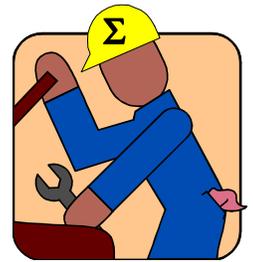


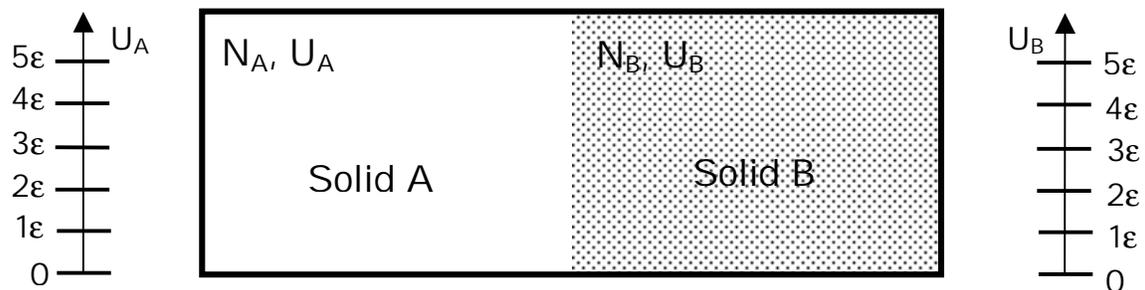
Fundamentals of Statistical Mechanics and the Boltzmann Equation



Name: _____

Section: _____ TA: _____

Lab Date: _____



Exercise #1: COUNTING MICROSTATES

In the first 'experiment' in this laboratory, you will use a model of two 'Einstein Solids' in thermal contact to evaluate the distribution of microstates in a closed thermodynamic system. Recall that in the Einstein model of the solid, the allowed energy levels are quantized with an equal energy spacing of ϵ . In class you considered the 1D version of this model system, but in this laboratory you will consider the slightly more complicated 3D version of the Einstein solid. The difference between the 1D and 3D versions of the Einstein model is simply that each particle has 3 spatial degrees of freedom (x, y, and z) in the 3D Einstein solid (as opposed to only 1 spatial degree of freedom in the 1D Einstein solid), and thus the total number of oscillators in an N particle system is 3N (compared to only N oscillators in the 1D solid). Consequently, in the 3D Einstein solid, the total number of microstates, $\Omega(N, q)$, associated with the macrostate having N particles and a total energy $U=q\epsilon$ is given by:

$$\Omega(N, q) = \frac{(q + 3N - 1)!}{q!(3N - 1)!}$$

Question #1: Consider a 3D Einstein solid system with $N=1$ particle (3 independent oscillators) and total energy $U = 3\varepsilon$. How many microstates are associated with this macrostate?

What is the entropy associated with this macrostate?

For this ($N=1, U=3\varepsilon$) macrostate above, write out all the microstates in the form (q_1, q_2, q_3) , where q_i is the energy level of the i th oscillator (one of the microstates is given as an example):

Possible microstates, (q_1, q_2, q_3) : $(0, 0, 3)$,

Question #2: Now, consider two Einstein solids (A and B) in thermal contact with $N_A=1, N_B=1$, and $U=6\varepsilon$. Write out the distribution of states among the various configurations (macropartitions) by completing the table below (the first is given):

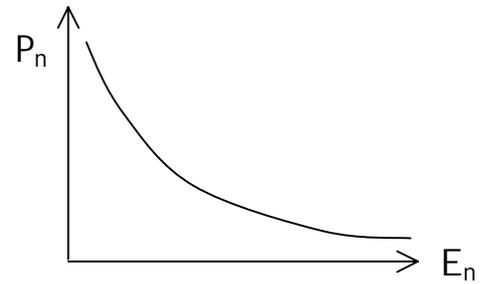
Configuration (Macro-partition)	Energy in solid A U_A (= $q_A \varepsilon$)	Energy in solid B U_B (= $q_B \varepsilon$)	# of micro- states in solid A $\Omega_A =$ $\Omega(N_A, q_A)$	# of micro- states in solid B $\Omega_B =$ $\Omega(N_B, q_B)$	Total # of micro- states in configur- ation $\Omega_{AB} = \Omega_A * \Omega_B$	Percentage of total microstates in configur- ation $\Omega_{AB} / \Omega_{AB}^{total}$
1	0ε	6ε	1	28	28	6%
2	1ε	5ε				
3	2ε	4ε				
4	3ε	3ε				
5	4ε	2ε				
6	5ε	1ε				
7	6ε	0ε				
$\Omega_{AB}^{total} =$					462	

What is the 'equilibrium' (i.e., most probable) configuration for this system?

What is the probability that this system will "fluctuate" at some particular time into a nonequilibrium configuration in which all the energy is in one solid or the other?

Exercise #2: THE BOLTZMANN DISTRIBUTION

In the second 'experiment' in this laboratory, you will use a simulation of the 1D Einstein model to study the important Boltzmann distribution of states for a small system in thermal equilibrium with a very large (reservoir) system. For a sufficiently large reservoir, the Boltzmann distribution is given by,



$$P_n = C e^{-E_n / k_B T}$$

This equation means that the probability of finding a particle in the n th state is proportional to the exponential of $-E$ (minus the state's energy) divided by the product of k_B (Boltzmann's constant) and T (the temperature in degrees Kelvin).

Question #3: Consider an Einstein solid in thermal contact with a reservoir. In the table below, write the ratio P_2/P_1 , i.e., the ratio of the probability for finding a particle with an energy E_2 , to that for finding a particle with an energy $E_1 = k_B T$.

$E_2 (k_B T)$	P_2/P_1
0.1	
0.5	
1	1
2	
3	

Sketch below your results for P_2/P_1 as a function of E_2 . Is this what you expect?

