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

Plan for Lecture 14:

Finish reading Chapter 6

Modern example of analysis using Lagrangian and Hamiltonian formalisms

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/28/2013	Chap. 1	Review of basic principles,Scattering theory	#1
2	Fri, 8/30/2013	Chap. 1	Scattering theory continued	#2
3	Mon, 9/02/2013	Chap. 1	Scattering theory continued	#3
4	Wed, 9/04/2013	Chap. 2	Accelerated Coordinate Systems	#4
5	Fri, 9/06/2013	Chap. 3	Calculus of variations	#5
6	Mon, 9/09/2013	Chap. 3	Calculus of variations -- continued	
7	Wed, 9/11/2013	Chap. 3	Calculus of variations applied to Lagrangians	#6
8	Fri, 9/13/2013	Chap. 3	Lagrangian mechanics	#7
9	Mon, 9/16/2013	Chap. 3 & 6	Lagrangian mechanics	#8
10	Wed, 9/18/2013	Chap. 3 & 6	Lagrangian mechanics	#9
11	Fri, 9/20/2013	Chap. 3 & 6	Lagrangian & Hamiltonian mechanics	#10
12	Mon, 9/23/2013	Chap. 3 & 6	Hamiltonian formalism	#11
13	Wed, 9/25/2013	Chap. 3 & 6	Hamiltonian formalism	#12
14	Fri, 9/27/2013	Chap. 3 & 6	Hamiltonian formalism	#13
15	Mon, 9/30/2013	Chap. 4	Small Oscillations	#14

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 $q_\sigma(t)$

Hamiltonian picture

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

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

$\Rightarrow$ Coupled first order differential equations for $q_\sigma(t)$ and $p_\sigma(t)$

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

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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.

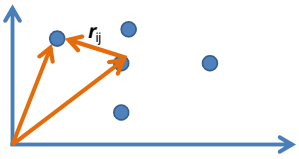
"Molecular dynamics" is a subfield of computational physics focused on analyzing the motions of atoms in fluids and solids with the goal of relating the atomistic and macroscopic properties of materials. Ideally molecular dynamics calculations can numerically realize the statistical mechanics viewpoint.

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

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

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

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



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

➔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

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

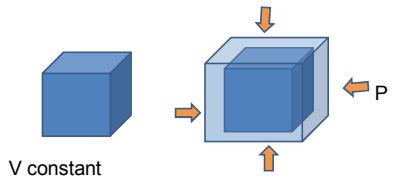
$$\mathbf{p}_i = m_i \dot{\mathbf{r}}_i$$

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

Canonical equations :

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

H. C. Andersen wanted to adapt the formalism for modeling an (N,V,E) ensemble to one which could model a system at constant pressure (P).



Andersen's clever transformation :

PV contribution to potential energy

Let $\boldsymbol{\rho}_i = \mathbf{r}_i / Q^{1/3}$

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

$$L = L(\{\boldsymbol{\rho}_i(t)\},\{\dot{\boldsymbol{\rho}}_i(t)\},Q,\dot{Q}) = Q^{2/3}\sum_i \tfrac{1}{2} m_i |\dot{\boldsymbol{\rho}}_i|^2 - \sum_{i<j} u(Q^{1/3}|\boldsymbol{\rho}_i - \boldsymbol{\rho}_j|) + \tfrac{1}{2} M\dot{Q}^2 - \alpha Q$$

kinetic energy of "balloon"

$$L = L\left(\{\boldsymbol{\rho}_i(t)\},\{\dot{\boldsymbol{\rho}}_i(t)\},Q,\dot{Q}\right) = Q^{2/3}\sum_i \tfrac{1}{2}m_i\left|\dot{\boldsymbol{\rho}}_i\right|^2 - \sum_{i<j} u\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right) + \tfrac{1}{2}M\dot{Q}^2 - \alpha Q$$

$$\boldsymbol{\pi}_i = \frac{\partial L}{\partial \dot{\boldsymbol{\rho}}_i} = mQ^{2/3}\dot{\boldsymbol{\rho}}_i$$

$$\Pi = \frac{\partial L}{\partial \dot{Q}} = M\dot{Q}$$

$$H = \sum_i \frac{\left|\boldsymbol{\pi}_i\right|^2}{2m_iQ^{2/3}} + \sum_{i<j} u\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right) + \frac{\Pi^2}{2M} + \alpha Q$$

$$\frac{d\boldsymbol{\rho}_i}{dt} = \frac{\boldsymbol{\pi}_i}{2m_iQ^{2/3}} \qquad \frac{dQ}{dt} = \frac{\Pi}{M}$$

$$\frac{d\boldsymbol{\pi}_i}{dt} = -Q^{1/3}\sum_{i<j} u'\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right)\frac{\boldsymbol{\rho}_i-\boldsymbol{\rho}_j}{\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|}$$

$$\frac{d\Pi}{dt} = \frac{2}{3Q}\sum_i \frac{\left|\boldsymbol{\pi}_i\right|^2}{2m_iQ^{2/3}} - \frac{1}{3Q^{2/3}}\sum_{i<j} u'\left(Q^{1/3}\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right|\right)\left|\boldsymbol{\rho}_i-\boldsymbol{\rho}_j\right| - \alpha$$

Relationship between system representations

Scaled		Original
$Q(t)$	=	$V(t)$
$Q^{1/3}\boldsymbol{\rho}_i(t)$	=	$\mathbf{r}_i(t)$
$\boldsymbol{\pi}_i / Q^{1/3}$	=	$\mathbf{p}_i$

Equations of motion in "original" coordinates:

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m_i} + \frac{1}{3}\mathbf{r}_i\frac{d\ln V}{dt}$$

$$\frac{d\mathbf{p}_i}{dt} = -\sum_{j<i}\frac{\mathbf{r}_i-\mathbf{r}_j}{\left|\mathbf{r}_i-\mathbf{r}_j\right|}u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right) - \frac{1}{3}\mathbf{p}_i\frac{d\ln V}{dt}$$

$$M\frac{d^2V}{dt^2} = -\alpha + \frac{1}{V}\left(\frac{2}{3}\sum_i\frac{\mathbf{p}_i\cdot\mathbf{p}_i}{m_i} - \frac{1}{3}\sum_{j<i}\left|\mathbf{r}_i-\mathbf{r}_j\right|u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)\right)$$

Physical interpretation:

$\alpha \Leftrightarrow$ Imposed (target) pressure

$$\frac{1}{V}\left(\frac{2}{3}\sum_i\frac{\mathbf{p}_i\cdot\mathbf{p}_i}{m_i} - \frac{1}{3}\sum_{j<i}\left|\mathbf{r}_i-\mathbf{r}_j\right|u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)\right) \Leftrightarrow \text{Internal pressure of system}$$

Time dependence

$$M\frac{d^2V}{dt^2} = -\alpha + \frac{1}{V}\left(\frac{2}{3}\sum_i\frac{\mathbf{p}_i\cdot\mathbf{p}_i}{m_i} - \frac{1}{3}\sum_{j<i}\left|\mathbf{r}_i-\mathbf{r}_j\right|u'\left(\left|\mathbf{r}_i-\mathbf{r}_j\right|\right)\right)$$

Digression on numerical evaluation of differential equations

Example differential equation (one dimension);

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

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

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 :

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

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