The Bhatia–Thornton Structure Factor

“Number Density – Concentration” for Hard-Core Fluid in the Random Phase Approximation

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Abstract

The expression for the Bhatia-Thornton partial structure factor “number density – concentration” for arbitrary two-component hard-core fluid in the random phase approximation is obtained.

Keywords: Hard-core mixture, random phase approximation, Bhatia-Thornton partial structure factors

As we noted in previous papers, the Ashcroft-Langreth (AL) partial structure factors \[ S_{ij}(q), \] can be written for the hard-core (HC) model potential in the random phase approximation (RPA) [2]:

\[
S_{ij}^{\text{RPA-HC}}(q) = \frac{1 - c_i \rho \rho_{ij}^{\text{HS}}(q) + c_i \rho \beta \phi_{ij}(q)}{Z(q)}, \quad (1)
\]

\[
S_{ij}^{\text{RPA-HC}}(q) = \frac{c_i c_j \rho \rho_{ij}^{\text{HS}}(q) - c_i \rho \beta \phi_{ij}(q)}{Z(q)}, \quad (2)
\]

\[
Z(q) = \prod_{k=1,2} \left(1 - c_k \rho \rho_{ik}^{\text{HS}}(q)\right) - c_i c_j \rho^2 \rho_{ij}^{\text{HS}}(q) + \prod_{k=1,2} \left(1 + c_k \rho \beta \phi_{ik}(q)\right) - c_i c_j \rho^2 \beta^2 \phi_{ij}(q) - \right.
\]

\[
-1 - c_i c_j \rho^2 \beta \left(\sum_{k,l} c_{ik}^{\text{HS}}(q)\phi_{jl}(q) - 2c_{ij}^{\text{HS}}(q)\phi_{ij}(q)\right), \quad (3)
\]

where \( c_i \) is the concentration of the \( i \)-th component, \( \rho \) - the mean atomic...
density of a binary mixture, $\beta = (k_B T)^{-1}$, $k_B$ - Boltzmann constant, $T$ - temperature, $c_{ij}^{\text{HS}}(q)$ and $c_{ii}^{\text{HS}}(q)$ - hard-sphere (HS) model partial direct correlation functions, $\phi_{ij}(q)$ and $\phi_{ii}(q)$ - Fourier transforms of the HC-outside parts of the HC partial pair potentials, $i,j=1,2$ ($i \neq j$).

The Bhatia-Thornton [3] structure factor “number density – concentration”, $S_{nc}(q)$, is usually expressed via AL structure factors by the following way:

$$S_{nc}(q) = c_1 c_2 \left[ S_{11}(q) - S_{22}(q) + \frac{(c_2 - c_1)S_{12}(q)}{\sqrt{c_1 c_2}} \right]. \quad (4)$$

In terms of the work [2] Eq. (4) can be rewritten as

$$S_{nc}(q) = c_i c_j \left[ S_{ii}(q) - S_{jj}(q) + \frac{(c_j - c_i)S_{ii}(q)}{\sqrt{c_i c_j}} \right]. \quad (5)$$

Combining Eq. (5) with Eqs. (1)-(3) we obtain the RPA-HC expression for $S_{nc}(q)$:

$$S_{nc}^{\text{RPA-HC}}(q) = c_i c_j \rho \left\{ c_i c_j^{\text{RPA-HC}}(q) - c_i c_j^{\text{RPA-HC}}(q) + 2(c_j - c_i)c_j^{\text{RPA-HC}}(q) \right\} \frac{Z(q)}{Z(q)} \quad (6)$$

where

$$c_i^{\text{RPA-HC}}(r) = c_i^{\text{HS}}(r) - \beta \phi_{ii}(r), \quad (7)$$

and

$$c_j^{\text{RPA-HC}}(q) = c_j^{\text{HS}}(q) - \beta \phi_{jj}(q). \quad (8)$$

References


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