Basics of Quantum Mechanics

Basics of Quantum Mechanics

- Why Quantum Physics? -

Basics of Quantum Mechanics
- Classical Point of View -

- In Newtonian mechanics, the laws are written in terms of PARTICLE TRAJECTORIES.
- 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.
- All properties of a particle can be known to infinite precision.

- **Conclusions:**
  - TRAJECTORY ➔ state descriptor of Newtonian physics,
  - EVOLUTION OF THE STATE ➔ Use Newton's second law
  - PRINCIPLE OF CAUSALITY ➔ Two identical systems with the same initial conditions, subject to the same measurement will yield the same result.

Basics of Quantum Mechanics
- Quantum Point of View -

- Quantum particles can act as both particles and waves → WAVE-PARTICLE DUALITY
- Quantum state is a conglomeration of several possible outcomes of measurement of 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.
- QUANTIZATION of energy is yet another property of "microscopic" particles.

Basics of Quantum Mechanics
- Heisenberg Uncertainty Principle -

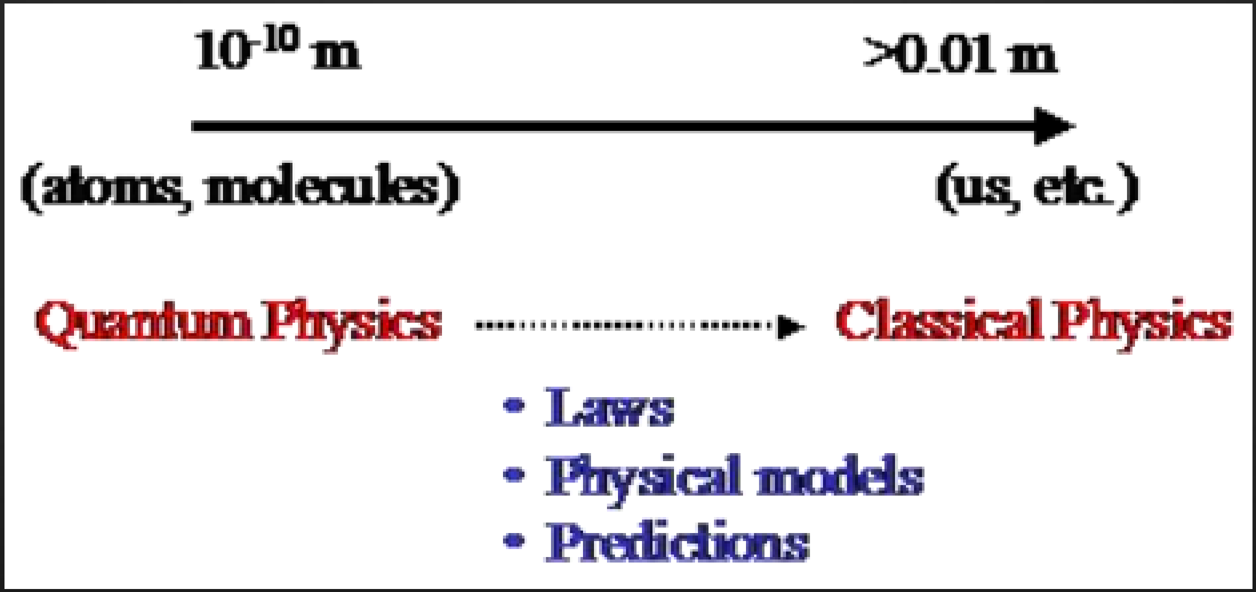
- One cannot unambiguously specify the values of particle's position and its momentum for a microscopic particle, i.e.

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

- 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.

Basics of Quantum Mechanics
- The Correspondence Principle -

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



Basics of Quantum Mechanics
- 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 DIFRACTION and INTERFERENCE.
- Maxwell's theory of electromagnetic radiation can explain these two phenomena, which was the reason why the corpuscular theory of light was abandoned.

Basics of Quantum Mechanics
- Particle-Wave Duality -

- Waves as particles:
  - Max Plank work 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 wavefront, but instead is localized in individual clumbs - quanta. Each quantum of frequency n travels through space with speed of light, carrying a discrete amount of energy and momentum =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.
  - Aharonov-Bohm effect

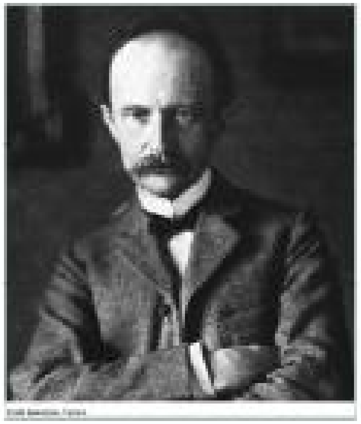
Check this link for Particle-Wave Duality explanation

http://www.youtube.com/watch?v=DfPeprQ7oGc

Waves as Particles

Basics of Quantum Mechanics
- 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: 550ºC
  - Bright red: 700ºC
  - Then: orange, yellow and finally white (really hot !)
- The emission spectrum depends on the material
- Theoretical description: simplifications necessary
  Blackbody



Max Plank
1858-1947

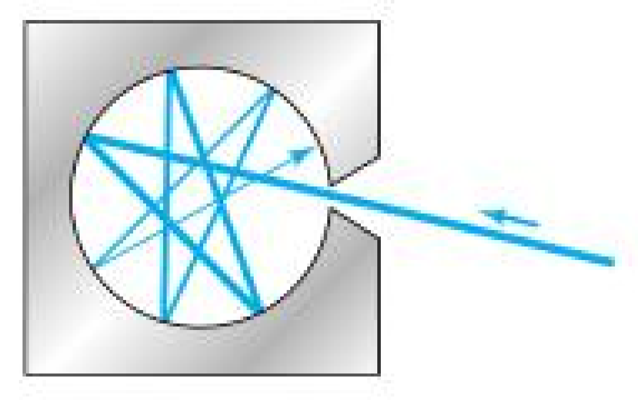
Nobel Prize in Physics 1918

Blackbody?

- A material is constantly exchanging heat with its surrounding (to remain at a constant temperature):
  - It absorbs and emits radiations
  - Problem: it can reflect incoming radiations, which makes a theoretical description more difficult (depends on the environment)
- A blackbody is a perfect absorber:
  - Incoming radiations is totally absorbed and none is reflected

Blackbody Radiation

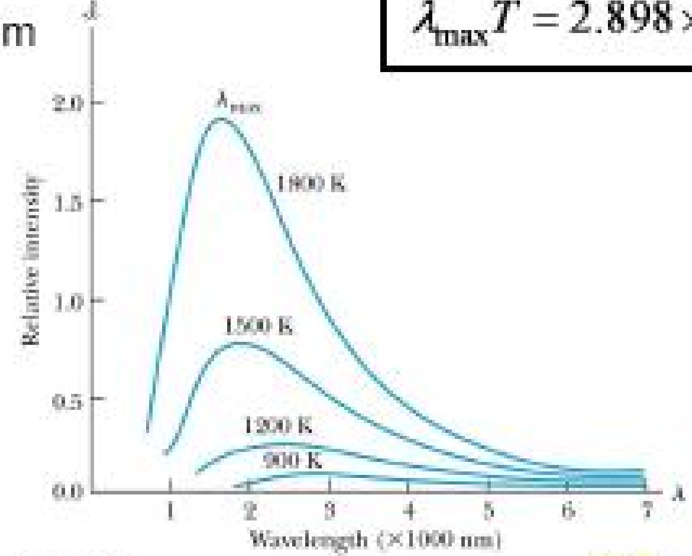
- Blackbody = a cavity, such as a metal box with a small hole drilled into it.
  - Incoming radiations entering the hole keep bouncing around inside the box with a negligible change of escaping again through the hole => Absorbed.
  - The hole is the perfect absorber, e.g. the blackbody Radiation emission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



Wien’s displacement law

- The intensity $\mathscr{I}(\lambda, T)$ 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



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

Empirical Formula

Wilhem Wien: Nobel Prize 1911

Stefan-Boltzmann Law

- The total power radiated increases with the temperature:

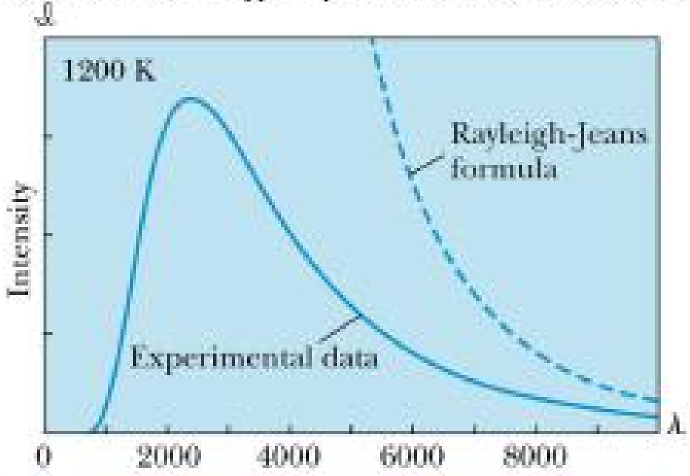
$$R(T) = \int_0^\infty \mathcal{I}(\lambda, T)\, d\lambda = \in \sigma T^4$$

- This is known as the Stefan-Boltzmann law, with the constant σ experimentally measured to be 5.6705×10^{-8} W / ($m^2 \cdot K^4$).

- 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: $\mathcal{I}(\lambda,T)=\frac{2\pi ckT}{\lambda^4}$ Rayleigh-Jeans formula
- Major flaw at short wavelength ("Ultraviolet catastrophe")

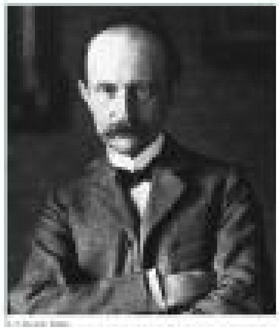


Describing the blackbody emission spectra:
one of the outstanding problems at the beginning of the 20th century

Two Catastrophes?

- Classical physics:
  - Emission spectrum: a superposition of electromagnetic waves of different frequencies
  - Frequencies allowed: standing waves inside the cavity
- Equipartition of the energy:
  - Every standing wave carries kT of energy
  - Flaw: when $\lambda \rightarrow 0$, the number of standing waves ↑, 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.
  - 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

1918 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 Boltzman's statistical methods to arrive at the following formula:

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

Planck's radiation law

- Planck made two modifications to the classical theory:
  1) 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.

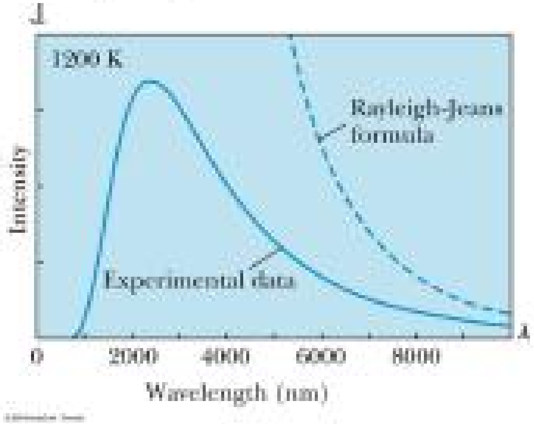
     $h = 6.6261 \times 10^{-34}$ J·s.

  2) 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 ←→ 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: <u>no ultraviolet catastrophe.</u>

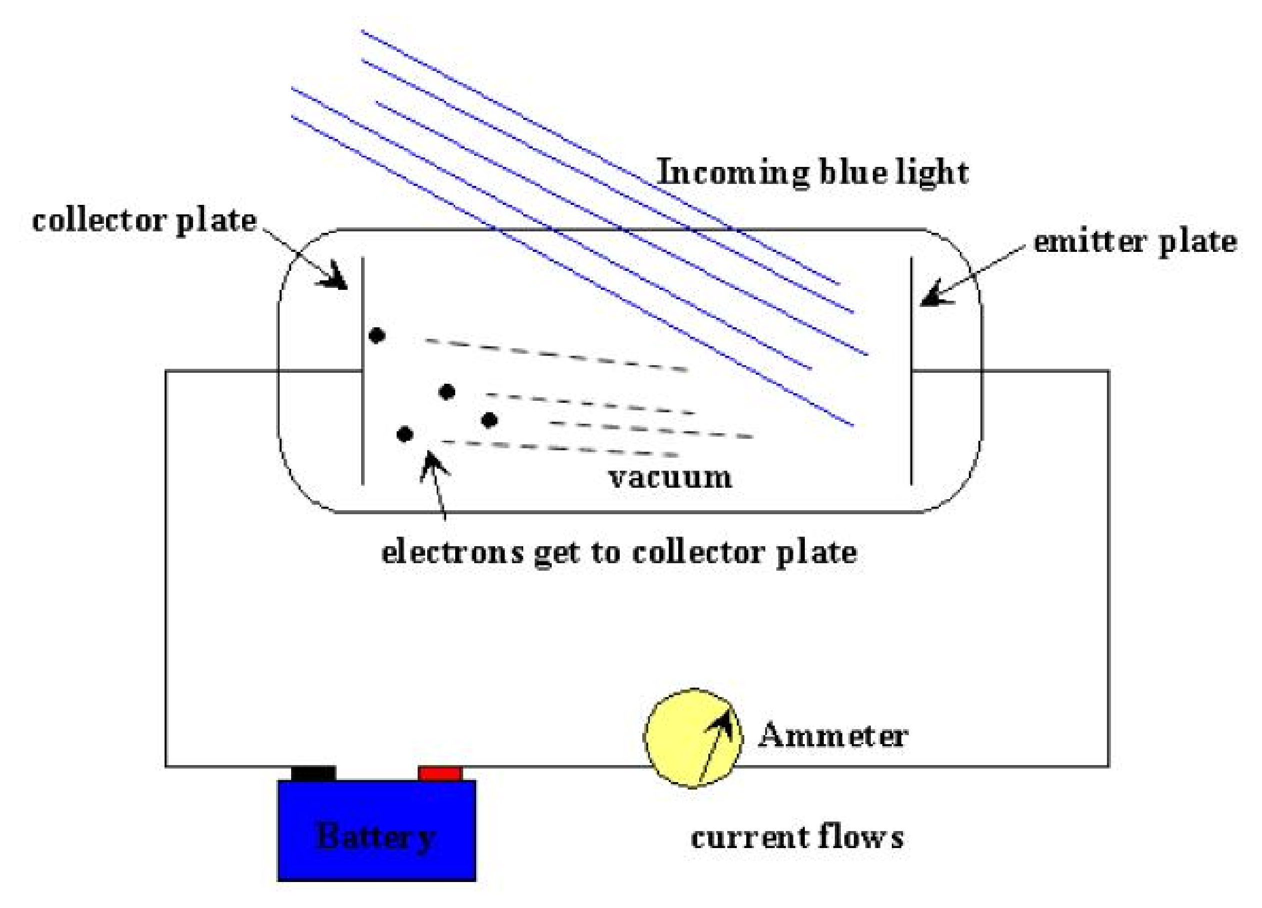


- Very disputed

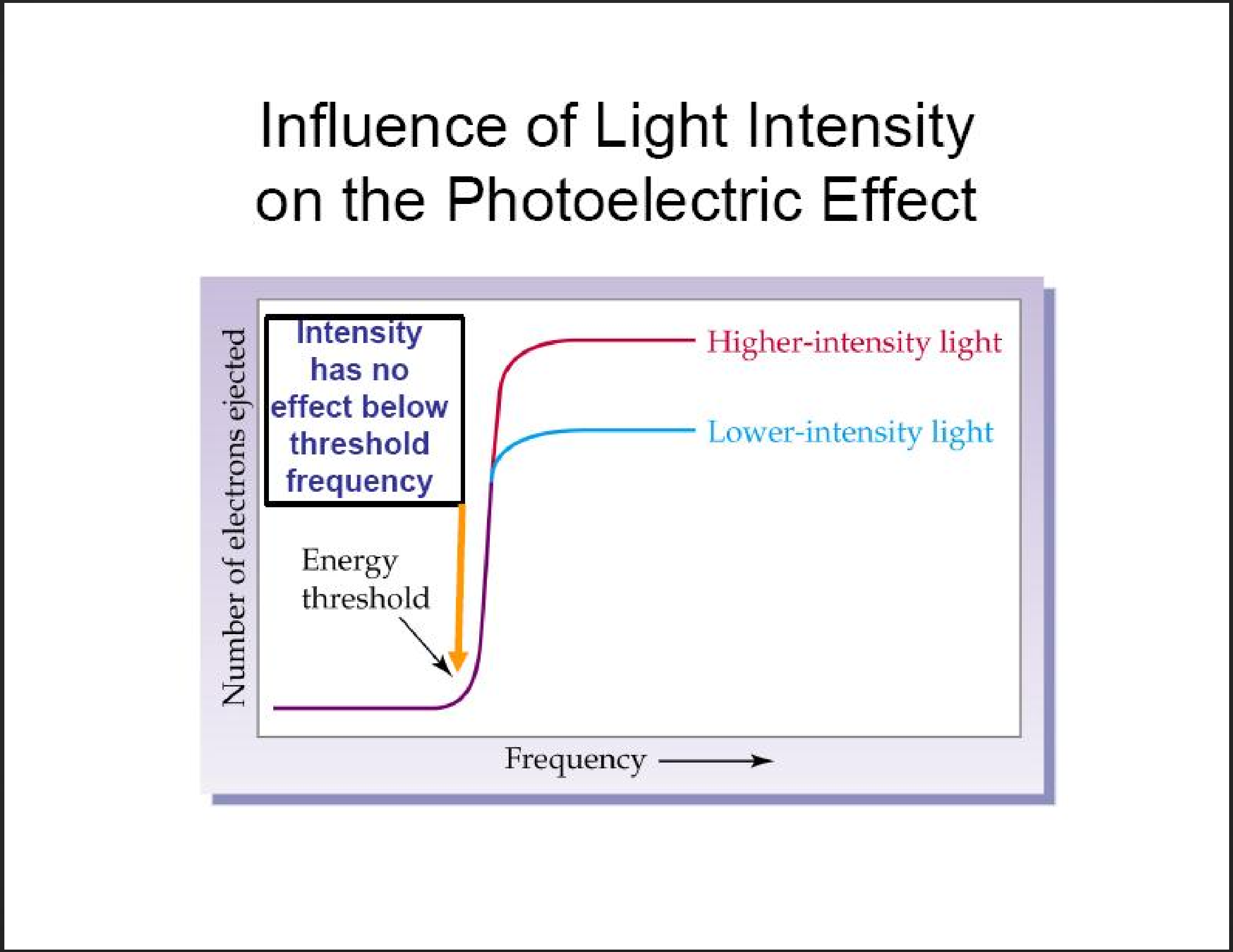
- Planck himself looked for a few years in ways to get h→0 without success.

Basics of Quantum Mechanics
- Photoelectric Effect -

A Photocell is Used to Study the Photoelectric Effect

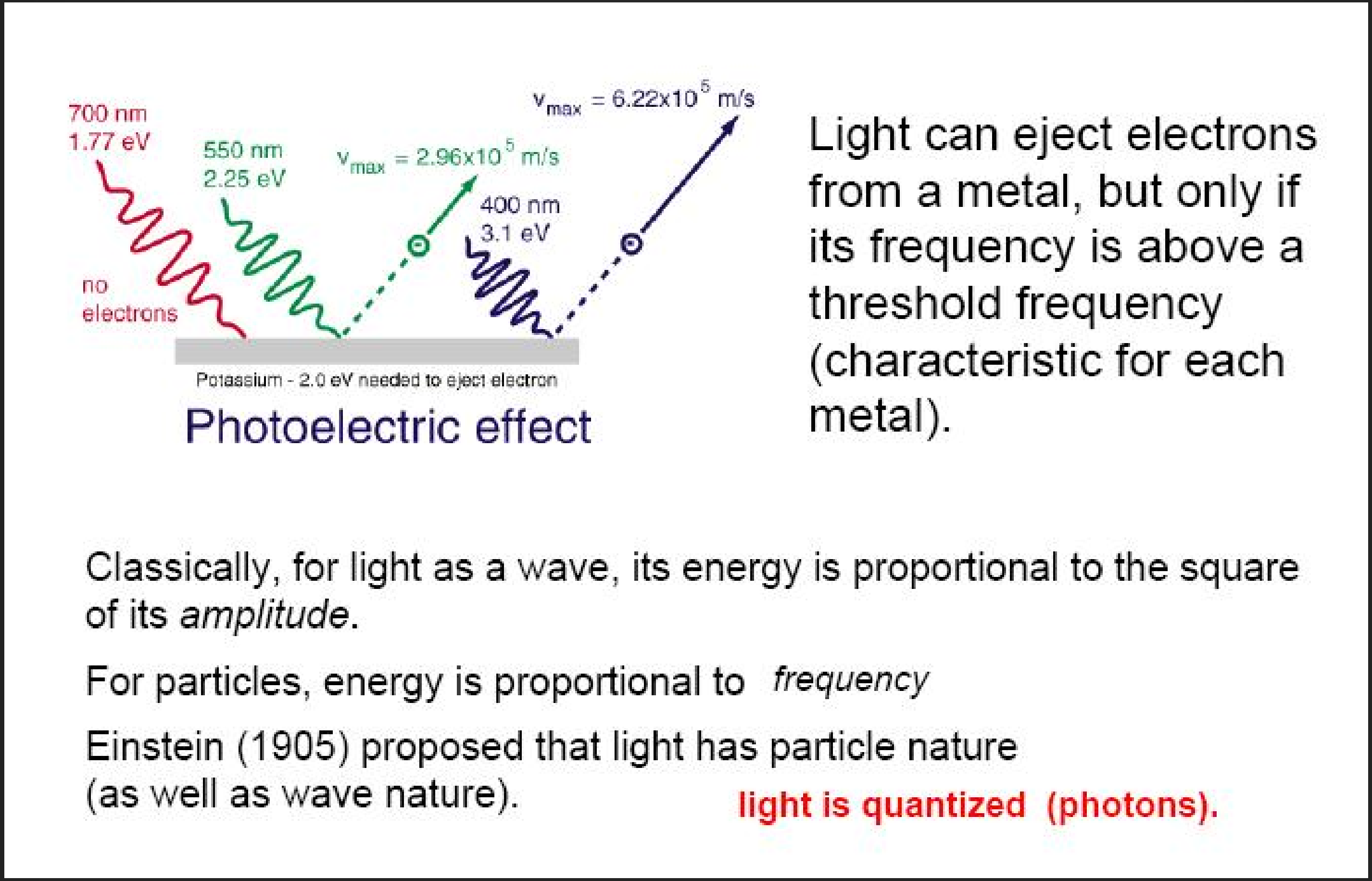


Basics of Quantum Mechanics
- Photoelectric Effect -



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

Basics of Quantum Mechanics
- Photoelectric Effect -



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).

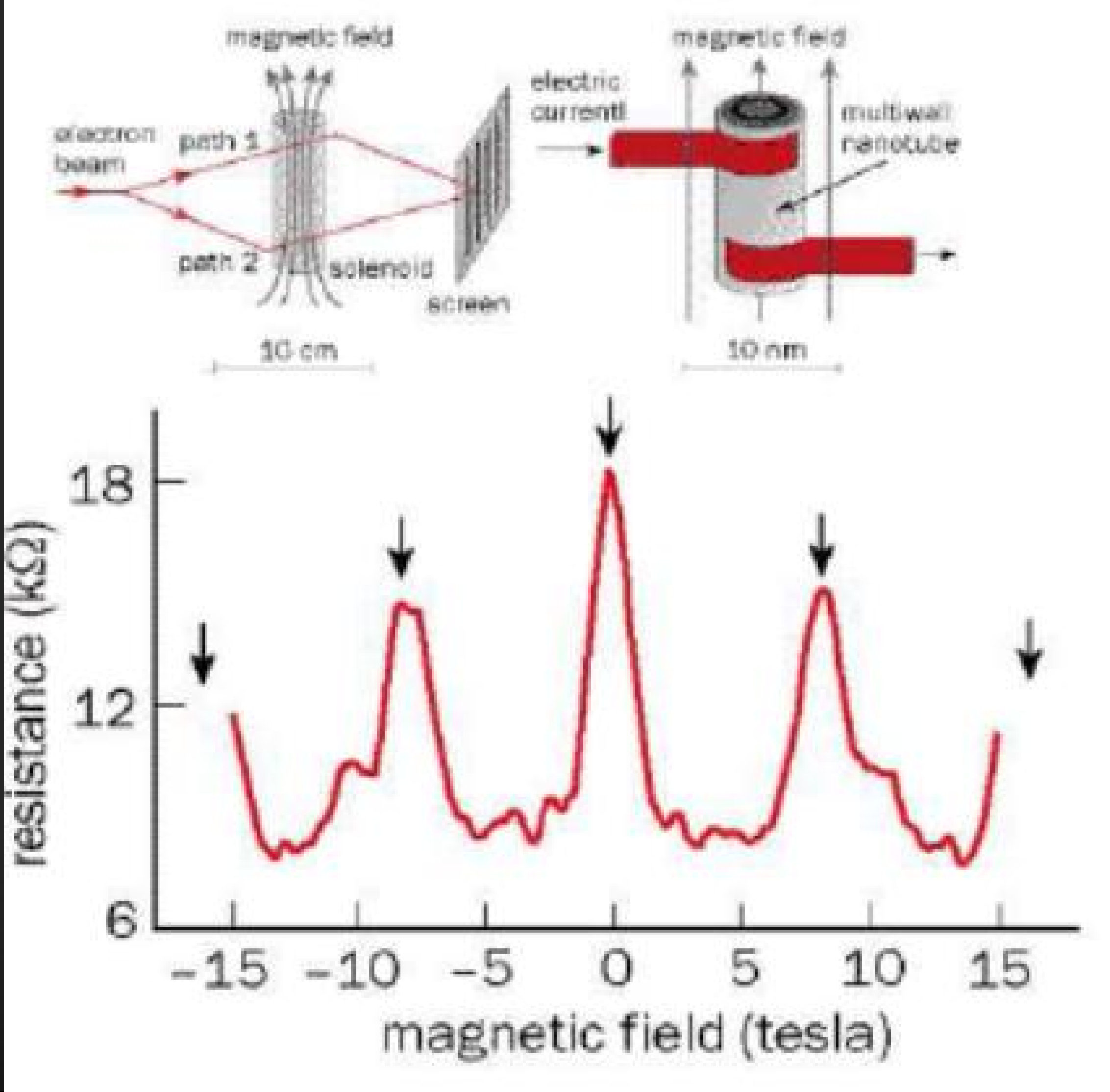
Larger frequency, means smaller wavelength, and larger Energy=hf.

Basics of Quantum Mechanics
- 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.

Particles as waves

Basics of Quantum Mechanics
- Aharonov – Bohm Effect -



Postulates of Quantum Mechanics

Basics of Quantum Mechanics
- 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

Basics of Quantum Mechanics
- First Postulate of Quantum Mechanics -

Quantum physicists are interested in all kinds of physical systems (photons, conduction electrons in metals and semiconductors, atoms, etc.). State of these rather diverse systems are represented by the same type of functions ➔ STATE FUNCTIONS.

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
- **Accesible information ➔** the information we can extract from the wavefunction
- **State function ➔** function of position, momentum, energy that is spatially localized.

Basics of Quantum Mechanics
- First Postulate of Quantum Mechanics -

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 of the system.

Note:

Wavefunction $\psi(x,t)$ ➔ position and time probability amplitude

Quantum mechanics describes the outcome of an 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.

Basics of Quantum Mechanics
- Second Postulate of Quantum Mechanics -

If a system is in a quantum state represented by a wavefunction 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 d*V*.

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.

Basics of Quantum Mechanics
- Second Postulate of Quantum Mechanics -

Therefore, the normalization condition for the wavefunction is:

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

Limitations on the wavefunction:

- 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).

Basics of Quantum Mechanics
- Third Postulate of Quantum Mechanics -

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

Basics of Quantum Mechanics
- 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:

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

- The product of two operators implies succesive operation:

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

- 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:

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

Basics of Quantum Mechanics
- 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:

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

and can be generalized for any pair of observables.

Basics of Quantum Mechanics
- Fourth Postulate of Quantum Mechanics -

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:

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

Basics of Quantum Mechanics
- Fourth Postulate of Quantum Mechanics -

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.