Adv. Studies Theor. Phys., Vol. 8, 2014, no. 15, 661 - 662
HIKARI Ltd, www.m-hikari.com
http://dx.doi.org/10.12988/astp.2014.4557

The Bhatia–Thornton Structure Factor "Number Density – Number Density" for the Hard-Core Fluid in Random Phase Approximation

S. P. Kazantsev

Ural Federal University, Mira str. 19, 620002, Ekaterinburg, Russia

Abstract

The expression for the Bhatia-Thornton partial structure factor "number density – number density" 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

The Bhatia-Thornton [1] structure factor "number density – number density", $S_{NN}(q)$, is connected with the Ashcroft-Langreth (AL) partial structure factors [2], $S_{ij}(q)$ (where *i*,*j*=1,2), by the following way:

$$S_{NN}(q) = c_1 S_{11}(q) + c_2 S_{22}(q) + 2\sqrt{c_1 c_2}\, S_{12}(q) \quad . \tag{1}$$

Here, c_i is the concentration of the *i*-th component.

The random phase approximation (RPA) for a classical binary fluid is formulated as follows:

$$c_{ij}^{\mathrm{RPA}}(r) = c_{0ij}(r) - \beta\varphi_{1ij}(r) \quad , \tag{2}$$

where $c_{ij}(r)$ is the partial direct correlation function, $\varphi_{ij}(r)$ - partial pair interatomic potential, $\beta = (k_{\mathrm{B}}T)^{-1}$, k_{B} - Boltzmann constant, T - temperature, symbols "0" and "1" are attributes of a reference system and perturbation, respectively.

Arbitrary hard-core (HC) model potential, $\varphi_{ij}^{\mathrm{HC}}(r)$, can be written as follows:

$$\varphi_{ij}^{\mathrm{HC}}(r)=\begin{cases}\infty, & r<\sigma_{ij}\\ \phi_{ij}(r), & r\geq\sigma_{ij}\end{cases}\quad, \tag{3}$$

where σ_{ij} are the partial HC diameters. For this case, the hard-sphere (HS) model is the reference system and Eq. (2) is being rewritten as follows:

$$c_{ij}^{\mathrm{RPA\text{-}HC}}(r)=c_{ij}^{\mathrm{HS}}(r)-\beta\phi_{ij}(r)\quad. \tag{4}$$

In the wave space Eq. (4) is

$$c_{ij}^{\mathrm{RPA\text{-}HC}}(q)=c_{ij}^{\mathrm{HS}}(q)-\beta\phi_{ij}(q)\quad. \tag{5}$$

Recently, for the potential (3) within the RPA, the expressions for AL partial structure factors were obtained [3]:

$$S_{ii}^{\mathrm{RPA\text{-}HC}}(q)=\frac{1-c_j\rho c_{jj}^{\mathrm{HS}}(q)+c_j\rho\beta\phi_{jj}(q)}{Z(q)}\quad, \tag{6}$$

$$S_{ij}^{\mathrm{RPA\text{-}HC}}(q)=\frac{\sqrt{c_ic_j}\,\rho c_{ij}^{\mathrm{HS}}(q)-\sqrt{c_ic_j}\,\rho\beta\phi_{ij}(q)}{Z(q)}\quad, \tag{7}$$

where ρ - mean atomic density of a mixture, $i\neq j$,

$$Z(q)=\prod_{k=1,2}\left(1-c_k\rho c_{kk}^{\mathrm{HS}}(q)\right)-c_ic_j\rho^2c_{ij}^{\mathrm{HS}2}(q)+\prod_{k=1,2}\left(1+c_k\rho\beta\phi_{kk}(q)\right)-c_ic_j\rho^2\beta^2\phi_{ij}^2(q)-$$
$$-1-c_ic_j\rho^2\beta\left(\sum_{i,j}c_{ii}^{\mathrm{HS}}(q)\phi_{jj}(q)-2c_{ij}^{\mathrm{HS}}(q)\phi_{ij}(q)\right)\quad. \tag{8}$$

Here, we combine Eq. (1) with Eqs. (6)-(8) to obtain the RPA-HC expression for $S_{NN}(q)$:

$$S_{NN}^{\mathrm{RPA\text{-}HC}}(q)=\frac{1+c_1c_2\rho\left\{2c_{12}^{\mathrm{HS}}(q)-c_{11}^{\mathrm{HS}}(q)-c_{22}^{\mathrm{HS}}(q)+\beta\nu(q)\right\}}{Z(q)}\quad, \tag{9}$$

where $\nu(q)$ is the Fourier transform of the ordering potential,

$$\nu(r)=\phi_{11}(r)+\phi_{22}(r)-2\phi_{12}(r)\quad. \tag{10}$$

References

[1] A.B. Bhatia, D.E. Thornton, Structural aspects of the electrical resistivity of binary alloys, Phys. Rev. B, 2 (1970), 3004-3012.

[2] N.W.Ashcroft, D.C.Langreth, Structure of binary liquid mixtures. II., Phys. Rev., 156 (1967), 685-692.

[3] A.B. Finkel’shtein, The Random Phase Approximation for Binary Hard-Core Mixture, Adv. Studies Theor. Phys., 8 (2014), 387-388.

Received: May 11, 2014