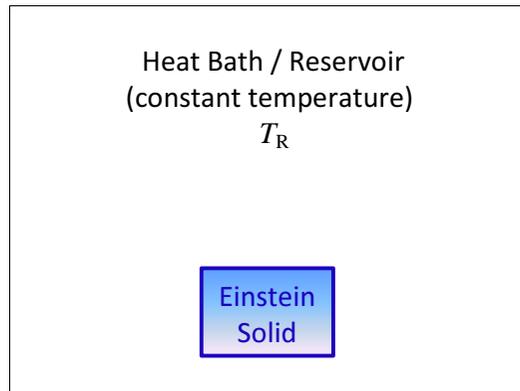


Guided Inquiry Worksheet 4:

Einstein Solid & Heat Bath / Reservoir

In this activity, we will consider the case of an Einstein solid in thermal contact with a *large reservoir* or *heat bath*. Energy is continually exchanged between the bath and the solid, but the bath is so large that its temperature remains constant.

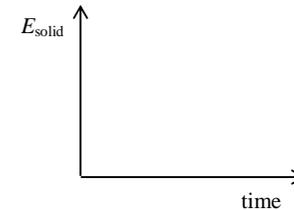
Considering a system (the Einstein solid in this case) under such conditions (energy exchange with a bath of constant temperature, while volume and particle number are held fixed) constitutes the *canonical ensemble* (also known as the *TVN ensemble*).



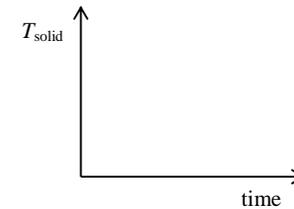
Although neither the solid nor the bath is isolated, the composite system of solid and bath is, and so the equal a priori probability postulate can be applied to the combined solid-bath system.

Assuming that the Einstein solid initially has no energy, answer the following questions:

A) How does the solid's energy change with time (if at all)?
(Include a sketch graph)



B) How does the solid's temperature change with time (if at all)?
(Include a sketch graph)



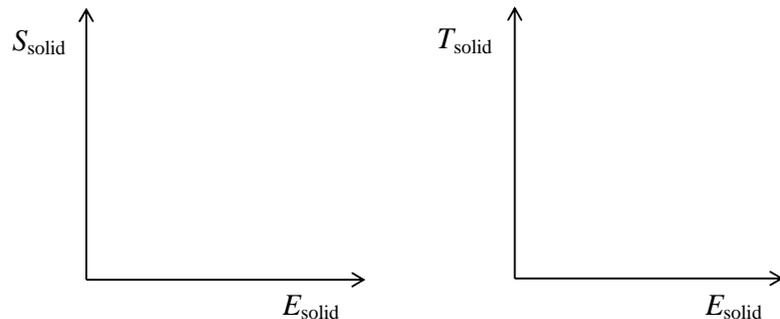
C) Is equilibrium ever reached?
If so, indicate on your graphs the point at which equilibrium is attained. How would you characterise equilibrium?

Activity 1: Small Einstein Solid & Heat Bath

Consider an Einstein solid containing 25 oscillators in contact with a large heat bath of constant temperature $T_R = 2.5\varepsilon/k$ (where ε is the energy spacing between the single oscillator states)

1.1) How many energy macrostates are available to the Einstein solid? Explain.

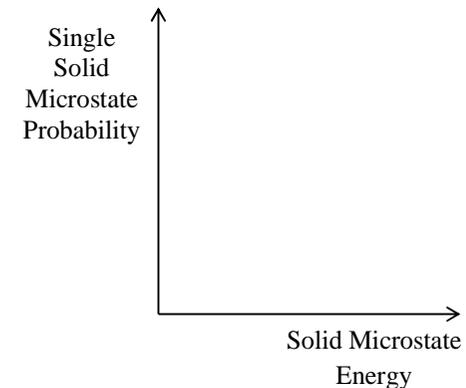
1.2) Draw sketch graphs of the entropy and temperature of the Einstein solid energy macrostates.



1.3) At equilibrium, would a solid microstate corresponding to a large solid energy be more, less or equally likely to a solid microstate corresponding to a small solid energy? Explain.

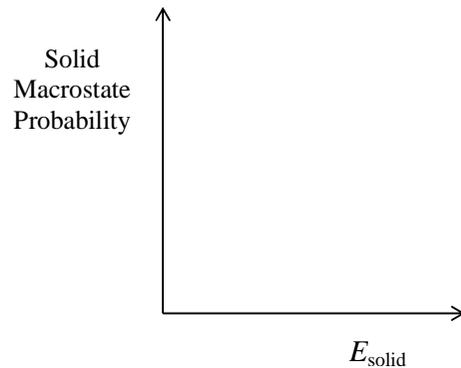
Is your answer above in violation of the Fundamental Assumption of Statistical Mechanics? Explain.

Draw a sketch graph showing the probability of single Einstein solid microstates (at equilibrium) as a function of the microstate energy:



Indicate on the graph above how this probability would change if the heat bath in contact with the Einstein solid had a higher temperature (label your sketch graphs clearly).

1.4) The previous graph showed the equilibrium probability of single Einstein solid microstates. Now, draw a sketch graph of the equilibrium probability of the Einstein solid having a particular energy content (i.e. the probability of each Einstein solid macrostate).



Explain exactly how you arrived at this prediction:

Indicate on the graph above how this probability is affected by a higher heat bath temperature. Explain your reasoning.

How would this manifest itself experimentally?

Now, turn back to predictions **A** and **B**. Are they consistent with the probability distribution drawn above?

Based on your earlier responses, which of the statements below best describe the equilibrium state of the solid? Explain all responses.

At equilibrium ...

- ... the solid energy is constant
- ... all solid energies are equally likely
- ... the average solid energy is constant, while the solid energy fluctuates about this average
- ... the solid temperature is constant
- ... the solid temperature fluctuates about the value of the heat bath's temperature

Now, consider the EJS simulation No4_EinsteinSolidHeatBath.jar.

- You are able to adjust the temperature of the heat bath by editing the temperature field (remember to press RETURN for changes to take effect) or else by moving the corresponding slider (note the colour of the background).
- The Einstein solid initially contains no energy and so its temperature is very low (note the colour). You can change its size by adjusting the “number of oscillators” slider.
- Press PLAY to allow the heat bath and solid to interact (i.e. exchange energy). What do you notice about the colours (temperatures) of the heat bath and solid?

1.5) Use the simulation to confirm your earlier predictions for the entropy, temperature and macrostate probability (**1.2** and **1.4**). You will need to check the boxes in the “Display” panel. Are these three plots in agreement? If not, explain the discrepancies.

1.6) By checking the “Show System Evolution” box, you are able to observe the solid’s energy and temperature evolution. Also shown, are their average values and standard deviations.

Are these in agreement with your earlier statements regarding equilibrium? Explain.

NOW EXIT THE SIMULATION

You should have observed that the Einstein solid energy and temperature fluctuate about well-defined averages and that the standard deviations also settle to well-defined values at equilibrium.

1.7) Predict how the heat bath temperature and Einstein solid size affect the Einstein solid energy and temperature averages and standard deviations (**don't use the simulation**).

Effect of heat bath temperature:

Predictions for averages:

Predictions for standard deviations:

Effect of Einstein solid size:

Predictions for averages:

Predictions for standard deviations:

1.8) Now use the simulation to test your predictions in **1.7** with the aid of the tables below. Describe your findings and note any discrepancies with your earlier predictions.

Effect of heat bath temperature:

$N =$

| T_R | $\langle E_{\text{solid}} \rangle$ | σ_E | $\langle T_{\text{solid}} \rangle$ | σ_T | $\sigma_E / \langle E \rangle$ | $\sigma_T / \langle T \rangle$ |
|-------|------------------------------------|------------|------------------------------------|------------|--------------------------------|--------------------------------|
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Findings and explanation of discrepancies with predictions:

Effect of Einstein solid size:

$T_R =$

| N | $\langle E_{\text{solid}} \rangle$ | σ_E | $\langle T_{\text{solid}} \rangle$ | σ_T | $\sigma_E / \langle E \rangle$ | $\sigma_T / \langle T \rangle$ |
|-----|------------------------------------|------------|------------------------------------|------------|--------------------------------|--------------------------------|
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Findings and explanation of discrepancies with predictions:

1.9) Based on the observed Einstein solid size dependence, what do you expect for a really large macroscopic solid in contact with a heat bath?