807 Final exam (40 points). 12/13/16, 12:30 p.m. - 3:30 p.m.

Problem 1.

Consider a system of N non-interacting particles moving in one dimension x (i.e., on a line) confined by a quartic potential $\sim x^4$. The Hamiltonian of the system is

$$H(x_1, x_2, ...x_N; p_1, p_2, ...p_N) \;=\; \sum_{i=1}^{N} \Big[\frac{p_i^2}{2m} + \alpha(\frac{x_i}{L})^4\Big]$$

where p_i are the momenta and x_i the positions of the particles labeled by $i = 1, 2, ...N$. The constants determining the strength of the potential are energy $\alpha > 0$ and length L. Assume that the system is in thermal equilibrium at temperature T and that classical statistical mechanics is applicable.

Find

(a) classical partition function of the system

(b) entropy and specific heat of the system. (Note that L is one-dimensional analog of volume V).

Solution:

From Eqs. (2.65) and (4.40)

$$\mathcal{Z} = \int \prod_{i=1}^{N} dx_i \, dp_i e^{-\beta \sum_{i=1}^{N} \left(\frac{p_i^2}{2m} + \alpha \frac{x_i^4}{L^4}\right)} \;=\; z^N,$$

where

$$z = \int dx \, dp \, e^{-\beta \frac{p^2}{2m} - \beta\alpha \frac{x^4}{L^4}} = \sqrt{\frac{2\pi m}{\beta}} \int dx \; e^{-\beta\alpha \frac{x^4}{L^4}} \;=\; \sqrt{\frac{2\pi m}{\beta}} \frac{L}{4} \frac{\Gamma(1/4)}{(\alpha\beta)^{1/4}}$$

is the one-particle partition function. Finally,

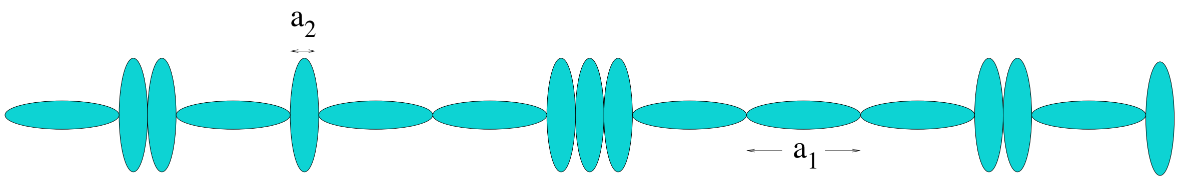
$$\mathcal{Z} = (L/4)^N \Big(\frac{2\pi m}{\beta}\Big)^{N/2} \Big(\frac{\Gamma(1/4)}{(\alpha\beta)^{1/4}}\Big)^N$$

The entropy is given by Eq. (4.36)

$$S = k_B\Big(\ln \mathcal{Z} - \beta \frac{\partial}{\partial \beta} \ln \mathcal{Z}\Big) \;=\; N k_B \Big(\ln z - \beta \frac{\partial}{\partial \beta} \ln z\Big) \;=\; N k_B (\ln L + \frac{3}{4} \ln k_B T) + \text{const},$$

the energy by Eq. (4.35) and the specific heat by Eq. (4.53)

$$E \;=\; -\frac{\partial}{\partial \beta} \ln Z \;=\; \frac{3}{4} N k_B T \;\;\Rightarrow\;\; c_V \;=\; \frac{1}{L} \frac{\partial E}{\partial T}\Big|_L \;=\; \frac{3}{4} \frac{N}{L} k_B$$



Problem 2.

A simple model of a polymer is a one-dimensional chain consisting of $N \gg 1$ linked segments as shown in Fig. 1. Each segment has two possible states: horizontal with length a_1 and energy E_1 and vertical with length a_2 and energy E_2. The segments are linked such that they cannot come apart. The chain is in thermal equilibrium at temperature T.

Find:

(a) Partition function of the chain, and

(b) Average length of the chain.

Solution:

The state with n horizontal links and $N-n$ vertical links has energy $nE_1 + (N-n)E_2$. There are $C_N^n = \frac{N!}{n!(N-n)!}$ different states with such energy so the partition function is

$$Z_N = \sum_{\text{states}} e^{-\beta E_i} = \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} e^{-\beta n E_1 - \beta(N-n)E_2} = \left(e^{-\beta E_1} + e^{-\beta E_2}\right)^N$$

The average length is given by

$$\begin{aligned}
\langle L \rangle &= \frac{1}{Z_N} \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} [a_1 n + a_2(N-n)] e^{-\beta n E_1 - \beta(N-n)E_2} \\
&= -\frac{1}{Z_N} \Big(\frac{a_1}{\beta} \frac{\partial}{\partial E_1} \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} e^{-\beta n E_1 - \beta(N-n)E_2} + \frac{a_2}{\beta} \frac{\partial}{\partial E_2} \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} e^{-\beta n E_1 - \beta(N-n)E_2} \Big] \\
&= -\frac{a_1}{\beta} \frac{\partial}{\partial E_1} \ln Z_N - \frac{a_2}{\beta} \frac{\partial}{\partial E_2} \ln Z_N = N \frac{a_1 e^{-\beta E_1} + a_2 e^{-\beta E_2}}{e^{-\beta E_1} + e^{-\beta E_2}}
\end{aligned}$$

Quick check: if $E_1 = E_2$ $\langle L \rangle = N\frac{a_1+a_2}{2}$ and if $a_1 = a_2 = a$ $\langle L \rangle = Na$.

Problem 3.

A gas composed of large number of non-interacting spin-0 particles is in thermal equilibrium with the reservoir at temperature T. The particles can be only in two states: ground state with energy E_0 and excited state with energy E_1. Assume that the gas can be described as grand canonical ensemble with chemical potential $\mu < E_0$.

How many particles we expect in the ground state and how many in the excited state?

Solution:

The grand partition function of Bose gas ins given by Eq. (9.49). In our case, instead of states with different $n_{\vec{k}}$ and energies $\epsilon_{\vec{k}}$ we have only two states with energies $_0$ and E_1 so Eq. (9.49) turns to

$$Z_G \;=\; \frac{1}{1-e^{-\beta(E_0-\mu)}}\frac{1}{1-e^{-\beta(E_1-\mu)}}$$

The average occupation numbers can be read from Eq. (9.58):

$$\langle n_0\rangle \;=\; \frac{e^{-\beta(E_0-\mu)}}{1-e^{-\beta(E_0-\mu)}}, \qquad \langle n_1\rangle \;=\; \frac{e^{-\beta(E_1-\mu)}}{1-e^{-\beta(E_0-\mu)}}.$$

Problem 4.

A certain solid contains $N \gg 1$ mutually non-interacting nuclei of spin one. Each nucleus can therefore be in any of three quantum states labeled by the quantum number $m = 1, 0, -1$. Because of electric field gradients within the solid interact with electric quadrupole moment of these nuclei, a nucleus in the state with $m = 1$ and $m = -1$ has the same energy $\epsilon > 0$ while its energy in the state $m = 0$ is zero. The solid has a temperature T.

(a) Find the partition function and the entropy of the nuclei in this solid (hint: Eq. (7.8) from the lecture notes).

(b) Find the average number of nuclei in the state $m = 0$.

(c) What happens with this average number if $T \to \infty$ and $T \to 0$?

Solution:

From Eq. (7.8)

$$Z \;=\; z^N$$

where z is a partition function for one nucleus

$$z \;=\; \sum_m e^{-\beta E_m} \;=\; 2e^{-\beta\epsilon}+1$$

so

$$Z \;=\; (2e^{-\beta\epsilon}+1)^N$$

and the entropy is given by Eq. (4.36)

$$S \;=\; k_B(\ln Z - \beta\frac{\partial}{\partial\beta}\ln Z) \;=\; Nk_B\Big[\ln\left(2e^{-\beta\epsilon}+1\right) + \frac{2\beta\epsilon e^{-\beta\epsilon}}{2e^{-\beta\epsilon}+1}\Big]$$

The probability for one particle to be in the state with $m = 0$ is

$$\frac{1}{1 + 2e^{-\beta\epsilon}}$$

so the average number of particles in $m = 0$ state is

$$N_0 \;=\; \frac{N}{1 + 2e^{-\beta\epsilon}}$$

As $T \to 0$ ($\beta \to \infty$) $N_0 \to N$ so all the particles are in the ground state. Conversely, as $T \to \infty$ ($\beta \to 0$) $N_0 = \frac{N}{3}$ so the particles are distributed uniformly between states with $m = 1$, $m = 0$, and $m = -1$.

Problem 5:

Suppose that the Hamiltonian of a system of non-interacting atoms with spin s placed in the uniform magnetic field pointing in z direction can be written as

$$\hat{H} \;=\; \hat{H}_0 - \hat{M}B$$

where the first term does not depend explicitly on the magnetic field B and $\hat{M} = \mu \sum_i \hat{s}_z^{(i)}$ ($\hat{s}^{(i)}$ is the spin operator for an atom and μ is Bohr magneton).

Express the susceptibility

$$\chi \;=\; \frac{\partial \mathcal{M}}{\partial B}$$

in terms of temperature, average magnetization $\langle M\rangle$ and average $\langle M^2\rangle$.

Solution.

The partition function is

$$Z \;=\; \mathrm{Tr}(e^{-\beta\hat{H}_0 + \beta B\hat{M}})$$

The magnetization is given by Eq. (11.4)

$$\mathcal{M} \;=\; \frac{1}{\beta V}\frac{\partial}{\partial B}\ln Z \;=\; \frac{1}{V}\frac{\mathrm{Tr}(\hat{M}e^{-\beta\hat{H}_0 + \beta B\hat{M}})}{\mathrm{Tr}(e^{-\beta\hat{H}_0 + \beta B\hat{M}})}$$

and therefore the susceptibility has the form

$$\chi \;=\; \frac{\partial \mathcal{M}}{\partial B} \;=\; \frac{\beta}{V}\frac{\mathrm{Tr}(\hat{M}^2e^{-\beta\hat{H}_0 + \beta B\hat{M}})}{\mathrm{Tr}(e^{-\beta\hat{H}_0 + \beta B\hat{M}})} - \frac{\beta}{V}\left[\frac{\mathrm{Tr}(\hat{M}e^{-\beta\hat{H}_0 + \beta B\hat{M}})}{\mathrm{Tr}(e^{-\beta\hat{H}_0 + \beta B\hat{M}})}\right]^2 \;=\; \frac{\langle M^2\rangle - \langle M\rangle^2}{k_B T V}$$