PHY 4523 Spring 2001 – Homework 1

Due at the start of class on Friday, January 26.

Answer both questions. To gain full credit you should explain your reasoning and show all working. Please write neatly and remember to include your name on the front page of your answers.

1. *Binary probabilities.* This problem generalizes the example of three spins discussed in class. It provides practice in using Stirling's formula, and illustrates the sharpness of the probability distribution for unconstrained variables in large systems.

   Consider a collection of N spins, each of which is equally likely to be in either of two possible orientations, up and down (or $\uparrow$ and $\downarrow$).

   (a) Find $\Omega(N)$, the total number of possible microstates for this system.

   (b) Show that the number of microstates of this system in which exactly $N_\uparrow$ of the spins point up (and $N_\downarrow = N - N_\uparrow$ point down) is

   $$\Omega(N; N_\uparrow) = \frac{N!}{N_\uparrow! \, (N - N_\uparrow)!}.$$

   (c) Calculate the probability $P(N_\uparrow)$ of finding the system in a microstate having $N_\uparrow$ up electrons.

   (d) Using the simplified form of Stirling's formula, $\ln n! = n \ln n - n$, calculate the leading terms in $\ln P(N_\uparrow)$ for situations in which both $N_\uparrow$ and $N_\downarrow$ are much bigger than one.

   (e) Show that there is a maximum in $\ln P(N_\uparrow)$ and hence in $P(N_\uparrow)$ at a particular value, $N_\uparrow = \tilde{N}_\uparrow$.

   (f) Using the formula $\ln(1 + x) = x - \frac{1}{2}x^2 + \ldots$ for $|x| \ll 1$, expand $\ln P(N_\uparrow)$ about $N_\uparrow = \tilde{N}_\uparrow$ in powers of $N_\uparrow - \tilde{N}_\uparrow$. Retain the first two nonzero terms in the expansion.

   (g) Use your result from (f) to write down an expression for $P(N_\uparrow)$ valid for $N_\uparrow \approx \tilde{N}_\uparrow$. Estimate the probability of finding $N_\uparrow = 1.01\tilde{N}_\uparrow$ for a system of one million spins ($N = 10^6$). You need only give your answer to the nearest power of ten.

2. *A collection of quantum harmonic oscillators.* This problem asks you to examine in more detail a model introduced in lectures. Parts (a) and (b) provide additional practice in working with Stirling's formula. Parts (c)–(f) illustrate the way in which the probabilistic results of statistical mechanics reduce, in the limit of large system size, to the "exact" results of classical thermodynamics.

   (a) Consider a collection of N quantum harmonic oscillators, each having the same frequency ω and an energy of the form $\epsilon = n\hbar\omega$, $n = 0, 1, 2, \ldots$. (We are neglecting the zero-point energy $\frac{1}{2}\hbar\omega$.) Let the system have a total energy $E =$

$M\hbar\omega$, where M is a positive integer. As shown in class, the multiplicity function for this system is

$$\Omega(E, N) = \frac{(M + N - 1)!}{M!\,(N - 1)!}.$$

Focus on the macroscopic limit in which $M > N \gg 1$ with $M/N = \bar{n}$, a finite constant greater than one (say, 10). Use the full version of Stirling's formula, $\ln n! = (n + \frac{1}{2}) \ln n - n + \ln\sqrt{2\pi} + O(1/n)$, to write $\ln\Omega(E, N)$ in terms of N, $\bar{n}$, and constants (*not* E or M).

(b) Take your result from (a) and wherever possible apply the formula $\ln(1 + x) = x - \frac{1}{2}x^2 + \ldots$ for $|x| \ll 1$. For example, $\ln[M/(N - 1)] = \ln[\bar{n}/(1 - 1/N)] = \ln\bar{n} - \ln(1 - 1/N) \approx \ln\bar{n} + 1/N + 1/(2N^2)$.

In this way, expand $\ln\Omega(E, N)$ as a sequence of terms of decreasing magnitude. First order all terms by their N dependence (e.g., $N \ln N > N > \ln N > 1 > 1/\ln N > 1/N$), then order each set of terms having the same N dependence by their $\bar{n}$ dependence.

In this and all the remaining parts of this problem, you may neglect any term which (i) vanishes when $N \longrightarrow \infty$ with $\bar{n}$ held constant and/or (ii) is less than $1/\bar{n}$ times the largest term with a given N dependence. For example, you should reduce $N + N/\bar{n} - N/\bar{n}^2 + 1/\bar{n}^3 + 1/\ln N$ to $N + N/\bar{n} + 1/\bar{n}^3$.

(c) Now consider a composite system consisting of two subsystems, labeled $\alpha = 1, 2$. Each subsystem contains N oscillators. Initially, each subsystem is closed and has the same total energy $E^{(\alpha)} = M\hbar\omega$ (with $M > N \gg 1$). Use your answer to (a) to write down an expansion for $\ln\Omega_i$, where Ω_i is the initial number of microstates accessible to the composite system.

(d) Now let the two subsystems be brought into thermal contact, so that a total energy $E = 2M\hbar\omega$ is distributed among $2N$ oscillators. Write down an expansion for $\ln\Omega_f$, where Ω_f is the new number of accessible microstates.

(e) Calculate the value of $\ln(\Omega_f/\Omega_i)$. Your answer should be positive because the microstates accessible in the final equilibrium state include all microstates accessible initially plus many others (all those with $E^{(1)} + E^{(2)} = 2M\hbar\omega$ but $E^{(1)} \neq M\hbar\omega$).

(f) Note that according to statistical mechanics, $\ln(\Omega_f/\Omega_i) \equiv (S_f - S_i)/k_B$, where S is the entropy. In classical thermodynamics, the entropy of a macroscopic system is supposed to be extensive, i.e., proportional to the size of the system. Thus the entropy of a system of $2N$ oscillators should be just twice that of a system of N oscillators of the same type. This reasoning suggests that Ω_f should equal Ω_i, or $\ln(\Omega_f/\Omega_i) = 0$.

Resolve the apparent contradiction with (d) by showing that in the "thermodynamic limit" ($N \to \infty$, $M \to \infty$, but $M/N = \bar{n} = $ finite and nonzero), the initial and final entropies per oscillator are the same, i.e., $S_f/N = S_i/N$. This gives precise meaning to the rather loose statement "entropy is extensive".