"HOMEWORK" 5 Solution

1) $V(r) = \begin{cases} \infty & \text{if } r \leq a \\ 0 & \text{if } r > a \end{cases}$

The virial coefficients are found by utilizing the cluster expansion,

$$a_3(T) \equiv -\frac{1}{3\lambda^6}\int_0^\infty\int_0^\infty f_{12} f_{23} f_{13}\, d^3r_{12}\, d^3r_{13} \qquad \text{(Pathria 9.2.5)}$$

$f_{ij} \equiv e^{-\beta u_{ij}} - 1$ where u_{ij} is the potential between particles i and j

With this $V(r)$,

$$f_{ij} = \begin{cases} -1 & \text{if } r_{ij} \leq a \\ 0 & \text{if } r_{ij} > a \end{cases}$$

So f_{ij} just puts boundaries on the integral,

$$a_3(T) = \frac{1}{3\lambda^6}\int_0^\infty d^3r_{12}\int_0^\infty d^3r_{13}\,(r_{12} \leq a)(r_{13} \leq a)(r_{23} \leq a)$$

$$= \frac{1}{3\lambda^6}\int_0^a dr_{12}\, r_{12}^2 \int d\Omega_{12} \int_0^a dr_{13}\, r_{13}^2 \int d\Omega_{13}\,(r_{23} \leq a)$$

where,

$$r_{23} = |\vec{r}_{23}| = |\vec{r}_{12} - \vec{r}_{13}| = \sqrt{(\vec{r}_{12}-\vec{r}_{13})\cdot(\vec{r}_{12}-\vec{r}_{13})} = \sqrt{r_{12}^2 + r_{13}^2 - 2r_{12}r_{13}\cos\theta}$$

The integral only contains the angle between the vectors, so integrate out one of the solid angles, and let the z-axis of the other be chosen to lie in the direction of the first angle,

$$= \frac{4\pi}{3\lambda^6}\int_0^a dr_{12}\, r_{12}^2 \int_0^a dr_{13}\, r_{13}^2 \int_{-1}^1 d(\cos\theta)\int_0^{2\pi} d\phi\,(r_{23} \leq a)$$

$$r_{23} \leq a \Rightarrow r_{12}^2 + r_{13}^2 - 2r_{12}r_{13}\cos\theta \leq a^2$$

$$\cos\theta \geq \frac{r_{12}^2 + r_{13}^2 - a^2}{2r_{12}r_{13}}$$

If $r_{12} + r_{13} \leq a$, there is no constraint on the angle θ, but if $r_{12} + r_{13} > a$, the angle is constrained (since $|\vec{r}_{12} - \vec{r}_{13}| \leq |\vec{r}_{12}| + |\vec{r}_{13}|$), so we break the integral in to two parts,

$$= \frac{8\pi^2}{3\lambda^6}\int_0^a dr_{12}\, r_{12}^2 \left[\int_0^{a-r_{12}} dr_{13}\int_{-1}^1 d\cos\theta + \int_{a-r_{12}}^a dr_{13}\int_{\frac{r_{12}^2+r_{13}^2-a^2}{2r_{12}r_{13}}}^1 d(\cos\theta)\right] r_{13}^2 \qquad \begin{matrix} r_{12} \to r \\ r_{13} \to x \end{matrix}$$

$$= \frac{8\pi^2}{3\lambda^6}\int_0^a dr\, r^2 \left[\frac{2}{3}(a-r)^3 + \int_{a-r}^a \left(1 - \frac{r^2+x^2-a^2}{2rx}\right) x^2\, dx\right]$$

$$= \frac{\pi^2 a^6}{\lambda^6}\,\frac{5}{18} \qquad \text{after integrating a bunch of polynomials}$$

This problem is also worked with Pathria in §9.3 where he uses a slightly different method to work the integral.

2) For the general 1D Ising model,

$$H = \sum_{ij} J_{ij}\sigma_i\sigma_j + \sum_i h\sigma_i \qquad \text{with } \sigma_i = \pm 1$$

We can write down the partition function,

$$Z = \sum_{\{\sigma_i\}} e^{-\beta H(\{\sigma_i\})} \qquad \text{where } \sum_{\{\sigma_i\}} = \left(\prod_i \sum_{\sigma_i}\right)$$

The free energy,

$$A = -kT \log Z$$

The susceptibility $\chi = -\frac{d^2 A}{dh^2}$, so,

$$\frac{\partial}{\partial h}\left(\frac{A}{-kT}\right) = \frac{1}{Z}\frac{\partial Z}{\partial h} = \frac{1}{Z}\sum_{\{\sigma_i\}}\sum_j \sigma_j e^{-\beta H(\{\sigma_i\})}(-\beta)$$

$$= -\beta \sum_j \langle\sigma_j\rangle$$

$$\frac{\partial^2}{\partial h^2}\left(\frac{A}{-kT}\right) = \frac{-1}{Z^2}\left(\frac{\partial Z}{\partial h}\right)^2 + \frac{\partial^2 Z}{\partial h^2}\Big/ Z$$

$$= \sum_{ij}\left(-\beta^2\langle\sigma_i\rangle\langle\sigma_j\rangle\right) + \frac{-\beta}{Z}\sum_{\{\sigma_i\}}\sum_j \sigma_j\left(\sum_k \sigma_k\right)e^{-\beta H(\{\sigma_i\})}(-\beta$$

$$= -\beta^2\sum_{ij}\langle\sigma_i\rangle\langle\sigma_j\rangle + \beta^2\sum_{ij}\langle\sigma_i\sigma_j\rangle$$

Remember that $\langle x\rangle = \frac{1}{Z}\sum_{\{\sigma_i\}} x e^{-\beta H(\{\sigma_i\})}$. So, plugging this into

$$\chi = -\left(-kT\right)\frac{\partial^2}{\partial h^2}\left(\frac{A}{-kT}\right)$$

$$= \beta\sum_{ij}\left(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle\right)$$