CHEM-GA 2600: Statistical Mechanics
Spring 2016, T & Th 9:30 - 10:45 am, LL1 40 Bobst

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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.

- 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 Statistical Mechanics
   A. Newton’s Laws of motion (Chapter 1, Sections 1.1 & 1.2)
   B. Phase spaces and the Lagrangian and Hamiltonian formulations (Chapter 1, Sections 1.3 – 1.6)
   C. The Liouville equation and equilibrium solutions (Chapter 2)
   D. Basic ensembles
      1. Microcanonical ensemble and introduction to molecular dynamics (Chapter 3)
      2. Canonical ensemble, thermostats (Chapter 4, except 4.6 and 4.7)
      3. Isothermal-isobaric ensemble, barostats (Chapter 5, except 5.6 and 5.7)
      4. Grand canonical ensemble (Chapter 6)

II. Distribution functions and liquid structure
     1. Spatial distribution functions, the radial distribution function and the Virial equation of state (Chapter 4, Section 4.6).
     2. Perturbation theory and the Van der Waals equation (Chapter 4, Section 4.7).

III. Molecular crystals and polymorphism
     1. Structure prediction as a statistical mechanical problem
     2. Fully flexible cells in molecular dynamics (Chapter 5, Sections 5.6 and 5.7)
     3. Navigating the phase diagram and solid-solid phase transitions

IV. Rare events and the sampling problem
     1. Free-energy perturbation theory (Chapter 8, Section 8.1)
     2. Adiabatic switching and thermodynamic integration (Chapter 8, Section 8.2)
     3. Jensen’s inequality and Jarzynski’s equality: Nonequilibrium methods (Chapter 8, Section 8.4)
     4. Reaction coordinates and rare events (Chapter 8, Section 8.6)
     5. The “blue moon” ensemble (Chapter 8, Section 8.7)
     6. Driving variables: Adiabatic dynamics, metadynamics, and how they can be combined (Chapter 8, 8.10 & 8.11)

V. 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.
VI. **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

VII. **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

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

1. Perturbative solution of the Liouville equation (Chapter 13, Section 13.1 & 13.2)
2. Linear response, Green-Kubo theory, and transport properties (Chapter 13, Section 13.3)
3. Classical time-correlation functions (Chapter 13, Section 13.4)

IX. **Time-dependent processes (Quantum case)** (Chapter 14, Sections 14.1 – 14.4)

A. Theory of spectroscopy
B. Examples of IR spectra
   1. Rigid rotor
   2. Harmonic and anharmonic oscillators
   3. Approximate quantum dynamics with path integrals
      i. Centroid and ring-polymer molecular dynamics (Chapter 14, Section 14.6)

X. **The Langevin and generalized Langevin equations** (Chapter 15)

1. The harmonic bath model.
2. Definitions of friction and random forces.
3. Exactly solvable cases.
5. Modern uses.
XI. Advanced Sampling Techniques

A. Transition path sampling (Chapter 7, Section 7.7)
B. Replica-exchange Monte Carlo (Chapter 7, Section 7.5)
C. Continuous-tempering

Grading basis

Homework (analytical):......20%
Homework (coding):.........20%
Midterm:...........................20%
Final:..............................20%
Final coding project:.........20%

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