Using *StatMech* to Calculate Entropy, Temperature and Heat Capacity

Spring 2024

Introduction

In the following exercises you will use Moore's *StatMech* program to calculate the entropy, temperature and heat capacity of a set of Einstein solids.

Experiment

1. *Starting the program*

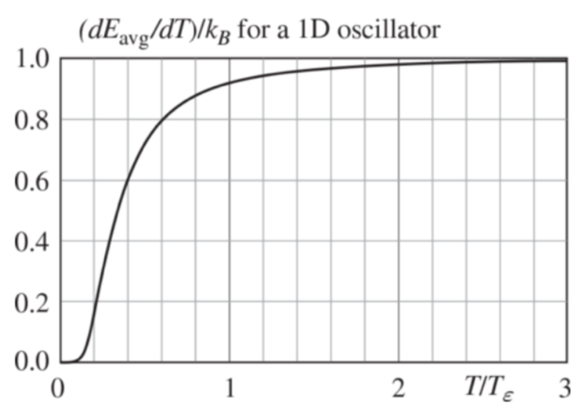
You can run Moore's StatMech program directly from *his Six Ideas That Shaped Physics* website using the following link: http://physics.pomona.edu/sixideas/StatMech/

2. *Setting up the number of oscillators*

In what follows it shall prove to be useful to specify how many independent oscillators a given Einstein solid has, rather than the number of atoms N. Recall that each atom can move in three independent directions, so an Einstein solid with N atoms has $H = 3N$ independent oscillators. What matters to us is that you can set the number of oscillators H in the two solids by selecting the drop-down menu on the upper left corner of *StatMech*.

3. *Exercises*

A. Use *StatMech* to create the macropartition table for a system consisting of two Einstein solids with $H_A = H_B = 50$ and $U = 1000\varepsilon$. Note that in this case the number of oscillators in each solid is the same.
   - (a) Identify the most likely macropartition of the combined system.
   - (b) What are the entropies of the combined system, solid *A* and solid *B*? Quote your answers in units of k_B. Can you find any macropartitions with a larger total entropy? Are there any macropartitions where the entropy of solid *A* is larger than in the most likely macropartition?
   - (c) Use the definition of temperature that you have seen in class to separately estimate the temperature of solids *A* and solid B in the most likely macropartition. *Hint: Recall how you calculated derivatives in Lab 2 – The Potential Field of an Electric Dipole*. Note that you can only calculate the temperature in units of ε/k_B. How do the two temperatures compare with each other?
   - (d) Repeat step (c) with a different macropartition (not the most likely one.) Are the temperatures the same? If not, which one is larger, the one of the solid with the largest or the smallest internal energy?
   - (e) Calculate the ratio T/T_ε, where $T_\varepsilon = \varepsilon/k_B$ is the solid's Einstein temperature (see equation T4.38.) Do you expect the solid to behave "classically"? Using the attached figure, predict what the heat capacity of the solid should be.
   - (f) Estimate the heat capacity of the system directly, namely, by adding and/or subtracting energy from the system. Is your estimate close to your answer in part (e)?



B. Repeat exercise A but use this time two Einstein solids with $H_A = 20, H_B = 80$, and $U = 1000\varepsilon$. In part (b), you can skip all but the first question. Observe that in this case the number of oscillators in each solid is *not* the same. For each of the parts, (a) through (f), comment on what is common and different in your answers to exercises A and B.

C. Repeat exercise A but use this time two Einstein solids with $H_A = H_B = 500$, and $U = 100\varepsilon$. In part (b), you can skip all but the first question. Note that in this case the number of oscillators in each solid is again the same. For each of the parts, (a) through (f), comment on what is common and different in your answers to exercises A and C.

4. *Discussion*

Discuss the most important/relevant observations you have made, particularly in regard to the equilibrium properties of the system and the relation between internal energy and temperature. Do your results match the theoretical predictions of the solid's heat capacity?

Equations needed:

Definition of entropy: $S = k_B \ln \Omega$

Definition of temperature: $\frac{1}{T} = \frac{\partial S}{\partial U} = \frac{1}{\varepsilon}\frac{\partial S}{\partial q}$, where $q = U/\varepsilon$.

Definition of specific heat: $c = \frac{\partial U}{\partial T}$