CHM 650: Statistical Mechanics and its applications to Chemistry

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Lectures: M 1415-1530 Th 1400-1515 FB 426
Course description: Thermodynamics, Statistical Mechanics of noninteracting systems, interacting systems, and nonequilibrium systems

Course Details

1. **Equilibrium Thermodynamics:** Thermodynamic Equilibrium state, laws of thermodynamics, axiomatic formulation of thermodynamics, thermodynamic potentials, stability criteria, phase equilibria (4 lectures)

2. **Ensembles in Statistical Mechanics:** Ensemble postulate and ergodicity, microcanonical, canonical and grand canonical ensembles, quantum and classical partition functions, phase space, fluctuations (6 lectures)

3. **Noninteracting systems:** Factorization of the partition function, quantum correlations, collective modes, occupation numbers, collections of fermions, bosons, photons, classical deal gas of spinless particles, molecular partition functions, ideal paramagnets. (6 lectures)

4. **Interacting Systems 1: Classical Liquids** Interparticle potentials, Configurational Partition functions, distributions, pair correlation function, neutron scattering experiments, Virial equation, Meyer cluster diagrams (6 lectures)

5. **Interacting Systems 2: Computer Simulations** Ensemble averages, ergodicity, random numbers, Monte Carlo methods, Molecular Dynamics, constant temperature MD. (5 lectures)

6. **Interacting Systems 3: Phase Transitions in Lattice models** Lattice gas, Ising Model, order parameter, Mean Field theory, Renormalization group theory (6 lectures)

7. **Nonequilibrium Statistical Mechanics** (6 lectures) Linear Response theory, fluctuation dissipation theorem, time correlation functions, applications to transport phenomena.

Books: There is no text book for this course. However, I will be basing a large part of my teaching from the first two references below.

1. D.A. McQuarrie, *Statistical Mechanics*
2. David Chandler, *Introduction to Modern Statistical Mechanics*
3. K.L. Huang, *Statistical Mechanics*
4. Benjamin Widom, *Statistical Mechanics: A concise introduction for chemists*

Internet Resources: There are many online resources, but there is no guarantee that they provide the correct information. You are encouraged to search on the internet. Some resources that might be useful are given below.

1. http://ocw.mit.edu/: This is the MIT open course ware.
2. http://www.wolfram.com/mathematica : This is the homepage of the software and programming language Mathematica. It has many good mathematical tips too.
3. http:/www.mathworks.com/MATLAB: Another mathematical software and an associated programming language.
4. http://pages.physics.cornell.edu/ sethna/StatMech/: James Sethna's page on his book, Statistical Mechanics: Entropy, Order and Complexity. You can download the entire book online. Lots of exercises, links, etc. Very interesting to see a modern view of statistical mechanics.
5. http://www.itp.phys.ethz.ch/education/lectures_hs11/StatPhys : Prof Manfred Sigrist's course on Statistical Physics. Complete with notes, exercises and downloadable programs.
6. http://www.nyu.edu/classes/tuckerman/stat.mech/index.html: Prof Mark E. Tuckerman's lecture notes. He is an excellent teacher and has also authored a very good book in Statistical Mechanics.

Grading System

1. Homework Assignments: (50 points total) : These will consist of 5 assignments. These will take a considerable amount of time and will involve a lot of reading and some programming, mathematical manipulations. This is really the most important part of the course.
2. Mid Semester : (20 points): In-class 2 hour exam
3. Final Exam : (30 points): In-class 3 hour exam

Letter Grades: Letter grades will be awarded based on the total points out of 100. The grades will be given based on average(A) and standard deviations(σ) from average. You have to score minimum 40 points out of 100 to pass the course; anyone above 80 points will automatically get an A grade.