

This homework focused on calculating the most probable macrostate of a system based on the thermodynamic probability. The total energy of the system, or internal energy is defined as

$$U = \sum_{i=1}^{\# \text{ levels}} N_i \epsilon_i$$

Where  $N_i$  is the number of particles in energy state  $\epsilon_i$ . Similarly, the total number of particles is as follows:

$$N = \sum_{i=1}^{\# \text{ levels}} N_i$$

The thermodynamic probability function is a measure of the most likely macrostate present in a system, where a macrostate is a specification of the number of particles in each energy level that satisfies the above two equations. The macrostate, or arrangement of  $N_i$ , that can be made up of the greatest number of microstates (greatest  $\Omega$ ) is the most likely macrostate. The value of  $\Omega$  was calculated as follows:

$$\ln(\Omega) = \sum_{i=1}^{\# \text{ levels}} N_i \ln\left(\frac{g_i}{N_i}\right) + N$$

With an internal energy of 1000 units, number of particles  $N=2000$ , degeneracy  $g_i = 10,000$ , and available energy levels of 0,1,2 the most probable macrostate consisted of  $N_0 = 1232$ ,  $N_1 = 536$ ,  $N_2 = 232$  with a thermodynamic probability  $\Omega = \exp(7021)$ .

This was found by iteration over all possible combinations of  $N_i$ , and each combination was found using the first two equations of this summary. To calculate the entropy of the most likely macrostate Boltzmann's Law was used:

$$S = k \ln(\Omega)$$

The most likely macrostate is coincident with the macrostate with the highest entropy and was found to be  $S = 9.694 \times 10^{-23} \text{ kJ/K}$

If the total energy of the system is increased then we would expect the distribution of particles in each energy level to shift toward the higher energy levels; the percentage increase of  $N_2$  would increase significantly,  $N_1$  would increase to a lesser extent, and  $N_0$  would decrease. At the same time, the number of possible microstates  $\Omega$  that correspond to the most likely macrostate would increase, as seen in Figure 1.

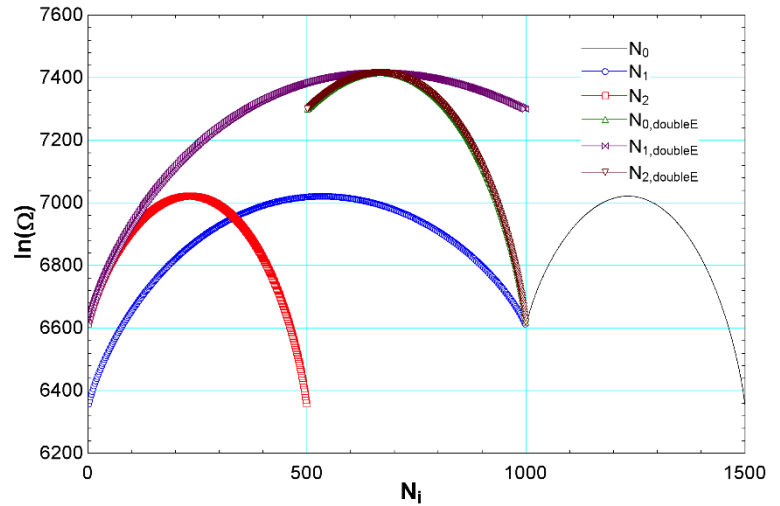


Figure 1: thermodynamic probability as a function of all three particle distributions. Curves are shown for  $N_1$ ,  $N_2$ , and  $N_3$  with internal energies at both 1000 and 2000 units to demonstrate trends of increasing energy. Note that each curve for a given energy level has the same maximum value of  $\Omega$ , which corresponds to the macrostate with the greatest number of possible microstates which is therefore the most probable macrostate.