Physics 114 **Statistical Mechanics** **Spring 2021**

Week 5 Reading and Problem Assignment

Overview:

This is a big week, where we begin to do statistical mechanics in earnest. One major topic this week is the statistical definition of the entropy and, as a consequence, the temperature. Section 14.8 of B&B calls $S = -k\ P_i\ lnP_i$ the *Gibbs entropy* of a thermodynamic system. B&B Ch. 15 defines the *Shannon entropy*, which applies beyond thermodynamics, to fields like cryptography, data compression and quantum mechanics.

Another major concept is the *partition function*. Partition functions are "just" a normalizing factor ... but this is a crucial thing. We need the right normalization when taking thermodynamic averages. By counting states, the partition function and its derivatives tell us every thermodynamic quantity we might want to know. This week, we practice this state counting, and next week we'll make the thermodynamic connection.

We'll discuss 2 kinds of collections of states; that is, two kinds of *ensemble*. The first is the *Microcanonical ensemble*, in which E, V, N are the fixed quantities. Though sometimes people don't call it a "partition function" the total number of microstates, $\Omega(E, V, N)$, plays an equivalent role in this ensemble. The other is the *Canonical ensemble*, in which T, V, N are the fixed quantities. Such a system would have solid, diathermal walls and be immersed in a heat bath. In the canonical ensemble, the partition function is commonly written as $Z(T, V, N)$. The Canonical partition function is such a big player in stat mech that we will continue to study it next week. At that time, we will use it to derive the free energies and bulk properties we've learned about in thermo. We'll also utilize Z to derive the law of *equipartition of energy* and for the *Maxwell-Boltzmann* distribution of velocities.

Suggested Reading:

G&T Sections

- Section 3.4.2
- Sections 4.2-4.6
- Sections 4.13, 4.14.1, 4.14.2

B&B sections

- Sections 4.1-4.6
- Sections 14.5-14.8

- Ch 15
- Appendix C.8

Optional Reading:

If you are intrigued by the topic, there are some very readable papers on information entropy under the Resources section of our Moodle Site. The original link to Claude Shannon's paper in information entropy is here: `http://math.harvard.edu/~ctm/home/text/others/shannon/entropy/entropy.pdf`

Warmup Problems:

1: Counting states for an electron in a 1D box
G&T Problem 4.11

2: Statistical basis for the 3rd law
G&T Problem 4.27
Also ... What value do you think $S(T)$ would approach as $T \to 0$ if there were a small magnetic field present?

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: Statistical definition of entropy
Do B&B Problem 14.8. Also ...
We learned a week ago that $F = U - TS$ was the definition of the Helmholtz free energy. If this is true, what is the relationship between Z and F?

2: Counting states for gas particles in a box
G&T Problem 4.14

3*: Einstein solids in thermal contact
G&T Problem 4.6

4: More about Einstein solids in thermal contact
G&T Problem 4.7

5*: A thermally isolated Einstein solid: G&T Problem 4.22

6: Relative abundance of isomers: G&T Problem 4.24

7: Maximizing the Shannon entropy B&B Problem 15.3

8: Bayesian Statistics
i) The Monty Hall Problem: B&B Problem 15.6

ii) Suppose that there are two different communities. In community A, COVID-19 occurs in 1 out of 100 people. In community B, it occurs in 1 out of 10,000 people. A pharmaceutical company has come up with a super-rapid test with accuracy x. Accuracy is defined the usual way: With probability x the test will be positive if the person tested actually has COVID-19. With probability $1 - x$ the test will be positive if the person *does not* have the disease. (In other words, with probability $1 - x$ it gives a "false positive".)

What does x need to be in community A in order to signify that with probability of 50% or greater, a person *does* have COVID-19 after they test positive? Same question for community B?

9*: The entropy of a monatomic ideal gas ... or is it?
Do G&T 4.18.
Then, please substitute $E = \frac{3}{2}kT$ and answer these questions:

- Does ΔS agree with what we found back doing thermo? Namely:

$$\Delta S = \frac{3}{2}Nk\ ln\frac{T_2}{T_1} + Nk\ ln\frac{V_2}{V_1}$$

- Does $S(T) \to 0$ as $T \to 0$? (It's OK if the answer is 'no', but if so, why?)