

PHY5524 Problem Set 2: Solution

Problem 1

(a) The partition function for a single one-dimensional quantum oscillator is

$$Q_1(T) = \sum_n e^{-\beta E_n} \quad (1)$$

$$= \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega_0} \quad (2)$$

$$= e^{-\beta\hbar\omega_0/2} \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega_0} \quad (3)$$

$$= e^{-\beta\hbar\omega_0/2} \sum_{n=0}^{\infty} (e^{-\beta\hbar\omega_0})^n \quad (4)$$

$$= e^{-\beta\hbar\omega_0/2} \frac{1}{1 - e^{-\beta\hbar\omega_0}} \quad (5)$$

If we have N three-dimensional quantum oscillators the total partition function is then

$$Q_N(T) = Q_1(T)^{3N} = \left(\frac{e^{-\beta\hbar\omega_0/2}}{1 - e^{-\beta\hbar\omega_0}} \right)^{3N} \quad (6)$$

(b) Given Q_N the Helmholtz free energy is easily found to be

$$A = -k_B T \ln Q_N(T) = 3N k_B T \ln \left(1 - e^{-\hbar\omega_0/k_B T} \right) + \frac{3}{2} N \hbar\omega_0. \quad (7)$$

(c) To find the specific heat we can first compute the internal energy

$$E = -\frac{\partial}{\partial \beta} \ln Q_N(T) \quad (8)$$

$$= 3N \hbar\omega_0 \left(\frac{1}{2} + \frac{1}{e^{\beta\hbar\omega_0} - 1} \right) \quad (9)$$

The specific heat is then

$$C(T) = \frac{\partial \langle E \rangle}{\partial T} = 3N k_B \left(\frac{\hbar\omega_0}{k_B T} \right)^2 \frac{e^{\beta\hbar\omega_0}}{(e^{\beta\hbar\omega_0} - 1)^2} \quad (10)$$

In the limit $k_B T \gg \hbar\omega_0$ we have $e^{\hbar\omega_0/k_B T} \simeq 1 + \frac{\hbar\omega_0}{k_B T}$ and

$$C(T) \simeq 3N k_B \left(\frac{\hbar\omega_0}{k_B T} \right)^2 \frac{1}{\left(1 + \frac{\hbar\omega_0}{k_B T} - 1 \right)^2} = 3N k_B \quad (11)$$

(the correct classical result) while in the limit $k_B T \ll \hbar\omega_0$,

$$C(T) \simeq 3N k_B \left(\frac{\hbar\omega_0}{k_B T} \right)^2 e^{-\hbar\omega_0/k_B T} \quad (12)$$

which goes to 0 exponentially as $T \rightarrow 0$.

Problem 2

(a) Each electric dipole has four states, two with energy $+aeE/2$ and two with energy $-aeE/2$. The partition function for a single dipole is then

$$Q_1(T) = 4 \cosh \frac{ea\mathcal{E}/2}{k_B T} \quad (13)$$

and for $N = nA$ noninteracting dipoles

$$Q_N(T) = Q_1^N = \left(4 \cosh \frac{ea\mathcal{E}/2}{k_B T} \right)^N \quad (14)$$

(b) Once we have Q_N we can immediately find the Helmholtz free energy,

$$A = -k_B T \ln Q_N = -k_B T N \ln \left(4 \cosh \frac{ea\mathcal{E}}{2k_B T} \right) \quad (15)$$

(c) As in the previous problem, the easiest way to work out the specific heat of the system is to first compute the internal energy E and then take the derivative w.r.t. temperature T . The internal energy E is

$$E = -\frac{\partial}{\partial \beta} \ln Q_N \quad (16)$$

$$= -\frac{\partial}{\partial \beta} N \ln(4 \cosh \beta ea\mathcal{E}/2) \quad (17)$$

$$= -N \frac{ea\mathcal{E}}{2} \tanh(\beta ea\mathcal{E}/2) \quad (18)$$

from which it follows that the specific heat is

$$C(T) = \frac{\partial E}{\partial T} = k_B \left(\frac{eaE}{2k_B T} \right)^2 \frac{1}{\cosh^2 \left(\frac{ea\mathcal{E}}{2k_B T} \right)} \quad (19)$$

(d) We can find the x component of the dipole moment per unit area by using the fact that the total energy E is equal to $-\vec{P} \cdot \vec{E} = -D_x \mathcal{E}$, where \vec{P} is the total dipole moment of the system. The dipole moment per unit area is then $d_x = -D_x/A$ or

$$d_x = n \frac{ea}{2} \tanh(\beta ea\mathcal{E}/2) \quad (20)$$

which, for $k_B T \gg eaE$ goes as

$$d_x \simeq n \left(\frac{ea}{2} \right)^2 \frac{1}{k_B T} \quad (21)$$

(this is the Curie-Weiss behavior we will study later for magnetic moments) and for $k_B T \ll eaE$ is approximately

$$d_x \simeq \frac{ea}{2} \quad (22)$$