Lab 6

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.

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 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 6.1. In this microstate there is 1 unit of energy in subsystem A, and sub-system B has 3 units of energy. 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.

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

In Figure 6.2, 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.
Figure 6.2: List of all possible microstates for our small model system.

Table 6.1: Multiplicities of the macrostates of the system with \( N_A = 1 \), \( N_B = 4 \), and \( q_{\text{total}} = 4 \).

<table>
<thead>
<tr>
<th>( q_A )</th>
<th>( q_B )</th>
<th>( \Omega_{AB} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td></td>
</tr>
</tbody>
</table>

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 6.1 by counting the number of possible microstates that have a given distribution of energy between systems A and B — we call this number \( \Omega_{AB} \).

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 6.1 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 \( q_A = 1 \).

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
In the Supplemental Reading (PDF on the PHYS 211 Lab Info site), 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:

\[ \Omega = \frac{(q + N - 1)!}{q!(N - 1)!}, \tag{6.1} \]

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

2. Use Eq. (6.1) to fill in the entries of Table 6.2. The third column, \( \Omega_A \), 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, \( \Omega_B \), 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 \( \Omega_{AB} \) in the column on the right should agree with your results in the far right column of Table 6.1, but this time they come from a formula that we can use (with the aid of a computer) for larger systems.

Notice that in our ridiculously small system, no outcome for the distribution of energy between the two subsystems is certain, nor is any outcome prohibited, but some distributions 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 ‘teach’ a computer to do the calculations.

3. Develop an Excel spreadsheet that reproduces Table 6.2. 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 \( \text{COMBIN} \) that will evaluate the multiplicities using Eq. (6.1). The syntax for calculating a multiplicity \( \Omega \) is \( \text{COMBIN}(Q+N-1,Q) \).

Make a graph of \( \Omega_{AB} \) vs. \( q_A \), and put a copy in your notebook. Make sure to indicate your values for \( N_A, N_B \), and \( q \) on or beside your 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 \( N_A \rightarrow 10, N_B \rightarrow 40 \), and \( q_{\text{tot}} \rightarrow 40 \), and rerun your spreadsheet calculations. Make a graph of \( \Omega_{AB} \) 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 \( q_{\text{tot}} \) 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 \( N_A \rightarrow 100, N_B \rightarrow 400 \), and \( q_{\text{tot}} \rightarrow 400 \), and rerun your spreadsheet. Make a graph of \( \Omega_{AB} \) 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 \( \Omega_{AB} \) vs. \( q_A \).

As you have seen, multiplicities grow very large for any but the very smallest systems.

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:

\[
\frac{1}{T} = \frac{dS}{dE_{\text{therm}}} \simeq \frac{\Delta S}{\Delta E_{\text{therm}}},
\]

(6.2)

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 \( \Omega \):

\[
S = k_B \ln \Omega.
\]

(6.3)

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 \( \Omega \)) and it also has the nice property that the entropy of two systems is additive:

\[
S_{\text{total}} = k_B \ln \Omega_{AB} = k_B \ln(\Omega_A \Omega_B) = k_B (\ln \Omega_A + \ln \Omega_B) = S_A + S_B.
\]

(6.4)

7. Add three more columns for your spreadsheet: one for \( S_A \), one for \( S_B \), and one for \( S_{\text{total}} \). Insert formulas into the cells of these columns to calculate values for \( S_A \), \( S_B \), and \( S_{\text{total}} \). For this lab, use units in which \( k_B \equiv 1 \).

8. Make a graph of \( S_A \) vs. \( q_A \), and on this same graph include a plot of \( S_B \) vs. \( q_A \). 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.

9. 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.

10. Now add a plot of \( S_{\text{total}} \) to your previous graph. Does the maximum in \( S_{\text{total}} \) correspond to the point of no spontaneous energy flow that you identified in the previous step? Put this graph in your lab notebook.

STOP

Show your graph to your instructor or TA, and discuss the regions you have identified in the previous two steps.
We can get an expression for temperature $T$ from Eq. (6.2):

$$\Delta S \rightleftharpoons \Delta E_{\text{therm}}.$$  \hspace{1cm} (6.5)

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

11. Add 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:

$$T_A \rightleftharpoons \frac{E_{\text{therm}}(q) - E_{\text{therm}}(q - 1)}{S_A(q) - S_A(q - 1)}.$$  \hspace{1cm} (6.6)

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, enter the value $T_A = 0$.)

Make a graph with plots of $T_A$ vs. $q_A$ and $T_B$ vs. $q_A$. 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 $\Omega_{AB}$ (a maximum in $S_{\text{total}}$)? Copy your graph and include it in your lab notebook.

12. In writing a conclusion for this lab, summarize some of the observations you have made. In particular, consider the graphs you made in Step 8 and analyzed in Step 9. 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?

(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?