Lecture 1:
Historical Overview, Statistical Paradigm, Classical Mechanics

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Historical Overview

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- In the 19th century Clausius introduced the concept of the mean free path of molecules in gases. He also stated that heat is the kinetic energy of molecules. In 1859 Maxwell applied molecular hypothesis to calculate the distribution of gas molecules over their velocities.
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- The statistical mechanics in its modern form was formulated as a complete theory by an American physicist Josiah Willard Gibbs in 1875-1902. The Gibbs formulation is the summit of the statistical physics. It provides rational justification of thermodynamics and requires only a minor modification to describe quantum statistics.
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In 1900 Max Planck formulated and presented his theory of blacks-body radiation based on a revolutionary quantum hypothesis. This theory started a new era of quantum physics in general and, in particular, the era of quantum statistical mechanics.
Statistical Paradigm

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- We need a new paradigm, recognizing that statistical laws resulting from the very presence of the huge number of particles cannot be in any way reduced to purely mechanical laws.
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*The goal of the statistical mechanics is to define these variables and to justify the laws of thermodynamics*
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The number $s$ depends on a particular system, e.g. for a system of $N$ particles in 3D space $s = 3N$. 

For any mechanical system a definite function:

$$L = L(q_1, q_2, \ldots, q_s, \dot{q}_1, \dot{q}_2, \ldots, \dot{q}_s, t) \equiv L(q, \dot{q}, t)$$

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Least Action Principle

The equations of motion can be obtained from the least action principle stating that the integral (action)

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$$ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0 \quad i = 1, \ldots, s \quad (1) $$

These are $s$ second order differential equations connecting $\ddot{q}$, $\dot{q}$, and $q$. 
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These are \( s \) second order differential equations connecting \( \ddot{q}, \dot{q} \), and \( q \). For conservative systems

\[ L(q, \dot{q}, t) = T(q, \dot{q}) - U(q), \]

where \( T = \sum_i m_i v_i^2 / 2 \) is the total kinetic energy and \( U(q) \) is the potential energy.
Hamilton’s (Canonical) Equations

In statistical mechanics another form of equations of motion is used (Hamilton’s equations). Introducing generalized momenta:

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and Hamiltonian function (using Legendre transformation):

\[ H(q, p, t) = \sum_{i=1}^{s} p_i \dot{q}_i - L(q, \dot{q}, t) \]  \hspace{1cm} (3)
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we obtain a set of 2s first-order differential equations (Hamilton’s equations):

\[ \dot{p}_i = -\frac{\partial H}{\partial q_i} \]  

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(5)
Conservations Laws (Integrals of Motion)

A general solution of a system of $2s$ first order differential equations depends on $2s$ arbitrary constants. For a conservative, isolated (closed) system the system of equations of motion does not contain the time $t$ (independent variable) explicitly (autonomous system). It means that the equations of motion are time-invariant, i.e. the origin of time $t_0$ is arbitrary. Since we can always eliminate $t_0$ there are only $2s - 1$ combinations of $q_i$ and $p_i$ that remain constant. These constants are called integrals of motion. There are seven integrals of motion that are of the most significance for statistical mechanics:
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- Three projections of Angular Momentum $\vec{M}$ resulting from isotropy of space
Conservation of Energy

Conservation of energy can be proven from time independence of the Hamiltonian at the Hamilton’s equations (4). Indeed, for any $H(p, q, t)$:

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \sum_{i=1}^{s} \left( \frac{\partial H}{\partial q_i} \dot{q}_i + \frac{\partial H}{\partial p_i} \dot{p}_i \right)$$

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Thus $H(p, q) = E$ where $E$ is the constant of motion identified as the energy of the system.
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