PHY 337/637 Analytical Mechanics
12:30-1:45 PM MWF in Olin 103

Discussion of Lecture 6 – Chap. 7 & 8 in Cline

Lagrangian and Hamiltonian analysis -- continued

1. Review of Lagrangian and Hamiltonian formalisms
2. Examples
3. Brief comments about phase space

WFU Physics Department

Physics Career Coffee Chat

Join our casual coffee chat with WFU Physics alum and Duke Univeristy faculty member Dr. Salman Azhar

Thursday
1:30 - 2:30 PM
Olin 105
Questions? jurchescu@wfu.edu

Physics Colloquium

Thursday

.

September 14th, 2023

Fantastic Frameworks From Physics

Dr. Salman Azhar is a co-founder or a co-investor in over 125 startups. He has scaled organizations by forming teams and solving enigmatic problems. Dr. Azhar has 35 years of experience in industry and academia, during which he has crafted and led talented teams in developing and launching innovative technical solutions with a wide range of applications. Dr. Azhar is a Faculty member and Executive in Residence at Duke University's Fuqua School of Business. He is a Charter Life Member of OPEN Global and a venture partner at SAP.io and the University of Minnesota. Dr. Azhar is an advisor to several companies, including Regiment Securities. His former business partners and clients include Toyota, Sony, SAP, and others. He is currently developing innovative technology initiatives and mentoring leaders. Dr. Azhar earned his MS and PhD in Computer Science from Duke as a James B. Duke Fellow and a BS in Math and Physics from Wake Forest University as a Carswell Scholar. In Thursday's talk, Dr. Salman plans to go over how he develops frameworks from physics to lead a more fulfilling life by making better decisions and solving real-world problems. He will share his thinking process and invite

Salman Azhar, PhD

WFU Alum, Faculty Member and
Executive in Residence
Fuqua School of Business
Duke University

4 pm - Olin 101

Refreshments will be served in Olin Lobby beginning at 3:30pm.

PHY 337/637 Analytical Mechanics

TR 12:30 -1:45 PM	OPL 103	http://www.wfu.edu/~natalie/f23phy337/

Instructor: Natalie Holzwarth	Office:300 OPL	e-mail:natalie@wfu.edu

Course schedule

In the table below, **Reading** refers to the chapters in the Cline textbook , **PP** refers to textbook section listing practice problems to be discussed at the course tutorials, and **Assign** is a link to the graded homework for the lecture. The graded homeworks are due each Tuesday following the associated lecture.

(Preliminary schedule -- subject to frequent adjustment.)

	Date	Reading	Topic	PP	Assign
1	Tu, 8/29/2023	Ch. 1 & 2	Introduction, history, and motivation	2E	#1
2	Th, 8/31/2023	Ch. 5	Introduction to Calculus of variation	5E	#2
3	Tu, 9/05/2023	Ch. 5	More examples of the calculus of variation	5E	#3
4	Th, 9/07/2023	Ch. 6	Lagrangian mechanics	6E	#4
5	Tu, 9/12/2023	Ch. 7 & 8	Hamiltonian mechanics	8E	#5
6	Th, 9/14/2023	Ch. 7 & 8	Hamiltonian mechanics	8E	
7	Tu, 9/19/2023				
8	Th, 9/21/2023				
9	Tu, 9/26/2023				
10	Th, 9/28/2023				

Review of Lagrangian and Hamiltonian formalisms

Particle dynamics using the Lagrangian formalism, thanks to Hamilton's principle –

Hamilton's principle states that the dynamical trajectory of a system is given by the path that extremizes the action integral

$$S = \int_{t_1}^{t_2} L\left(q, \dot{q}, t\right) dt$$

for a system with a single generalized coordinate *q(t)*

$$S = \int_{t_1}^{t_2} L\left(\{q_\sigma\}, \{\dot{q}_\sigma\}, t\right) dt$$

for a system with multiple dimensions and/or particles with generalized coordinates $q_\sigma(t)$

$$L\left(\{q_\sigma\}, \{\dot{q}_\sigma\}, t\right) = T\left(\{q_\sigma\}, \{\dot{q}_\sigma\}, t\right) - U\left(\{q_\sigma\}, \{\dot{q}_\sigma\}, t\right)$$

Kinetic energy **Potential energy**

Lagrangian picture

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

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

Lagrangian equations of motion: $$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} = 0$$

Alternate form of Euler-Lagrange equations: $$\frac{d}{dt}\left(L - \sum_\sigma \frac{\partial L}{\partial \dot{q}_\sigma}\dot{q}_\sigma\right) = \frac{\partial L}{\partial t}$$

Switching variables – Legendre transformation

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

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

Note that: $$\frac{dH}{dt} = \frac{\partial H}{\partial t}$$

Canonical equations: $$\dot{q}_\sigma = \frac{\partial H}{\partial p_\sigma} \qquad \dot{p}_\sigma = -\frac{\partial H}{\partial q_\sigma}$$

In the Hamiltonian formulation --

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

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

Why are these equations known as the “canonical equations”?

a. Because they are beautiful.
b. The term is meant to elevate their importance to the level of the music of J. S. Bach
c. To help you remember them
d. No good reason; it is just a name

Recipe for constructing the Hamiltonian and analyzing the equations of motion

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

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

Constants of the motion in Hamiltonian formalism

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

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \quad \Rightarrow \text{constant } q_\sigma \equiv \bar{q}_\sigma \text{ if } \frac{\partial H}{\partial p_\sigma} = 0$$

$$\frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma} \quad \Rightarrow \text{constant } p_\sigma \equiv \bar{p}_\sigma \text{ if } \frac{\partial H}{\partial q_\sigma} = 0$$

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

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

$$\Rightarrow \text{ constant } H \equiv \bar{H} \text{ if } \frac{\partial H}{\partial t} = 0$$

Example: one-dimensional potential:

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

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

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

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

Constants: $\overline{p}_x, \overline{p}_y, \overline{H}$ (using bar to indicate constant)

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

Example: Motion in a central potential

$$L = \tfrac{1}{2} m\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - V(r)$$

$$p_r = m\dot{r} \qquad p_\varphi = mr^2\dot{\varphi}$$

$$H = m\dot{r}^2 + mr^2\dot{\varphi}^2 - \left(\tfrac{1}{2} m\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - V(r)\right)$$

$$= \tfrac{1}{2} m\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) + V(r)$$

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

Note that:

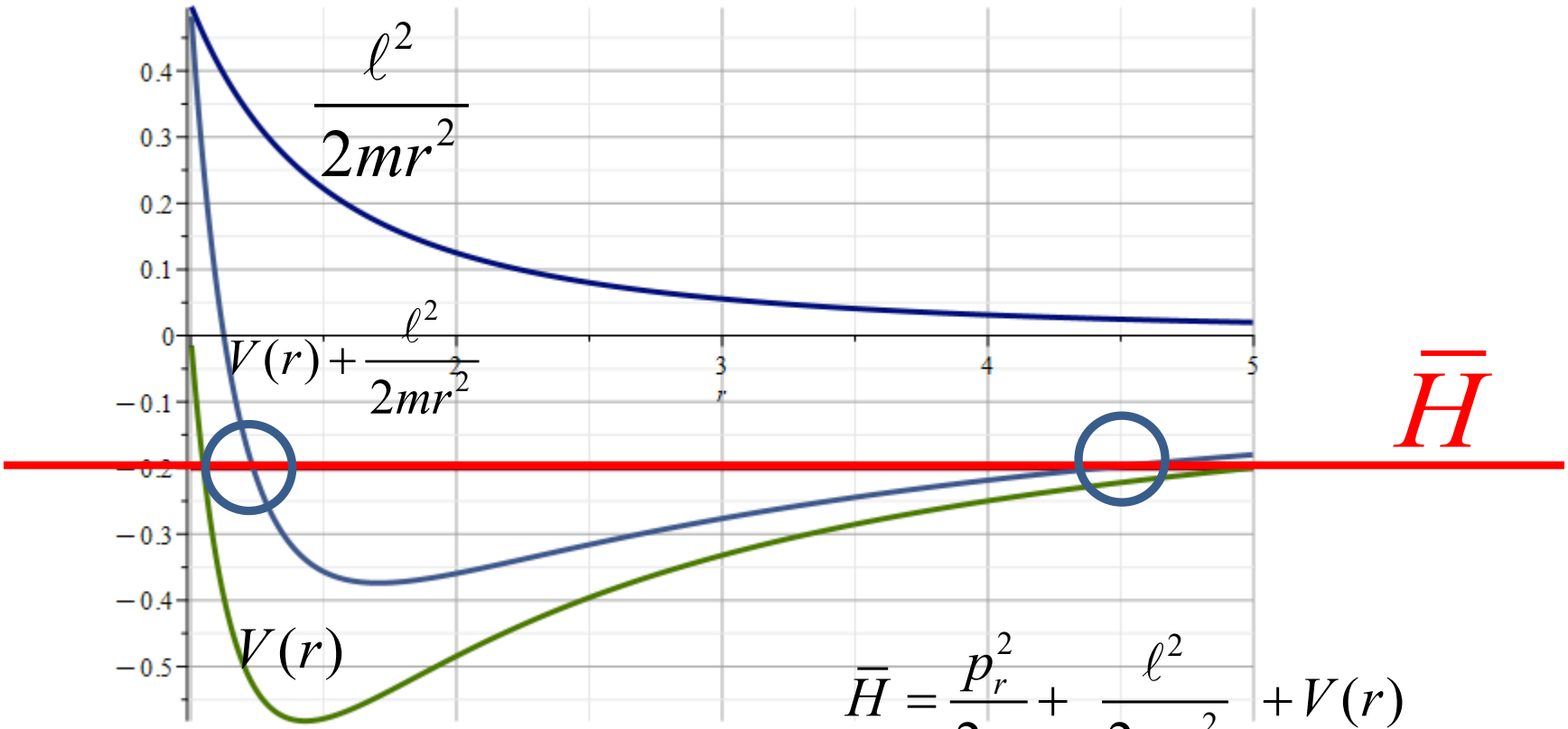
Constants: $\bar{p}_\varphi, \bar{H}$

$\bar{p}_\varphi \to \ell$ (angular momentum)

Equations of motion:

$$\frac{dr}{dt} = \frac{p_r}{m} \qquad \frac{dp_r}{dt} = -\frac{\partial H}{\partial r} = \frac{\bar{p}_\varphi^2}{mr^3} - \frac{\partial V}{\partial r}$$

Example of motion in a central potential



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

$$\bar{H} = \frac{m}{2}\left(\frac{dr}{dt}\right)^2 + \frac{\ell^2}{2mr^2} + V(r)$$

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

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

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

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

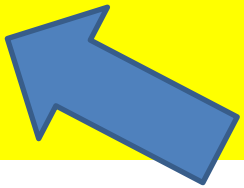
Hamiltonian: $\mathbf{p}=\frac{\partial L}{\partial\dot{\mathbf{r}}}=m\dot{\mathbf{r}}+\frac{q}{c}\mathbf{A}(\mathbf{r},t)$

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

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

$$=\frac{1}{2}m\dot{\mathbf{r}}^2+U(\mathbf{r})+q\Phi(\mathbf{r},t)$$

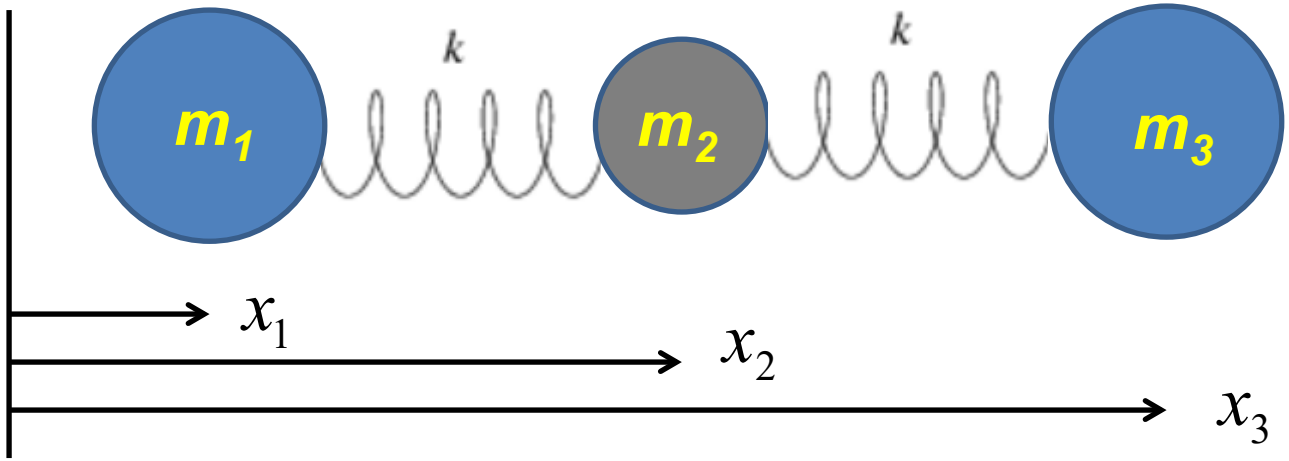
$$H(\mathbf{r},\mathbf{p},t)=\frac{1}{2m}\left(\mathbf{p}-\frac{q}{c}\mathbf{A}(\mathbf{r},t)\right)^2+U(\mathbf{r})+q\Phi(\mathbf{r},t)$$



Canonical form

Some more examples of using Lagrangian and/or Hamiltonian formalism for analyzing motion --

Example – linear molecule



$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2$$

$$-\frac{1}{2}k\left(x_2 - x_1 - \ell_{12}\right)^2 - \frac{1}{2}k\left(x_3 - x_2 - \ell_{23}\right)^2$$

Let: $x_1 \to x_1 - x_1^0 \quad x_2 \to x_2 - x_1^0 - \ell_{12} \quad x_3 \to x_3 - x_1^0 - \ell_{12} - \ell_{23}$

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k\left(x_2 - x_1\right)^2 - \frac{1}{2}k\left(x_3 - x_2\right)^2$$

Coupled equations of motion :

$$m_1\ddot{x}_1 = k\left(x_2 - x_1\right)$$

$$m_2\ddot{x}_2 = -k\left(x_2 - x_1\right) + k\left(x_3 - x_2\right) = k\left(x_1 - 2x_2 + x_3\right)$$

$$m_3\ddot{x}_3 = -k\left(x_3 - x_2\right)$$

Let $x_i(t) = X_i^\alpha e^{-i\omega_\alpha t}$

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Coupled linear equations:

$$-\omega_\alpha^2 m_1 X_1^\alpha = k\left(X_2^\alpha - X_1^\alpha\right)$$

$$-\omega_\alpha^2 m_2 X_2^\alpha = k\left(X_1^\alpha - 2X_2^\alpha + X_3^\alpha\right)$$

$$-\omega_\alpha^2 m_3 X_3^\alpha = -k\left(X_3^\alpha - X_2^\alpha\right)$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix} \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

Matrix form:

$$\begin{pmatrix} k-\omega_\alpha^2 m_1 & -k & 0 \\ -k & 2k-\omega_\alpha^2 m_2 & -k \\ 0 & -k & k-\omega_\alpha^2 m_3 \end{pmatrix} \begin{pmatrix} X_1^\alpha \\ X_2^\alpha \\ X_3^\alpha \end{pmatrix} = 0$$

More convenient form:

Let $Y_i \equiv \sqrt{m_i} X_i$ Equations for Y_i take the form:

$$\begin{pmatrix} \kappa_{11}-\omega_\alpha^2 & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22}-\omega_\alpha^2 & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33}-\omega_\alpha^2 \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = 0$$

where $\kappa_{ij} = \kappa_{ji} \equiv \dfrac{k}{\sqrt{m_i m_j}}$

Rearranging the equation to an eigenvalue problem:

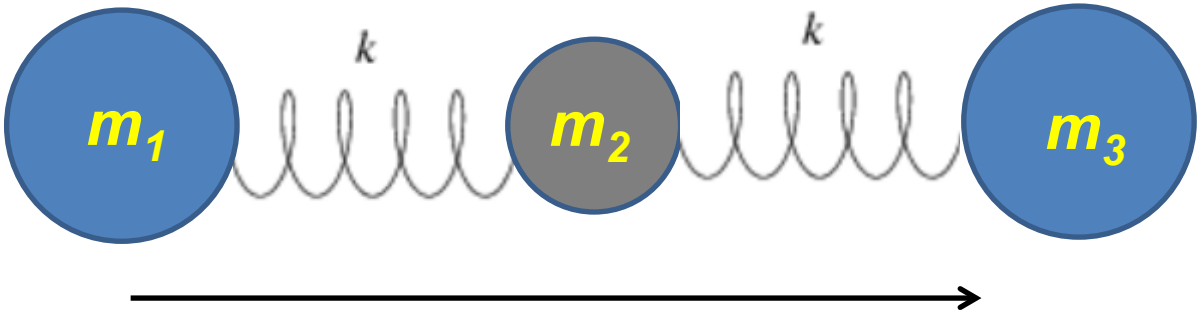
$$\begin{pmatrix} \kappa_{11} & -\kappa_{12} & 0 \\ -\kappa_{12} & 2\kappa_{22} & -\kappa_{23} \\ 0 & -\kappa_{23} & \kappa_{33} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

Special case for CO_2 molecule -- $m_1 = m_3 \equiv m_O$ and $m_2 \equiv m_C$

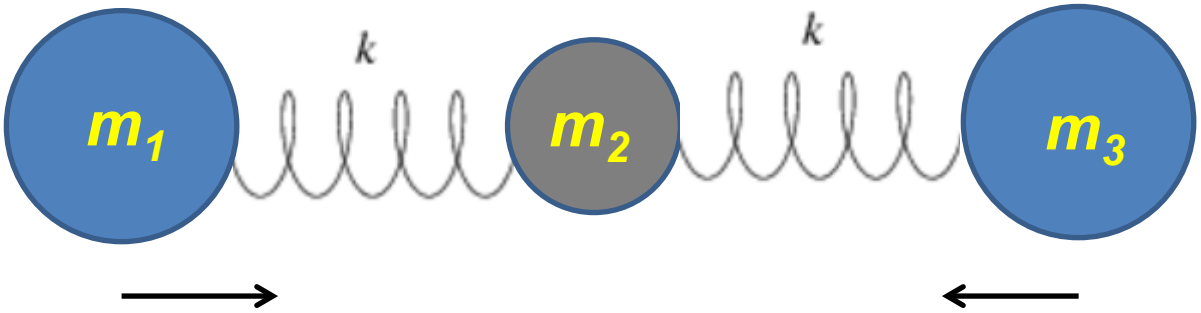
$$\begin{pmatrix} \kappa_{OO} & -\kappa_{OC} & 0 \\ -\kappa_{OC} & 2\kappa_{CC} & -\kappa_{OC} \\ 0 & -\kappa_{OC} & \kappa_{OO} \end{pmatrix} \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix} = \omega_\alpha^2 \begin{pmatrix} Y_1^\alpha \\ Y_2^\alpha \\ Y_3^\alpha \end{pmatrix}$$

For $m_1 = m_3 \equiv m_O$

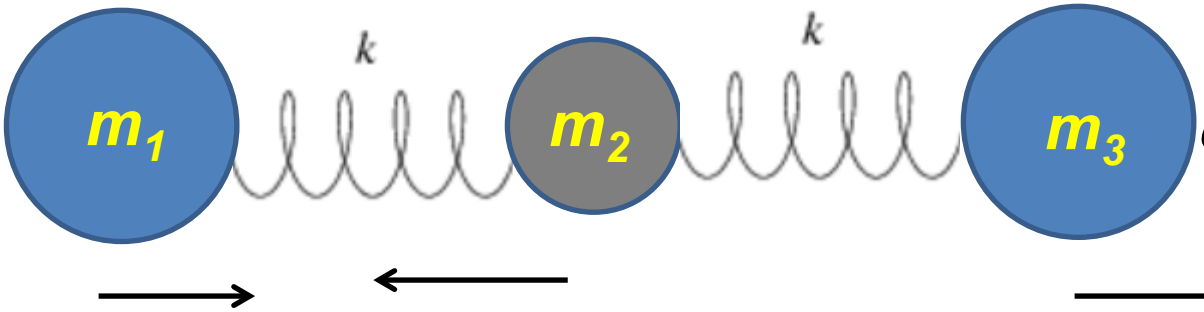
and $m_2 \equiv m_C$



$\omega_1 = 0$



$\omega_2 = \sqrt{\dfrac{k}{m_O}}$



$\omega_3 = \sqrt{\dfrac{k}{m_O} + \dfrac{2k}{m_C}}$

(with help from Maple)

Eigenvalues and eigenvectors:

***N,N'* are normalization constants.**

$$\omega_1^2 = 0 \qquad \begin{pmatrix} Y_1^1 \\ Y_2^1 \\ Y_3^1 \end{pmatrix} = N_1 \begin{pmatrix} \sqrt{\frac{m_O}{m_C}} \\ 1 \\ \sqrt{\frac{m_O}{m_C}} \end{pmatrix}, \quad \begin{pmatrix} X_1^1 \\ X_2^1 \\ X_3^1 \end{pmatrix} = N'_1 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\omega_2^2 = \frac{k}{m_O} \qquad \begin{pmatrix} Y_1^2 \\ Y_2^2 \\ Y_3^2 \end{pmatrix} = N_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} X_1^2 \\ X_2^2 \\ X_3^2 \end{pmatrix} = N'_2 \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\omega_3^2 = \frac{k}{m_O} + \frac{2k}{m_C} \qquad \begin{pmatrix} Y_1^3 \\ Y_2^3 \\ Y_3^3 \end{pmatrix} = N_3 \begin{pmatrix} 1 \\ -2\sqrt{\frac{m_O}{m_C}} \\ 1 \end{pmatrix}, \quad \begin{pmatrix} X_1^3 \\ X_2^3 \\ X_3^3 \end{pmatrix} = N'_3 \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

What about Hamiltonian formulation → notion of phase space.

Phase space

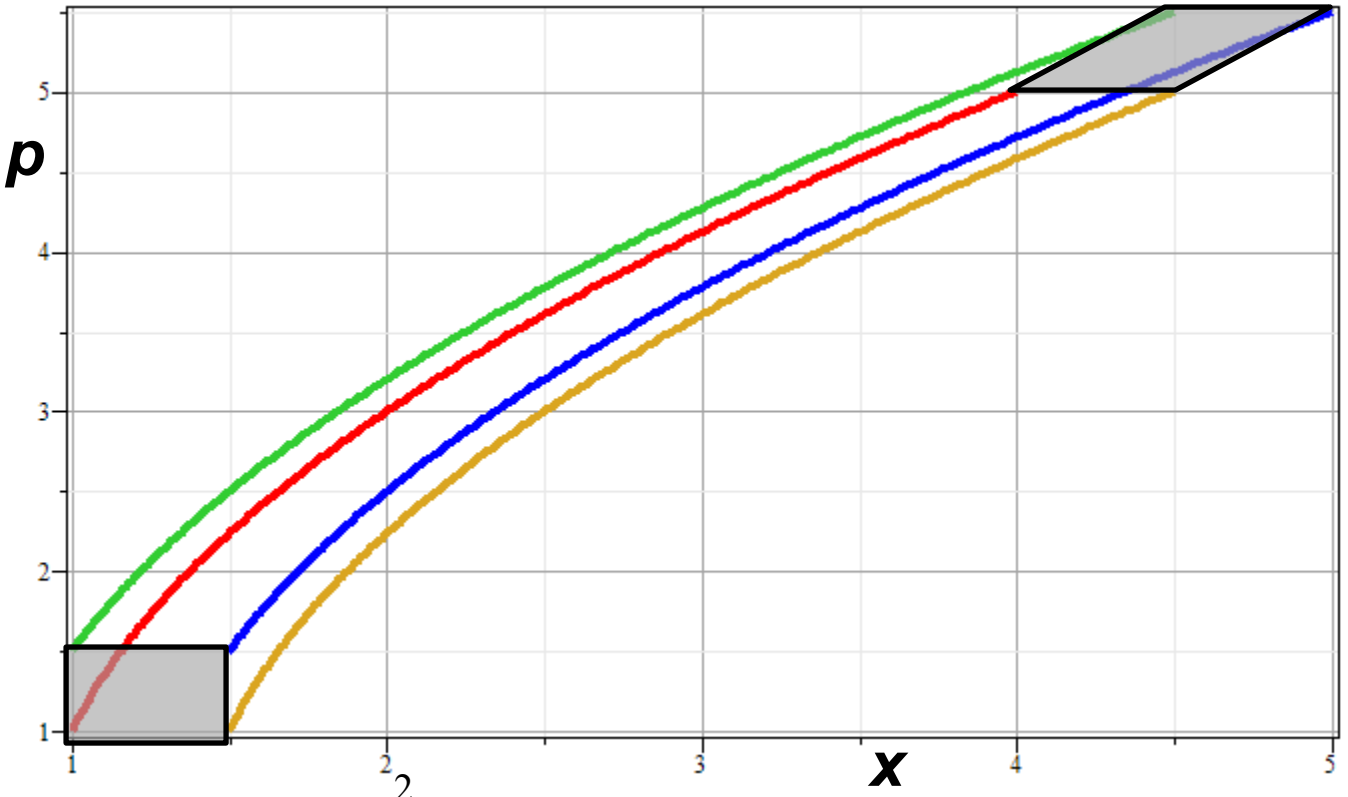
Phase space is defined at the set of all coordinates and momenta of a system:

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

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

The notion of density of particles in phase space is simply the ratio of the number of particles per unit phase space volume. It seems reasonable that under conditions where there are no sources or sinks for the particles, that the density should remain constant in time.

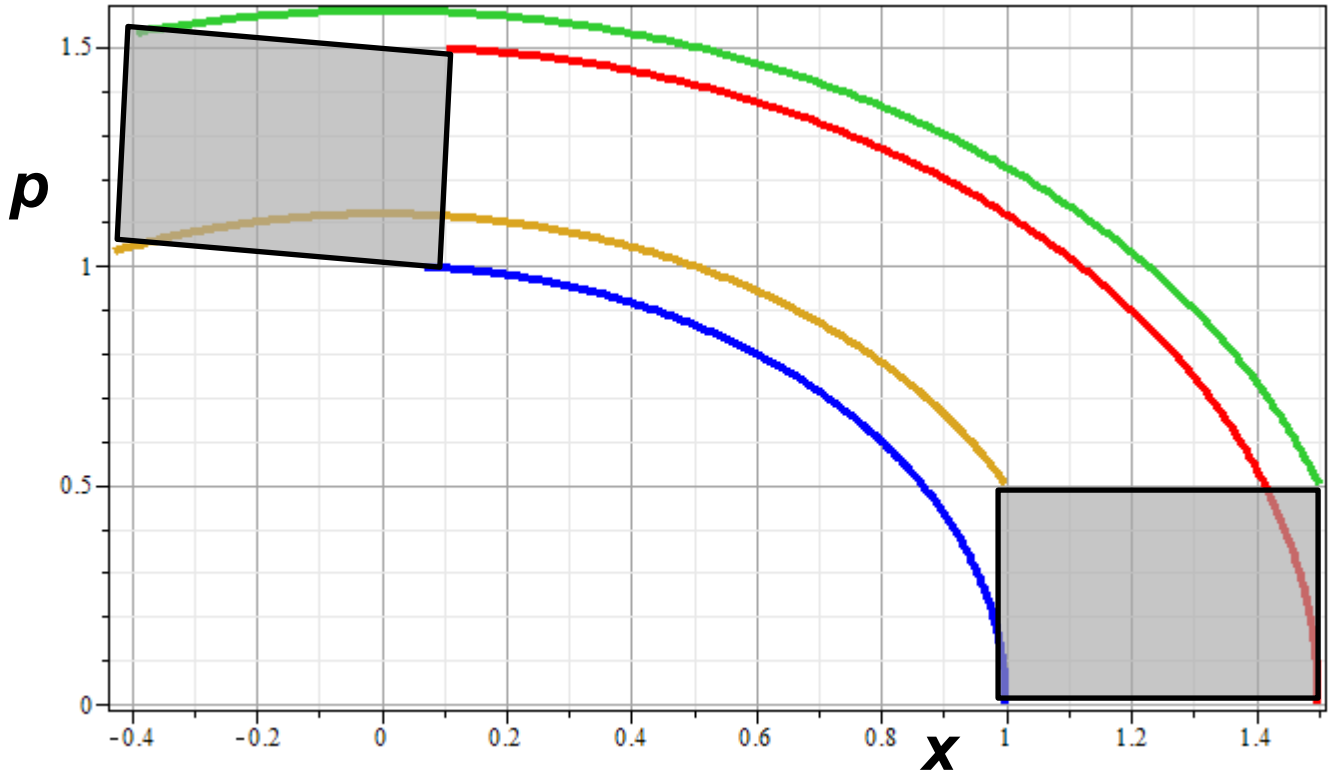
Phase space diagram for one-dimensional motion due to constant force



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

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

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



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

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

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.

Joseph Liouville

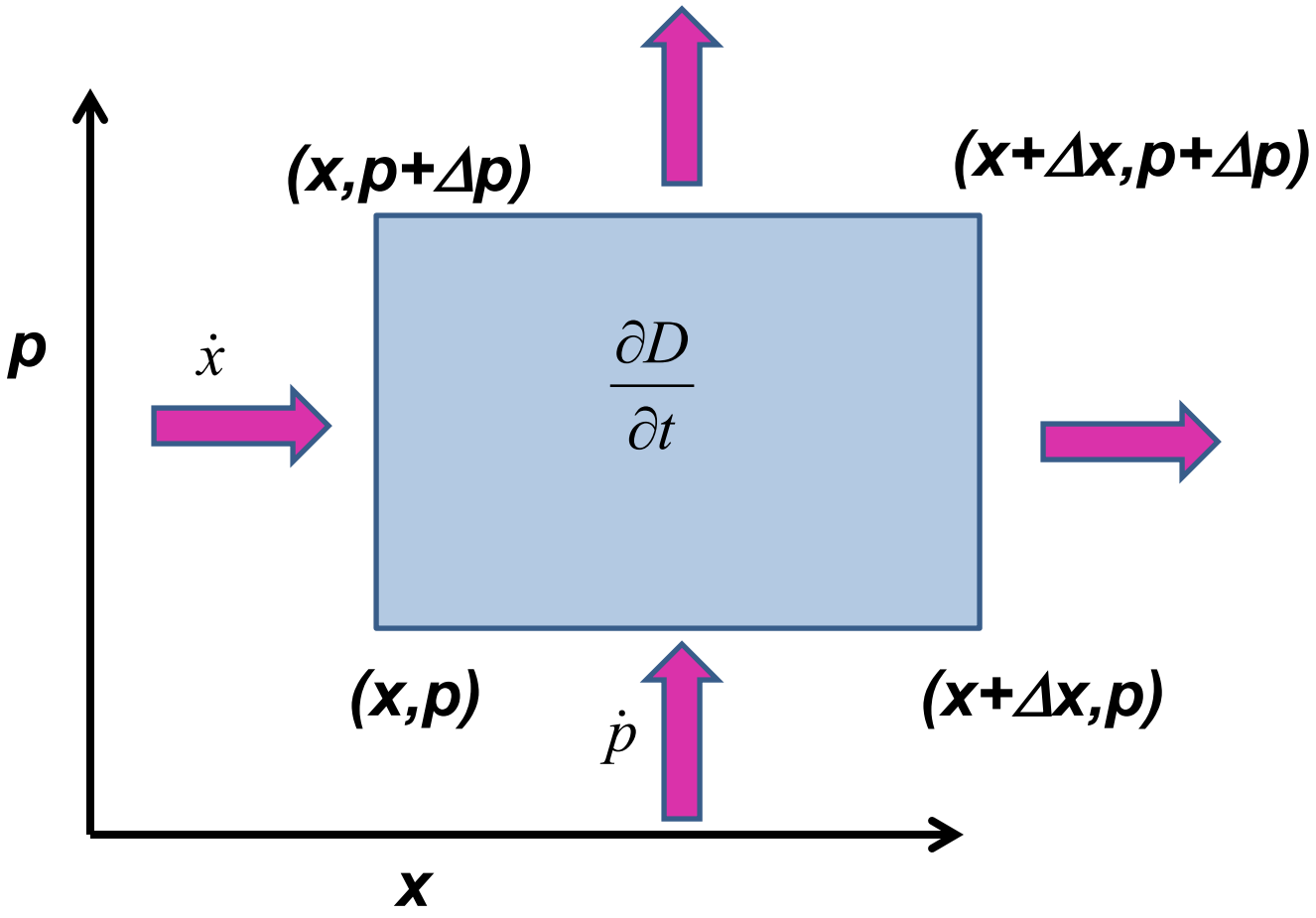
lived from 1809 to 1882

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

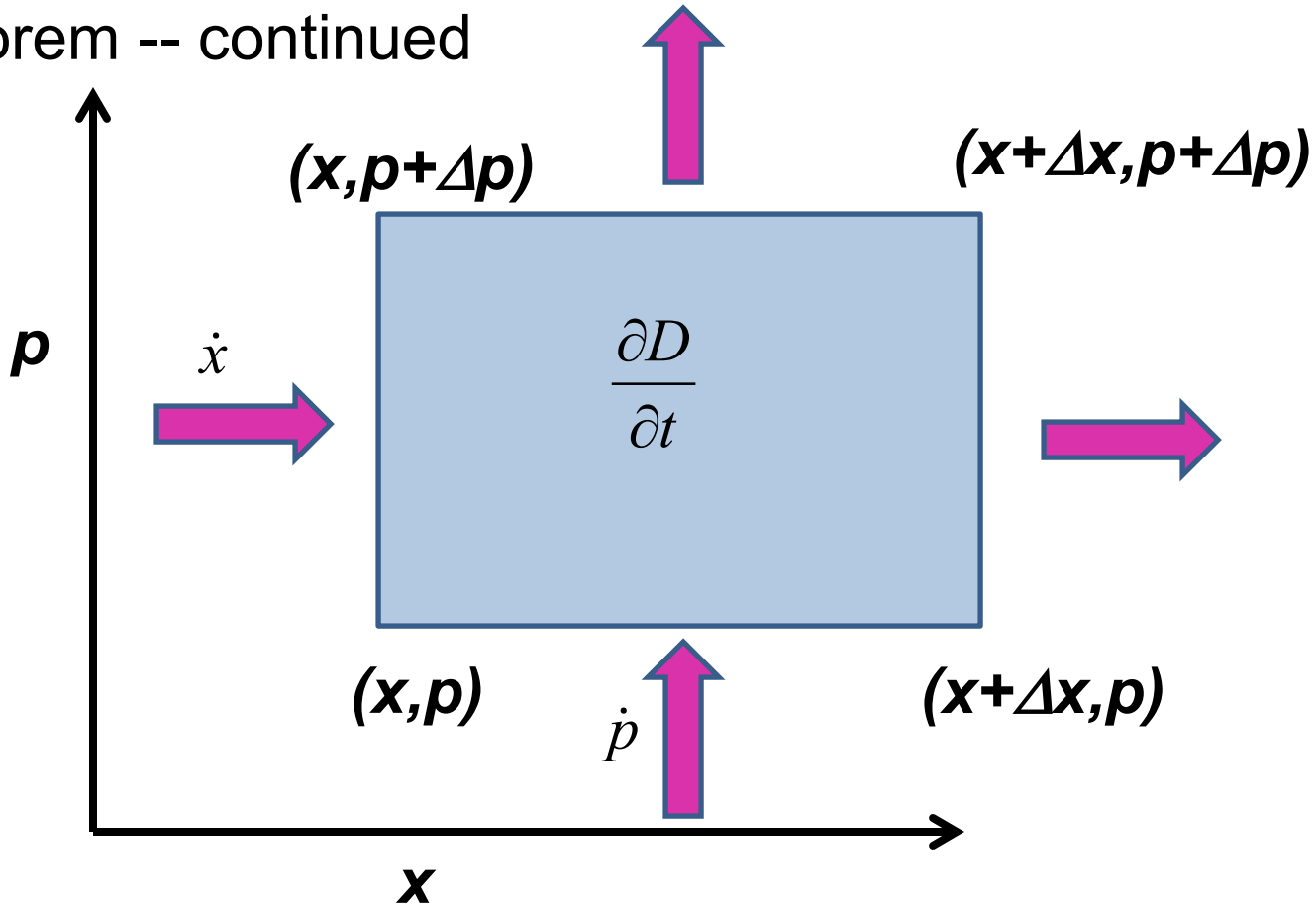
$$\frac{dD}{dt} = \sum_\sigma \left(\frac{\partial D}{\partial q_\sigma} \dot{q}_\sigma + \frac{\partial D}{\partial p_\sigma} \dot{p}_\sigma \right) + \frac{\partial D}{\partial t}$$

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

Liouville's theorem



Liouville's theorem -- continued

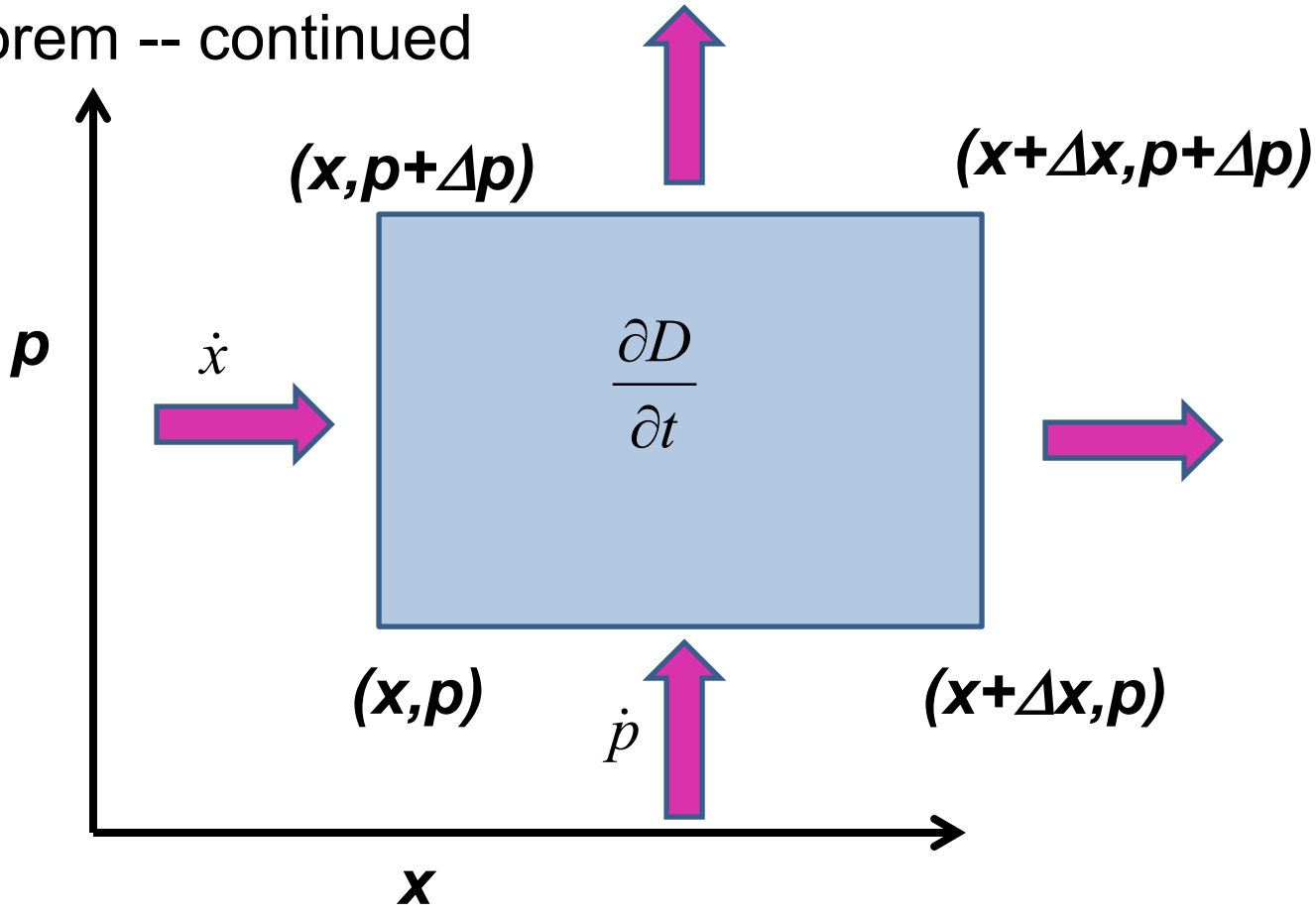


$$\frac{\partial D}{\partial t} \Rightarrow \text{time rate of change of particles within volume}$$

$$= \text{time rate of particle entering minus particles leaving}$$

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

Liouville's theorem -- continued



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

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

Summary:

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:

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

Liouville's theorm shows that:

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

Note that we are assuming that no particles are created or destroyed in these processes.

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

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. Computationally this can be approximated using molecular dynamics or sampling methods.

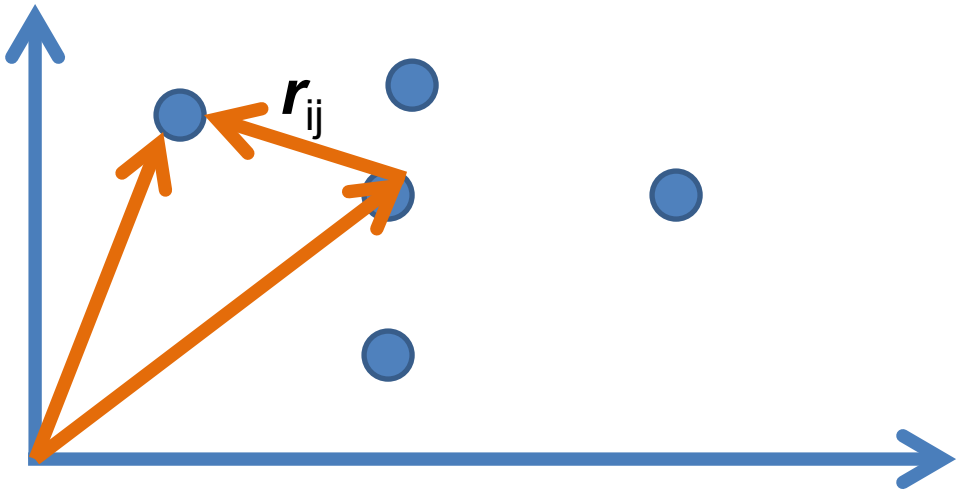
"Molecular dynamics" is a subfield of computational physics focused on analyzing the motions of atoms in fluids and solids with the goal of relating the atomistic and macroscopic properties of materials. Ideally molecular dynamics calculations can numerically realize the statistical mechanics viewpoint.

Imagine that the generalized coordinates $\{q_\sigma(t)\}$ represent N atoms, each with 3 spacial coordinates:

$$L = L\left(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t\right) = T - U$$

For simplicity, it is often assumed that the potential interaction is a sum of pairwise interactions:

$$U(r^N) = \sum_{i<j} u(r_{ij}) \,. \qquad (2.1)$$



$$L = L\left(\{\mathbf{r}_i(t)\},\{\dot{\mathbf{r}}_i(t)\}\right) = \sum_i \tfrac{1}{2} m_i \left|\dot{\mathbf{r}}_i\right|^2 - \sum_{i<j} u\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)$$

➔From this Lagrangian, can find the 3N coupled 2nd order differential equations of motion and/or find the corresponding Hamiltonian, representing the system at constant energy, volume, and particle number N (N,V,E ensemble).

Lagrangian and Hamiltonian forms

$$L = L\left(\{\mathbf{r}_i(t)\},\{\dot{\mathbf{r}}_i(t)\}\right) = \sum_i \tfrac{1}{2} m_i \left|\dot{\mathbf{r}}_i\right|^2 - \sum_{i<j} u\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)$$

Euler-Lagrange equations:

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = -\sum_{i<j} u'\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)\frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}$$

Hamiltonian formulation:

$$\mathbf{p}_i = m_i \dot{\mathbf{r}}_i$$

$$H = \sum_i \frac{\left|\mathbf{p}_i\right|^2}{2m_i} + \sum_{i<j} u\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)$$

Canonical equations:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m_i} \qquad \frac{d\mathbf{p}_i}{dt} = -\sum_{i<j} u'\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|\right)\frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|}$$

By solving these coupled equations, we can use our atomic scale ideas to model macroscopic systems…

Digression on numerical evaluation of differential equations

Example differential equation (one dimension);

$$\frac{d^2x}{dt^2} = f(t) \qquad \text{Let} \quad t = nh \qquad (n = 1, 2, 3\ldots)$$

$$x_n \equiv x(nh); \qquad f_n \equiv f(nh)$$

Euler's method :

$$x_{n+1} = x_n + hv_n + \frac{1}{2}h^2 f_n$$

$$v_{n+1} = v_n + hf_n$$

Velocity Verlet algorithm :

$$x_{n+1} = x_n + hv_n + \frac{1}{2}h^2 f_n$$

$$v_{n+1} = v_n + \frac{1}{2}h(f_n + f_{n+1})$$