Using *StatMech* to Calculate Macrostate Multiplicities
Spring 2024

Introduction

The following exercise uses Moore's *StatMech* program to automate the creation of macropartition tables for Einstein solids.

Experiment

1. *Starting the program*

You can run Moore's *StatMech* program directly from his *Six Ideas That Shaped Physics* website using the following link: http://physics.pomona.edu/sixideas/StatMech/

2. *Exercises*

Read the description of the program and its operation in section T2.6 (p. 27). Do the following exercises:

A. (a) When you start *StatMech*, you will notice that the default setting is for the case $N_A = N_B = 1$ and $U = 6\varepsilon$. Examine the data produced and verify that the program reproduces table T2.1. Also look at the graph of the macropartition probabilities.

(b) Click the **×10** button in the upper part of the program window to multiply each variable by 10. Click the **Update Table** button to examine the case where $N_A = N_B = 10$ and $U = 60\varepsilon$. What is different about the table (*besides the fact that it is longer*)? How has the graph changed?

(c) Now scale everything up by a factor of 10 again, to $N_A = N_B = 100$ and $U = 600\varepsilon$. (Note that the program now begins to arrange the table into *bins* of macropartitions, since it is limited to displaying 100 lines of data.) What else has changed about the table? How has the graph changed?

B. (a) Use *StatMech* to generate a macropartition table for two Einstein solids in contact where $N_A = N_B = 5$ and $U = 20\varepsilon$ and answer the following questions.

(1) How many total microstates are available to the system?

(2) Which is the most probably macropartition, and how many microstates are available to the system in this macropartition?

(3) What is the average energy per atom (U/N) in each solid in this macropartition?

(4) What range of values of the ratio U_A/U corresponds to macropartitions whose probabilities are at least one-half as large as the most probable macropartition? (*Hint*: *Move your cursor along the graph and estimate the values of* U_A/U.)

(b) Answer the same set of questions as in (a) for the case $N_A = N_B = 50$ and $U = 200\varepsilon$. Note that all variables are scaled up by a factor of ten, so that the energy per atom remains fixed.

(c) Describe any trends you see in how the answers to these questions change as the system becomes larger.

C. Run the *StatMech* program for two Einstein solids in contact with $N_A = N_B = 100$ and $U = 200\varepsilon$ and note the message **U was adjusted to yield equal bin sizes**. Answer the following questions:

(1) Recall from the book's description of the program that the final column of the table lists the number of microstates for each macrostate expressed as a fraction of the total number accessible microstates. According to the fundamental assumption of statistical mechanics, this is also the probability of that macrostate's occurring. Any macropartition that has a probability above 0.0001 means that these macrostates comprise about 99.98% of the system's total microstates.

Look at the *Bin Probability* column of the table and determine the range of values that U_A is likely to have more than 99.98% of the time.

(2) How many times more likely is the system to be found in the center macropartition where $U_A = 100\varepsilon$ and $U_B = 99\varepsilon$, than in the extreme macropartition where $U_A = 0$ and $U_B = 199\varepsilon$? *Hint: Calculate the ratio of the probability of the center macropartition to that of the extreme macropartition*.

(3) Change the program setting for the number of bins from two to *one* macropartition and update the table. Look at the graph and you will see that now only the first half of the graph is displayed, from $U_A = 0$ to $U_A = 99\varepsilon$.

If U_A were initially to have the extreme value 0, how many times more likely is it to move to the next macropartition ($U_A = 1$) nearer the center than to remain in the extreme one? *Hint: Again, calculate the ratio of probabilities*.