CHM 421/621
Statistical Mechanics

Lecture 1
Introduction to Course

Course Plan

Phase 1: Introduction and Review

- **Introduction**: Macroscopic and microscopic states, limitations of thermodynamics and the need for a statistical approach.
- **Review of Thermodynamics**: A theoretical approach
- **Probability**: Definitions, probability of compound events, distribution functions, averages, variance, uncertainty.

Phase 2: Formalism of Statistical Mechanics

- **Basic Postulates**
- **Ensemble approach to counting**: The micro-canonical (NVE) ensemble, application to ideal gas
- **Boltzmann equation for entropy**: Connection to uncertainty

Course Plan

Phase 3: Ensembles

- **Canonical Distribution**: Derivation and discussion.
- **Canonical partition function**: Important relations, molecular partition function.
- **Applications**: Ideal gas molecules in a box, 2-level quantum system, harmonic oscillator
- **Other ensembles**: Grand-canonical, isothermal-isobaric, generalisations
- **Fluctuations and Response Functions**: C_V, κ_T, etc.

Phase 4: Applications of Statistical Mechanics (exact models)

- **Equipartition theorem**
- **Rigid rotors**: Review, canonical distribution, effect of nuclear spins - ortho and para hydrogen.
- **Harmonic oscillators**: Review, lattice of oscillators, heat capacities of solids - Einstein and Debye models.

Course Plan

Phase 5: Statistics of Indistinguishable particles

- **Fermi-Dirac distribution**: Bloch electrons in solids
- **Bose-Einstein distribution**: Phonons and photons

Phase 6: Applications to Chemical equilibrium

- **Ideal gas mixtures**
- **Calculation of Equilibrium constants**

Phase 7: Advanced applications (if time and interest permit)

- **Phase transitions**

Assessment Plan

Learning through active participation
Discussions and Problem Solving (in class)

Assessment Aspects
Quizzes (2) - 10%
Homework Assignments - 10%
Mid-sem Exam - 30%
End-sem Exam - 50%

Books and Resources

Suggested Reading

Statistical Mechanics - D. A. MacQuarrie
Physical Chemistry - P. W. Atkins
Equilibrium Statistical Mechanics - E. Atlee Jackson
Thermodynamics and an Introduction to Thermostatistics - H. B. Callen
Introduction to Modern Statistical Mechanics - D. Chandler
Statistical Mechanics for Chemistry and Materials Science - B. Bagchi

TAs: Rashid, Yogesh (AB2-201)
Instructor: V. Srinivasan (AB2-225)
Course Website: https://helios.iiserb.ac.in/~vardha/Courses/CHM421