Stat Mech I HW4

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1 Problem 1

a) The multiplicity W(n,N) to put n quanta into N harmonic oscillators is $\binom{n}{N} = \frac{(N-1)!}{n!(N-1)!}$. Planck proved this using the generating function $g(t) = t^n$. We start with $W(n,1)$, which is clearly equal to 1. Using the generating function:

$$\sum_{n=0}^{\infty} W(n,1)t^n = \sum_{n=0}^{\infty} t^n = \frac{1}{1-t} \tag{1.1}$$

For N harmonic oscillators we take the generating function to the Nth power.

$$\left(\frac{1}{1-t}\right)^N = \sum_{n=0}^{\infty} W(n,N)t^n = a_0 + a_1 t + a_2 t^2 + ... \tag{1.2}$$

We can now solve for the coefficients of the series which are the W(n,N). To find W(n,N) we differentiate n times and set t=0.

$$\frac{d^n}{dt^n}\sum_{n=0}^{\infty} W(n,N)t^n = \frac{1}{n!}W(n,N) \tag{1.3}$$

$$W(n,N) = \lim_{t\to\ 0} \frac{1}{n!}\frac{d^n}{dt^n}\left(\frac{1}{1-t}\right)^n \tag{1.4}$$

$$W(n,N) = \lim_{t\to\ 0} \frac{1}{n!} N(N+1)(N+2)...(N+n-1)(1-t)^{-N-m} \tag{1.5}$$

$$W(n,N) = \frac{N(N+1)...(N+n-1}{n!}\frac{(N-1)!}{(N-1)!} = \frac{(N+n-1)!}{n!(N-1)!} \tag{1.6}$$

b) Using the microcanonical ensemble approach we can now calculate the entropy.

$$S = k\ln W = k\ln\left(\frac{(N+n-1)!}{n!(N-1)!}\right) \tag{1.7}$$

Using the Stirling approximation this simplifies to:

$$S = k((N+n)\ln(N+n) - n\ln n - N\ln N) \tag{1.8}$$
$$\tag{1.9}$$

c) We now use Planck's expression for the total energy $U = n\hbar\omega$. Substituting $n = \frac{U}{\hbar\omega}$ we then have:

$$S = k((N+n)\ln(N+n) - n\ln n - N\ln N) \tag{1.10}$$
$$S = k((N+\frac{U}{\hbar\omega})\ln(N+\frac{U}{\hbar\omega}) - \frac{U}{\hbar\omega}\ln\frac{U}{\hbar\omega} - N\ln N) \tag{1.11}$$

d) The temperature is $\frac{1}{T} = \frac{\partial S}{\partial U}$. We take $\frac{\partial S}{\partial n}\frac{\partial n}{\partial U}$, with $\frac{\partial n}{\partial U} = \frac{1}{\hbar\omega}$.

$$\frac{\partial S}{\partial n} = k(\ln(N+n) + 1 - \ln n - 1) = k\ln\frac{N+n}{n} \tag{1.12}$$
$$\frac{1}{kT} = \frac{1}{\hbar\omega}\ln\frac{N+\frac{U}{\hbar\omega}}{\frac{U}{\hbar\omega}} \tag{1.13}$$
$$e^{\frac{\hbar\omega}{kT}} = \frac{N+\frac{U}{\hbar\omega}}{\frac{U}{\hbar\omega}} = \frac{N\hbar\omega}{U} + 1 \tag{1.14}$$
$$U = \frac{N\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1} \tag{1.15}$$

2 Problem 2

a) Call the number of quanta in SHO 1 by n_1, then the number of quanta in SHO 2 is $n' - 1 - n_1$. We see that n_1 completely determines the system state, and can range from 0 to $n' - 1$. There are therefore n' microstates available to the system, and the entropy is $S = k\ln n'$.
b) We follow the same argument as part A, but now the total energy constrains the number of quanta in the second oscillator to $\frac{n''}{2} - 1 - n_1$. Now n_1 can range from 0 to $\frac{n''}{2}$ so there are $\frac{n''}{2}$ microstates (which is fine since n'' is even). The entropy is $S = k\ln(\frac{n''}{2})$.
c) S is an extensive parameter so we simply add the results from part A and part B. Expressed in terms of the energies:

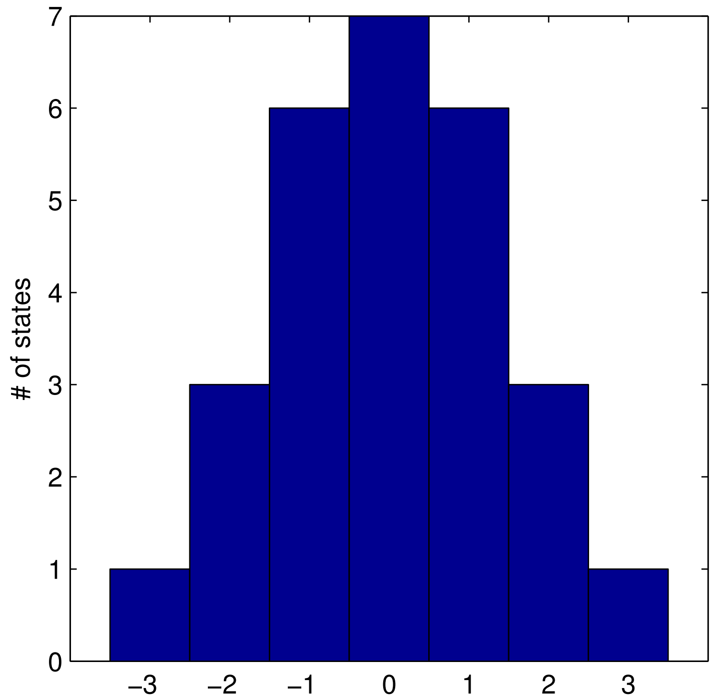
$$S = k\left(\ln\frac{E'}{\hbar\omega} + \ln\frac{E''}{2(2\hbar\omega)}\right) \tag{2.1}$$
$$S = k\left(\ln\frac{E'}{\hbar\omega} + \ln\frac{E''}{2\hbar\omega} - \ln 2\right) \tag{2.2}$$
$$S = k\left(\ln\frac{E'}{2\hbar\omega} + \ln\frac{E''}{2\hbar\omega}\right) \tag{2.3}$$

3 Problem 3

The complete enumeration of all states (M=1) is:

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & -1 & 0 \\ -1 & -1 & 1 \\ -1 & 0 & -1 \\ -1 & 0 & 0 \\ -1 & 0 & 1 \\ -1 & 1 & -1 \\ -1 & 1 & 0 \\ -1 & 1 & 1 \\ 0 & -1 & -1 \\ 0 & -1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & 0 \\ 1 & -1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 0 \\ 1 & 1 & 1 \end{bmatrix} \tag{3.1}$$

The figure below shows the number of states with each possible value of M_z.



a) With all state having probability $\frac{1}{27}$ the entropy is 3.2958.
b) The entropy when only $M_z = 0$ is possible is 1.9549.
c) The entropy when only $M_z = M$ is possible is 1.7918.
d) There is only one state with $M_z = 3M$, so the entropy is 0.
e) We minimize the entropy using Lagrange multipliers to incorporate the constraints $\sum f_i = 1$ and $\sum f_i M_{zi} = \gamma M$.

$$F = \sum f_i \ln f_i - \lambda_1 (\sum f_i - 1) - \lambda_2 (\sum f_i M_{zi} - \gamma M) \tag{3.2}$$

$$\frac{\partial F}{\partial f_i} = 1 + \ln f_i - \lambda_1 - \lambda_2 M_{zi} = 0 \tag{3.3}$$

$$f_i = e^{\lambda_1 + \lambda_2 M_{z_i} - 1} \tag{3.4}$$

$$\sum f_i = e^{\alpha} \sum e^{\lambda_2 M_{zi}} = 1, \alpha \equiv \lambda_1 - 1 \tag{3.5}$$

$$e^{-\alpha} = \sum e^{\lambda_2 M_{zi}} \tag{3.6}$$

4 Problem 4

In class it was shown that $\frac{\partial U}{\partial \beta} =< (\Delta E)^2 >$. To work out $< (\Delta E)^3 >$ we find $\frac{\partial^2 U}{\partial \beta^2}$.

$$d\beta = -\frac{1}{kT^2} dT \tag{4.1}$$

$$\frac{\partial U}{\partial \beta} = \frac{\partial U}{\partial T}\frac{\partial T}{\partial \beta} = kT^2 \frac{\partial U}{\partial T} = kT^2 C_v \tag{4.2}$$

$$\frac{\partial^2 U}{\partial \beta^2} = \frac{\partial}{\partial T}(\frac{\partial U}{\partial \beta})\frac{\partial T}{\partial \beta} \tag{4.3}$$

$$\frac{\partial^2 U}{\partial \beta^2} = \left(2kTC_v + kT^2 \frac{\partial C_v}{\partial T}\right) kT^2 \tag{4.4}$$

$$\frac{\partial^2 U}{\partial \beta^2} = k^2 \left(2T^3 C_v + T^4 \frac{\partial C_v}{\partial T}\right) \tag{4.5}$$

For an ideal gas $U = \frac{3}{2}NkT$ and $C_v = \frac{3}{2}Nk$. So we have:

$$< (\Delta E)^2 >= kT^2 C_v = \frac{3}{2}Nk^2T^2 \tag{4.6}$$

$$< U^2 >= (\frac{3}{2}NkT)^2 \tag{4.7}$$

$$< (\frac{\Delta E}{U})^2 >= \frac{2}{3N} \tag{4.8}$$

$$< (\Delta E)^3 >= k^2(2T^3(\frac{3}{2}Nk) + T^4(0)) = 3Nk^3T^3 \tag{4.9}$$

$$< U^3 >= \frac{3^3}{2^3}N^3k^3T^3 \tag{4.10}$$

$$< (\frac{\Delta E}{U})^3 >= \frac{2^3}{3^3}\frac{1}{N^2} = \frac{8}{9N} \tag{4.11}$$

5 Problem 5

For an ideal gas the entropy is $S = Nk\left(\ln \frac{V}{N\lambda^3} + \frac{5}{2}\right)$. We show that:

$$\frac{S}{Nk} = \ln(\frac{Q_1}{N}) + T(\frac{\partial \ln Q_1}{\partial T})_P \tag{5.1}$$

The partition function for an ideal gas is $Q_n(V,T) = \frac{1}{N!}(\frac{V}{\lambda^3})^N$. Q_1 is $\frac{V}{\lambda^3}$. We expand Q_1 and find $(\frac{\partial \ln Q_1}{\partial T})_P$.

$$Q_1 = \frac{V}{h^3}(2\pi mkT)^{3/2} \tag{5.2}$$

$$(\frac{\partial \ln Q_1}{\partial T})_P = \frac{1}{Q_1}\frac{\partial Q_1}{\partial T} \tag{5.3}$$

$$(\frac{\partial \ln Q_1}{\partial T})_P = \frac{3}{2}\frac{1}{T} \tag{5.4}$$

We see that $\frac{S}{Nk} = \ln\left(\frac{Q_1}{N}\right) + T\left(\frac{\partial \ln Q_1}{\partial T}\right)_P = \ln\frac{V}{N\lambda^3} + \frac{3}{2}$.