Basics of Quantum Mechanics

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Why we need to study Quantum Mechanics

- Classical mechanics (Newton's mechanics) and Maxwell's equations (electromagnetics theory) are mainly applicable for macroscopic systems.
- Quantum mechanics is used to explain microscopic phenomena such as photon-atom scattering and flow of the electrons in semiconductors.
- 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

- 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.

Quantum Point of View

- Quantum particles acts as both particles as well as wave i.e. show Wave-Particle Duality.
- Quantum state is a collection of variety of possible outcomes of measurement of physical properties.
- Quantum mechanics largely depends on the phenomena of probability.
- QUANTIZATION of energy is yet another property of "microscopic" particles.

Heisenberg Uncertainty Principle

- It is impossible to simultaneously 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.

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)
- Maxwell's theory of electromagnetic radiation can explain these two phenomena, which was the reason why the other theories of light were discarded.

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

Blackbody Radiation

- Given by Max Planck (1858-1947).
- 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 mainly depends on the material.

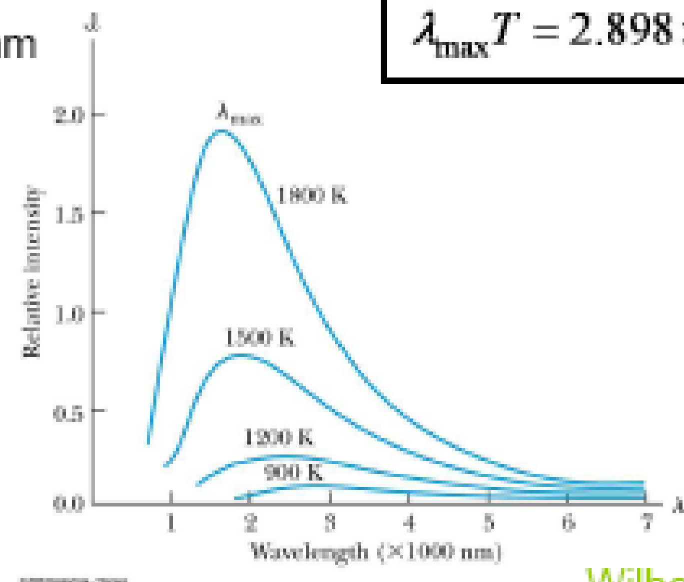
Blackbody

- A material is constantly exchanging heat with its surrounding (to remain at a constant temperature).
- A blackbody is a perfect absorber. Incoming radiations is totally absorbed and none is reflected

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



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

Empirical Formula

Wilhem Wien: Nobel Prize 1911

Stefan-Boltzmann Law

- The total power radiated increases with the temperature:

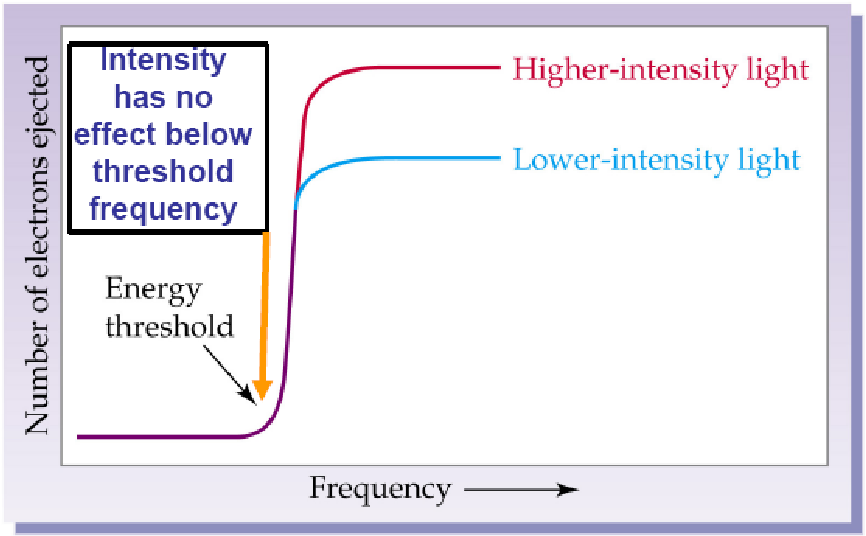
$$R(T) = \int_0^{\infty} \mathcal{I}(\lambda, T)\, d\lambda = \epsilon\, \sigma T^4$$

- 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** (ϵ = 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.

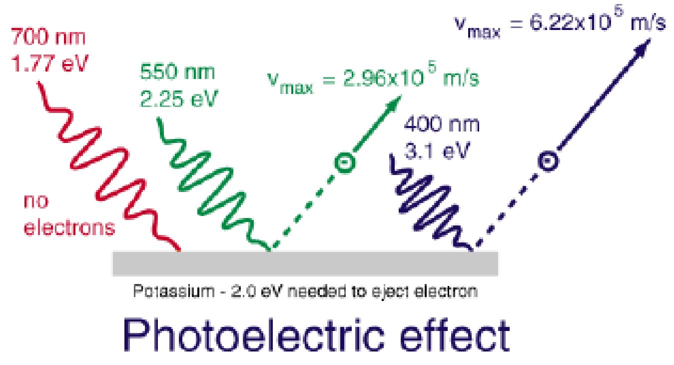
Photoelectric Effect

Influence of Light Intensity on the Photoelectric Effect



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

Basics of Quantum Mechanics - 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 -

- It confirms the particle nature of light and 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.

First Postulate of Quantum Mechanics

Quantum physicists study 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.

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.

- 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.

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*.
- $|\psi(x,t)|^2$ position and time probability density
- 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.

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

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).

Third Postulate of Quantum Mechanics

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

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:

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

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 $\widehat{H}\psi = i\hbar\partial\psi/\partial t$, where $\widehat{H}=\widehat{T}+\widehat{V}$ 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.