PHYS 542 Statistical Mechanics II - Fall 2012

(December 27, 2012)

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Lectures: M 14:40-16:30 FENS L058
T 12:40-13:30 FENS L058

Course Description:

This course aims to introduce the basic physical concepts and mathematical formalism for treating many-particle systems that are not in thermal equilibrium. The presentation of physical concepts is preceded by a short review of random variables and stochastic processes. The main theme of the first part of the course is the Boltzmann equation. Here, we present concepts necessary to introduce the Boltzmann equation as well as some of the implications of this equation. To develop intuition about many of the abstract concepts in this part, students will be introduced to the technique of molecular dynamics (MD) simulations. After writing their own simple MD code, they will have a chance to visually examine the motion of a simple fluid of spherical particles and obtain numerical estimates for some of the properties of this fluid. The main theme of the third part of the course is the ensemble description of systems obeying the quantum mechanics. Here, we will introduce the density matrix and obtain its equation of motion. The utility of the density matrix will be illustrated by focusing on spin degrees of freedom and examining the phenomenon of magnetic resonance.

Evaluation:

Homework and quizzes		15 %
Exam I	(Nov 13)	25 %
Exam II	(Dec 25)	25 %
Take-home final exam		35 %

Detailed Course Content:

I. Random variables and stochastic processes

A. *Random variables*: characteristic function, moments, cumulants, Gaussian distribution, marginal and conditional probability densities, random variable transformation theorem

B. *Stochastic processes:* Markov processes, Chapman-Kolmogorov equation, Wiener process

II. Gibbsian ensembles of classical systems

A. *Classical mechanics*: molecular dynamics simulations, dynamical functions

B. Statistical ensembles: macroscopic vs. microscopic, ensembles in phase space, density of the phase fluid and its evolution

III. Reduced distribution functions and their evolution

A. Reduced distribution functions and local variables: one- and two-particle dynamical functions and connection with macroscopic descriptions.

B. The BBGKY hierarchy: evolution of the reduced distribution functions, Vlasov equation, and Boltzmann equation

IV. The Boltzmann equation

A. Heuristic derivation of the Boltzmann equation: binary collisions, conservations laws, and collision integral

B. The Boltzmann H-theorem and thermodynamics

V. From molecular to fluid dynamics

A. Boltzmann equation's approach to equilibrium: local equilibrium, linearized collision integral

B. Hydrodynamics from the Boltzmann equation: zeroth and first order hydrodynamics, linearized hydrodynamic equations and sound.

VI. Gibbsian ensemble of quantum systems

A. *Quantum ensembles*: the density matrix, its evolution, the pictures of Schrödinger and Heisenberg

B. Phenomenological and density matrix description of *magnetic resonance spectroscopy*

References:

BOOKS

1. Noëlle Pottier, *Nonequilibrium Statistical Physics: Linear Irreversible Processes*, Oxford University Press, 2010.
2. Radu Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics*, John Wiley & Sons, 1975.
3. Kerson Huang, *Statistical Mechanics*, 2$^{\text{nd}}$ edition, John Wiley & Sons, 1987.
4. Radu Balescu, *Statistical Dynamics: Matter out of Equilibrium*, Imperial College Press, 1997.
5. Arnab Rai Choudhuri, *The Physics of Fluids and Plasmas: An Introduction for Astrophysicists*, Cambridge University Press, 1998.
6. Daan Frenkel and Berend Smit, *Understanding Molecular Simulation*, 2$^{\text{nd}}$ edition, Academic Press, 2002.
7. Dennis C. Rapaport, *The Art of Molecular Dynamics Simulation*, 2$^{\text{nd}}$ edition, Cambridge University Press, 2004.