Physics 375: Thermal & Statistical Physics; TΘ 10:30AM-12:00PM; Dennis 305

Instructor: Michael Lerner, Dennis 221, Phone: 727-LERNERM

Office Hours: T 9-10, Θ 1:30-3:30 and by appointment. I also have an open-door policy, and you're encouraged to stop in to ask questions whenever my door is open. That's most of the time.

Course goals

- Students will understand the basics of thermal physics: how do macroscopic quantities such as temperature relate to each other?
- Students will understand the statistical underpinnings of thermal physics from a molecular level, including foundational topics and modern formulations of the second "law" of thermodynamics.
- Students will understand and apply the concepts of statistical and thermal physics to a topic in their area of interest.
- Students will explore the wide range of applications of statistical mechanics by developing a Monte Carlo model to simulate and evaluate March Madness brackets.

Required Textbook: Schroeder, **Thermal Physics** It's extremely readable, and has a good selection of real-world problems.

Prerequisite Physics 345, modern physics.

Grading Policy

- Class preparation/participation, Moodle/Piazza participation: 10%
- Three in-class labs, each 4%
- Two midterms, each 9%, for a total of 18%
- One final, 15%
- Independent project, 10%
- Homework, 35%

Attendance Policy: Students are expected to attend classes regularly. A student who incurs an excessive number of absences may have some or all of the class preparation/participation grade (10%) deducted at the discretion of the instructor.

Piazza: http://piazza.com/earlham/spring2015/phys375

Academic Integrity: http://www.earlham.edu/policies-and-handbooks/community/student-code-of-conduct/

Important Dates:

Drop Deadline	4/3/2015
Project Topics Due	4/7/2015
First exam	2/17/2015
Second exam	4/14/2015
Final Exam, Comprehensive emphasis on later topics	5/4/2015

Class time There will be two class meetings each week. The class meetings will generally consist of lectures, discussion of assignments, and student presentation of assigned problems. The longer meetings will allow us to work through longer computational exercises in class.

It is very important that you study the appropriate text assignments before coming to class. I will repeat and re-emphasize material from the book, but you'll find that you understand and internalize the material much better if the class discussion is your second exposure. In this class, in particular, there is a huge variety of applied problems that we'd love to discuss. The more you've read before class, the more we can delve into new material in class.

You are required to post to the Piazza site by 9PM the day before class. Your post should include what you thought was most interesting and important from the reading. You should mention any parts of the reading that were particularly hard to understand. You can also comment to ask a question or answer someone else's question in lieu of mentioning the most interesting/important things. This counts for **HALF** of your reading/participation grade!

Homework As you surely know by now, your understanding will be significantly greater if you work problems throughout the week rather than saving them all for Sunday night. So, homework will be assigned each class period. You are actively encouraged to work cooperatively on them. **Understanding someone else's solution to a problem is not nearly as useful as being able to solve the problem yourself.** Therefore, I ask that you attempt each problem on your own before discussing it with your peers. You may then compare answers and discuss strategies, but the solution you turn in should be written entirely by you. If you are using online solutions as part of your study, you should inform me so that we can work out guidelines for such usage.

Several of the problems assigned in this class are quite challenging. Others are rote computation. For the more challenging problems, my goal is to have you make the strongest possible effort towards **understanding** the solution. Thus, if you cannot fully solve the problem, say whatever you can about the way in which a solution would proceed from where you stop; say what you can about the qualitative behavior of a solution; say what you can about the physical meaning of the solution.

Due dates Homework assigned on Thursday is due at the start of class the following Tuesday. Homework assigned on Tuesday is due at 5:00 PM (in the box outside my office) on Friday.

Resubmission If you get a homework problem wrong, you may redo it for half of the missed credit. If you choose this option, you must have a friend grade it (using the solution set in the library) and then submit the re-graded work to me. The goal here is to encourage you to keep thinking about these problems until you understand them while still giving credit to work done on time. Resubmissions can be turned in any time before the final.

Late work In an ideal world, all homework would be done on time. We seem not to inhabit that world, so how will I deal with late homework?

1) On the due date, submit something whatever you have done, even if its only a few problems. You may then submit additional work late. However, unless you submit something on the due day, your late work wont be accepted at all. Solutions will be available in the library as soon as the homework is due. If you consult these while completing late work (A) you must mention that fact on your assignment (B) you must use "real" late days, no the ten "free" late days described below.

2) The part of the homework that is submitted late will penalized; later work $\Rightarrow$ larger penalty.

3) During the semester your have 10 free "late days" for homework. Don't use them early in the semester for frivolous reasons; you may need them toward the end of the semester.

4) Each student has a maximum of 20 late days. Once youve used those up, your homework will not be accepted unless its on time. Please put a date on any work you submit. Late penalties are usually 10% per day late, with Saturday/Sunday counting as one "day." Homework that is more than 1 week late generally will not be accepted for grading.

Homework problems will be graded on roughly the same scale as used in Physics 125 and 235:

5 Solution is complete and well-written

4 Solution is missing minor parts or some important explanations

3 Solution is missing major parts and/or has few if any explanations

2 At least one major portion of the problem correct

1 Very little coherent initial effort was expended

0 No initial solution was submitted

Books and Resources

Additional Textbooks

Gould and Tobochnik, Statistical and Thermal Physics It was a close decision between this and Schroeder. I went with Schroeder for several reasons, but this book is free and good. http://www.compadre.org/stp/

An Introduction to Statistical Mechanics and Thermodynamics An extremely well-written modern introduction. Paced a bit faster than we'll go, this would be a good intro grad text, or 475-level text.

Sethna, Entropy, Order Parameters, and Complexity This is a freely-available, modern, advanced, applied statistical mechanics textbook. Its main strengths include the broad range of problems (statistical mechanics, in its modern form, is an extremely broad, applied subject) and the extremely up-to-date content. You can download it from Sethna's website (http://www.lassp.cornell.edu/sethna/). On the other hand, it has a reputation as a book that's "fantastic if you already know the subject matter" but difficult to learn from on your own at the advanced undergraduate level. The plan is to supplement Schroeder with bits and pieces of Sethna. Please start pawing through Sethna ASAP so that you can pick out interesting topics that we may use.

Required Software

The Anaconda Python Distribution We'll do several computational exercises throughout the class. If you have a laptop, please install the Anaconda Python Distribution. If you do not have a laptop, please contact me ASAP. http://continuum.io/downloads

Recommended Textbooks

Kusse and Westwig, Mathematical Physics This text is extremely well written. It's a good reference for the math you may have forgotten.

Schey, div grad curl and all that This is an extremely conversational introduction to/refresher on vector calculus.

Bridging the Vector Calculus Gap This is a fantastic resource for vector calculus that focuses on actually using the material in practice, rather than just learning it in a mathematical context. http://www.math.oregonstate.edu/bridge/

Styer, Statistical Mechanics I just found this recently, but it looks like a nice attempt at integrating modern material into a Stat Mech course. Note that it is not yet a complete book. http://www.oberlin.edu/physics/dstyer/StatMech/book.pdf

Labs Statistical Mechanics is one of the most active areas of modern physics research, and we'll supplement the class with at least three labs:

Diffusion Statistical mechanics is also concerned with predicting diffusion constants of grains of pollen floating on water (think Einstein's famous 1905 paper) or proteins moving about in cell membranes. We will team up with Adam Hoppe at South Dakota State University to use a web-controlled TIRF (total internal reflection) microscope to measure the diffusion constant of individual lipids (actually, we'll be looking at quantum dots attached to lipids) in cell membranes. This will give us a way of calculating Boltzmann's constant. This lab is also of interest to biochemistry students, so I've invited several of them to watch and perhaps participate.

Non-equilibrium Statistical Mechanics Think for a minute about moving your hand around under water. If you move your hand infinitely slowly (called "quasistatically"), you would say that the work required to move your hand from one place (state A) to another (state B) is equal to the free energy difference between A and B. What if you move your hand quickly? Until very recently (1997), the most definite general answer we could give is that the work required would be greater than or equal to the free energy difference (you'd burn up some energy in friction), but performing several non-equilibrium processes like this would not be able to tell you exactly the free energy difference between A and B. In this lab, we will study one of the most shocking results of statistical mechanics, the Jarzynski equality, which allows us to average *nonequilibrium* processes to determine the exact energy difference between two *equilibrium* states. This lab involves computer simulations of proteins, and will be done in two parts, separated by several weeks.

Entropy of Unknotting In this lab, we will model the unknotting of a small beaded chain via random walks, and make both quantitative and qualitative measurements of the entropy involved of unknotting.

The entropy of unkotting is a self-directed lab. You may begin it at any point after spring break.

Tests All will be self-scheduled exams, to be picked up and turned in at the front desk of the science library.

Independent project The applications of modern statistical mechanics are so broad that we cannot hope to cover even a reasonable sampling of them in a single course. However, I don't want you to miss out on the parts that happen to be most interesting to you. Therefore, you'll each pick either an interesting problem to model or an interesting technique to learn. You'll write a short paper and present the results to the class. You'll be expected to start on this halfway through the semester, and we'll discuss it in more detail at that point. Sethna's book provides a wealth of such problems, and I'm certainly available to provide background material that you may be missing if needed.

Topics are largely at your discretion, but may include

- Information Theory and Statistical Mechanics
- Foundations of the Zeroth and Second "Laws" of thermodynamics
- Coarsening
- Time correlation functions
- Statistical Mechanics/Thermodynamics of small systems
- Further work with Monte Carlo simulations
- Thermal ratchets, theory and practice
- Order parameters and critical exponents (often an in-class topic!, see Sethna)

Course Outline

My plan is to move fairly quickly through the first part of the book, assuming it's mostly review. Later sections are up for discussion: should we spend more time on heat engines, or more time on statistical mechanics and applications?

In any case, we'll be doing several computational simulations throughout. In order to make things standard, we'll do them all in Python.

In addition to the focus on simulation, we'll focus more on statistical mechanics than on thermodynamics, so we will skip straight from Chapter 3 to Chapter 6, giving us time to set up Monte Carlo simulations of March Madness. The syllabus is fairly flexible, but we need to get to MD simulations *before* March, and we need to get through diffusion before the lab is scheduled. I expect this class to be a lot of work, and an enormous amount of fun.

Tuesday	Thursday
Jan 13th Winter break	15th **1** Read through Schroeder p. 28 (§1.1-1.4) What is Statistical Physics?; Thermal equilibrium; Microscopic model of ideal gas; equipartition theorem; heat and work Problems in class: 1.4, 1.14, 1.18 HW #1: 1.7(a), 1.8, 1.16, 1.17, 1.20
20th **2** Read through Schroeder p. 48 (§1.5-1.7) Compressive work; Heat capacities; Rates of processes Problems in class: 1.37, 1.45 HW #2: 1.22 (a,b,c,e - give radius), 1.31, 1.34, 1.36, 1.43	22nd **3** Read through p. 59 (§2.1-2.3) Two-State Systems; Einstein model of a solid; Interacting systems Problems in class: Class choice HW #3: 2.4, 2.5, 2.6, 2.8
27th **4** Read through p. 73(§2.4-2.5) Large Systems; Ideal Gas Problems in class: One of the below. Class votes. HW #4: 2.11, 2.16, 2.17, 2.18, 2.19, 2.21	29th **5** Read through p. 92 (§2.6, 3.1) ENTROPY!; Temperature Problems in class: class choice! HW #5: 2.29, 2.31, 2.33, 2.35, 2.37
Feb 3rd **6** Read through p. 107 (§3.2, 3.3) Entropy and Heat; Paramagnetism Problems in class: class choice! HW #6: 2.38, 3.3, 3.6, 3.13, 3.14 Additional problem from class.	5th **7** Read through p. 121 (§3.4, 3.5, 3.6) Mechanical Equilibrium and Pressure; Diffusive Equilibrium and Chemical Potential Problems in class: class choice! HW #7: 3.24, 3.30, 3.32, 3.35, 3.36a

<table>
<tr><th>Tuesday</th><th>Thursday</th></tr>
<tr><td>10th 8
Guest Lecture
Read through p. 220-237 (§6.1-6.2)<hr>The Boltzmann Factor, Average values<hr>Problems in class: class choice!<hr>HW #8: 6.3 (it's easier to define some dimensionless variable $t = kT/\epsilon$ and plot $Z(t)$), 6.4, 6.11, 6.12, 6.13, 6.22ab
Extra Credit: the rest of 6.22 (we'll do the rest of the problem in class, so you can earn extra credit only by bringing this to class finished)</td><td>12th 9
Read through p. 327-356 (§8.2)<hr>Ising models<hr>Problems in class: class choice!<hr>HW #9: 8.15, 8.17, 8.25, 8.26</td></tr>
<tr><td>17th 10
First test through §6.2, due the Wednesday after break
Read additional assigned material (Ising.pdf) and §8.2<hr>Continue §8.2, more about MC; MC Pi estimation, Monte Carlo Simulation Coding; March Madness code.<hr>Problems in class:<hr>HW #10: 8.16, 8.18, 8.23</td><td>19th
Early Semester Break
yay!!!</td></tr>
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<tr><th>Tuesday</th><th>Thursday</th></tr>
<tr><td>24th **11**
Read through p. (§1.7)

Diffusion, rates

Problems in class: class choice!

HW #11: 1.56, 1.68 (hint: you can make life easier by reading page 47 and assuming that the perfume has spread to half of the room), report on one interesting topic from Sethna. March Madness Monte Carlo problems 1-3 (see the github site)
Extra credit: finish 1.57,</td><td>26th **12**
Read through p. 149-165 (§5.1-5.2)

Free energy available as work; Free Energy as a force towards equilibrium
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Problems in class: 5.7, class choice!

HW #12: 5.4, 5.8, 5.9, 1.40, March Madness Monte Carlo problems 4-5.</td></tr>
<tr><td>Mar 3rd **13**
Read through p. 166-185 (§5.3)

Phase Transformations of Pure Substances

Problems in class: class choice!

HW #13: 5.26, 5.32, 5.48, 5.52
Extra credit: 5.51</td><td>5th **14**
Read through p. 122-148 (§4.1-4.4) **More than most days, you must have done the reading ahead of class**

Heat Engines and Refrigerators (§4.1-4.2)
For discussion, but not as important: §4.3-4.4

Problems in class: class choice!

HW #14: 4.7, 4.8, 4.12, 4.14</td></tr>
<tr><td>10th **15**
Read lab handout

Lab #1: Simulation of free energy 1

Problems in class: lab!

HW #15: Finish lab!</td><td>12th **16**
Read through p. 186-199 (§5.4)

Phase Transitions of Mixtures

Problems in class: class choice!

HW #16: 5.35</td></tr>
<tr><td>17th
Spring Break</td><td>19th
Spring Break</td></tr>
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TUESDAY	THURSDAY
24th **17** **Read lab handout** **Lab #2: Diffusion& modern microscopy** Problems in class: start analysis! HW #17: finish analysis	26th **18** **You may begin Lab #3: Entropy of Unknotting at any point after this lecture.** Read through p. 200-207, 238-246 (§5.5, §6.3-6.4) Dilute Solutions; Equipartition; Maxwell Speed Distribution Problems in class: class choice! HW #18: 5.75, 5.76, 5.82, 6.31, 6.38 Extra Credit: 5.81, 6.39
31st **19** Read through p. 247-256 (§6.5-6.7) Partition Functions, Free Energy and Composite Systems Also catch up Problems in class: class choice! HW #19: work on your papers Extra credit: 6.43, 6.48, 6.53(!)	Apr 2nd **20** Read provided additional material Student choice: The new fluctuation theorems *or* project workday. Problems in class: class choice! HW #20: Extra credit: Jarzynski problem from Tuckerman.

<table>
<tr><th>Tuesday</th><th>Thursday</th></tr>
<tr><td>7th 21

Project Topics Due

Read lab handout We'll be working through the "Stretching Deca-alanine" tutorial from the Computational Biophysics folks at UIUC. We'll work through the in-class portions in class, but you'll need to read the three emailed PDFs ahead of time.

Lab #4: Simulation of free energy 2

Problems in class: lab!

HW #21: Finish lab!</td><td>9th 22

Project Paragraph Due

Read through p. 257-270 (§7.1-7.2)
Class Handout: VariousQMDistributions.PDF

The Gibbs Factor; Bosons and Fermions

Problems in class: class choice!

HW #22: 7.8, 7.10, 7.11ace, 7.13
Extra Credit: 7.9, 7.13 the rest, 7.18</td></tr>
<tr><td>14th 23

Second test

Read through p. 271-287 (§7.3)

Degenerate Fermi Gases, Density of States

Problems in class: class choice!

HW #23: 7.23fg, 7.41 (i.e. "how lasers work")
Extra Credit: 7.22, 7.23abcde, 7.42 (if you do not do these for extra credit, ask Michael for the solutions, as they're required for the other problems.)</td><td>16th 24
Read through p. 271-287 (§7.3)

Density of States
catch up

Problems in class: class choice!

HW #24: work on your papers
Extra credit: 7.33, 7.34, 7.35</td></tr>
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Tuesday	Thursday
21st **25** **Project Workday!**	23rd **26** Read through p. 307-326 (§7.5-7.6) Debye Theory of Solids; Bose-Einstein Condensation Problems in class: class choice! HW #25: work on your papers Extra credit: 7.58, 7.60, 7.64
28th **27** **PROJECT PRESENTATIONS!**	30th **28** **PROJECT PRESENTATIONS!**
May 5th Reading Day	7th Finals