Lab 9

Entropy, Temperature, and Heat Flow

Continuing Objectives

6. Be able to make a good graph either in your notebook or with a computer (label, scales, units, dependent, and independent variables).

8. Use a computer to collect and analyze data.

Lab-specific Objectives

1. Understand the statistical explanation of entropy.

2. Learn the relationships between entropy, heat flow, and temperature.

Introduction

In class you have been introduced to a definition of *entropy* based on the number of possible ways to distribute energy within a system. This definition illustrates that entropy S is a measure of probability: the more probable a state, the higher its entropy. In this lab we will explore the concept of *microstates*, *macrostates*, *probability*, *entropy*, the *direction of heat flow*, and *temperature*, all in the context of a simple physical model with which you are already familiar: the Einstein solid. (In this lab we will assume that the energy units of our solid have magnitude one, i.e., $\epsilon = 1$.)

We will start by looking at a small system — in fact, it's a **ridiculously** small system. Our system will be two Einstein solids whose oscillators can exchange energy: Einstein solid **A** consists of a single oscillator, and Einstein solid **B** consists

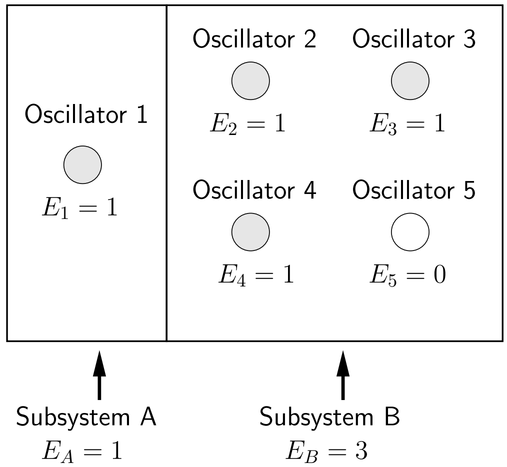
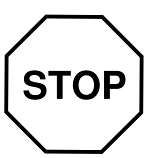


Figure 9.1: An example of a microstate of our small model system. (There are 19 other microstates that are also in the same macrostate with $E_A = 1$.)

of four oscillators. And, to keep things simple, we will initially limit consideration to a system with only four units of energy.

- The *macrostate* of the system is characterized simply by the number of units of energy in subsystem **A** and the number of units of energy in subsystem **B**.
- In a *microstate* description we know exactly how much energy there is in each labeled oscillator.

A specific microstate of this small system of two Einstein solids is illustrated in Figure 9.1. In this microstate there is 1 unit of energy in subsystem **A**, and 3 units of energy in subsystem **B**. We will describe this microstate with the notation [1:1,1,1,0]. The number to the left of the colon gives the number of units of energy in oscillator 1 (i.e., subsystem **A**); the numbers to the right of the colon indicate the energies in each of the oscillators in subsystem **B**.



The *macrostate* of the example microstate [1:1,1,1,0] is $E_A = 1$. Can you think of other arrangements (that is, microstates) that satisfy this macrostate? Write down at least three and explain your results to your instructor or TA.

Energy can be exchanged between the two subsystems via exchanges of energy between individual oscillators. One of the questions we will address is the following: *What is the most likely way that the energy will be distributed between subsystems* **A** *and* **B** *after a large number of random energy-redistributing interactions?*

Prediction

Make a prediction: After many exchanges of energy between the two subsystems, are we more likely to find subsystem **A** with more than one unit of energy, exactly one unit of energy, or less than one unit of energy? Write down your prediction, and a brief justification for your prediction.

Statistical Description of Einstein Solid

[0 : 4, 0, 0, 0] [0 : 0, 4, 0, 0] [0 : 0, 0, 4, 0] [0 : 0, 0, 0, 4] [0 : 3, 1, 0, 0] [0 : 3, 0, 1, 0] [0 : 3, 0, 0, 1] [0 : 1, 3, 0, 0] [0 : 0, 3, 1, 0] [0 : 0, 3, 0, 1]

[0 : 1, 0, 3, 0] [0 : 0, 1, 3, 0] [0 : 0, 0, 3, 1] [0 : 1, 2, 1, 0] [0 : 1, 2, 0, 1] [0 : 0, 2, 1, 1] [0 : 1, 0, 0, 3] [0 : 0, 1, 0, 3] [0 : 0, 0, 1, 3] [0 : 2, 2, 0, 0]

[0 : 2, 0, 2, 0] [0 : 2, 0, 0, 2] [0 : 0, 2, 2, 0] [0 : 0, 2, 0, 2] [0 : 0, 0, 2, 2] [0 : 2, 1, 1, 0] [0 : 2, 1, 0, 1] [0 : 2, 0, 1, 1] [0 : 1, 0, 2, 1] [0 : 0, 1, 2, 1]

[0 : 1, 1, 0, 2] [0 : 1, 0, 1, 2] [0 : 0, 1, 1, 2] [0 : 1, 1, 2, 0] [0 : 1, 1, 1, 1]

[1 : 0, 0, 0, 3] [1 : 3, 0, 0, 0] [1 : 0, 3, 0, 0] [1 : 0, 0, 3, 0] [1 : 2, 1, 0, 0] [1 : 2, 0, 1, 0] [1 : 2, 0, 0, 1] [1 : 1, 2, 0, 0] [1 : 0, 2, 1, 0] [1 : 0, 2, 0, 1]

[1 : 1, 0, 2, 0] [1 : 0, 1, 2, 0] [1 : 0, 0, 2, 1] [1 : 1, 0, 0, 2] [1 : 0, 1, 0, 2] [1 : 0, 0, 1, 2] [1 : 1, 1, 1, 0] [1 : 1, 1, 0, 1] [1 : 1, 0, 1, 1] [1 : 0, 1, 1, 1]

[2 : 2, 0, 0, 0] [2 : 0, 2, 0, 0] [2 : 0, 0, 2, 0] [2 : 0, 0, 0, 2] [2 : 1, 1, 0, 0] [2 : 1, 0, 1, 0] [2 : 1, 0, 0, 1] [2 : 0, 1, 1, 0] [2 : 0, 1, 0, 1] [2 : 0, 0, 1, 1]

[3 : 1, 0, 0, 0] [3 : 0, 1, 0, 0] [3 : 0, 0, 1, 0] [3 : 0, 0, 0, 1] [4 : 0, 0, 0, 0]

Figure 9.2: List of all possible microstates for our small model system.

In Figure 9.2, a list of all 70 possible microstates for the total system described is shown. The number before the colon is the number of units of energy in subsystem **A**.

We have listed every possible microstate of the system with a total of 5 oscillators and 4 units of energy. Fill in the blank entries of Table 9.1 by counting the number of possible microstates that have a given distribution of energy between systems **A** and **B** — we call this number Ω_{AB}.

q_A	q_B	Ω_{AB}
0	4	
1	3	
2	2	
3	1	
4	0	

Table 9.1: Multiplicities of the macrostates of the system with $N_A = 1$, $N_B = 4$, and $q_{\text{total}} = 4$.

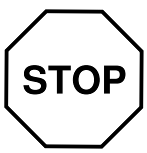
1. Let's assume that the random energy exchanges result in visiting every microstate with equal probability. (This is a *major* assumption in real physical systems, and it's called the *ergodic hypothesis*.) Assuming that this is true, use the data in Table 9.1 to calculate

   (a) the probability that the system will be found in a microstate in which subsystem **A** has $q_A = 2$, $q_A = 3$, or $q_A = 4$. (These are microstates with more energy in subsystem **A** than was the case in our initial microstate.)

   (b) the probability that the system will be found in a microstate in which subsystem **A** has $q_A = 0$. (These are microstates with less energy in subsystem **A** than was the case in our initial microstate.)

   (c) the probability that the system will be found in a microstate in which subsystem **A** has the original energy of $q_A = 1$.

   Question. Based on these probabilities, are you more likely to find subsystem **A** with more than one unit of energy, exactly one unit of energy, or less than one unit of energy? Does this agree with your prediction?



Show your table to your instructor or TA and discuss your results.

In the Supplemental Reading (PDF in the Lab 9 Entropy folder on the netspace), you were introduced to a formula that allows you to calculate the number of microstates of an Einstein solid (or subsystem of an Einstein solid) based on the number of oscillators and the number of units of energy in that solid (or subsystem). This is called the *multiplicity*:

$$\Omega = \frac{(q + N - 1)!}{q!\,(N-1)!}, \tag{9.1}$$

where N is the number of oscillators in the system (or subsystem), and q is the number of energy units.

2. Use Eq. (9.1) to fill in the entries of Table 9.2. The third column, Ω_A, is just the number of ways to distribute the q_A units of energy in subsystem **A** between the N_A oscillators of the subsystem, and the fourth column, Ω_B, is just the number of ways to distribute the q_B units of energy in subsystem **B** between its N_B oscillators. The results for Ω_{AB} in the column on the right should agree with your results in the far right column of Table 9.1, but this time they come from a formula that we can use (with the aid of a computer) for larger systems.

q_A	q_B	Ω_A	Ω_B	$\Omega_{AB} = \Omega_A \times \Omega_B$
0	4			
1	3			
2	2			
3	1			
4	0			

Table 9.2: Multiplicities of the macrostates of the system with $N_A = 1$, $N_B = 4$, and $q_{\text{total}} = 4$. You should perform the calculations to fill in the empty entries of this table "by hand," and then reproduce the table with a computer spreadsheet.

Notice that in our ridiculously small system, no outcome for the distribution of energy (i.e., macrostate) between the two subsystems is certain, nor is any outcome prohibited, but some macrostates are much more likely than others.

Generalization to Systems with Many Oscillators

In this section, you will develop a spreadsheet to explore what happens in a system with many more oscillators than the ridiculously small Einstein solids considered in the previous section. But first you must prepare a computer to do the calculations. Since you will be exploring systems of increasing size and total energy, as much as possible, use absolute referencing for fixed quantities.

3. Open the Excel template in the netspace Lab 09 Entropy folder. You will see it has a section where you can reproduce Table 9.2. You should be able to fill in the first two entries, $q_A = 0$ and $q_B = 4$, and the rest of the cells should be automatically filled by formulas that you have entered. Excel has a built-in function `COMBIN` that will evaluate the multiplicities using Eq. (9.1). The syntax for calculating a multiplicity in Excel:

   $$\Omega = \frac{(q+N-1)!}{q!\,(N-1)!} \quad \text{is} \quad \texttt{COMBIN(Q+N-1,Q)}.$$

   Once you fill in the table, a graph of Ω_{AB} vs. q_A will appear below the data. Print this and put a copy in your notebook.

   Task: Write a sentence or two describing what information you can extract about the system and its preferred macrostates by looking at this graph.

STOP Show your spreadsheet and graph to your instructor or TA.

4. Increase the size of your system by a factor of 10, so that $N_A \to 10$, $N_B \to 40$, and $q_{tot} \to 40$. Fill in the formulae (and copy to complete the columns) in the corresponding section of the spreadsheet. Study the graph of Ω_{AB} vs. q_A for this larger system, and put a copy in your notebook. Make sure to indicate your values for N_A, N_B, and q_{tot} on your graph, and determine the most likely value for q_A, the energy in subsystem **A**, from your data.

5. Increase the size of your system by another factor of 10, so that $N_A \to 100$, $N_B \to 400$, and $q_{\text{tot}} \to 400$. Fill in the formulae (and copy to complete the columns of Ω_A, Ω_B, and Ω_{AB}) in the corresponding section of the spreadsheet. Study this graph of Ω_{AB} vs. q_A for this larger system, and put a copy in your notebook. Comment on the similarities and differences in your three plots of Ω_{AB} vs. q_A.

   Task: Summarize your observations. What trends do you notice as you increase the size if your system and its available energy?

Entropy, Temperature, and Equilibrium

In the previous section, you saw that certain distributions of energy between the two subsystems are much more likely than others, and that the peak in the distribution of probabilities narrows as the size of the system increases. When systems become macroscopic, with $\sim 10^{23}$ particles, the peak becomes incredibly narrow, and there is an extremely well-defined value of q_A that is overwhelmingly favored; this preferred arrangement gives what we know as the *equilibrium* value of the thermal energy of subsystem **A**. But how is all of this related to temperature?

Recall that in class we introduced a definition based on statistical mechanics:

$$\frac{1}{T} = \frac{dS}{dE_{\text{therm}}} \simeq \frac{\Delta S}{\Delta E_{\text{therm}}}, \tag{9.2}$$

where S is the entropy.

Let's start by investigating entropy itself. The entropy of a system is proportional to the logarithm of the multiplicity Ω:

$$S = k_B \ln \Omega. \tag{9.3}$$

Because it is a logarithm, S is much easier to work with on a computer (it's smaller than the incredibly huge multiplicities given by Ω) and it also has the nice property that the entropy of two systems is additive:

$$\begin{aligned} S_{\text{total}} &= k_B \ln \Omega_{AB} \\ &= k_B \ln(\Omega_A \Omega_B) \\ &= k_B (\ln \Omega_A + \ln \Omega_B) \\ &= S_A + S_B. \end{aligned} \tag{9.4}$$

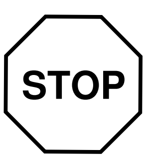
6. For your largest system, there are three more columns in your spreadsheet: one for S_A, one for S_B, and one for S_{total}. Insert formulas into the cells of these columns to calculate values for S_A, S_B, and S_{total}. For this lab, use units in which $k_B \equiv 1$.

7. A graph of S_A vs. q_A and S_B vs. q_A will appear below the multiplicity graph. You should see the entropy curve of S_B vs. q_A "flipped over" so that it is increasing to the left, since that's the direction of increasing q_B. This graph should be similar to the graph displayed in Figure 9.5 of the Supplementary Reading. Paste this graph into your notebook document and use it in the next step.

8. To help you understand the implications of your graph, review Section 9.6 of the Supplementary Reading. On your entropy graph, indicate three regions: **Region I** where energy would spontaneously flow from subsystem **A** to subsystem **B**, **Region II** where energy would spontaneously flow from subsystem **B** to subsystem **A**, and **Region III** where no energy would spontaneously flow.

   Task. Without using the definition of temperature, describe the physical principle that allows you to figure out the spontaneous direction of energy flow.

9. Now study the line for S_{total} on your graph. Does the maximum in S_{total} correspond to the point of no spontaneous energy flow that you identified in the previous step? Put this graph in your lab notebook.



Show your graph to your instructor or TA, and discuss the regions you have identified in the previous two steps.

We can obtain an expression for temperature T from Eq. (9.2):

$$T \simeq \frac{\Delta E_{\text{therm}}}{\Delta S}. \tag{9.5}$$

We will use this relationship to approximate the temperatures in our two subsystems.

10. There are two columns in your spreadsheet, one for T_A and one for T_B. For a given row, or value of q_A, you can approximate the value of the temperature using information from the previous row as follows:

$$T_A \simeq \frac{E_{\text{therm}}(q) - E_{\text{therm}}(q-1)}{S_A(q) - S_A(q-1)}. \tag{9.6}$$

    The numerator is simply the energy level spacing of the Einstein solid, $\epsilon = 1$, and the denominator we can get from the entropy column. (This calculation won't work for the $q_A = 0$ row, since there are no $q - 1$ values to use. For this cell, do not enter a value.)

    A graph with plots of T_A vs. q_A and T_B vs. q_A will appear under the entropy plot. Check the regions where you said energy should flow from subsystem **A** to subsystem **B** — which is larger, T_A or T_B? Check the regions where you said energy should flow from subsystem **B** to subsystem **A** — which is larger, T_A or T_B? How do the values of T_A and T_B compare at the value of q_A that gave a peak in the multiplicity Ω_{AB} (a maximum in S_{total})? Print your graph and include it in your lab notebook.

11. In writing a conclusion for this lab, summarize some of the observations you have made. In particular, consider the graphs you made in Step 7 and analyzed in Step 8. You identified a region (**Region I**) of this graph in which energy would spontaneously flow from subsystem **A** to subsystem **B**. Your conclusion should address the following issues:

    (a) How is the direction of energy flow in **Region I** of your graph connected to the concept of multiplicities of macrostates? Why does energy flow in that particular way? In other words, explain the direction of energy flow without referring to the definition of temperature.

    (b) Use the statistical interpretation of temperature given in Eq. (9.2) to explain why subsystem **A** has a higher temperature than subsystem **B** in **Region I** of your graph. Why does this definition of temperature imply that energy will flow from **A** to **B**?

Reflection

Please reflect on today's lab in your notebook.

Look back at today's lab-specific objectives (beginning of the lab).

1. What activities did you do today that helped understand those topics?
2. How has your understanding of those topics changed through today's lab?