PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF Olin 103

Plan for Lecture 12:

Continue reading Chapter 3 & 6

1. **Hamiltonian formalism**
2. **Phase space**
3. **Liouville's theorem**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/27/2014	Chap. 1	Review of basic principles	#1
2	Fri, 8/29/2014	Chap. 1	Scattering theory	#2
3	Mon, 9/01/2014	Chap. 1	Scattering theory continued	#3
4	Wed, 9/03/2014	Chap. 2	Accelerated coordinate systems	#4
5	Fri, 9/05/2014	Chap. 3	Calculus of variations	#5
6	Mon, 9/08/2014	Chap. 3	Calculus of variations	#6
7	Wed, 9/10/2014	Chap. 3	Hamilton's principle	#7
8	Fri, 9/12/2014	Chap. 3 & 6	Hamilton's principle	#8
9	Mon, 9/15/2014	Chap. 3 & 6	Lagrangians with constraints	#9
10	Wed, 9/17/2014	Chap. 3 & 6	Lagrangians and constants of motion	#10
11	Fri, 9/19/2014	Chap. 3 & 6	Hamiltonian formalism	#11
12	Mon, 9/22/2014	Chap. 3 & 6	Hamiltonian formalism	#11
13	Wed, 9/24/2014	Chap. 3 & 6	Hamiltonian Jacobi transformations	
14	Fri, 9/26/2014			

Hamiltonian formalism

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

Canonical equations of motion

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma}$$

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

Hamiltonian formalism and time evolution:

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

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

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

Hamiltonian formalism and time evolution:

Poisson brackets:

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 :

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

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

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 :

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

Phase space

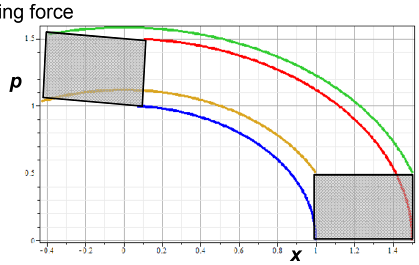
Phase space is defined at the set of all coordinates and momenta of a system :
$\left(\{q_\sigma(t)\},\{p_\sigma(t)\}\right)$
For a d dimensional system with N particles, the phase space corresponds to $2dN$ degrees of freedom.

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

$$H(x,p)=\frac{p^2}{2m}-F_0x \qquad \dot{p}=F_0 \qquad \dot{x}=\frac{p}{m}$$

$$p_i(t)=p_{0i}+F_0t \qquad x_i(t)=x_{0i}+\frac{p_{0i}}{m}t+\frac{1}{2}F_0t^2$$

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



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

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

Liouville's Theorem (1838)

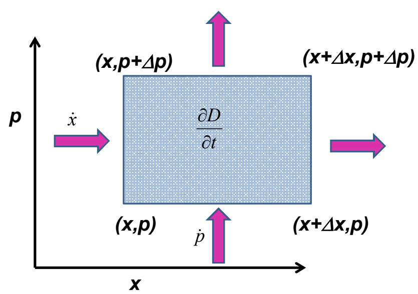
The density of representative points in phase space corresponding to the motion of a system of particles remains constant during the motion.

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

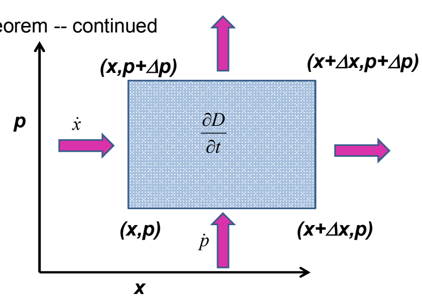
$$\frac{dD}{dt} = \sum_\sigma \left(\frac{\partial D}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial D}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial D}{\partial t}$$

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

Liouville's theorem



Liouville's theorem -- continued

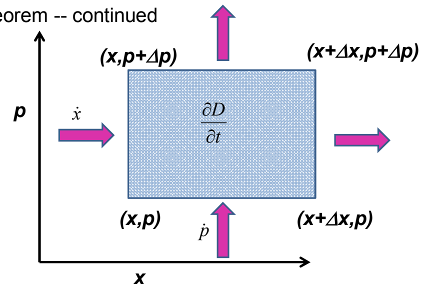


$\frac{\partial D}{\partial t} \Rightarrow$ time rate of change of particles within volume

= time rate of particle entering minus particles leaving

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

Liouville's theorem -- continued



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

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

Review:
Liouville's theorem:
Imagine a collection of particles obeying the Canonical equations of motion in phase space.

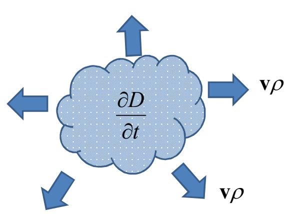
Let D denote the "distribution" of particles in phase space:

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

Liouville's theorm shows that:

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

Proof of Liouville'e theorem:



Continuity equation:

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

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

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

We also have a $6N$ dimensional gradient:

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

$$\frac{\partial D}{\partial t} = -\nabla \cdot (\mathbf{v}D)$$
$$= -\sum_{j=1}^{3N}\left[\frac{\partial}{\partial q_j}(\dot{q}_j D) + \frac{\partial}{\partial p_j}(\dot{p}_j D)\right]$$
$$= -\sum_{j=1}^{3N}\left[\frac{\partial D}{\partial q_j}\dot{q}_j + \frac{\partial D}{\partial p_j}\dot{p}_j\right] - D\sum_{j=1}^{3N}\left[\frac{\partial \dot{q}_j}{\partial q_j} + \frac{\partial \dot{p}_j}{\partial p_j}\right]$$
$$\frac{\partial \dot{q}_j}{\partial q_j} + \frac{\partial \dot{p}_j}{\partial p_j} = \frac{\partial^2 H}{\partial q_j \partial p_j} + \left(-\frac{\partial^2 H}{\partial p_j \partial q_j}\right) = 0$$

0

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

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

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

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.

Molecular dynamics simulations at constant pressure and/or temperature[a)]

Hans C. Andersen

Department of Chemistry, Stanford University, Stanford, California 94305

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In the molecular dynamics simulation method for fluids, the equations of motion for a collection of particles in a fixed volume are solved numerically. The energy, volume, and number of particles are constant for a particular simulation, and it is assumed that time averages of properties of the simulated fluid are equal to microcanonical ensemble averages of the same properties. In some situations, it is desirable to perform simulations of a fluid for particular values of temperature and/or pressure or under conditions in which the energy and volume of the fluid can fluctuate. This paper proposes and discusses three methods for performing molecular dynamics simulations under conditions of constant temperature and/or pressure, rather than constant energy and volume. For these three methods, it is shown that time averages of properties of the simulated fluid are equal to averages over the isoenthalpic–isobaric, canonical, and isothermal–isobaric ensembles. Each method is a way of describing the dynamics of a certain number of particles in a volume element of a fluid while taking into account the influence of surrounding particles in changing the energy and/or density of the simulated volume element. The influence of the surroundings is taken into account without introducing unwanted surface effects. Examples of situations where these methods may be useful are discussed.

Virial theorem (Clausius ~ 1860)

$$2\langle T\rangle = -\left\langle \sum_\sigma \mathbf{F}_\sigma \cdot \mathbf{r}_\sigma \right\rangle$$

Proof :

Define : $A \equiv \sum_\sigma \mathbf{p}_\sigma \cdot \mathbf{r}_\sigma$

$$\frac{dA}{dt} = \sum_\sigma \left(\dot{\mathbf{p}}_\sigma \cdot \mathbf{r}_\sigma + \mathbf{p}_\sigma \cdot \dot{\mathbf{r}}_\sigma\right) = \sum_\sigma \mathbf{F}_\sigma \cdot \mathbf{r} + 2T$$

$$\left\langle \frac{dA}{dt} \right\rangle = \left\langle \sum_\sigma \mathbf{F}_\sigma \cdot \mathbf{r} \right\rangle + 2\langle T\rangle$$

$$\left\langle \frac{dA}{dt} \right\rangle = \frac{1}{\tau}\int_0^\tau \frac{dA(t)}{dt}\,dt = \frac{A(\tau) - A(0)}{\tau} \Rightarrow 0$$