

**PHY 711 Classical Mechanics and
Mathematical Methods**
10-10:50 AM MWF Online or (occasional)
in Olin 103

Plan for Lecture 12 – Chap. 3&6 (F&W)

- 1. Constructing the Hamiltonian**
- 2. Hamilton's canonical equation**
- 3. Examples**

This lecture shows how to “derive” the Hamiltonian formalism from the Lagrangian.

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Wed, 8/26/2020	Chap. 1	Introduction	#1	8/31/2020
2	Fri, 8/28/2020	Chap. 1	Scattering theory	#2	9/02/2020
3	Mon, 8/31/2020	Chap. 1	Scattering theory	#3	9/04/2020
4	Wed, 9/02/2020	Chap. 1	Scattering theory		
5	Fri, 9/04/2020	Chap. 1	Scattering theory	#4	9/09/2020
6	Mon, 9/07/2020	Chap. 2	Non-inertial coordinate systems		
7	Wed, 9/09/2020	Chap. 3	Calculus of Variation	#5	9/11/2020
8	Fri, 9/11/2020	Chap. 3	Calculus of Variation	#6	9/14/2020
9	Mon, 9/14/2020	Chap. 3 & 6	Lagrangian Mechanics	#7	9/18/2020
10	Wed, 9/16/2020	Chap. 3 & 6	Lagrangian & constraints	#8	9/21/2020
11	Fri, 9/18/2020	Chap. 3 & 6	Constants of the motion		
12	Mon, 9/21/2020	Chap. 3 & 6	Hamiltonian equations of motion	#9	9/23/2020



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There is a short homework problem due Wednesday.

PHY 711 – Assignment #9

September 21, 2020

1. Consider a Lagrangian describing one dimensional motion of a particle of mass m in a mechanical potential $V(x)$ with an addition time dependent function $s(t)$ and extra constants Q and K having the form

$$L(x, \dot{x}, s, \dot{s}) = \frac{1}{2}m\dot{x}^2 - V(x) + Q\dot{s}^2 - K \ln(s).$$

- (a) Find the constants of motion for this system.
- (b) Find the corresponding Hamiltonian if canonical form $H(x, p_x, s, p_s)$.

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Homework due Wednesday.

Lagrangian picture

For independent generalized coordinates $q_\sigma(t)$:

$$L = L(\{q_\sigma(t)\}, \{\dot{q}_\sigma(t)\}, t)$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} = 0$$

\Rightarrow Second order differential equations for $q_\sigma(t)$

Switching variables – Legendre transformation

Define: $H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$

$$H = \sum_\sigma \dot{q}_\sigma p_\sigma - L \quad \text{where } p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$$

$$dH = \sum_\sigma \left(\dot{q}_\sigma dp_\sigma + p_\sigma d\dot{q}_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt$$

Starting with the Lagrangian and then performing a Legendre transformation.

Hamiltonian picture – continued

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

$$H = \sum_{\sigma} \dot{q}_\sigma p_\sigma - L \quad \text{where} \quad p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$$

$$\begin{aligned} dH &= \sum_{\sigma} \left(\dot{q}_\sigma dp_\sigma + p_\sigma d\dot{q}_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt \\ &= \sum_{\sigma} \left(\frac{\partial H}{\partial q_\sigma} dq_\sigma + \frac{\partial H}{\partial p_\sigma} dp_\sigma \right) + \frac{\partial H}{\partial t} dt \\ \Rightarrow \dot{q}_\sigma &= \frac{\partial H}{\partial p_\sigma} \quad \frac{\partial L}{\partial q_\sigma} = \frac{d}{dt} \quad \frac{\partial L}{\partial \dot{q}_\sigma} \equiv \dot{p}_\sigma = -\frac{\partial H}{\partial q_\sigma} \quad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t} \end{aligned}$$

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Finding the Hamiltonian equations of motion.

Direct application of Hamiltonian's principle using the Hamiltonian function --



Generalized coordinates :

$$q_\sigma(\{x_i\})$$

Define -- Lagrangian: $L \equiv T - U$

$$L = L(\{q_\sigma\}, \{\dot{q}_\sigma\}, t)$$

$$\Rightarrow \text{Minimization integral: } S = \int_{t_i}^{t_f} L(\{q_\sigma\}, \{\dot{q}_\sigma\}, t) dt$$

Expressed in terms of Hamiltonian:

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

$$H = \sum_\sigma \dot{q}_\sigma p_\sigma - L \quad \Rightarrow L = \sum_\sigma \dot{q}_\sigma p_\sigma - H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

Showing that Hamilton's principle can be formulated with the Hamiltonian formulation.

Hamilton's principle continued:
Minimization integral:

$$S = \int_{t_i}^{t_f} \left(\sum_{\sigma} \dot{q}_{\sigma} p_{\sigma} - H(\{q_{\sigma}(t)\}, \{p_{\sigma}(t)\}, t) \right) dt$$

$$\delta S = \int_{t_i}^{t_f} \left(\sum_{\sigma} \left(\dot{q}_{\sigma} \delta p_{\sigma} + \delta \dot{q}_{\sigma} p_{\sigma} - \frac{\partial H}{\partial q_{\sigma}} \delta q_{\sigma} - \frac{\partial H}{\partial p_{\sigma}} \delta p_{\sigma} \right) \right) dt = 0$$

$$\Rightarrow \dot{q}_{\sigma} = \frac{\partial H}{\partial p_{\sigma}}$$

$$\Rightarrow \dot{p}_{\sigma} = -\frac{\partial H}{\partial q_{\sigma}}$$

Canonical equations

Detail:

$$\int_{t_i}^{t_f} \left(\sum_{\sigma} (\delta \dot{q}_{\sigma} p_{\sigma}) \right) dt = \int_{t_i}^{t_f} \left(\sum_{\sigma} \left(\frac{d(\delta q_{\sigma} p_{\sigma})}{dt} - \delta q_{\sigma} \dot{p}_{\sigma} \right) \right) dt = \sum_{\sigma} \delta q_{\sigma} p_{\sigma} \Big|_{t_i}^{t_f} - \int_{t_i}^{t_f} \left(\sum_{\sigma} (\delta q_{\sigma} \dot{p}_{\sigma}) \right) dt$$

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So called “Canonical” equations.

Constants of the motion in Hamiltonian formalism

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$
$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \Rightarrow \text{constant } q_\sigma \text{ if } \frac{\partial H}{\partial p_\sigma} = 0$$
$$\frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma} \Rightarrow \text{constant } p_\sigma \text{ if } \frac{\partial H}{\partial q_\sigma} = 0$$
$$\frac{dH}{dt} = \sum_{\sigma} \left(\frac{\partial H}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial H}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial H}{\partial t}$$
$$\frac{dH}{dt} = \sum_{\sigma} (-\dot{p}_\sigma \dot{q}_\sigma + \dot{q}_\sigma \dot{p}_\sigma) + \frac{\partial H}{\partial t} = \frac{\partial H}{\partial t}$$
$$\Rightarrow \text{constant } H \text{ if } \frac{\partial H}{\partial t} = 0$$

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Finding constants of the motion within the Hamiltonian formalism.

Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function : $L = L(\{q_\sigma(t)\}, \{\dot{q}_\sigma(t)\}, t)$
2. Compute generalized momenta : $p_\sigma \equiv \frac{\partial L}{\partial \dot{q}_\sigma}$
3. Construct Hamiltonian expression : $H = \sum_\sigma \dot{q}_\sigma p_\sigma - L$
4. Form Hamiltonian function : $H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$
5. Analyze canonical equations of motion :

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \quad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

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Important recipe. Tape this to your wall!!!

Example 1: one-dimensional potential :

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(z)$$

$$p_x = m\dot{x} \quad p_y = m\dot{y} \quad p_z = m\dot{z}$$

$$H = mx^2 + my^2 + mz^2 - \left(\frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(z) \right)$$

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + V(z)$$

Constants : p_x, p_y, H

Equations of motion : $\frac{dz}{dt} = \frac{\partial H}{\partial p_z} = \frac{p_z}{m} \quad \frac{dp_z}{dt} = -\frac{dV}{dz}$

Example.

Example 2 : Motion in a central potential

$$L = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) - V(r)$$

$$p_r = m\dot{r} \quad p_\phi = mr^2\dot{\phi}$$

$$\begin{aligned} H &= m\dot{r}^2 + mr^2\dot{\phi}^2 - \left(\frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) - V(r)\right) \\ &= \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) + V(r) \end{aligned}$$

$$H = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V(r)$$

Constants : p_ϕ, H

Equations of motion :

$$\frac{dr}{dt} = \frac{p_r}{m} \quad \frac{dp_r}{dt} = -\frac{\partial H}{\partial r} = \frac{p_\phi^2}{mr^3} - \frac{\partial V}{\partial r}$$

Another example

Other examples

Lagrangian for symmetric top with Euler angles α, β, γ :

$$L = L(\alpha, \beta, \gamma, \dot{\alpha}, \dot{\beta}, \dot{\gamma}) = \frac{1}{2} I_1 (\dot{\alpha}^2 \sin^2 \beta + \dot{\beta}^2) + \frac{1}{2} I_3 (\dot{\alpha} \cos \beta + \dot{\gamma})^2 - Mgh \cos \beta$$

$$p_\alpha = I_1 \dot{\alpha} \sin^2 \beta + I_3 (\dot{\alpha} \cos \beta + \dot{\gamma}) \cos \beta$$

$$p_\beta = I_1 \dot{\beta}$$

$$p_\gamma = I_3 (\dot{\alpha} \cos \beta + \dot{\gamma})$$

$$H = \frac{1}{2} I_1 (\dot{\alpha}^2 \sin^2 \beta + \dot{\beta}^2) + \frac{1}{2} I_3 (\dot{\alpha} \cos \beta + \dot{\gamma})^2 + Mgh \cos \beta$$

$$H = \frac{(p_\alpha - p_\gamma \cos \beta)^2}{2I_1 \sin^2 \beta} + \frac{p_\beta^2}{2I_1} + \frac{p_\gamma^2}{2I_3} + Mgh \cos \beta$$

Constants : p_α, p_γ, H

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Another example

Other examples

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) + \frac{q}{2c}B_0(-\dot{xy} + \dot{yx})$$

$$p_x = m\dot{x} - \frac{q}{2c}B_0y$$

$$p_y = m\dot{y} + \frac{q}{2c}B_0x$$

$$p_z = m\dot{z}$$

$$H = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)$$

$$H = \frac{\left(p_x + \frac{q}{2c}B_0y\right)^2}{2m} + \frac{\left(p_y - \frac{q}{2c}B_0x\right)^2}{2m} + \frac{p_z^2}{2m}$$

Constants : p_z, H

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Example with magnetic field.

Canonical equations of motion for constant magnetic field:

$$H = \frac{\left(p_x + \frac{q}{2c} B_0 y \right)^2}{2m} + \frac{\left(p_y - \frac{q}{2c} B_0 x \right)^2}{2m} + \frac{p_z^2}{2m}$$

Constants : p_z, H

$$\frac{dx}{dt} = \frac{p_x + \frac{q}{2c} B_0 y}{m} \quad \frac{dy}{dt} = \frac{p_y - \frac{q}{2c} B_0 x}{m}$$

$$\frac{dp_x}{dt} = -\frac{\partial H}{\partial x} = \frac{qB_0}{2mc} \left(p_y - \frac{q}{2c} B_0 x \right)$$

$$\frac{dp_y}{dt} = -\frac{\partial H}{\partial y} = -\frac{qB_0}{2mc} \left(p_x + \frac{q}{2c} B_0 y \right)$$

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Working out the equations of motion.

Canonical equations of motion for constant magnetic field
-- continued:

$$\begin{aligned}\frac{dx}{dt} &= \frac{p_x + \frac{q}{2c} B_0 y}{m} & \frac{dy}{dt} &= \frac{p_y - \frac{q}{2c} B_0 x}{m} \\ \frac{dp_x}{dt} &= \frac{qB_0}{2mc} \left(p_y - \frac{q}{2c} B_0 x \right) = \frac{qB_0}{2c} \frac{dy}{dt} \\ \frac{dp_y}{dt} &= -\frac{qB_0}{2mc} \left(p_x + \frac{q}{2c} B_0 y \right) = -\frac{qB_0}{2c} \frac{dx}{dt} \\ \frac{d^2x}{dt^2} &= \frac{\dot{p}_x}{m} + \frac{q}{2mc} B_0 \dot{y} = \frac{qB_0}{mc} \frac{dy}{dt} \\ \frac{d^2y}{dt^2} &= \frac{\dot{p}_y}{m} - \frac{q}{2mc} B_0 \dot{x} = -\frac{qB_0}{mc} \frac{dx}{dt}\end{aligned}$$

More evaluation of the equations of motion.

General treatment of particle of mass m and charge q moving in 3 dimensions in an potential $U(\mathbf{r})$ as well as electromagnetic scalar and vector potentials $\Phi(\mathbf{r},t)$ and $\mathbf{A}(\mathbf{r},t)$:

Lagrangian:
$$L(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{1}{2}m\dot{\mathbf{r}}^2 - U(\mathbf{r}) - q\Phi(\mathbf{r}, t) + \frac{q}{c}\dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}, t)$$

Hamiltonian:
$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} + \frac{q}{c}\mathbf{A}(\mathbf{r}, t)$$

$$\begin{aligned} H(\mathbf{r}, \mathbf{p}, t) &= \mathbf{p} \cdot \dot{\mathbf{r}} - L(\mathbf{r}, \dot{\mathbf{r}}, t) \\ &= \frac{1}{2m} \left(\mathbf{p} - \frac{q}{c} \mathbf{A}(\mathbf{r}, t) \right)^2 + U(\mathbf{r}) + q\Phi(\mathbf{r}, t) \end{aligned}$$

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Recap of treatment of electromagnetic interactions in the Lagrangian and Hamiltonian formulations.

Some details: $L(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{1}{2}m\dot{\mathbf{r}}^2 - U(\mathbf{r}) - q\Phi(\mathbf{r}, t) + \frac{q}{c}\dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}, t)$

Hamiltonian: $\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} + \frac{q}{c}\mathbf{A}(\mathbf{r}, t)$

$$H(\mathbf{r}, \mathbf{p}, t) = \mathbf{p} \cdot \dot{\mathbf{r}} - L(\mathbf{r}, \dot{\mathbf{r}}, t)$$

$$\begin{aligned} &= \left(m\dot{\mathbf{r}} + \frac{q}{c}\mathbf{A}(\mathbf{r}, t) \right) \cdot \dot{\mathbf{r}} - \left(\frac{1}{2}m\dot{\mathbf{r}}^2 - U(\mathbf{r}) - q\Phi(\mathbf{r}, t) + \frac{q}{c}\dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}, t) \right) \\ &= \frac{1}{2}m\dot{\mathbf{r}}^2 + U(\mathbf{r}) + q\Phi(\mathbf{r}, t) \end{aligned}$$

$$H(\mathbf{r}, \mathbf{p}, t) = \frac{1}{2m} \left(\mathbf{p} - \frac{q}{c}\mathbf{A}(\mathbf{r}, t) \right)^2 + U(\mathbf{r}) + q\Phi(\mathbf{r}, t)$$



Canonical form

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Continued.

Other properties of Hamiltonian formalism –
Poisson brackets:

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \Rightarrow \text{constant } q_\sigma \text{ if } \frac{\partial H}{\partial p_\sigma} = 0$$

$$\frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma} \Rightarrow \text{constant } p_\sigma \text{ if } \frac{\partial H}{\partial q_\sigma} = 0$$

$$\frac{dH}{dt} = \sum_{\sigma} \left(\frac{\partial H}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial H}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial H}{\partial t}$$

Similarly for an arbitrary function : $F = F(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$

$$\frac{dF}{dt} = \sum_{\sigma} \left(\frac{\partial F}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial F}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial F}{\partial t} = \sum_{\sigma} \left(\frac{\partial F}{\partial q_\sigma} \frac{\partial H}{\partial p_\sigma} - \frac{\partial F}{\partial p_\sigma} \frac{\partial H}{\partial q_\sigma} \right) + \frac{\partial F}{\partial t}$$

Now a interesting addition property of the Hamiltonian formulation.

Poisson brackets -- continued:

For an arbitrary function : $F = F(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$

$$\frac{dF}{dt} = \sum_{\sigma} \left(\frac{\partial F}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial F}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial F}{\partial t} = \sum_{\sigma} \left(\frac{\partial F}{\partial q_\sigma} \frac{\partial H}{\partial p_\sigma} - \frac{\partial F}{\partial p_\sigma} \frac{\partial H}{\partial q_\sigma} \right) + \frac{\partial F}{\partial t}$$

Define :

$$[F, G]_{PB} \equiv \sum_{\sigma} \left(\frac{\partial F}{\partial q_\sigma} \frac{\partial G}{\partial p_\sigma} - \frac{\partial F}{\partial p_\sigma} \frac{\partial G}{\partial q_\sigma} \right) = -[G, F]_{PB}$$

$$\text{So that : } \frac{dF}{dt} = [F, H]_{PB} + \frac{\partial F}{\partial t}$$

Poisson bracket continued.

Poisson brackets -- continued:

$$[F, G]_{PB} \equiv \sum_{\sigma} \left(\frac{\partial F}{\partial q_{\sigma}} \frac{\partial G}{\partial p_{\sigma}} - \frac{\partial F}{\partial p_{\sigma}} \frac{\partial G}{\partial q_{\sigma}} \right) = -[G, F]_{PB}$$

Examples :

$$[x, x]_{PB} = 0 \quad [x, p_x]_{PB} = 1 \quad [x, p_y]_{PB} = 0$$
$$[L_x, L_y]_{PB} = L_z$$

Liouville theorem

Let D \equiv density of particles in phase space :

$$\frac{dD}{dt} = [D, H]_{PB} + \frac{\partial D}{\partial t} = 0$$

Example.

Phase space

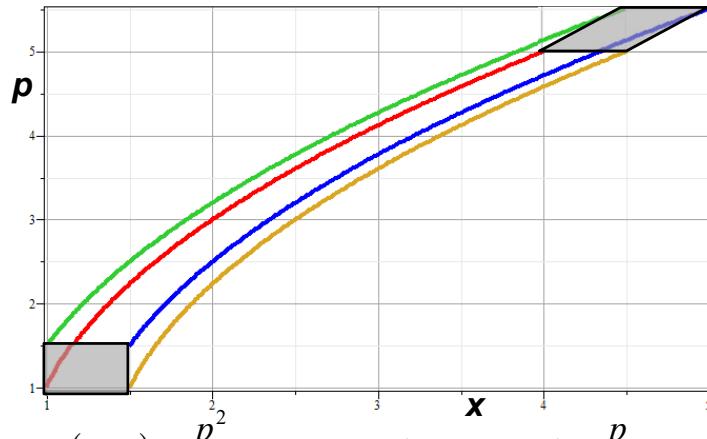
Phase space is defined at the set of all coordinates and momenta of a system :

$$(\{q_\sigma(t)\}, \{p_\sigma(t)\})$$

For a d dimensional system with N particles, the phase space corresponds to $2dN$ degrees of freedom.

Notion of phase space

Phase space diagram for one-dimensional motion due to constant force



$$H(x, p) = \frac{p^2}{2m} - F_0 x \quad \dot{p} = F_0 \quad \dot{x} = \frac{p}{m}$$

$$p_i(t) = p_{0i} + F_0 t \quad x_i(t) = x_{0i} + \frac{p_{0i}}{m} t + \frac{1}{2} F_0 t^2$$

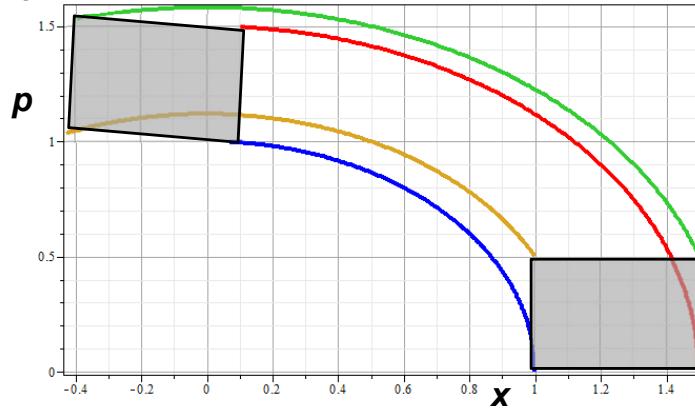
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Example of time evolution of phase space.

Phase space diagram for one-dimensional motion due to spring force



$$H(x, p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \quad \dot{p} = -m\omega^2x \quad \dot{x} = \frac{p}{m}$$

$$p_i(t) = p_{0i} \cos(\omega t + \theta_{0i}) \quad x_i(t) = \frac{p_{0i}}{m\omega} \sin(\omega t + \theta_{0i})$$

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Another example of time evolution of phase space.

Liouville's Theorem (1838)

The density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion.

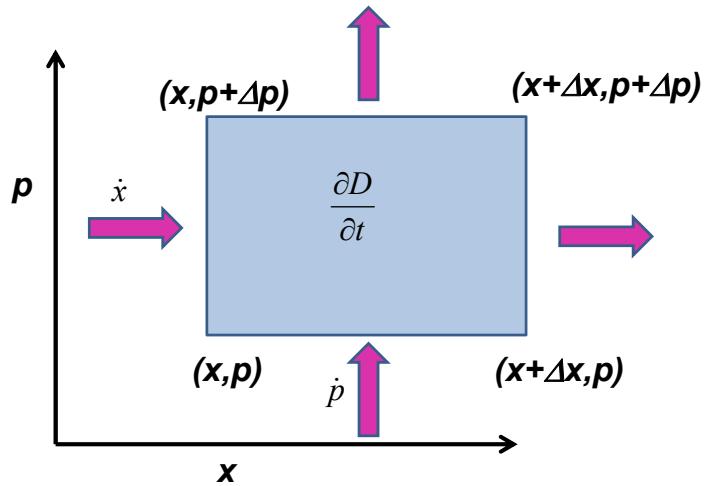
Denote the density of particles in phase space : $D = D(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$

$$\frac{dD}{dt} = \sum_{\sigma} \left(\frac{\partial D}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial D}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial D}{\partial t}$$

According to Liouville's theorem : $\frac{dD}{dt} = 0$

Application to the density of phase space – Liouville theorem.

Liouville's theorem



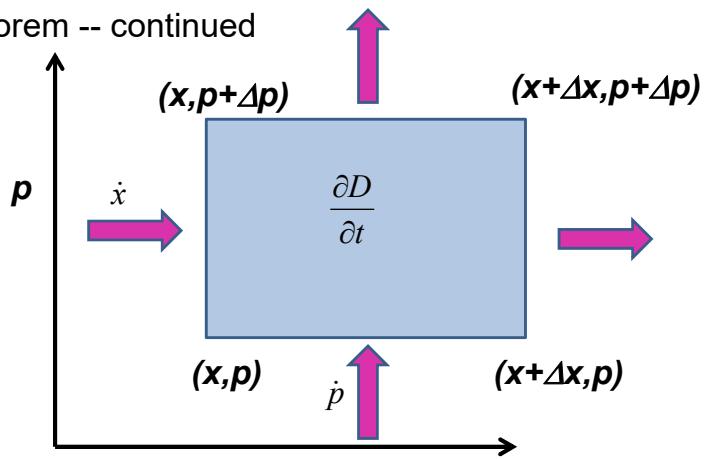
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Diagram of flow in phase space.

Liouville's theorem -- continued



$$\begin{aligned}\frac{\partial D}{\partial t} &\Rightarrow \text{time rate of change of particles within volume} \\ &= \text{time rate of particle entering minus particles leaving} \\ &= -\frac{\partial D}{\partial x} \dot{x} - \frac{\partial D}{\partial p} \dot{p}\end{aligned}$$

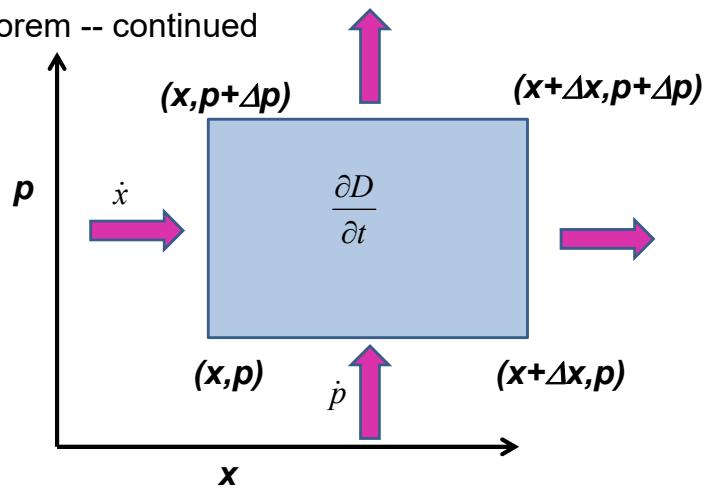
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Some details.

Liouville's theorem -- continued



$$\frac{\partial D}{\partial t} = -\frac{\partial D}{\partial x} \dot{x} - \frac{\partial D}{\partial p} \dot{p}$$

$$\frac{\partial D}{\partial t} + \frac{\partial D}{\partial x} \dot{x} + \frac{\partial D}{\partial p} \dot{p} = 0 = \frac{dD}{dt}$$

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More details.

Review:

Liouville's theorem:

Imagine a collection of particles obeying the Canonical equations of motion in phase space.

Let D denote the "distribution" of particles in phase space :

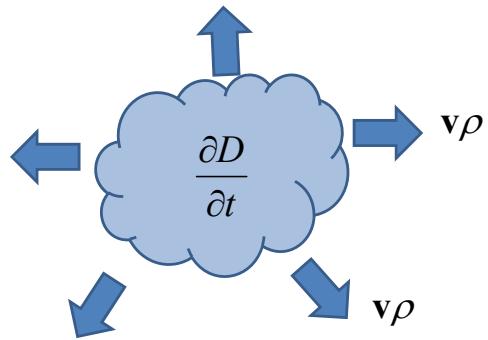
$$D = D(\{q_1 \cdots q_{3N}\}, \{p_1 \cdots p_{3N}\}, t)$$

Liouville's theorem shows that :

$$\frac{dD}{dt} = 0 \quad \Rightarrow D \text{ is constant in time}$$

Summary of Liouville theorem.

Proof of Liouville's theorem:



Continuity equation :

$$\frac{\partial D}{\partial t} = -\nabla \cdot (\mathbf{v}D)$$

Note : in this case, the velocity is the $6N$ dimensional vector :

$$\mathbf{v} = (\dot{\mathbf{r}}_1, \dot{\mathbf{r}}_2, \dots, \dot{\mathbf{r}}_N, \dot{\mathbf{p}}_1, \dot{\mathbf{p}}_2, \dots, \dot{\mathbf{p}}_N)$$

We also have a $6N$ dimensional gradient :

$$\nabla = (\nabla_{\mathbf{r}_1}, \nabla_{\mathbf{r}_2}, \dots, \nabla_{\mathbf{r}_N}, \nabla_{\mathbf{p}_1}, \nabla_{\mathbf{p}_2}, \dots, \nabla_{\mathbf{p}_N})$$

Another more formal derivation of Liouville

$$\frac{\partial D}{\partial t} = -\nabla \cdot (\mathbf{v}D)$$

$$\begin{aligned} &= -\sum_{j=1}^{3N} \left[\frac{\partial}{\partial q_j} (\dot{q}_j D) + \frac{\partial}{\partial p_j} (\dot{p}_j D) \right] \\ &= -\sum_{j=1}^{3N} \left[\frac{\partial D}{\partial q_j} \dot{q}_j + \frac{\partial D}{\partial p_j} \dot{p}_j \right] - D \sum_{j=1}^{3N} \left[\frac{\partial \dot{q}_j}{\partial q_j} + \frac{\partial \dot{p}_j}{\partial p_j} \right] \\ &\frac{\partial \dot{q}_j}{\partial q_j} + \frac{\partial \dot{p}_j}{\partial p_j} = \frac{\partial^2 H}{\partial q_j \partial p_j} + \left(-\frac{\partial^2 H}{\partial p_j \partial q_j} \right) = 0 \end{aligned}$$

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More details.

$$\frac{\partial D}{\partial t} = - \sum_{j=1}^{3N} \left[\frac{\partial D}{\partial q_j} \dot{q}_j + \frac{\partial D}{\partial p_j} \dot{p}_j \right] - D \sum_{j=1}^{3N} \left[\frac{\partial \dot{q}_j}{\partial q_j} + \frac{\partial \dot{p}_j}{\partial p_j} \right]$$

$$\begin{aligned} \frac{\partial D}{\partial t} &= - \sum_{j=1}^{3N} \left[\frac{\partial D}{\partial q_j} \dot{q}_j + \frac{\partial D}{\partial p_j} \dot{p}_j \right] \\ \Rightarrow \frac{\partial D}{\partial t} + \sum_{j=1}^{3N} \left[\frac{\partial D}{\partial q_j} \dot{q}_j + \frac{\partial D}{\partial p_j} \dot{p}_j \right] &= \frac{dD}{dt} = 0 \end{aligned}$$

0

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Derivation of Liouville theorem

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

Importance of Liouville's theorem to statistical mechanical analysis:

In statistical mechanics, we need to evaluate the probability of various configurations of particles. The fact that the density of particles in phase space is constant in time, implies that each point in phase space is equally probable and that the time average of the evolution of a system can be determined by an average of the system over phase space volume.

Comment.