Statistical Mechanics PHY540 Midterm solution

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1 Cerium phase diagram:

We start from Clausius Clapeyron equation:

$$\frac{dp}{dT} = \frac{s_{\alpha} - s_{\alpha'}}{v_{\alpha} - v_{\alpha'}}$$

for molecular volumes and entropies. Evaluate on the coexistence seam:

$$\frac{dp}{dT} = -\frac{30Kbar}{1000K}$$

we find:

$$s_{\alpha} - s_{\alpha'} = \left(-0.044 \times 2.65 \times 10^{-29} \frac{m^3}{atom}\right) \times \left(-\frac{30 Kbar}{1000 K}\right) = 3.5 \times 10^{-24} \frac{J}{K~atom}$$

the heat could be obtained from dQ = TdS and is:

$$400K \times \Delta s = 1.4 \frac{J}{atom} = 0.009 \frac{eV}{atom}$$

which should be absorbed on the transition $\alpha \to \alpha'$.

2 d = 2 gas:

The one particle partition function is:

$$z_1 = \frac{A}{\lambda^2} = \frac{2\pi m AkT}{h^2}$$

and the full partition function is therefore:

$$Z(T,V,N) = \frac{1}{N!} z_1^N = \frac{1}{N!} \left(\frac{2\pi m AkT}{h^2} \right)^N$$

Following the advice we ignore Gibbs factor as we are not concerned with explicit N-derivatives of the partition function (though it DOES change the entropy!).

The free energy reeds:

$$F = -kT \log Z = -NkT \log \left(\frac{2\pi mAkT}{h^2}\right)$$

The pressure is:

$$p = -\frac{dF}{dA} = \frac{NkT}{A}$$

which is analogous to the ideal gas in d = 3.

The entropy is given by:

$$S = -\frac{dF}{dT} = Nk \log \left(\frac{2\pi mAkT}{h^2}\right) + Nk$$

the Energy could be calculated by:

$$U = F + TS = NkT$$

which is what we expect from equipartition. This result IS independent of the question weather Gibbs factor is introduced in the calculation.

3 Magnetisation issues:

The one particle partition function is:

$$z_1 = e^{-\beta E_0} + e^{-\beta (E_0 + \Delta - \mu H)} + e^{-\beta (E_0 + \Delta)} + e^{-\beta (E_0 + \Delta + \mu H)}$$

the magnetisation would not be effected by Gibbs factor issues and we can write:

$$Z_N = z_1^N \Rightarrow F = -NkT \log \left(e^{-\beta E_0} + e^{-\beta (E_0 + \Delta - \mu H)} + e^{-\beta (E_0 + \Delta)} + e^{-\beta (E_0 + \Delta + \mu H)} \right)$$

or using the more convenient formulation:

$$F = -NkT \log \left(e^{-\beta(E_0 + \Delta)} \left[1 + e^{\beta \Delta} + 2 \cosh(\beta \mu H) \right] \right)$$

the magnetisation is:

$$M = -\frac{dF}{dH} = \frac{2N\mu\sinh(\beta\mu H)}{1 + e^{\beta\Delta} + 2\cosh(\beta\mu H)}$$

the susceptibility is:

$$\lim_{H \to 0} \frac{M}{H} = \frac{2N\mu}{3 + e^{\beta\Delta}} \lim_{H \to 0} \frac{\sinh(\beta\mu H)}{H} = \frac{2N\mu}{3 + e^{\beta\Delta}} \beta\mu$$