Hamiltonian Mechanics

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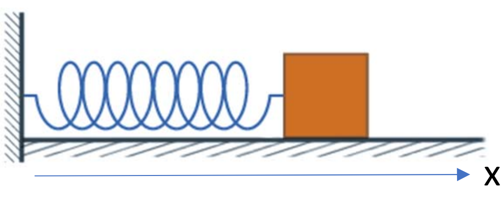
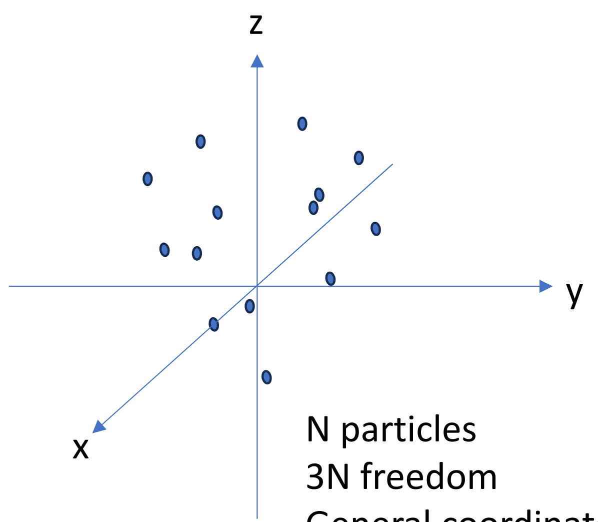
General coordinates and configuration space

- Generalized Coordinates: any n quantities $(q_1, q_2, \ldots, q_n)$ which completely define the position of a system with n degrees of freedom are called generalized coordinates of the system.

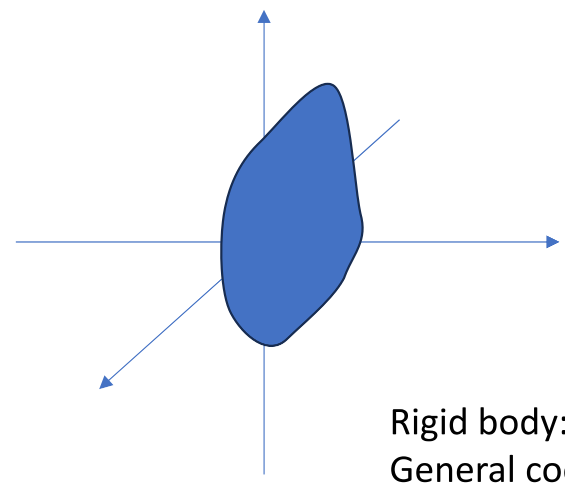


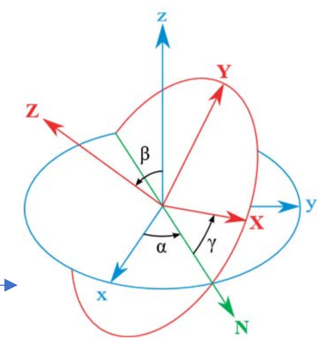
a hormonic oscillator
1 freedom
General coordinates: x



N particles
3N freedom
General coordinates:

$$(x_1, y_1, z_1, x_2, y_2, z_2, \ldots, x_n, y_n, z_n)$$





Rigid body: 6 freedom
General coordinates:

$$(x, y, z, \alpha, \beta, \gamma)$$

- The space defined by the generalized coordinates is called the configuration space of the physical system.

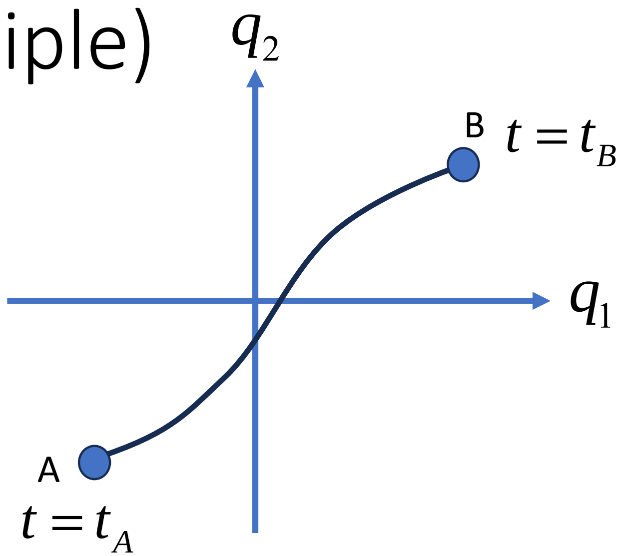
Hamilton's Principle (Least Action Principle)

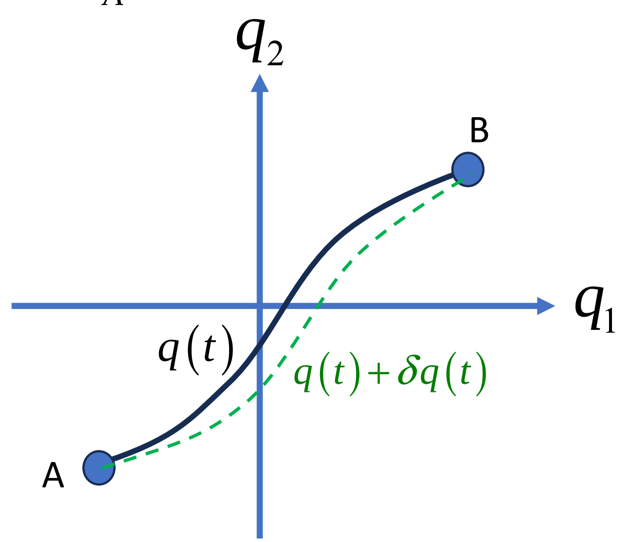
- Since the position of a mechanical system is fully determined by the generalized coordinates, its evolution/motion can be described by a path in the configuration space.
- The Hamilton's principle describes the path that the mechanical system takes to move from point A to point B:

Every mechanical system is characterized by a definite function, $L(q_1, q_2, \ldots \dot{q}_1, \dot{q}_2 \ldots, t)$, and the system moves in such a way that the integral

action → $$S = \int_{t_A}^{t_B} L\left(q_1(t), q_2(t)\ldots, \dot{q}_1(t), \dot{q}_2(t)\ldots, t\right) dt$$

has a stationary value, i.e. $\delta S = 0$ for any infinitesimal deviation from the actual path.





Lagrange's equation

- From the Hamilton principal, we can derive explicitly the equation of motion in terms of second order differential equation, i.e. the Lagrange's equation.

$$\delta S = \int_{t_A}^{t_B} L\left(q_1(t)+\delta q_1(t),\ldots,\dot{q}_1(t)+\delta\dot{q}_1(t),\ldots,t\right)dt - \int_{t_A}^{t_B} L\left(q_1(t),\ldots,\dot{q}(t),\ldots,t\right)dt$$

$$= \int_{t_A}^{t_B}\sum_i \frac{\partial L}{\partial q_i}\delta q_i dt + \int_{t_A}^{t_B}\sum_i \frac{\partial L}{\partial \dot{q}_i}\delta \dot{q}_i dt$$

$$= \int_{t_A}^{t_B}\sum_i \frac{\partial L}{\partial q_i}\delta q_i dt + \int_{t_A}^{t_B}\frac{d}{dt}\left(\sum_i \delta q_i \frac{\partial L}{\partial \dot{q}_i}\right)dt - \int_{t_A}^{t_B}\sum_i \delta q_i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)dt$$

Vanishes since $\delta q_i(t_A)$=0 and $\delta q_i(t_B)$=0

$$= \int_{t_A}^{t_B}\sum_i \left[\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right]\delta q_i dt + \sum_i\left(\delta q_i(t_A)\left.\frac{\partial L}{\partial \dot{q}_i}\right|_{t=t_A} - \delta q_i(t_B)\left.\frac{\partial L}{\partial \dot{q}_i}\right|_{t=t_B}\right)$$

$$= \sum_i \int_{t_A}^{t_B}\left[\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right]\delta q_i dt$$

The Hamilton principle requires δS=0 and δq(t) is arbitrary.

Lagrange's equation

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0$$

Explicitly, this represents a set of n second-order equations

$$\frac{d}{dt}\frac{\partial L(q,\dot{q},t)}{\partial \dot{q}_i} = \frac{\partial L(q,\dot{q},t)}{\partial q_i} \quad \Leftrightarrow \quad \sum_{j=1}^{n}\left(\ddot{q}_j\frac{\partial^2 L(q,\dot{q},t)}{\partial \dot{q}_i\,\partial \dot{q}_j} + \dot{q}_j\frac{\partial^2 L(q,\dot{q},t)}{\partial \dot{q}_i\,\partial q_j} + \frac{\partial^2 L(q,\dot{q},t)}{\partial \dot{q}_i\,\partial t}\right) = \frac{\partial L(q,\dot{q},t)}{\partial q_i}.$$

Some examples of Lagrange's equation

- Free space: $L(x, y, z, \dot{x}, \dot{y}, \dot{z}, t) = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right)$

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0 \Longrightarrow \quad \ddot{x} = 0 \qquad \ddot{y} = 0 \qquad \ddot{z} = 0$$

- A particle in a potential $U(x, y, z)$ $\quad L(x, y, z, \dot{x}, \dot{y}, \dot{z}, t) = \frac{1}{2}m\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right) - U(x, y, z)$

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0 \Longrightarrow \quad m\ddot{x} = -\frac{\partial U}{\partial x} \equiv F_x \quad m\ddot{y} = -\frac{\partial U}{\partial y} \equiv F_y \quad m\ddot{z} = -\frac{\partial U}{\partial z} \equiv F_z$$

- 1D Harmonic oscillator $\quad L(x, \dot{x}, t) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0 \Longrightarrow \quad m\ddot{x} = -kx$$

Energy of a mechanical system

- Although $q_i(t)$ and $\dot{q}_i(t)$ change with time, the combinations of them can be unchanged with time and these combinations are called integrals of the motion (or conserved quantities).
- One of such conserved quantities is the energy of the system.

$$\frac{dL}{dt} = \sum_i \left.\frac{\partial L}{\partial q_i}\right|_{\dot{q}_i,t} \dot{q}_i + \sum_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} \ddot{q}_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} = \sum_i \dot{q}_i \frac{d}{dt}\left(\left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t}\right) + \sum_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} \ddot{q}_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} = \sum_i \frac{d}{dt}\left(\dot{q}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t}\right) + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i}$$

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) = 0$$

$$\sum_i \frac{d}{dt}\left(\dot{q}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} - L\right) = -\left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i}$$

If Lagrangian does not explicitly depend on time, i.e $\frac{\partial}{\partial t} L = 0$

$$\frac{d}{dt}\sum_i \left(\dot{q}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} - L\right) = 0$$

Hence the energy of the system is conserved if the Lagrangian does not explicitly depends on time (homogeneity of time).

$$E(q_i, \dot{q}_i) = \sum_i \left(\dot{q}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} - L\right)$$

← Energy of the system

Momentum of the Mechanical System

- A second conservation quantity follows from the homogeneity of space: the mechanical properties of a closed system are unchanged by any parallel displacement of the entire system in space.
- For simplicity, let's consider a system consisting of N particles

$a = 1 \ldots N$ is the index for different particle.

$$\delta L = L\left(\vec{r}_a + \vec{\varepsilon}, \dot{\vec{r}}_a, t\right) - L\left(\vec{r}_a, \dot{\vec{r}}_a, t\right) = \vec{\varepsilon} \cdot \sum_a \frac{\partial L}{\partial \vec{r}_a} = 0 \Rightarrow \sum_a \frac{\partial L}{\partial \vec{r}_a} = 0$$

$$\Rightarrow \begin{cases} \sum_a \frac{\partial L}{\partial x_a} = 0 \\ \sum_a \frac{\partial L}{\partial y_a} = 0 \\ \sum_a \frac{\partial L}{\partial z_a} = 0 \end{cases}$$

$$\frac{\partial L}{\partial x_a} = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}_a}, \quad \frac{\partial L}{\partial y_a} = \frac{d}{dt}\frac{\partial L}{\partial \dot{y}_a}, \quad \frac{\partial L}{\partial z_a} = \frac{d}{dt}\frac{\partial L}{\partial \dot{z}_a}$$

$$\Rightarrow \begin{cases} \frac{d}{dt}\sum_a \frac{\partial L}{\partial \dot{x}_a} = 0 \\ \frac{d}{dt}\sum_a \frac{\partial L}{\partial \dot{y}_a} = 0 \\ \frac{d}{dt}\sum_a \frac{\partial L}{\partial \dot{z}_a} = 0 \end{cases} \Rightarrow \begin{cases} \frac{d}{dt}\sum_a p_{a,x} = 0 \\ \frac{d}{dt}\sum_a p_{a,y} = 0 \\ \frac{d}{dt}\sum_a p_{a,z} = 0 \end{cases}$$

Momentum

$$p_{a,x} \equiv \frac{\partial}{\partial \dot{x}_a} L, \quad p_{a,y} \equiv \frac{\partial}{\partial \dot{y}_a} L, \quad p_{a,z} \equiv \frac{\partial}{\partial \dot{z}_a} L$$

Hamiltonian system

- The Lagrangian and Lagrange's equation completely describe the system by specifying the generalized coordinates and its derivatives, i.e. velocities. However, it is not the only way to describe the system.
- There are advantages to describe the system in terms of generalized coordinates and generalized momentum (in stead of velocities).

$$(q_i, \dot{q}_i) \Rightarrow (q_i, p_i) \qquad p_i \equiv \frac{\partial}{\partial \dot{q}_i} L(q_i, \dot{q}_i, t)\Big|_{q_i, t}$$

- The passage from one set of independent variables to another is called in mathematics Legendre's transformation.

Hamilton's equations

- For a system with n degrees of freedom, the Hamilton's equations are a set of 2n first-order differential equations for the 2n unknown functions, P(t) and q(t). (while Lagrange's equations are n second order differential equations).
- Hamilton's equation treat variable P and q in a more symmetric form than the Lagrange's equation. They are also called canonical equations.

$$dL = \sum_i \left.\frac{\partial L}{\partial q_i}\right|_{\dot{q}_i,t} dq_i + \sum_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} d\dot{q}_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt$$

$$= \sum_i \frac{d}{dt}\left(\left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t}\right) dq_i + \sum_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{q_i,t} d\dot{q}_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt$$

$$= \sum_i \dot{p}_i dq_i + \sum_i p_i d\dot{q}_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt$$

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

Hamiltonian of the system (energy of the system)

$$= \sum_i \dot{p}_i dq_i + \sum_i d(p_i \dot{q}_i) - \sum_i \dot{q}_i dp_i + \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt \Rightarrow d\left(\sum_i p_i \dot{q}_i - L\right) = \sum_i \dot{q}_i dp_i - \sum_i \dot{p}_i dq_i - \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt$$

$$dH(q_i, p_i, t) = \sum_i \dot{q}_i dp_i - \sum_i \dot{p}_i dq_i - \left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i} dt$$

From chain rule → $dH(q_i, p_i, t) = \sum_i \left.\frac{\partial H}{\partial q_i}\right|_{p_i,t} dq_i + \sum_i \left.\frac{\partial H}{\partial p_i}\right|_{q_i,t} dp_i + \left.\frac{\partial H}{\partial t}\right|_{q_i,p_i} dt$

Hamilton's equations

$$\dot{q}_i = \left.\frac{\partial H}{\partial p_i}\right|_{q_i,t}$$

$$\dot{p}_i = -\left.\frac{\partial H}{\partial q_i}\right|_{p_i,t}$$

$$\left.\frac{\partial H}{\partial t}\right|_{q_i,p_i} = -\left.\frac{\partial L}{\partial t}\right|_{q_i,\dot{q}_i}$$

Deriving the Hamilton's equations from the Hamilton's principle

$$\delta S = \delta\int_{t_A}^{t_B} L dt \quad \leftarrow \quad L = \sum_i p_i\dot{q}_i - H(q_i, p_i, t) \quad \leftarrow \quad H(q_i, p_i, t) \equiv \sum_i p_i\dot{q}_i - L$$

$$= \delta\int_{t_A}^{t_B}\left(\sum_i p_i\dot{q}_i - H(q_i, p_i, t)\right)dt$$

$$= \int_{t_A}^{t_B}\left(\sum_i (p_i + \delta p_i)(\dot{q}_i + \delta\dot{q}_i) - H(q_i + \delta q_i, p_i + \delta p_i, t)\right)dt - \int_{t_A}^{t_B}\left(\sum_i p_i\dot{q}_i - H(q_i, p_i, t)\right)dt$$

$$= \int_{t_A}^{t_B}\left(\sum_i (p_i\delta\dot{q}_i + \dot{q}_i\delta p_i) - \frac{\partial H}{\partial q_i}\delta q_i - \frac{\partial H}{\partial p_i}\delta p_i\right)dt$$

$$= \int_{t_A}^{t_B}\left(\sum_i \left(\frac{d}{dt}(p_i\delta q_i) - \delta q_i\dot{p}_i + \dot{q}_i\delta p_i\right) - \frac{\partial H}{\partial q_i}\delta q_i - \frac{\partial H}{\partial p_i}\delta p_i\right)dt$$

$$= \int_{t_A}^{t_B}\left(\sum_i -\left(\frac{\partial H}{\partial q_i} + \dot{p}_i\right)\delta q_i + \left(\dot{q}_i - \frac{\partial H}{\partial p_i}\right)\delta p_i\right)dt \qquad \delta S = 0 \Rightarrow$$

$$\dot{q}_i = \left.\frac{\partial H}{\partial p_i}\right|_{q_i, t} \qquad \dot{p}_i = -\left.\frac{\partial H}{\partial q_i}\right|_{p_i, t}$$

Some examples of Hamilton's equation

- Free space: $L(x,y,z,\dot{x},\dot{y},\dot{z},t)=\frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right)$ $\quad p_x=\frac{\partial}{\partial\dot{x}}L\Big|_{x,y,z,t}=m\dot{x}$

$$H\left(x,y,z,p_x,p_y,p_z,t\right)=p_x\dot{x}+p_y\dot{y}+p_z\dot{z}-L=\frac{p_x^2+p_y^2+p_z^2}{2m} \qquad \dot{x}=\frac{\partial H}{\partial p_x}=\frac{p_x}{m} \qquad \dot{p}_x=-\frac{\partial H}{\partial x}=0$$

- A particle in a potential $U(x,y,z)$ $\quad L(x,y,z,\dot{x},\dot{y},\dot{z},t)=\frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right)-U(x,y,z)$

$$H\left(x,y,z,p_x,p_y,p_z,t\right)=p_x\dot{x}+p_y\dot{y}+p_z\dot{z}-L=\frac{p_x^2+p_y^2+p_z^2}{2m}+U(x,y,z) \qquad \dot{x}=\frac{\partial H}{\partial p_x}=\frac{p_x}{m} \qquad \dot{p}_x=-\frac{\partial H}{\partial x}=-\frac{\partial U}{\partial x}$$

- 1D Harmonic oscillator $\quad L(x,\dot{x},t)=\frac{1}{2}m\dot{x}^2-\frac{1}{2}kx^2$

$$H\left(x,p_x,t\right)=p_x\dot{x}-L=\frac{p_x^2}{2m}+\frac{1}{2}kx^2 \qquad \dot{x}=\frac{\partial H}{\partial p_x}=\frac{p_x}{m} \qquad \dot{p}_x=-\frac{\partial H}{\partial x}=-kx$$

What is canonical transformation?

- Since the choice of the generalized coordinates is arbitrary, the form of the Lagrange's equations and the Hamilton's equations do not change when we transfer from one set of generalized coordinates to another set.

$$Q_i = Q_i\left(q_1, q_2, \ldots t\right)$$

- For Hamiltonian system, we would like to extend the transformation such that
  - ✓1. both the generalized coordinates and generalized momentum are included into the transformation and
  - ✓2. preserves the form of the Hamilton's equations when new variables (momentum and coordinates) are used (transformation preserving the form of the Hamilton's equations are called canonical transformation)

$$\left.\begin{aligned} Q_i &= Q_i\left(q_1, q_2, \ldots, p_1, p_2, \ldots, t\right) \\ P_i &= P_i\left(q_1, q_2, \ldots, p_1, p_2, \ldots, t\right) \end{aligned}\right\} \xrightarrow{\text{If the transformation is canonical}} \left\{\begin{aligned} \dot{Q}_i &= \frac{\partial \tilde{H}\left(Q_i, P_i, t\right)}{\partial P_i} \\ \dot{P}_i &= -\frac{\partial \tilde{H}\left(Q_i, P_i, t\right)}{\partial Q_i} \end{aligned}\right.$$

How to find canonical transformation?

- The Hamilton's equation can be derived from the stationary action principle:

$$\delta\int_{t_A}^{t_B}\left(\sum_i p_i\dot{q}_i - H\right)dt = 0 \quad \Rightarrow \quad \dot{q}_i = \left.\frac{\partial H}{\partial P_i}\right|_{q_i,t} \qquad \dot{P}_i = -\left.\frac{\partial H}{\partial q_i}\right|_{P_i,t}$$

- If the new variables satisfy $\delta\int_{t_A}^{t_B}\left(\sum_i P_i\dot{Q}_i - \tilde{H}\right)dt = 0$ (*)

then they also satisfy $\dot{P}_i = -\frac{\partial\tilde{H}(Q_i,P_i,t)}{\partial Q_i}$ $\quad \dot{Q}_i = \frac{\partial\tilde{H}(Q_i,P_i,t)}{\partial P_i}$, i.e. they are canonical.

- The obvious way to guarantee (*) is valid is if

$$\sum_i p_i\dot{q}_i - H = \sum_i P_i\dot{Q}_i - \tilde{H} + \frac{dF}{dt}$$

with F(p,q,P,Q,t) being some arbitrary function of generalized coordinates, generalized momentum and time since $\delta\int_{t_A}^{t_B}\frac{dF}{dt}dt = \delta F(t_A) - \delta F(t_B) = 0$ Starting and ending points are fixed.

Find canonical transformation using generating function

It turns out that F can be used to find some of the canonical transformation, and it is called the generating function.

- If F is a function q and Q, i.e. $F\left(q_i, Q_i\right)$ ← Type I generating function

$$\sum_i p_i \dot{q}_i - H = \sum_i P_i \dot{Q}_i - \tilde{H} + \frac{dF}{dt}$$

$$\frac{dF}{dt} = \sum_i p_i \dot{q}_i - \sum_i P_i \dot{Q}_i + \left(\tilde{H} - H\right)$$

$$\frac{dF}{dt}\left(q_i, Q_i, t\right) = \sum_i \left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial q_i}\right|_{Q_i, t} \dot{q}_i + \sum_i \left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial Q_i}\right|_{q_i, t} \dot{Q}_i + \left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial t}\right|_{q_i, Q_i}$$

$$p_i = \left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial q_i}\right|_{Q_i, t}$$

$$P_i = -\left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial Q_i}\right|_{q_i, t}$$

$$\tilde{H} = H + \left.\frac{\partial F\left(q_i, Q_i, t\right)}{\partial t}\right|_{q_i, Q_i}$$

More types of generating function

$$F(q,\tilde{q},t) \quad \Rightarrow dF = P_i dq_i - \tilde{P}_i d\tilde{q}_i + (H' - H)dt;\ P_i = \frac{\partial F}{\partial q_i};\ \tilde{P}_i = -\frac{\partial F}{\partial \tilde{q}_i};\ H' = H + \frac{\partial F}{\partial t}.$$

$$\Phi(q,\tilde{P},t) = F + \tilde{q}_i \tilde{P}_i \quad \Rightarrow d\Phi = P_i dq_i + \tilde{q}_i d\tilde{P}_i + (H' - H)dt;\ P_i = \frac{\partial \Phi}{\partial q_i};\ \tilde{q}_i = \frac{\partial \Phi}{\partial \tilde{P}_i};\ H' = H + \frac{\partial \Phi}{\partial t};$$

$$\Omega(P,\tilde{q},t) = F - P_i q_i \quad \Rightarrow d\Omega = -q_i dP_i - \tilde{P}_i d\tilde{q}_i + (H' - H)dt;\ q_i = -\frac{\partial \Omega}{\partial P_i};\ \tilde{P}_i = -\frac{\partial \Omega}{\partial \tilde{q}_i};\ H' = H + \frac{\partial \Omega}{\partial t};$$

$$\Lambda(P,\tilde{P},t) = \Phi - P_i q_i \quad \Rightarrow d\Lambda = \tilde{q}_i d\tilde{P}_i - q_i dP_i + (H' - H)dt;\ q_i = -\frac{\partial \Lambda}{\partial P_i};\ \tilde{q}_i = \frac{\partial \Lambda}{\partial \tilde{P}_{ii}};\ H' = H + \frac{\partial \Lambda}{\partial t};$$