Guided Inquiry Worksheet 2:

Interacting Einstein Solids

&

Entropy

According to the fundamental assumption of statistical mechanics,

**AT EQUILIBRIUM,
ALL ALLOWED MICROSTATES OF AN
ISOLATED SYSTEM ARE EQUALLY LIKELY**

When we consider interacting systems, some energy divisions or *macropartitions* have more *microstates* corresponding to them than others (i.e. they offer more microscopic arrangements). These macropartitions are more probable than those with fewer microstates.

So …

**AT EQUILIBRIUM,
NOT ALL MACROPARTITIONS ARE EQUALLY LIKELY**

Activity 1: Two Interacting Tiny Einstein Solids

*Consider two interacting Einstein solids A and B,
each with three oscillators. The combined system of A and B
is isolated with a total of three quanta of energy*

1.1) What does it mean for two objects to "interact"?

This system was considered in "Worksheet 1: Activity 2". In that activity, we constructed the following table, showing the 4 possible *macropartitions* of the system:

q_A	q_B	$\Omega_A (q_A)$	$\Omega_B (q_A)$	$\Omega_{total} (q_A)$
0	3	1	10	10
1	2	3	6	18
2	1	6	3	18
3	0	10	1	10
				56

We concluded that although all 56 microstates of the isolated system are equally likely, the macropartition corresponding to 1 unit of energy in solid A has a probability of 18/56 = 32%, while the macropartition with no energy in solid A has a probability of only 10/56 = 18%.

1.2) Using the definition of *entropy* given in class, $S = k \ln \Omega$, complete the following table for this system:

Keep entropies in units of k

q_A	q_B	S_A	S_B	S_{total}	Prob
0	3		2.30 k		18%
1	2				32%
2	1				32%
3	0				18%

Assume that these two solids are initially in a state that has all of the energy in solid A, (i.e. $q_A (t = 0) = 3$ and $q_B (t = 0) = 0$). The two solids are then brought into contact and allowed to interact.

1.3) What will happen to the system as time evolves and A & B interact? Explain fully.

1.4) Based on your explanation above, draw a sketch graph of your prediction for the number of quanta in solid A as a function of time:

q_A

t
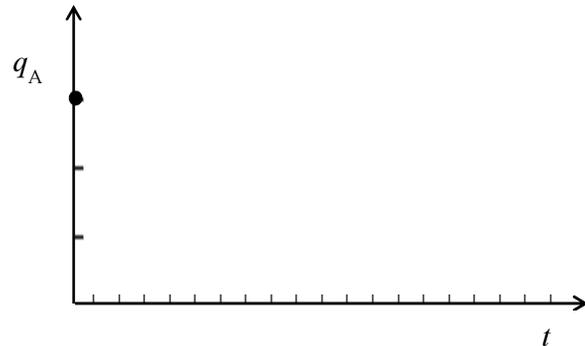
Explain your reasoning:

Is it easy to see the point at which equilibrium is reached?
If so, indicate this point on your sketch above. If not, discuss.

Suppose that we allow our two solids to interact for a long time (such that any effect of the initial arrangement of energy is gone, and equilibrium is reached). We then make regular measurements of the energy contents of each solid over a long period of time.

1.5) Sketch the **energy histograms** for solids A and B built up over a long period of time from the onset of equilibrium:
(label the axes appropriately)

A :   B :

q_A q_B
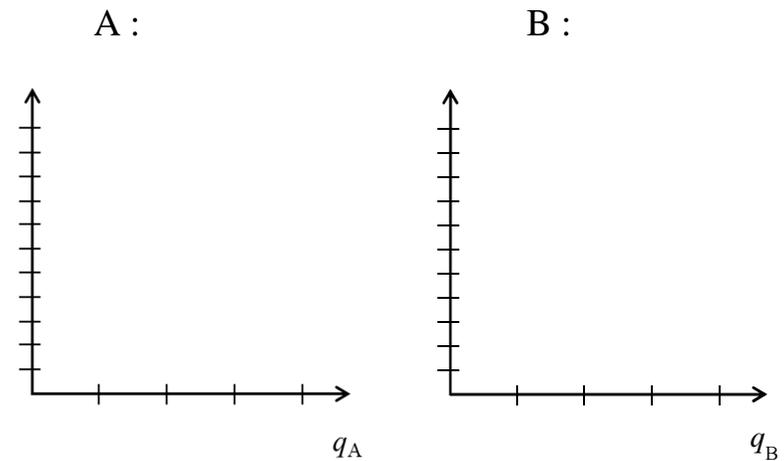
Using the fundamental assumption, we can simulate interaction at equilibrium by allowing energy to randomly distribute itself over the combined system of A and B in such a way that all microstates are treated equally. We will use such an applet to investigate the behaviour of our system of two tiny Einstein solids and to test our earlier predictions. Open **No2_TwoInteractingEinsteinSolids.jar** and edit the fields to correspond to the situation currently under consideration.

1.6) **Before pressing "Evolve"**

i) Compare your table (**1.2**) with the applet's table. Do they agree?

ii) … select the initial condition with all of the energy in solid A. How is this initial condition displayed in the applet's entropy graph?

1.7) **Now press "Evolve"**

i) Spend some time exploring the output. Make sure you can explain exactly what is shown in each frame.
(check the "display boxes" for more output)

ii) Does your earlier prediction in (**1.4**) agree with the output of this applet? If not, how does it differ?

(you may need to reset the simulation and then press "Evolve" with the energy evolution window displayed)

iii) Why does it only make sense to compare the applet with your prediction for the period after equilibrium is reached?

1.8) Now, answer the following questions based on the applet's output:

i) Does entropy ever decrease in this system? Explain.

ii) Is the 2nd Law of Thermodynamics violated? Explain.

1.9) i) Study the applet's energy histograms. Do they agree with your predictions in (**1.5**). If not, how do they differ?

ii) You should see reasonable agreement between analytic predictions (black markers) and the simulation's energy histograms. How are the analytic predictions determined?

Pause the applet and confirm your answer above by calculating one of the analytic predictions (show all working):

(right click the mouse with the cursor over a marker and select "Analyze data" to view marker co-ordinates)

iii) Can you see the effect of the initial conditions in the histograms? Explain.

iv) Clear the histograms and allow them to build up again. Do you see the effect of the initial conditions now? Explain.

v) What happens to the histograms after the system is allowed to evolve for a long period of time? Be specific.

Activity 2: Two Interacting Small Einstein Solids

Consider the somewhat larger system of
10 oscillators in solid A and 30 oscillators in solid B,
sharing a total of 48 quanta of energy

2.1) Use the applet to determine the entropies of each macropartition.

      i) Which macropartition is the most probable?
      (use the graph to estimate it by eye, and then the table to confirm the estimate)

What is the total entropy and probability of this macropartition?

      ii) Which macropartition is the least probable?
      What is its total entropy and probability?

(the applet may display a probability of zero for some macropartitions, but this is simply due to the limited
number of digits in the display- use the entropy values to compute such probabilities)

    iii) Calculate the ratio of the probabilities of the most likely and
least likely macropartitions? Comment on the result.

2.2) If the system is initially in a state with all of its energy in solid A,
sketch a graph of the energy content of A as time evolves:

q_A

t

Indicate the point at which equilibrium is reached

Now, use the applet to investigate this system's evolution from its initial state with all of the energy in solid A.

2.3) i) Are your predictions confirmed? If not, how do they differ?

    ii) What do you notice about the evolution of the system's energy
content? Does the system approach a single macropartition?

iii) In what way(s) is the behaviour of this system a) similar to, and b) different from, that observed for the smaller system in Activity 1? Remember to consider the energy histograms too.

a) Similar:

b) Different:

iv) Does entropy ever decrease in this system?

v) Has the 2nd Law of Thermodynamics been violated? Explain.

Activity 3: Two Interacting Medium Einstein Solids

Consider the somewhat larger system of
100 oscillators in solid A and 300 oscillators in solid B,
sharing a total of 480 quanta of energy

3.1) Use the applet to determine the entropies of each macropartition.

        i) Which macropartition is the most probable?

What is the total entropy and probability of this macropartition?

        ii) Which macropartition is the least probable?
          What is its total entropy and probability?

(you will need to work with logs or else your calculator will simply return a result of zero)

    iii) Calculate the ratio of the probabilities of the most likely and
           least likely macropartitions? Comment on the result.

3.2) If the system is initially in a state with all of its energy in solid A, sketch a graph of the energy content of A as time evolves:

Indicate the point at which equilibrium is reached

Now, use the applet to investigate this system's evolution from its initial state with all of the energy in solid A.

3.3) i) Are your predictions confirmed? If not, how do they differ?

    ii) What do you notice about the evolution of the system's energy content? Does the system approach a single macropartition?

iii) In what way(s) is the behaviour of this system a) similar to, and
b) different from, that observed in Activities 1 & 2?
Remember to consider the energy histograms too.

a) Similar:

b) Different:

iv) Does entropy ever decrease in this system?

v) Has the 2nd Law of Thermodynamics been violated? Explain.

Activity 4: Effect of System Size

Use the applet to investigate the effect of system size on the equilibrium state of an isolated system of two Einstein solids

4.1) Using the results of Activities 1, 2 & 3, comment on the effect that system size has on an isolated system's equilibrium state.

i) In particular, how is equilibrium different for medium systems compared to very small systems? Include sketch graphs.

Very Small System	Medium System

q_A t q_A t
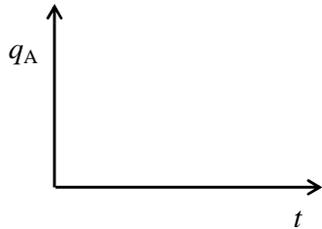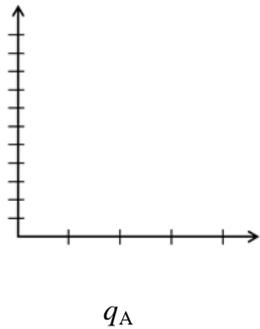
Energy Histogram of A	Energy Histogram of A
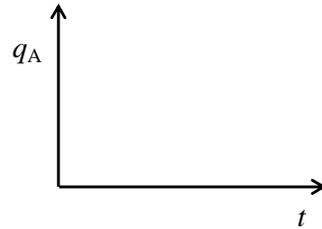
q_A q_A
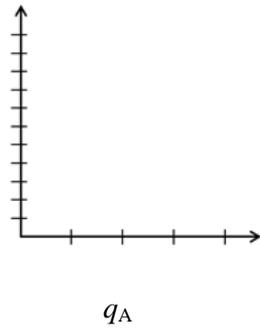
ii) How would you define equilibrium in a way that makes sense for tiny, small and medium sized systems? Your response should be a definition for equilibrium that you would happily defend!

iii) Unfortunately, it is not possible to simulate a system of "Avogadro-size". However, based on your observations of medium-sized systems, what can you conclude for really large systems containing Avogadro's number of particles and energy units?