Statistical Physics Tutorial 2 March 6, 2022

1. a)

$$H_N\{s_i\} = -h\sum_{i=1}^N s_i$$

Thus:

$$Z_{N} = \sum_{s_{1}=\pm 1} \sum_{s_{2}=\pm 1} \cdots \sum_{s_{N}=\pm 1} \exp\left\{-\beta h \sum_{i=1}^{N} s_{i}\right\}$$

$$= \sum_{s_{1}=\pm 1} \sum_{s_{2}=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \exp\left\{-\beta h \sum_{i=1}^{N-1} s_{i}\right\} \left(\sum_{S_{N}=\pm 1} \exp\left\{-\beta h s_{N}\right\}\right)$$

$$= \sum_{s_{1}=\pm 1} \sum_{s_{2}=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \exp\left\{-\beta h \sum_{i=1}^{N-1} s_{i}\right\} \left(e^{\beta h} + e^{-\beta h}\right)$$

$$= \sum_{s_{1}=\pm 1} \sum_{s_{2}=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \exp\left\{-\beta h \sum_{i=1}^{N-1} s_{i}\right\} 2 \cosh(\beta h)$$

$$= 2 \cosh(\beta h) \sum_{s_{1}=\pm 1} \sum_{s_{2}=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \exp\left\{-\beta h \sum_{i=1}^{N-1} s_{i}\right\}$$

$$= 2 \cosh(\beta h) Z_{N-1}$$

And $Z_1 = e^{\beta h} + e^{-\beta h} = 2 \cosh(\beta h)$. It follows that:

$$Z_N = [2\cosh(\beta h)]^N$$

Now for the average magnetization $\langle s_i \rangle$:

$$\langle s_{i} \rangle = \frac{1}{Z_{N}} \sum_{s_{1}=\pm 1} s_{1} \sum_{s_{2}=\pm 1} s_{2} \cdots \sum_{s_{N}=\pm 1} s_{N} \exp \left\{ -\beta h \sum_{i=1}^{N} s_{i} \right\}$$

$$= \frac{1}{Z_{N}} \sum_{s_{1}=\pm 1} s_{1} \sum_{s_{2}=\pm 1} s_{2} \cdots \sum_{s_{N-1}=\pm 1} \exp \left\{ -\beta h \sum_{i=1}^{N-1} s_{i} \right\} \sum_{s_{N}=\pm 1} s_{N} \exp \left\{ -\beta h s_{N} \right\}$$

$$= \frac{1}{Z_{N}} \sum_{s_{1}=\pm 1} s_{1} \sum_{s_{2}=\pm 1} s_{2} \cdots \sum_{s_{N-1}=\pm 1} \exp \left\{ -\beta h \sum_{i=1}^{N-1} s_{i} \right\} [-2 \sinh(\beta h)]$$

$$\vdots$$

$$= \frac{[-2 \sinh(\beta h)]^{N}}{Z_{N}}$$

$$= [- \tanh(\beta h)]^{N}$$

2. The cannonical partition function for an ideal gas is:

$$Z_N = \frac{1}{h^3 N!} \int d^{3N} p \ d^{3N} q e^{-\beta H}$$

$$= \frac{1}{\lambda^{3N} N!} \int d^{3N} q \exp\left\{-\beta \sum_{i < j} u_{ij}\right\}$$

$$= \frac{1}{\lambda^{3N} N!} \int d^{3N} q e^{-\beta \times 0}$$

$$= \frac{1}{\lambda^{3N} N!} \int d^{3N} q$$

$$= \frac{V^N}{\lambda^{3N} N!}$$

Since there is no interaction between ideal gas molecules. We can use this to evaluate the grand partion function for an ensemble of ideal gas samples:

$$3 = \sum_{N=0}^{\infty} z^N \frac{V^N}{\lambda^{3N} N!}$$
$$= \sum_{N=0}^{\infty} \frac{(zV/\lambda^3)^N}{N!}$$
$$= e^{zV/\lambda^3}$$

We also have that:

$$P = \frac{k_B T}{V} \ln \mathfrak{Z} = z \frac{k_B T}{\lambda^3} \Rightarrow \frac{P}{k_B T} = \frac{z}{\lambda^3}$$

and:

$$\langle N \rangle = z \frac{\partial}{\partial z} \left[\frac{zV}{\lambda^3} \right] = \frac{zV}{\lambda^3} \Rightarrow \frac{\langle N \rangle}{V} = \frac{z}{\lambda^3}$$

From which we deduce:

$$\frac{P}{k_BT} = \frac{\langle N \rangle}{V} \Rightarrow PV = \langle N \rangle k_BT$$

3. We have:

$$\frac{1}{\lambda^3} \sum_{l=1}^{\infty} b_l z^l = \frac{P}{k_B T} = \frac{1}{\lambda^3} \sum_{l=1}^{\infty} a_l \times \left(\lambda^3 \frac{\langle N \rangle}{V}\right)^l$$

$$\Rightarrow \sum_{l=1}^{\infty} b_l z^l = \sum_{l=1}^{\infty} a_l \times \left(\sum_{k=1}^{\infty} k b_k z^k\right)^l$$

Now we match coefficients of z. The only way to get a z term on the right handside is if l = k = 1:

$$b_1 z = a_1 \times b_1 z \Rightarrow a_1 = 1$$

Also note that:

$$b_1 = \frac{1}{V} \int_V d^3 r = 1 \Rightarrow a_1 = b_1 = 1$$

For the z^2 terms, the only way to get z^2 on the right is if l=1 and k=2 or if l=2 and k=1

$$b_2 z^2 = a_1 \times (2b_2 z^2) + a_2 \times (b_1 z^1)^2$$

 $\Rightarrow b_2 = 2b_2 + a_2$
 $\Rightarrow a_2 = -b_2$

Where I used the fact that $a_1 = b_1 = 1$. For the z^3 terms, the only way to get z^3 on the right is if l = l and k = 3 or if l = 2 and k = 1, 2 (cross multiplied terms) and l = 3. This is because 3 is a prime number.

$$b_3 z^3 = a_1 \times (3b_3 z^3) + a_2 \times (b_1 z \times 2b_2 z^2 + 2b_2 z^2 \times b_1 z) + a_3 \times (b_1 z)^3$$

$$\Rightarrow b_3 = 3b_3 + (-b_2)(4b_2) + a_3$$

$$\Rightarrow a_3 = 4b_2^2 - 2b_3$$

4. We wish to find $a_2 = -b_2$, to this end note that:

$$\begin{split} b_2 &= \frac{\lambda^3}{2! V \lambda^{3 \times 2}} \int d^3 q_1 \int d^3 q_2 f_{12} \\ &= \frac{1}{2 V \lambda^3} \int d^3 q_1 \int d^3 (q_2 - q_1) \left[e^{-\beta V(|q_2 - q_1|)} - 1 \right] \\ &= \frac{1}{2 V \lambda^3} \int d^3 q_1 \int d^3 x \left[e^{-\beta V(|x|)} - 1 \right] \end{split}$$

Where $x = q_2 - q_1$. Provided that the interaction range of the potential is short the integrals can be treated as approximately independent. This follows from the fact that if q_1 starts differing largely from q_2 , the integrand dependent on x becomes negligible ($V \rightarrow 0$). Thus the integral over x cannot vary much with changing q_1 . Hence:

$$b_{2} \approx \frac{1}{2V\lambda^{3}} \left(\int d^{3}q_{1} \right) \left(\int d^{3}x \left[e^{-\beta V(|x|)} - 1 \right] \right)$$

$$= \frac{1}{2\lambda^{3}} \int d^{3}x \left[e^{-\beta V(|x|)} - 1 \right]$$

$$= \frac{1}{2\lambda^{3}} \int_{0}^{2\pi} d\phi \int_{0}^{\pi} \sin\theta d\theta \int_{0}^{\infty} r^{2} dr \left[e^{-\beta V(|r|)} - 1 \right]$$

$$= \frac{2\pi}{\lambda^{3}} \int_{0}^{\infty} r^{2} dr \left[e^{-\beta V(|r|)} - 1 \right]$$

Now we can use this to evaluate a_2 .

$$a_2 = -b_2 = -\frac{2\pi}{\lambda^3} \int_0^\infty (e^{-\beta V(r)} - 1) r^2 dr$$

$$= -\frac{2\pi}{\lambda^3} \int_0^\alpha (0 - 1) r^2 dr - \frac{2\pi}{\lambda^3} \int_\alpha^\infty (1 - 1) r^2 dr$$

$$= \frac{2\pi}{\lambda^3} \int_0^\alpha r^2 dr$$

$$= \frac{2\pi \alpha^3}{3\lambda^3}$$

5. Doing a similar calculation to the above:

$$a_{2} = -\frac{2\pi}{\lambda^{3}} \int_{0}^{\infty} (e^{-\beta V(r)} - 1)r^{2} dr$$

$$= -\frac{2\pi}{\lambda^{3}} \left[\int_{0}^{\alpha} (0 - 1)r^{2} dr + \int_{\alpha}^{2\alpha} (e^{\beta v_{0}/kT} - 1)r^{2} dr - \int_{2\alpha}^{\infty} (1 - 1)r^{2} dr \right]$$

$$= -\frac{2\pi}{\lambda^{3}} \left[-\frac{\alpha^{3}}{3} + (e^{\beta v_{0}} - 1) \left(\frac{8\alpha^{3}}{3} - \frac{\alpha^{3}}{3} \right) \right]$$

$$= -\frac{2\pi\alpha^{3} (7e^{v_{0}/kT} - 8)}{3\lambda^{3}}$$

It can been seen from this that a_2 is negative for low T, and is positive for high T when the exponential is large and small respectively. Thus a_2 does change sign with temperature.