DEPARTMENT OF CHEMISTRY

CONTENTS:

Classical Mechanics:

"Classical Mechanics describe the motion of macroscopic objects such as space crafts, planets, stars and glaxies."

The classical Mechanics also known as "Newtonian Mechanics" provides extremely accurate results as long as the domain of study is restricted to large objects and speeds involved do not approach the speed of light.

The classical theories are simple, but this branch of mechanics cannot be applied to extremely small particles moving at very high speed, as the results may be inaccurate.

→ According to NMR Theory the classical Mechanics is:

- based on mass and charge of nucleus.
- Represents the nucleus as a bar magnet.
- Usefull as a pictorial model but has limited theoretical utility.

Introduction:

There are few phenomenon which the classical Mechanics failed to explain.

(i) Stability of an atom

(ii) Spectral series of Hydrogen atom.

(iii) Black body radiations.

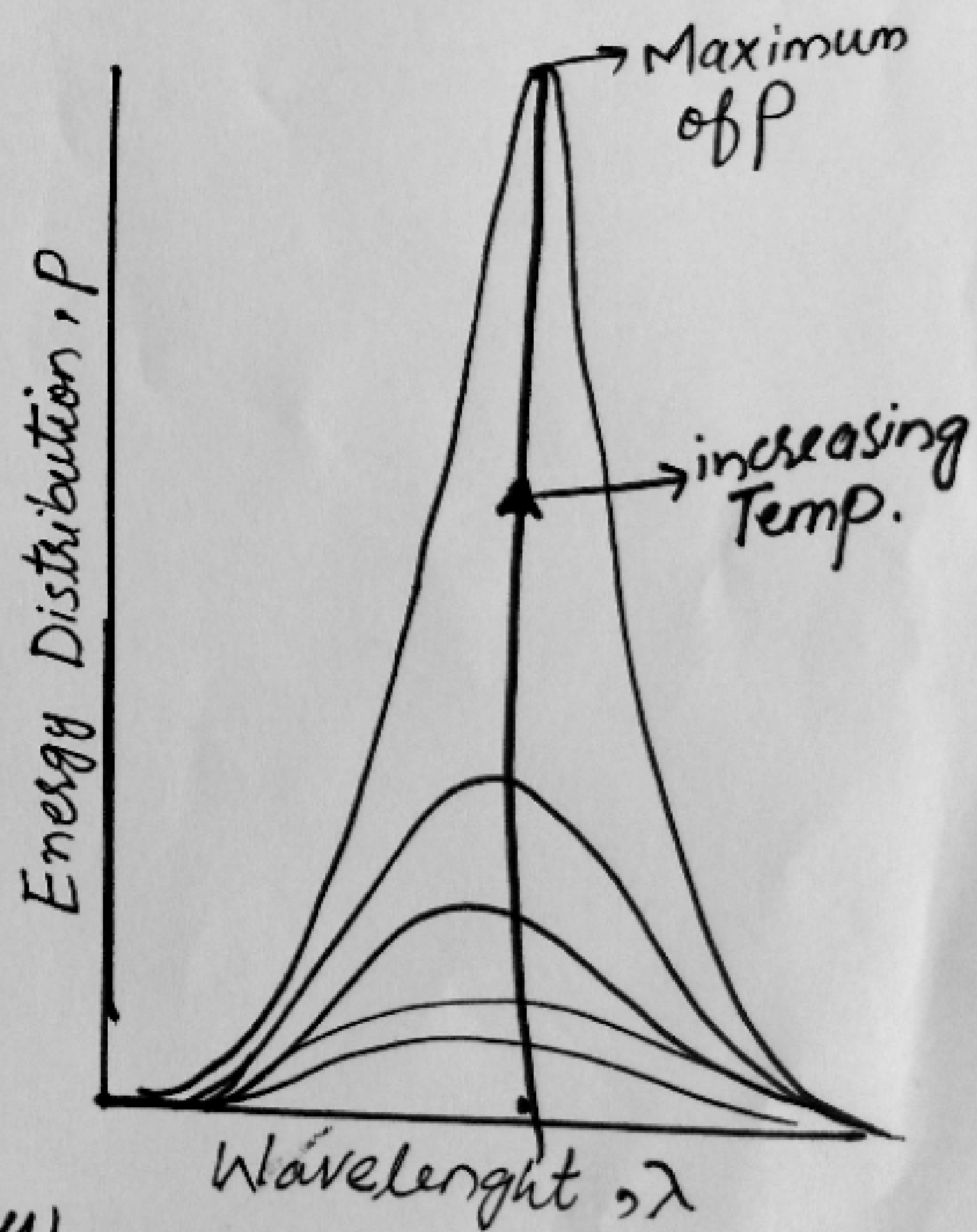
The Failures of classical Physics:

- **Black body Radiation:**
  - A hot object emits light (consider hot metals)
  - At higher Temperature the radiations becomes of shorter wave lenght. (Red → White → blue).
  - Black body: "An object capable of emitting and absorbing all frequencies uniformly"
- **Experimental Observations:**
  - As the temperature raised, the peak in the energy Out-put shifts to shorter wave lenghts.
  - Wien Displacement law.

$$T\lambda_{max} = \frac{1}{5}c_2 \quad (C_2 = 1.44\,cmK)$$

  - Stefan-Boltzmann Law:

$$E = E/V = aT^4 \qquad M = aT^4$$



  - Rayleigh – Jeans law:
    - First attempted to describe energy distribution.
    - Used classical Mechanics and equi-partition principle.

$$dE = \rho d\lambda \quad \left(\rho = \frac{8\pi kT}{\lambda^4}\right)$$

    - Although successful at high wavelenght, it fails badly at low wavelenght.
  - Even cool objects emits visible to UV region.

Quantum Mechanics:

"Quantum mechanics Science dealing with the behaviour of matter and light on the atomic and sub-atomic scale."

- It attempts to describe and account for the properties of molecules and atoms and their constituents, electrons, protons and neutrons etc.
- These properties includes the interaction of the particles With One another and withe Electro-magnetic Radiations (i.e Light, X-Rays and gamma rays).
- Quantum Mechanics deals with the motion of micro-scopic particles or quantum particles.

Introduction:

Quantum mechanics has much more Complicated theories than classical mechanics but provides accurate results for particles of even very small sizes.

- Quantum mechanics handles the wave-particle duality of atoms and molecules.
- Special theory of of relativity by Einstein (1905) deals with particles of extremly small sizes. While General theory of relativity by Einstein (1916) can be used to study all particles in general. i.e. Even particles of macroscopic sizes.

Following **Essential ideas** are used in Quantum Mechanics.

(1) **Uncertainity Principle:**

Conjugate quantities of particles (For exemple. Position and momementum) Cannot be known simultaneously with in a certain accuracy limit.

(2) **Quantization:**

The measurements of a physical quantity in a confined system results in quanta (The measured values are discreate.

(3) **Wave-particle Duality:**

All particles can be described as waves (travelling both in space and in time). The state of a particle is given by a wave-function ψ.

(4) **Extrapolation to classical Mechanics:**

The laws of classical newtonian Mechanics are the extrapolation of the laws of quantum mechanics for large systems with very large number of particles..

Difference between classical and Quantum Mechanics.

• **Introduction:**

The difference between quantum and classical physics is the difference between ramp and a staircase.

• In classical mechanics, events (in general) are continuous, which is to say they move in smooth, orderly and predicable patterns.

Projectile motion is a good exemple of classical mechanics. Or the colours, of the rainbow, where frequencies progress continuously from red through violet.

Events, in other words, proceed incremently up a ramp.

• In quantum mechanics, events (in particular) are unpredictable, which is to say "jumps" occur that involve seemingly random transitions between states : hence the term "quantum leaps" More Over a quantum leap is an all or nothing proposition, sort of like jumping from the roof of One building Onto another. You either make it or you break it.

Events in the quantum world, jumps from One stair to the next and are seemingle dis contiuous

For exemple, Transitions in electrons between energy levels in an atom by making quantum leaps from One level to the next.

Some **Common differences** between classical and quantum mechanics are given below.

Classical Mechanics	Quantum Mechanics
(i) It deals with macroscopic particles.	(i) It deals with microscopic particles.
(ii) It is based upon Newton's laws of motions.	(ii) It takes into account's Heisenberg uncertainity principle and de-Broglie concept of dual nature of matter.
(iii) It is based on Maxwell's electromagnetic wave theory according to which any amount of energy ~~can~~ may be absorbed or emitted continuously.	(iii) It is based on plank's Quantum theory according to which only discrete values of energy are emitted or absorbed.
(iv) The state of system is defined by specifying all the forces acting on the particles as well as their positions and velocities (moment). The future state can be predicted with certainity.	(iv) It gives propabilities of finding the particles at various locations in space.
(v) Partical state is described by six numbers x, y, z, P_x, P_y, P_z in given time.	(v) Particle state is fully described by complex functions ($\psi_{(x,y,z)}$) given in whole space.

(vi) Time dependent of state is described by Hamilton's equation. $dr/dt = \partial H/\partial p \quad dp/dt = -\partial H/\partial r$	(vi) Time dependent of state is described by Schrodinger equation. $i\hbar \partial \psi/\partial t = \hat{H}\psi$ where $\hat{H}$ is Hamilton Operator.
(vii) Quantities x and p describing states are directly measurable.	(vii) Function ψ is not directly measurable quantity
(viii) Classical Mechanics is dynamical Theory.	(viii) Quantum mechanics has stochastic character. Values of $\lvert\psi(r)\rvert^2$ gives propability of particle presence in the point r. Physical quantities are their mean values.

Explained Differences

- Classical physics is casual, compelete knowledge of past allows computation of future. Compelete knowledge of future allows precise computation of past.
- Not so in "Quantum physics" Objects in quantum physics are not particles nor waves, they are a strange combination of both.
- In classical physics: two bombs with identical fuses would explode at the same time. In Quantum physics two absolutly identical radioactive atoms can and generally will explode at very different times.
- Most physicists beleive that quantum physics is the right theory, even though many details are yet to be worked out, Classical physics can be derived from quantum physics in the limit that the quantum properties are hidden. that fact is called correspondence principle.

The differences between classical and Quantum mechanics can be given as follows.

For classical physics/Mechanics:

According to classical mechanics:

(1) Particles and feilds possess well defined dynamic Variables at all times:

Dynamic variable are the quantities used to describe the motion of objects, such as

position velocity, momentum and energy.
Classical physics presupposes that the dynamic Variables are well defined and can be measured to perfect precision.

According to Quantum mechanics:

- Particles posses a wave function (ψ) at all Times.

The wave function assign a complex number to each point in space at each moment in time. This function contain with in it all information about the particle. Everything that can be known about particle's motion is extracted from $\psi(x,t)$. To recover dynamic information we use Born's rule and calculate $\psi\psi_*$ to get the propability density of particle's position and we calculate $\phi\phi_*$ to get the propability density of particle's momentum.
This is the different approach than the classical mechanics.

(2) In Classical Mechanics,

- Particles as point-like objects following Predictable Trajectories.

In classical mechanics, a particle is treated as dimensionless point. This point travels from $A \rightarrow B$ by tracing out a continuous path through the intermediate space. A billiard ball traces out a straight line as it rolls across the table. The idea of definite trajectory well defined the dynamic variables. The idea of definite trajectory must be discarded as well..

In Quantum Mechanics:

- <u>Trajectories are replaced by wave function Evolution:</u>

As the wave function changes in time, so do the propabilities of observing particular position and momentum for the particle.

The evolution equation is time dependend Schrodinger equation

$i\hbar\Psi_{(x,t)} = H\Psi_{(x,t)}\, i\hbar\Psi_{(x,t)} = H\,\Psi_{(x,t)}$. 'H' is the Hamiltonian operator for the system i.e a self-adjoint Operator corresponding to total energy of the system.

(3) In classical Mechanics.

- <u>Dynamic Variables as Continuous real numbers:</u>

In classical physics, dynamic variables are smoothly varying continuous values.

According to Quantum Mechanics.

- <u>Dynamic variables are Hermitian metrices:</u>

Instead of real values, continuously evolving dynamic variables. Schrodinger uses fixed

Hermitian metrices (or self adjoint operators) to represent ~~dyno~~ observable quantities. Each observable such as position, momentum energy etc. has a corresponding operator.

The Eigen values of the operators determine the allowed values of corresponding observable. The energy levels of atoms ~~are~~ for example are eigen values of Hamiltonian operator.

(4) In classical Mechanics.

- **Particles and waves as seperate Phenomenon:**

Classical Physics has One framework for particles and a different framework for waves and feilds. It ~~ca~~ means that a billiard ball and a water waves move in a very different fashion from A ⟶ B.

According to Quantum Mechanics.

- **Unification of particles and waves:**

A mathematical analysis of schrodinger analysis reveals that it has wave like solution and particles behave ~~ф~~. Propagate as waves. This means we should not picture particle as Tiny spheres bouncing around their environment. The closest you can get to visualizing a particle is by visualizing its wave function

According to classical Mechanics.

(5) Newtons Second Law:

With out the four kinemetic features mentioned above $\sum F = ma$ is more than wrong, it's nonsensical. A radically different dynamics must be developed that is governed by a very different equation of motion.

In Quantum Mechanics

- **The time dependent schrodinger wave equation replaces Newton's Second law.**

Schrodinger wave equation:

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

$$i\hbar \frac{\partial^2 \psi}{\partial x^2} = \hat{H}\psi$$

$$E\psi = \hat{H}\psi$$

$\hat{H}$ → Hamiltonian Operator.

In classical Mechanics

(6) Predictability of measurement outcomes.

In classical physics the outcomes of measurements can be predicted perfectly assuming full knowledge of system beforehand.

In Quantum Mechanics, even if you have full knowledge of the system, the outcomes of certain measurents are impossible to Predict.

- ## Measurement is Random:

In quantum mechanics, even if you have full knowledge of a quantum system prior to measurements i.e $\psi(x,t)$ you still will not able to predict the outcomes of measurements in general. The Outcome of the measurement is probabilistic. The possible outcomes are determined by eigenvalues of the operator you are observing and probability of each outcome is determined by the projection of the wave function onto the eigenvector of that operator.

Some other **Important differences** between classical and Quantum Mechanics are given below.

Difference between Classical physics and Quantum Physics.

Classical Mechanics.	Quantum Mechanics.
(i) **Determinism** If the initial state is known, One can predict the physical state at another moment of space-Time. The classical object is localized in space time and is used to describe reality.	(i) **Indeterminism:** It is impossible to assign a well defined trajectory to a quantum particle. The quantum particle is not localized in space Time and is part of reality.

(ii) **Reality:**

The is One level of reality, the empirical (physical) reality.

(ii) **Levels of Reality**

There are multiple levels of reality, including the empirical, that are accessible to humans due to the existance of Multiple Levels of perception.

(iii) **Continuity:**

One cannot pass from One point of space and time with out passing through all intermediate points.

(iii) **Discontinuity**

Between Two points their is nothing. Save for the quantum notion of the vaccum, a gap of potentialities.

(iv) **Relativity:**

~~Relativity~~ Reality is single referential, the doctrine that measurements and preceptions are true only in relation to a given observer at a given place and time.

(iv) **New Relativity:**

Reality is multi-refrential, no level of reality constitutes a priviledge place from where One could understand all the other levels of reality.

(v) **Resistance:**

To oppose, experience unwillingness and/or unresponsiveness to movement (change in state of motion or rest).

(v) ~~Re~~ **Non-Resistance**

Become Open to other prespectives, ideologies value premises and belief systems, inherently letting go of aspects.

<u>Quantum Mechanics</u> is able to describe

(1) Photo-electric effect.

(2) Black body radiation.

(3) Compton effect.

(4) Emission of line Spectra.

where the Classical Mechanics cannot explain all these phenomenon.

The most outstanding development in modern science was ~~Quan~~ the conception of Quantum mechanics. This new approach was highly successfull in explaining about the behaviour of atoms, molecules and nuclei.

De Broglie Waves:

The Quantum mechanics follows the concept of De-Broglie i.e every particle which may be electron, proton etc.. exhibit wave-particle dual nature.

Energy of photon is

$$E = h\nu$$

for a particle, mass 'm'

$$E = mc^2$$

$$mc^2 = h\nu$$

$$mc^2 = \frac{hc}{\lambda}$$

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

Suppose a particle of mass 'm' is moving with velocity 'v' then the wavelenght is given by

$$\lambda = \frac{h}{mv} \quad \text{or} \quad \lambda = \frac{h}{p}$$

- De-Broglie wave does not depend on whether the moving particle is charged or uncharged. It means matter waves are not electromegnetic in nature.

- ## Heisenberg Uncertainity Principle.

In classical mechanics the position and momentum of particle is certain. but in Quantum mechanics the position and momentum of a particle is uncertain

According to Heisenberg Uncertainity principle.

"It is impossible to measure both the position and momentum simultaneously with unlimited accuracy"

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2} \qquad \because \hbar = \frac{h}{2\pi}$$

$\Delta x \rightarrow$ Uncertainity in position

$\Delta p_x \rightarrow$ Uncertainity in momentum.

The product of $\Delta x, \Delta p_x$ of an object is greater than or equal to $\frac{\hbar}{2}$.