Chemistry 175/273: Outline

Statistical Mechanics
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Additional reading material for each lecture is specified as Author-Chapter-Section. For example, Chandler, Chapter 3, Section 2 is rendered Chandler-3-2. Most of the lectures are not based directly on these materials, so you may find that the presentation differs a bit.

1. Statistical Mechanics as the connection between microscopic and macroscopic
    - Counting states at equal probability
    - Microcanonical postulate
    - *Reference:* Chandler-3-1, Chandler-3-2
2. Computing the microcanonical partition function and Derivation of the Boltzmann distribution
    - Defining ensemble averages
    - Dilute solution and scaling of the partition function
    - Stirling's approximation
    - *Reference:* McQuarrie-1-5, McQuarrie-2-2
    - Perturbative expansion around the microcanonical ensemble
    - Thermodynamic limit, fluctuations disappear
    - *Reference:* Widom-1-3, Chandler-3-2
3. Canonical partition function and fluctuations & response
    - Dynamics and averaging (ergodicity)
    - Free energies as cumulant generating functions
    - Heat-capacity via a fluctuation response relation
    - *Reference:* Chandler-3-3
4. Partition function a non-interacting monoatomic gas
    - Derivation of q_{trans} from particle in a box
    - *Reference:* McQuarrie-5-1
5. Rotational partition function and vibrational partition function
    - Derivation of q_{rot}
    - Derivation of q_{vib}
    - *Reference:* McQuarrie-6-1 / 6-2 / 6-3
6. From the molecular partition function to the ideal gas law
    - Combining all the QM contributions to the molecular energy
    - Deriving the ideal gas law
    - *Reference:* McQuarrie-6-1 / 6-2 / 6-3

7. Entropy of mixing
    - Sackur-Tetrode Equation
    - Gibbs' Paradox
    - *Reference:* Sethna-5-1, McQuarrie-5-2
8. Moving between ensembles
    - Grand canonical ensemble
    - NpT ensemble
    - Legendre transforms recovering thermodynamic potentials
    - *Reference:* McQuarrie-3
9. Equilibrium constants from Statistical Mechanics!
    - contributions to heat capacity from molecular partition function
    - *Reference:* Chandler-4-6, McQuarrie-9-1
10. Recap for simple particles, Bose-Einstein and Fermi-Dirac statistics
    - Condensation
    - *Reference:* Chandler-4-4, Chandler-4-5, McQuarrie-7
11. Bose-Einstein and Fermi-Dirac statistics (II)
    - Free electron model
    - Classical limit
    - *Reference:* Chandler-4-4, Chandler-4-5, McQuarrie-7
12. Free electron model
    - Free electron model
    - Low temperature scaling of the heat capacity
    - *Reference:* Chandler-4-4, Chandler-4-5, McQuarrie-7
13. Phase transitions
    - Necessity of long range correlations
    - *Reference:* Chandler-5-1
14. Phase transitions in the Ising model
    - Analytical solution in 1D
    - *Reference:* Chandler-5
15. Modern approaches to the theory of phase transitions
    - Mean-field theory
    - Renormalization group
    - The necessity of computer simulations

- *Reference:* Chandler-5

16. Computation: Sampling the Boltzmann Distribution
    - Metropolis Criterion & Detailed Balance
    - Markov Chain Monte Carlo (MCMC) algorithms
    - *Reference:* Chandler-6, Krauth-1
17. Computing radial distribution functions
    - Hard Disk MCMC
    - Introduction to the radial distribution function
    - *Reference:* Widom-6, 7
    - Virial expansion, second virial coefficient from $g(r)$
18. Molecular Dynamics I
    - Ergodicity recap, Initialization
    - Force fields, where do they come from?
    - Lennard-Jones potential, multipole expansion
    - *Reference:* Chandler-6, Krauth-1
19. Molecular Dynamics II
    - Hamilton's equations
    - Symplectic integration and energy conservation
20. Conserving energy during integration
    - Velocity verlet algorithm
    - Constant temperature simulation
21. Dynamical properties and collision theory
    - Computing the diffusion coefficient
    - Langevin equation
22. Transport phenomena
    - Phenomenology
    - Continuity equation
23. Transport phenomena II
    - Fokker-Planck equation
    - Onsager reciprocity
24. Diffusion in liquids
    - Stokes-Einstein
    - Caging effects

25. Transition State Theory
    - Eyring equation
    - Limitations
26. Linear Response Theory and beyond
    - Response functions
    - High-level description of fluctuation theorems