Physics 313 Problem Set 3

Important concepts from lectures 5-7

Two state system: every 'particle' (or site) has exactly two possible states, which we have denoted with $\uparrow$ and $\downarrow$.

The energy of each site is 0 when the site is in the $\downarrow$ state and ϵ_0 when it is in the $\uparrow$ state. For N sites, the total energy is $E = \epsilon_0 q$ where q is the number of sites in the $\uparrow$ state. We think of q as the number of available quanta of energy.

There are

$$\Omega(N, q) = \binom{N}{q}$$

ways to distribute q quanta of energy among the N sites (or $\Omega(N, q)$ configurations with total energy $\epsilon_0 q$).

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Einstein solid: this is made up of N copies of the quantum harmonic oscillator (QHO). The QHO has energy levels labeled by non-negative integers, $n = 0, 1, 2, \ldots$.

The energy of each oscillator is $(hf)n$ where f is the frequency and h is the Planck's constant. The total energy E of N QHOs is the sum of all individual energies. If there are q quanta of energy to be distributed, $E = (hf)q$, and there are

$$\Omega(N, q) = \binom{N + q - 1}{q}$$

configurations with this energy.

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Fundamental assumption of stat mech:

If a system is isolated and in equilibrium inside, then all microstates (microscopic configurations) are equally probable.

Consequence:

The probability of any macrostate (a state with well defined macroscopic quantities: N, E, etc...) is proportional to the number of microstates with those macroscopic quantities.

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The spontaneous flow of energy stops when the system is at or near its most likely macrostate (the macrostate with the greatest multiplicity).

Another way to put it: systems tend towards the most likely macrostate. This is a version of the Second Law Of Thermodynamics.

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Stirling's Approximation (or Formula)

$$N! \approx N^N e^{-N} \sqrt{2\pi N} \tag{1}$$

$$N! \approx N^N e^{-N} \tag{2}$$

where the first version is more accurate than the second. You can use the second, simpler version as long as it does not all cancel.

The second formula can also be written

$$\ln N! \approx N \ln N - N$$

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For 2 weakly coupled Einstein solids A and B, the total multiplicity of a macrostate given by N_A, N_B, q_A and $q_B = q_{TOT} - q_A$ (where q_{TOT} is the total number of quanta of energy in the A+B system) is

$$\Omega(N_A, N_B, q_{TOT}, q_A) = \binom{N_A + q_A - 1}{q_A} \binom{N_B + q_B - 1}{q_B}$$

Now, setting $N_A = N_B = N$, $q_{TOT} = q$, $q_A = q/2 + x$ and $q_B = q/2 - x$, with $N \ll q$ and $x \ll q$, we derived in class that

$$\Omega(N_A, N_B, q_{TOT}, q_A) = \Omega_{max}\ e^{-N\left(\frac{2x}{q}\right)^2}$$

This is a narrow Gaussian peak, whose width is $\Delta x = q/\sqrt{N}$. Relative to the entire range of x (which is q) we have

$$\frac{\Delta x}{q} = \frac{1}{\sqrt{N}} \ll 1$$

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In a large enough system, once it has reached its equilibrium state, the fluctuations away from the most likely macrostate are too small to be measured. This is called the Thermodynamic Limit, where we recover laws of ordinary thermodynamics from statistical mechanics.

Problem Set

Due at the end of class, Wednesday September 24^{th} (late assignments will not be accepted).

1. For an Einstein solid with three oscillators and 4 units of energy, list all microstates and represent each as a series of dots and vertical lines like we did in class. Check that the general formula for the number of microstates works in this case.

2. **(a)** What is the probability that a two-state paramagnet with $N = 10$ will have *exactly* 5 dipoles pointing up and 5 dipoles pointing down? Give a numerical answer in addition to the formula.
(b) Repeat part (a) with $N = 10,000$ and exactly 5000 dipoles pointing up and 5000 dipoles pointing down? You will need to use Stirling's Formula. You will need to keep the $\sqrt{2\pi N}$ terms for this one!

3. Let $y \ll x$. Recall from the first problem set that $\ln(x - y) \approx \ln x - y/x$.
(a) Use Stirling's Formula to argue that

$$\ln \binom{x}{y} \approx y \ln\left(\frac{ex}{y}\right)$$

(b) Consider
(i) a two-state paramagnet
(ii) an Einstein solid
each with N sites and a small number of quanta of energy $q \ll N$. Use your answer in part (b) to find approximate expressions for the corresponding multiplicities
(i) $\Omega(N, q) = \binom{N}{q}$
(ii) $\Omega(N, q) = \binom{N-q+1}{q}$
Comment on the similarity between to answers: explain why these two systems, in the limit $q \ll N$ are essentially the same.

4. In this question, we will do a computation similar to the one we did in class with two Einstein solids, only for two-state paramagnets. As this is a longish computation, I have broken it down into lots of steps.

Let's take two paramagnets, A and B. Assume they are weakly coupled to each other, and isolated from their environment, Let A and B have N sites each. Denote with q_A the number of energy quanta in A and with q_B the number of energy quanta in B. The total energy is conserved, so $q = q_A + q_B$ is fixed, but A and B can pass energy between them, so q_A and q_B fluctuate.

We will find it useful to define $\beta = q/(2N)$, $\alpha_A = q_A/N$ and $\alpha_B = q_B/N$. We will assume that β, α_A and α_B are numbers between 0 and 1 and are neither large nor small.

(a) Write down $\Omega(N, \alpha_A, \alpha_B)$, which is the total number of microstates of the A+B system with the macroscopic numbers N, $q_A = N\alpha_A$ and $q_B = N\alpha_B$. Write your answer in terms of N, α_A, and α_B.

(b) Using Stirling's formula, show that

$$\ln \binom{N}{\alpha N} \approx -N\left[\alpha \ln \alpha + (1-\alpha)\ln(1-\alpha)\right]$$

(c) Using your answers from parts (a) and (b), show that

$$\ln \Omega(N, \alpha_A, \alpha_B) = -N\left[\alpha_A \ln \alpha_A + (1-\alpha_A)\ln(1-\alpha_A) + \alpha_B \ln \alpha_B + (1-\alpha_B)\ln(1-\alpha_B)\right]$$

(d) As a preparation step for part (e), show that, to second order in $x \ll \gamma$,

$$(\gamma + x)\ln(\gamma + x) = \gamma \ln \gamma + x(\ln \gamma + 1) + \frac{x^2}{2\gamma}$$

You will need to use this formula 4 times in the next part.

(e) Let $\alpha_A = \beta + x$ and $\alpha_B = \beta - x$, with $x \ll \beta$ and $x \ll (1-\beta)$, and expand your answer in part (c) to second order in x (i.e., keep terms up to x^2).

You should get

$$\begin{aligned} \ln \Omega(N, \beta - x, \beta + x) &= \\ -N\left[2\beta \ln \beta + 2(1-\beta)\ln(1-\beta) + \frac{x^2}{\beta(1-\beta)}\right] \end{aligned}$$

(f) Now exponentiate your answer in part (c) and show that

$$\Omega(N, \beta - x, \beta + x) = \left(\beta^\beta (1-\beta)^{1-\beta}\right)^{-2N} \exp\left(\frac{-Nx^2}{\beta(1-\beta)}\right)$$

(g) For what x does the answer to part (d) reach its maximum? Evaluate the value of $\Omega(N, \beta - x, \beta + x)$ at that point, and call it Ω_{max}.

(h) Plot

$$\frac{\Omega(N, \beta - x, \beta + x)}{\Omega_{max}}$$

as a function of x for $\beta = 1/3$ and x from $-1/3$ to $1/3$. Do this for three different values of N: N=10, 100, and 10,000. You may use your favourite computer program to generate the plot, or you may sketch it by hand. Don't forget to label everything.

(i) Comment on the behaviour of the distribution as a function of N in the context of the thermodynamic limit.