B.Sc. (Semester - 5)
Subject: Physics
Course: US05CPHY21
Classical Mechanics

UNIT- IV Hamiltonian Formulation

Introduction:

The Lagrangian formulation is alternate method of Newtonian formulation to solve some physical problems. There exists another powerful theory known as the Hamiltonian formulation which is an alternative to the Lagrangian formulation. It is convenient and useful particularly in dealing with problems of modern physics. No new physical concept is introduced in this formulation but we get another tool to work on the problem in physics.

In this formulation, we obtain Hamilton's equations of motion for a system with n degrees of freedom. We shall assume that the constraints are holonomic and the forces are derivable from potentials which depend either on position or velocity dependent.

Hamilton's Equations of Motion:

We know that

$$H = \sum p_i \dot{q}_i - L(q_i, \dot{q}_i, t) \qquad \ldots (4.1)$$

Let the Hamiltonian be the function of generalised coordinate q_i and generalised momenta $p_i = \frac{\partial L}{\partial \dot{q}_i}$, i.e. $\dot{q}_i$ is replaced by p_i.

$$\therefore \; H = H(q_i, p_i, t) \qquad \ldots (4.2)$$

$$\therefore dH = \sum_k \frac{\partial H}{\partial p_k} dp_k + \sum_k \frac{\partial H}{\partial q_k} dq_k + \frac{\partial H}{\partial t} dt \qquad \ldots (4.3)$$

The differentiation of equation (4.1) is

$$dH = \sum_k p_k d\dot{q}_k + \sum_k \dot{q}_k dp_k - dL \qquad \ldots (4.4)$$

Since, $\qquad L = L(q_i, \dot{q}_i, t)$

$$\therefore dL = \sum_k \frac{\partial L}{\partial q_k} dq_k + \sum_k \frac{\partial L}{\partial \dot{q}_k} d\dot{q}_k + \frac{\partial L}{\partial t} dt$$

But, $\quad p_k = \frac{\partial L}{\partial \dot{q}_k}$

$$\therefore dL = \sum_k \frac{\partial L}{\partial q_k} dq_k + \sum_k p_k d\dot{q}_k + \frac{\partial L}{\partial t} dt \qquad \ldots (4.5)$$

Using equation (4.5) in (4.4), we get

$$dH = \sum_k p_k d\dot{q}_k + \sum_k \dot{q}_k dp_k - \sum_k \frac{\partial L}{\partial q_k} dq_k - \sum_k p_k d\dot{q}_k - \frac{\partial L}{\partial t} dt$$

$$\therefore dH = \sum_k \dot{q}_k dp_k - \sum_k \frac{\partial L}{\partial q_k} dq_k - \frac{\partial L}{\partial t} dt$$

$$\therefore dH = \sum_k \dot{q}_k dp_k - \sum_k \dot{p}_k dq_k - \frac{\partial L}{\partial t} dt \qquad \dots (4.6)$$

Comparing the coefficients of dp_k and dq_k in equations (4.3) and (4.6), we get

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \qquad \dots (4.7)$$

and ,

$$\dot{p}_k = \frac{\partial H}{\partial q_k} \qquad \dots (4.8)$$

Equations (4.7) and (4.8) are called Hamilton's equations or Hamilton's canonical equations of motion. They are a set of $2n$ first order differential equations of motion.

Also comparing the coefficients of dt in equations (4.3) and (4.6), we get

$$-\frac{\partial L}{\partial t} = \frac{\partial H}{\partial t} \qquad \dots (4.9)$$

- If H does not involve a particular coordinate q_k, then $\frac{\partial H}{\partial q_k} = 0$

$$\therefore \; \dot{p}_k = 0$$
$$\therefore \; \dot{p}_k = const.$$

Such a coordinate q_k is called *cyclic* or *ignorable coordinate*. Thus, a cyclic coordinate in the Lagrangian will be absent in the Hamiltonian.

Since,

$$H = H(p_k, q_k, t)$$

The total time derivative of H gives,

$$\therefore \frac{dH}{dt} = \sum_k \frac{\partial H}{\partial q_k} \dot{q}_k + \sum_k \frac{\partial H}{\partial p_k} \dot{p}_k + \frac{\partial H}{\partial t} \qquad \dots (4.10)$$

Using Hamilton's equations (4.7) & (4.8) in above equation (4.10), we have

$$\frac{dH}{dt} = -\sum_k \dot{p}_k \dot{q}_k + \sum_k \dot{q}_k \dot{p}_k + \frac{\partial H}{\partial t}$$

$$\therefore \frac{dH}{dt} = \frac{\partial H}{\partial t} \qquad \dots (4.11)$$

Using equation (4.9) & (4.11), we get

$$\therefore \frac{dH}{dt} = \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \qquad \dots (4.12)$$

If the Lagrangian does not involve time explicitly, then $\frac{\partial L}{\partial t} = 0$

$$\therefore \frac{dH}{dt} = 0$$

$$\therefore H = const. \qquad \dots (4.13)$$

Thus, the Hamiltonian H is a constant of the motion.

For conservative system, when the potential energy is not a function of velocities , i.e. $\frac{\partial V}{\partial \dot{q}_k} = 0$, then

$$H = T + V = const. \qquad \dots (4.14)$$

Hence, H is the total energy of the system.

Applications of the Hamiltonian Formulation:

(a) A Simple Pendulum with Moving Support:

A pendulum of mass m is suspended from a support which is moving along a straight horizontal line as shown if Fig.(4.1)

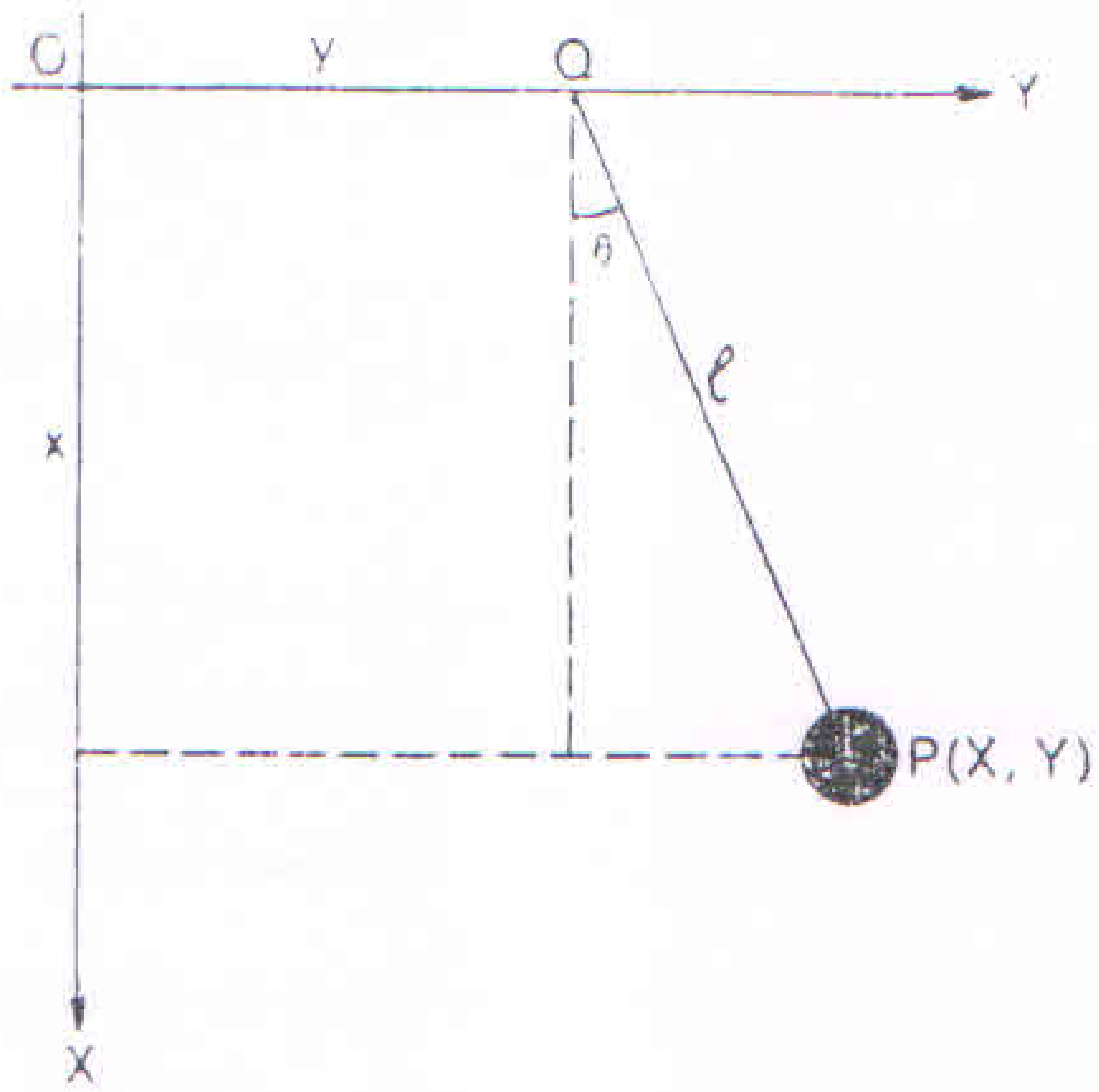

Fig:4.1

Let, $PQ = l$, then the coordinates of P are

$$X = l\ \cos\theta \quad and \quad Y = y + l\ \sin\theta$$

$$\therefore\ \dot{X} = -l\dot{\theta}\sin\theta \quad and \quad \dot{Y} = \dot{y} + l\dot{\theta}\cos\theta$$

Now, the kinetic energy of the pendulum is

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m(\dot{X}^2 + \dot{Y}^2)$$

$$\therefore\ T = \frac{1}{2}m\left[l^2\dot{\theta}^2\sin^2\theta + \dot{y}^2 + 2l\dot{y}\dot{\theta}\cos\theta + l^2\dot{\theta}^2\cos^2\theta\right]$$

$$\therefore\ T = \frac{1}{2}m\left(\dot{y}^2 + l^2\dot{\theta}^2 + 2l\dot{y}\dot{\theta}\cos\theta\right) \qquad ...(4.15)$$

Its potential energy with respect to its vertical position when $\theta = 0$ is,

$$V = mgl(1 - \cos\theta) \qquad ...(4.16)$$

Hence, the Lagrangian is given by

$$L = T - V$$

$$\therefore L = \frac{1}{2}m\left(\dot{y}^2 + l^2\dot{\theta}^2 + 2l\dot{y}\dot{\theta}\cos\theta\right) - mgl(1 - \cos\theta) \qquad ....(4.17)$$

The Hamiltonian function is

$$H = \sum_k p_k\dot{q}_k - L$$

$$\therefore H = p_y\dot{y} + p_\theta\dot{\theta} - L \qquad ...(4.18)$$

But,

$$p_y = \frac{\partial L}{\partial \dot{y}} = m\dot{y} + ml\dot{\theta}\cos\theta$$

$$\therefore\ p_y = m(\dot{y} + l\dot{\theta}\cos\theta) \qquad \dots(4.19)$$

And

$$p_\theta = \frac{\partial L}{\partial\dot{\theta}} = ml^2\dot{\theta} + ml\dot{y}\cos\theta$$

$$\therefore\ p_\theta = ml(l\dot{\theta} + \dot{y}\cos\theta) \qquad \dots(4.20)$$

Using equations (4.19) , (4.20) & (4.17) in (4.18), we get

$$H = m\dot{y}\,(\dot{y} + l\dot{\theta}\cos\theta) + ml\dot{\theta}(l\dot{\theta} + \dot{y}\cos\theta) - \frac{1}{2}m\,(\dot{y}^2 + l^2\dot{\theta}^2 + 2l\dot{y}\dot{\theta}\cos\theta)$$
$$+\ mgl(1 - \cos\theta)$$

$$\therefore H = m[\dot{y}^2 + \dot{y}l\dot{\theta}\cos\theta + l^2\dot{\theta}^2 + l\dot{\theta}\dot{y}\cos\theta] - \frac{1}{2}m\,(\dot{y}^2 + l^2\dot{\theta}^2 + 2l\dot{y}\dot{\theta}\cos\theta)$$
$$+\ mgl(1 - \cos\theta)$$

$$\therefore H = \frac{1}{2}m\,(\dot{y}^2 + l^2\dot{\theta}^2 + 2l\dot{y}\dot{\theta}\cos\theta) +\ mgl(1 - \cos\theta) \qquad \dots(4.21)$$

Substituting the values of $\dot{y}$ and $l\dot{\theta}$ from equations (4.19) & (4.20), we get

$$H = \frac{1}{2m\sin^2\theta}\left[p_y^2 + \frac{p_\theta^2}{l^2} - \frac{2p_yp_\theta}{l}\cos\theta\right] +\ mgl(1 - \cos\theta) \qquad \dots(4.22)$$

Since y is cyclic, the momentum p_y is a constant of motion. Equation (4.22) is Hamilton's equation of motion in terms of momenta.

(b) Charged Particle in an Electromagnetic Field:

The Lagrangian for a charged particle in an electromagnetic field is

$$L = T - V = \frac{1}{2}mv^2 - q\phi + q(\vec{v}\cdot\vec{A}) \qquad \dots(4.23)$$

Hence, the canonical momenta are given by

$$p_k = \frac{\partial L}{\partial v_k} = mv_k + qA_k$$

Thus,

$$\vec{p} = \sum_k \hat{e}_k p_k = \sum_k \hat{e}_k(mv_k + qA_k)$$

$$\therefore\ \vec{p} = m\vec{v} + q\vec{A} \qquad \dots(4.24)$$

The Hamiltonian function is given by

$$H = \sum_k p_k\dot{q}_k - L$$

$$\therefore\ H = \sum_k p_k v_k - L$$

$$\therefore\ H = \sum_k (mv_k + qA_k)v_k - \left[\frac{1}{2}mv^2 - q\phi + q(\vec{v}\cdot\vec{A})\right]$$

$$\therefore\ H = \frac{1}{2}mv^2 + q\phi \qquad \dots(4.25)$$

From equation (4.24), we have

$$\vec{v} = \frac{1}{m}(\vec{p} - q\vec{A})$$

Substituting this value of $\vec{v}$ in equation (4.25), we get

$$\therefore\ H = \frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 + q\phi \qquad \dots(4.26)$$

This is the Hamiltonian in terms of momenta.

Now, the Hamilton's canonical equations in this case can be written as,

$$\dot{r}_i = \frac{\partial H}{\partial p_i}, i = 1,2,3$$

However, this can be written as

$$\dot{\vec{r}} = \frac{\partial H}{\partial \vec{p}} = \frac{\partial}{\partial \vec{p}}\left[\frac{1}{2m}\left(\vec{p} - q\vec{A}\right)^2 + q\phi\right]$$

$$\therefore\ \vec{v} = \frac{1}{m}\left(\vec{p} - q\vec{A}\right) \qquad \dots(4.27)$$

Similarly,

$$\dot{\vec{p}} = -\vec{\nabla}H = -q\vec{\nabla}\phi + q\vec{\nabla}\left(\vec{v}\cdot\vec{A}\right) \qquad \dots(4.28)$$

Here, $\vec{p}$ depends only on time and not on space coordinates.

Let us now consider the motion of a charge q in a uniform magnetic field $\vec{B}$ along z-axis. Then the vector potential is give by $\vec{B} = \vec{\nabla} \times \vec{A}$, has the magnitude $B = \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}$

The components of vector potential in this case is

$$A_x = A_z = 0 \quad and \quad A_z = xB$$

The Hamiltonian in this case is

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2m}\left(p_y - qxB\right)^2 \qquad \dots(4.29)$$

Since H does not depend on y and z, we have

$$p_y = const. \quad and \quad p_z = const.$$

Now, putting $\omega = \frac{qB}{m}$ and $x_0 = \frac{p_y}{qB}$ in equation (4.29), we get

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{2}m\omega^2(x - x_0)^2 \qquad \dots(4.30)$$

Hamilton's equations of motion are

$$\dot{p}_x = -m\omega^2(x - x_0),\ \dot{p}_y = 0,\ \dot{p}_z = 0 \qquad \dots(4.31)$$

or $\quad p_y = const.\ and\ \ p_z = const.$

Here,

$$\dot{p}_x = -m\omega^2(x - x_0) \qquad \dots(4.32)$$

This is the equation of motion of simple harmonic oscillator.

$$\therefore\ \ddot{x} = -\omega^2(x - x_0) \qquad \dots(4.33)$$

The solution of above equation is

$$x = a\ \cos(\omega t + \alpha) + x_0 \qquad \dots(4.34)$$

It should be noted that x_0 is not a fixed point but moves with a velocity p_y/m parallel to the y –axis.

To determine y and z , we use

$$\dot{y} = -\frac{\partial H}{\partial p_y} = -\frac{1}{m}\left(p_y - qxB\right) = \omega(x - x_0)$$

$$\therefore\ \dot{y} = a\ \omega \cos(\omega t + \alpha) \qquad \dots(4.35)$$

and, $$\dot{z} = \frac{p_z}{m} \qquad \text{... (4.36)}$$

The solutions of equations (4.35) & (4.36) are

$$y = a\ \sin(\omega t + \alpha) + y_0 \qquad \text{... (4.37)}$$

and, $$z = \frac{p_z}{m}t + z_0 \qquad \text{... (4.38)}$$

Thus, the particle moves along a spiral of radius a with its axis that is parallel to $\vec{B}$.

Phase Space:

In Lagrangian formulation the motion of the system with n degrees of freedom represented by $3n$ dimensional space is known as *configuration space*. The motion of any point in the configuration space is called *system point*. As the system point moves, its n coordinates will change and the system point in the configuration space will describe a curve which give the trajectory or path of the system.

In the Hamiltonian formulation n coordinates $q_i$and n momenta p_i are taken as independent variables. In only n momenta are used as axes in n -dimensional space, we will get the *momentum space*. Any point in the momentum space will describe the state of the motion of the whole system and the locus of the point is called the *hodograph*. A combination of coordinate and momentum space is described by a function $H(q,p)$. This $2n$- dimensional space having n coordinates q_i and n momenta p_i is known as ***phase space***. A single point in this phase space will fix all the position coordinates and momenta. Thus, the point describes the state of motion of the system besides giving its position.

Illustration:

Let us consider one dimensional simple harmonic oscillator. The total energy of the oscillator is,

$$E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \qquad \text{... (4.39)}$$

This can be written in the form

$$\frac{p^2}{(2E/m\omega^2)} + \frac{p^2}{2mE} = 1 \qquad \text{... (4.40)}$$

This is the equation of ellipse in two-dimensional space with p and x- axes as shown in fig.(4.2)

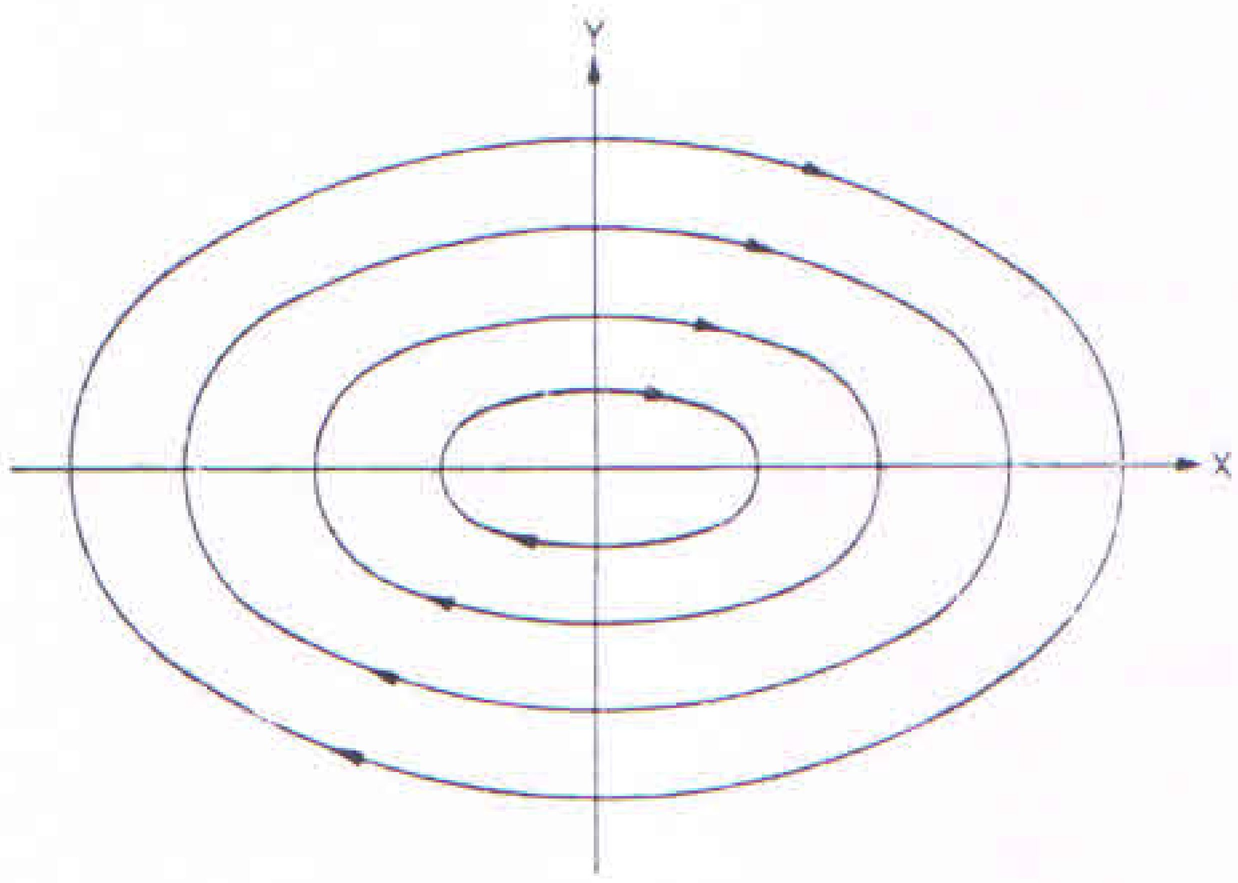

Fig: 4.2

The ellipse has semi-axis $\sqrt{2E/m\omega^2}$ and $\sqrt{2mE}$ and the area of ellipse is $2\pi E/\omega$.The ellipses show various possible paths of the oscillator at different energies in the phase space. These paths are called the *phase diagrams*.

Two paths in the phase space can never cross. If they do, it will mean that there are two possible momenta. For the given amplitude of the oscillator, the energy is constant. The paths in fig.(4.1) will always be clockwise.

Comments on The Hamiltonian Formulation:

- In the Lagrangian formulation the Lagrangian L is a function of generalised coordinates q_j and generalised velocities $\dot{q}_j$. They are not independent variables. For a system of n -degree of freedom, motion is considered in an n- dimensional coordinate space called configuration space. Since the Lagrange's equations are second order differential equations. We required $2n$ initial values to obtain the solutions.
- While in Hamiltonian formulation, the generalised momenta p_i and the generalised coordinates q_i are the independent variables. The system of n- degree of freedom has $2n$ independent variables. The motion of the system decided by the $2n$-independent variables is called the phase space. There are $2n$ Hamilton's equations each of being first order differential equation and their solutions will need $2n$ initial values.
- The Hamilton's equations fall in two groups corresponding to generalised momenta and coordinates having an almost symmetrical relationship.
- The Hamiltonian formulation is particularly useful in making a transition from classical mechanics to quantum mechanics in which the action is quantized.

Gauge Transformation:

The Lagrangian and Hamiltonian are related by the relation

$$H(p_i, q_i, t) = \sum p_i \dot{q}_i - L(q_i, \dot{q}_i, t) \qquad \dots (4.41)$$

Now, consider an arbitrary function as

$$f = f(q_1, q_2, \dots \dots \dots, q_n, t)$$

Its total time derivative is given by

$$\frac{df}{dt} = \sum_i \frac{\partial f}{\partial q_i} \dot{q}_i + \frac{\partial f}{\partial t} \qquad \dots (4.42)$$

Differentiation of equation (4.42) with respect to $\dot{q}_j$ gives

$$\frac{\partial}{\partial \dot{q}_j} \frac{df}{dt} = \frac{\partial f}{\partial q_i} \qquad \dots . (4.43)$$

Further differentiation with respect to t gives

$$\frac{d}{dt} \frac{\partial}{\partial \dot{q}_j} \left(\frac{df}{dt}\right) = \frac{d}{dt} \left(\frac{\partial f}{\partial q_i}\right) = \frac{\partial}{\partial q_i} \left(\frac{df}{dt}\right) \qquad \dots (4.44)$$

Above equation is Lagrange's equation satisfied by $\frac{df}{dt}$. Thus, we can define a new Lagrangian as

$$L' = L + \frac{df(q_1, q_2, \dots \dots \dots . q_n, t)}{dt} \qquad \dots . (4.45)$$

Thus, the Lagrangian is not unique but it is always uncertain by a term $\frac{df}{dt}$. This transformation equation of Lagrangian is known as ***gauge transformation***.

The new canonical momenta are

$$p_j' = \frac{\partial L'}{\partial \dot{q}_j} = \frac{\partial L}{\partial \dot{q}_j} + \frac{\partial}{\partial \dot{q}_j}\frac{df}{dt} = p_j + \frac{\partial f}{\partial q_j} \qquad \dots (4.46)$$

We now introduce a coordinate transformation from old coordinates q_j to a new set of coordinates $Q_k (k = 1,2, \dots \dots . , n)$

$$q_j = q_j(Q_1, Q_2, \dots \dots \dots , Q_n, t) \qquad \dots (4.47)$$

This is known as *point transformation*.

Hence, the new Lagrangian becomes

$$L'(Q_k, \dot{Q}_k, t) = L(q_j, \dot{q}_j, t) \pm \frac{df(Q_k, t)}{dt} \qquad \dots (4.48)$$

In order to transform variables q_i to Q_i, we can take the arbitrary function in above equation (4.48) as a function of both the new and old coordinates. Thus, $F \equiv F(q_i, Q_i, t)$ is a function of $2n$ variables besides time, in which only n variables are independent.

We can write, by using the transformation equation (4.47), as

$$F = F(q_j, Q_k, t) = F[q_j(Q_1, Q_2, \dots \dots \dots , Q_n, t), Q_k, t]$$

$$\therefore F = F(Q_1, Q_2, \dots \dots \dots , Q_n, t)$$

Then, transformation equation (4.48) becomes

$$L'(Q_k, \dot{Q}_k, t) = L(q_j, \dot{q}_j, t) \pm \frac{dF(q_j, Q_k, t)}{dt} \qquad \dots (4.49)$$

Since $\frac{dF}{dt}$ of $\frac{df}{dt}$ identically satisfies Lagrange's equations. In the theory of the canonical transformations, we shall use

$$L(q, \dot{q}, t) = L'(Q, \dot{Q}, t) + \frac{dF(q, Q, t)}{dt} \qquad \dots (4.50)$$

Thus, function F, whose total time derivative satisfies Lagrange's equations, relates the new and old Lagrangian and is said to generate the transformation. Hence, F is called the ***generating function***.

- **Illustration:**

Consider the Lagrangian for a simple harmonic oscillator

$$L = \frac{1}{2}m(\dot{q}^2 - \omega^2 q^2) \qquad \dots (4.51)$$

Transform it with the generating function

$$F = \frac{1}{2}im\omega^2 q^2 \qquad \dots (4.52)$$

The transformed Lagrangian from equation (4.49) with the positive sign is

$$L' = L + \frac{dF}{dt}$$

$$\therefore L' = \frac{1}{2}m(\dot{q}^2 - \omega^2 q^2) + 2im\omega^2 q\dot{q}$$

$$\therefore L' = \frac{1}{2}m(\dot{q} + i\omega q)^2 \qquad \text{... (4.53)}$$

Canonical Transformation:

If a coordinate is cyclic in the Lagrangian, it is also cyclic in the Hamiltonian. Then, the equation with conjugate momentum becomes

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = 0 \qquad \text{... (4.54)}$$

$$\therefore p_i = \alpha_i = const. \qquad \text{... (4.55)}$$

The Hamilton's equation for $\dot{q}_i$ gives

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \frac{\partial H}{\partial \alpha_i} = \omega_i = \omega_i(\alpha_i) \qquad \text{... (4.56)}$$

$$\therefore q_i = \omega_i t + \beta_i \qquad \text{... (4.57)}$$

Where β_i, are determined from initial conditions.

When q_k and p_k are the position and momentum coordinates, and Q_k and P_k are the new position and momentum coordinates such that

$$\left.\begin{aligned} P_k &= P_k(p_1, p_2, \dots\dots, p_n, q_1, q_2 \dots\dots q_n, t) \\ Q_k &= Q_k(p_1, p_2, \dots\dots, p_n, q_1, q_2 \dots\dots q_n, t) \end{aligned}\right\} \qquad \text{... (4.58)}$$

We can also write as,

$$\left.\begin{aligned} & P_k = P_k(p_j, q_j, t) \\ and\,, \quad & Q_k = Q_k(p_j, q_j, t) \end{aligned}\right\} \qquad \text{... (4.59)}$$

then, if there exists a Hamiltonian $K = K(Q_k, P_k, t)$ in the new coordinates such that

$$\dot{P}_k = -\frac{\partial K}{\partial Q_k} \quad and \ \dot{Q}_k = \frac{\partial K}{\partial P_k} \qquad \text{... (4.60)}$$

Equations (4.60) are known as ***canonical transformations***.

This is also called ***contact transformations***. The coordinates Q_k and P_k are referred to as the canonical coordinates.

The Hamiltonian function H and K in terms of the two sets of coordinates are given by

$$\left.\begin{aligned} & H = \sum p_k \dot{q}_k - L(q, \dot{q}, t) \\ and, \quad & K = \sum_k P_k \dot{Q}_k - L'(Q, \dot{Q}, t) \end{aligned}\right\} \qquad \text{... (4.61)}$$

We have

$$L(q, \dot{q}, t) = L'(Q, \dot{Q}, t) + \frac{dF_1(q, Q, t)}{dt}$$

$$\therefore L(q_j, \dot{q}_j, t) = L'(Q_k, \dot{Q}_k, t) + \sum_l \left(\frac{\partial F_1}{\partial q_l}\dot{q}_l + \frac{\partial F_1}{\partial Q_l}\dot{Q}_l\right) + \frac{\partial F_1}{\partial t} \qquad \text{... (4.62)}$$

where we have used F_1 to denote $F(q_i, Q_i, t)$ which is a function of $2n$ independent variables.

Differentiating equation (4.62) with respect to q_m and $\dot{Q}_m$, we get

$$\frac{\partial L}{\partial \dot{q}_m} = +\frac{\partial F_1}{\partial q_m} = +p_m \qquad \text{.... (4.63)}$$

where p_m is the old generalised momentum, and

$$\frac{\partial L'}{\partial \dot{Q}_m} = -\frac{\partial F_1}{\partial Q_m} = +P_m \qquad \text{.... (4.64)}$$

where P_m is the generalised momentum for the new Lagrangian L'.

Similarly, the transformed Hamiltonian is

$$K = \sum_i P_i \dot{Q}_i - L'$$

$$\therefore \quad K = \sum_i P_i \dot{Q}_i - L + \sum_l \left(\frac{\partial F_1}{\partial q_l}\dot{q}_l + \frac{\partial F_1}{\partial Q_l}\dot{Q}_l\right) + \frac{\partial F_1}{\partial t} \qquad \text{... (4.65)}$$

Hence, canonical equation (4.60) becomes,

$$\dot{P}_j = -\frac{\partial K}{\partial Q_j} \quad and \ \dot{Q}_j = \frac{\partial K}{\partial P_j} \qquad \text{... (4.66)}$$

Now, using equations (4.63) & (4.64) in equation (4.65), we get

$$K = \sum_i \left(-\frac{\partial F_1}{\partial Q_i}\right)\dot{Q}_i - L + \sum_i p_i \dot{q}_i + \sum_i \frac{\partial F_1}{\partial Q_i}\dot{Q}_i + \frac{\partial F_1}{\partial t}$$

$$\therefore K = \sum_i p_i \dot{q}_i - L + \frac{\partial F_1}{\partial t}$$

$$\therefore K = H + \frac{\partial F_1}{\partial t} \qquad \text{.... (4.67)}$$

Thus, we get a set of relations for the generating function $F_1 = F_1(q_i, Q_i, t)$ to canonical transformation as

$$p_i = \frac{\partial F_1}{\partial q_i} \qquad \text{... (4.68)}$$

$$P_i = -\frac{\partial F_1}{\partial Q_i} \qquad \text{... (4.69)}$$

$$and \qquad K = H + \frac{\partial F_1}{\partial t} \qquad \text{.... (4.70)}$$

Using generating function $F_1(q_i, Q_i, t)$, we can find the coordinates p_i and P_i. Above equations (4.68) & (4.69) gives the relation between q_i to p_i and Q_i to P_i. Equation (4.70) gives the relation between the new and the old Hamiltonian.

Here we have chosen $F_1 = F_1(q_i, Q_i, t)$, i.e. F is a function of $2n$ old and new coordinates. We can choose any one of the functions of new and old coordinates and momenta as

$$F_1(q, Q, t), F_2(q, P, t), F_3(p, Q, t), F_4(p, P, t)$$

The exact form of the generating function depends upon the nature of the problem. For example, for a transformation $P_k = P_k(p, t)$, p and P are dependent variables and we must exclude F_4.

Consider a generating function $F_1(q, Q)$ for the harmonic oscillator is given by

$$F_1 = \frac{1}{2} m\omega q^2 \cot Q \qquad \text{... (4.71)}$$

$$Then, \qquad p = \frac{\partial F_1}{\partial q} = m\omega q \ \cot Q \qquad \text{... (4.72)}$$

$$and, \qquad P = -\frac{\partial F_1}{\partial Q} = -\frac{1}{2} m\omega q^2 \text{cosec}^2 Q \qquad \dots (4.73)$$

From equation (4.73), we have

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q \qquad \dots (4.74)$$

With this substitution, equation (4.72) becomes

$$p = \sqrt{2mP\omega} \cos Q \qquad \dots (4.75)$$

Since F_1 does not involve t explicitly, the Hamiltonian is unaffected by the transformation. In order to express H in terms of Q and P, we proceed as follows:

The Hamiltonian H for the oscillator is

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \qquad \dots (4.76)$$

Substituting the values of p and q in above equation, we get

$$H = \omega P \cos^2 Q + \omega P \sin^2 Q = \omega P \qquad \dots (4.77)$$

Equation (4.77) shows that the Hamiltonian is cyclic in Q. Hence, the conjugate momentum P must be constant. Now,

$$P = \frac{H}{\omega} = \frac{E}{\omega}$$

Where E is the total energy. Further,

$$\dot{Q} = \frac{\partial H}{\partial P} = \omega$$

Hence, $Q = \omega t + \alpha$, where α is a constant of integration. Thus, the transformation has changed the problem of the oscillator in such a way that the new P is a constant of motion and the new Q gives translational motion of the oscillator and the transformation is equivalent to changing the oscillatory motion into a translational one.

Since,

$$q = \sqrt{\frac{2P}{m\omega}} \sin Q$$

$$\therefore \; q = \sqrt{\frac{2P}{m\omega}} \sin(\omega t + \alpha) \qquad \dots. (4.78)$$

This is the solution for a harmonic oscillator.

If generating function F_2 is chosen, then the transformation from (q, Q) to (q, P) has to carried out. Since, we have equation (4.69)

$$\frac{\partial F_1}{\partial Q_k} = -P_k$$

The generating function F_2 can be written as

$$F_2(q, P, t) = F_1(q, Q, t) + \sum P_k Q_k \qquad \dots (4.79)$$

Equation (4.79) can be solved for F_1. Substituting this value of F_1 in equation (4.50), wherein we write L and L' in terms of H and K, we get

$$\sum p_i q_i - H = \sum P_i \dot{Q}_i - K + \frac{d}{dt}\left\{F_2(q, P, t) - \sum P_i Q_i\right\}$$

$$\therefore K = H - \sum \dot{P}_i Q_i - \sum p_i \dot{q}_i + \frac{d}{dt} F_2(q, P, t) \qquad \dots (4.80)$$

Expressing the total time derivative $\frac{dF_2(q,P,t)}{dt}$ in terms of the derivatives of its argument, we obtain

$$K = H - \sum p_i \dot{q}_i - \sum \dot{P}_i Q_i + \sum \frac{\partial F_2}{\partial q_i} \dot{q}_i + \sum \frac{\partial F_2}{\partial P_i} \dot{P}_i + \frac{\partial F_2}{\partial t}$$

$$\therefore K = H + \frac{\partial F_2}{\partial t} - \sum \left(p_i - \frac{\partial F_2}{\partial q_i}\right) \dot{q}_i - \sum \left(Q_i - \frac{\partial F_2}{\partial P_i}\right) \dot{P}_i \qquad \dots (4.81)$$

As we are making q and P independent variables, the coefficients of $\dot{q}_i$ and $\dot{P}_i$ must be identically zero. Thus, we get

$$p_i = \frac{\partial F_2}{\partial q_i} \qquad \dots (4.82a)$$

$$Q_i = \frac{\partial F_2}{\partial P_i} \qquad \dots (4.82b)$$

and

$$K = H + \frac{\partial F_2}{\partial t} \qquad \dots (4.82c)$$

By following the same procedure as in the previous two cases, we get for F_3 and F_4

$$q_i = -\frac{\partial F_3}{\partial p_i} \qquad \dots (4.83a)$$

$$P_i = -\frac{\partial F_2}{\partial Q_i} \qquad \dots (4.83b)$$

and

$$K = H + \frac{\partial F_3}{\partial t} \qquad \dots (4.83c)$$

and

$$q_i = -\frac{\partial F_4}{\partial p_i} \qquad \dots (4.84a)$$

$$Q_i = \frac{\partial F_4}{\partial p_i} \qquad \dots (4.84b)$$

and

$$K = H + \frac{\partial F_4}{\partial t} \qquad \dots (4.84c)$$

Condition for Transformation to be Canonical:

It can be shown that a transformation

$$P_i = P_i(q_k, p_k, t), Q_k = Q_k(q_k, p_k, t)$$

is canonical only if the expression

$$\sum_i p_i \, dq_i - \sum_i P_i dQ_i \qquad \dots (4.85)$$

is an exact differential.

For example, consider the generating function which transforms variables q_i, p_i to variables Q_i, P_i when time is held fixed:

$$p_i = \frac{\partial F_1}{\partial q_i}$$

and

$$P_i = -\frac{\partial F_1}{\partial Q_i}$$

Now, since $F_1 = F_1(q_i, Q_i)$, we can write

$$dF_1 = \sum_k \frac{\partial F_1}{\partial q_k} dq_k + \sum_k \frac{\partial F_1}{\partial Q_k} dQ_k$$

$$\therefore\ dF_1 = \sum_k p_k\, dq_k - \sum_k P_k\, dQ_k \qquad \text{... (4.86)}$$

But, dF_1 is an exact differential. Hence, the expression

$$\sum_k p_k\, dq_k - \sum_k P_k\, dQ_k$$

must also be an exact differential. This result can be obtained by using any generating function. The condition of an exact differential can also be written as:

The transformation (p_i, q_i) to (P_i, Q_i) is canonical if $\sum q_i\, dp_i - \sum Q_i\, dP_i$ is an exact differential.

It should also be remembered that for canonical transformations not involving t, then

$$H(p_k, q_k) = K(P_k, Q_k) \qquad \text{... (4.87)}$$

Illustrations of Canonical Transformations:

1. Consider a generating function of the type

$$F_2 = \sum_k q_k P_k \qquad \text{... (4.88)}$$

Then, from equation (4.82), we have

$$p_k = \frac{\partial F_2}{\partial q_k} = P_k$$

$$Q_k = \frac{\partial F_2}{\partial P_k} = q_k$$

and , $$H = K$$

Thus, the old and new coordinates are the same. Hence, the function $F_2 = \sum_k q_k p_k$ generates identity transformation.

2. A more general function of the above type is

$$F_2 = \sum_k f_k(q_1, q_2, \dots, q_n, t) P_k \qquad \text{... (4.89)}$$

Then, new coordinates Q_k are given by

$$Q_k = \frac{\partial F_2}{\partial P_k} = f_k(q, t) \qquad \text{... (4.90)}$$

Equation (4.90) show that new coordinates Q_k are the functions of old coordinate q_k. A transformation of this type is called a point transformation. The functions f_k appearing in equation (4.89) are completely arbitrary and hence all the point transformations are canonical.

3. We show that transformation

$$P = \frac{1}{2}(p^2 + q^2) \text{ and } Q = \tan^{-1}\frac{q}{p} \text{ is canonical}$$

The transformation is canonical if $(p\,dq - PdQ)$ is an exact differential. In the present case

$$p\,dq - P\,dQ = p\,dq - \frac{1}{2}(p^2 + q^2)\frac{p\,dq - q\,dp}{p^2 + q^2}$$

$$= p\,dq - \frac{1}{2}(p\,dq - q\,dp) \quad = \frac{1}{2}(p\,dq + q\,dp)$$

$$\therefore\ p\,dq - P\,dQ = d\left(\frac{1}{2}pq\right) \qquad \dots (4.91)$$

Thus, $p\,dq - P\,dQ$ is an exact differential and hence the transformation is canonical.

4. We now show that $\sum_k q_k Q_k$ generates the exchange transformation in which position coordinates and the momenta can be interchanged.

The given generating function is of the type

$$F_i = \sum_k q_k Q_k$$

Hence, from equation (4.68) & (4.69),

$$p_k = \frac{\partial F_1}{\partial q_k} = Q_k \qquad \dots (4.92)$$

and,

$$P_k = -\frac{\partial F_1}{\partial Q_k} = -q_k \qquad \dots (4.93)$$

Thus, the coordinates and the momenta are interchanged by the transformation.

5. In the case of canonical transformations given by equation (4.58), we can obtain the following relations:

$$\text{(i)}\quad \frac{\partial q_j}{\partial Q_k} = \frac{\partial P_k}{\partial p_j}, \qquad \text{(ii)}\quad \frac{\partial q_j}{\partial P_k} = -\frac{\partial Q_k}{\partial p_j}$$

To prove relation (i), we use equations (4.83a) and (4.83b) as

$$q_j = -\frac{\partial F_3}{\partial p_j} \quad \text{and} \quad P_k = -\frac{\partial F_3}{\partial Q_k}$$

Hence,

$$\frac{\partial q_j}{\partial Q_k} = -\frac{\partial^2 F_3}{\partial Q_k \partial p_j}$$

and,

$$\frac{\partial P_k}{\partial p_j} = -\frac{\partial^2 F_3}{\partial p_j \partial Q_k}$$

Hence

$$\frac{\partial q_j}{\partial Q_k} = \frac{\partial P_k}{\partial p_j} \qquad \dots (4.94)$$

Relation (ii) can be proved in a similar manner using equations (4.84a) and (4.84b).

Two more relations of this type can also be proved. These are

$$\frac{\partial p_j}{\partial Q_k} = -\frac{\partial P_k}{\partial q_j} \quad \text{and} \quad \frac{\partial p_j}{\partial P_k} = \frac{\partial Q_k}{\partial q_j} \qquad \dots (4.95)$$

Poisson Brackets:

We now consider the useful representation of Poisson brackets in which the equations of motion can be written in a symmetric form. The Poisson brackets are found to be a very useful tool in quantum mechanics and field theory.

The Poisson brackets are defined by the equation

$$[u,v]_{q,p} = \sum_k \left(\frac{\partial u}{\partial q_k}\frac{\partial v}{\partial p_k} - \frac{\partial u}{\partial p_k}\frac{\partial v}{\partial q_k}\right) \quad \text{... (4.96)}$$

or
$$[u,v]_{Q,P} = \sum_k \left(\frac{\partial u}{\partial Q_k}\frac{\partial v}{\partial P_k} - \frac{\partial u}{\partial P_k}\frac{\partial v}{\partial Q_k}\right) \quad \text{... (4.97)}$$

It is obvious from the definition of the Poisson brackets that

$$[u,v] = -[v,u] \quad \text{... (4.98)}$$

i.e. , the Poisson brackets are anti-commutative.

Similarly, the Poisson bracket of a function with itself is identically zero. Thus,

$$[u,u] = 0, \quad [v,v] = 0 \quad \text{... (4.99)}$$

Moreover,
$$[u,c] = 0 = [v,c] \quad \text{... (4.100)}$$

Where c is independent of q or p.

The Poisson bracket obeys the distributive law of algebra.

$$[u+v,w] = [u,w] + [v,w] \quad \text{... (4.101)}$$

Similarly
$$[u,vw] = [u,v]w + v[u,w] \quad \text{... (4.102)}$$

The above properties can be proved by using the definition and the elementary properties of differentiation and are left to the reader as an exercise.

Another important property of the Poisson brackets is

$$[q_j, p_k] = \delta_{jk}$$

Where δ_{jk} is the Kronecker delta.

To prove this property, we write the expansion

$$[u,v] = \sum_l \left(\frac{\partial u}{\partial q_l}\frac{\partial v}{\partial p_l} - \frac{\partial u}{\partial p_l}\frac{\partial v}{\partial q_l}\right)$$

as
$$[q_j, p_k] = \sum_l \left(\frac{\partial q_j}{\partial q_l}\frac{\partial p_k}{\partial p_l} - \frac{\partial q_j}{\partial p_l}\frac{\partial p_k}{\partial q_l}\right)$$

But, $\dfrac{\partial q_j}{\partial q_l} = \delta_{jl}$, $\dfrac{\partial p_k}{\partial p_l} = \delta_{kl}$ and $\dfrac{\partial q_j}{\partial p_l} = 0 = \dfrac{\partial p_k}{\partial q_l}$, and $\sum_l \delta_{jl}\delta_{kl} = \delta_{jk}$

Hence, we are left with

$$[q_j, p_k] = \delta_{jk} \quad \text{... (4.103)}$$

It can also be proved that

$$[u, q_j] = -\frac{\partial u}{\partial p_j} \quad \text{and} \quad [u, p_j] = +\frac{\partial u}{\partial q_j} \quad \text{... (4.104)}$$

Let us consider a very important identity called Jacobi's identity satisfied by Poisson brackets. The identity is

$$[u,[v,w]] + [v,[w,u]] + [w,[u,v]] = 0 \quad \text{... (4.105)}$$

The definition of the Poisson bracket can be written as

$$[u,v] = \sum_{k=1}^{n} \left(\frac{\partial u}{\partial q_k}\frac{\partial v}{\partial p_k} - \frac{\partial u}{\partial p_k}\frac{\partial v}{\partial q_k}\right) v$$

$$\equiv D_u v \equiv \sum_{i=1}^{2n} \alpha_i \frac{\partial v}{\partial \xi_i} \quad \text{... (4.106)}$$

Where D_u is an operator defined by

$$D_u = \sum_{i=1}^{2n} \alpha_i \frac{\partial}{\partial \xi_i} \qquad \dots (4.107)$$

and ξ_i represents a set of q_i and p_i variables. Similarly

$$D_v = \sum_{j=1}^{2n} \beta_j \frac{\partial}{\partial \xi_j}$$

The first two terms of the identity (equation 4.105) are

$$\begin{aligned}[u,[v,w]] + [v,[w,u]] &= [u,[v,w]] - [v,[u,w]] \\ &= D_u(D_v w) - D_v(D_w w) \\ &= (D_u D_v - D_v D_u) w \\ &= \sum_{i,j} \alpha_i \frac{\partial}{\partial \xi_i}\left(\beta_j \frac{\partial w}{\partial \xi_j}\right) - \sum_{i,j} \beta_j \frac{\partial}{\partial \xi_j}\left(\alpha_i \frac{\partial w}{\partial \xi_i}\right)\end{aligned}$$

$$\therefore [u,[v,w]] + [v,[w,u]] = \sum_{i,j} \alpha_i \beta_j \frac{\partial^2 w}{\partial \xi_i \partial \xi_j} - \sum_{i,j} \alpha_i \beta_j \frac{\partial^2 w}{\partial \xi_j \partial \xi_i} + \sum_{i,j}\left(\alpha_i \frac{\partial \beta_j}{\partial \xi_i}\frac{\partial w}{\partial \xi_j} - \beta_j \frac{\partial \alpha_i}{\partial \xi_j}\frac{\partial w}{\partial \xi_i}\right) \qquad \dots (4.108)$$

The first two terms on the RHS of equation (4.108) cancel each other since the order of differentiation is unimportant. Further, by using the property that the sum is not affected if the indices are interchanged (that is why they are sometimes called the *dummy* indices), we can write the above expression as

$$\begin{aligned}[u,[v,w]] + [v,[w,u]] &= \sum_{i,j}\left(\alpha_i \frac{\partial \beta_j}{\partial \xi_i} - \beta_j \frac{\partial \alpha_i}{\partial \xi_i}\right)\frac{\partial w}{\partial \xi_j} \\ &\equiv \sum_i \left(A_j \frac{\partial w}{\partial p_i} + B_j \frac{\partial w}{\partial q_i}\right) \qquad \dots (4.109)\end{aligned}$$

Where we have now used variables q_i and p_i, and the coefficients of partial derivatives of w are expressed through constants A_j and B_j. Let us determine the constants by taking $w = p_j$. We have

$$[u,[v,p_j]] - [v,[u,p_j]] = A_j$$

Or

$$A_j = \left[u, \frac{\partial v}{\partial q_j}\right] - \left[v, \frac{\partial u}{\partial q_i}\right]$$

$$\therefore A_j = \left[u, \frac{\partial v}{\partial q_j}\right] + \left[\frac{\partial u}{\partial q_j}, v\right]$$

$$\therefore A_j = \frac{\partial}{\partial q_j}[u, v] \qquad \dots (4.110)$$

Where we have used equation (4.104). Similarly, when we take $w = q_j$, we get, by using equation (4.104),

$$B_j = [u,[v,q_j]] - [v,[u,q_j]]$$

$$\therefore B_j = -\left[u, \frac{\partial v}{\partial p_j}\right] + \left[v, \frac{\partial u}{\partial p_j}\right]$$

$$\therefore B_j = -\frac{\partial}{\partial p_j}[u, v] \qquad \dots(4.111)$$

Substituting coefficients A_j and B_j in equation (4.109), we get

$$[u, [v, w]] + [v, [w, u]] = \sum_i \left(\frac{\partial w}{\partial p_i}\frac{\partial}{\partial q_j}[u, v] - \frac{\partial w}{\partial q_i}\frac{\partial}{\partial p_j}[u, v]\right)$$
$$= -[w, [u, v]]$$

This is the Jacobi's identity.

We now prove that the Poisson brackets are also invariant under canonical transformations. Let $F$and G be any two arbitrary functions. Then,

$$[F, G]_{q,p} = \sum_j \left(\frac{\partial F}{\partial q_j}\frac{\partial G}{\partial p_j} - \frac{\partial F}{\partial p_j}\frac{\partial G}{\partial q_j}\right) \qquad \dots(4.112)$$

Suppose that, q_j, p_j are functions of new coordinates Q_k, P_k, then equation (4.112) becomes

$$[F, G]_{q,p} = \sum_{jk}\left[\frac{\partial F}{\partial q_j}\left(\frac{\partial G}{\partial Q_k}\frac{\partial Q_k}{\partial p_j} + \frac{\partial G}{\partial P_k}\frac{\partial P_k}{\partial p_j}\right) - \frac{\partial F}{\partial p_j}\left(\frac{\partial G}{\partial Q_k}\frac{\partial Q_k}{\partial q_j} + \frac{\partial G}{\partial P_k}\frac{\partial P_k}{\partial q_j}\right)\right]$$

$$\therefore [F, G]_{q,p} = \sum_k \left\{\frac{\partial G}{\partial Q_k}[F, Q_k]_{q,p} + \frac{\partial G}{\partial P_k}[F, P_k]_{q,p}\right\} \qquad \dots(4.113)$$

When we consider a special case of $F = Q_k$, we get by changing G to F from equation (4.113)

$$[Q_k, F]_{q,p} = \sum_j \frac{\partial F}{\partial Q_j}[Q_k, Q_j] + \sum_j \frac{\partial F}{\partial P_j}[Q_k, P_j] \qquad \dots(4.114)$$

$$\therefore [Q_k, F]_{q,p} = \sum_j \frac{\partial F}{\partial P_j}\delta_{jk} \qquad \dots(4.115)$$

Where we have used equation (4.103). We can write

$$[F, Q_k] = -\frac{\partial F}{\partial P_k} \qquad \dots(4.116)$$

Similarly, we can prove that

$$[F, P_k] = \frac{\partial F}{\partial Q_k} \qquad \dots(4.117)$$

Hence, the expression for $[F, G]_{q,p}$ becomes

$$[F, G]_{q,p} = \sum_k \left(\frac{\partial F}{\partial Q_k}\frac{\partial G}{\partial P_k} - \frac{\partial G}{\partial Q_k}\frac{\partial F}{\partial P_k}\right) = [F, G]_{Q,P} \qquad \dots(4.118)$$

Equation (4.118) shows that the Poisson bracket is also invariant under canonical transformation in the phase space. Hence, there is no need of writing the subscripts (q, p) or (Q, P) on the Poisson brackets.