Quantum Chemistry

-First lecture-

Quantum Chemistry

Reference

Principle of Quantum Mechanic (Dr. Salam . M 1982)

Fundamental of quantum chemistry and spectrum (Dr. Essam . A 1990)

Quantum Chemistry and Molecular spectroscopy 1. Dr. Qais Abdul Karim 1988.

Quantum chemistry and molecular spectrometer.

Dr. kais A,K Ibrahim 1988.

Quantum Chemistry quantum chemistry Dr. Mohammed Saleh 1982.

P.W. Atkins 1988.

we studying in the course

1. Mathematical and physical foundations.

The origin of quantum theory.

Quantum theory hypotheses.

Solutions to the Schrodenker equation.

Mathematical and physical foundations

1. Mathematical and physical foundation

General Introduction

The purpose of the basic principles in mathematics and quantum physics is to know (function and its types, calculus, coordinates and types, opeartors, linear algebra, eigenvalue -function and eigenvalue -worth).

In quantum mechanics, you need three things.

(function, opeartors, eigenvalue).

a. function

A mathematical expression that contains one or more variables and its value depends on the value of the variables receiving, for example.

1)$2x+1$ A function based on one variable which is x

2)x^2+2y Depends on two variables x, y So you should note.

$y=2x+1$

Thus, the function depends on two independent and non-independent variables. $\therefore y=f(x)$

So it's a function of.yx

For example, if energy is a function of pressure and temperature.

$$E = f(p, T)$$

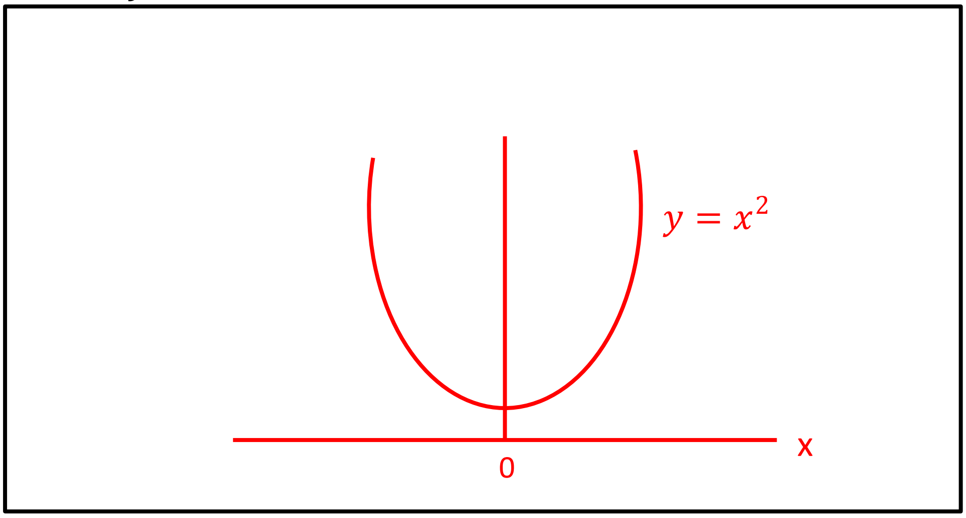
Function types: - 1.

Continuous function

$y = x^2$

dy

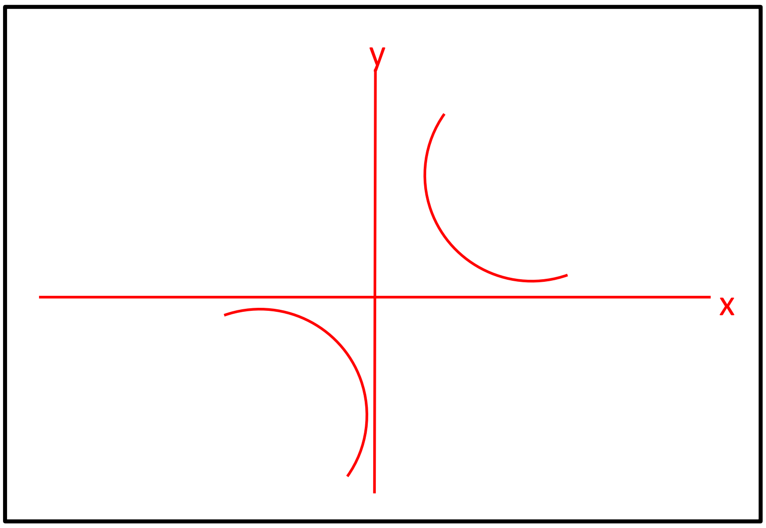
$\_\_\_ = finit\ dx$



2. non-continuous function

$$y = \frac{1}{x}$$

$$\frac{dy}{dx} = \infty$$

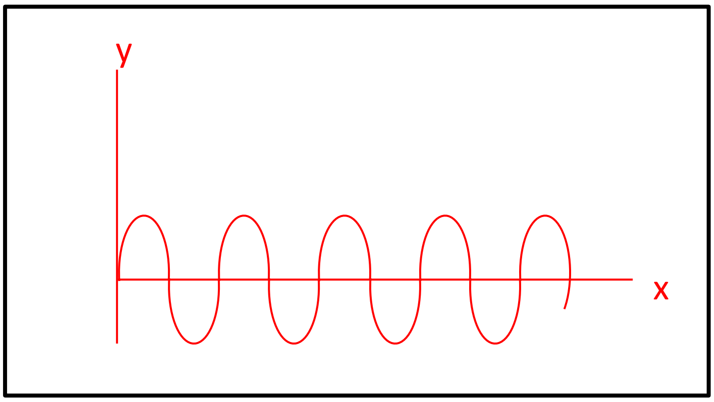


3. periodic and continuous function

A continuous periodic is inside the sin angle and selected.

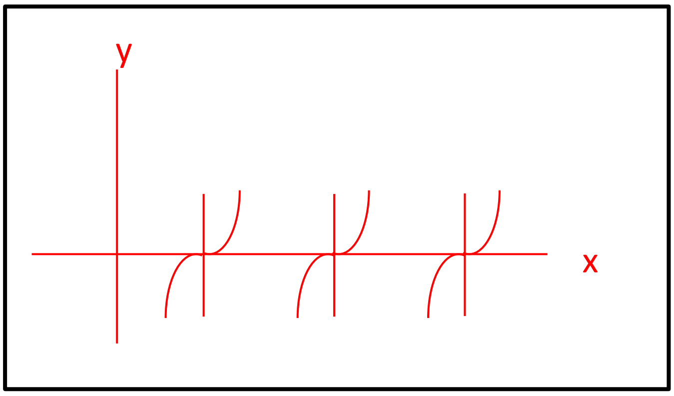
$$y = \sin(\mathrm{x})$$

$$\frac{dy}{} = finit\ dx$$



4. periodic and dic Continuous function

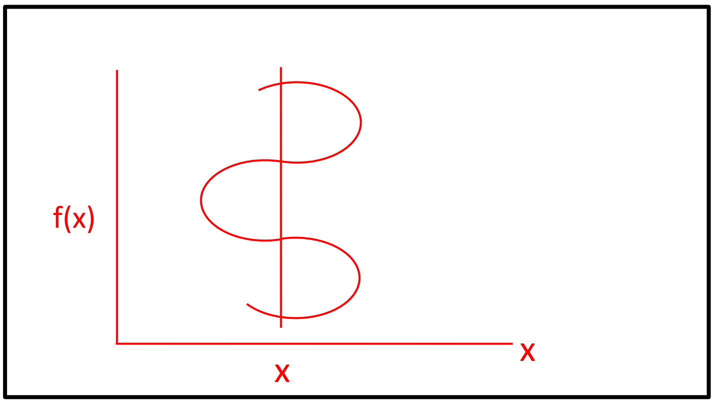
$y = \tan(x)$



5. accept able function

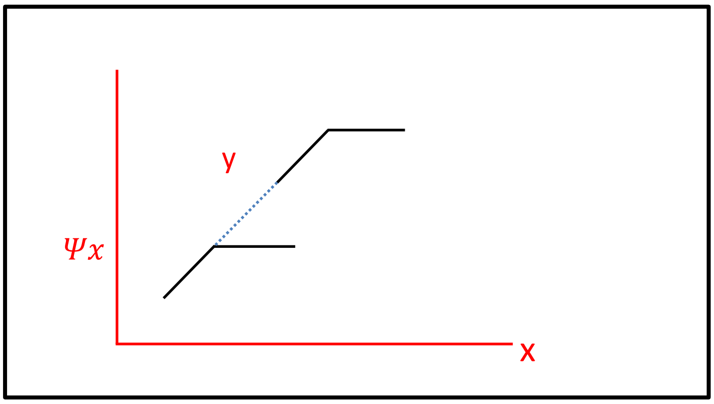
It is a function consistent with the physical reality to which the following conditions must apply:

a) Being one-value for any point means that the function does not bend over itself as in the following drawing:

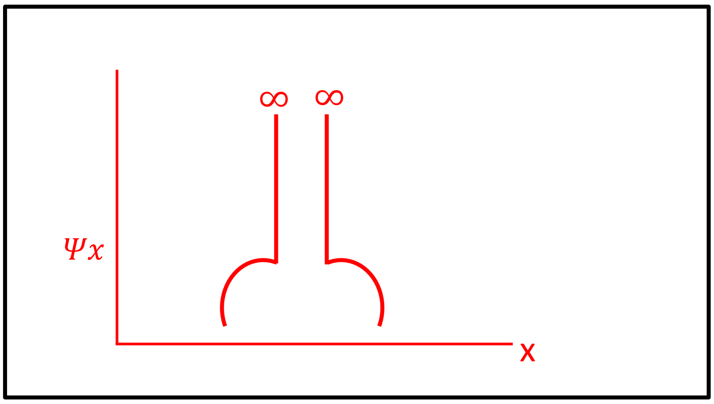


An unacceptable function because it cannot exist in more than one place and because it bends over itself and therefore has more than one value at the same location (x).

b) The function should be continuous as well as itsslope, i.e. the second derivative continues as in:



c) To be infinity and to have an integratable box as in:



b. Differential

The rate of change and we need in quantum chemistry represents the rate of change in electronic density with the distance $(r)$from the nucleus. $\left(\frac{dP}{dr}\right)$

For example, the following function can be found the first differential and the second differential where the

$y = x^2 + 1$ ______1

$\rightarrow x + \Delta x$ Change in x

} ____(2)

$\rightarrow y + \Delta y$ Change in y

Substitute 2 in 1

$y + \Delta y = (x + \Delta x)^2 + 1$ ____(3)

$$y + \Delta y = \underbrace{x^2 + 2x * \Delta x + \Delta x^2 + 1}_{y} \_\_\_\_(4)$$

Since y= x^2+1

$$\therefore y + \Delta y = y + 2x\Delta x + \Delta x^2 \_\_\_\_ 5$$

$$\Delta y = 2x\Delta x + \Delta x^2 \_\_\_\_(6)$$

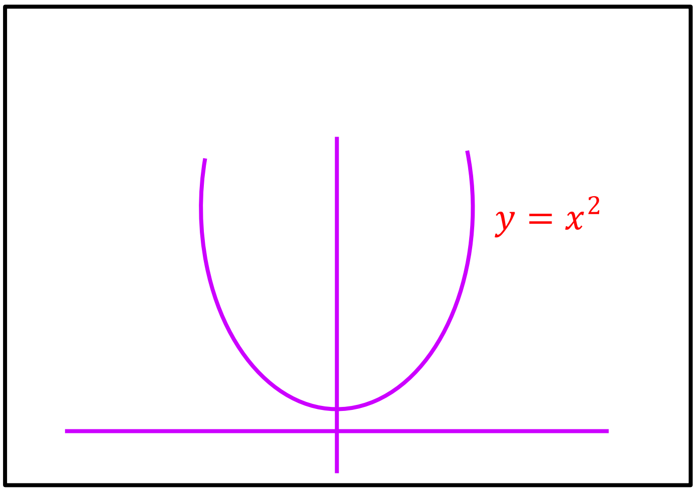
And by dividing Δx

$\frac{\Delta y}{\Delta x} = 2x + \Delta x$ A small value that can be neglected →

First differentiation $= \frac{\Delta y}{\Delta x} = 2x$ or $y' = 2x'$

The second differential is a positive value

$y'' = \frac{\Delta^2 y}{\Delta x^2} = 2$ or $y'' = 2$



Partical Differential

In this case, molecular differentiation represents two or more variables (i.e. when the function contains more than one variable), for example energy is a function of pressure and temperature to find molecular differentiation.

$$E = f(p, T)$$

$$dE = \left(\frac{dE}{dp}\right)_T dp + \left(\frac{dE}{dT}\right)_p dT$$

c. Plural and multiplication symbols product and summation symbols

In plural and multiplication codes, they are used to simplify the writing of collections and multiplications, which are as follows:

a) $\boldsymbol{Sigma} \sum \boldsymbol{summtion}$

gather$X = a_1 + a_2 + a_3 + \cdots + a_n$

$$X = \sum_{i=1}^{n} a$$

ex//

$$X = \sum_{i=3}^{6} a$$

$$\sum_{i=3}^{6} a_3 + a_4 + a_5 + a_6$$

One of the most important characteristics of plural codes is:

a) $\sum^{n}{}_{i=1} Cai$ C = Constant

*When there is a hard conveys out of the plural limits

$$X = c\sum_{i=1}^{n} ai$$

b)

$$\sum_{i=1}^{n}(ai + bi) = \sum_{i=1}^{n} ai + \sum_{i=1}^{n} bi$$

$$\sum_{i=1}^{n}(ai - bi) = \sum_{i=1}^{n} ai - \sum_{i=1}^{n} bi$$

b) Multiplication code (∏) product

It is symbolized by(∏).

$$y = a_1 * a_2 * a_3 \dots . a_n$$

$$y = \prod_{i=1}^{n} a$$

ex//

$$y = \prod^{3} i^2$$

$$i=1$$

Borders from 3

$$y=\prod_{i=1}^{3}(1)^2*(2)^2*(3)^2$$

d. complex number

It's the number that contains its symbol, the $(\sqrt{-1})$ complex number consists of two molecules, a real part, and an imaginary part that contains so$(i)(\sqrt{-1})$

$$C=A+iB$$

Compou

immajonray part

real part

$$if\ iB\neq 0\ then\ C\ complex\ number$$

$$if\ iB=0\ then\ C\ real\ part$$

ex//

$2.1 + i3$

$2.1 + 3\sqrt{-1}$

complex conjugate

For each composite number such as (c) there are installation facilities that are coded (c*) and result from compensating each (i) by the number compounded by (-i) ex//

$C = A + iB$The number of compounds we want to turn into installation facilities is as follows: $C^{*} = A - iB$Installation facilities

Where the product of multiplying the complex number with the installation facilities represents a real positive number

CC* = positive real no.

e. linear algebra

a) linear space

We take a set of items a, b, c, ... Those subject to collection and beatings can achieve the following rules:

1) $A + B = B + A$

2) $(A + B) + C = A + (B + C)$

3) $a(A + B) = aA + aB$

b) Effects or opeartors factors (op)

It is a symbol that refers to a mathematical process that takes place on the function that comes after the influencer to change it to a new function that is different from the quantity of examples of effects:

$$(x \frac{d}{dx} f, \frac{d}{dx} f, \sqrt{f})$$

$\frac{d}{dx}$ **Differential influencer differention op**

Coded with Q^ or p^

There are two types of effects:

1) Linear op linear effects

Differential linear effects are used in quantum mechanics, which have the two characteristics:

1- $\frac{dx}{dy}(f+g) = \frac{d}{dx} f + \frac{d}{dx} g$

2- $\frac{d}{dx} a f = a \frac{d}{dx} f$ where a is constant

2) Non-linear op effects

ex//

$\sqrt{f+g} \neq \sqrt{f} + \sqrt{g}$

One of the most important influences of the famous quantum mechanics is an influence called Laplas.

$$\nabla^2 = \left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{dz^2}\right] F$$

del sequare

Order of op Arrangement effects

Influences are not subject to the exchange law and when arranged, there are more than two effects according to the exchange:

1- Commute op mutual effects

In this type of effect we get the same value so the difference between them = 0,

That is, if it's

$$P^\wedge Q^\wedge = Q^\wedge P^\wedge$$

Effects have commute if the difference between them is equal to zero.

$$P^\wedge Q^\wedge - Q^\wedge P^\wedge = 0$$

2- Non-reciprocal effects not commute op

In this type of influence we get different values and so the difference between them is not equal to zero. So:

$P^\wedge Q^\wedge \neq Q^\wedge P^\wedge$

Thus, the effects do not have the replacement property (not commute) because

$P^\wedge Q^\wedge - Q^\wedge P^\wedge \neq 0$

ex//

if $P^\wedge = 5+$, $Q^\wedge = C$, $f(x) = a$

Find the exchange   Explain The function commute

whether the function is commute or not

Sol//

$Q^\wedge P^\wedge f(x) = P^\wedge Q^\wedge f(x)$

First influencer $Q^\wedge P^\wedge f(x) = a$

$c(5 + a) = 5c + ac \rightarrow (1)$

$P^{\wedge}Q^{\wedge}f(x) = a$

$(5 + c)a = 5a + ac \rightarrow (2)$

$\because Q^{\wedge}P^{\wedge}f(x) \neq P^{\wedge}Q^{\wedge}f(x)$

That is,$Q^{\wedge}P^{\wedge}(x) - P^{\wedge}Q^{\wedge}(x) \neq 0$

So the function is not reciprocal. since

the function not commute