Liouville's Theorem & Ergodicity

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Hamiltonian Mechanics

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}. \tag{1}$$

William Rowan Hamilton (1805 $\sim$ 1865)

Lagrangian Mechanics

Action minimization:

$$\delta S = \delta \int L dt. \tag{2}$$

Lagrangian:

$$L = T - V. \tag{3}$$

Lagrange Equation:

$$\frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = 0. \tag{4}$$

Energy Conservation

We consider the Lagrangian, $L(q, \dot{q}, t)$. The time derivative of the Lagrangian is given by

$$\begin{aligned}\frac{dL}{dt} &= \frac{\partial L}{\partial q}\frac{dq}{dt} + \frac{\partial L}{\partial \dot{q}}\frac{d\dot{q}}{dt} + \frac{\partial L}{\partial t}, \\ &= \frac{\partial L}{\partial q}\dot{q} + \frac{\partial L}{\partial \dot{q}}\ddot{q} + \frac{\partial L}{\partial t}.\end{aligned}$$

Since the generalized momentum is $p = \frac{\partial L}{\partial \dot{q}}$,

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}} = \frac{d}{dt}p = \dot{p}.$$

Energy Conservation

It leads

$$\frac{dL}{dt} = \dot{p}\dot{q} + p\ddot{q} + \frac{\partial L}{\partial t} = \frac{d}{dt}(p\dot{q}) + \frac{\partial L}{\partial t}.$$

Lagrangian is not conserved with time. But, if we define the Hamiltonian as

$$H = p\dot{q} - L, \tag{5}$$

the equation becomes:

$$\frac{dH}{dt} = -\frac{\partial L}{\partial t}.$$

Then, Hamiltonian is conserved if Lagrangian does not depend on time explicitly.

Hamilton's Equation

Hamiltonian is given by

$$H = p\dot{q} - L.$$

The variation of the Hamiltonian is

$$\begin{aligned} \delta H &= \dot{q}\delta p + p\delta\dot{q} - \delta L \\ &= \dot{q}\delta p + p\delta\dot{q} - \frac{\partial L}{\partial q}\delta q - \frac{\partial L}{\partial \dot{q}}\delta\dot{q}. \end{aligned}$$

Since $p = \frac{\partial L}{\partial \dot{q}}$ and $\dot{p} = \frac{\partial L}{\partial q}$,

$$\delta H = \dot{q}\delta p - \dot{p}\delta q.$$

Considering that H is a function of p and q,

$$\delta H = \frac{\partial H}{\partial p}\delta p + \frac{\partial H}{\partial q}\delta q.$$

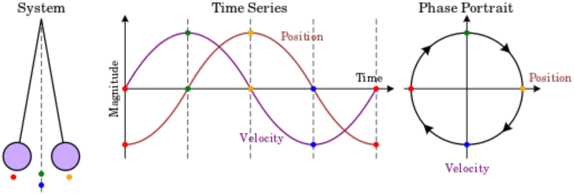
Hamilton's Equation

Finally, we obtain Hamilton's equations (two first order equations):

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}.$$

Phase Space

$$\frac{dq}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H}{\partial q}.$$



Simple Harmonic Motion (from Wikipedia)

Simple Harmonic Oscillators

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2.$$
$$2mH = p^2 + (m\omega q)^2.$$

Simple harmonic motion corresponds to a circular motion in phase space (p, q).

Liouville (Liouville-Gibbs) Theorem

Hamiltonian Mechanics

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \quad H(p,q) = \Delta E.$$

We consider (p,q) as fluids with the density ρ and current J in phase space. Then, the continuity equation is

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot J,$$

where the divergence is

$$\boldsymbol{\nabla} \cdot v = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0.$$

Liouville (Liouville-Gibbs) Theorem

The current in phase space is $J = \rho\vec{v}$. Then, the continuity equation gives

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\boldsymbol{\nabla} \cdot J \\ &= -\sum_i \left[\frac{\partial \rho \dot{q}_i}{\partial q_i} + \frac{\partial \rho \dot{p}_i}{\partial p_i}\right] \\ &= -\sum_i \left[\frac{\partial \rho}{\partial q_i}\dot{q}_i + \rho\frac{\partial \dot{q}_i}{\partial q_i} + \frac{\partial \rho}{\partial p_i}\dot{p}_i + \rho\frac{\partial \dot{p}_i}{\partial p_i}\right] \\ &= -\sum_i \left[\frac{\partial \rho}{\partial q_i}\dot{q}_i + \frac{\partial \rho}{\partial p_i}\dot{p}_i\right].\end{aligned}$$

Note that

$$\frac{\partial \dot{q}}{\partial q} = \frac{\partial^2 H}{\partial q \partial p} = \frac{\partial^2 H}{\partial p \partial q} = -\frac{\partial \dot{p}}{\partial p}.$$

Liouville (Liouville-Gibbs) Theorem

$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot J = -\sum_i \left[\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right].$$

Rearranging the equation:

$$\begin{aligned} 0 &= \frac{\partial \rho}{\partial t} + \sum_i \left[\frac{\partial \rho}{\partial q_i} \dot{q}_i + \frac{\partial \rho}{\partial p_i} \dot{p}_i \right] \\ &= \frac{\partial \rho}{\partial t} + \sum_i \left[\frac{\partial \rho}{\partial q_i} \frac{\partial H}{\partial p_i} - \frac{\partial \rho}{\partial p_i} \frac{\partial H}{\partial q_i} \right] \\ &= \frac{\partial \rho}{\partial t} + \{\rho, H\} = \frac{d\rho}{dt}, \end{aligned}$$

where the Poisson bracket $\{A, B\}$ is

$$\{A, B\} = \sum_i \left[\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right]. \tag{6}$$

Liouville (Liouville-Gibbs) Theorem

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \{\rho, H\} = 0.$$

- incompressible flow
- volume in phase space is conserved
- no attractors
- microcanonical ensembles are time independent

Ergodicity

- Ergodicity: energy surface in phase space is thoroughly stirred by the time evolution.
- time average = ensemble average

$$\langle f \rangle = \frac{\int f(q,p)\rho(q,p)dqdp}{\int \rho(q,p)dqdp}.$$

$$\bar{f} = \frac{1}{T}\int_0^T f(q,p)dt.$$

Can we show that our systems are ergodic? Well, usually not.

Where to go next. . .

Let us go to microcanonical ensemble.