Discussion 3

Name and section: ____________________

1. Consider a lattice with N sites and n green particles. Consider another lattice, adjacent to the first, with M sites and m red particles. Assume that the green and red particles cannot switch lattices. This is state A.

   (a) What is the total number of configurations W_A of the system in state A?

$$\begin{aligned} W_A &= \binom{N}{n}\binom{M}{m} \\ &= \frac{N!}{n!(N-n)!}\frac{M!}{m!(M-m)!} \end{aligned}$$

   (b) Now assume that all $N+M$ sites are available to all the green and red particles. The particles remain distinguishable by their color. This is state B. Now what is the total number of configurations W_B of the system?

$$W_B = \frac{(N+M)!}{n!m!(N+M-m-n)!}$$

   Now take $N = M$ and $n = m$ for the following two problems.

   (c) Using Stirling's approximation ($N! \sim N^N/\mathrm{e}^N$), what is the ratio of W_A/W_B?

$$\begin{aligned} W_A &\to \left(\frac{N!}{n!(N-n)!}\right)^2 \\ &\to \left(\frac{N^N/\mathrm{e}^N}{(n^n/\mathrm{e}^n)[(N-n)^{N-n}/\mathrm{e}^{N-n}]}\right)^2 \\ &= \frac{N^{2N}}{n^{2n}(N-n)^{2N-2n}} \\ W_B &\to \frac{(2N!)}{(n!)^2(2N-2n)!} \\ &\to \frac{(2N)^{2N}/\mathrm{e}^{2N}}{(n^{2n}/\mathrm{e}^{2n})[(2N-2n)^{2N-2n}/\mathrm{e}^{2N-2n}]} \\ &= \frac{(2N)^{2N}}{n^{2n}(2N-2n)^{2N-2n}} \\ \frac{W_A}{W_B} &= \frac{\frac{N^{2N}}{n^{2n}(N-n)^{2N-2n}}}{\frac{(2N)^{2N}}{n^{2n}(2N-2n)^{2N-2n}}} \\ &= \frac{2^{2N-2n}}{2^{2N}} \\ &\boxed{\frac{W_A}{W_B} = \frac{1}{4^n}} \end{aligned}$$

(d) Which state, A or B, has the greatest entropy? Calculate the entropy difference given by

$$\Delta S = S_A - S_B = -k_B \ln \frac{W_A}{W_B}.$$

B has greater entropy.

$$\Delta S = -k_B \ln \frac{1}{4^n}$$
$$\boxed{\Delta S = 2nk_B \ln 2}$$

2. Consider two systems, A and B. System A has $N_A = 10$ particles and system B has $N_B = 4$ particles. Each particle has two possible energies, $\varepsilon = 0$ or $\varepsilon = 1$. Suppose that system A starts with $n_A = 2$ particles with $\varepsilon = 1$ and $(N_A - n_A)$ particles with $\varepsilon = 0$ (so system A energy $U_A = 2$) and system B starts with $n_B = 2$ particles with $\varepsilon = 1$ and $(N_B - n_B)$ particles with $\varepsilon = 0$ (system B energy $U_B = 2$ also). This situation is shown in fig. 1. The two systems are brought in thermal contact and the total energy $U = U_A + U_B$ is conserved.

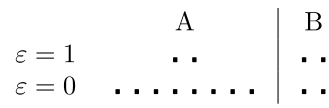

Figure 1: Depiction of the initial configuration of systems A and B before thermal equilibration

(a) What are all possible configurations of this system if energy can pass between A and B, but particles cannot? Draw them in the figure below.

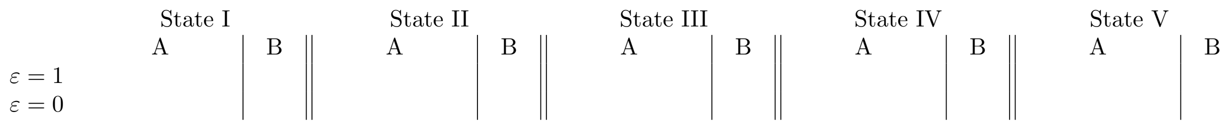

Figure 2: All possible configurations of the system following thermal contact

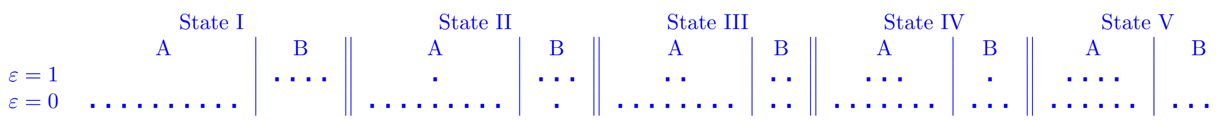

Figure 3: Answer of all possible configurations of the system following thermal contact

(b) What are the multiplicities of each system in each of the states drawn above? What are the overall multiplicities of each state?

State	W
I	1
II	40
III	270
IV	480
V	210

(c) Based on the multiplicities, which is the most likely state?

The most likely state is state IV because it has the highest multiplicity.

(d) What are the probabilities of finding a particle with energy $\varepsilon = 0$ or $\varepsilon = 1$ for each system in each of the states above? For example, in system B in fig. 1, $p_0 = \frac{1}{2}$ and $p_1 = \frac{1}{2}$.

	State I		State II		State III		State IV		State V	
	A	B	A	B	A	B	A	B	A	B
p_0	1	0	0.9	0.25	0.8	0.5	0.7	0.75	0.6	1
p_1	0	1	0.1	0.75	0.2	0.5	0.3	0.25	0.4	0

(e) Is there any relationship between the probabilities calculated in part (d) and the most likely state found in (c)?

Yes: the probabilities between systems is most similar in state IV which is also the state with highest multiplicity.

(f) Since there is only exchange of energy and no exchange of particles between systems A and B (i.e., N_A and N_B are fixed), W_A is a function only of the variable n_A and W_B is a function only of the variable n_B, the numbers of particles in the $\varepsilon = 1$ level in systems A and B respectively. The total multiplicity $W(n_A, n_B) = W_A(n_A)W_B(n_B)$ is a multidimensional function. Write down an expression for $\ln W$ and its total differential $\mathrm{d}\ln W$ in terms of $\mathrm{d}n_A$ and $\mathrm{d}n_B$.

$$\begin{aligned} W(n_A, n_B) &= \binom{N_A}{n_A}\binom{N_B}{n_B} \\ \ln W(n_A, n_B) &= \ln N_A!N_B! - \ln n_A!n_B!(N_A - n_A)!(N_B - n_B)! \\ \mathrm{d}\ln W &= \frac{\partial \ln W_A}{\partial n_A}\,\mathrm{d}n_A + \frac{\partial \ln W_B}{\partial n_B}\,\mathrm{d}n_B \end{aligned}$$

(g) Write down an expression for the total energy of the system U in terms of n_A and n_B give its total differential $\mathrm{d}U$. If U is constant what does this imply about $\mathrm{d}n_A$ and $\mathrm{d}n_B$?

$$\begin{aligned} U &= n_A + n_B \\ \mathrm{d}U &= \mathrm{d}n_A + \mathrm{d}n_B \end{aligned}$$

If $\mathrm{d}U = 0$, then

$$\mathrm{d}n_A = -\,\mathrm{d}n_B$$

(h) Use your last finding in (g) to simplify your expression for $\mathrm{d}\ln W$ from (f).

$$\mathrm{d}\ln W = \mathrm{d}n_A\left(\frac{\partial \ln W_A}{\partial n_A} - \frac{\partial \ln W_B}{\partial n_B}\right)$$

(i) Set your simplified expression for $\mathrm{d}\ln W$ from (h) equal to zero to maximize $\ln W$ (and hence maximize W) and then use Stirling's approximation to obtain a relationship between the numbers of particles in the different levels in the different systems when they reach thermal equilibrium (i.e., they maximize the total entropy and multiplicity).

$$\begin{aligned} 0 &= \frac{\partial \ln W_A}{\partial n_A} - \frac{\partial \ln W_B}{\partial n_B} \\ \frac{\partial \ln W_A}{\partial n_A} &= \frac{\partial \ln W_B}{\partial n_B} \\ \frac{\partial}{\partial n_A}\left(-n_A \ln n_A + n_A - (N_A - n_A)\ln(N_A - n_A) + N_A - n_A\right) &= \frac{\partial \ln W_B}{\partial n_B} \\ -\ln n_A + \ln(N_A - n_A) &= -\ln n_B + \ln(N_B - n_B) \\ \boxed{\frac{n_A}{N_A} = \frac{n_B}{N_B}} \end{aligned}$$

(j) Explain how this is consistent with your findings from above.
This is exactly the same as the result from (c): the probabilities or proportions of particles in the higher energy level will be the same for both systems in the most probable state.