

✓ Lagrange Equation for small oscillation -

Those molecule whose motion lies b/w the motion of stable and unstable molecules known as small molecule and whose oscillation is known as small oscillation which also lies b/w stable and unstable oscillation.

A system of particle is said to be in equilibrium if all particles remain in rest that is net force acting on the particle is very high.

Let us consider a generalized force acting on each particle is given as

$$Q_j = - \left[\frac{\partial V}{\partial q_j} \right]_0 \quad \text{--- (1)}$$

If we assume the equilibrium to be stable then condition of equilibrium can be written as

$$q_j = q_{0j} + u_j$$

Where q_{0j} is the displacement of generalized coordinate in stable position (it is fixed)
 u_j is the displacement of the generalized coordinate from the stable position (as generalized coordinate)

Let potential energy is the function of u_j & q_{0j} then its expanded form as may be written as

$$\begin{aligned} V(q_1, q_2, \dots, q_n) &= V(u_1, u_2, \dots, u_n) \\ &= V(q_{01}, q_{02}, \dots, q_{0n}) \end{aligned}$$

In expanded form the above eqⁿ may be written as, (Taylor series's expansion)

$$V = V(q_0, q_0, \dots, q_0) + \sum_j \left(\frac{\partial V}{\partial q_j} \right)_0 u_j + \frac{1}{2} \sum_{jk} \left(\frac{\partial^2 V}{\partial q_j \partial q_k} \right)_0 u_j u_k + \dots$$

all the condition in above equation show unstable condition except the third term from the potential energy can be expressed as

$$V = \frac{1}{2} \sum_{jk} \left(\frac{\partial^2 V}{\partial q_j \partial q_k} \right) u_j u_k$$

$$V = \frac{1}{2} \sum_{jk} V_{jk} u_j u_k \quad \text{--- (2)}$$

$$V_{jk} = \frac{\partial^2 V}{\partial q_j \partial q_k}$$

Now from the definition of K.E

$$T = \frac{1}{2} \sum_{jk} m_{jk} \dot{u}_j \dot{u}_k \quad \text{--- (3)}$$

where u_j, u_k and q_j and q_k are the displacements

then above eq also be written as

$$\begin{cases} u_j = q_j \\ u_k = q_k \\ \dot{u}_j = \dot{q}_j \\ \dot{u}_k = \dot{q}_k \end{cases}$$

$$T = \frac{1}{2} \sum_{jk} m_{jk} \dot{q}_j \dot{q}_k \quad \text{--- (4)}$$

$$T = \frac{1}{2} \sum_{jk} T_{jk} \dot{q}_j \dot{q}_k \quad \text{--- (5)}$$

from the definition of Lagrangian

$$L = T - V$$

$$L = \frac{1}{2} \sum_{jk} T_{jk} \dot{q}_j \dot{q}_k - \frac{1}{2} \sum_{jk} V_{jk} q_j q_k$$

--- (6)

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0 \quad \text{--- (7) Lagrange's eqn}$$

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_K} \right) = \frac{1}{2} T_{JK} \ddot{q}_K$$

$$\frac{\partial L}{\partial q_j} = -\frac{1}{2} V_{JK} q_K$$

by eq (7)

$$\frac{1}{2} \frac{d}{dt} (T_{JK} \ddot{q}_K) + \frac{1}{2} q_K V_{JK} = 0$$

$$T_{JK} \ddot{q}_K + V_{JK} q_K = 0 \quad \text{--- (8)}$$

This is the required Expression for the Lagrange eq which can be expressed in matrix form for n-co-ordinate as follows

$$\begin{bmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{nn} \end{bmatrix} \begin{bmatrix} \ddot{q}_1 \\ \ddot{q}_2 \\ \vdots \\ \ddot{q}_n \end{bmatrix} + \begin{bmatrix} V_{11} & V_{12} & \dots & V_{1n} \\ V_{21} & V_{22} & \dots & V_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ V_{n1} & V_{n2} & \dots & V_{nn} \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \end{bmatrix} = 0$$

In General form it may be written as

$$T\ddot{q} + Vq = 0$$

This is the required Expression of small oscillation in K.E + P.E.

* Normal Coordinate And Normal Frequency of Vibration :-

The Generalized Coordinate which is used to describe the oscillation of single frequency is known as Normal frequency of Vibration And such as Generalized Coordinate is known as Normal Coordinate. the Transformation of motion of such Coordinate (Normal Coordinate) is described by a Term And in such Condition the displacement of the Normal Coordinate can be expressed as

$$L_j = \sum_{jk} Q_{jk} n_{jk} \quad \text{--- (1)}$$

Where Q_{jk} is a constant which change the Normal Coordinate into Another Coordinate. If i^{th} And j^{th} Molecules are same then the above eq. can be written as

$$\mu = a_n \quad \text{--- (2)}$$

Again the P.E of the molecule can be expressed as

$$V = \frac{1}{2} \sum_{jk} V_{jk} V_j V_k$$

$$V = \frac{1}{2} \sum_{jk} \mu_j V_{jk} \mu_k$$

Then by the Transformation matrix the above Equation reduced in the form of

$$V = \frac{1}{2} \dot{u}^T V \dot{u}$$

Also from Eq. (2) the above equation reduced in the form of

$$V = \frac{1}{2} (\dot{q}_n)^T V \dot{q}_n$$

$$V = \frac{1}{2} \dot{q}^T n^T V n \dot{q}$$

$$V = \frac{1}{2} n^T \dot{q}^T V n \dot{q}$$

And from the general formula we know that

$$\dot{q}^T V n = \Omega$$

The above equation reduced in the form of

$$V = \frac{1}{2} n^T \Omega n \quad \text{--- (3)}$$

Now K.E can be written as

$$T = \frac{1}{2} \sum_{j,k} T_{jk} \dot{x}_j \dot{x}_k$$

$$T = \frac{1}{2} \sum_{j,k} \dot{x}_j T_{jk} \dot{x}_k$$

Then Again by the matrix transformation the above equation reduced in the form of

$$T = \frac{1}{2} \dot{x}^T T \dot{x}$$

Again from Eq. (2) the above equation reduced in the form of

$$T = \frac{1}{2} n^T \dot{q}^T T n \dot{q}$$

Also from the general formula we know that

$$a^T a = 1$$

The above equation reduced in the form of

$$T = \frac{1}{2} \dot{h}^T h$$

$$T = \frac{1}{2} \dot{h}_x^2 \quad (4)$$

where $\dot{h}_x = \dot{h}$

Now the Lagrangian of the system can be expressed as

$$L = T - V$$

$$L = \frac{1}{2} \dot{h}_x^2 - \frac{1}{2} h^T \Omega h \quad (5)$$

The p.e of the small coordinate can be written in the quadratic form and can be expressed as

$$V = \frac{1}{2} h^T \Omega h = \frac{1}{2} \omega_x^2 h_x^2 \quad (6)$$

Then from eq (5) & (6) we get

$$L = \frac{1}{2} (\dot{h}_x^2 - \omega_x^2 h_x^2) \quad (7)$$

Now from the Lagrangian equation of the motion we know that

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{h}_x} \right) - \frac{\partial L}{\partial h_x} = 0$$

Again from eq (7) we get

$$\frac{\partial L}{\partial \dot{h}_x} = \dot{h}_x \quad \text{And} \quad \frac{\partial L}{\partial h_x} = -\omega_x^2 h_x$$

then the above equation can be written as

$$\frac{d}{dt}(\dot{n}_i) + \omega_i^2 n_i = 0$$

$$\ddot{n}_i + \omega_i^2 n_i = 0$$

where ω_i is the frequency of vibration and n_i is the normal coordinate for different coordinate.

$$\ddot{n}_1 + \omega_1^2 n_1 = 0$$

$$\ddot{n}_2 + \omega_2^2 n_2 = 0$$

$$\ddot{n}_3 + \omega_3^2 n_3 = 0$$

These are the equation of vibration of different molecules.

with various conditions with different molecules and different frequencies of vibration.

These are the normal coordinates of vibration of molecules.

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