraction measurements, Davisson and Germer calculated λ to be

$$\lambda = (2.15\ \text{Å})(\sin 50.0°) = 1.65\ \text{Å}$$

in excellent agreement with the de Broglie formula.

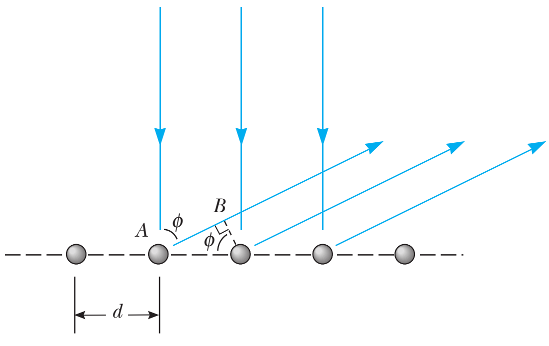


Figure 5.6 Constructive interference of electron matter waves scattered from a single layer of atoms at an angle ϕ.

Figure 5.7 Diffraction of 50-kV electrons from a film of Cu_3Au. The alloy film was 400 Å thick. (*Courtesy of the late Dr. L. H. Germer*)

It is interesting to note that while the diffraction lines from low-energy reflected electrons are quite broad (see Fig. 5.5), the lines from high-energy electrons transmitted through metal foils are quite sharp (see Fig. 5.7). This effect occurs because hundreds of atomic planes are penetrated by high-energy electrons, and consequently Equation 5.9, which treats diffraction from a surface layer, no longer holds. Instead, the Bragg law, $2d \sin \theta = n\lambda$, applies to high-energy electron diffraction. The maxima are extremely sharp in this case because if $2d \sin \theta$ is not exactly equal to $n\lambda$, there will be no diffracted wave. This occurs because there are scattering contributions from so many atomic planes that eventually the path length difference between the wave from the first plane and some deeply buried plane will be *an odd multiple of* $\lambda/2$, resulting in complete cancellation of these waves (see Problem 13).

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If de Broglie's postulate is true for all matter, then any object of mass m has wavelike properties and a wavelength $\lambda = h/p$. In the years following Davisson and Germer's discovery, experimentalists tested the universal character of de Broglie's postulate by searching for diffraction of other "particle" beams. In subsequent experiments, diffraction was observed for helium atoms (Estermann and Stern in Germany) and hydrogen atoms (Johnson in the United States). Following the discovery of the neutron in 1932, it was shown that neutron beams of the appropriate energy also exhibit diffraction when incident on a crystalline target (Fig. 5.8).

EXAMPLE 5.3 Thermal Neutrons

What kinetic energy (in electron volts) should neutrons have if they are to be diffracted from crystals?

Solution Appreciable diffraction will occur if the de Broglie wavelength of the neutron is of the same order of magnitude as the interatomic distance. Taking $\lambda = 1.00$ Å, we find

$$p = \frac{h}{\lambda} = \frac{6.63 \times 10^{-34}\,\text{J}\cdot\text{s}}{1.00 \times 10^{-10}\,\text{m}} = 6.63 \times 10^{-24}\,\text{kg}\cdot\text{m/s}$$

The kinetic energy is given by

$$K = \frac{p^2}{2m_\text{n}} = \frac{(6.63 \times 10^{-24}\,\text{J}\cdot\text{s})^2}{2(1.66 \times 10^{-27}\,\text{kg})}$$
$$= 1.32 \times 10^{-20}\,\text{J} = 0.0825\text{ eV}$$

Note that these neutrons are nonrelativistic because K is much less than the neutron rest energy of 940 MeV, and so our use of the classical expression $K = p^2/2m_\text{n}$ is justified. Because the average thermal energy of a particle in thermal equilibrium is $\frac{1}{2}k_\text{B}T$ for each independent direction of motion, neutrons at room temperature (300 K) possess a kinetic energy of

$$K = \tfrac{3}{2}k_\text{B}T = (1.50)(8.62 \times 10^{-5}\text{ eV/K})(300\text{ K})$$
$$= 0.0388\text{ eV}$$

Thus "thermal neutrons," or neutrons in thermal equilibrium with matter at room temperature, possess energies of the right order of magnitude to diffract appreciably from single crystals. Neutrons produced in a nuclear reactor are far too energetic to produce diffraction from crystals and must be slowed down in a graphite column as they leave the reactor. In the graphite moderator, repeated collisions with carbon atoms ultimately reduce the average neutron energies to the average thermal energy of the carbon atoms. When this occurs, these so-called thermalized neutrons possess a distribution of velocities and a corresponding distribution of de Broglie wavelengths with average wavelengths comparable to crystal spacings.

to the radiation given off by any charged particle when it is decelerated. The minimum continuous x-ray wavelength, $\lambda_{\min}$, is found to be independent of target composition and depends only on the tube voltage, V. It may be explained by attributing it to the case of a head-on electron–atom collision in which all of the incident electron's kinetic energy is converted to electromagnetic energy in the form of a single x-ray photon. For this case we have

$$eV = hf = \frac{hc}{\lambda_{\min}}$$

or

$$\lambda_{\min} = \frac{hc}{eV} \tag{3.26}$$

where V is the x-ray tube voltage.

Superimposed on the continuous spectrum are sharp x-ray lines labeled K_α and K_β, which are like sharp lines emitted in the visible light spectrum. The sharp lines depend on target composition and provide evidence for discrete atomic energy levels separated by thousands of electron volts, as explained in Chapter 9.

The Compton Effect

Let us now turn to the year 1922 and the experimental confirmation by Arthur Holly Compton that x-ray photons behave like particles with momentum hf/c. For some time prior to 1922, Compton and his coworkers had been accumulating evidence that showed that classical wave theory failed to explain the scattering of x-rays from free electrons. In particular, classical theory predicted that incident radiation of frequency f_0 should accelerate an electron in the direction of propagation of the incident radiation, and that it should cause forced oscillations of the electron and reradiation at frequency f', where $f' \leq f_0$ (see Fig. 3.22a).[15] Also, according to classical theory, the frequency or wavelength of the scattered radiation should depend on the length of time the electron was exposed to the incident radiation as well as on the intensity of the incident radiation.

Imagine the surprise when Compton showed experimentally that the wavelength shift of x-rays scattered at a given angle is absolutely independent of the intensity of radiation and the length of exposure, and depends only on the scattering angle. Figure 3.22b shows the quantum model of the transfer of momentum and energy between an individual x-ray photon and an electron. Note that the quantum model easily explains the lower scattered frequency f', because the incident photon gives some of its original energy hf to the recoiling electron.

A schematic diagram of the apparatus used by Compton is shown in Figure 3.23a. In the original experiment, Compton measured the dependence of scattered x-ray intensity on wavelength at three different scattering angles

[15]This decrease in frequency of the reradiated wave is caused by a double Doppler shift, first because the electron is receding from the incident radiation, and second because the electron is a moving radiator as viewed from the fixed lab frame. See D. Bohm, *Quantum Theory*, Upper Saddle River, NJ, Prentice-Hall, 1961, p. 35.

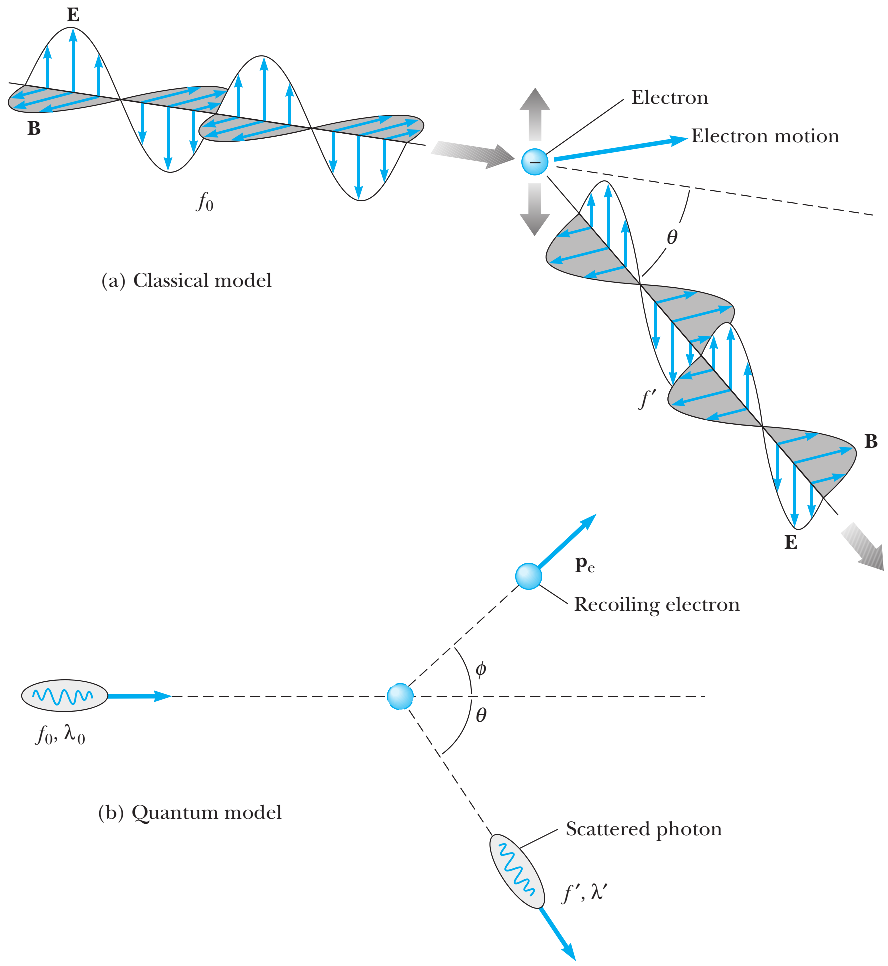

Figure 3.22 X-ray scattering from an electron: (a) the classical model, (b) the quantum model.

of 45°, 90°, and 135°. The wavelength was measured with a rotating crystal spectrometer, and the intensity was determined by an ionization chamber that generated a current proportional to the x-ray intensity. Monochromatic x-rays of wavelength $\lambda_0 = 0.71$ Å constituted the incident beam. A carbon target with a low atomic number, $Z = 12$, was used because atoms with small Z have a higher percentage of loosely bound electrons. The experimental intensity versus wavelength plots observed by Compton for scattering angles of 0°, 45°, 90°, and 135° are shown in Figure 3.23b. They show two peaks, one at λ_0 and a shifted peak at a longer wavelength λ'. The shifted peak at λ' is caused by the scattering of x-rays from nearly free electrons. Assuming that x-rays behave like particles, λ' was predicted by Compton to depend on scattering angle as

Compton effect

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta) \qquad (3.27)$$

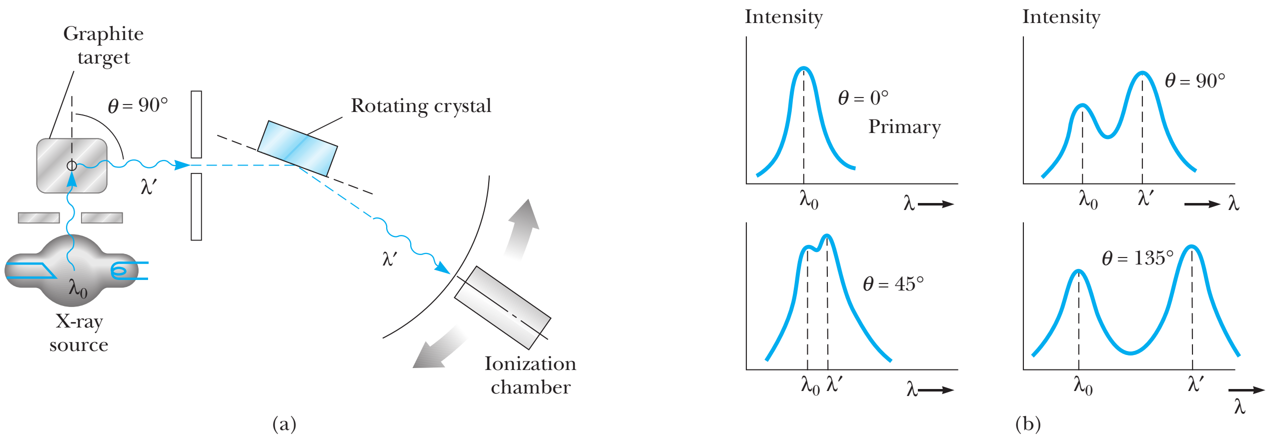

Figure 3.23 (a) Schematic diagram of Compton's apparatus. The wavelength was measured with a rotating crystal spectrometer using graphite (carbon) as the target. The intensity was determined by a movable ionization chamber that generated a current proportional to the x-ray intensity. (b) Scattered x-ray intensity versus wavelength of Compton scattering at $\theta = 0°$, 45°, 90°, and 135°.

where m_e = electron mass; the combination of constants h/m_ec is called the Compton wavelength of the electron and has a currently accepted value of

$$\frac{h}{m_ec} = 0.0243 \text{ Å} = 0.00243 \text{ nm}$$

Compton's careful measurements completely confirmed the dependence of λ' on scattering angle θ and determined the Compton wavelength of the electron to be 0.0242 Å, in excellent agreement with the currently accepted value. It is fair to say that these results were the first to really convince most American physicists of the basic validity of the quantum theory!

The unshifted peak at λ_0 in Figure 3.23 is caused by x-rays scattered from electrons tightly bound to carbon atoms. This unshifted peak is actually predicted by Equation 3.27 if the electron mass is replaced by the mass of a carbon atom, which is about 23,000 times the mass of an electron.

Let us now turn to the derivation of Equation 3.27 assuming that the photon exhibits particle-like behavior and collides elastically like a billiard ball with a free electron initially at rest. Figure 3.24 shows the photon–electron collision for which energy and momentum are conserved. Because the electron typically recoils at high speed, we treat the collision relativistically. The expression for conservation of energy gives

$$E + m_ec^2 = E' + E_e \tag{3.28}$$

Energy conservation

where E is the energy of the incident photon, E' is the energy of the scattered photon, m_ec^2 is the rest energy of the electron, and E_e is the total relativistic energy of the electron after the collision. Likewise, from momentum conservation we have

$$p = p' \cos \theta + p_e \cos \phi \tag{3.29}$$

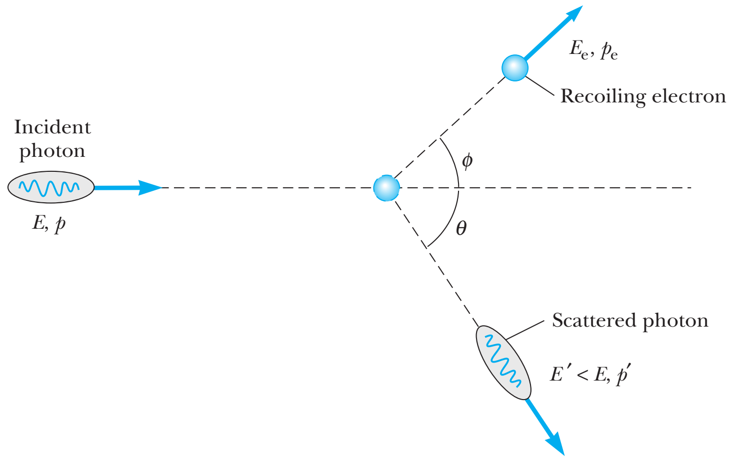

Figure 3.24 Diagram representing Compton scattering of a photon by an electron. The scattered photon has less energy (or longer wavelength) than the incident photon.

$$p' \sin\theta = p_e \sin\phi \tag{3.30}$$

where p is the momentum of the incident photon, p' is the momentum of the scattered photon, and p_e is the recoil momentum of the electron. Equations 3.29 and 3.30 may be solved simultaneously to eliminate ϕ, the electron scattering angle, to give the following expression for p_e^2:

$$p_e^2 = (p')^2 + p^2 - 2pp' \cos\theta \tag{3.31}$$

At this point it is necessary, paradoxically, to use the wave nature of light to explain the particle-like behavior of photons. We have already seen that the energy of a photon and the frequency of the associated light wave are related by $E = hf$. If we assume that a photon obeys the relativistic expression $E^2 = p^2c^2 + m^2c^4$ and that a photon has a mass of zero, we have

$$p_{\text{photon}} = \frac{E}{c} = \frac{hf}{c} = \frac{h}{\lambda} \tag{3.32}$$

Here again we have a paradoxical situation; a particle property, the photon momentum, is given in terms of a wave property, λ, of an associated light wave. If the relations $E = hf$ and $p = hf/c$ are substituted into Equations 3.28 and 3.31, these become respectively

$$E_e = hf - hf' + m_e c^2 \tag{3.33}$$

and

$$p_e^2 = \left(\frac{hf'}{c}\right)^2 + \left(\frac{hf}{c}\right)^2 - \frac{2h^2 ff'}{c^2}\cos\theta \tag{3.34}$$

Because the Compton measurements do not concern the total energy and momentum of the electron, we eliminate E_e and p_e by substituting Equations 3.33 and 3.34 into the expression for the electron's relativistic energy,

$$E_e^2 = p_e^2c^2 + m_e^2c^4$$

After some algebra (see Problem 33), one obtains Compton's result for the increase in a photon's wavelength when it is scattered through an angle θ:

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta) \tag{3.27}$$

EXAMPLE 3.7 The Compton Shift for Carbon

X-rays of wavelength $\lambda = 0.200$ nm are aimed at a block of carbon. The scattered x-rays are observed at an angle of 45.0° to the incident beam. Calculate the increased wavelength of the scattered x-rays at this angle.

Solution The shift in wavelength of the scattered x-rays is given by Equation 3.27. Taking $\theta = 45.0°$, we find

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

$$= \frac{6.63 \times 10^{-34}\,\text{J}\cdot\text{s}}{(9.11 \times 10^{-31}\,\text{kg})(3.00 \times 10^8\,\text{m/s})}(1 - \cos 45.0°)$$

$$= 7.11 \times 10^{-13}\,\text{m} = 0.00071\,\text{nm}$$

Hence, the wavelength of the scattered x-ray at this angle is

$$\lambda = \Delta\lambda + \lambda_0 = 0.200711\,\text{nm}$$

Exercise 6 Find the fraction of energy lost by the photon in this collision.

Answer Fraction $= \Delta E/E = 0.00355$.

EXAMPLE 3.8 X-ray Photons versus Visible Photons

(a) Why are x-ray photons used in the Compton experiment, rather than visible-light photons? To answer this question, we shall first calculate the Compton shift for scattering at 90° from graphite for the following cases: (1) very high energy γ-rays from cobalt, $\lambda = 0.0106$ Å; (2) x-rays from molybdenum, $\lambda = 0.712$ Å; and (3) green light from a mercury lamp, $\lambda = 5461$ Å.

Solution In all cases, the Compton shift formula gives $\Delta\lambda = \lambda' - \lambda_0 = (0.0243\,\text{Å})(1 - \cos 90°) = 0.0243\,\text{Å} = 0.00243$ nm. That is, regardless of the incident wavelength, the same small shift is observed. However, the fractional change in wavelength, $\Delta\lambda/\lambda_0$, is quite different in each case:

γ-rays from cobalt:

$$\frac{\Delta\lambda}{\lambda_0} = \frac{0.0243\,\text{Å}}{0.0106\,\text{Å}} = 2.29$$

X-rays from molybdenum:

$$\frac{\Delta\lambda}{\lambda_0} = \frac{0.0243\,\text{Å}}{0.712\,\text{Å}} = 0.0341$$

Visible light from mercury:

$$\frac{\Delta\lambda}{\lambda_0} = \frac{0.0243\,\text{Å}}{5461\,\text{Å}} = 4.45 \times 10^{-6}$$

Because both incident and scattered wavelengths are simultaneously present in the beam, they can be easily resolved only if $\Delta\lambda/\lambda_0$ is a few percent or if $\lambda_0 \leq 1$ Å.

(b) The so-called free electrons in carbon are actually electrons with a binding energy of about 4 eV. Why may this binding energy be ignored for x-rays with $\lambda_0 = 0.712$ Å?

Solution The energy of a photon with this wavelength is

$$E = hf = \frac{hc}{\lambda} = \frac{12\,400\,\text{eV}\cdot\text{Å}}{0.712\,\text{Å}} = 17\,400\,\text{eV}$$

Therefore, the electron binding energy of 4 eV is negligible in comparison with the incident x-ray energy.

Engineering Physics

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

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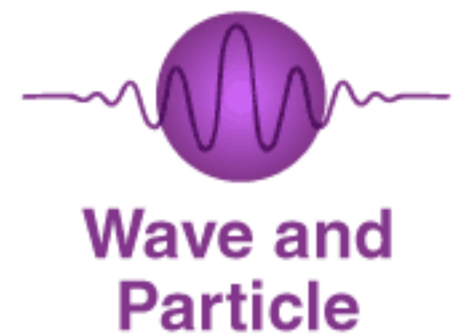
Classical …to…Quantum



- 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.

$$\Psi\ (x,t),\ \text{Psi}$$

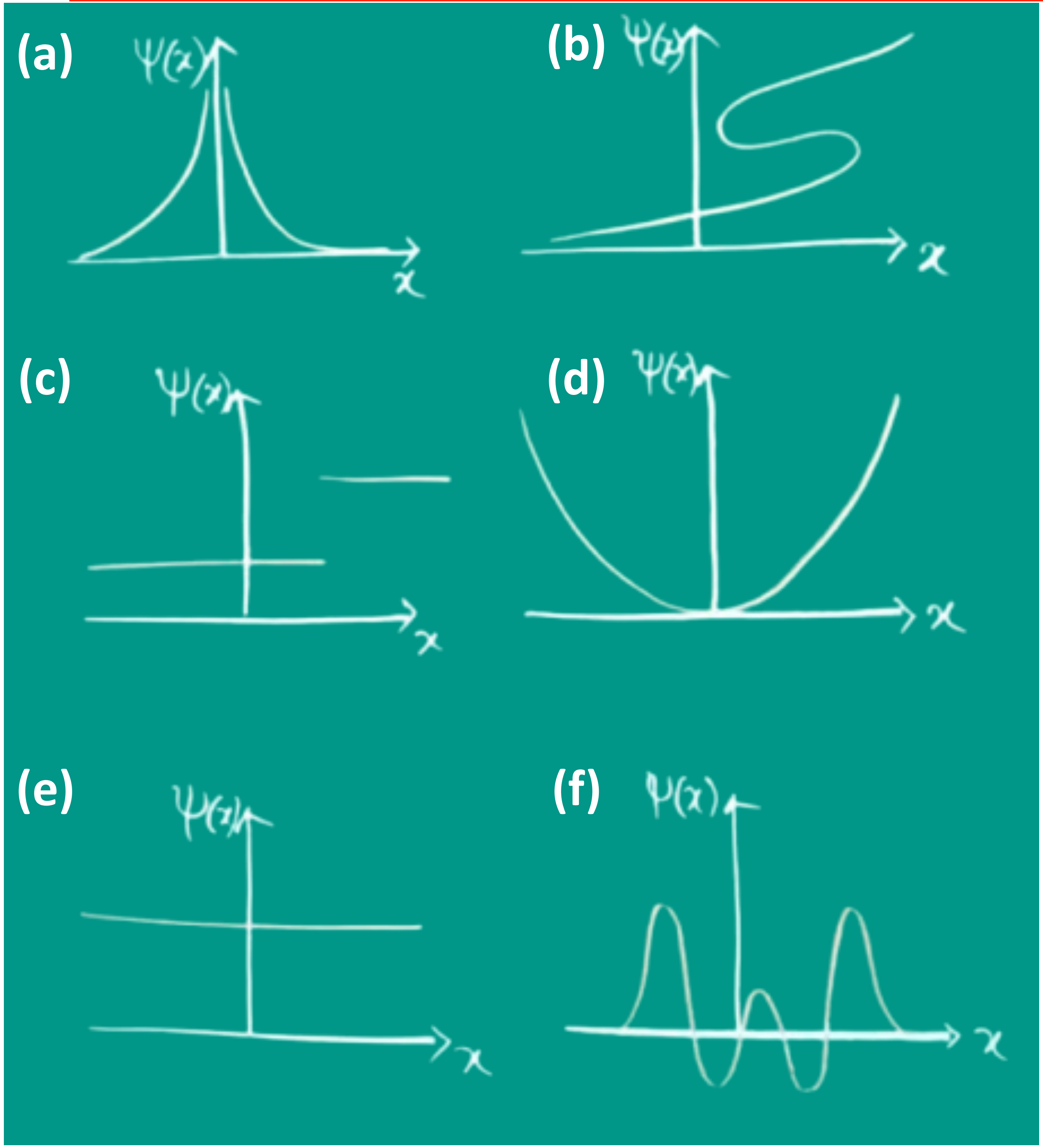
It is generally represented as $\Psi(x,t)$ where x is the position and t is the time

- **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

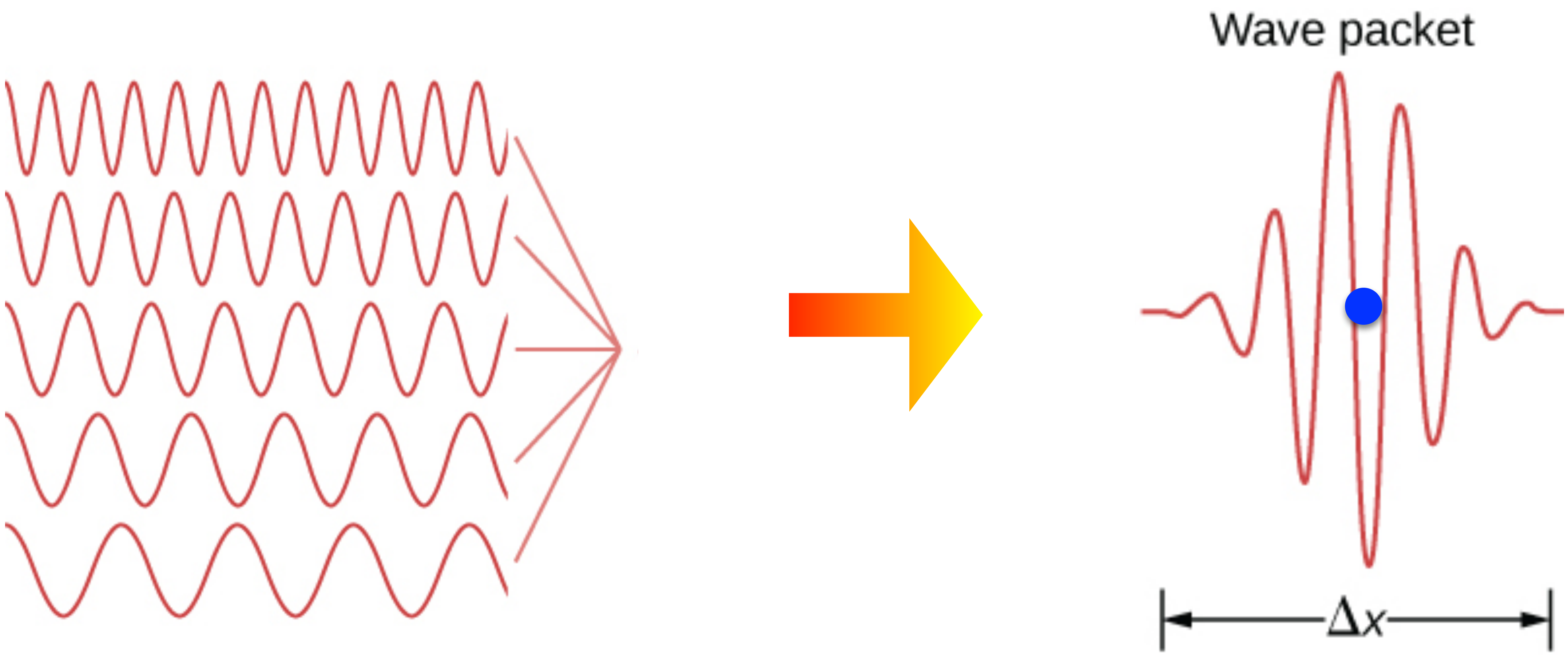
(c). NO- Not Continuous

(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

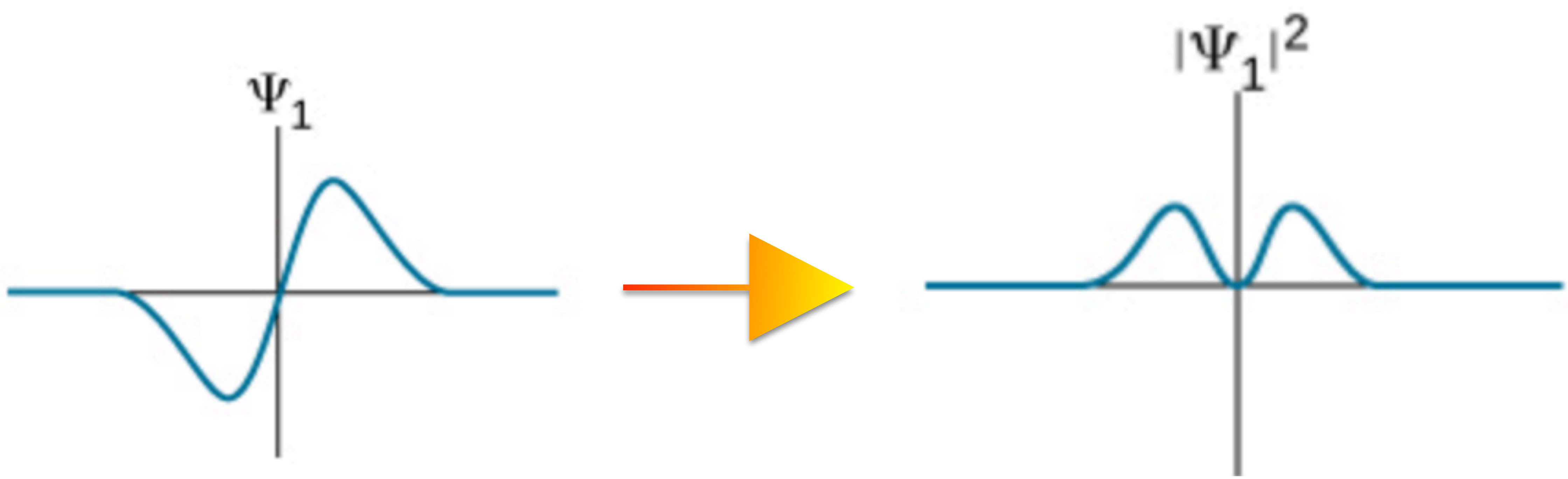
The mathematical expression that satisfy all the condition, which represent the wave packet corresponds to a quantum particle is a wave function

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

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

$$\Downarrow$$

Normalisation of a wave function

Normalisation of Wave Function ψ

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

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

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

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

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

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

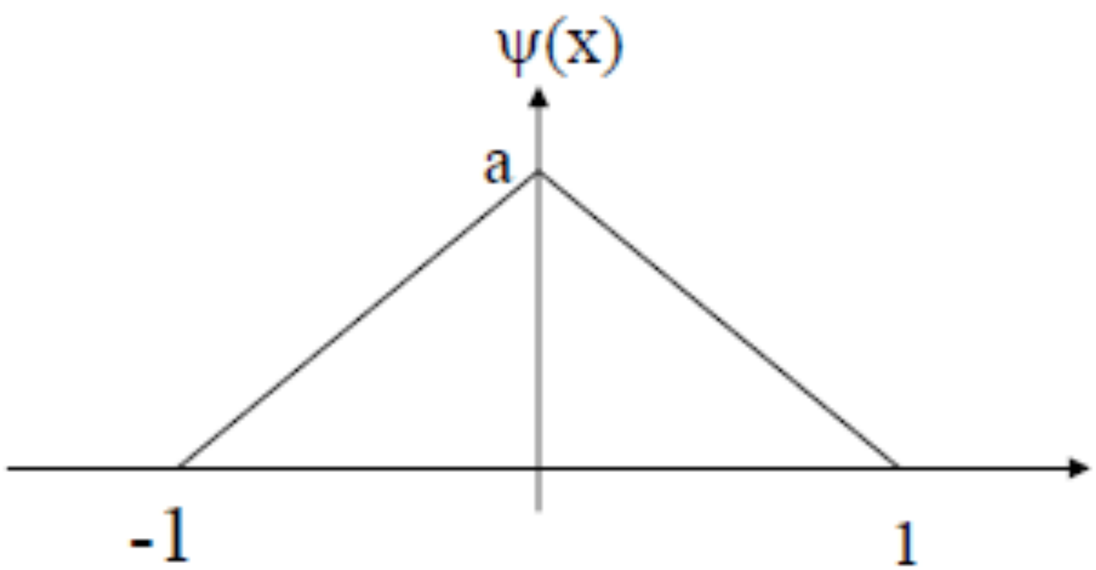
$$\Rightarrow A = \left(\frac{2\lambda}{\pi}\right)^{1/4}$$

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

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.



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

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

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

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

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

Possible Questions

1. **Define Wave function? What are the characteristics of a well behaved wavefunction?**

2. Numerical on Normalisation and its importance?

3. The wavefunction for a quantum particle of mass m confined to move in the range 0 ≤ x ≤ L is given by $\Psi(x) = N\ Sin(\frac{4\pi x}{L})$**.**

Calculate N

Although the Bohr theory of the atom, which can be extended further than was done in Chap. 4, is able to account for many aspects of atomic phenomena, it has a number of severe limitations as well. First of all, it applies only to hydrogen and one-electron ions such as He^+ and Li^{2+}—it does not even work for ordinary helium. The Bohr theory cannot explain why certain spectral lines are more intense than others (that is, why certain transitions between energy levels have greater probabilities of occurrence than others). It cannot account for the observation that many spectral lines actually consist of several separate lines whose wavelengths differ slightly. And perhaps most important, it does not permit us to obtain what a really successful theory of the atom should make possible: an understanding of how individual atoms interact with one another to endow macroscopic aggregates of matter with the physical and chemical properties we observe.

The preceding objections to the Bohr theory are not put forward in an unfriendly way, for the theory was one of those seminal achievements that transform scientific thought, but rather to emphasize that a more general approach to atomic phenomena is required. Such an approach was developed in 1925 and 1926 by Erwin Schrödinger, Werner Heisenberg, Max Born, Paul Dirac, and others under the apt name of **quantum mechanics.** "The discovery of quantum mechanics was nearly a total surprise. It described the physical world in a way that was fundamentally new. It seemed to many of us a miracle," noted Eugene Wigner, one of the early workers in the field. By the early 1930s the application of quantum mechanics to problems involving nuclei, atoms, molecules, and matter in the solid state made it possible to understand a vast body of data ("a large part of physics and the whole of chemistry," according to Dirac) and—vital for any theory—led to predictions of remarkable accuracy. Quantum mechanics has survived every experimental test thus far of even its most unexpected conclusions.

5.1 QUANTUM MECHANICS

Classical mechanics is an approximation of quantum mechanics

The fundamental difference between classical (or Newtonian) mechanics and quantum mechanics lies in what they describe. In classical mechanics, the future history of a particle is completely determined by its initial position and momentum together with the forces that act upon it. In the everyday world these quantities can all be determined well enough for the predictions of Newtonian mechanics to agree with what we find.

Quantum mechanics also arrives at relationships between observable quantities, but the uncertainty principle suggests that the nature of an observable quantity is different in the atomic realm. Cause and effect are still related in quantum mechanics, but what they concern needs careful interpretation. In quantum mechanics the kind of certainty about the future characteristic of classical mechanics is impossible because the initial state of a particle cannot be established with sufficient accuracy. As we saw in Sec. 3.7, the more we know about the position of a particle now, the less we know about its momentum and hence about its position later.

The quantities whose relationships quantum mechanics explores are *probabilities.* Instead of asserting, for example, that the radius of the electron's orbit in a ground-state hydrogen atom is always exactly 5.3×10^{-11} m, as the Bohr theory does, quantum mechanics states that this is the *most probable* radius. In a suitable experiment most trials will yield a different value, either larger or smaller, but the value most likely to be found will be 5.3×10^{-11} m.

Quantum mechanics might seem a poor substitute for classical mechanics. However, classical mechanics turns out to be just an approximate version of quantum mechanics. The certainties of classical mechanics are illusory, and their apparent agreement with experiment occurs because ordinary objects consist of so many individual atoms that departures from average behavior are unnoticeable. Instead of two sets of physical principles, one for the macroworld and one for the microworld, there is only the single set included in quantum mechanics.

Wave Function

As mentioned in Chap. 3, the quantity with which quantum mechanics is concerned is the **wave function** Ψ of a body. While Ψ itself has no physical interpretation, the square of its absolute magnitude $|\Psi|^2$ evaluated at a particular place at a particular time is proportional to the probability of finding the body there at that time. The linear momentum, angular momentum, and energy of the body are other quantities that can be established from Ψ. The problem of quantum mechanics is to determine Ψ for a body when its freedom of motion is limited by the action of external forces.

Wave functions are usually complex with both real and imaginary parts. A probability, however, must be a positive real quantity. The probability density $|\Psi|^2$ for a complex Ψ is therefore taken as the product $\Psi^*\Psi$ of Ψ and its **complex conjugate** Ψ^*. The complex conjugate of any function is obtained by replacing $i(=\sqrt{-1})$ by $-i$ wherever it appears in the function. Every complex function Ψ can be written in the form

Wave function $$\Psi = A + iB$$

where A and B are real functions. The complex conjugate Ψ^* of Ψ is

Complex conjugate $$\Psi^* = A - iB$$

and so $$|\Psi|^2 = \Psi^*\Psi = A^2 - i^2B^2 = A^2 + B^2$$

since $i^2 = -1$. Hence $|\Psi|^2 = \Psi^*\Psi$ is always a positive real quantity, as required.

Normalization

Even before we consider the actual calculation of Ψ, we can establish certain requirements it must always fulfill. For one thing, since $|\Psi|^2$ is proportional to the probability density P of finding the body described by Ψ, the integral of $|\Psi|^2$ over all space must be finite—the body is *somewhere,* after all. If

$$\int_{-\infty}^{\infty} |\Psi|^2\, dV = 0$$

the particle does not exist, and the integral obviously cannot be ∞ and still mean anything. Furthermore, $|\Psi|^2$ cannot be negative or complex because of the way it is defined. The only possibility left is that the integral be a finite quantity if Ψ is to describe properly a real body.

It is usually convenient to have $|\Psi|^2$ be *equal* to the probability density P of finding the particle described by Ψ, rather than merely be proportional to P. If $|\Psi|^2$ is to equal P, then it must be true that

Normalization

$$\int_{-\infty}^{\infty} |\Psi|^2 \, dV = 1 \tag{5.1}$$

since if the particle exists somewhere at all times,

$$\int_{-\infty}^{\infty} P \, dV = 1$$

A wave function that obeys Eq. (5.1) is said to be **normalized.** Every acceptable wave function can be normalized by multiplying it by an appropriate constant; we shall shortly see how this is done.

Well-Behaved Wave Functions

Besides being normalizable, Ψ must be single-valued, since P can have only one value at a particular place and time, and continuous. Momentum considerations (see Sec. 5.6) require that the partial derivatives $\partial\Psi/\partial x$, $\partial\Psi/\partial y$, $\partial\Psi/\partial z$ be finite, continuous, and single-valued. Only wave functions with all these properties can yield physically meaningful results when used in calculations, so only such "well-behaved" wave functions are admissible as mathematical representations of real bodies. To summarize:

1 Ψ must be continuous and single-valued everywhere.
2 $\partial\Psi/\partial x$, $\partial\Psi/\partial y$, $\partial\Psi/\partial z$ must be continuous and single-valued everywhere.
3 Ψ must be normalizable, which means that Ψ must go to 0 as $x \to \pm\infty$, $y \to \pm\infty$, $z \to \pm\infty$ in order that $\int |\Psi|^2 \, dV$ over all space be a finite constant.

These rules are not always obeyed by the wave functions of particles in model situations that only approximate actual ones. For instance, the wave functions of a particle in a box with infinitely hard walls do not have continuous derivatives at the walls, since $\Psi = 0$ outside the box (see Fig. 5.4). But in the real world, where walls are never infinitely hard, there is no sharp change in Ψ at the walls (see Fig. 5.7) and the derivatives are continuous. Exercise 7 gives another example of a wave function that is not well-behaved.

Given a normalized and otherwise acceptable wave function Ψ, the probability that the particle it describes will be found in a certain region is simply the integral of the probability density $|\Psi|^2$ over that region. Thus for a particle restricted to motion in the x direction, the probability of finding it between x_1 and x_2 is given by

Probability

$$P_{x_1 x_2} = \int_{x_1}^{x_2} |\Psi|^2 \, dx \tag{5.2}$$

We will see examples of such calculations later in this chapter and in Chap. 6.

5.2 THE WAVE EQUATION

It can have a variety of solutions, including complex ones

Schrödinger's equation, which is the fundamental equation of quantum mechanics in the same sense that the second law of motion is the fundamental equation of Newtonian mechanics, is a wave equation in the variable Ψ.

The de Broglie wavelength of a particle of momentum p is $\lambda = h/p$ and the corresponding wave number is

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

In terms of wave number the particle's momentum is therefore

$$p = \frac{hk}{2\pi}$$

Hence an uncertainty Δk in the wave number of the de Broglie waves associated with the particle results in an uncertainty Δp in the particle's momentum according to the formula

$$\Delta p = \frac{h\,\Delta k}{2\pi}$$

Since $\Delta x\, \Delta k \geq \frac{1}{2}$, $\Delta k \geq 1/(2\Delta x)$ and

Uncertainty principle

$$\Delta x\, \Delta p \geq \frac{h}{4\pi} \tag{3.21}$$

This equation states that the product of the uncertainty Δx in the position of an object at some instant and the uncertainty Δp in its momentum component in the x direction at the same instant is equal to or greater than $h/4\pi$.

If we arrange matters so that Δx is small, corresponding to a narrow wave group, then Δp will be large. If we reduce Δp in some way, a broad wave group is inevitable and Δx will be large.

Werner Heisenberg (1901–1976) was born in Duisberg, Germany, and studied theoretical physics at Munich, where he also became an enthusiastic skier and mountaineer. At Göttingen in 1924 as an assistant to Max Born, Heisenberg became uneasy about mechanical models of the atom: "Any picture of the atom that our imagination is able to invent is for that very reason defective," he later remarked. Instead he conceived an abstract approach using matrix algebra. In 1925, together with Born and Pascual Jordan, Heisenberg developed this approach into a consistent theory of quantum mechanics, but it was so difficult to understand and apply that it had very little impact on physics at the time. Schrödinger's wave formulation of quantum mechanics the following year was much more successful; Schrödinger and others soon showed that the wave and matrix versions of quantum mechanics were mathematically equivalent.

In 1927, working at Bohr's institute in Copenhagen, Heisenberg developed a suggestion by Wolfgang Pauli into the uncertainty principle. Heisenberg initially felt that this principle was a consequence of the disturbances inevitably produced by any measuring process. Bohr, on the other hand, thought that the basic cause of the uncertainties was the wave-particle duality, so that they were built into the natural world rather than solely the result of measurement. After much argument Heisenberg came around to Bohr's view. (Einstein, always skeptical about quantum mechanics, said after a lecture by Heisenberg on the uncertainty principle: "Marvelous, what ideas the young people have these days. But I don't believe a word of it.") Heisenberg received the Nobel Prize in 1932.

Heisenberg was one of the very few distinguished scientists to remain in Germany during the Nazi period. In World War II he led research there on atomic weapons, but little progress had been made by the war's end. Exactly why remains unclear, although there is no evidence that Heisenberg, as he later claimed, had moral qualms about creating such weapons and more or less deliberately dragged his feet. Heisenberg recognized early that "an explosive of unimaginable consequences" could be developed, and he and his group should have been able to have gotten farther than they did. In fact, alarmed by the news that Heisenberg was working on an atomic bomb, the U.S. government sent the former Boston Red Sox catcher Moe Berg to shoot Heisenberg during a lecture in neutral Switzerland in 1944. Berg, sitting in the second row, found himself uncertain from Heisenberg's remarks about how advanced the German program was, and kept his gun in his pocket.

These uncertainties are due not to inadequate apparatus but to the imprecise character in nature of the quantities involved. Any instrumental or statistical uncertainties that arise during a measurement only increase the product $\Delta x\, \Delta p$. Since we cannot know exactly both where a particle is right now and what its momentum is, we cannot say anything definite about where it will be in the future or how fast it will be moving then. *We cannot know the future for sure because we cannot know the present for sure.* But our ignorance is not total: we can still say that the particle is more likely to be in one place than another and that its momentum is more likely to have a certain value than another.

H-Bar

The quantity $h/2\pi$ appears often in modern physics because it turns out to be the basic unit of angular momentum. It is therefore customary to abbreviate $h/2\pi$ by the symbol $\hbar$ ("h-bar"):

$$\hbar = \frac{h}{2\pi} = 1.054 \times 10^{-34}\ \mathrm{J \cdot s}$$

In the remainder of this book $\hbar$ is used in place of $h/2\pi$. In terms of $\hbar$, the uncertainty principle becomes

Uncertainty principle

$$\Delta x\, \Delta p \geq \frac{\hbar}{2} \tag{3.22}$$

Example 3.6

A measurement establishes the position of a proton with an accuracy of $\pm 1.00 \times 10^{-11}$ m. Find the uncertainty in the proton's position 1.00 s later. Assume $v \ll c$.

Solution

Let us call the uncertainty in the proton's position Δx_0 at the time $t = 0$. The uncertainty in its momentum at this time is therefore, from Eq. (3.22),

$$\Delta p \geq \frac{\hbar}{2\Delta x_0}$$

Since $v \ll c$, the momentum uncertainty is $\Delta p = \Delta(mv) = m\, \Delta v$ and the uncertainty in the proton's velocity is

$$\Delta v = \frac{\Delta p}{m} \geq \frac{\hbar}{2m\, \Delta x_0}$$

The distance x the proton covers in the time t cannot be known more accurately than

$$\Delta x = t\, \Delta v \geq \frac{\hbar t}{2m\, \Delta x_0}$$

Hence Δx is inversely proportional to Δx_0: the *more* we know about the proton's position at $t = 0$, the *less* we know about its later position at $t > 0$. The value of Δx at $t = 1.00$ s is

$$\Delta x \geq \frac{(1.054 \times 10^{-34}\ \mathrm{J \cdot s})(1.00\ \mathrm{s})}{(2)(1.672 \times 10^{-27}\ \mathrm{kg})(1.00 \times 10^{-11}\ \mathrm{m})}$$

$$\geq 3.15 \times 10^{3}\ \mathrm{m}$$

This is 3.15 km—nearly 2 mi! What has happened is that the original wave group has spread out to a much wider one (Fig. 3.16). This occurred because the phase velocities of the component waves vary with wave number and a large range of wave numbers must have been present to produce the narrow original wave group. See Fig. 3.14.

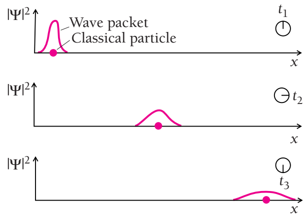


Figure 3.16 The wave packet that corresponds to a moving packet is a composite of many individual waves, as in Fig. 3.13. The phase velocities of the individual waves vary with their wave lengths. As a result, as the particle moves, the wave packet spreads out in space. The narrower the original wavepacket—that is, the more precisely we know its position at that time—the more it spreads out because it is made up of a greater span of waves with different phase velocities.

3.8 UNCERTAINTY PRINCIPLE II

A particle approach gives the same result

The uncertainty principle can be arrived at from the point of view of the particle properties of waves as well as from the point of view of the wave properties of particles.

We might want to measure the position and momentum of an object at a certain moment. To do so, we must touch it with something that will carry the required information back to us. That is, we must poke it with a stick, shine light on it, or perform some similar act. The measurement process itself thus requires that the object be interfered with in some way. If we consider such interferences in detail, we are led to the same uncertainty principle as before even without taking into account the wave nature of moving bodies.

Suppose we look at an electron using light of wavelength λ, as in Fig. 3.17. Each photon of this light has the momentum h/λ. When one of these photons bounces off the electron (which must happen if we are to "see" the electron), the electron's

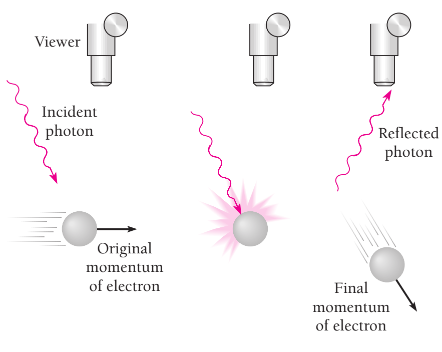


Figure 3.17 An electron cannot be observed without changing its momentum.

original momentum will be changed. The exact amount of the change Δp cannot be predicted, but it will be of the same order of magnitude as the photon momentum h/λ. Hence

$$\Delta p \approx \frac{h}{\lambda} \tag{3.23}$$

The longer the wavelength of the observing photon, the smaller the uncertainty in the electron's momentum.

Because light is a wave phenomenon as well as a particle phenomenon, we cannot expect to determine the electron's location with perfect accuracy regardless of the instrument used. A reasonable estimate of the minimum uncertainty in the measurement might be one photon wavelength, so that

$$\Delta x \geq \lambda \tag{3.24}$$

The shorter the wavelength, the smaller the uncertainty in location. However, if we use light of short wavelength to increase the accuracy of the position measurement, there will be a corresponding decrease in the accuracy of the momentum measurement because the higher photon momentum will disturb the electron's motion to a greater extent. Light of long wavelength will give a more accurate momentum but a less accurate position.

Combining Eqs. (3.23) and (3.24) gives

$$\Delta x \, \Delta p \geq h \tag{3.25}$$

This result is consistent with Eq. (3.22), $\Delta x \, \Delta p \geq \hbar/2$.

Arguments like the preceding one, although superficially attractive, must be approached with caution. The argument above implies that the electron can possess a definite position and momentum at any instant and that it is the measurement process that introduces the indeterminacy in $\Delta x \, \Delta p$. On the contrary, *this indeterminacy is inherent in the nature of a moving body*. The justification for the many "derivations" of this kind is first, they show it is impossible to imagine a way around the uncertainty principle; and second, they present a view of the principle that can be appreciated in a more familiar context than that of wave groups.

3.9 APPLYING THE UNCERTAINTY PRINCIPLE

A useful tool, not just a negative statement

Planck's constant h is so small that the limitations imposed by the uncertainty principle are significant only in the realm of the atom. On such a scale, however, this principle is of great help in understanding many phenomena. It is worth keeping in mind that the lower limit of $\hbar/2$ for $\Delta x \, \Delta p$ is rarely attained. More usually $\Delta x \, \Delta p \geq \hbar$, or even (as we just saw) $\Delta x \, \Delta p \geq h$.

Example 3.7

A typical atomic nucleus is about 5.0×10^{-15} m in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is to be part of a nucleus.

Solution

Letting $\Delta x = 5.0 \times 10^{-5}$ m we have

$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq \frac{1.054 \times 10^{-34}\ \text{J} \cdot \text{s}}{(2)(5.0 \times 10^{-15}\ \text{m})} \geq 1.1 \times 10^{-20}\ \text{kg} \cdot \text{m/s}$$

If this is the uncertainty in a nuclear electron's momentum, the momentum p itself must be at least comparable in magnitude. An electron with such a momentum has a kinetic energy KE many times greater than its rest energy mc^2. From Eq. (1.24) we see that we can let KE $= pc$ here to a sufficient degree of accuracy. Therefore

$$\text{KE} = pc \geq (1.1 \times 10^{-20}\ \text{kg} \cdot \text{m/s})(3.0 \times 10^{8}\ \text{m/s}) \geq 3.3 \times 10^{-12}\ \text{J}$$

Since 1 eV $= 1.6 \times 10^{-19}$ J, the kinetic energy of an electron must exceed 20 MeV if it is to be inside a nucleus. Experiments show that the electrons emitted by certain unstable nuclei never have more than a small fraction of this energy, from which we conclude that nuclei cannot contain electrons. The electron an unstable nucleus may emit comes into being at the moment the nucleus decays (see Secs. 11.3 and 12.5).

Example 3.8

A hydrogen atom is 5.3×10^{-11} m in radius. Use the uncertainty principle to estimate the minimum energy an electron can have in this atom.

Solution

Here we find that with $\Delta x = 5.3 \times 10^{-11}$ m.

$$\Delta p \geq \frac{\hbar}{2\Delta x} \geq 9.9 \times 10^{-25}\ \text{kg} \cdot \text{m/s}$$

An electron whose momentum is of this order of magnitude behaves like a classical particle, and its kinetic energy is

$$\text{KE} = \frac{p^2}{2m} \geq \frac{(9.9 \times 10^{-25}\ \text{kg} \cdot \text{m/s})^2}{(2)(9.1 \times 10^{-31}\ \text{kg})} \geq 5.4 \times 10^{-19}\ \text{J}$$

which is 3.4 eV. The kinetic energy of an electron in the lowest energy level of a hydrogen atom is actually 13.6 eV.

Energy and Time

Another form of the uncertainty principle concerns energy and time. We might wish to measure the energy E emitted during the time interval Δt in an atomic process. If the energy is in the form of em waves, the limited time available restricts the accuracy with which we can determine the frequency ν of the waves. Let us assume that the minimum uncertainty in the number of waves we count in a wave group is one wave. Since the frequency of the waves under study is equal to the number of them we count divided by the time interval, the uncertainty $\Delta\nu$ in our frequency measurement is

$$\Delta\nu \geq \frac{1}{\Delta t}$$