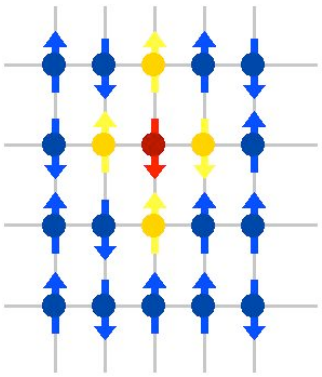
CHEM 60642 – Statistical Mechanics II

Spring 2008, 3 Credits
Offered by the Department of Chemistry & Biochemistry
Instructor: Dan Gezelter
Time: MWF 9:35 – 10:25 a.m.

Summary:
This is a graduate-level course that surveys advanced topics in statistical mechanics with a special emphasis on chemically interesting applications. The topics covered include: phase transitions, lattice models, and renormalization group theory; liquid theory and the molecular simulation of fluids; chemical reactions in solution phase; theoretical aspects of supercritical fluids, supercooled and glassy materials.

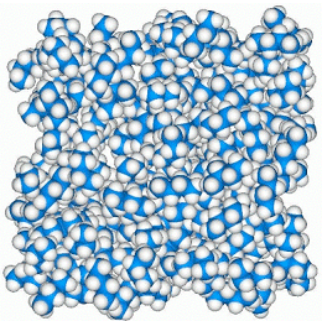
Main Texts

- Introduction to Modern Statistical Mechanics, by David Chandler
- Statistical Mechanics, by Donald A. McQuarrie

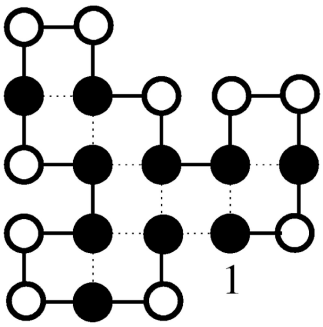


Course Outline

I. Review of Statistical Mechanical concepts
II. Ising models and lattice gases
  A. Independent spins in a field and equivalent lattice gas.
  B. Interacting spins on a line, the transfer matrix.
  C. Correlation functions.
  D. Reversible work.
  E. Spins with random fields, influence functionals.
  F. Spins on a plane, phase transitions, broken symmetry, interfacial fluctuations.
  G. Monte Carlo simulations of the 2D Ising model.
  H. Mean field theory, Gibbs-Bogoliubov bound.



III. Atomic and continuum models of liquids
  A. The Lennard-Jones Fluid.
  B. Molecular dynamics simulation.
  C. Correlation functions and measurements, elements of linear response theory.
  D. Linear models
    1. Langevin equations (diffusion, friction and memory).
    2. Gaussian fields (Debye-Huckel and beyond).
  E. The hard sphere model, WCA theory.
  F. Chemical equilibrium and relaxation.



IV. Special topics
  A. Free energy perturbation
  B. The Jarzynski Equality
  C. Electron transfer, quantum rare events, golden rule, Marcus theory.
  D. Path integrals.
  E. Tunneling, instantons
  F. Ising model / Quantum correspondence
  G. Biased Monte Carlo methods