STATISTICAL THERMODYNAMICS WITH NUMERICAL APPLICATIONS

Chemistry 448 Spring Semester 2000
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COURSE OUTLINE

1. INTRODUCTION

2. SOME DEFINITIONS AND ASSORTED MATHEMATICAL METHODS
permutations, configurations, system quantum states
boltzons bosons fermions
ensemble average
the most probable distribution
Lagrange multipliers
Stirling's approximation

3. STATISTICAL MECHANICS OF A SYSTEM OF ONE KIND OF PARTICLES, NON-INTERACTING
the molecular partition function
the nature of alpha and beta
interpretation of heat and work
interpretation of entropy

4. ATOMS AND DIATOMIC MOLECULES
energy levels & partition functions
distribution laws & thermodynamic functions
nuclear spin statistics

5. STATISTICAL MECHANICS AND CHEMICAL EQUILIBRIUM

6. POLYATOMIC MOLECULES
symmetry number
vibrations
classical partition functions without internal rotation

7. CANONICAL AND GRAND CANONICAL ENSEMBLES
thermodynamic functions
systems with more than one component

8. FLUCTUATIONS
density fluctuations in the grand ensemble
the random walk
diffusion and random walk

9. IMPORTANCE SAMPLING
Metropolis

Rouse algorithm
Norman-Filinov algorithm for grand canonical ensemble
Finite size problem, periodic boundary conditions

10. SYSTEMS OF INTERACTING PARTICLES
canonical partition function
distribution functions
pair correlation functions
the assumption of pair potentials
the Lennard-Jones fluid
ensemble averages of dynamical variables and molecular properties
more on intermolecular potentials
phase transformations

11. MIXTURES
the reference state
distributions of the molecules of a binary mixture
average properties in a binary mixture

12. SAMPLING METHODS
why not use Boltzmann sampling?
umbrella sampling

13. MOLECULAR DYNAMICS SIMULATIONS
what types of information do we expect to retrieve from MC & MD simulations?

14. CRYSTALS
Einstein's model
Debye model
entropy and disorder in crystals

15. STATISTICAL MECHANICS OF MAGNETIC SYSTEMS
non-interacting magnets
N interacting magnets
Ising model