CHEM-GA 2600: Statistical Mechanics

Fall, 2016, Location: 429 Waverly

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Books

The main text for the course is *Statistical Mechanics: Theory and Molecular Simulation* by M. E. Tuckerman, published by Oxford University Press.

In addition, I have compiled a list of other excellent books on the subject (listed below), which can provide alternative explanations and supplementary information.

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*

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*
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*
M. Boas, *Mathematical Methods in the Physical Sciences*

Material will also be drawn from current literature in statistical mechanics.

Course Outline

I. **Classical mechanics** (Chapter 1, Sections 1-3, 6)
   - A. Newton's laws of motion
   - B. Phase spaces and the Lagrangian and Hamiltonian formulations

II. **Foundations of classical statistical mechanics** (Chapter 2)
   - A. The ensemble concept
   - B. Liouville's Theorem
   - C. The Liouville equation
   - D. Equilibrium solutions

III. **The microcanonical ensemble** (Chapter 3, Sections 1-10)
   - A. Basic thermodynamic relations
   - B. Phase space distribution and the partition function
   - C. Applications: Free particles and harmonic oscillators
   - D. Introduction to molecular dynamics calculations
     - i. Integrators from Taylor expansions
     - ii. Integrators from the Liouville operator
     - iii. Trajectories and the calculation of observables: Ergodicity

IV. **The canonical ensemble** (Chapter 4, Sections 1-5, 8, 9, 11)
   - A. Basic thermodynamic relations
   - B. Phase space distribution and the partition function
   - C. Energy fluctuations
   - D. Applications: Free particles, harmonic oscillators, and the Gaussian random chain model
   - E. Canonical molecular dynamics
     - i. Generalized Liouville theorem and non-Hamiltonian algorithms
     - ii. Nosé-Hoover and Nosé-Hoover chains
     - iii. The isokinetic ensemble and isokinetic molecular dynamics

V. **The isothermal-isobaric ensemble** (Chapter 5, Sections 1-10)
   - A. Basic thermodynamic relations
   - B. Phase space distribution and the partition function
   - C. Virial theorems and volume fluctuations
   - D. Applications: Free particles and periodic potentials
   - E. Isothermal-isobaric molecular dynamics
     - i. Isotropic volume fluctuations
     - ii. Anisotropic cell fluctuations

VI. **The grand canonical ensemble** (Chapter 6 plus literature)

A. Basic thermodynamic relations
B. Phase space distribution and the partition function
C. Particle number fluctuations
D. Applications: Free particles and harmonic oscillators
D. Adaptive resolution molecular dynamics

VII. **Distribution functions and liquid structure** (Chapter 4, Sections 6, 7)

A. Spatial distribution functions, the radial distribution function, and the Virial equation of state
B. Diffraction experiments and radial distribution functions
C. Thermodynamics from radial distribution functions
D. Perturbation theory and the Van der Waals equation

VIII. **Rare-event sampling and free energy calculations** (Chapter 8, Sections 1-3, 6-11)

A. Free-energy perturbation theory
B. Adiabatic switching and thermodynic integration
C. Adiabatic free energy dynamics and metadynamics
D. Collective variables, reactions, and conformational changes
E. The "blue moon" ensemble
F. Umbrella sampling
G. Adiabatic free energy dynamics and metadynamics

IX. **Review of the basic postulates of quantum mechanics** (Chapter 9)

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
G. Spin and wave functions for identical particles.

X. **Foundations of quantum statistical mechanics** (Chapter 10)

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

XI. **Introduction to path integrals in quantum mechanics and quantum statistical mechanics** (Chapter 12)

   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
   F. Numerical evaluation of path integrals

XII. **Time-dependent processes: Classical case** (Chapter 13, Sections 1-4)

   A. Perturbative solution of the Liouville equation
   B. Linear response, Green-Kubo theory, and transport properties
   C. Classical time-correlation functions

XIII. **Time-dependent processes: Quantum case** (Chapter 14)

   A. Theory of spectroscopy
   B. Quantum linear response theory
   C. Quantum time correlation functions
      i. Exact formulations in energy and path integral representations
      ii. Imaginary time approximations

XIV. **The Langevin and generalized Langevin equations** (Chapter 15, Sections 1-5)

   A. The harmonic bath model.
   B. Definitions of friction and random forces.
   C. Exactly solvable cases.
   D. Numerical integration and ensembles.
   E. Modern uses.

Grading basis

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

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

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

Web resources

Lecture material can be found on the course web page:

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