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

Plan for Lecture 13:

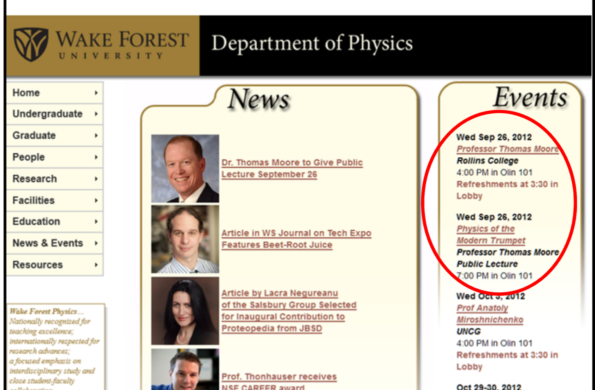
Continue reading Chapter 6

- **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, 8/29/2012	Chap. 1	Review of basic principles;Scattering theory	#1
2	Fri, 8/31/2012	Chap. 1	Scattering theory continued	#2
3	Mon, 9/03/2012	Chap. 1	Scattering theory continued	#3
4	Wed, 9/05/2012	Chap. 1 & 2	Scattering theory/Accelerated coordinate frame	#4
5	Fri, 9/07/2012	Chap. 2	Accelerated coordinate frame	#5
6	Mon, 9/10/2012	Chap. 3	Calculus of Variation	#6
7	Wed, 9/12/2012	Chap. 3	Calculus of Variation continued	
8	Fri, 9/14/2012	Chap. 3	Lagrangian	#7
9	Mon, 9/17/2012	Chap. 3 & 6	Lagrangian	#8
10	Wed, 9/19/2012	Chap. 3 & 6	Lagrangian	#9
11	Fri, 9/21/2012	Chap. 3 & 6	Lagrangian	#10
12	Mon, 9/24/2012	Chap. 3 & 6	Lagrangian and Hamiltonian	#11
13	Wed, 9/26/2012	Chap. 6	Lagrangian and Hamiltonian	#12



FOREST SITY | Department of Physics

WFU Physics Colloquium

TITLE: The Physics of the Modern Trumpet

SPEAKER: Professor Thomas Moore,

Department of Physics,
Rollins College

TIME: Wednesday September 26, 2012 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

The modern trumpet has developed over the past 500 years into a highly specialized instrument that takes advantage of some very subtle physics. This presentation will include an overview of the physics of the trumpet, a discussion of the variables in trumpet design, and the results of some new research into how small vibrations of the metal affect the sound.

WFU Physics Public Lecture

TITLE: Trumpet Lessons: The physics of the modern trumpet and what it can teach us about art and science

SPEAKER: Dr. Thomas Moore,

Department of Physics,
Rollins College

TIME: Wednesday September 26, 2012 at **7:00 PM**

PLACE: Room 101 Olin Physical Laboratory

ABSTRACT

The modern trumpet is the result of a centuries-long process of trial and error. Since it was not designed using established scientific theories, an understanding of how the trumpet actually works has lagged far behind its development. This presentation will explain the science behind how trumpets are designed and what makes them sound as they do. Some myths about what makes a good trumpet will be investigated, and the relationship between the scientist and artist will be discussed.

Dr. Moore is the Archibald Granville Bush Professor of Science at Rollins College in Winter Park, FL. He earned his PhD at the Institute for Optics at the University of Rochester. He also served in the U.S. Army for twenty-one years in many capacities, among them commanding a combat arms unit, serving as a research scientist at Lawrence Livermore National Laboratory, and teaching physics at the U.S. Military Academy at West Point. His current research in musical acoustics focuses on the physics of the piano and brass instruments, and his research interests include a variety of other instruments.

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 $p_\sigma(t)$

J. Chem. Physics **72** 2384-2393 (1980)

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

Hans C. Andersen

Department of Chemistry, Stanford University, Stanford, California 94305

(Received 10 July 1979; accepted 31 October 1979)

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.

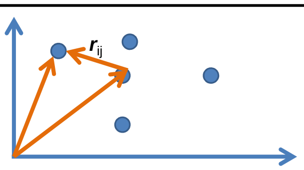
"Molecular dynamics" is a subfield of computational physics focused on analyzing the motions of atoms in fluids and solids with the goal of relating the atomistic and macroscopic properties of materials. Ideally molecular dynamics calculations can numerically realize the statistical mechanics viewpoint.

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).

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

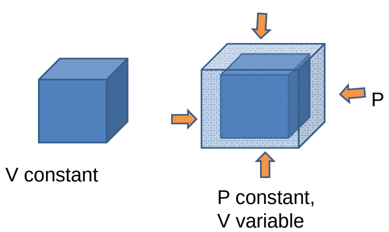
$$\mathbf{p}_i = m_i \dot{\mathbf{r}}_i$$

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

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).



PV contribution to potential energy

Andersen's clever transformation:

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"

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

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

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

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

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

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

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