Phys316 Exploration 1 *Boltzmann Distribution* *Name:*

Preliminary

A microstate is a state of a physical system described at the finest level of detail. A macrostate is a state of a physical system that is described in terms of the systems overall or average properties at a macroscopic level. A macrostate will generally consist of many different microstates. In defining a macrostate we ignore what is going on at the microscopic (atomic/molecular) level.

1. Please give a brief physical description of what entropy is to you.

The entropy of a particular macrostate is just the (natural) logarithm of that macrostate's multiplicity. If we denote the entropy by S, then

$$S = k \ln \Omega.$$

2. The ln denotes the natural logarithm, which is a function that is built into any decent scientific calculator. Hopefully you are already familiar with this function, but if not you should plot a graph of lnx vs. x on a graphing calculator or computer plotting program. Make a sketch of ln(x) in the space below.

Project 1: *CoinFlips*

Take 4 coins and align them in a row. The coins cannot change positions, and are therefore are distinguishable. In the columns below please list all possible macrostates and their multiplicities. I have listed the case for all coins being heads as an example.

Macrostate	**Multiplicity**	**Entropy**	**Probability**
H H H H	1	0	

3. Now add up the probabilities you found in the previous table. What do you get? Is this what you expected? Why?

Project 1: *CoinFlips*

We have a program which allows you to simulate the random flipping of coins. Please calculate the following values for 10 coins.

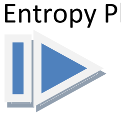
Macrostate	Multiplicity	Probability
10 H, 0T	1	
9 H, 1 T		
8 H, 2 T		
7 H, 3 T		
6 H, 4 T		
5 H, 5 T		
4 H, 6 T		
3 H, 7 T		
2 H, 8 T		
1 H, 9 T		
0 H, 10 T		

3. Which statement below best describes the relationship between probability and entropy for the macrostates we have considered?
   a. The most probable macrostates have the lowest entropy.
   b. The most probable macrostates have the highest entropy.
   c. There is no clear relationship between entropy and probability for these macrostates.

4. If you put ten coins in a cup and then dump them out onto the table, the probability that you would get values between 3 and 7 tails (inclusive of 3 & 7) is?

   The probability that you would get less than 3 tails or more than 7 tails is?

5. In question 4 you should have found that roughly 90% of the probability is concentrated into 5 of the 11 macrostates. Based on these results you can conclude that as you increase the number of coins in the system the probability:
    a. becomes more spread out among a larger fraction of the macrostates
    b. becomes more concentrated into a smaller fraction of the macrostates
    c. remains about the same for a given fraction of the macrostates

Now that you have a handle on multiplicities and entropy, let's perform a little "experiment" with our model. What would happen if we start with a row of 20 coins that are all showing heads and then we began flipping coins over at random? This may seem like a strange thing to investigate, but we will see later on that the behavior of this system provides us with a qualitative understanding of how real systems (like gases) behave. We will use a Java program to simulate the following experiment. We will start with all 20 coins heads up and then we will randomly choose which coin to turn over, in reality this could be accomplished by rolling a 20-sided die. To begin set the number of coins to 20, select "Show Entropy Plot" and "Show Histogram". Make individual coin flips one at a time by pressing the  button.

6. Describe what happens to the number of heads in your sequence of coins as you flip more and more coins.

7. Consider a situation in which your sequence of 20 coins is in a macrostate with 15 heads and 5 tails. How many different results from the die roll would lead to a macrostate with 16 heads and 4 tails?

8. If the macrostate is 15 H, 5 T then how many different results from the die roll would lead to the macrostate 14 H, 6 T?

9. Based on the answer to the previous two questions, if the current macrostate is 15 H, 5 T then what is the most likely macrostate for the model system after the next die roll? How much more likely is this macrostate than the alternative?

10. If the current macrostate is 4 H, 16 T then what is the most likely macrostate for the model system after the next die roll? How much more likely is this macrostate than the alternative?

Click the Start button to run the simulation. Let the simulation run until it has done at least 200 flips, then click Pause. Look at the Number of Heads/Tails graph. Sketch a graph of the Entropy vs. the number of coin flips and the resulting histogram on the grids below.

11. Look carefully at the Entropy plot. Describe the overall behavior of the model system's entropy. Does the entropy ever decrease, even just briefly?

12. Change the number of coins to 200. Run the simulation until it has done at least 400 flips. In what way are these results similar to the results for 20 coins? In what way are they different?

Project 3: *Connecting Multiplicity to Entropy in an Ideal Gas*

Now let's look at something a little closer to the real world. We will consider an ideal gas in a box. An ideal gas consists of molecules that don't interact with each other in any way, but simply fly around exhibiting inertial motion until they hit a wall and bounce off. We will assign each molecule a random initial velocity (with completely random direction and random speed assigned according to something called the Maxwell-Boltzmann distribution). Now let's try to see how the increase of entropy connects to another version of the Second Law of Thermodynamics, namely:

Energy will only flow spontaneously from an object with a higher temperature to an object with a lower temperature. It will not spontaneously flow in the opposite direction.

We will stick with the ideal gas in a box, but this time we are going to have two gases. We will examine a system that starts off with a cold gas in the left side of the box and a hot gas (composed of the same type of molecules, for simplicity) in the right side, with a barrier between the two. Recall that temperature is really a measure of the average kinetic energy of the molecules in the gas, so the molecules on the left will be moving slower on average than the molecules in the right side. What happens when we remove the barrier?

Open the Java Program for HotAndColdIdealGases. The Hot/Cold Gas window shows an animation of the gas, which starts off with the cold (black) particles on the left and the hot (green) particles on the right. Set the number of green and black particles to 200. Click the Temp Plots box to show a plot of the temperature of the gas in each side of the box (the temperature of the left side is in red, that of the right side in blue). The temperature of each side is calculated by first finding the average kinetic energy of all the molecules in that side of the box.

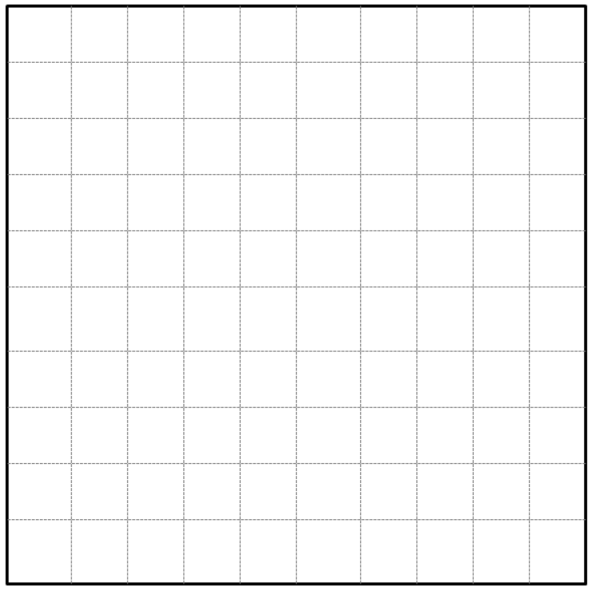
13. Click Start to run the animation and let it run until the time reaches about 50. (Note: you can speed up the simulation by moving the Speed slider to the right.) What happens to the temperatures of the two sides?

14. Once the two sides of the box reach the same temperature, do they both stay at that temperature or does the temperature fluctuate?

15. Did the entropy of the hot gas increase during this simulation? Did the entropy of the cold gas increase? The entropy of the whole system is just the sum of the entropies of the two gases. So did the entropy of the system increase? In other words, did the behavior of this system conform to the entropy version of the Second Law?

16. Real gases don't behave like ideal gases except under certain restrictive conditions (very low density). Instead, the molecules of real gases interact with each other and exchange energy. If a fast-moving molecule collides with a slow-moving molecules is it more likely that the fast-moving molecule will give some energy to the slow-moving molecule, or that the slow-moving molecule will give some energy to the fast-moving molecule? After MANY such interactions, what will happen to the speed of the molecules in the gas?

17. Please sketch a plot of the entropy as a function of time might look like for this system on the graph below. What parameters does the entropy of an ideal gas depend upon?



Historical Objections to Boltzmann's Ideas

Boltzmann originally used the motion of molecules to derive the second law in 1872. This derivation made it appear that the second law is absolute, that the entropy of an isolated system can never decrease. But as we have seen Boltzmann's later ideas about entropy (first presented in 1877) indicate that the second law is only very likely to hold true. In fact, we have seen violations of the second law in the models we have studied.

18. One objection to Boltzmann's theorem was presented by Josef Loschmidt in 1876. He pointed out that the law of Newtonian mechanics are time reversible, which means that they work equally well backwards in time as they do forwards. If a certain set of motions leads to an increase in entropy, then the time-reversed motion will lead to a decrease in entropy. Both sets of motions are allowed by Newton's Laws. One way to produce these time-reversed motions is to reverse the direction of motion of each molecule. The motion of the system after the reversal will be a time-reversed version of the motion before the reversal. To visualize this effect run the HotAndColdIdealGases simulation again. Let the simulation run until the gas reaches equilibrium, then hit the Reverse button. Let the simulation run for longer than you let it run before hitting Reverse. Describe what happens to the gas.

19. This and other objections led Boltzmann to reformulate his interpretation of the Second Law. In 1877 he presented the statistical approach to entropy that we have been examining. He admitted that violations of the second law are possible but argued that such violations would be highly unlikely and would be short-lived in any macroscopic system. Based on what you have seen in the coin flip model and the computer simulations, would you agree that violations of the Second Law are unlikely to occur in a gas with 10^{24} molecules? Are such violations possible?

20. Consider what a radical shift this is in the concept of a "law of nature." Are we really justified in calling the Second Law of Thermodynamics a "Law" if it is just a statement of probability? Defend your answer.

21. Evolution of life on Earth shows a clear tendency to produce more organized (ordered) structures over time. Does this violate the Second Law? If the entropy of all living things on Earth is decreasing over time, what else must be happening according to the Second Law?