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

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

\[
\phi(r) = \begin{cases} 
\infty & \text{for } r < a \\
e^\frac{\epsilon r}{c-a} & a < r < b \\
0 & r > b
\end{cases}
\] (2-4)

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 \( \kappa_T \) 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.