G25.2651: Advanced Statistical Mechanics

Spring 2009, MW 9:30-10:45

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Books

The main text for the course is a book in progress to be published by Oxford University press entitled, *Statistical Mechanics: Theory and Practice through Molecular Simulation* by M. E. Tuckerman (CDs to be given out on the first day). This is a project in development that is maybe 95% complete. There are still some missing sections, figures, and appendices, and there might be a few typos. In general, any feedback on this book that you wish to provide would be greatly appreciated and taken into account in the finalization process. **IMPORTANT**: Since the book is not complete, I am providing it to you for use in this course exclusively. Please DO NOT distribute your copy to anyone outside the course.

Because the main text is not yet complete, I have compiled a list of other excellent books on the subject (listed below). These are also highly useful references for the course:

R. K. Pathria, *Statistical Mechanics.* Oxford, New York
D.A. McQuarrie, *Statistical Thermodynamics*
K. Huang, *Statistical Mechanics, 2nd edition*
W. Greiner, L. Neise and H. Stöcker, *Thermodynamics and Statistical Mechanics*
R.P. Feynman, *Statistical Mechanics, A set of lectures*
D. Chandler, *Introduction to Modern Statistical Mechanics*
M. Kardar, *Statistical Physics of Particles*

There are also detailed lecture notes posted on the course Web site given at the end of this syllabus.

When needed, we will cover some basic principles from quantum mechanics, wherein, we will draw from the following references:

R. Shankar, *Principles of Quantum Mechanics*
C. Cohen-Tannoudji, *Quantum Mechanics* (Volume 2)
R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*

For further reading and background to the mathematics used in this course, I highly recommend:

G. Arfken, *Mathematical Methods for Physicists*
M. E. Starzak, *Mathematical Methods in Chemistry and Physics*

Often, material will be drawn from current literature in statistical mechanics.

Course Outline

I. **Review of Classical Statistical Mechanics**

A. Microscopic equations of motion
B. Phase space, phase space vectors, and Liouville's Theorem
C. The Liouville equation and equilibrium solutions
D. Review of the basic ensembles
  1. Microcanonical ensemble
  2. Canonical ensemble
  3. Isothermal-isobaric ensemble
  4. Grand canonical ensemble

II. **Distribution functions and liquid structure**

1. Spatial distribution functions and the radial distribution function
2. Virial equation of state
3. Perturbation theory and the Van der Waals equation

III. **Calculating the free energy**

1. Free-energy perturbation theory
2. Adiabatic switching and thermodynic integration
3. Jensen's inequality and Jarzynski's equality: Nonequilibrium methods
4. Reaction coordinates and rare events
5. The "blue moon" ensemble
6. Transforming the partition function
7. Driving variables: Adiabatic dynamics and metadynamics

IV. **Review of the basic postulates of quantum mechanics**

A. Hilbert space and state vectors
B. Operators, eigenvalues and observables
C. Measurement
D. Microscopic dynamics and the Schrödinger equation
E. Representations: Momentum and coordinate basis wave functions
F. The Heisenberg picture

V. **Foundations of quantum statistical mechanics**

A. Quantum ensembles and the density matrix
B. Properties of the density matrix
C. Time evolution of the density matrix and the quantum Liouville equation
D. Equilibrium solutions of the Liouville equation
E. Density matrix for the basic quantum ensembles

1. Canonical ensemble
2. Isothermal-isobaric ensemble
3. Grand canonical ensemble

VI. **Introduction to path integrals in quantum mechanics and quantum statistical mechanics**

A. Trotter theorem and derivation of the path integral for the canonical density matrix

B. Path integrals for the time-evolution operator

C. Continuous and discrete path integrals:

1. Functional integration
2. Most probable path and derivation of classical mechanics

D. Thermodynamics from path integrals

E. Example applications:

1. The free particle
2. The harmonic oscillator
3. Quantum tunneling

VII. **Quantum mechanics of systems of N identical particles**

A. Introduction to spin and spin operators

B. Spin and symmetries of the N-particle wave function

C. Fermions and Bosons

VIII. **Path integrals for N-particle systems**

A. Boltzmann statistics

B. Fermions and Bosons (2-particle case)

C. Fermions and Bosons (General case)

IX. **Time-dependent processes (Classical case)**

1. Perturbative solution of the Liouville equation
2. Linear response and Green-Kubo theory
3. Classical time-correlation functions
4. Examples of transport properties
5. Reaction rates and transition state theory

X. **Time-dependent perturbation theory**

A. Interaction picture

B. Time-ordered product form of the propagator

C. Derivation of Fermi's Golden Rule

XI. **Time-dependent processes (Quantum case)**

A. Theory of spectroscopy

B. Examples of IR spectra

C. Quantum linear response theory

1. Rigid rotor
2. Harmonic and anharmonic oscillators
3. Emergence of selection rules

D. Quantum transition state theory

XII. **The Langevin and generalized Langevin equations**

XIII. **Critical phenomena**

A. Overview

B. Perturbation theory and the Van der Waals equation

C. Critical behavior of the Van der Waals equation

D. The Ising model and mean-field theory

E. Exact solutions of the Ising model

F. Wang-Landau sampling

G. Introduction to the renormalization group and scaling theory

Grading basis

Homework:............20%

Midterm:...............40%

Final:....................40%

Web resources

Notes for all lectures can be found on the course web page:

http://www.nyu.edu/classes/tuckerman/stat.mech
http://www.nyu.edu/classes/tuckerman/stat.mechII