Analytical structure factors for colloidal fluids with size and interaction polydispersities

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The hard sphere M Yukawa fluid is considered as a model for a colloidal fluid. On the basis of the mean spherical approximation solution of the Ornstein-Zernike equation, for the case of the closure relation consisting of the sum of the M Yukawa terms with the factorizable coefficients, compact and useful expressions of static structure factors are presented. The expressions are tractable for the hard sphere M Yukawa fluid with intrinsic size and interaction polydispersities as well as for the fluid with an arbitrary number of components. [S1063-651X(98)04609-1]

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I. INTRODUCTION

Many colloidal fluids are polydisperse in size, shape, or interaction, due to the mesoscopic or macroscopic nature of colloidal particles. Knowledge of polydispersity effects on measurable quantities would be essential for us to understand properties of colloids. Since such a colloidal fluid has in general a number of components of a many body system, many workers approached the fluid by analytical methods with the employment of the appropriate models. In particular, analytical expressions for the static structures have been the matters of concern and studied in the models of a polydisperse hard sphere fluid [1–5], a polydisperse charged hard sphere fluid [6,7], and a polydisperse hard sphere Yukawa fluid [8,9].

A polydisperse hard sphere M Yukawa (HSMY) fluid, which is considered below, is one of the most extensive-models, including all the models above as special cases. As far as the present authors are aware, no analytical expression for static structures has been studied yet for the polydisperse HSMY fluid. The aim of the present paper is to present analytical expressions of the partial structure factor, the total structure factor, and the scattering function of the fluid. The expressions are based on the mean spherical approximation (MSA) solution of the Ornstein-Zernike (OZ) equation in the HSMY fluid with an arbitrary number of components.

Now, in the HSMY fluid the MSA is defined by the following closure relation for the OZ equation:

$$g_{ij}(r)=0, \quad r<\sigma_{ij}=(\sigma_i+\sigma_j)/2, \tag{1.1a}$$

$$c_{ij}(r)=\sum_{n=1}^{M} \frac{K_{ij}^{(n)}}{r}\, e^{-z_n r}, \quad r>\sigma_{ij} \tag{1.1b}$$

where $g_{ij}(r)$ and $c_{ij}(r)$ are the radial distribution function and the direct correlation function, respectively, and σ_i is the diameter of a hard-spherical particle of the i component of the fluid. The formal solution of the OZ equation with the closure above is given in terms of the coefficients that are defined to be the physical solution of the system of nonlinear algebraic equations [10,11].

Since the system of equations is too difficult to solve generally, one of the present authors considered the following factorizable case [12–14]:

$$K_{ij}^{(n)}=K^{(n)}d_i^{(n)}d_j^{(n)}. \tag{1.2}$$

In fact, this case gives considerable simplifications for solving the system of equations and has been useful [12–14]. In addition, the simple analytical expressions have been obtained by many workers for thermodynamic quantities [15–19]. Originally, the expressions are due to the special algebraic form of Eq. (1.2). Such an investigation still has been progressing [20].

Now, such an investigation of the effect of the special algebraic form of Eq. (1.2) would be interesting in a structural aspect of the fluid as well. As seen below, the pursuit of the effect results in compact and useful expressions for the static structures: The expressions are tractable even for the fluid with intrinsic size and interaction polydispersities. In Sec. II, we review briefly the MSA solution. Section III gives the expressions of the static structure factors. A discussion is given in Sec. IV.

II. BRIEF REVIEW ON THE SOLUTION

Let us consider the HSMY fluid consisting of spherical particles with the number density of the j component, ρ_j. In the Baxter formalism, the formal solution of the OZ equation with the closure of Eqs. (1.1a) and (1.1b) is given in terms of the Baxter function $Q_{ij}(r)$ as follows [10,11]:

$$Q_{ij}(r)=Q_{ij}^0(r)+\sum_{n=1}^{M} D_{ij}^{(n)}e^{-z_n r}, \tag{2.1a}$$

where

$$Q_{ij}^0(r)=\begin{cases} 0, & r>\sigma_{ij} \text{ or } r<\lambda_{ji}=(\sigma_j-\sigma_i)/2 \\ \frac{1}{2}(r-\sigma_{ij})(r-\lambda_{ji})A_j+(r-\sigma_{ij})\beta_j & \\ \quad +\sum_{n=1}^{M} C_{ij}^{(n)}(e^{-z_n r}-e^{-z_n\sigma_{ij}}), & \lambda_{ji}<r<\sigma_{ij}. \end{cases} \tag{2.1b}$$

The Laplace transform of $Q_{ij}(r)$ is introduced by the definition as [10,11]

$$\tilde{Q}_{ij}(is)=\int_{\lambda_{ji}}^{\infty}dr Q_{ij}(r)e^{-sr}$$
$$=e^{s\lambda_{ij}}\Bigg[\sigma_i^3\psi_1(s\sigma_i)A_j+\sigma_i^2\varphi_1(s\sigma_i)\beta_j+\sum_{n=1}^{M}C_{ij}^{(n)}$$
$$\times e^{-z_n\sigma_{ij}}\left(\frac{e^{z_n\sigma_i}-e^{-s\sigma_i}}{s+z_n}-\frac{1-e^{-s\sigma_i}}{s}\right)$$
$$+\sum_{n=1}^{M}D_{ij}^{(n)}\frac{e^{-z_n\lambda_{ji}}}{s+z_n}\Bigg], \tag{2.2}$$

where $\psi_1(x)\equiv[1-x/2-(1+x/2)e^{-x}]/x^3$, $\varphi_1(x)\equiv(1-x-e^{-x})/x^2$, and $\varphi_0(x)\equiv(1-e^{-x})/x$.

In order to give the most simple expressions for the coefficients A_j, β_j, $C_{ij}^{(n)}$, and $D_{ij}^{(n)}$ above, let us follow our previous work [12,13]. The special form of Eq. (1.2) and the basic assumption of the Baxter formalism permit us to write the following expression for $D_{ij}^{(n)}$:

$$D_{ij}^{(n)}=-d_i^{(n)}a_j^{(n)}e^{z_n\sigma_j/2}, \tag{2.3a}$$

where $a_j^{(n)}$ is determined later. This is the key expression to make the problem remarkably simple. As in the previous paper, we get the following:

$$C_{ij}^{(n)}=(d_i^{(n)}-B_i^{(n)}/z_n)a_j^{(n)}e^{z_n\sigma_j/2}, \tag{2.3b}$$

$$\beta_j=\frac{\pi}{\Delta}\sigma_j+\sum_{n=1}^{M}\Delta^{(n)}a_j^{(n)}, \tag{2.3c}$$

$$A_j=\frac{2\pi}{\Delta}\left(1+\frac{\pi\zeta_2}{2\Delta}\sigma_j\right)+\frac{\pi}{\Delta}\sum_{n=1}^{M}P^{(n)}a_j^{(n)}, \tag{2.3d}$$

where $\zeta_m=\Sigma_l\rho_l\sigma_l^m$, $\Delta=1-\pi\zeta_3/6$,

$$B_i^{(n)}=2\pi\sum_l\rho_l d_l^{(n)}\int_0^{\infty}dr\ re^{-z_nr}g_{il}(r), \tag{2.4}$$

$$\Delta^{(n)}=-\frac{2\pi}{\Delta}\sum_l\rho_l\sigma_l^2\Bigg[\psi_1(z_n\sigma_l)\sigma_lB_l^{(n)}e^{z_n\sigma_l/2}$$
$$+\frac{1+z_n\sigma_l/2}{(z_n\sigma_l)^2}d_l^{(n)}e^{-z_n\sigma_l/2}\Bigg], \tag{2.5}$$

$$P^{(n)}=\sum_l\rho_l\sigma_lX_l^{(n)}-\frac{\Delta}{\pi}z_n\Delta^{(n)} \tag{2.6}$$

with

$$X_j^{(n)}=d_j^{(n)}e^{-z_n\sigma_j/2}+\sigma_jB_j^{(n)}e^{z_n\sigma_j/2}\varphi_0(z_n\sigma_j)+\sigma_j\Delta^{(n)}. \tag{2.7}$$

As is seen from Eqs. (2.3a)–(2.7), our problem is reduced to determining the set $\{a_j^{(n)},B_j^{(n)}\}$. This set is determined by the following equations [13,20]:

$$-\Pi_j^{(n)}=\sum_{m=1}^{M}\frac{a_j^{(m)}}{z_n+z_m}\sum_l\rho_l[z_mX_l^{(n)}X_l^{(m)}$$
$$+X_l^{(m)}\Pi_l^{(n)}-X_l^{(n)}\Pi_l^{(m)}], \tag{2.8}$$

$$\frac{2\pi K^{(n)}}{z_n}d_j^{(n)}e^{-z_n\sigma_j/2}+\sum_l a_l^{(n)}\mathcal{I}_{jl}^{(n)}$$
$$-\sum_{m=1}^{M}\frac{1}{z_n+z_m}\left(\sum_k\rho_ka_k^{(n)}a_k^{(m)}\right)$$
$$\times\sum_l[\mathcal{J}_{jl}^{(n)}(\Pi_l^{(m)}-z_mX_l^{(m)})-\mathcal{I}_{jl}^{(n)}X_l^{(m)}]=0, \tag{2.9}$$

where

$$\mathcal{J}_{jl}^{(n)}=\delta_{jl}\sigma_j\varphi_0(z_n\sigma_j)-\frac{2\pi}{\Delta}\rho_l\sigma_l\sigma_j^3\psi_1(z_n\sigma_j), \tag{2.10}$$

$$\mathcal{I}_{jl}^{(n)}=\delta_{jl}+\sigma_j^2\varphi_0(z_n\sigma_j)\frac{\pi}{2\Delta}\rho_l\sigma_l$$
$$-\frac{2\pi}{\Delta}\rho_l\sigma_j^3\psi_1(z_n\sigma_j)\left[1+\frac{\pi\zeta_2}{2\Delta}\sigma_l+\frac{z_n\sigma_l}{2}\right], \tag{2.11}$$

$$\Pi_j^{(n)}\equiv B_j^{(n)}e^{z_n\sigma_j/2}+\left(1+\frac{z_n\sigma_j}{2}\right)\Delta^{(n)}+\frac{\pi}{2\Delta}\sigma_j\sum_l\rho_l\sigma_lX_l^{(n)}. \tag{2.12}$$

Equations (2.8) and (2.9) are equivalent to Eqs. (29) and (31) in Ref. [13], respectively.

Since $\Delta^{(n)}$ and $P^{(n)}$ are functions of $\{B_j^{(n)}\}$ as seen from Eqs. (2.5)–(2.7), we can solve Eq. (2.8) and get $\{a_j^{(n)}\}$ in terms of $\{B_j^{(n)}\}$. The substitution of this result into Eq. (2.9) gives us equations for $\{B_j^{(n)}\}$. However, the equations obtained still would be too complicated to solve. As a matter of fact, in the 1 Yukawa case the simple method of solution of the equations has been given by Blum [21] and by Ginoza [12–14]. Such methods of solution have been progressing in the M Yukawa case as well [20,22].

III. EXPRESSIONS OF STATIC STRUCTURE FACTORS

The partial structure factor related to i and j components, $S_{ij}(k)$, is calculated from the following general formula [6,9]:

$$S_{ij}(k)=\delta_{ij}-2\,\mathrm{Re}[\{\hat{\gamma}_s(ik)\}_{ij}], \tag{3.1}$$

where the ij element of the symmetric matrix $\hat{\gamma}_s(s)$ is defined by

$$\{\hat{\gamma}_s(s)\}_{ij}\equiv\frac{2\pi}{s}(c_ic_j)^{1/2}\rho\tilde{g}_{ij}(s) \tag{3.2}$$

with the concentration $c_j=\rho_j/\rho$, ρ being the total number density, and the Laplace transform defined by

$$\tilde{g}_{ij}(s)\equiv\int_0^\infty dr\ r g_{ij}(r)e^{-sr}. \tag{3.3}$$

The total structure factor $S(k)$ is defined by

$$S(k)=\sum_{ij}(c_ic_j)^{1/2}S_{ij}(k). \tag{3.4}$$

Therefore, the calculation of the structure factors is reduced to that of $\hat{\gamma}_s(s)$. Below, we shall present MSA expressions of $S_{ij}(k)$ and $S(k)$.

Now, the Laplace transform of the OZ equation in the Baxter formalism yields with the use of the MSA solution above [10,11]

$$\sum_l 2\pi\tilde{g}_{il}(s)[\delta_{lj}-c_l\rho\tilde{Q}_{lj}(is)]$$
$$=\left\{\left(1+\frac{s\sigma_i}{2}\right)A_j+s\beta_j\right\}\frac{e^{-s\sigma_{ij}}}{s^2}$$
$$-\sum_{n=1}^{M}\frac{z_n}{s+z_n}e^{-(s+z_n)\sigma_{ij}}C_{ij}^{(n)}. \tag{3.5}$$

With the use of Eq. (3.2), this equation can be written in a matrix form as

$$\hat{\gamma}_s(s)\hat{Q}(is)=\hat{\Lambda}(s), \tag{3.6}$$

where the ij elements of the matrices $\hat{Q}(is)$ and $\hat{\Lambda}(s)$ are given by

$$\{\hat{Q}(is)\}_{ij}\equiv\delta_{ij}-(c_ic_j)^{1/2}\rho\tilde{Q}_{ij}(is), \tag{3.7}$$

$$\Lambda_{ij}(s)\equiv\rho\frac{(c_ic_j)^{1/2}}{s}e^{-s\sigma_{ij}}\left[\left\{\left(1+\frac{s\sigma_i}{2}\right)A_j+s\beta_j\right\}\right.$$
$$\left.\times\frac{1}{s^2}-\sum_{n=1}^{M}\frac{z_n}{s+z_n}e^{-z_n\sigma_{ij}}C_{ij}^{(n)}\right]. \tag{3.8}$$

From Eq. (3.6), we get

$$\hat{\gamma}_s(s)=\hat{\Lambda}(s)\hat{R}(s), \tag{3.9}$$

where $\hat{R}(s)$ is defined by

$$\hat{Q}(is)\hat{R}(s)=1. \tag{3.10}$$

Now, with the use of Eqs. (2.3a)–(2.3d), Eq. (3.8) gives

$$\Lambda_{ij}(s)\equiv(c_ic_j)^{1/2}e^{-s\sigma_{ij}}\sum_{n=1}^{M+2}w_i^{(n)}(s)\alpha_j^{(n)}, \tag{3.11}$$

where

$$\alpha_j^{(1)}=1, \tag{3.12a}$$

$$\alpha_j^{(2)}=\sigma_j, \tag{3.12b}$$

$$\alpha_j^{(n+2)}=a_j^{(n)}, \tag{3.12c}$$

$$w_i^{(1)}(s)=\rho\frac{2\pi}{\Delta s^3}\left(1+\frac{s\sigma_i}{2}\right), \tag{3.13a}$$

$$w_i^{(2)}(s)=\rho\frac{\pi}{\Delta s^3}\left\{s+\frac{\pi\zeta_2}{\Delta}\left(1+\frac{s\sigma_i}{2}\right)\right\}, \tag{3.13b}$$

$$w_i^{(n+2)}(s)=\rho\left\{\frac{\pi P^{(n)}}{\Delta s^3}\left(1+\frac{s\sigma_i}{2}\right)+\frac{\Delta^{(n)}}{s^2}\right.$$
$$\left.-\frac{z_n}{s(s+z_n)}\left(Z_i^{(n)}-\frac{e^{-z_n\sigma_i}}{z_n}B_i^{(n)}e^{z_n\sigma_i/2}\right)\right\}, \tag{3.13c}$$

with $n=1,2,\ldots,M$ and

$$Z_j^{(n)}=d_j^{(n)}e^{-z_n\sigma_j/2},$$

while the substitution of Eq. (2.2) into Eq. (3.7) and the use of Eqs. (2.3a)–(2.3d) yield

$$\{\hat{Q}(is)\}_{ij}=\delta_{ij}-(c_ic_j)^{1/2}e^{s\lambda_{ij}}\sum_{n=1}^{M+2}Y_i^{(n)}(s)\alpha_j^{(n)}, \tag{3.14}$$

where

$$Y_i^{(1)}(s)=\frac{2\pi\rho}{\Delta}\sigma_i^3\psi_1(s\sigma_i), \tag{3.15a}$$

$$Y_i^{(2)}(s)=\frac{\pi\rho}{\Delta}\left\{\frac{\pi\zeta_2}{\Delta}\sigma_i^3\psi_1(s\sigma_i)+\sigma_i^2\varphi_1(s\sigma_i)\right\}, \tag{3.15b}$$

$$Y_i^{(n+2)}(s)=\rho\left\{\frac{\pi P^{(n)}}{\Delta}\sigma_i^3\psi_1(s\sigma_i)+\Delta^{(n)}\sigma_i^2\varphi_1(s\sigma_i)\right.$$
$$+\left(Z_i^{(n)}-\frac{e^{-z_n\sigma_i}}{z_n}B_i^{(n)}e^{z_n\sigma_i/2}\right)$$
$$\left.\times\left(\frac{e^{z_n\sigma_i}-e^{-s\sigma_i}}{s+z_n}-\frac{1-e^{-s\sigma_i}}{s}\right)-\frac{Z_i^{(n)}e^{z_n\sigma_i}}{s+z_n}\right\} \tag{3.15c}$$

with $n=1,2,\ldots,M$.

Equations (3.10) and (3.14) give

$$R_{ij}(s)=\delta_{ij}+(c_ic_j)^{1/2}e^{s\lambda_{ij}}\sum_{n=1}^{M+2}Y_i^{(n)}(s)L_j^{(n)}(s), \tag{3.16}$$

where $R_{ij}(s)$ is the ij element of $\hat{R}(s)$ and

$$L_j^{(n)}(s)\equiv c_j^{-1/2}\sum_l c_l^{1/2}e^{s\lambda_{jl}}\alpha_l^{(n)}R_{lj}(s). \tag{3.17}$$

From Eqs. (3.16) and (3.17), we get

$$L_j^{(n)}(s)=\alpha_j^{(n)}+\sum_{m=1}^{M+2}F^{(n,m)}(s)L_j^{(m)}(s), \tag{3.18}$$

where

$$F^{(n,m)}(s)=\sum_i c_i\alpha_i^{(n)}Y_i^{(m)}(s), \tag{3.19}$$

Therefore

$$L_j^{(n)}(s)=\sum_{m=1}^{M+2} G^{(n,m)}(s)\alpha_j^{(m)}, \tag{3.20}$$

where $G^{(n,m)}(s)$ is the (n,m) element of matrix $\hat{G}(s)$ defined by

$$\hat{G}(s)[1-\hat{F}(s)]=1, \tag{3.21}$$

the (n,m) element of the matrix $\hat{F}(s)$ being $F^{(n,m)}(s)$.

Therefore, from Eqs. (3.9), (3.11), and (3.16), with the use of Eqs. (3.18), (3.19), and (3.20) we get

$$\{\hat{\gamma}_s(s)\}_{ij}=(c_ic_j)^{1/2}e^{-s\sigma_{ij}}\sum_{n=1}^{M+2}\sum_{m=1}^{M+2} w_i^{(n)}(s)G^{(n,m)}(s)\alpha_j^{(m)}.$$

Substitution of this equation into Eq. (3.1) gives

$$S_{ij}(k)=\delta_{ij}-(c_ic_j)^{1/2}2\times\mathrm{Re}\left[e^{-s\sigma_{ij}}\sum_{n=1}^{M+2}\sum_{m=1}^{M+2} w_i^{(n)}(s)G^{(n,m)}(s)\alpha_j^{(m)}\right]_{s=ik}. \tag{3.22}$$

From Eqs. (3.4) and (3.22), we get

$$S(k)=1-2\,\mathrm{Re}\left[\sum_{n=1}^{M+2}\sum_{m=1}^{M+2} F_w^{(n)}(s)G^{(n,m)}(s)F_\alpha^{(m)}(s)\right]_{s=ik}, \tag{3.23}$$

where

$$F_w^{(n)}(s)\equiv\sum_i c_ie^{-s\sigma_i/2}w_i^{(n)}(s), \tag{3.24a}$$

$$F_\alpha^{(m)}(s)\equiv\sum_i c_ie^{-s\sigma_i/2}\alpha_i^{(n)}. \tag{3.24b}$$

The substitutions of Eqs. (3.12a)–(3.12c) into (3.24b) and Eqs. (3.13a)–(3.13c) into (3.24a) give explicit expressions of $F_\alpha^{(n)}$ and $F_w^{(n)}$, respectively. On the other hand, from Eq. (3.21) the expression of $G^{(n,m)}$ is obtained in terms of $F^{(n,m)}$, which is calculated with the substitution of Eqs. (3.12a)–(3.12c) and Eqs. (3.15a)–(3.15c) into Eq. (3.19). Thus, from Eqs. (3.22) and (3.23) we now obtain explicit analytical expressions of the static structure factors.

IV. DISCUSSION

In Sec. III, for the HSMY fluid with an arbitrary number of components we gave analytical expressions of the partial static structure factor and the total static structure factor, given by Eqs. (3.22) and (3.23), respectively. As for the coherent scattering intensity $I(k)$, it can be written in terms of $S_{ij}(k)$ as [23]

$$I(k)=\rho\sum_{ij}(c_ic_j)^{1/2}F_i(k)F_j(k)S_{ij}(k), \tag{4.1}$$

where $F_j(k)$ is the form factor of the spherical particle of the j component. The substitution of Eq. (3.22) into Eq. (4.1) yields

$$I(k)=\rho\sum_j c_j|F_j(k)|^2-2\rho\times\mathrm{Re}\left[\sum_{n=1}^{M+2}\sum_{m=1}^{M+2} I_w^{(n)}(k)G^{(n,m)}(ik)I_\alpha^{(m)}(k)\right], \tag{4.2}$$

where

$$I_w^{(n)}(k)\equiv\sum_j c_je^{-ik\sigma_j/2}F_j(k)w_j^{(n)}(ik), \tag{4.3a}$$

$$I_\alpha^{(n)}(k)\equiv\sum_j c_je^{-ik\sigma_j/2}F_j(k)\alpha_j^{(n)}. \tag{4.3b}$$

Thus, the main result of the paper is the compact and useful expressions of $S_{ij}(k)$, $S(k)$, and $I(k)$. The expressions are very tractable in applications since the applications become possible by simply performing the component sums independently for each components, as seen from Eqs. (3.19), (3.24a), (3.24b), (4.3a), and (4.3b). It is obvious from the derivation in Sec. III that the origin of such characteristics of the expressions is the special algebraic form of Eq. (1.2). The application has been reported already in the intrinsically polydisperse hard sphere Yukawa fluid [9].

Recently, the MSA formula for the scattering intensity from multicomponent mixtures of charged hard spheres has been reported [7]. The formula is obtained from

$$S_{ij}(k)=\{[\hat{Q}(k)\hat{Q}(-k)]^{-1}\}_{ij},$$

where $\hat{Q}(k)$ is the Baxter's matrix. This route is somewhat different from that in Sec. III. Both routes, however, must be equivalent as long as the Baxter's basic assumption on $\hat{Q}(k)$ is satisfied.

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