# FALL 2001

<table>
<thead>
<tr>
<th>THERMODYNAMICS and STATISTICAL THERMODYNAMICS 3150:635-001</th>
<th>STATISTICAL MECHANICS 3650:661-001</th>
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<tbody>
<tr>
<td>Instructor: David S. Perry</td>
<td>Instructor: Jutta Luettmer-Strathmann</td>
</tr>
<tr>
<td>Office: KNCL 103</td>
<td>Office: Ayer 211</td>
</tr>
<tr>
<td>Phone: 972-7372</td>
<td>Phone: 972-8029</td>
</tr>
<tr>
<td>Email: <a href="mailto:DPerry@UAkron.edu">DPerry@UAkron.edu</a></td>
<td>Email: <a href="mailto:jutta@UAkron.edu">jutta@UAkron.edu</a></td>
</tr>
<tr>
<td>Office Hours: 1:00 pm to 6:00 pm daily. If I am not immediately available, ask the secretary for an appointment. I will ask the office staff to give students priority where possible.</td>
<td>Office Hours: M W 2-4pm and by appointment.</td>
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Lectures: T Th 12:15 – 1:00 pm KNCL 401
Homework Sessions: TBA

Course homepage: [http://physics.uakron.edu/dept/faculty/jutta/statmech/statmech.htm](http://physics.uakron.edu/dept/faculty/jutta/statmech/statmech.htm)
Electronic reserve: through the library website
Password: statmech

Scope: Thermodynamics (review)
Statistical Thermodynamics/Statistical Mechanics
Applications

Credit: Homework and Class Participation 30
Classical Thermodynamics Exam 20
Statistical Mechanics 20
Individual Project 30

Texts: D. A. McQuarrie, *Statistical Thermodynamics*, Univ. Science Books, 1985, (principal text). An alternative text is *Statistical Mechanics* by the same author. This text is virtually identical to the former except it contains several chapters on modern topics including non-equilibrium statistical mechanics. Although it about twice the price, it is recommended for serious students of this subject.
I. Thermodynamics
   This will be a fairly fast-paced review designed to bring your understanding up to
   a graduate level. This part of the course will, in part, be defined by the problems
   and will take about one third of the lecture time.
   Preliminaries
   The Laws of Thermodynamics
   Maxwell's Relationships
   The Euler equation and Thermodynamic Potentials
   Conditions of Equilibrium
   Thermodynamic Stability
   Classical Theory of Phase Transitions

II. Statistical Thermodynamics – Statistical Mechanics
   This part of the course will follow to a large extent the presentation of McQuarrie,
   *Statistical Thermodynamics*, Chapters 1-10. In addition we will discuss the Ising
   model and Monte Carlo Simulations.

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 which 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 two weeks 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

Scope

• Library research including up-to-date material OR computer simulation
• Essay not more than 10 typed double spaced pages. Try for 6 to 8 pages plus figures and references. For a computer simulation project, the essay may be replaced by a single page outline plus references, annotated program and copies of the transparencies of your presentation.
• 20 minute talk. Use about a dozen transparencies. Be sure to enlarge (about 2 x) literature figures.

Content for library research projects:

• A solid explanation of the phenomena 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.
• Hand in your literature search strategy (e.g., search phrases used in SciFinder) and a printout of the relevant references that you found. Hint: Always save your search results to disk and edit them down later with a word processor.

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, molecular dynamics simulations),
• 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),
• statistical spectroscopy (random matrix theory, cross-correlation, Fourier transform analysis),
• nonequilibrium statistical mechanics (pick a specific case or application)
• an application of the Monte Carlo method
• an application of the molecular dynamics method
• Brownian motion

Content for computer simulation projects:
• A computer simulation of a simple physical system of interest to you.
• Several topics for simulation projects are suggested below but you are welcome to explore your own. Some of the topics require very little experience in programming, for example those that build on the Monte Carlo simulation of the Ising model that you will perform in your homework. For others, experience in Matlab, Fortran, or C will be very helpful. Please stop by to discuss your possible projects.
• Your outline should consist of a title and short descriptions of the physical system, the effects you are looking for, and the simulation method.
• Include literature references as appropriate for a scientific paper.
• Your presentation should include an Introduction that expands on the outline and motivates your work followed by a qualitative description of the simulation method. Present your simulation results in appropriately labeled figures and conclude with a discussion of your results. Please make sure that your talk is understandable to all of us.
• Please submit your program electronically (by email or on floppy disk) and hand in an annotated printout.

Topics
• Choose from these or come and discuss your own ideas
  • Finite size-scaling in the two-dimensional Ising model – investigate a continuous phase transition and determine the critical exponents.
  • The role of spatial dimensions – the Ising model in one, two, three (and maybe even four) dimensions
  • First order phase transitions in the two-dimensional Ising model – hysteresis
  • Dynamic aspects of the Ising model – domain formation, interfaces
  • Antiferromagnetic Ising model on a triangular lattice – frustration
  • Self-avoiding random walk in dimensions 2 and/or 3 – a model for polymers in solution
  • Collapse transition of self-interacting polymer chains – a first taste of protein folding
  • Molecular beam epitaxy (MBE) – explore how the growth mode changes when you vary parameters like interaction energies, barrier heights, etc.
  • Diffusion limited aggregation
  • Percolation
  • Structure of a hard-disk fluid – a molecular dynamics simulation
CHEM 635 and PHYS 661 Reserve Reading List (2 day)  
3150:635 and 3650:661  
Profs. David Perry and Jutta Luettmer-Strathmann

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

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

3. H. L. Freidman, A Course in Statistical Mechanics,  
   QC 174.8 .F75 1985

4. David Chandler, Introduction to Modern Statistical Mechanics,  
   QC 174.8 .C47 1987

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

6. Norman Davidson, Statistical Mechanics,  
   QC 175 .D3

7. M. Berry, S. Rice, and J. Ross, Physical Chemistry  
   QD 435.2 .B48 1980b

   1st edition was the classic by Lewis and Randall QC 311 .L4 (1923),  

   QC 175.P35 1996

10. L. D. Landau and E. M. Lifshitz, Statistical Physics  
    QC 175.L32 1980

11. Kerson Huang, Statistical Mechanics  
    QC 174.8 H83 1987

12. W. Greiner, L. Neiser, and H. Stöcker, Thermodynamics and Statistical Mechanics  
    QC 311 G74 1995

13. H. B. Callen, Thermodynamics : an introduction to the physical theories of  
    equilibrium thermostatics and irreversible thermodynamics  
    QC311 .C25 1960