



A Quick Guide to Quantum World

Lesson 2

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Why Quantum Mechanics?

- Classical mechanics by Newton-Lagrange-Hamilton-Dirac and Maxwell's electro-magnetic theory of light can explain all macroscopic phenomena such as motion of billiard balls or rockets, but fails in the microscopic world.
- Quantum mechanics is used to explain microscopic phenomena such as photon-atom scattering, flow of electrons in a semiconductor etc.
- Quantum Mechanics is a collection of postulates based on a huge number of experimental observations.
- The differences between the classical and quantum mechanics can be understood by examining both
 - **The classical point of view**
 - **The quantum point of view**



Classical Point of View

- ✓ In classical mechanics, the laws are written in terms of **particle trajectories**.
- ✓ Here a **PARTICLE** is an indivisible mass point object that has a variety of properties that can be measured, which we call **observables**. The observables specify the state of the particle (position and momentum).
- ✓ A **system** is a collection of particles, which interact among themselves via internal forces, and can also interact with the outside world via external forces. The **state of a system** is a collection of the states of the particles that comprise the system.
- ✓ **Note:** Here all properties of a particle can be known to infinite precision.
- ✓ **Conclusions:**
 - ✓ **TRAJECTORY** → State descriptor of Newtonian physics,
 - ✓ **EVOLUTION OF THE STATE** → Use of Newton's second law
 - ✓ **PRINCIPLE OF CAUSALITY** → Two identical systems with same initial conditions, subject to the same measurements, will yield the same result.



Quantum Point of View

- Quantum particles can act as **both particles and waves** → that means **wave-particle duality** becomes important.
- Quantum state is a conglomeration of several possible outcomes of measurement of different physical properties → Quantum mechanics uses the language of **probability** theory (random chance)
- An observer cannot observe a microscopic system **without altering some of its properties**. Neither one can predict how the state of the system will change. So an inherent **uncertainty** prevails in the quantum world.
- **Quantization** of energy is yet another property of "microscopic" particles that arises from several restrictions in their movement. So a **discontinuity** rules in this area and nothing is continuous here.



Heisenberg Uncertainty Principle

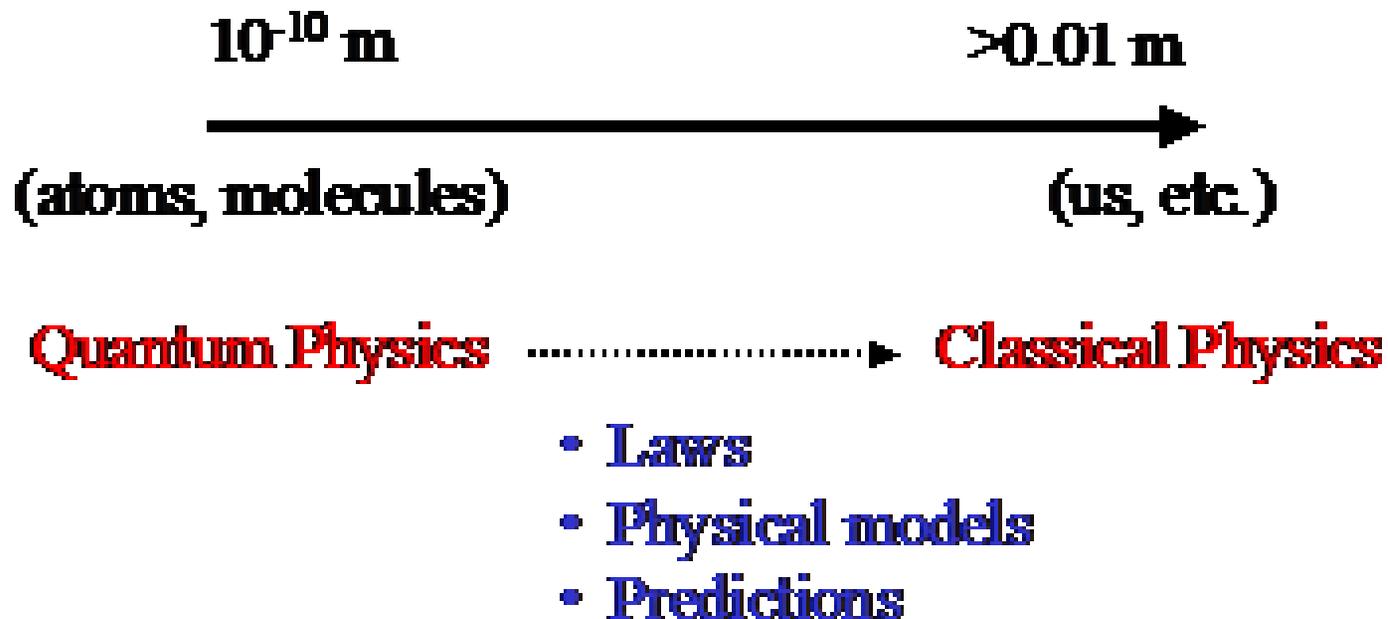
- One cannot unambiguously specify the values of particle's position and its momentum for a microscopic particle, i.e.

$$\Delta x(t_0) \cdot \Delta p_x(t_0) \geq \frac{1}{2} \frac{h}{2\pi}$$

- Position and momentum are, therefore, considered as incompatible variables.
- The Heisenberg uncertainty principle strikes at the very heart of the classical physics => the particle trajectory.
- Same is true for energy-time pair too.

The Correspondence Principle

When Quantum mechanics is applied to macroscopic systems, it **must reduce to the classical physics**. Therefore, the non-classical phenomena, such as uncertainty and duality, must become undetectable. Niels Bohr codified this requirement into his **Correspondence Principle**:





Particle-Wave Duality

- ✓ The behavior of a "microscopic" particle is very different from that of a classical particle:
 - ✓ → in some experiments it resembles the behavior of a classical wave (not localized in space)
 - ✓ → in other experiments it behaves as a classical particle (localized in space)
- ✓ Corpuscular theories of light treat light as though it were composed of particles, but can not explain diffraction and interference.
- ✓ Maxwell's theory of electromagnetic radiation can explain these two (diffraction and interference) phenomena, which was the reason why the corpuscular theory of light was abandoned.



Particle-Wave Duality

Waves as particles:

- ✓ Max Plank worked on black-body radiation, in which he assumed that the molecules of the cavity walls, described using a simple oscillator model, can only exchange energy in quantized units.
- ✓ 1905 Einstein proposed that the energy in an electromagnetic field is not spread out over a spherical wave front, but instead is localized in individual clump - quanta. Each quantum of frequency ν travels through space with speed of light, carrying a discrete amount of energy and momentum called as PHOTON used to explain the photoelectric effect, later to be confirmed by the x-ray experiments of Compton.

Particles as waves

- ✓ Double-slit experiment, in which instead of using a light source, one uses the electron gun. The electrons are diffracted by the slit and then interfere in the region between the diaphragm and the detector indicating the wave behavior of electrons, i.e., particles.

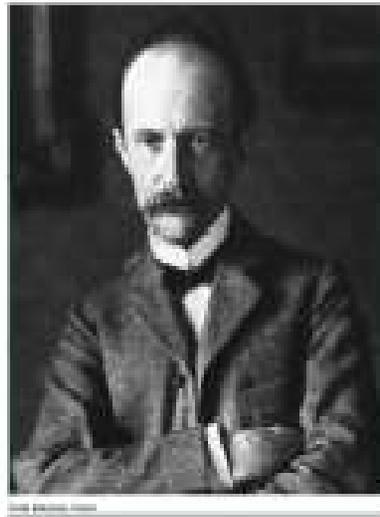


Wave as Particle

Some Examples

Blackbody Radiation

- Known since centuries that when a material is heated, it radiates heat and its color **depends on its temperature**
- Example: heating elements of a stove:
 - – Dark red: 550°C
 - – Bright red: 700°C
 - – Then: orange, yellow and finally white (**really hot !**)
- The emission spectrum **depends on the material**
- Theoretical description: simplifications necessary: An ideal model needed - that is Blackbody



Max Planck
1858-1947

Nobel Prize in Physics 1918

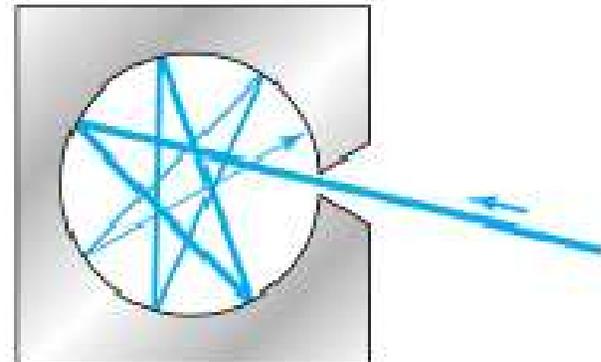


What is a Blackbody?

- ✓ A material that is constantly exchanging heat with its surrounding (to remain at a constant temperature) [Isothermal]:– It absorbs and emits radiations.
- ✓ **Problem:** it can reflect incoming radiations, which makes a theoretical description more difficult (depends on the environment).
- ✓ **Solution:** A blackbody, that is a perfect absorber: where incoming radiations are totally absorbed and none is reflected.

Blackbody Radiation

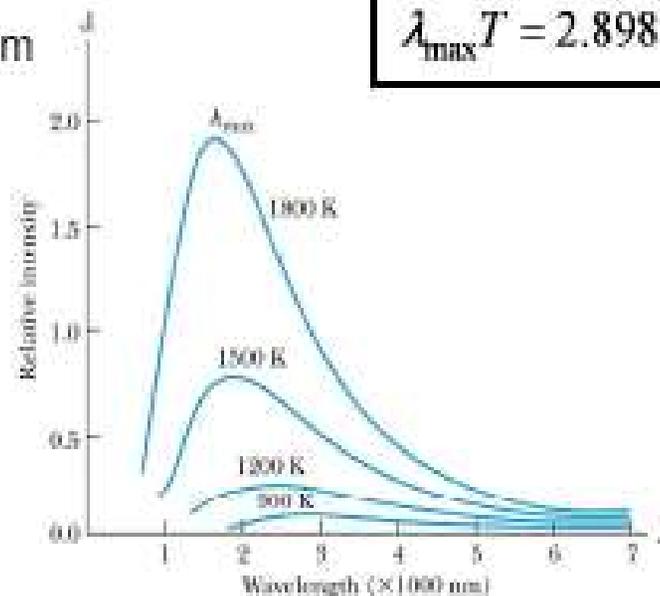
- ✓ Blackbody = a cavity, such as a metal box with a small hole drilled into it.
- ✓ Incoming radiations entering the hole keep bouncing around inside the box with a negligible change of escaping again through the hole => Absorbed.
- ✓ The hole is the perfect absorber, e.g. the blackbody radiation emission does not depend on the material the box is made of => Universal in nature



Wien's displacement law

- The intensity $\mathcal{I}(\lambda, T)$ is the total power radiated per unit area per unit wavelength at a given temperature
- **Wien's displacement law:** The maximum of the distribution shifts to smaller wavelengths as the temperature is increased.

Visible light: 400 – 700 nm
UltraViolet: <400 nm
Infrared: >700 nm



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

Empirical Formula

Wilhem Wien: Nobel Prize 1911



Stefan-Boltzmann Law

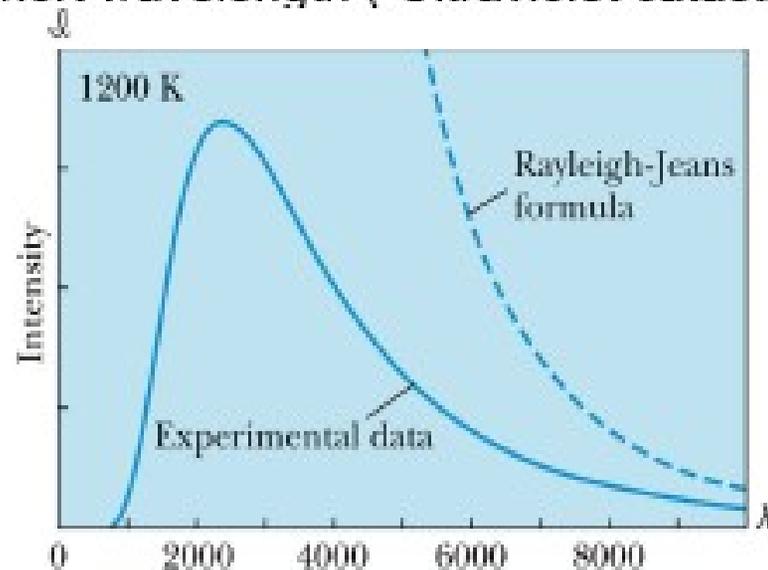
- The total power radiated increases with the temperature:

$$R(T) = \int_0^{\infty} \mathcal{L}(\lambda, T) d\lambda = \epsilon \sigma T^4$$

- This is known as the **Stefan-Boltzmann law**, with the constant σ experimentally measured to be $5.6705 \times 10^{-8} \text{ W / (m}^2 \cdot \text{K}^4)$.
- The **emissivity ϵ** ($\epsilon = 1$ for an idealized blackbody) is simply the ratio of the emissive power of an object to that of an ideal blackbody and is always less than 1.

Understanding the blackbody radiation spectrum

- Attempts to fit the low and high wavelength part of the spectrum
- Using classical theory of electromagnetism and thermodynamics, Lord Rayleigh comes up with:
$$j(\lambda, T) = \frac{2\pi ckT}{\lambda^4}$$
 Rayleigh-Jeans formula
- Major flaw at short wavelength (“Ultraviolet catastrophe”)



Describing the blackbody emission spectra:
one of the outstanding problems at the beginning of the 20th century



Two Catastrophes?

- **Classical physics:**

- Emission spectrum: a superposition of electromagnetic waves of different frequencies
- Frequencies allowed: standing waves inside the cavity

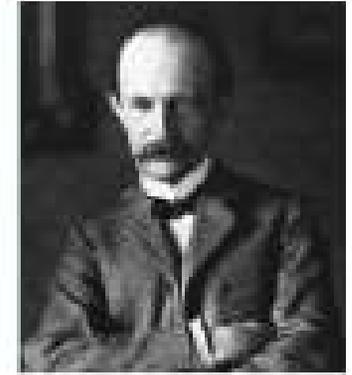
- **Equi-partition of the energy:**

- Every: standing wave carries kT of energy
- Flaw: when $l \rightarrow 0$, the number of standing waves \uparrow , leading to $E \rightarrow \infty$

- **[Ultraviolet Catastrophe] Failure of classical theories:**

- The work of Rayleigh-Jeans was considered as state-of-the-art, using well tested theories, which were in very good agreement with experimental results in many other circumstances.
- **So need for a new theory.....**

Max Planck and the blackbody problem



- **Max Planck** 1858-1947

- Expert in thermodynamics and statistical mechanics
- Around 1900: Proposes first an empirical formula (based on real physics) to reproduce both the high and low wavelength parts of the emission spectrum
 - Remarkable agreement with experimental results
- Then, works on a theoretical basis of the formula

1910 Nobel Prize

Planck's radiation law

- Planck assumed that the radiation in the cavity was emitted (and absorbed) by some sort of "oscillators" contained in the walls. He used Boltzmann's statistical methods to arrive at the following formula:

$$I(\lambda, T) = \frac{2\pi c^2 h}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$

Planck's radiation law

- Planck made two modifications to the classical theory:
 - The oscillators (of electromagnetic origin) can only have certain discrete energies determined by $E_n = nh\nu$, where n is an integer, ν is the frequency, and h is called Planck's constant.

$$h = 6.6261 \times 10^{-34} \text{ J}\cdot\text{s}$$

- The oscillators can absorb or emit energy in discrete multiples of the fundamental quantum of energy given by

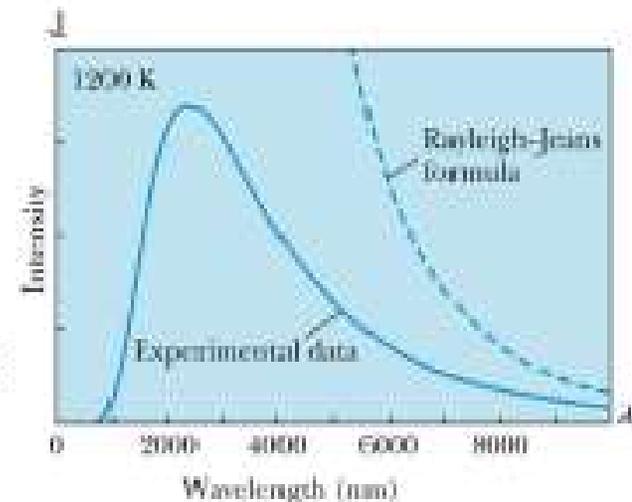
$$\Delta E = h\nu$$

Quantization !

- Blackbody emission spectrum explained by introducing quantization of energy transfers, resolves the ultraviolet catastrophe
 - Low wavelength \leftrightarrow High frequency ($\nu = c/\lambda$)
 - At small λ , the energy $E=h\nu$ needed to fill up the “oscillator” states increases. Their probability to be occupied decreases rapidly, e.g. faster than the rate found in the Rayleigh-Jeans formula: no ultraviolet catastrophe.

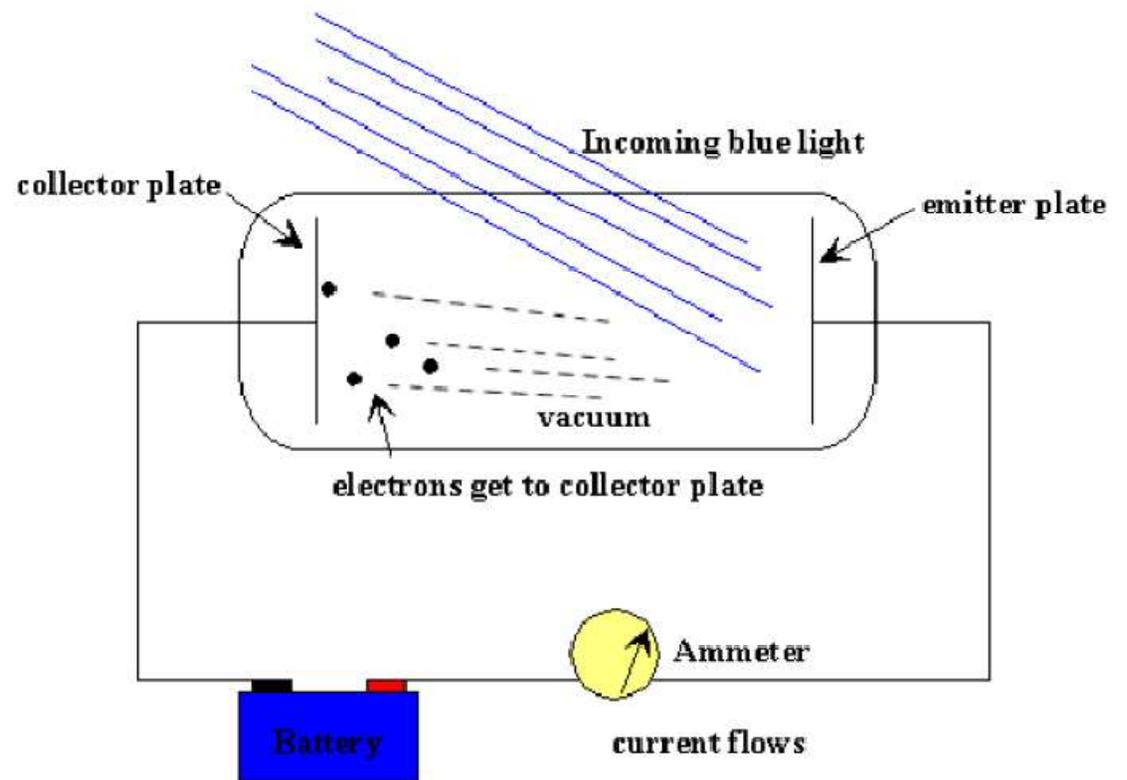
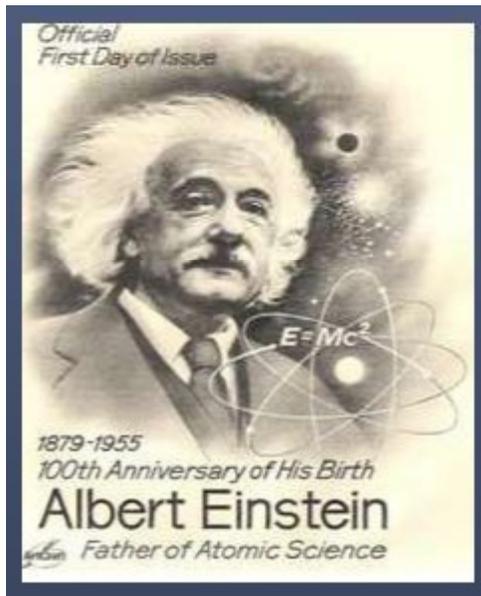
- Very disputed

- Planck himself looked for a few years in ways to get $h \rightarrow 0$ without success.



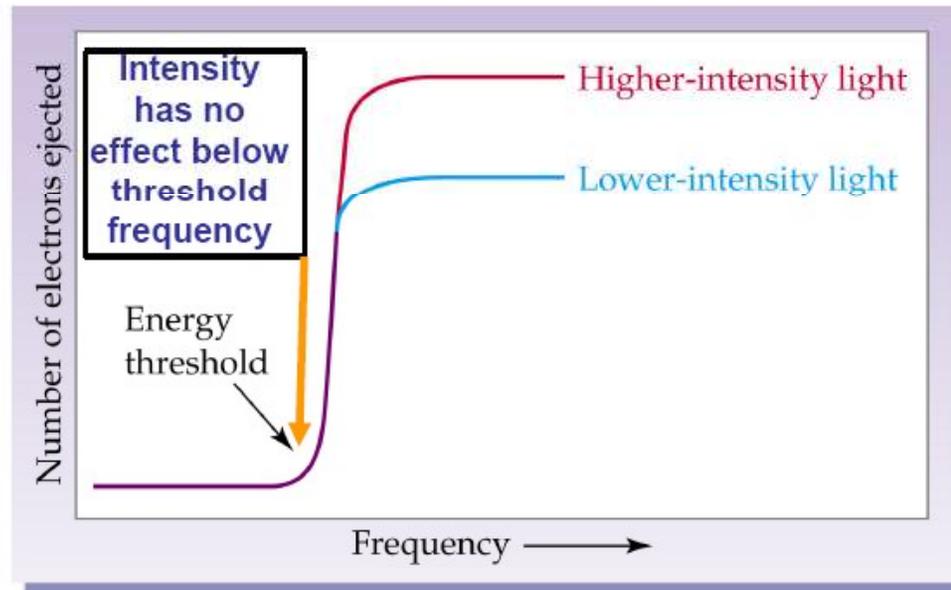
Photoelectric Effect

A Photocell is Used to Study the Photoelectric Effect



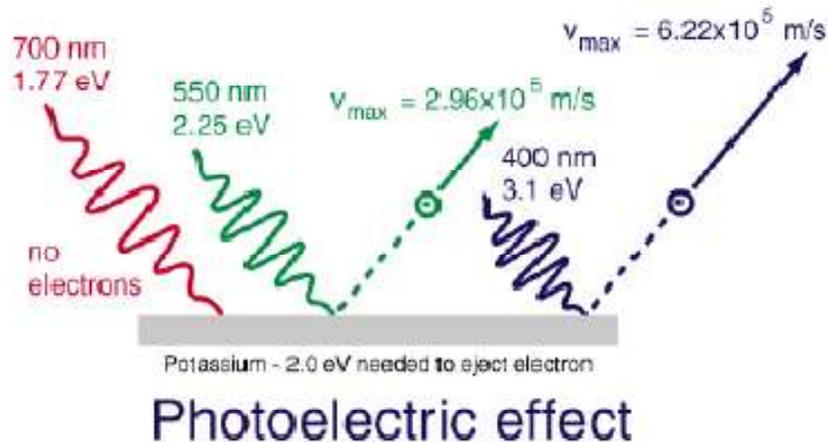
Photoelectric Effect

Influence of Light Intensity on the Photoelectric Effect



Larger light intensity means larger number of photons at a given frequency (Energy)

Photoelectric Effect



Light can eject electrons from a metal, but only if its frequency is above a threshold frequency (characteristic for each metal).

Classically, for light as a wave, its energy is proportional to the square of its *amplitude*.

For particles, energy is proportional to *frequency*

Einstein (1905) proposed that light has particle nature (as well as wave nature).

light is quantized (photons).

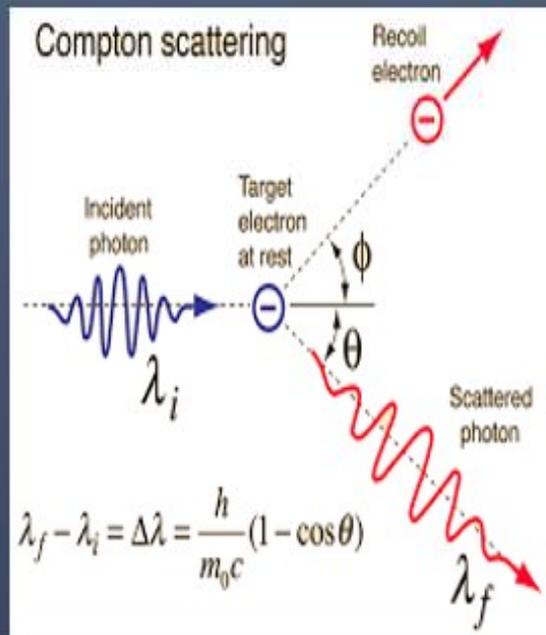
Larger frequency, means smaller wavelength and larger Energy = $h\nu$



Photoelectric Effect

- ✓ The photoelectric effect provides evidence for the **particle nature of light**.
- ✓ It also provides evidence for **quantization**.
- ✓ If light shines on the surface of a metal, there is a point at which electrons are ejected from the metal.
- ✓ The electrons will only be ejected once the **threshold frequency** is reached .
- ✓ Below the threshold frequency, no electrons are ejected.
- ✓ Above the threshold frequency, the number of electrons ejected **depend on the intensity** of the light.

The Compton effect



- The Compton effect (also called Compton scattering) is the result of high-energy photon colliding with an electron, which releases loosely bound electrons from the other shell of the atom or molecule.
- The scattered radiation experienced a wavelength shift that cannot be explained in terms of classical wave theory, thus lending support to Einstein's photon theory.

Einstein's photoelectric equation

$$h\nu = h\nu_0 + \frac{1}{2}mv^2$$

$$\frac{1}{2}mv^2 = h(\nu - \nu_0)$$

Compton shift expression

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0} \frac{(1 - \cos \theta)}{c}$$



All these **three** problems; **Black Body, Photoelectric and Compton**; that are excellent proofs of **Particle nature of Light** would be discussed in details in the coming lessons one by one elaborately.

So don't worry in case of any doubts!!



Particle as wave

Experimental Proof

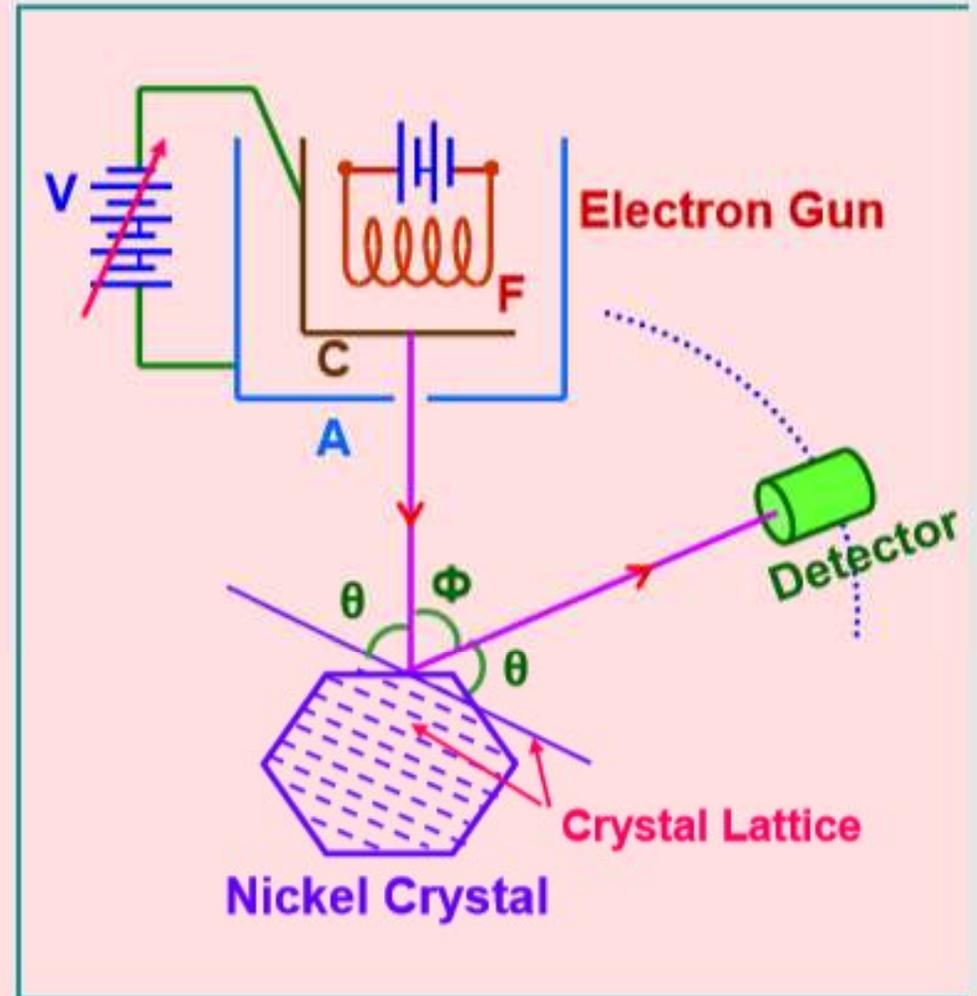
Davisson and Germer Experiment:

A beam of electrons emitted by the electron gun is made to fall on Nickel crystal cut along cubical axis at a particular angle.

The scattered beam of electrons is received by the detector which can be rotated at any angle.

The energy of the incident beam of electrons can be varied by changing the applied voltage to the electron gun.

Intensity of scattered beam of electrons is found to be maximum when angle of scattering is 50° and the accelerating potential is 54 V .



$$\theta + 50^\circ + \theta = 180^\circ \quad \text{i.e.} \quad \theta = 65^\circ$$

For Ni crystal, lattice spacing
 $d = 0.91 \text{ \AA}$

For first principal maximum, $n = 1$

Electron diffraction is similar to X-ray diffraction.

\therefore Bragg's equation $2d\sin\theta = n\lambda$ gives

$$\lambda = 1.65 \text{ \AA}$$



George Thomson

Wave nature of Particle;

“electron” here, was confirmed independently by **Clinton Davisson & Germer (USA) and George Thomson (UK) in 1927.** Ironically his Dad (**J.J. Thomson**) demonstrated that the same electron was a particle!

Time flies and changes too, right?



JJ Thomson won the Nobel Prize for Physics in **1906** for demonstrating that **electron is a particle**.

GP Thomson (son of JJ) won it in **1937** for demonstrating that **electron is a wave**.

And they were both right!



Postulates of Quantum Mechanics

A Brief Overview



What is Quantum Mechanics?

- Quantum Mechanics is nothing more but linear algebra and Hilbert spaces.
- What makes quantum mechanics quantum mechanics is the physical interpretation of the results that are obtained.



First Postulate

First postulate of Quantum mechanics:

Every physically-realizable state of the system is described in quantum mechanics by a state function ψ that contains all accessible physical information about the system in that state.

- ✓ **Physically realizable states** → states that can be studied in laboratory
- ✓ **Accessible information** → all the possible information we can extract from the wave function
- ✓ **State function** → function of position, momentum, energy that is spatially localized.



First Postulate

If ψ_1 and ψ_2 represent two physically-realizable states of the system, then the linear combination

$$\Psi = c_1\psi_1 + c_2\psi_2$$

where c_1 and c_2 are arbitrary complex constants, represents a third physically realizable state ψ of the system.

Note:

Wave function $\psi(x, t) \rightarrow$ position and time probability amplitude

Quantum mechanics describes the outcome of an set or ensemble of measurements, where an ensemble of measurements consists of a very large number of identical experiments performed on identical non-interacting systems, all of which have been identically prepared so as to be in the same state.

Second Postulate

If a system is in a quantum state represented by a wave function ψ , then

$$PdV = |\psi|^2 dV$$

is the probability that in a position measurement at time t the particle will be detected in the infinitesimal volume dV .

Note: $|\psi(x, t)|^2$ → position and time probability density

The importance of normalization follows from the Born interpretation of the state function as a position probability amplitude. According to the second postulate of quantum mechanics, the integrated probability density can be interpreted as a probability that in a position measurement at time t , we will find the particle anywhere in space.



Second Postulate

Therefore, the normalization condition for the wave function is:

$$\int P dV = \int |\psi(x, y, z)|^2 dV = \int \psi^*(x, y, z)\psi(x, y, z)dV = 1$$

Limitations on the wave function:

- Only normalizable functions can represent a quantum state and these are called physically admissible functions.
- State function must be continuous and single valued function.
- State function must be a smoothly-varying function (continuous derivative).

Third Postulate

Every observable in quantum mechanics is represented by an operator which is used to obtain physical information about the observable from the state function. For an observable that is represented in classical physics by a function $Q(x,p)$, the corresponding operator is $Q(\hat{x}, \hat{p})$.

Observable	Operator
Position	\hat{x}
Momentum	$\hat{p} = -\frac{\hbar}{i} \frac{\partial}{\partial x}$
Energy	$E = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$

More on Operators

- An operator is an instruction, a symbol which tells us to perform one or more mathematical acts on a function, say $f(x)$. The essential point is that they act on a function.
- Operators act on everything to the right, unless the action is constrained by brackets.
- Addition and subtraction rule for operators:

$$(\hat{Q}_1 \pm \hat{Q}_2)f(x) = \hat{Q}_1 f(x) \pm \hat{Q}_2 f(x)$$

- The product of two operators implies successive operation:

$$\hat{Q}_1 \hat{Q}_2 f(x) = \hat{Q}_1 [\hat{Q}_2 f(x)]$$

- The product of two operators is a third operator:

$$\hat{Q}_3 = \hat{Q}_1 \hat{Q}_2$$

- Two operators commute if they obey the simple operator expression:

$$[\hat{Q}_1, \hat{Q}_2] = \hat{Q}_1 \hat{Q}_2 - \hat{Q}_2 \hat{Q}_1 = 0 \Rightarrow \hat{Q}_1 \hat{Q}_2 = \hat{Q}_2 \hat{Q}_1$$

More on Operators

The requirement for two operators to be commuting operators is a very important one in quantum mechanics and it means that we can simultaneously measure the observables represented with these two operators. The non-commutivity of the position and the momentum operators (the inability to simultaneously determine particles position and its momentum) is represented with the Heisenberg uncertainty principle, which in mathematical form is expressed as:

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} = \frac{1}{2} |\langle [\hat{x}, \hat{p}] \rangle|$$

and can be generalized for any pair of observables.

Fourth Postulate

1926 Erwin Schrödinger proposed an equation that describes the evolution of a quantum-mechanical system → SWE which represents quantum equations of motion, and is of the form:

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

This work of Schrödinger was stimulated by a 1925 paper by Einstein on the quantum theory of ideal gas, and the de Broglie theory of matter waves.

Note:

Examining the time-dependent SWE, one can also define the following operator for the total energy:

$$\hat{E} = i\hbar \frac{\partial}{\partial t}$$

Fourth (Fundamental) postulate of Quantum mechanics:

The time development of the state functions of an isolated quantum system is governed by the time-dependent SWE $\hat{H}\psi = i\hbar\partial\psi / \partial t$, where $\hat{H} = \hat{T} + \hat{V}$ is the Hamiltonian of the system.

Note on isolated system:

The TDSWE describes the evolution of a state provided that no observations are made. An observation alters the state of the observed system, and as it is, the TDSWE can not describe such changes.



Fourth Postulate

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Note on isolated system:

The TDSWE describes the evolution of a state provided that no observations are made. An observation alters the state of the observed system, and as it is, the TDSWE can not describe such changes.



These **Four Postulates** are the four pillars of **Quantum Mechanics**.

The ideas are completely new, that may make you baffled right now.

But don't worry! They would be discussed in details in the coming lessons!

THANK YOU!

ANY QUESTION ?

