Quantum Mechanics

In the late seventeenth century Newton discovered classical mechanics .

The laws of motion of macroscopic objects . In the earth twentieth century physicists found that classical mechanics does not correctly describe the behavior of very small particles such as the electrons and nuclei of atoms and molecules .

The behavior of such particles is described by a set of laws called quantum mechanics.

Quantum chemistry applies quantum mechanics to problems in chemistry

The influence of quantum chemistry is evident in all branches of chemistry .physical chemists use quantum mechanics to calculate thermodynamic properties (for example , entropy , heat capacity) of gases , to interpret molecular spectra ,thereby allowing experimental determination of molecular properties (for example , bond lengths and bond angles , dipole moments , energy differences) to calculate molecular properties theoretically :to calculate properties of transition states in chemical reactions , thereby allowing estimation of rate contants to understand intermolecular forces, and to deal with bonding in solids .

The development of quantum mechanics began 1900 with planck study of the light emitted by heated solids so we start by discussing the nature of light.

Max planck developed a theory that gave excellent agreement with the observed black body –radiation curves and assumed that the atoms of the black body could emit light energy only in amounts given by hv. Where v is the radiations frequency :

$v = c / \lambda$	$\lambda v = c$

h is planck constant	$=6.6 \times 10^{-34}$ J.s
C is speed of light	$=2.99 \times 10^{8}$ m/s
λ	wave length
1 nm	$= 10^{-9}$ m
$1^{0}A$	$= 10^{-10}$ m

In 1905 Eintein showed that these observations could be explained by regarding light as compased of particlelike entities called photons with each photon having an energy .

$E._{photon} = h\nu$

In the late nineteenth century , investigations of electric discharge tubes and natural radioactivity showed that atoms and molecules are composed of charged particles .

Electrons have a negative charge .the proton has a positive charge equal in magnitude but opposite in sign to the electron charge and is 1836 times as heavy as the electron.

The third constituent of atoms, the neutron is uncharged and slightly heavier than the proton.

The chemical properties of atoms and molecules are determined by their electronic structure, and so the question arises as to the nature of the motions and energies of the electrons.

Since the nucleus is much more massive than the electron we expect the motion of the nucleus to be slight compared with the electron motions .

Quantum Mechanics: including quantum field theory in a fundamental theory in physics which described nature at the smallest scales of energy levels of atoms and subatomic particles.

Quantum Mechanics cannot predict the exact location of a particle in space only the probability of finding it at different locations.

Coordinates Systems

1-Cartesian Coordinates

2-Spherical polar Coordinates

3-Cylindrical Coordinates

4-Confocal ellipsoidal Coordinates

1-Cartesian Coordinates

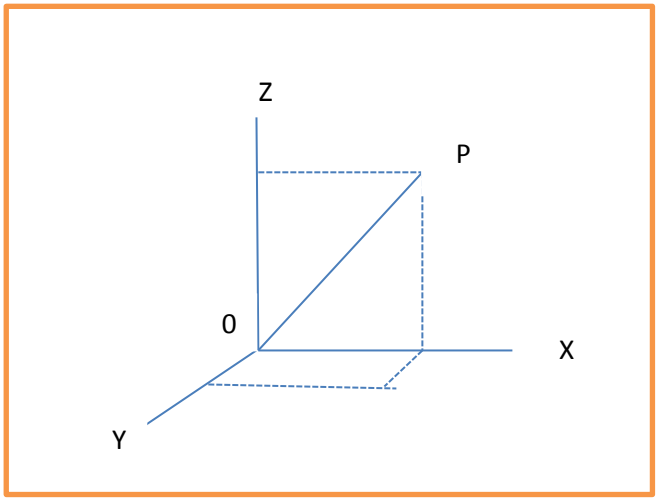
Position any point in space .

dt=dx dy dz

$-\infty \leq X \leq +\infty$

$-\infty \leq Y \leq +\infty$

$-\infty \leq Z \leq +\infty$



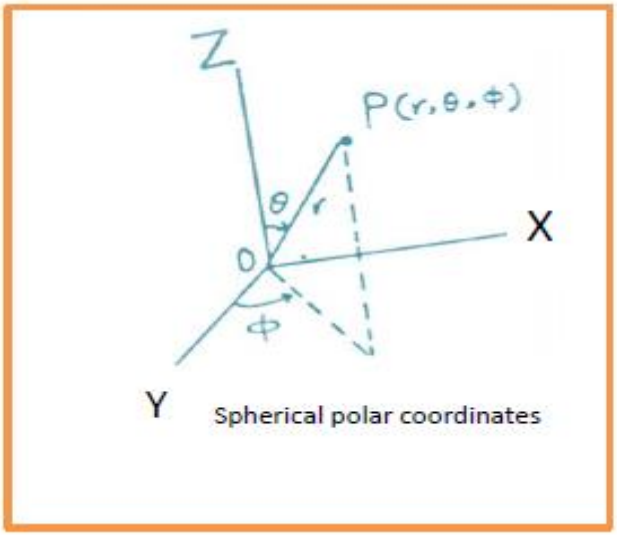
2-Spherical polar Coordinates

Point in space determined (r) the radius , Θ the colatitude , and ϕ the azimuth .

$0 \leq r \leq +\infty$

$0 \leq \Theta \leq \pi$

$0 \leq \phi \leq 2\pi$



$X = r \sin \Theta \cos \phi$

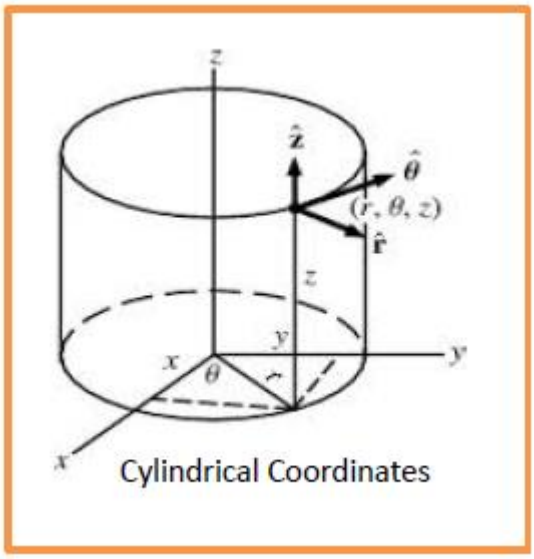
$Y = r \sin \Theta \sin \phi$

$Z = r \cos \Theta$

$dt = r^2 \sin \Theta \, dr \, d\Theta \, d\phi$

3- Cylindrical Coordinates

Determinate two distance and angle (r, Z, ∅)



Cylindrical Coordinates

$0 \leq r \leq +\infty$

$0 \leq \phi \leq 2\pi$

$-\infty \leq Z \leq +\infty$

$X = r \cos \phi$

$Y = r \sin \phi$

$Z = Z$

$dt = r\, dr\, d\phi\, dZ$

Example 1: Equation to change from Cartesian to spherical ?

$$x = r \sin\theta \cos\phi$$
$$Y = r \sin\theta \sin\phi$$
$$z = r \cos\theta$$

Example 2: Equation to change from Cartesian to : Cylindrical?

$$x = r \cos\phi$$
$$y = r \sin\phi$$
$$z = z$$

.....