Ministry of Higher Education
and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

- Second lecture -

Stage 4

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Eigen value equation

In quantum mechanics, some physical amounts can possess certain values, i.e. there are values allowed, as experiments show, so it's called eigen value.

Necessary sports accountability To find certain subjective values are called self-worth accountability and are formulated in an equation called Eigen value equation And write In the following form

$$\hat{P} f = a f$$

where

- a - Eigen value
- P^- Differential opearators
- F- Function

This equation is characterizedby its containing the same function on both ends [f]

A group of Eigen -functions can have the same Eigen-value, for example.

The three functions

$P^\wedge f_1 = a\ f_1$

$P^\wedge f_2 = a\ f_2$

$P^\wedge f_3 = a\ f_3$

This Eigen value is called degenerate and in the case of a number of Eigen functions called the degree of degenerate

*It is a number of different functions that, if influenced by the same operators, give similar energies.

Like the energy-equal orbits .

So we deduce the eigen -function when a mathematical effect operators a particular function, it often leads to the production of a new function, for example.

1_ $\frac{d}{dx}$ $\sin_\theta = \cos\theta$

So $\sin \emptyset$ it's a function that's not eigen to the worker. $\frac{d}{dx}$

2- $\frac{d}{dx}\cos\times = -\sin\times$

∴ The function $\cos x$ is not eigen -contained for the worker. $\frac{d}{dx}$

But in other cases, the differential output is the same function multiplied by the constant, such a function is called a eigen function of the operators, i.e. any function such as [f]is a eigen function of the effectsuch as p^

If it achieves an equation in the following way

$$\hat{P}f = af$$

a eigen function of the operators

Q/Prove that the function e^{ax}eigen value for$\frac{d}{dx}$

Sol/

$\frac{d}{dx}$ ^{xa}e =ae^{ax}

It is a eigen -function of the worker $\frac{d}{dx}$ because the same eigen -value was obtained

Coordinate systems

Lend classifies a point, curve or surface in space } vacuum{ it is used to simplify mathematical equations and exist in types.

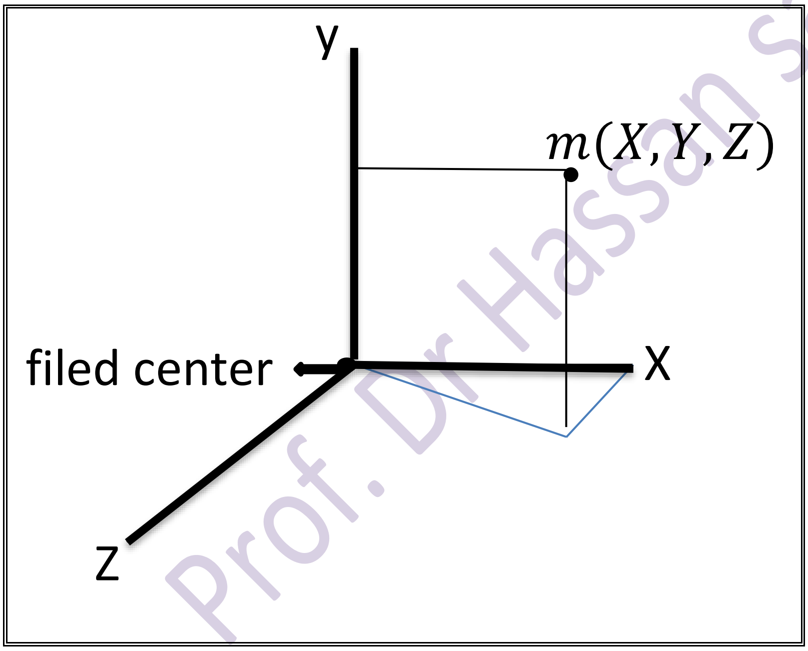
1- dynamic coordinates or cartesin coordinate

2. Spherical polar coordinate

3. Cylindrical coordinate

4. Eilptical coordinate

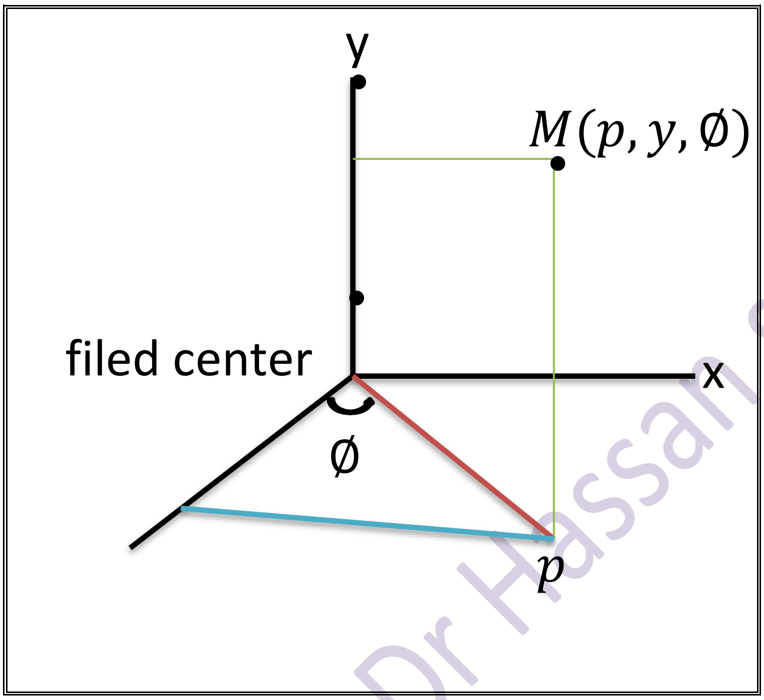
1- Dynamic coordinate (three axes) three axis



A point such as M is described by distances located in the direction of three perpendicular axes, X.Y.Z. where the M point(X.Y.Z) has a point away from the coordinate center (0) in the direction of the three axes (X.Y.Z).

-2 Cylindrical coordinate

Tow dimentional and one angle



*Any point such as M is assigned by two distances: (P.y),angle (Ø)confined between theaxis(Z) and the *drop of the line* P (OP) *in the level* (Zy)

The relationship between cartesian and cylindrical coordinates is

$Z = p \cos \emptyset$

$x = p \sin \emptyset$

$y = y$

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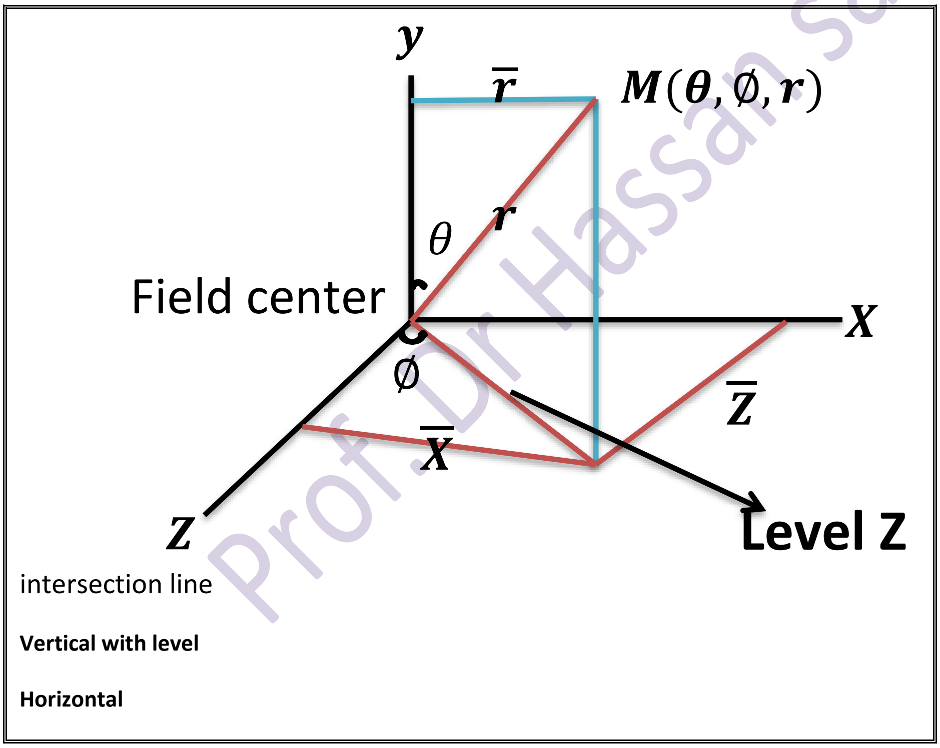
3. *Spherical polar coordinate*

Tow angle and one dimentional and one after one



Quantu

It is the process of describing a point using two angle and distance. One angle and the other angle (p$o$and axis (y) are confined between the axis ()θwhich is

(x.y.z)The three coordinates are related to (ø)

It's called where (p) is drawn from the point of origin to (op)where the line

(Ø Polar angleiscalled the polar angle. θØ

Azimuthal in the toxic ankle

In OPand Muscat (Z)where this angleis confined between the axis

So you should note the dimensions of the threechanges (Xy)level

1- Represents the radius of the ball through which the size of the ball determines the size of the ball -: r

$0 \leq r \leq +\infty$

2- And it's the angle that determines any of the ball rings: θangle

$0 \leq \theta \leq 180(\pi)$

3- Is the angle that determines the location of the body on the ring-: $\emptyset$ angle

$0 \leq \emptyset \leq 2\pi$

The Cartesian modernism to Convert,so it can be converted

Spherical coordinates instead of the following equations

1: Z= $r \sin\theta \cos\emptyset$

2: X =$r \sin\theta \sin\emptyset$

3: y= $r \cos\theta$

Ex //

Z=$r \sin\theta \cos\emptyset$

Prove that

$\cos\emptyset = \frac{\text{المجاور}}{\text{الوتر}}$. $\frac{adja\ \ cent}{tenson}$

$$\cos \emptyset = \frac{z}{ř}$$

$\therefore Z = ř \cos \emptyset$ —— 1

$$\sin \theta = \frac{\text{المقابل}}{\text{الوتر}} \frac{interviewer}{tenson}$$

$\sin \theta = \frac{ř}{r} \rightarrow ř = r \sin \theta$ —— 2

2 Substitute in 1

$$\mathbf{Z = r \sin \theta \cos \emptyset}$$