CHEM-GA 2600: Statistical Mechanics

Glen Hocky

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Class Hours: M/W 9:30 AM-10:45 AM
Class Room: GCASL 379

Course Description

This course will be a modern introduction to the topic of *statistical mechanics*, that is, the way in which the interactions between sufficiently large sets of molecules give rise to experimentally observable properties of a system.

I will strive to make this course as directly useful for understanding research going on in the department, be it in theoretical, physical, materials, or biological chemistry. Hence special emphasis will be given to how theory and computation connects to experiments, e.g. in the areas of phase transitions, spectroscopy, self-assembly, polymers, etc.

Books

The main text for the course is **Statistical Mechanics: Theory and Molecular Simulation by Mark E. Tuckerman**.

There are many other great books worth looking at. These can provide alternative explanations, derivations, and many practice problems.

- B.J. Berne and R. Pecora, Dynamic Light Scattering
- D. Chandler, Introduction to Modern Statistical Mechanics
- R.P. Feynman, Statistical Mechanics, A set of lectures
- J.-P. Hansen, and I.R. McDonald, Theory of Simple Liquids
- T.L. Hill, Statistical Mechanics
- D.A. McQuarrie, Statistical Mechanics
- R. Zwanzig, Nonequilibrium statistical mechanics

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Course Structure

Logistics

Class will generally be every Monday and Wednesday. There is no class scheduled for Monday September 30 or Wednesday October 9 (Jewish Holidays). There will not be class the Wednesday of Thanksgiving (November 27), but there is class scheduled on November 25.

Due to NYU Fall recess on Monday October 14, there will be no class on that day, but instead we will meet on Tuesday October 15 at the usual time.

I will be hosting three Seminar Speakers who are both Statmech Experts this semester. Hence, you should attend the talks of Suri Vaikuntanathan (Tuesday Sept 24, 11am), Andrew White (Tuesday October 22, 11 am), and David Reichman (Friday Nov 1, 11:15am). I may assign a homework question pertaining to their talk. There is another computational talk (Avner Schlessinger, Tues Sept 17, 11 am) that you may want to attend.

The midterm will be Oct 23, 28 or 30, depending on where we are in the course. The final will happen or be assigned around the week of December 9th (final week of regular classes).

Grading

There will be weekly problem sets. These will be graded for completeness but not accuracy. They are for your own benefit, but I will to collect them every week to see how the class is doing.

Some computational exercises may be found at https://github.com/hockyg/chem-ga-2600.

Grading will be based on the midterm and the final (the form of the final, whether it is an exam, final project/paper, or a combination of these, will be determined later).

- Homeworks, 20%
- Midterm, 35%
- Final, 45%

Topics Outline

Topics that will be covered:

Connection between classical mechanics and thermodynamics, statistical definition of thermodynamic quantities, the concept of thermodynamic ensembles, molecular dynamics simulations, Monte Carlo sampling, enhanced sampling for thermodynamic quantities, phase transitions, linear-response theory, and fluctuation dissipation theorems.

Topics that may be covered:

Theory of simple liquids, non-ideal liquids, time correlation functions, generalized Langevin equation, random walks and diffusion, polymer theory.