Physics 114 Statistical Mechanics Spring 2021

Week 6 Reading and Problem Assignment

Overview:

The Canonical partition function is a topic of continued study this week. We will use it for two important purposes: deriving the law of *equipartition of energy* and for the *Maxwell-Boltzmann* distribution of velocities. We'll exploit the simple relationship between $Z(T,V,N)$ and the Helmoltz free energy, $F(T,V,N)$. We'll practice calculating thermodynamic variables from Z: ones that are easy to measure and control (like P), easy to measure but not control (like C_V) and difficult to control (like E and S). We'll do problems that bridge the gap between microcanonical and canonical statistics - showing that for thermodynamically large systems, these provide two roads to the same destination. Finally, we will study how one simulates a system of interacting particles using *Monte Carlo*.

Suggested Reading:

G&T Sections

- Section 4.7-4.11
- Sections 6.1, 6.2

B&B Sections

- Section 4.7
- Ch. 5
- Chs. 19, 20, 21
  As usual, these B&B chapters are pretty short and very readable.

Warmup Problems:

1: Beautiful, simple way to write a partition function: B&B 21.1

2: The Maxwellian distribution: What's the rms speed $\sqrt{< v^2 >}$ of nitrogen N_2 at room temperature? How different is your answer if you approximate its speed as $< v >$ instead?

Problems to discuss in our meeting

Note: The * means that these problems are to be handed in. They are due the day after we meet.

1*: High T limits of partition functions: B&B problem 20.1

2: Harmonic Oscillators
(Last week we did G&T 4.22 for microcanonical oscillators. Now, canonical :-)
i) G&T Problem 4.28
ii) G&T Problem 4.50
Hint: Much of this is done in B&B ... please fill in any gaps in math or logic for yourself.

3: Noninteracting Magnets: B&B Problem 20.6

4: A 2-state system with degeneracy:
B&B Problem 21.4
Also: Please compare what you derived, which is B&B Eq. (21.46), with the heat capacity shown in part (a) of Figure 20.4 (p. 225). That graph applies to a slightly different 2-state system. Any salient differences? If so, can you explain why?

5*: Entropy of mixing
i) G&T Problem 6.8
ii) G&T Problem 6.9

6: Equipartition B&B Problem 19.5

7: Rotational heat capacity G&T Problem 6.46

8: Maxwell-Boltzman velocities and speeds
i) Simulation: Do part (a) of G&T Problem 6.11
ii) Calculation: Do G&T Problem 6.12

9*: MC simulation:
You have two options and only need to pick one.
Option 1: **Demon thermometer and ideal gas:** Do G&T Problem 1.8 parts (a), (b), (c), (d), and (g)

OR

Option 2: **Construct your own MC simulation in Python**
Here is a suggested protocol that would simulate an Einstein solid:

1. Decide on a temperature. That is, let $1/kT = \beta$ and pick a value of β. I suggest a value not too different from $\beta = 1$, but you can try a couple of different values, and see what difference it makes.

2. Initialize: Create an array of N numbers representing the energies of a set of N particles. Let them each start with 0 energy.

3. Pick a random particle (That is, choose a random integer between 1 and N to determine your particle of interest.)

4. Trial move: Toss a "coin" (That is, choose another random integer, now either 0 or 1.) If heads, consider adding $\Delta E = +1$ to the energy of the particle. If tails, think about adding $\Delta E = -1$ to its energy.

5. Accept or reject the move:

   - Definitely accept the move if it would lower the particle's energy, but not below zero.
   - Definitely reject the move if it would lower the energy of the particle below 0.
   - Accept the move with probability $e^{-\beta \Delta E}$ if it would raise the energy. (To do this, you need to generate a real random number between 0 and 1, which G&T call r.)

6. Go back to step 3 and iterate a lot of times ... you want each of the N particles to experience many moves.

As the simulation proceeds, measure something interesting. Average energy? A histogram of energies? Other ...?