Course on "Advanced Statistical Physics"
Spring Semester (2016)
School of Nano Science, Institute for Research in Fundamental Sciences (IPM), Tehran, Iran
Lecturer: Ali Naji (School of Physics, IPM)
Tutor: Bahman Roostaei (School of Physics, IPM)

Homework #7: Virial Expansion Due: May 21, 2016

Note: *References from which some of the following problems have been taken are available upon request.*

1: A gas in d dimensions has pairwise interaction potential $\Phi(|\mathbf{r}_i - \mathbf{r}_j|)$ between its constituent particles given by

$$\Phi(r) = \begin{cases} \infty & 0 < r < a \\ -\varepsilon & a < r < b \\ 0 & b < r < \infty \end{cases}$$

(i) Compute the second virial coefficient $B_2(T)$ and interpret its behavior in the limits $T \to \infty$ and $T \to 0$, both for $\varepsilon > 0$ and $\varepsilon < 0$.

(ii) Using $\Phi(r)$ as a model for the potential between two argon atoms in three dimensions, find suitable values of ε and of the ratio a/b, given that argon has a Boyle temperature of 410 K and a maximum Joule-Kelvin inversion temperature of 720 K.

2: Compute the second virial coefficient for the weakly coupled particles with potential $V(r) = V_0$ for $r < R$ and $V(r) = 0$ for $r > R$.

3: The third virial coefficient can be written as

$$B_3 = -\frac{1}{3}\int d\mathbf{r}_{12}\int d\mathbf{r}_{13} f(\mathbf{r}_{12}) f(\mathbf{r}_{13}) f(\mathbf{r}_{13} - \mathbf{r}_{12}) \tag{1}$$

where $f(\mathbf{r}) = e^{-\beta V(\mathbf{r})} - 1$ and $V(\mathbf{r})$ is the interaction potential between particles with relative position $\mathbf{r}$.

(i) Show that the third virial coefficient can be written as

$$B_3 = -\frac{1}{3}\frac{1}{(2\pi)^3}\int d\mathbf{k}\ \tilde{f}(\mathbf{k})\tilde{f}(-\mathbf{k})\tilde{f}(-\mathbf{k}), \tag{2}$$

where the Fourier transform of $f(\mathbf{r})$ is defined as $\tilde{f}(\mathbf{k}) = \int e^{i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{r})$.

(ii) Compute $\tilde{f}(\mathbf{k})$ for a gas of hard spheres with radius R.

(iii) Use part (ii) to compute the third virial coefficient for a hard-sphere gas.

4: The second virial coefficient $B_2(T)$ has been measured for nitrogen as a function of T (although nitrogen is diatomic, it can be shown that the single atom arguments still hold). Calculate $B_2(T)$ numerically for the Lennard-Jones potential

$$U(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{3}$$

with the values $\epsilon/k_B = 95$ K and $\sigma = 3.74$ Å. Search for the published values and compare your results with them. Don't forget to mention the references.