Ministry of Higher Education and Scientific Research

Al-Muthanna University

College of Science

Department of Chemistry

Quantum Chemistry

-The fourth lecture-

Stage 4

Prof. Dr Hassan sabih

2) Laqrang equations

The Lagrange equation is correct formovement, whether the movement is linear, circular or cylindrical.

To understand these equations, you know the L function called the Lakrange function.

$L = X_1 , Y_1 , Z1 + X2 , Y_2 , Z_2 +$ ---------------(1

It is a function of all engineering coordinates (Xi) and speed of movement (X•) of objects in the mechanical system and this function equals the difference between motor and latent energy

L = T – V _____(2)

Where the Lakrange function is a function of the variable (speed, coordinate, time)

*The Lakrange equation of non-conservative systems is

$$L(\dot{q}, q, t) = T(q \bullet, q, t) - V(qt)$$

*In conservative systems

$$L(\dot{q}, q) = T(\dot{q}, q) - V(q)$$

Since kinetic energy is a function of speed only

$T = f(\dot{X}, \dot{Y}, \dot{Z})$ ----------(3

So the potential energy is a function of coordinates only.

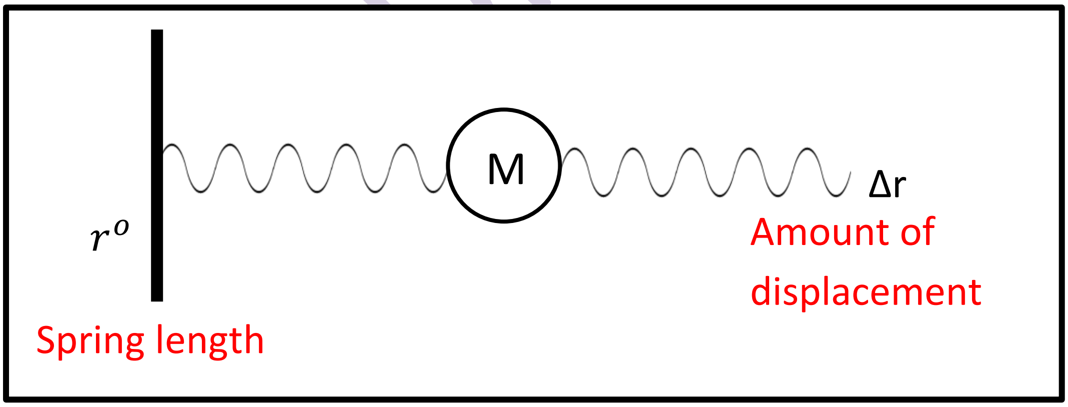
$V = f(X, Y, Z)$ -----------(4

So by compensating for the lakrange diplex in Newton's motion equations, we get a total of motor rates for several bodies (after abbreviation and order) where we deal with vertical coordinates as well as several energies for many objects.

So we take the difference to make it easier for several bodies to function.

$$\left.\begin{aligned} \frac{d}{dt}\cdot\frac{dL}{d\dot{x}} - \frac{dL}{dx} = 0 \\ \frac{d}{dt}\cdot\frac{dL}{d\dot{y}} - \frac{dL}{dy} = 0 \\ \frac{d}{dt}\cdot\frac{dL}{d\dot{z}} - \frac{dL}{dz} = 0 \end{aligned}\right\} \text{Laqrang equation dynamic}$$

One of the most important applications of the Lakrange equations is harmonic oscillator in the ego system



This system consists of a mass (m) attracted to the center by mechanical pull force (if the spring is frictionless) and the force of attraction (R) is known as restor force resulting from multiplying the value of the constant force"C"in the geometric displacement under the position of the mass from its stable state(r_0) so the restor force can be found in the relationship

$$R = C * \Delta r \_\_\_\_\_(1$$

Through this, the energy of the effort can be known from the relationship.

$$v = \frac{1}{2} C \ r^2 \_\_\_\_\_\_\_(2$$

But when using the area of cartesian coordinates and taking the three directions in the direction of the underlying and dynamic energy, the following

$$v = \frac{1}{2} C \left(X^2 + Y^2 + Z^2 \right) \_\_\_\_\_(3 \qquad \text{latent})$$

$$T = \frac{1}{2} m \left(\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2 \right) \_\_\_\_\_ (4 \qquad \text{kinetics})$$

It describes the Lakrange function of this system as follows:

$$\because L = T - V$$

$$\therefore L = \frac{1}{2} m \left(\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2 \right) - \frac{1}{2} C \left(X^2 + Y^2 + Z^2 \right) \_\_\_5$$

By compensating for equation 5 in the main Lakrange equations (withorder and abbreviation), we get a set of equations for the application of the harmonic vibrator.

$$\left. \begin{aligned} M\ddot{x} + cx &= 0 \\ M\ddot{y} + cy &= 0 \\ M\ddot{Z} + cz &= 0 \end{aligned} \right\}$$

Where:

$-\ddot{x}$ Ground acceleration

$-x$ Coordinate

$-c$ Constant strength

So when you start the measurement experiment for the coordinates of the harmonic vibrator for the purpose of describing the change in the position of the mass in the time allowance and by describing the change of the three cartesian coordinates in the field can be found the constant of strength in the relationship known as physics and it concerns the application of the harmonic vibrator

$$\left(\left(\, C \;=\; 4\,\pi^2 m\, v_o^2\,\right)\right)$$

v_o : vibration frequency

3) Hamilton equation

Hamilton's equation includes:

1) It's one of the general equations.
2) Includes the Hamilton (H) function, which represents the total power of the system
   H = T + V
   Hamilton's function also includes the L-function.
3) Hamilton's function is a function of speed and momentum general ness .

$$H = \dot{P}i\, \dot{q}i - L$$

But if there are multiple particles, hamilton's function becomes

$H = \sum_{i=1}^{3N} \dot{P}i\, \dot{q} - L$, N = X , Y , Ƶ

Hamilton's function is momentum-based and does not rely on L.

4) In hamilton's equation.

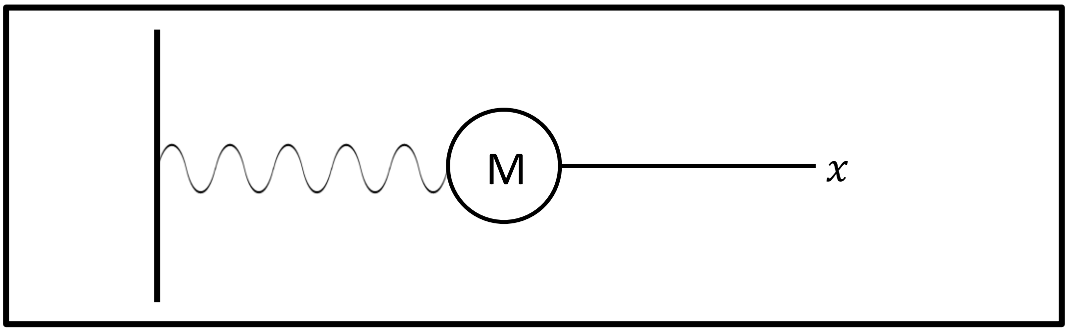
أ) We're deriving speed for momentum in Hamilton's function.

$$\frac{\partial H}{\partial Pi} = \partial \dot{q}i$$

$$\frac{\partial H}{\partial qi} - \frac{\partial L}{\partial qi} = -pi$$

One of the most important applications of the Hamilton equation

We take a spiral spring body that fixes one end of it with am body mass when it sheds strength on the body and pulls it towards the x axis.



This force will be countered by other forces called restor fource, equal to the amount and in contrast to the direction, so that the movement can be described according to Newton's equation and Hawke's law.

F = m a Newton law

F = - k x Howk law

equally

((m a = - k x))

This can be proven according to the Lagrange equation.

$$\frac{\delta}{\delta t} \cdot \frac{\delta L}{\delta \dot{q} i} = \frac{\delta L}{\delta q i} \quad \text{.............(1}$$

By expressing the Lakrange function of the retention system

$$L(\dot{q}\ , q) = T\ (\dot{q}\ , q) - v\ (q) \quad \text{..........(2}$$

$$Where\ (q = x\ , \dot{q} = \dot{x}\ , a = \ddot{x})$$

$$L\ (\dot{x}\ , x) = T\ (\dot{x}\ , x) - v\ (x) \quad \text{...... (3}$$

$$T = \frac{1}{2} m\ \dot{x}^2 \quad \text{.......(4}$$

$$v = \frac{1}{2} K\ X^2 \quad \text{.......(5}$$

We make up for 4,5 in equation 3.

$$L\left(\dot{X},X\right)=\frac{1}{2}m\,\dot{X}^2-\frac{1}{2}K\,X^2 \;\ldots\ldots\ldots (6$$

We make up for 6 in equation 1.

$$\frac{\partial}{\partial t}\cdot\frac{\partial(\dot{x},x)}{\partial \dot{x}i}=\frac{dL(\dot{x},x)}{\partial xi}\;\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7$$

We make up 7 in 6.

$$\frac{\partial}{\partial t}\cdot\frac{\partial\left(\frac{1}{2}m\dot{x}^2-\frac{1}{2}KX^2\right)}{\partial \dot{x}}=\frac{\partial\left(\frac{1}{2}m\dot{x}^2-\frac{1}{2}KX^2\right)}{\partial x}\ldots .(8$$

$$\frac{\partial}{\partial t}\cdot\frac{\partial}{\partial \dot{x}}\left(\frac{1}{2}m\dot{x}^2-\frac{1}{2}K\,X^2\right)=\frac{d}{dx}\left(\frac{1}{2}m\dot{x}^2-\frac{1}{2}KX^2\right)\ldots\ldots (9$$

$$\frac{\partial}{\partial t}\cdot(m\ddot{x}-0)=(0-kx)\quad\ldots ..(10$$

$$\left.\begin{array}{r} ma=-kx \\ \therefore m\ddot{x}=-KX \end{array}\right\}\ldots\ldots(11$$

Ex : Prove that Hamilton function rearesentation total energy in con serative System ?

Solu:-

$$H=\sum_{i=1}^{3N} pi\dot{q}i-L \;\underline{\hspace{3cm}}(1)$$

$$H=\sum_{i=1}^{3N} pi\dot{q}i-(T-V)\;\underline{\hspace{3cm}}(2)$$

$$H = \sum_{i=1}^{3N} p i \dot{q} i - T + V \_\_\_\_\_\_(3)$$

$$\because \frac{dL}{d\dot{q}i} = Pi \_\_\_\_(4)$$

We make up 4 in 3.

$$H = \sum_{i=1}^{3N} \dot{q}i \cdot \frac{\partial L}{\partial \dot{q}i} - T + V \_\_\_\_\_\_(5)$$

$$H = \sum_{i=1}^{3N} \dot{q}i \left(\frac{T - V}{\partial \dot{q}i}\right) - T + V \_\_\_\_\_\_(6)$$

In the portfolio system, we deal with kinetic energy, so it's neglected. $\frac{\partial v}{\partial \dot{q}i}$

$$H = \sum_{i=1}^{3N} \dot{q}i \left(\frac{\partial T}{\partial \dot{q}i}\right) - T + V \_\_\_\_\_\_(7)$$

$$T = \frac{1}{2} m\dot{q}i^2 \_\_\_\_\_\_ (8)$$

$$2T = m\dot{q}i^2 \_\_\_\_\_\_ (9)$$

Energy derived relative to relative speed

$$\frac{\partial T}{\partial \dot{q}i} = m\dot{q}i \_\_\_\_\_\_(10)$$

We make up 10 in 7.

$$H = \sum_{i=1}^{3N} \dot{q}i\, m\dot{q} - T + v \text{ \_\_\_\_\_\_ } (11)$$

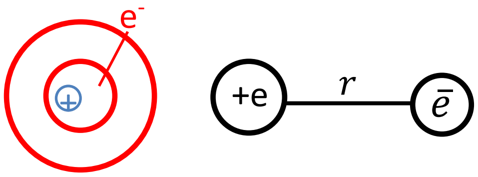
$$H = \sum_{i=1}^{3N} m\dot{q}^2 i - T + V \text{ \_\_\_\_\_\_ } (12)$$

$$H = \sum_{i=1}^{3N} 2T - T + V \text{ \_\_\_\_\_\_ } (13)$$

$$\therefore H = \sum_{i=1}^{3N} T + V$$

$H = T + v$ Total energy

Q/ Write Hamilton for H_2 with digram



$H = T + v$

$$T = \frac{1}{2} m v^2$$

$$= \frac{mv^2}{2} = \frac{m^2v^2}{2m} = \frac{P^2}{2M}$$

Changing by changing the number of e-$N = \frac{charge\ squared}{distance} = \frac{+e\ \bar{e}}{r} = -\frac{e^2}{r}$

$$H = T + v$$

$$\therefore H = \frac{P^2}{2m} - \frac{e^2}{r}$$