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The Random Phase Approximation for Binary Hard-Core Mixture

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Abstract

Expressions of the Ashcroft-Langreth partial structure factors for an arbitrary two-component hard-core fluid in the random phase approximation are presented.

Keywords: Hard-core mixture, random phase approximation, partial structure factor

In general case, the random phase approximation (RPA) for classical binary fluid is formulated as follows:

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

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, i,j=1,2.

For any hard-core (HC) $\varphi_{ij}(r)$,

$$\varphi_{ij}^{\mathrm{HC}}(r) = \begin{cases} \infty, & r < \sigma_{ij} \\ \phi_{ij}(r), & r \geq \sigma_{ij} \end{cases} \quad , \tag{2}$$

where σ_{ij} is the partial HC diameter,

$$c_{ij}^{\mathrm{RPA\text{-}HC}}(r) = c_{ij}^{\mathrm{HS}}(r) - \beta\phi_{ij}(r) \quad . \tag{3}$$

Here, "HS" denotes the hard-sphere model, which for a mixture is described by the following $\varphi_{ij}(r)$:

$$\varphi_{ij}^{\mathrm{HS}}(r)=\begin{cases}\infty, & r<\sigma_{ij}\\ 0, & r\geq\sigma_{ij}\end{cases}\quad, \tag{4}$$

In the wave space Eq. (3) is being rewritten as

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

The Lebowitz exact solution [1] obtained for the additive HS binary mixture in the Percus-Yevick approximation [2] can be used to calculate $c_{ij}^{\mathrm{HS}}(r)$ and $c_{ij}^{\mathrm{HS}}(q)$.

The Ashcroft-Langreth (AL) partial structure factors [3] are expressed as follows ($i\neq j$):

$$S_{ii}(q)=\frac{1-c_j\rho c_{jj}(q)}{\prod\limits_{k=1,2}\left(1-c_k\rho c_{kk}(q)\right)-c_ic_j\rho^2c_{ij}^2(q)}\quad, \tag{6}$$

$$S_{ij}(q)=\frac{\sqrt{c_ic_j}\,\rho c_{ij}(q)}{\prod\limits_{k=1,2}\left(1-c_k\rho c_{kk}(q)\right)-c_ic_j\rho^2c_{ij}^2(q)}\quad, \tag{7}$$

where c_i is the concentration of the *i*-th component, ρ - mean atomic density of a mixture. Combining Eqs. (6) and (7) with Eq. (5) one can obtain after some transformations the expressions of AL partial structure factors within the RPA for an arbitrary $\phi_{ij}(r)$ in a general form:

$$S_{ii}^{\mathrm{RPA\text{-}HC}}(q)=\frac{1-c_j\rho c_{jj}^{\mathrm{HS}}(q)+c_j\rho\beta\phi_{jj}(q)}{\mathrm{Z}(q)}\quad, \tag{8}$$

$$S_{ij}^{\mathrm{RPA\text{-}HC}}(q)=\frac{\sqrt{c_ic_j}\,\rho c_{ij}^{\mathrm{HS}}(q)-\sqrt{c_ic_j}\,\rho\beta\phi_{ij}(q)}{\mathrm{Z}(q)}\quad, \tag{9}$$

$$\mathrm{Z}(q)=\prod_{k=1,2}\left(1-c_k\rho c_{kk}^{\mathrm{HS}}(q)\right)-c_ic_j\rho^2c_{ij}^{\mathrm{HS}2}(q)+\prod_{k=1,2}\left(1+c_k\rho\beta\phi_{kk}(q)\right)-c_ic_j\rho^2\beta^2\phi_{ij}^2(q)-$$

$$-1-c_ic_j\rho^2\beta\left(\sum_{i,j}c_{ii}^{\mathrm{HS}}(q)\phi_{jj}(q)-2c_{ij}^{\mathrm{HS}}(q)\phi_{ij}(q)\right)\quad. \tag{10}$$

Expressions obtained can be used to describe the square-well, triangular-well, hard-core-Yukawa, charged-hard-sphere and other model binary mixtures.

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