Physics 114 Statistical Mechanics Spring 2018
Seminar 1

Break provided by: Amy

Overview:

Things fall. -Isaac Newton
Things fall apart. -William Butler Yeats; Chinua Achebe

We will revisit what you know of thermodynamics this week ... reminding ourselves of the 0th law (thermometers work) and 1st law (increase in energy of a system = work on it + heat into it), and allude to the 2nd law (things fall apart). Thermo is an extremely important field which brought about the industrialization of society and revolutionized transportation, power generation, chemical engineering ... It is a wholly self-consistent set of ideas and equations based on experimental definitions and multivariable calculus. Weirdly, thermo is largely immune to microscopic details of the gasses, liquids, solids and plasmas that it describes.

Why is thermodynamics valid? The answer lies in *statistical mechanics* which treats large systems comprised of small objects. Stat mech rests on some ridiculously simple postulates about these systems, like ergodicity and equal a priori probabilities. “From micro to macro” is the first theme in one of our texts, Gould and Tobochnik (G&T). The implication is that there are many microscopic details that we *do not need to know*, to calculate the macroscopic properties correctly. (Details that we *do* need include whether the objects obey classical or quantum mechanics, whether they are relativistic or not, and if there are constraints on what they can do ... like from walls, insulation, etc.) Thanks to the laws of probability, *stat mech provides the definitions and supports the equations that comprise thermodynamics.* Moreover, non-equilibrium stat mech takes us beyond thermo, to systems whose macroscopic properties evolve in time. Stat mech even applies to non-physics systems like biological and economic ones where the “laws of motion” are not Newtonian or the Schrodinger Equation, but particular to those disciplines. *Stat mech rocks!*

Our first job this week will be to go over the organization of the seminar and decide how you want it to run, how you want your grade to be determined, and so on. Usually, I like to have both presentations and problem-solving, both analytical and numerical work. As you can tell from the long “Concept checklist” part of this assignment, I feel compelled to *summarize in writing* the major ideas each week. Hopefully, this goes a long way toward helping you organize your learning, study for tests, ... I also like to take a little time during seminar to summarize a major idea - and even more importantly - to have you to comment on and and ask questions about what you’ve read.

Required Reading:

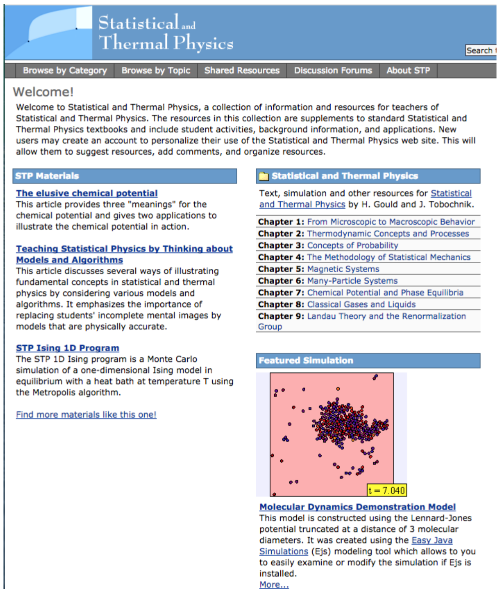
G&T sections

- chapter 1
- from chapter 2, sections 2.1 - 2.11

B&B sections

- from chapter 1, sections 1.1-1.3
- Appendices C.6 and C.7
- chapter 2
- chapter 11
- chapter 12

Computational Preparation: Be sure that whatever computer you typically use is able to run the simulations that go with G&T . One thing that might work is the G&T Statistical and Thermal Physics java website: `http://stp.clarku.edu/simulations/` . Redirect yourself, or else go directly to `https://www.compadre.org/STP/?` . Below is the Compadre page for “STP” (simulations in thermal physics). If you then follow that page’s link to “Chapter 1: From Microscopic to Macroscopic Behavior” and at the bottom of that next page, select a link saying “Simulations”, you’ll see



Welcome!

Welcome to Statistical and Thermal Physics, a collection of information and resources for teachers of Statistical and Thermal Physics. The resources in this collection are supplements to standard Statistical and Thermal Physics textbooks and include student activities, background information, and applications. New users may create an account to personalize their use of the Statistical and Thermal Physics web site. This will allow them to suggest resources, add comments, and organize resources.

STP Materials

The elusive chemical potential
This article provides three "meanings" for the chemical potential and gives two applications to illustrate the chemical potential in action.

Teaching Statistical Physics by Thinking about Models and Algorithms
This article discusses several ways of illustrating fundamental concepts in statistical and thermal physics by considering various models and algorithms. It emphasizes the importance of replacing students' incomplete mental images by models that are physically accurate.

STP Ising 1D Program
The STP 1D Ising program is a Monte Carlo simulation of a one-dimensional Ising model in equilibrium with a heat bath at temperature T using the Metropolis algorithm.

Find more materials like this one!

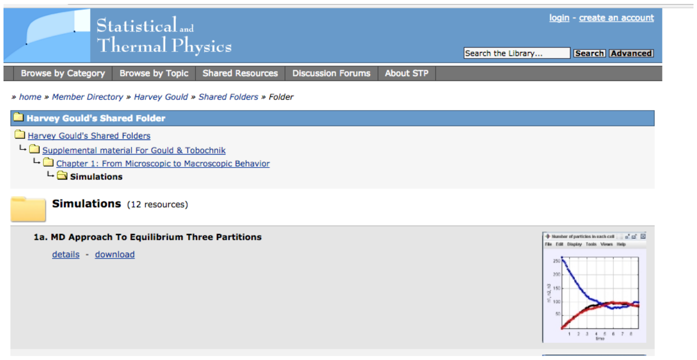
Statistical and Thermal Physics

Text, simulation and other resources for Statistical and Thermal Physics by H. Gould and J. Tobochnik.

Chapter 1: From Microscopic to Macroscopic Behavior
Chapter 2: Thermodynamic Concepts and Processes
Chapter 3: Concepts of Probability
Chapter 4: The Methodology of Statistical Mechanics
Chapter 5: Magnetic Systems
Chapter 6: Many-Particle Systems
Chapter 7: Chemical Potential and Phase Equilibria
Chapter 8: Classical Gases and Liquids
Chapter 9: Landau Theory and the Renormalization Group

Featured Simulation

Molecular Dynamics Demonstration Model
This model is constructed using the Lennard-Jones potential truncated at a distance of 3 molecular diameters. It was created using the Easy Java Simulations (Ejs) modeling tool which allows to you to easily examine or modify the simulation if Ejs is installed.
More...



Harvey Gould's Shared Folder

Harvey Gould's Shared Folders
- Supplemental material For Gould & Tobochnik
  - Chapter 1: From Microscopic to Macroscopic Behavior
    - **Simulations**

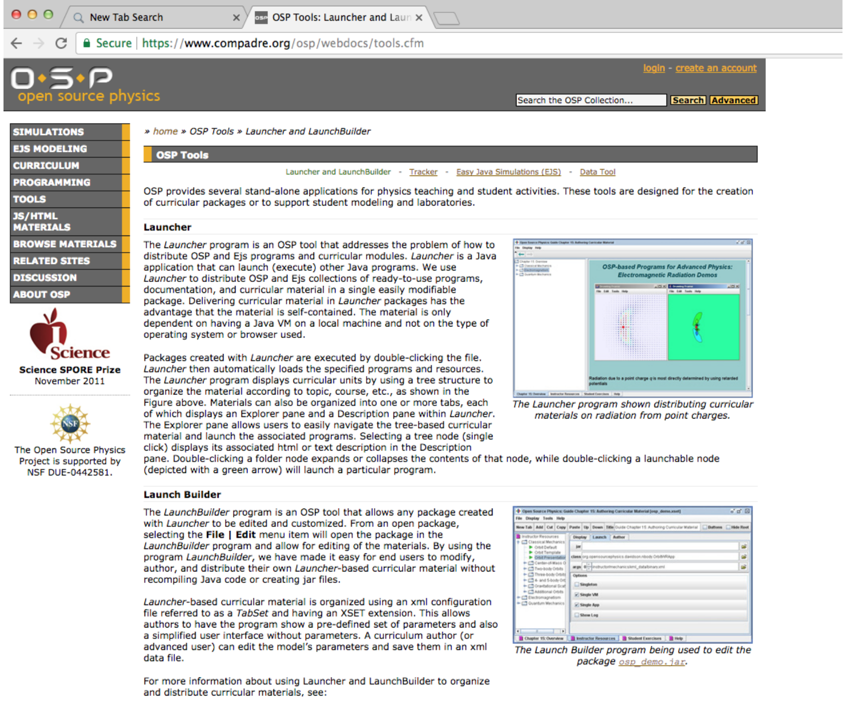
Simulations (12 resources)

1a. MD Approach To Equilibrium Three Partitions

details - download

Can you successfully open and use the application? Hope!

As an alternative, you may need to go to another Compadre page, the Open Source Physics page https://www.compadre.org/osp/webdocs/tools.cfm. You'll see the page as in the image below, from which you can download the *Launcher* package as in the second image. This will run standalone Java simulations. This may involve loading a new version of Java, and/or setting the Java security in your system preferences. Please check with ITS if this is giving you trouble.



OSP Tools

OSP provides several stand-alone applications for physics teaching and student activities. These tools are designed for the creation of curricular packages or to support student modeling and laboratories.

Launcher

The *Launcher* program is an OSP tool that addresses the problem of how to distribute OSP and Ejs programs and curricular modules. *Launcher* is a Java application that can launch (execute) other Java programs. We use *Launcher* to distribute OSP and Ejs collections of ready-to-use programs, documentation, and curricular material in a single easily modifiable package. Delivering curricular material in *Launcher* packages has the advantage that the material is self-contained. The material is only dependent on having a Java VM on a local machine and not on the type of operating system or browser used.

Packages created with *Launcher* are executed by double-clicking the file. *Launcher* then automatically loads the specified programs and resources. The *Launcher* program displays curricular units by using a tree structure to organize the material according to topic, course, etc., as shown in the Figure above. Materials can also be organized into one or more tabs, each of which displays an Explorer pane and a Description pane within *Launcher*. The Explorer pane allows users to easily navigate the tree-based curricular material and launch the associated programs. Selecting a tree node (single click) displays its associated html or text description in the Description pane. Double-clicking a folder node expands or collapses the contents of that node, while double-clicking a launchable node (depicted with a green arrow) will launch a particular program.

The Launcher program shown distributing curricular materials on radiation from point charges.

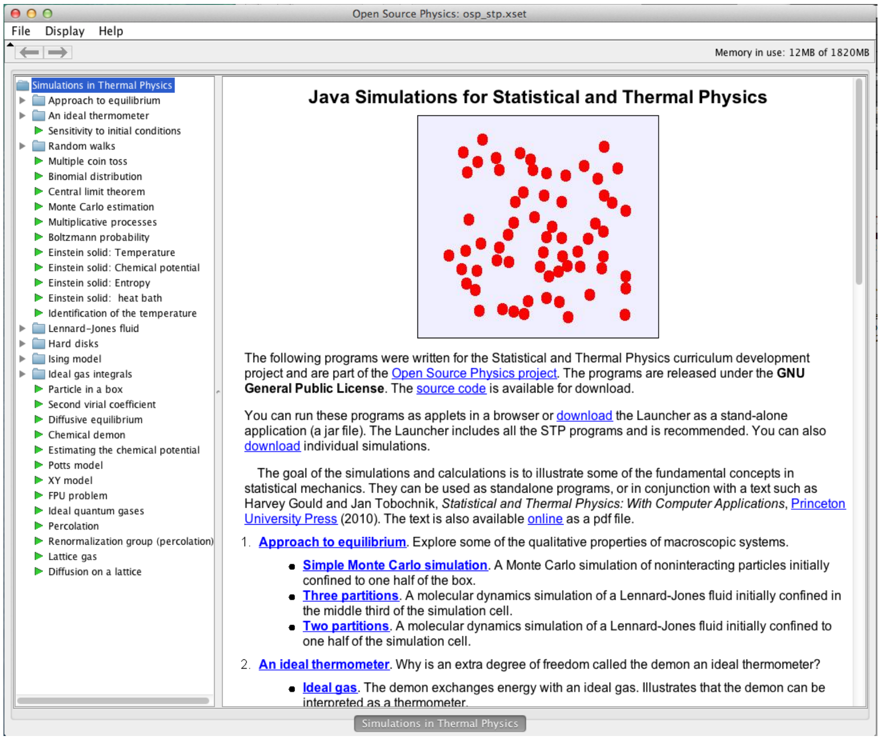
Launch Builder

The *LaunchBuilder* program is an OSP tool that allows any package created with *Launcher* to be edited and customized. From an open package, selecting the **File | Edit** menu item will open the package in the *LaunchBuilder* program and allow for editing of the materials. By using the program *LaunchBuilder*, we have made it easy for end users to modify, author, and distribute their own *Launcher*-based curricular material without recompiling Java code or creating jar files.

Launcher-based curricular material is organized using an xml configuration file referred to as a *TabSet* and having an XSET extension. This allows authors to have the program show a pre-defined set of parameters and also a simplified user interface without parameters. A curriculum author (or advanced user) can edit the model's parameters and save them in an xml data file.

The Launch Builder program being used to edit the package `osp_demo.jar`.

For more information about using Launcher and LaunchBuilder to organize and distribute curricular materials, see:



- Simulations in Thermal Physics
  - Approach to equilibrium
  - An ideal thermometer
  - Sensitivity to initial conditions
  - Random walks
  - Multiple coin toss
  - Binomial distribution
  - Central limit theorem
  - Monte Carlo estimation
  - Multiplicative processes
  - Boltzmann probability
  - Einstein solid: Temperature
  - Einstein solid: Chemical potential
  - Einstein solid: Entropy
  - Einstein solid: heat bath
  - Identification of the temperature
  - Lennard-Jones fluid
  - Hard disks
  - Ising model
  - Ideal gas integrals
  - Particle in a box
  - Second virial coefficient
  - Diffusive equilibrium
  - Chemical demon
  - Estimating the chemical potential
  - Potts model
  - XY model
  - FPU problem
  - Ideal quantum gases
  - Percolation
  - Renormalization group (percolation)
  - Lattice gas
  - Diffusion on a lattice

Java Simulations for Statistical and Thermal Physics

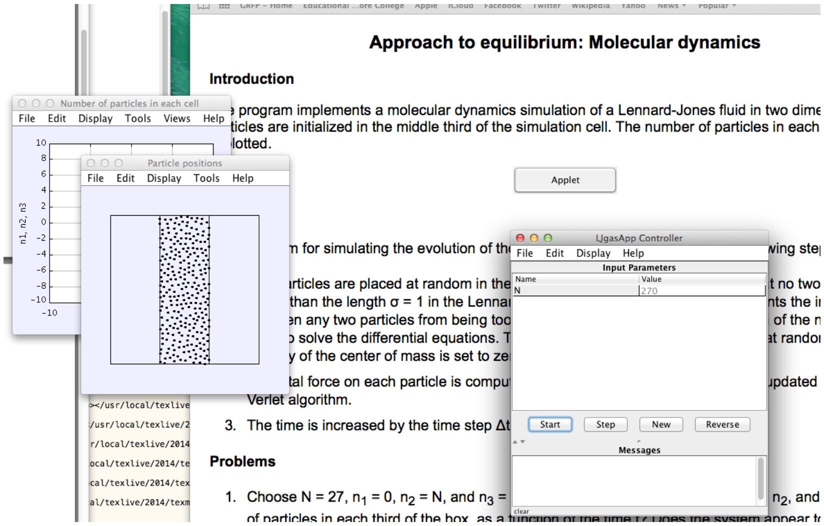
The following programs were written for the Statistical and Thermal Physics curriculum development project and are part of the Open Source Physics project. The programs are released under the **GNU General Public License**. The source code is available for download.

You can run these programs as applets in a browser or download the Launcher as a stand-alone application (a jar file). The Launcher includes all the STP programs and is recommended. You can also download individual simulations.

The goal of the simulations and calculations is to illustrate some of the fundamental concepts in statistical mechanics. They can be used as standalone programs, or in conjunction with a text such as Harvey Gould and Jan Tobochnik, *Statistical and Thermal Physics: With Computer Applications*, Princeton University Press (2010). The text is also available online as a pdf file.

1. **Approach to equilibrium**. Explore some of the qualitative properties of macroscopic systems.
   - **Simple Monte Carlo simulation**. A Monte Carlo simulation of noninteracting particles initially confined to one half of the box.
   - **Three partitions**. A molecular dynamics simulation of a Lennard-Jones fluid initially confined in the middle third of the simulation cell.
   - **Two partitions**. A molecular dynamics simulation of a Lennard-Jones fluid initially confined to one half of the simulation cell.
2. **An ideal thermometer**. Why is an extra degree of freedom called the demon an ideal thermometer?
   - **Ideal gas**. The demon exchanges energy with an ideal gas. Illustrates that the demon can be interpreted as a thermometer.

The goal is to hit the green arrow next to the "Three partitions" applet and see something like the image below, after hitting "Initialize", then "Start".



Approach to equilibrium: Molecular dynamics

Introduction

e program implements a molecular dynamics simulation of a Lennard-Jones fluid in two dime
ticles are initialized in the middle third of the simulation cell. The number of particles in each
lotted.

Name	Value
N	270

m for simulating the evolution of th … wing ste

rticles are placed at random in the … t no two
than the length σ = 1 in the Lenna … nts the i
en any two particles from being too … of the n
o solve the differential equations. T … t rando
y of the center of mass is set to ze

tal force on each particle is compu … updated
Verlet algorithm.

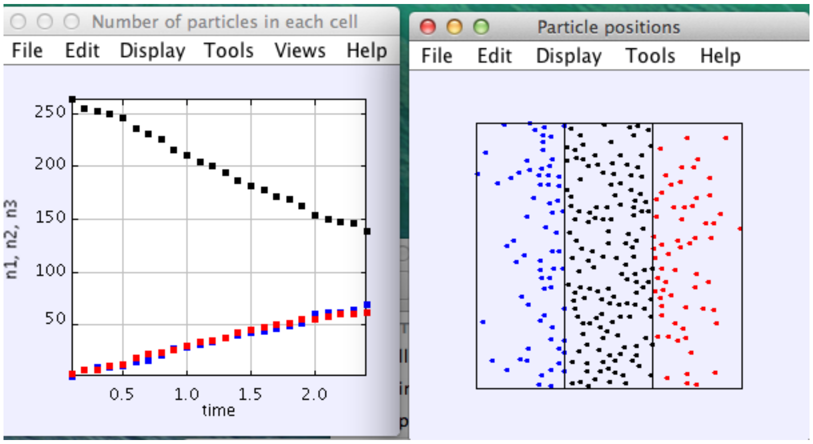
3. The time is increased by the time step Δt

Problems

1. Choose N = 27, n_1 = 0, n_2 = N, and n_3 = … n_2, and
of particles in each third of the box as a function of the time t? Does the system appear t

```
></usr/local/texlive
/usr/local/texlive/2
r/local/texlive/2014
ocal/texlive/2014/te
cal/texlive/2014/tex
al/texlive/2014/texm
```

Hopefully, one way or another you are now running the simulation and taking data! Below is what you should see once you hit "initialize" and start running `ApproachToEquilibriumThreePartitions`.



Concept checklist from Readings:

- Time has a direction for a large system ... "things fall apart"
- Energy naturally goes from a useful (able to do work) to a less useful (thermal energy) form.
- We might be tempted to say that energy goes from the form of work to the form of heat. But that's wrong ... why?
- How is heat, Q different from energy, E? How is it different from temperature, T?
- *Notation alert*: B&B uses U for energy, whereas G&T uses E. Look for other such notational differences as we read. Sigh.
- *System* and its surroundings: System can be open or closed; walls insulating or conducting.
- *Microstates* and *macrostates*: Their definition depends on what we are modeling (gas? magnet? black body?) For a classical, monatomic gas of N atoms, the macrostate for a closed system is characterized by three variables: P, V and T while a microstate has 6N variables, the positions and momenta of the atoms. N is large (on the computer, 10^6 and in real life, 10^{23}).
- Thermodynamic variables can be *intensive* or *extensive*.
- *Entropy* (whose rigorous definition is postponed for a future week) is something that increases in all real-world processes. It is also something that labels a macrostate. It is larger for macrostates that correspond to larger numbers of microstates.
- Simulations: A *molecular dynamics* simulation solves $\vec{F} = d\vec{p}_i/dt$ numerically, to find $\vec{r}_i(t)$ and $\vec{v}_i(t)$ for $i = 1, 2, ..., N$ particles.

- Systems *spontaneously approach equilibrium.* In equilibrium we observe a mean, or average, value of a macroscopic quantity. Yes, this definition is somewhat circular ... the system is in equilibrium when its macroscopic properties don't change and are described by the laws of (equilibrium) thermodynamics.

- Macroscopic properties are often called *functions of state* (or variables of state or state variables). Functions of state change if we change *parameters* of the system, and their change is always described as an exact differential. Thus, they are independent of the path in parameter space, depending only on the starting and ending values of the parameters.

- Equilibrium is not the same thing as being static. There are *equilibrium fluctuations* in equilibrium mean values. E.g. the simulation `ApproachToEquilibriumParticlesInBox` will show us a mean number on the left side, $\bar{n}$, but also a variance, $\sigma^2 = \overline{(n - \bar{n})^2}$.

  This week, I just want you to get a flavor for means and variances (which measure fluctuations around the mean). In later weeks, we will calculate these theoretically, and estimate them with simulations. We will also see how means and variances scale with system size, temperature, ...

- The postulates of *history independence* and *equal a priori probabilities.*

- Pressure arises from microscopic collisions of particles with walls.

  $$P = F/A = \frac{1}{A}\frac{dp_x}{dt}$$

  where just for argument's sake, we consider collisions with the area A of a wall in the $y - z$ plane, so the x component of momentum p_x is what changes during the collision.

- *The 0th law of thermodynamics*: One statement is that when two bodies are in thermal equilibrium with a third body, they are in thermal equilibrium with each other. “Thermal equilibrium” means same temperature. Two systems come to the same temperature when they are allowed to exchange energy. Of course, this might not be the original temperature of either system. A thermometer subtracts only a tiny amount of energy from a system. It thus does not change the system's original temperature, but merely reports on it.

- The *ensemble* concept : Many different systems, each one in equilibrium. On the other hand, simulations and experiments often involve just one system advancing in time. The *ergodic hypothesis* lets us equate the two pictures. Thus an ensemble of many equilibrium systems, and one system in equilibrium measured over time will show us the same physics.

- *Sensitivity to initial conditions* suggests that history independence and the ergodic hypothesis apply. As a system evolves, it eventually "forgets" the details of how it began.

- How long does the system take to forget its starting configuration? There will be some *relaxation time* - a time scale for reaching equilibrium. This time depends on the size of the system, the type of contact with its surroundings, etc. You can run G&T programs like `ApproachToEquilibrium...` or `SensitivityToInitialConditions` to get a sense of this for specific cases. G&T section 1.13.1 gives you the case of N particles in a box with two sides, and allows you in Problems 1.2 and Problem 1.10 to calculate the time scale, τ over which the system equilibrates. Here, $\tau = N/2$.

- Models of matter:
  - ideal gas particle
  - particles that interact via a pure repulsion as in G&T Eq. (1.5)
  - the LJ interaction
  - lattice models

- Important constants and their values: k, N_A and R.

- The Kelvin temperature scale. The ideal gas temperature scale is a related idea. We will talk about the "triple point later".

- A *pressure equation of state* is sometimes written $P = f(T, \rho)$ where $\rho = N/V$; though more casually we just write a function relating P, T, N and V. The ideal gas one is $PV = NkT$ (physicist-preferred) or $PV = nRT$. (chemist-preferred). The van der Waals equation of state corrects some assumptions about idealized gasses.

- An *energy equation of state* looks like $E = f(N, V, T)$. The ideal gas and van der Waals equations are found in G&T section 2.9. Note that energy of an ideal gas does not care about its density, $\rho = N/V$, but for the more realistic gas, energy changes - in the case of Eq. (2.24) it is lower - when density is higher.

- The monatomic ideal gas energy of state $E = \frac{3}{2}NkT$ will be derived later (though you may know it if you've already studied kinetic theory of gasses or the equipartition theorem).

- *Processes* take us from one thermodynamic macrostate to another. *Quasi static* means that the system passes through a set of equilibrium states at every stage. *Reversible* means that one can find a practical way to run the process in reverse. For example, any process where friction acts is irreversible. An irreversible process cannot be quasistatic. Subtle? Hell yes.

- The *work done on a gas* undergoing a quasi static process from state 1 to 2 is

  $$W_{1\to 2} = -\int_{V_1}^{V_2} PdV$$

  We can use this equation plus the equation of state for an ideal gas to find the work done on processes that are

  - isothermal
  - isochoric
  - isobaric

- Schroeder (Phys 13) called this kind of work "compression work" which is smart - it reminds you that there are other kinds, though this is the one we most often think of ... gas in cylinder acted upon by piston.

- An *adiabatic* process takes place when the system is insulated from its surroundings, so no heating or cooling happens. For an adiabatic process, $Q = 0$. Careful: this is not saying that the temperature of the system is constant on an adiabat. Rather, work done on the system, W, will change its thermal energy: $W = \Delta E$, and hence its temperature will change. (Exception: The system is undergoing a phase transition.)

- The net work *on* a gas is the negative of area of a cycle like Fig. 2.4 in G&T. If arrows would reversed, sign of work changes. For the work done *by* the gas, again the sign changes.

- *The 1st law of thermo:* $\Delta E = W + Q$.

- For an ideal gas, with the help of the 1st law, we can calculate Q, ΔE, and W for a process as shown on a PV diagram. In particular, know how to do this for the four fundamental kinds of processes: isochores, isobars, isotherms and adiabats.

- For adiabats we derive that $PV^{(f+2)/f} = const$ where G&T limits us to the case $f = 3$, true for monatomic gasses. Equivalently, $TV^{2/f} = const$. The abbreviation $\gamma = (f+2)/f$ is used. The symbol γ is called the "adiabatic index" or "adiabatic constant".

- We will talk more about *enthalpy*, H, later. For now, note that the definition of this function of state is $H = U + PV$. Schroeder (Phys 13) gave us this memorable way to think about the difference between H and U:

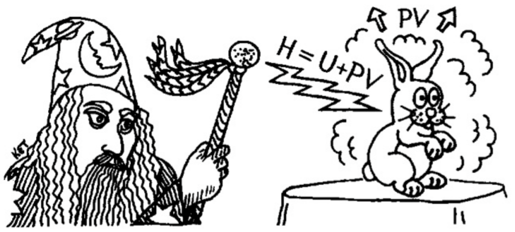


Figure 1.15. To create a rabbit out of nothing and place it on the table, the magician must summon up not only the energy U of the rabbit, but also some additional energy, equal to PV, to push the atmosphere out of the way to make room. The *total* energy required is the **enthalpy**, $H = U + PV$.

- *Heat capacity* is $C = \frac{Q}{\Delta T}$. Different processes might be involved as T changes, yielding different values of C. Two popular cases are isochoric and isobaric changes:

  $$C_V \equiv (\partial E/\partial T)_V \quad ; \quad C_P \equiv (\partial H/\partial T)_P$$

  The heat capacity for isobaric processes is higher because some of Q goes into work, not increasing E ... hence increasing T. It can be shown that $\gamma = \frac{C_p}{C_v}$. Similarly, $C_P - C_V = R$.

- The *specific heat capacity* is the heat capacity per unit mass of the substance. We often note specific heat as c. Sometimes people want the heat capacity of exactly one mole: this is called the *molar heat capacity*. (It can be a tiny bit confusing to read C_V in B&B and not know if it is for one mole or n moles, but the units give it away.)

Checklist: Math concepts to know this week:

- easy-to-evaluate integrals as in G&T 1.13.2
- given $f(x, y)$, how to take a partial derivative like $(\partial f(x, y)/\partial x)_y$.
- writing a Taylor series for a function
- the definition of an exact differential - for example that the integral of $f(x, y)$ is independent of the path between its endpoints, and that partial differentiation can occur in any order, so $(\partial^2 f/\partial x \partial y) = (\partial^2 f/\partial y \partial x)$

Presentation: *No student ones this week*

Amy will talk about states, equilibrium and temperature.

Warmup Problems: *Due before seminar, Monday at 5 pm*

Note: In future, you will have just one or two warmup problems!

1. Say which computing languages/environments you feel comfortable using in order to solve numerical problems and make graphs. Which computer languages or environments (if any) could you comfortably use to write a short numerical calculation or simulation?
2. Go to the G&T Statistical and Thermal Physics java website: `http://stp.clarku.edu/simulations/` . Try to run a simulation like `ApproachToEquilibriumThreePartitions`. (This simulation is discussed in Section 1.4 of G&T and I ask you to do a G&T problem using it below.) This might be run as an applet (perhaps necessitating a change in your Java security settings) or as a standalone Java program. Did you succeed? If not, ITS can help ... I hope the answer to this question is ultimately 'yes' :-)
3. **work** G&T Problem 2.7
4. **pressure equation of state** Write the van der Waals equation of state, which is G&T Eq. (2.12) in the form $P = f(T, \rho)$

Regular Problems: *For this first seminar, do as many as you comfortably have time for. For future seminars, we are going to assign problems to pairs of people. Each of you will get a chance to do the "introduction" to a problem, and to do the "solving" in another.*

1: reversible or not? G&T Problem 2.6

2: work G&T Problem 2.8

3: adiabatic and isothermal compression G&T Problem 2.17

4: transfer of heat between two bodies B&B Problem 2.5.

5: isothermal expansion B&B Problem 11.1

6: taking partial derivatives B&B Problem 11.4

7: partial derivatives for a thermal process B&B Problem 12.3

8: work, heat and thermal energy for different thermodynamic processes G&T Problem 2.56

9: free expansion (*part of G&T Problem 2.24, which we will come back to later)* An ideal gas of N particles in a box of volume V_2 is initially confined to only part of the box, with volume $V_1 < V_2$. The remaining volume of the box is empty - a vacuum. The gas has initial temperature T. The gas is then allowed to expand freely to fill the entire volume V_2. The box is thermally insulated from the outside world. What is the change in energy of the gas? What is the change in temperature of the gas?

10: modeling a bicycle pump G&T Problems 1.24 and 2.9

11: approach to equilibrium with three and two partitions G&T problem 1.1 parts (a) - (f)

If the `VideoCapture` feature of these applications doesn't work for you (It doesn't for me.) you can make a video some other way. E.g. Quicktime player does it on the Mac ... see under the File menu that you can do a New Screen Recording.

12: more about approach to equilibrium G&T problem 1.10

13: PV = NkT A cloud of neutral hydrogen atoms has a mass which is 100 times the mass of our sun, a temperature of T=50K and a number density of 500 atoms per cm^3. What is its pressure in Pa? What is its volume? (If you are an Astro person, feel free to convert the volume to ly^3 :-)