PHY5524
Problem Set 2: Solution

Problem 1

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

$$
\begin{aligned}
Q_1(T) &= \sum_n e^{-\beta E_n} && (1)\\
&= \sum_{n=0}^{\infty} e^{-\beta(n+1/2)\hbar\omega_0} && (2)\\
&= e^{-\beta\hbar\omega_0/2}\sum_{n=0}^{\infty} e^{-n\beta\hbar\omega_0} && (3)\\
&= e^{-\beta\hbar\omega_0/2}\sum_{n=0}^{\infty} (e^{-\beta\hbar\omega_0})^n && (4)\\
&= e^{-\beta\hbar\omega_0/2}\frac{1}{1-e^{-\beta\hbar\omega_0}} && (5)
\end{aligned}
$$

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

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

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

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

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

$$
\begin{aligned}
E &= -\frac{\partial}{\partial\beta}\ln Q_N(T) && (8)\\
&= 3N\hbar\omega_0\left(\frac{1}{2}+\frac{1}{e^{\beta\hbar\omega_0}-1}\right) && (9)
\end{aligned}
$$

The specific heat is then

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

In the limit $k_BT \gg \hbar\omega_0$ then $e^{\hbar\omega_0/k_BT} \simeq 1+\frac{\hbar\omega_0}{k_BT}$ and

$$C(T) \simeq 3Nk_B\left(\frac{\hbar\omega_0}{k_BT}\right)^2\frac{1}{\left(1+\frac{\hbar\omega_0}{k_BT}-1\right)^2} = 3Nk_B \tag{11}$$

while in the limit $k_BT \ll \hbar\omega_0$,

$$C(T) \simeq 3Nk_B\left(\frac{\hbar\omega_0}{k_BT}\right)^2 e^{-\hbar\omega_0/k_BT} \tag{12}$$

Problem 2

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

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

and for $N = nA$ noninteracting dipoles

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

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

$$A = -k_BT\ln Q_N = -k_BTN\ln\left(4\cosh\frac{ea\mathcal{E}}{2k_BT}\right) \tag{15}$$

(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

$$\begin{aligned} E &= -\frac{\partial}{\partial\beta}\ln Q_N && (16)\\ &= -\frac{\partial}{\partial\beta}N\ln(4\cosh\beta ea\mathcal{E}/2) && (17)\\ &= -N\frac{ea\mathcal{E}}{2}\tanh(\beta ea\mathcal{E}/2) && (18)\end{aligned}$$

from which it follows that the specific heat is

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

(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

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

which, for $k_BT \gg eaE$ goes as

$$d_x \simeq n\left(\frac{ea}{2}\right)^2\frac{1}{k_BT} \tag{21}$$

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

$$d_x \simeq \frac{ea}{2} \tag{22}$$