Hamilton's equation of motion

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In Lagrangian mechanics the system is represented by $\left(q_j, \dot{q}_j, t\right)$,i.e. generalized position and generalized velocities

$$L = L\left(q_i, \dot{q}_i, t\right)$$

In contrast **Hamiltonian mechanics** the system is represented by $\left(q_i, p_i, t\right)$ generalized position and generalized momenta

$$H = H\left(q_i, p_i, t\right) \longrightarrow$$ **Hamiltonian of the system**

In Lagrangian mechanics the generalized momenta is

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

The transformation is in between

$$L\left(q_i, \dot{q}_i, t\right) \Rightarrow H\left(q_i, \frac{\partial L}{\partial \dot{q}_i}, t\right) = H\left(q_i, p_i, t\right)$$

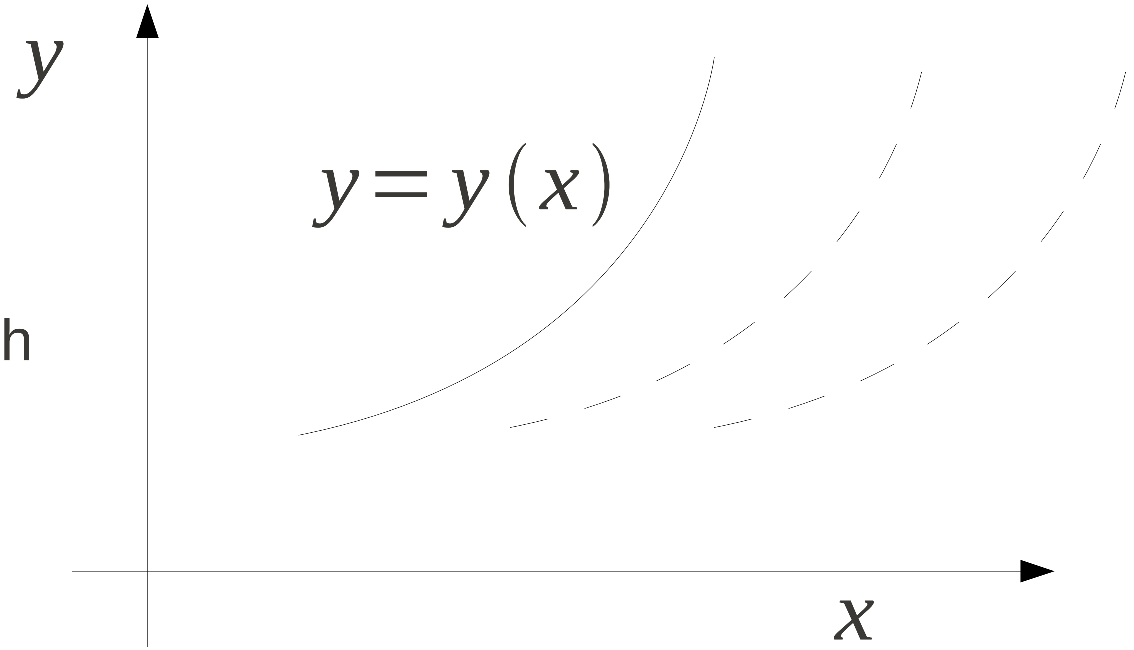
Such a transformation is achieved by **Legendre transforms**

Principles Legendre transformation

Legendre transformation can be explained by geometrical means

Consider a function of a single variable

$$y = y(x)$$



Represent the derivative of y with respect to x is given by

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

If we have to keep p as and independent variable

Eliminate x form the above two equations and obtain $y = y(p)$

For example let us choose a function $y(x) = k x^2 + g$

$$\frac{dy}{dx} = p = 2kx$$

Now from the new representation old representation cannot be obtained uniquely by integration

$$y = y(p)$$

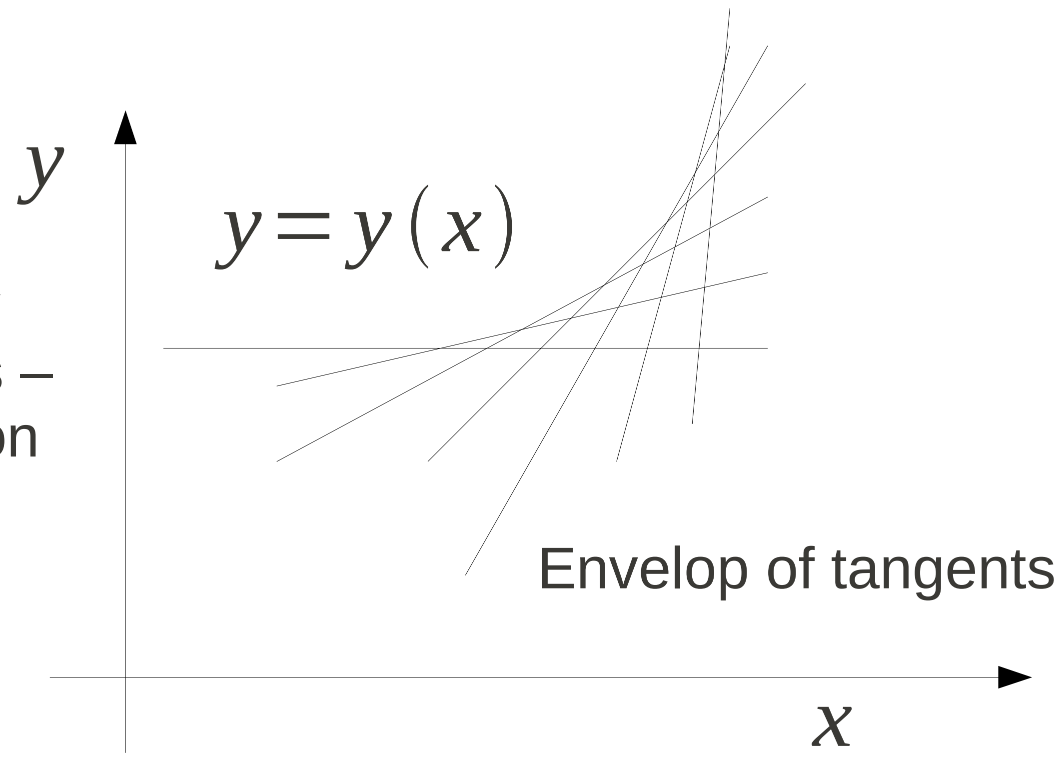
$$y(p) = 2kx$$

$$\int y(p)\,dx = k x^2$$

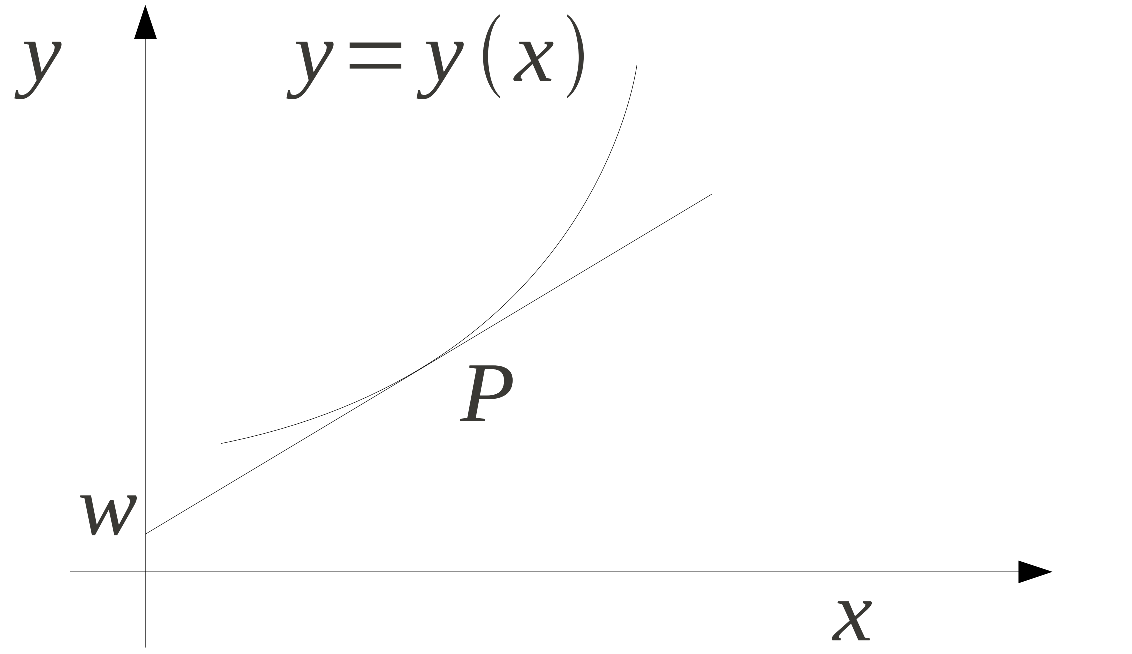
We get a family of curves – see the the lines

Therefore the representation is not unique so we do not get back the original representation

Every point if need to be represented by lines is given by slope and intercept on the y axis – equivalent representation position space is by point (x,y). In both cases two numbers need to represent same information



Let the slope be p and the intercept be w



$$p=\frac{y-w}{x-0}$$

$$w=y-p\,x$$

That is $w=w(p)$

$$d\,w=d\,y-dp\,x-p\,dx$$

We have the relations using this

$$\frac{d\,y}{d\,x}=p\,,\qquad d\,y=p\,dx$$

$$\Rightarrow d\,w=-dp\,x$$

$$\Rightarrow \frac{d\,w}{d\,p}=-x$$

That leads to relation $y=w+p\,x$

Forward transformation

$$y = y(x)$$

$$\frac{d\,y}{d\,x} = p$$

$$w = y - p\,x$$

Elimination of x and y yields

$$w = w(p)$$

Reverse transformation

$$w = w(p)$$

$$\frac{d\,w}{d\,p} = -x$$

$$y = w + p\,x$$

Elimination of p and w yields

$$y = y(x)$$

For the trial function we may perform the forward and backward transformation to get original function back

Let $y(x) = x^2 + g$

$$\frac{d\,y}{d\,x} = p \; = 2\,x$$

Let $y(x)=x^2+g$

$$w=y-px$$

$$\frac{dy}{dx}=p=2x$$

Using the relation $y(x)=x^2+g$

$$w=x^2+g-px$$

Using the relation $x=\frac{p}{2}$

$$w=\frac{p^2}{4}+g-\frac{p^2}{2} \quad =g-\frac{p^2}{4}$$

Now using reverse transformation of $w=y-px$

$$y=w+px$$

Using the relation $p=2x,$

$$y=-\frac{p^2}{4}+g+px$$

$$y=-4\frac{x^2}{4}+g+2x^2$$

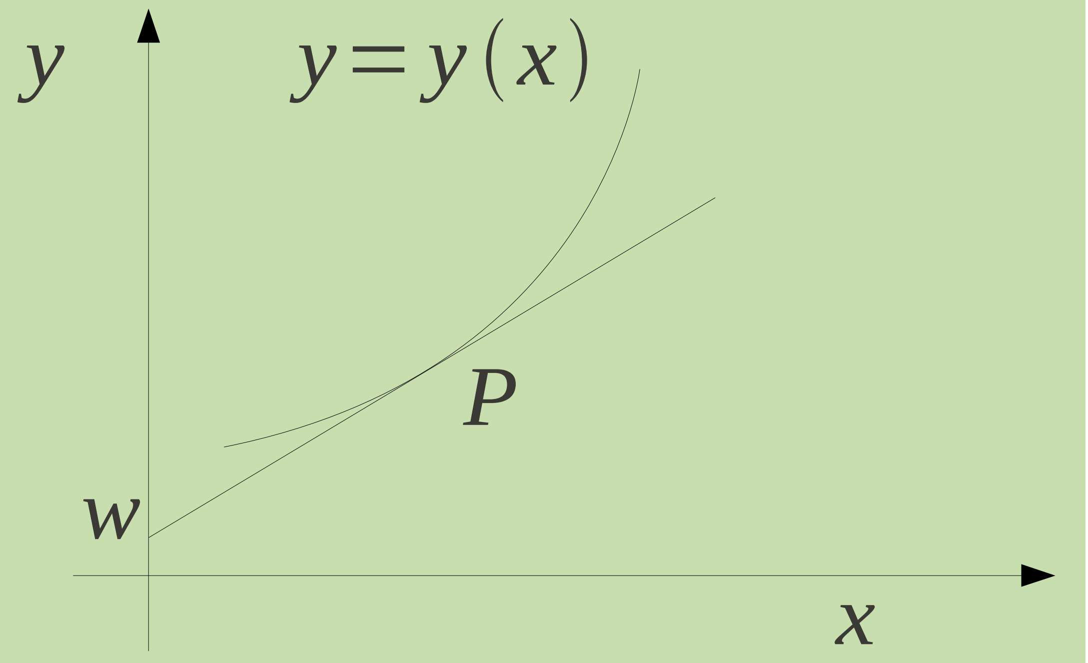
$$y=x^2+g$$

Legendre' transform of two variable

$$f(x,y) \Rightarrow g(x,u) \qquad u = \frac{\partial f}{\partial y}$$

$$f(x,y) \Rightarrow g\left(x, \frac{\partial f}{\partial y}\right)$$ with

Let the slope be p and the intercept be w



$$p = \frac{y-w}{x-0}$$

$$w = y - p\,x$$

That is $w = w(p)$

extending this relation to many variables $g(x,u) = u\,y - f(x,y)$

Legendre' transform of two variable

$$f(x,y) \Rightarrow g(x,u) \quad \text{with} \quad u = \frac{\partial f}{\partial y}$$

$$f(x,y) \Rightarrow g\left(x, \frac{\partial f}{\partial y}\right)$$

$$g(x,u) = u\,y - f(x,y)$$

$$d\,g = y\,d\,u + u\,dy - df$$

$$= y\,d\,u + u\,dy - \frac{\partial f}{\partial x}\,d\,x - \frac{\partial f}{\partial y}\,d\,y$$

$$= y\,d\,u + \cancel{u\,dy} - \frac{\partial f}{\partial x}\,d\,x \cancel{- u\,d\,y}$$

$$= y\,d\,u - \frac{\partial f}{\partial x}\,d\,x$$

$$g(x,u)=u\,y-f(x,y)$$

$$dg=y\,du-\frac{\partial f}{\partial x}dx$$

From this relation we can obtain the relations

$$\frac{\partial g}{\partial u}=y$$

$$\frac{\partial g}{\partial x}=\frac{\partial f}{\partial x}$$

Using these relation and extending this relation for n degrees of freedom the **Hamiltonian** of the system may be obtained from the **Lagrangian** of the system

$$H(q_i,p_i,t)=\sum_i p_i\dot{q}_i-L(q_i,\dot{q}_i,t)$$

The **Hamiltonian** of the system is now defined as

$$H(q_i, p_i, t) = \sum_i p_i \dot{q}_i - L(q_i, \dot{q}_i, t)$$

The equation of motion in the Hamiltonian formalism is obtained by taking first total derivative of the Hamiltonian

$$dH = \sum_i p_i d\dot{q}_i + \dot{q}_i d p_i - dL(q_i, \dot{q}_i, t)$$

In this relation the total differential of the Lagrangian is

$$dL = \sum_i \frac{\partial L}{\partial q_i} d q_i + \sum_i \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i + \frac{\partial L}{\partial t} dt$$

Substituting using terms of Lagrangian equation of motion and definition of generalized momentum

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \frac{\partial L}{\partial q_i} \qquad \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = \dot{p}_i$$

$$dL=\sum_i \frac{\partial L}{\partial q_i}dq_i+\sum_i \frac{\partial L}{\partial \dot{q}_i}d\dot{q}_i+\frac{\partial L}{\partial t}dt$$

$$dL=\sum_i \dot{p}_i dq_i+\sum_i p_i d\dot{q}_i+\frac{\partial L}{\partial t}dt$$

Combining with differential change in the Hamiltonian

$$dH=\sum_i p_i d\dot{q}_i+\dot{q}_i dp_i-dL(q_i,\dot{q}_i,t)$$

$$=\sum_i \cancel{p_i d\dot{q}_i}+\dot{q}_i dp_i-\sum_i \dot{p}_i dq_i-\sum_i \cancel{p_i d\dot{q}_i}-\frac{\partial L}{\partial t}dt$$

$$=\sum_i \dot{q}_i dp_i-\sum_i \dot{p}_i dq_i-\frac{\partial L}{\partial t}dt$$

The Hamiltonian only depends on position and momenta

$$H=H(q_i,p_i,t)$$

$$dH=\sum_i \dot{q}_i\, dp_i-\sum_i \dot{p}_i\, dq_i-\frac{\partial L}{\partial t}dt$$

If we take differential change of the Hamiltonian in terms of generalized momenta and generalized position.

$$dH=\sum_i \frac{\partial H}{\partial p_i}dp_i+\sum_i \frac{\partial H}{\partial q_i}dq_i+\frac{\partial H}{\partial t}dt$$

Now comparing these equations we arrive Hamilton's equation of motion

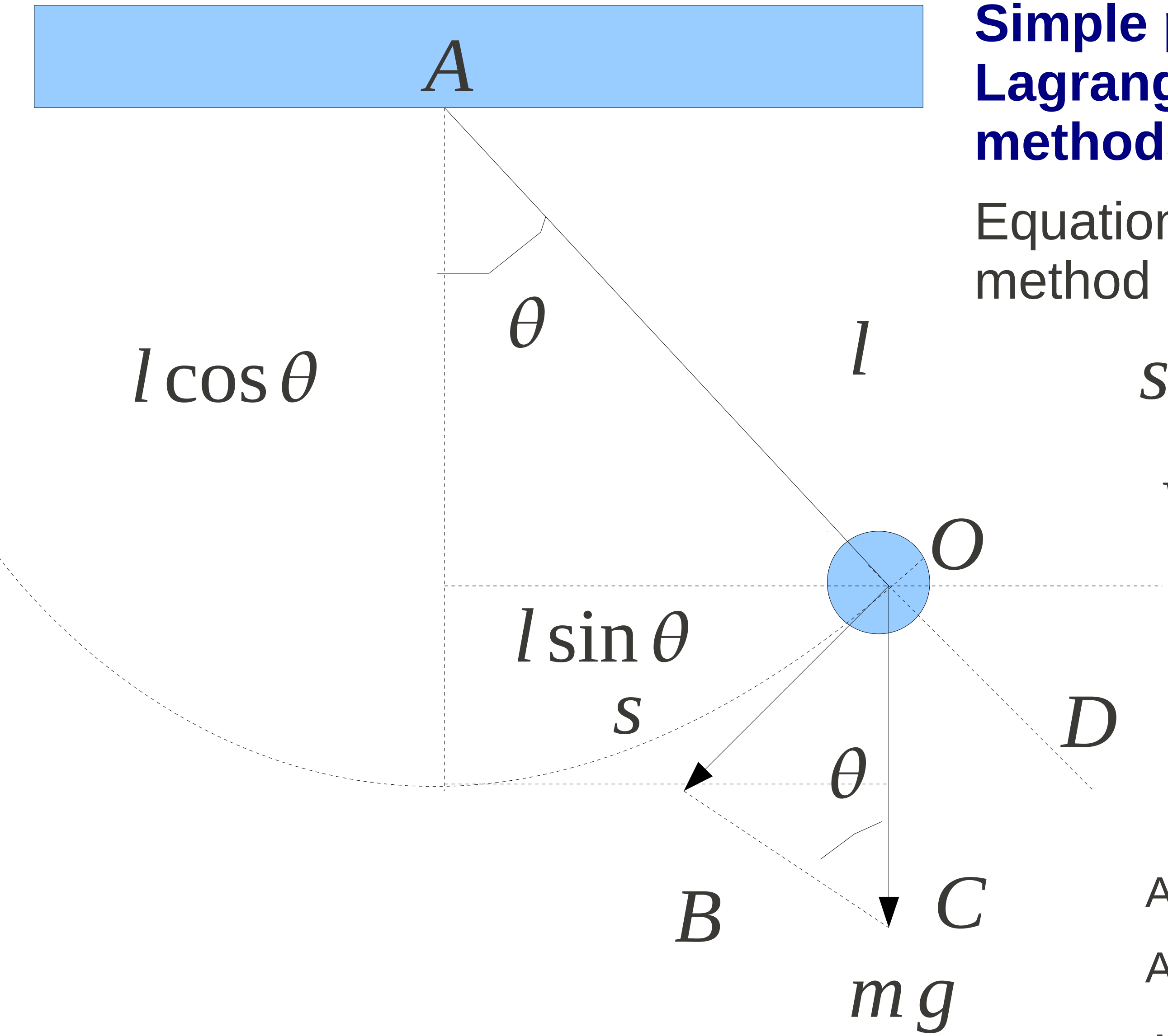
$$\dot{q}_i=\frac{\partial H}{\partial p_i} \qquad \dot{p}_i=-\frac{\partial H}{\partial q_i} \qquad \frac{\partial H}{\partial t}=-\frac{\partial L}{\partial t}$$

The Hamiltonian is constructed using the equation

$$H(q_i, p_i, t)=\sum_i p_i\dot{q}_i-L(q_i, \dot{q}_i, t)$$

In Lagrangian formalism there are N differential equations of second order. In contrast Hamiltonian formalism leads to 2N differential equation of first order.

Simple pendulum by Newtonian Lagrangian and Hamiltonian methods



Equation of motions by Newton's method

$$s = l\theta$$

$$v = \frac{ds}{dt} = l\frac{d\theta}{dt}$$

$$a = \frac{d^2 s}{dt^2} = l\frac{d^2\theta}{dt^2}$$

Angle AOB= angle DOB = 90

Angle COD is

Angle COB is $90^o - \theta$

Angle OCB is θ

Direction of l is perpendicular to θ

$$mg\sin\theta = -ml\frac{d^2\theta}{dt^2}$$

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$$\sin\theta = \theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} + \dots\dots\dots \qquad \frac{d^2\theta}{dt^2} = -\frac{g}{l}\theta$$

By Lagrangian methods

The Kinetic energy of the simple pendulum is given by

$$T = \frac{1}{2}mv^2 = \frac{1}{2}m(l\dot{\theta})^2 = \frac{1}{2}ml^2\dot{\theta}^2$$

The potential energy is given by

$$V = mgh = mgl(1-\cos\theta)$$

$$L = T - V$$ the Lagrangian

$$= \frac{1}{2}ml^2\dot{\theta}^2 - mgl(1-\cos\theta)$$

$$\frac{\partial L}{\partial\theta} = -mgl\sin\theta \qquad \left(\frac{\partial L}{\partial\dot{\theta}}\right) = ml^2\dot{\theta}$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial\dot{\theta}}\right) = \frac{\partial L}{\partial\theta} \qquad \ddot{\theta} = -\frac{g}{l}\sin\theta$$

By Hamiltonian methods

$$L=\frac{1}{2}ml^2\dot{\theta}^2-mgl(1-\cos\theta)$$

By Hamiltonian mechanics – the energy terms have to be expressed in terms of momentum

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

We know

$$T=\frac{1}{2}mv^2=\frac{1}{2}ml^2\dot{\theta}^2$$

The kinetic energy in terms of the generalized momenta

$$T=\frac{1}{2}ml^2\dot{\theta}^2=\frac{1}{2}\frac{(ml^2\dot{\theta})^2}{ml^2}=\frac{1}{2}\frac{p_\theta^2}{ml^2}$$

The Hamiltonian of the system is given by

$$H=\frac{1}{2}\frac{p_\theta^2}{ml^2}+mgl(1-\cos\theta)$$

The Hamiltonian of the system is given by

$$H = \frac{1}{2}\frac{p_\theta^2}{ml^2} + mgl(1 - \cos\theta)$$

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = -mgl\sin\theta$$ using $$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

$$\dot{\theta} = \frac{\partial H}{\partial p_\theta} = \frac{p_\theta}{ml^2}$$ using $$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

$$\Rightarrow \dot{\theta}ml^2 = p_\theta$$

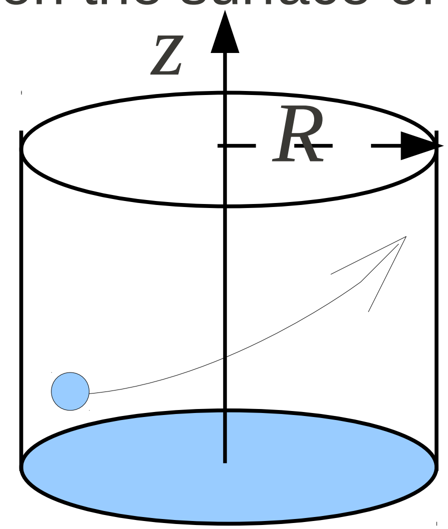
Differentiating once more

$$\Rightarrow \dot{p}_\theta = ml^2\ddot{\theta}$$

$$\Rightarrow ml^2\ddot{\theta} = -mgl\sin\theta$$

$$\ddot{\theta} = -\frac{g}{l}\sin\theta$$

Equation of motion of particle constrained to move on the surface of a cylinder. The Particle is subject a radial force



Mass of the particle m

Equation of the cylinder $x^2 + y^2 = R^2$

Central force $\vec{F} = -k\vec{r}$

Potential corresponding to the force $U = \frac{1}{2}kr^2 = \frac{1}{2}(x^2 + y^2 + z^2)$

$$U = \frac{1}{2}kr^2 = \frac{1}{2}k(R^2 + z^2)$$

The velocity in cylindrical coordinates

$$v^2 = \dot{R}^2 + R^2\dot{\theta}^2 + \dot{z}^2$$

Since R is a constant the kinetic energy is $T = \frac{1}{2}m(R^2\dot{\theta}^2 + \dot{z}^2)$

The Lagrangian is given by

$$L = T - V = \frac{1}{2} m \left(R^2 \dot{\theta}^2 + \dot{z}^2 \right) - \frac{1}{2} k \left(R^2 + z^2 \right)$$

Formulation Hamiltonian mechanics requires formulation of the problem in terms of momentum representation

Now the generalized momenta is given using Lagrangian mechanics

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = m R^2 \dot{\theta} \qquad p_z = \frac{\partial L}{\partial \dot{z}} = m \dot{z}$$

The Hamiltonian of the system can be expressed in terms of the generalized momentum representation as

$$H(z, p_\theta, p_z) = T + U \quad = \frac{p_\theta^2}{2 m R^2} + \frac{p_z^2}{2m} + \frac{1}{2} k z^2$$

The constant part is now suppressed

$$\dot{p}_\theta = -\frac{\partial H}{\partial \theta} = 0 \qquad \dot{p}_z = -\frac{\partial H}{\partial z} = -k z$$

$$H=\frac{p_\theta^2}{2mR^2}+\frac{p_z^2}{2m}+\frac{1}{2}kz^2$$

The Hamilton's equations also have

$$\dot{\theta}=\frac{\partial H}{\partial p_\theta}=\frac{p_\theta}{mR^2} \qquad \dot{z}=\frac{\partial H}{\partial p_z}=\frac{p_z}{m}$$

They are same as that obtained from generalized momenta from Lagrangian formalism

$$\dot{p}_\theta=-\frac{\partial H}{\partial \theta}=0 \qquad p_\theta=\frac{\partial L}{\partial \dot{\theta}}=mR^2\dot{\theta}$$

$$\Rightarrow p_\theta=mR^2\dot{\theta}=constant$$

Angular momentum about the symmetry axis is conserved. Now combine equations

$$\dot{p}_z=-\frac{\partial H}{\partial z}=-kz \qquad p_z=\frac{\partial L}{\partial \dot{z}}=m\dot{z}$$

$$\dot{p}_z = -\frac{\partial H}{\partial z} = -k\,z \qquad p_z = \frac{\partial L}{\partial \dot{z}} = m\,\dot{z}$$

combining $$m\,\ddot{z} = -k\,z$$

$$\ddot{z} + \omega^2 z = 0 \qquad \omega^2 = \frac{k}{m}$$

This is the equation for harmonic motion – that is, the particle exhibit harmonic motion along z direction.

Phase space dynamics (q, p)

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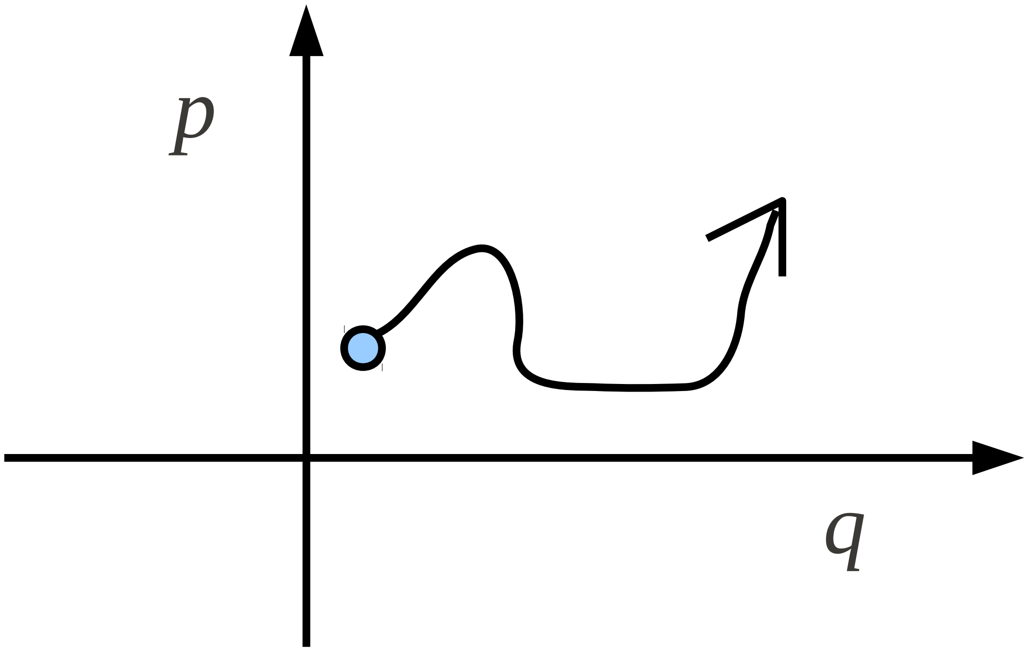
Hamiltonian dynamics is best represented in phase space which is similar to configuration space but include the momentum coordinates also

Representation of one dimensional motion in the phase space



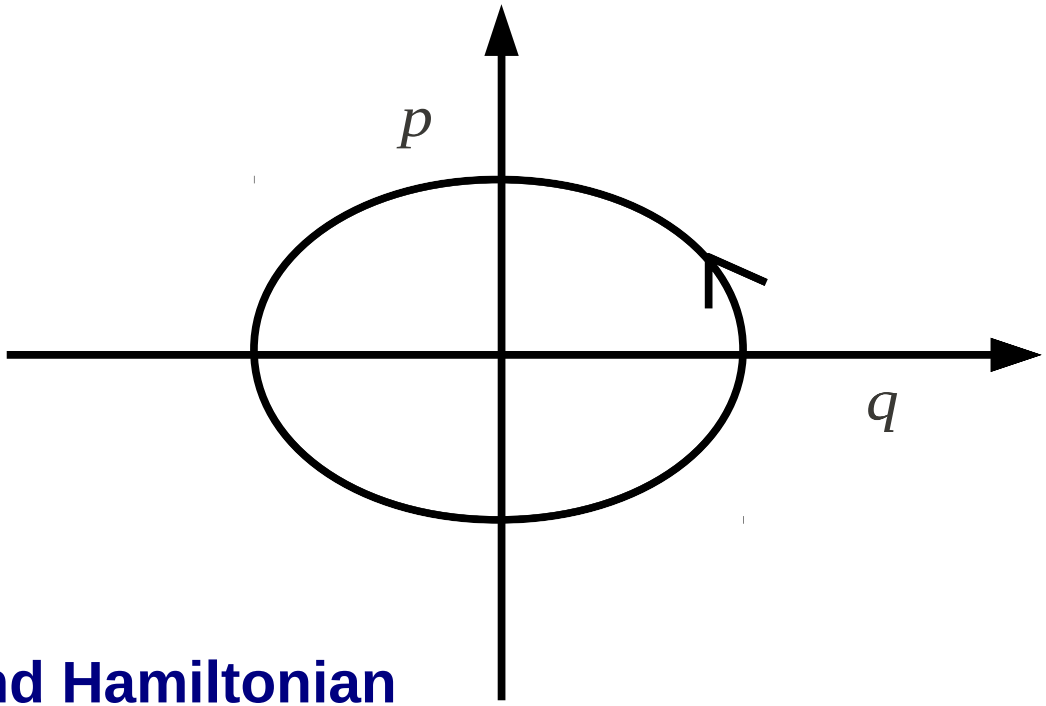
In phase space for system that have n degrees freedom is represented by a point that have 2n coordinates

$$(q_{1,} q_{2,} \dots q_n, p_{1,} p_{2,} \dots p_n)$$

Phase space of simple harmonic oscillator is defined by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2} k x^2$$

$$H=\frac{p^2}{2m}+\frac{1}{2}kq^2$$



Conservation of energy and Hamiltonian

When Hamiltonian has no explicit dependence on time it is a constant of motion

$$\frac{dH}{dt}=\sum_i\frac{\partial H}{\partial q_i}\dot{q}_i+\sum_i\frac{\partial H}{\partial p_i}\dot{p}_i$$

$$\dot{q}_i=\frac{\partial H}{\partial p_i}$$

$$\frac{dH}{dt}=\sum_i\frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i}-\sum_i\frac{\partial H}{\partial p_i}\frac{\partial H}{\partial q_i}$$

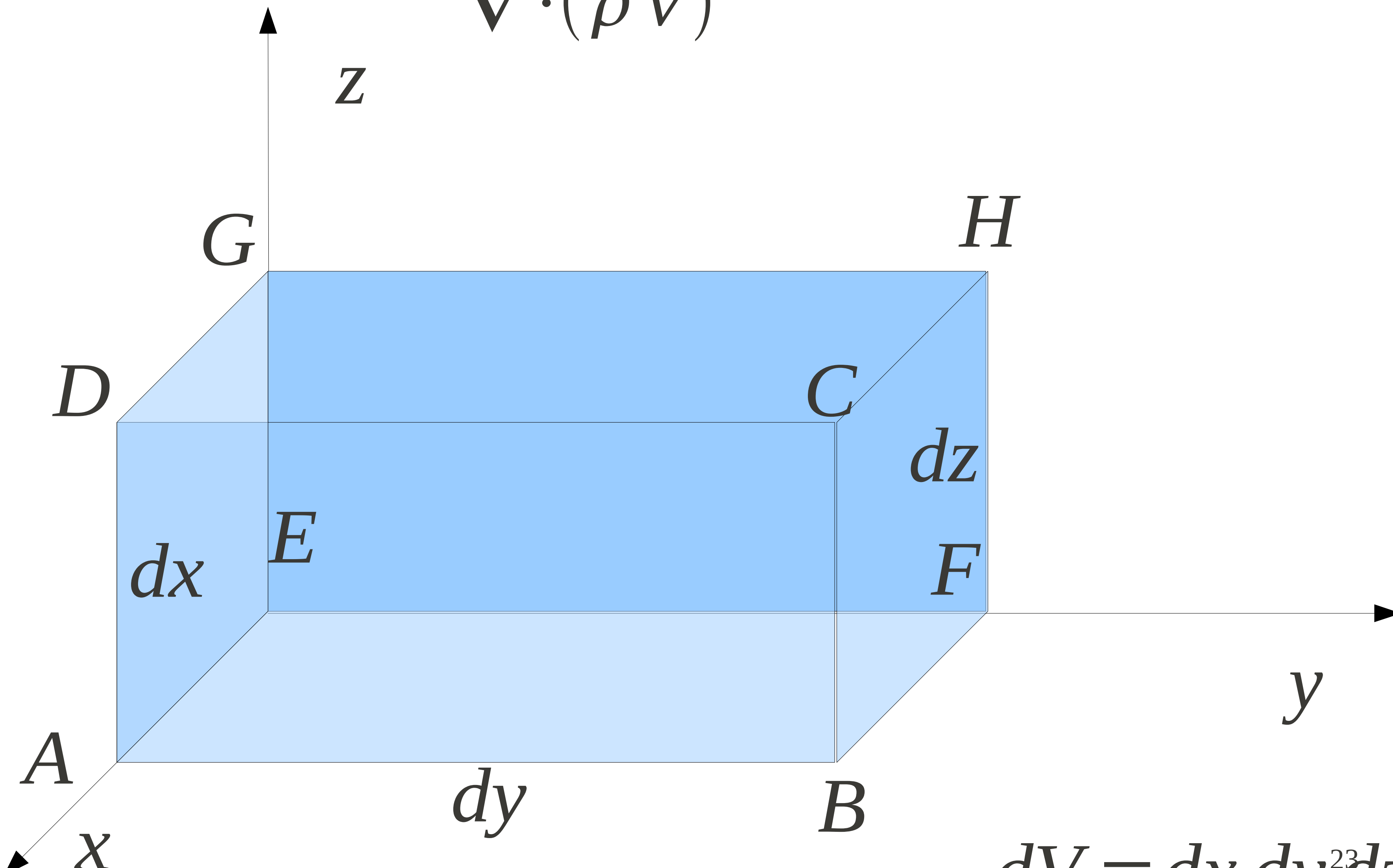
$$\dot{p}_i=-\frac{\partial H}{\partial q_i}$$

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

Physical meaning of divergence of fluid - from module I

Velocity of a compressible fluid with density $\rho(x, y, z)$ is $\vec{v}$

$$\vec{\nabla}\cdot(\rho\,\vec{v})$$



$$dV = dx\,dy\,dz$$

Consider a small volume defined by the element

$$dV = dx\,dy\,dz$$

The component of the flow are $\left(\rho v_x, \rho v_y, \rho v_z\right)$

fluid flowing into this volume through the face EFGH per unit time

$$\rho v_x\big|_{x=0} dy\,d\,z$$

other components $\rho v_y, \rho v_z$ have no contribution in this direction

fluid flowing into this volume through the face ABCD per unit time

$$\rho v_x\big|_{x=dx} dy\,d\,z$$

This quantity is expanded as

$$\rho v_x\big|_{x=dx} dy\,d\,z = \left[\rho v_x + \frac{\partial}{\partial x}(\rho v_x)\,dx\right]_{x=0} dy\,dz$$

Original flow　　　　Correction in the flow

The net flow out is at face ABCD $= \frac{\partial}{\partial x}(\rho v_x)\, dx\, dy\, dz$

We can arrive at the result as

$$= \lim_{\Delta x \to 0} \frac{\rho v_x(\Delta x, 0, 0) - \rho v_x(0,0,0)}{\Delta x}$$

$$= \frac{\partial}{\partial x}(\rho v_x(x, y, z))\Big|_{0,0,0}$$

The formulation in the x direction can adapted into y and z direction also

By change of the coordinates

$$x \rightarrow y \quad y \rightarrow z$$

Total net flow out the volume is

$$= \left(\frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial y}(\rho v_y) + \frac{\partial}{\partial z}(\rho v_z) \right) dx\, dy\, dz$$

$$= \vec{\nabla} \cdot (\rho \vec{v})\, dx\, dy\, dz$$

The net flow out the volume element $dx\,dy\,dz$ out of a compressible fluid is $= \vec{\nabla} \cdot (\rho \vec{v})$

Application of divergence: rate of change of density with respect time is equal to the divergence velocity field of that liquid element

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot (\rho \vec{v}) = 0$$

Phase space and the Liouville's theorem

The representative point moves in phase space along a unique path

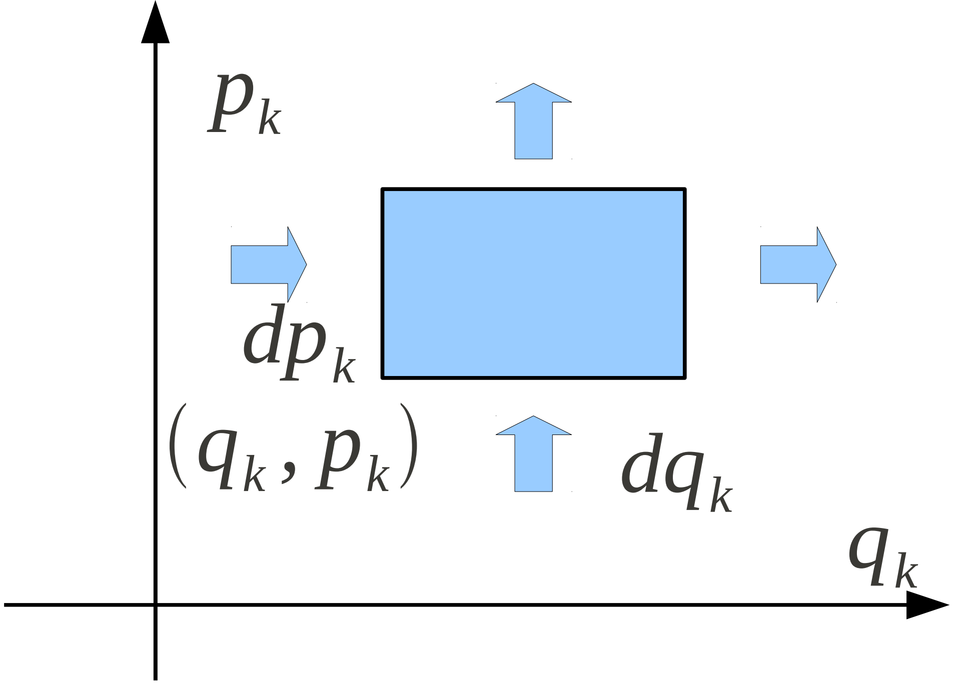
when the initial conditions are given it is possible to predict the future of the trajectory from the initial condition.

The trajectory can be obtained from the Hamiltonian of the system

As the degree of freedom increases in a system, for example in system of gas molecules, it is impossible to determine all initial conditions and therefore we need to devise a method to study the dynamics of such systems

Since representative points move along a unique path and these paths never intersect, therefore the paths covers the phase space sufficiently closely so that a dynamic density of such paths may give useful information regarding the dynamics of the system

Let us consider number of trajectories passing through a small area then the number of phase space points in that area



$$N = \rho\, dv$$

where $$dv = dq_1\, dq_2 \ldots\ldots dq_n\, dp_1\, dp_2 \ldots\ldots dp_n$$

Consider and element of area as shown in the figure

Number of phase space points entering the area from the left

$$\rho \frac{dq_k}{dt} dp_k = \rho\, \dot{q}_k\, dp_k$$

Number of phase space points entering the area from the bottom

$$\rho \frac{dp_k}{dt} dq_k = \rho\, \dot{p}_k\, dq_k$$

Total points entering the area is given by

$$\rho \left(\dot{p}_k\, dq_k + \dot{q}_k\, dp_k \right)$$

Total point exiting from the opposite side is given by

$$\left[\rho\, \dot{q}_k + \frac{\partial(\rho\, \dot{q}_k)}{\partial\, q_k} dq_k \right] dp_k + \left[\rho\, \dot{p}_k + \frac{\partial(\rho\, \dot{p}_k)}{\partial\, p_k} dp_k \right] dq_k$$

Net change of density in this in area in $d\, q_k\, d\, p_k$ per unit time is given by

$$\frac{\partial \rho}{\partial t} dq_k\, dp_k$$

$$\frac{\partial \rho}{\partial t} dq_k\, dp_k = \rho\left(\dot{p}_k\, dq_k + \dot{q}_k\, dp_k\right)$$

$$-\left[\rho\, \dot{q}_k + \frac{\partial(\rho\, \dot{q}_k)}{\partial q_k} dq_k\right] dp_k - \left[\rho\, \dot{p}_k + \frac{\partial(\rho\, \dot{p}_k)}{\partial p_k} dp_k\right] dq_k$$

That means

$$\frac{\partial \rho}{\partial t} dq_k\, dp_k = -\left[\frac{\partial(\rho\, \dot{q}_k)}{\partial q_k} + \frac{\partial(\rho\, \dot{p}_k)}{\partial p_k}\right] dq_k\, dp_k$$

In expanded form

$$\frac{\partial \rho}{\partial t} = -\left[\frac{\partial \rho}{\partial q_k} \dot{q}_k + \rho \frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \rho}{\partial p_k} \dot{p}_k + \rho \frac{\partial \dot{p}_k}{\partial p_k}\right]$$

$$\left[\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \dot{p}_k}{\partial p_k}\right]$$

The expression may be simplified using Hamilton's equation of motion

$$\left[\frac{\partial^2 H}{\partial q_k \partial p_k} - \frac{\partial^2 H}{\partial p_k \partial q_k}\right] = 0$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

$$\dot{q}_i = \frac{\partial H}{\partial p_i}$$

The expression may be simplified using Hamilton's equation of motion

$$\frac{\partial \rho}{\partial t} = -\left[\frac{\partial \rho}{\partial q_k}\dot{q}_k + \rho\frac{\partial \dot{q}_k}{\partial q_k} + \frac{\partial \rho}{\partial p_k}\dot{p}_k + \rho\frac{\partial \dot{p}_k}{\partial p_k}\right]$$

$$= -\left[\frac{\partial \rho}{\partial q_k}\dot{q}_k + \frac{\partial \rho}{\partial p_k}\dot{p}_k\right]$$

$$\frac{\partial \rho}{\partial t} = -\left[\frac{\partial \rho}{\partial q_k} \frac{d q_k}{dt} + \frac{\partial \rho}{\partial p_k} \frac{d p_k}{d t} \right]$$

$$\frac{\partial \rho}{\partial t} + \left[\frac{\partial \rho}{\partial q_k} \frac{d q_k}{dt} + \frac{\partial \rho}{\partial p_k} \frac{d p_k}{d t} \right] = 0$$

This is the expression for total time derivative of density

$$\frac{d \rho}{d t} = 0$$

This result is known as **Liouville's** theorem which states that the density of representative points in phase space corresponding to a system of particles remains a constant – This conservation law is valid for phase space. There is no equivalent problem exist in configuration space. This allows us to use probabilistic approach to mechanics, that is called **statistical mechanics** which links thermodynamics and mechanics of particles