Problem Set 8

Problem 1 (40)

The Ornstein-Zernike equation is the integral equation for the correlation function $h(r) = g(r) - 1$ which expresses it in terms of the so-called "direct correlation" $c(r)$ via

$$h(r_{12}) = c(r_{12}) + \rho \int d^3\vec{r}_3 c(r_{13}) h(r_{32}) \tag{1}$$

It may be regarded as the definition of $c(r)$ in terms of the radial distribution function $g(r)$. However, if one were to take $c(r) = f(r) = e^{-\beta\phi(r)} - 1$ which is the leading term in the low density expansion of $g(r) - 1$, O-Z equation would produce some approximation of $h(r)$. Generate a low density expansion (solving this equation by iteration) and show which diagrams are included. Compare with the result of problem #2 (PS#7).

Problem 2 (60) Consider potential

$$\phi(r) = \infty \quad for \quad r < a \tag{2}$$

$$= \epsilon \frac{c-r}{c-a} \quad a < r < b \tag{3}$$

$$= 0 \quad r > b \tag{4}$$

where $\epsilon > 0$ and $c > a$.

a) Sketch and comment briefly on the reasonableness of the potential as a model of liquid for $c = b/2$, $c = b$ and $c = 2b$.

b) Sketch $g(r)$ in the limit of low density for a couple of temperatures when $c = 2b$

c) In the same limit of low density calculate the scattering intensity $I(k)$ when $c = \infty$.

d) Determine corresponding compressibility κ_T from your results.

e) Sketch your answer as a function of k for the case $\epsilon = 0$ and find the 1st non-zero correction term in the expansion of $I(k)$ in powers of ka about $k = 0$.

f) By considering a general potential $\phi(r)$ and expanding $I(k)$ in the powers of k, determine what information about the potential is obtained by determining this leading correction term at low densities.