Statistical Mechanics - Homework 3

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PROBLEM 1

For a single particle, the Hamiltonian is

$$H = \frac{p^2}{2m} + mgh$$

which immediately leads to

$$dw = \frac{dx^3 dp^3}{(2\pi\hbar)^2} c e^{-\beta H}$$

The single-particle partition function is

$$Z_1 = \int \frac{d^3p\ d^3x}{(2\pi\hbar)^3} e^{-\frac{\beta p^2}{2m} - \beta mgh}$$

The p integral gives

$$\int d^3p\ e^{-\frac{\beta p^2}{2m}} = \left(\frac{2\pi m}{\beta}\right)^{3/2}$$

and we can evaluate the x integral in terms of the given dimensions of the air column:

$$Z_1 = \int_0^{h_0} dh\ \frac{S}{(2\pi\hbar)^3} \left(\frac{2\pi m}{\beta}\right)^{3/2} e^{-\beta mgh} = \frac{S\sqrt{m}}{(2\pi)^{3/2}\hbar^3 g \beta^{5/2}} \left(1 - e^{-\beta mgh_0}\right)$$

The full partition function is $Z = \frac{1}{N!} Z_1^N$. The free energy is

$$F = -T \ln Z = T \ln N! - NT \ln Z_1 = T(N \ln N - N) - NT \left[\ln \frac{S\sqrt{m}}{(2\pi)^{3/2}\hbar^3 g \beta^{5/2}} + \ln\left(1 - e^{-\beta mgh_0}\right)\right]$$

The internal energy is (after a bit of algebra)

$$E = -\frac{\partial \ln Z}{\partial \beta} = -\frac{N}{Z_1}\frac{\partial Z_1}{\partial \beta} = \frac{Nmgh_0}{1 - e^{\beta mgh_0}} + \frac{5N}{2\beta}$$

The height of the center of mass of the column is given by the expectation value of h:

$$\langle h \rangle = \frac{1}{Z} \int \frac{d^3p\ d^3x}{(2\pi\hbar)^3}\ h e^{-\frac{\beta p^2}{2m} - \beta mgh} = -\frac{1}{Z}\frac{1}{\beta m}\frac{\partial Z}{\partial g} = \frac{1}{\beta m}\left(\frac{1}{g} - \frac{\beta m h_0}{1 - e^{\beta mgh_0}}\right)$$

The heat capacity is

$$C = \frac{\partial E}{\partial T} = \frac{\partial}{\partial T}\left(\frac{Nmgh_0}{1 - e^{mgh_0/T}} + \frac{5NT}{2}\right) = -\frac{Nm^2g^2h_0^2}{T^2}\frac{e^{mgh_0/T}}{\left(1 - e^{mgh_0/T}\right)^2} + \frac{5N}{2}$$

If we take $mgh_0/T \gg 1$, then the 2nd power of the exponential in the denominator of the first term dominates, making this term irrelevant. Thus, $C \approx 5N/2$. If we take $mgh_0/T \ll 1$, then we can Taylor expand the exponentials in mgh_0/T, which gives

$$C \approx -\frac{N\left(\frac{mgh_0}{T}\right)^2\left(1+\frac{mgh_0}{T}\right)}{\left(1-1-\frac{mgh_0}{T}\right)^2} + \frac{5N}{2} = \frac{5N}{2} - N\left(1+\frac{mgh_0}{T}\right) \sim \frac{3N}{2}$$

For $\langle h\rangle$, $mgh_0/T \gg 1$ eliminates the second term, leaving $\langle h\rangle \approx \frac{T}{mg}$. When $mgh_0/T \ll 1$, we find

$$\langle h\rangle \approx \frac{T}{mg} - \frac{h_0}{1-1-\frac{mgh_0}{T}} = \frac{2T}{mg}$$

PROBLEM 2

Part (a)

The single-particle partition function is

$$Z_1 = \int \frac{d^3p\ d^3x}{(2\pi\hbar)^3}\ e^{-\beta c\,|p|} = \frac{V}{(2\pi\hbar)^3}\int dp_x\ dp_y\ dp_z e^{-\beta c\sqrt{px^2+p_y^2+p_z^2}}$$

Switching to polar coordinates:

$$Z_1 = \frac{V}{(2\pi\hbar)^3}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \int_0^{\infty} dr\ r^2 \sin\theta e^{-\beta cr} = \frac{VT^3}{\pi^2\hbar^3c^3}$$

so the multiparticle partition function is

$$Z = \frac{1}{N!}\left(\frac{VT^3}{\pi^2\hbar^3c^3}\right)^N$$

The free energy is

$$F = T\ln\frac{1}{Z} = T(N\ln N - N) + NT\ln\frac{\pi^2\hbar^3c^3}{VT^3}$$

The internal energy is

$$E = -\frac{\partial \ln Z}{\partial\beta} = -N\frac{\partial}{\partial\beta}\left[\ln\left(\frac{V}{\pi^2\hbar^3c^3\beta^3}\right)\right] = \frac{3N}{\beta}$$

Using $F = E - TS$ we find the entropy:

$$S = 4N - N\ln N - N\ln\frac{\pi^2\hbar^3c^3}{T^3V}$$

The pressure is

$$P = -\left(\frac{\partial F}{\partial V}\right)_T = \frac{NT}{V}$$

Part (b)

We previously saw that the equation of state is $PV = NT$. We want to calculate $\left(\frac{\partial P}{\partial V}\right)_S$ and $\left(\frac{\partial T}{\partial V}\right)_S$. From our expression for S, we see that for it to be constant, we must have $T^3 V = c$, where c is a constant. Solving for T, we find $T = (c/v)^{1/3}$, so we can substitute this into the equation of state to find

$$P(V) = Nc^{1/3}V^{-4/3} \implies \left(\frac{\partial P}{\partial V}\right)_S = -\frac{4}{3}V^{-7/3}Nc^{1/3} = -\frac{4}{3}\frac{NT}{V^2} = -\frac{4}{3}\frac{P}{V}$$

Now that we know this, the other derivative is easy to find:

$$\left(\frac{\partial T}{\partial V}\right)_S = \frac{1}{N}\left(V\frac{\partial P}{\partial V} + P\right) = -\frac{4}{3}\frac{T}{V} + \frac{P}{N} = -\frac{1}{3}\frac{T}{V}$$

PROBLEM 3

Since we only care about the angular probability distribution, we can get away with not integrating over all of phase space. The single particle partition function is

$$Z_1 = \int_0^\pi d\theta \ \sin\theta e^{\beta\vec{b}\cdot\vec{\varepsilon}} = \int_0^\pi d\theta \ \sin\theta e^{\beta b\varepsilon\cos\theta} = \frac{2\sinh(\beta b\varepsilon)}{\beta b\varepsilon}$$

This tells us that the angular distribution is

$$dw_\theta = \frac{1}{Z_1}d\theta e^{\beta\vec{b}\cdot\vec{\varepsilon}}$$

which gives

$$\frac{dw_\theta}{d\theta} = \frac{d}{d\theta}\left(\frac{e^{\beta b\varepsilon\cos\theta}\beta b\varepsilon}{2\sinh(\beta b\varepsilon)}\right) = -\frac{\sin\theta\,(\beta b\varepsilon)^2\, e^{\beta b\varepsilon\cos\theta}}{2\sinh(\beta b\varepsilon)}$$

In homework 2, we defined total magnetization as $E = -HM$. Defining polarization as the electric field analogue of this, we have

$$P = -\frac{E}{\varepsilon} = \frac{1}{\varepsilon}\frac{\partial\ln Z}{\partial\beta} = \frac{N}{\varepsilon}\frac{\partial}{\partial\beta}\left[\ln\frac{2\sinh(\beta b\varepsilon)}{\beta b\varepsilon}\right] = \frac{N}{\varepsilon}\left(\frac{b\varepsilon}{2\sinh(\beta b\varepsilon)}2\cosh(\beta b\varepsilon) - \frac{b\varepsilon}{\beta b\varepsilon}\right) = \frac{Nb}{\tanh(\beta b\varepsilon)} - \frac{N}{\beta\varepsilon}$$

As $\beta \to 0$, we can Taylor expand the first term to find

$$P = Nb\left(\frac{1}{\beta b\varepsilon} + \frac{\beta b\varepsilon}{3}\right) - \frac{N}{\beta\varepsilon} = \frac{N\beta b^2\varepsilon}{3} \to 0$$

PROBLEM 4

Part (a)

For a single dipole, the partition function is

$$Z_1 = \sum_{m=-J}^{J} e^{\frac{m\mu H}{JT}}$$

Since the dipoles are not interacting, their energies add linearly, so generalizing the one-dipole partition function gives

$$Z = \frac{1}{N!}\left(\sum_{m=-J}^{J} e^{\frac{m\mu H}{JT}}\right)^N = \frac{1}{N!}\left(\frac{e^{\frac{H\mu}{JT}(1+J)} - e^{-\frac{H\mu}{JT}}}{e^{\frac{H\mu}{JT}} - 1}\right)^N$$

where the factor of $1/N!$ accounts for the fact that the dipoles are indistinguishable. The free energy is

$$F = T\ln\frac{1}{Z} = T\ln N! - NT\ln\left[\frac{e^{\frac{H\mu}{JT}(1+J)} - e^{-\frac{H\mu}{JT}}}{e^{\frac{H\mu}{JT}} - 1}\right] = TN\ln N - TN - NT\ln\left[e^{\frac{H\mu}{JT}(1+J)} - e^{-\frac{H\mu}{JT}}\right] + NT\ln\left[e^{\frac{H\mu}{JT}} - 1\right]$$

The internal energy is

$$E = -\frac{\partial \ln Z}{\partial\beta} = -\frac{\partial}{\partial\beta}\left(N\ln\left[e^{\beta H\mu\frac{1+J}{J}} - e^{-\frac{H\mu\beta}{J}}\right] - N\ln\left[e^{\frac{H\mu\beta}{J}} - 1\right]\right)$$

$$= \frac{NH\mu}{J}\left[\frac{1}{1-e^{-\frac{H\mu\beta}{J}}} - \frac{(1+J)e^{\frac{\beta H\mu(1+J)}{J}} + e^{-\frac{H\mu\beta}{J}}}{e^{\frac{\beta H\mu(1+J)}{J}} - e^{-\frac{H\mu\beta}{J}}}\right] = \frac{NH\mu}{J}\left[\frac{1}{1-e^{-\frac{H\mu\beta}{J}}} - (J+1) - \frac{2+J}{e^{\frac{H\mu\beta}{J}(2+J)} - 1}\right]$$

Part (b)

The magnetization is defined by $E = -HM$, so

$$M = -\frac{J}{N\mu}\left[\frac{1}{1-e^{-\frac{H\mu\beta}{J}}} - (J+1) - \frac{2+J}{e^{\frac{H\mu\beta}{J}(2+J)} - 1}\right]^{-1}$$

The susceptibility is

$$\chi = \left(\frac{\partial M}{\partial H}\right)_T = \frac{\beta}{N}\left[\frac{(2+J)^2 e^{\frac{H\mu\beta}{J}(2+J)}}{\left(e^{\frac{H\mu\beta(2+J)}{J}} - 1\right)^2} - \frac{e^{-\frac{H\mu\beta}{J}}}{\left(1-e^{-\frac{H\mu\beta}{J}}\right)^2}\right]\left[\frac{1}{1-e^{-\frac{H\mu\beta}{J}}} - (J+1) - \frac{2+J}{e^{\frac{H\mu\beta}{J}(2+J)} - 1}\right]^{-2}$$

The dependence of M on T is

$$\left(\frac{\partial M}{\partial T}\right)_H = \frac{H}{4NT^2}\left(\frac{1}{\sinh^2\left(\frac{H\mu}{2JT}\right)} - \frac{(2+J)^2}{\sinh^2\left(\frac{H\mu(2+J)}{2JT}\right)}\right)\left[\frac{1}{1-e^{-\frac{H\mu}{JT}}} - (J+1) - \frac{2+J}{e^{\frac{H\mu}{JT}(2+J)} - 1}\right]^{-2}$$

Part (c)

The heat capacity is

$$\left(\frac{\partial E}{\partial T}\right)_H = \frac{NH^2\mu^2}{4J^2T^2}\left(\frac{1}{\sinh^2\left(\frac{H\mu}{2JT}\right)} - \frac{(2+J)^2}{\sinh^2\left(\frac{H\mu(2+J)}{2JT}\right)}\right)$$