PHY 293F – WAVES AND PARTICLES
DEPARTMENT OF PHYSICS, UNIVERSITY OF TORONTO

PROBLEM SET #6 - SOLUTIONS

Marked Q1 (out of 7 marks) and Q4 (out of 3 marks) for a total of 10.

1. Problem 2.11 on page 60 of Schroeder.

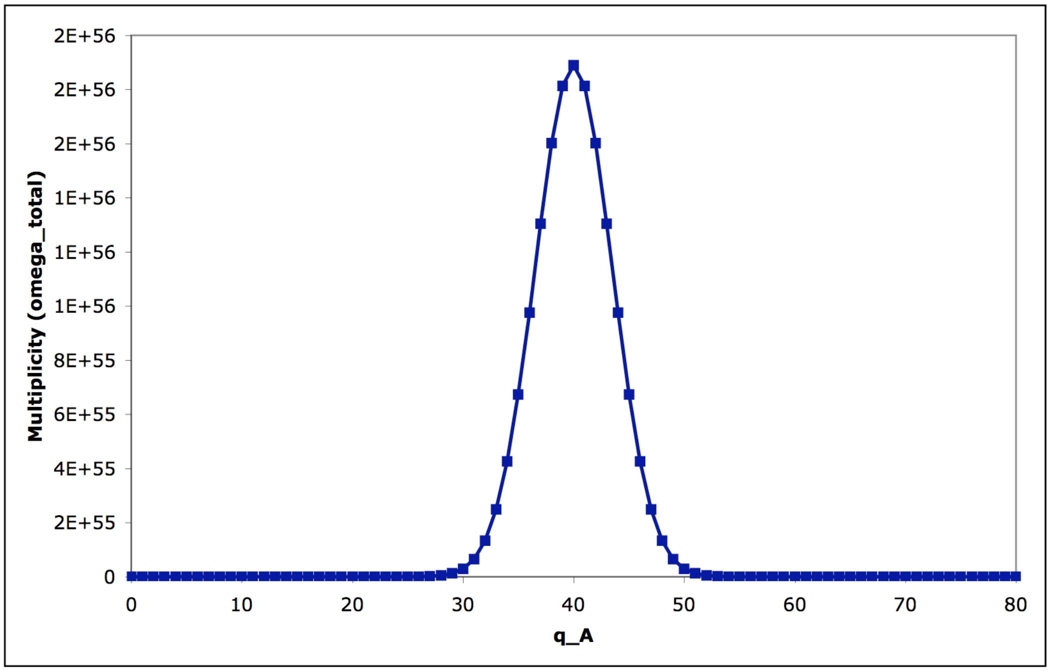
For two interacting two-state paramagnets, with N=100 dipoles in each, we have 80 energy units to share between the two paramagnets. The total number of macrostates available for this system is 81. This equation is used to calculate the multiplicity of each paramagnet in each macrostate and total multiplicity:

$$\Omega(N,q) = \binom{N}{q} = \frac{N!}{q!(N-q)!}.$$

Using a computer program, we can determine multiplicities of each paramagnet and system of two paramagnets. For brevity, some macrostates are omitted from table below.

Two two-state paramagnets			q_total =	80
N_A =	100	N_B =	100	
q_A	omega_A	q_B	omega_B	omega_total
0	1	80	5.35983E+20	5.35983E+20
1	100	79	2.04184E+21	2.04184E+23
2	4950	78	7.33207E+21	3.62937E+25
3	161700	77	2.48653E+22	4.02071E+27
4	3921225	76	7.97761E+22	3.1282E+29
…	…	…	…	…
37	3.42003E+27	43	3.81165E+28	1.3036E+56
38	5.67005E+27	42	2.82588E+28	1.60229E+56
39	9.01392E+27	41	2.01164E+28	1.81328E+56
40	1.37462E+28	40	1.37462E+28	1.88959E+56
41	2.01164E+28	39	9.01392E+27	1.81328E+56
42	2.82588E+28	38	5.67005E+27	1.60229E+56
43	3.81165E+28	37	3.42003E+27	1.3036E+56
44	4.93782E+28	36	1.9772E+27	9.76309E+55
45	6.14485E+28	35	1.09507E+27	6.72902E+55
46	7.3471E+28	34	5.80717E+26	4.26659E+55
47	8.44135E+28	33	2.94692E+26	2.4876E+55
48	9.32066E+28	32	1.43013E+26	1.33297E+55
49	9.89131E+28	31	6.63246E+25	6.56037E+54
50	1.00891E+29	30	2.93723E+25	2.96341E+54
51	9.89131E+28	29	1.24108E+25	1.2276E+54
52	9.32066E+28	28	4.99881E+24	4.65922E+53
53	8.44135E+28	27	1.91735E+24	1.6185E+53
…	…	…	…	…
78	7.33207E+21	2	4950	3.62937E+25
79	2.04184E+21	1	100	2.04184E+23
80	5.35983E+20	0	1	5.35983E+20

Also, we produced a graph of the multiplicity of the whole system (Ω_{total}) versus q_A the number of energy units in paramagnet A.



Using the results from above, the most probable macrostate of the whole system is when 40 units of energy are in each of the two-state paramagnets.

$$P(q_A = 40) = \frac{\Omega(q_A = 40)}{\Omega_{total}} = \frac{1.89\text{x}10^{56}}{1.65\text{x}10^{57}} = 11.5\%.$$

The least probable macrostate is when all the energy units are in one of the two-state paramagnets (either $q_A = 0$ or $q_B=0$).

$$P(q_A = 0) = \frac{\Omega(q_A = 0)}{\Omega_{total}} = \frac{5.36\text{x}10^{20}}{1.65\text{x}10^{57}} = 3.25\text{x}10^{-37}.$$

Note that the most probable state for the whole system is when the energy is evenly distributed between the two paramagnets (q_A and q_B=40). However, the most probable state for each individual paramagnet is when q_A (or q_B)=50 (not 40), the state where there are an equal number of spin-up and spin-down dipoles.

2. In class, we derived a formula for the multiplicity of a large Einstein solid in the "high temperature" limit by using Stirling's approximation. Using these same methods, derive a formula for the multiplicity of a large Einstein solid in the "low temperature" limit. In your derivation, remember to clearly state the approximations you made and justify why they could be made. Why is it sufficient to use the less exact form of Stirling's approximation?

Using expressions derived in class for a large Einstein solid where q and N are both large, we can omit "-1" from expression because of magnitudes of q and N:

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

Applying Stirling's approximation for the natural logarithm of the multiplicity, we get:

$$\begin{aligned}\ln\Omega &= \ln\left(\frac{(q+N)!}{q!N!}\right)\\ &= \ln(q+N)! - \ln q! - \ln N!\\ &\approx (q+N)\ln(q+N) - (q+N) - q\ln q + q - N\ln N + N\\ &= (q+N)\ln(q+N) - q\ln q - N\ln N.\end{aligned}$$

This can be done because both q and N are large.

Because q<<N, we can apply the same type of logarithm manipulation technique that was used in class with the Taylor expansion approximation. From here, we can simplify ln(q+N) to:

$$\begin{aligned}\ln(q+N) &= \ln N\left[\left(1+\frac{q}{N}\right)\right]\\ &= \ln N + \ln\left(1+\frac{q}{N}\right)\\ &\approx \ln N + \frac{q}{N}.\end{aligned}$$

*Then this can be plugged into the ln*Ω *expression. After collecting terms, we get:*

$$\begin{aligned}\ln\Omega &\approx (q+N)\left[\ln N + \frac{q}{N}\right] - q\ln q - N\ln N\\ &= q\ln N + \frac{q^2}{N} + N\ln N + q - q\ln q - N\ln N\\ &= q\ln\left(\frac{N}{q}\right) + q.\end{aligned}$$

For the low temperature case (q<<N), the q^2/N term is very small and can be neglected.

By exponentiating, we get:

$$\begin{aligned}\Omega &= e^{q\ln(N/q)}e^{q}\\ &= \left(\frac{Ne}{q}\right)^q.\end{aligned}$$

Here, we could use the less exact form of Stirling's approximation because of the difference in magnitude between q and N (q<<N). The additional factors cancel when the orders of magnitude of N and q are considered in the approximation.

3. For a single large two-state paramagnet, the multiplicity function is very sharply peaked about $N_\uparrow = N/2$.

   a. Estimate the height of the peak in the multiplicity function using Stirling's approximation.

   The most likely macrostate for the system is $N_\uparrow = N_\downarrow = N/2$. So the peak in the multiplicity function is:

$$\Omega_{\max} = \frac{N!}{N_\uparrow! N_\downarrow!} = \frac{N!}{\left(\frac{N}{2}!\right)^2}$$

$$\approx \frac{N^N e^{-N}\sqrt{2\pi N}}{\left(\left(\frac{N}{2}\right)^{N/2} e^{-N/2}\sqrt{2\pi N/2}\right)^2}$$

$$= 2^N \sqrt{\frac{2}{\pi N}}.$$

   Here you need to use the more exact form of Stirling's approximation because N and N/2 are both large and are of the same order of magnitude.

   b. Use the method that we used in class to derive a formula for the multiplicity function in the vicinity of the peak, in terms of $x \equiv N_\uparrow - N/2$. Verify that your formula agrees with your result for part (a) when $x = 0$.

   Using Stirling's approximation, the multiplicity of this system is:

$$\Omega = \frac{N!}{N_\uparrow! N_\downarrow!}$$

$$\approx \frac{N^N e^{-N}\sqrt{2\pi N}}{N_\uparrow^{N_\uparrow} e^{-N_\uparrow}\sqrt{2\pi N_\uparrow}\, N_\downarrow^{N_\downarrow} e^{-N_\downarrow}\sqrt{2\pi N_\downarrow}}$$

$$= \frac{N^N}{N_\uparrow^{N_\uparrow} N_\downarrow^{N_\downarrow}}\sqrt{\frac{N}{2\pi N_\uparrow N_\downarrow}}.$$

   Substituting in for $N_\uparrow$ and $N_\downarrow$ in terms of x and N/2, we get:

$$\Omega \approx \frac{N^N}{\left(\frac{N}{2}+x\right)^{N/2+x}\left(\frac{N}{2}-x\right)^{N/2-x}}\sqrt{\frac{N}{2\pi\left(\frac{N}{2}+x\right)\left(\frac{N}{2}-x\right)}}$$

$$= \frac{N^N}{\left(\left(\frac{N}{2}\right)^2 - x^2\right)^{N/2}\left(\frac{N}{2}+x\right)^{x}\left(\frac{N}{2}-x\right)^{-x}}\sqrt{\frac{N}{2\pi\left(\left(\frac{N}{2}\right)^2 - x^2\right)}}.$$

   Working with the natural logarithm is a little easier at this point, so we can express as lnΩ:

$$\ln\Omega = N\ln N - \frac{N}{2}\ln\left(\left(\frac{N}{2}\right)^2 - x^2\right) - x\ln\left(\frac{N}{2}+x\right) + x\ln\left(\frac{N}{2}-x\right) + \ln\sqrt{\frac{N}{2\pi}} - \frac{1}{2}\ln\left(\left(\frac{N}{2}\right)^2 - x^2\right)$$

Using the relative size of x and N (x<<N) and the Taylor expansion approximation for small values (as we have done before), we can simplify the expressions in the various ln terms:

$$\ln\left[\left(\frac{N}{2}\right)^2 - x^2\right] = \ln\left(\frac{N}{2}\right)^2 + \ln\left[1 - \left(\frac{2x}{N}\right)^2\right]$$

$$\approx 2\ln\frac{N}{2} - \left(\frac{2x}{N}\right)^2$$

$$\ln\left[\frac{N}{2} \pm x\right] = \ln\left(\frac{N}{2}\right) + \ln\left[1 \pm \frac{2x}{N}\right]$$

$$\approx \ln\frac{N}{2} \pm \frac{2x}{N}$$

Substituting these back into the expression for lnΩ and collecting terms, we get:

$$\ln\Omega \approx N\ln N - \frac{N}{2}\left(2\ln\frac{N}{2} - \left(\frac{2x}{N}\right)^2\right) - x\left[\ln\frac{N}{2} + \frac{2x}{N}\right] + x\left[\ln\frac{N}{2} - \frac{2x}{N}\right] + \ln\sqrt{\frac{N}{2\pi}} - \frac{1}{2}\left[2\ln\frac{N}{2} - \left(\frac{2x}{N}\right)^2\right]$$

$$\approx N\ln\left(\frac{N}{\frac{N}{2}}\right) + \ln\sqrt{\frac{N}{2\pi}\left(\frac{2}{N}\right)^2} - \frac{2x^2}{N} + \frac{2x^2}{N^2}$$

$$\approx N\ln 2 + \ln\sqrt{\frac{N}{2\pi}} - \frac{2x^2}{N} + \frac{2x^2}{N^2}.$$

From here, the term in $2x^2/N^2$ is omitted since it is very small compared to the rest of the terms. Exponentiating the expression to get the multiplicity expression, we get:

$$\Omega = 2^N\sqrt{\frac{2}{\pi N}}e^{-2x^2/N}, \text{ where } x << N.$$

This is a Gaussian function with the maximum value at x=0 (as we found in part (a)), $\Omega_{\max} = 2^N\sqrt{\frac{2}{\pi N}}$.

c. Calculate the width of the peak in the multiplicity formula using the width definition given in class.

The width of the peak is found when $\Omega = \frac{1}{e}\Omega_{\max}$. *So to find the width, we solve the relation* $-1 = -\frac{2x^2}{N}$ *for x to get* $x = \sqrt{\frac{N}{2}}$. *The full width of the peak is 2x or* $\sqrt{2N}$.

d. Consider a case where you flipped 1,000,000 fair coins. Would you be surprised to get 501,000 heads and 499,000 tails? Would you be surprised to get 510,000 heads and 490,000 tails? Explain why.

Since the two-state paramagnet is very similar to the coin flip, we can use the results from part (c) in this explanation.

For a set of $N=10^6$ coins, the half-width (x or the distance away from the most probable state where we are very likely to find the system) is $x = \sqrt{N} = \sqrt{500{,}000} \sim 700$.

So, obtaining a result that has 501,000 heads is not too far away from the half-width of the most probable states we calculated above. This is not really a surprising result.

Now, obtaining a result that has 510,000 heads (or x=10,000) is much more surprising. Using the expression for Ω *derived in part (b), we can compute the multiplicity of this state as a fraction of the maximum value:*

$$\frac{\Omega(\text{510,000 heads})}{\Omega_{\max}} = e^{-2x^2/N}$$

$$= e^{-200}.$$

To obtain this result is much more surprising (to the point of shock) because of how far from the peak in multiplicity this result lies.

4. Problem 2.29 on page 77 of Schroeder.

For a system of two Einstein solids, with $N_A=300$, $N_B=200$ and $q_{total}=100$. The total multiplicity of this system can be calculated for each of the macrostates using a computer program or it was given in the Schroeder in Sec. 2.3/Figure 2.5.

The most likely macrostate occurs at $q_A=60$, so the entropy in units of Boltzmann's constant is:

$$\frac{S}{k} = \ln(6.89\text{x}10^{114}) = 264.4.$$

The least likely macrostate occurs at $q_A=0$ (or $q_A=100$), so the entropy is:

$$\frac{S}{k} = \ln(2.77\text{x}10^{81}) = 187.5.$$

The difference in entropy is much smaller than the difference in probabilities.

Over long times scales all microstates are accessible, so need the sum over the multiplicity of all macrostates to calculate the entropy over long time scales. This is:

$$\frac{S}{k} = \ln(9.26\text{x}10^{115}) = 267.0.$$

It is not much larger than the entropy in the most probable macrostate!