THERMODYNAMICS and STATISTICAL THERMODYNAMICS
3150:635-001
Spring 2010

Instructor:      David S. Perry
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Scope:          Thermodynamics (review)  
                Statistical Thermodynamics
                Applications

Structure:      Lectures Tu Th  3:15 - 4:30 PM. in  KNCL 321
                3 credits
                Weekly problems
                2 examinations

Prerequisites:  3 to 4 semesters of college mathematics (excluding precalculus)
                1 semester of undergraduate thermodynamics, e.g., CHM 313.
                1 semester of quantum chemistry, e.g., CHM 314 (recommended).

Texts:          D. A. McQuarrie, Statistical Mechanics (principal text).
                Any basic text on chemical thermodynamics (supplementary text. Peter A. Rock,
                Chemical Thermodynamics is a good one!)

Credit:        Problems and Class Participation       20
                Classical Thermodynamics Exam           20
                Statistical Thermodynamics Exam        30
                Individual Project                     30
                TOTAL                                 100

The relative weight of the four components above and the dates of the exams can be
adjusted according to the background and interests of the class.

Individual projects will involve an essay or computation on a topic in statistical
thermodynamics that is at the frontier of current research. Each student will
undertake a different topic.

Class participation credit will be given for presentation and discussion of homework
problems and preparation of written solutions to homework problems for distribution
to the class.
I. Thermodynamics

This will be a fairly fast-paced review designed to bring your understanding up to a graduate level. The coverage of this part of the course will be defined by the problems; I will not lecture explicitly on every topic.

Preliminaries
The First Law
The Second Law
Maxwell's Relationships
The Third law
The Chemical Potential

II. Statistical Thermodynamics

This part of the course will follow the presentation of McQuarrie, *Statistical Mechanics*, Chapters 1-10 and 13 and will take almost half of the lecture time. This part of the course will cover the core concepts of Statistical Mechanics and applications to gases and liquids.

III. Applications

Many of the applications to be discussed are found in chapters 11-15 of McQuarrie. Important applications include

- non-ideal gases,
- crystals,
- liquids,
- first and second order phase transitions,
- systems in electric and magnetic fields,
- polymers,
- superconductivity,
- liquid crystals,
- ergodicity and chaos,
- statistical spectroscopy,
- nonequilibrium statistical mechanics

The applications that are covered and the emphasis placed on each will depend, in part, on the interests of the members of the class. Several topics will be covered by the oral presentation of projects by individual class members during the last week of the semester. It is the objective of this part of the course to impart at least some appreciation for the scope and power of modern research in statistical mechanics.
Individual Projects

Each student can choose to do a library research project or a computational project. Your topic must be distinct from your dissertation research. Please consult with me on your topic selection.

Library Research Project

Scope
- library research including up-to-date material
- essay not more than 10 typed double spaced pages. Try for 6 to 8 pages plus figures and references.
- 15 minute talk, and 5 minutes for questions. Use about a 10-12 slides to introduce the key concepts of your topic to the class. Be sure to enlarge literature figures to make them easily discernible and include the exact reference at the bottom.

Content
- A solid explanation of a phenomenon through statistical mechanical theory.
- One concrete application to a specific system.
- Include literature references as appropriate for a scientific paper.
- The level of the presentation should be appropriate for members of this class who are NOT familiar with the topic. The explanations should be qualitatively clear and not excessively mathematical. Part of your score will be for how well you communicate the important concepts to the class. Each member of the class will get a copy of your essay. Note that this level of presentation requires a deeper understanding of the material than does a fully technical presentation.
- According to standard professional practice, all material taken from another source must be explicitly referenced. This includes
  - any quoted text (which should be in quotation marks),
  - each equation,
  - each figure, and
  - each table taken from another source.
- Include figures and tables as needed for a clear exposition. Figures may be copied from books and articles, but be sure to write your own caption to make the figure understandable in the context of your essay and include the explicit reference for that figure in the caption.

Topics
Use these as ideas or choose your own topic.
- non-ideal gases,
- crystals (metals, insulators, semiconductors),
- liquids (water, hard spheres, argon, etc.),
- first or second order phase transitions,
- systems in electric or magnetic fields (Ising model, phase transitions),
- polymers (properties, formation, or molecular dynamics simulations),
- fractals (e.g., scaling properties of polymers)
- superconductivity (regular, high Tc materials),
- Bose condensation in ultracold gases
- liquid crystals (phases, phase transitions, molecular dynamics simulations),
- phase transitions in DNA
- critical phenomena (critical exponents, renormalization group theory, industrial applications)
- ergodicity and chaos (in kinetics, in molecules, in classical systems, quantum systems),
Computational Projects

Scope
- Use of statistical mechanics to compute useful thermodynamic quantities on a system of interest.
- Report including relevant background, procedure, data, and conclusions not more than 10 typed double spaced pages. Try for 6 to 8 pages plus figures and references.
- 15 minute talk, and 5 minutes for questions. Use about a 10-12 slides to introduce the key concepts of your topic to the class. Be sure to enlarge literature figures to make them easily discernible and include the exact reference at the bottom.

Content
- Use a combination of literature data and ab initio, semi-empirical, and molecular dynamics calculations to determine the molecular quantities needed to calculate the thermodynamic quantity of interest.
- Gaussian03 and Spartan have a built-in capability of calculating thermodynamic data.
- Where possible try more than one level of calculation for the molecular properties to evaluate the reliability of your result.
- Critically evaluate your results. It is not so important for this project to get the best possible result, but it is essential to understand the assumptions, flaws, and limitations of your calculation.

Topics
- Determine the equilibrium constant(s) between different conformations of a molecular system. Application to small peptides, organic or inorganic molecules.
- Calculate the thermodynamic properties of a molecular system that has many conformers under thermal equilibrium.
- Calculate the rate constant using transition state theory for the interconversion between certain molecular conformations.
- Predict the fragmentation pattern of a molecular ion at different energies, or as a function of energy.

In Class Presentations of Projects
- We will devote the last week of the semester to student presentations in class. Since we have 10 in the class this year we will have to plan on either extra-long class sessions that week lasting until about 5 PM or use of the official final exam time slot.
- I will assign the dates and ordering of the presentations to make - so far as possible - a coherent program for the class. The purpose is to give the class an overview of the diversity and power of modern statistical mechanics.
- The purpose of the oral presentation is to share with the class the key concepts of your project in a way that is meaningful to them. You need to introduce the under-lying concepts at the level the class member can appreciate. You should provide a “take-home” message that each class member
will likely remember well after the course is done. Your will only be able to present orally a small part of what you have researched.

- Because of the limited time for all of the presentations, the length restriction (15 minutes) will be rigorously enforced.
- Send me your presentation (.ppt, .pptx, or .pdf) by 5:00 PM the evening BEFORE your presentation so that I can load it onto my computer. That will give me a record of your presentation and it will allow a quick transition between talks.

**Grading of Projects**

**Written Essay (and documentation of calculations if applicable) - 20 points**

- Form - 10 points
  - organization
  - following the Scope and Content as specified above
  - clarity and lucidity
  - references & citations for figures and tables in the captions

- Effort and Insight - 10 points
  - How much productive work was spent on the project?
  - Where the key foundational concepts understood?
  - What insights into the field were obtained?

**Oral Presentation - 10 points**

- Form - 3 points
  - organization, clarity of slides, documentation on slides
  - Did I get a copy of the presentation on time?

- Communication to the Class - 7 points
  - Where the key concepts communicated clearly to the class?
  - Did the students get the take-home message?
  - Did the speaker meet the class at their level?
  - Was the excitement and impact of the topic communicated?
CHEM 635 Reserve Reading List
3150:635
SPRING 2010
Prof. David Perry

1. Peter A. Rock, Chemical Thermodynamics (2 copies on 2-hr reserve), QD 501 .R732 1983

2. D. A. McQuarrie, Statistical Mechanics, QC 174.8 .M3


Other useful texts:


J. G. Kirkwood and Oppenheim, Chemical Thermodynamics, QD 501 .K754

Charles E. Hecht, Statistical Thermodynamics and Kinetic Theory, QC 311.5 .H43 1990

Kenneth S. Pitzer, Thermodynamics (3rd edition 1995)
1st edition was the classic by Lewis and Randall QC 311 .L4 (1923),

Terrell L. Hill, An Introduction to Statistical Thermodynamics;
Richard Chace Tolman, The Principles of Statistical Mechanics;
Silvio R. A. Salinas, Introduction to Statistical Physics.
Name ............................................  Student ID .................................

Department .................................  Phone (lab) .................................

** Your UA Email address will be used **  (home) .................................
(class announcements will be sent by email)

Name of Research Advisor ....................

Undergraduate College .........................  Degree  .........................

Degree year ....................

List Mathematics Courses  ....................

List Quantum Courses  .........................

List Thermodynamics & Statistical Thermodynamics Courses

** Topics of particular Interest in Thermodynamics and Statistical Mechanics **

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