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LETTER TO THE EDITOR

An analytic structure factor for a multicomponent fluid with a screened Coulomb plus power series interaction

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Abstract
From our previous analytic solutions of the Ornstein–Zernike equation in the mean-spherical approximation (Yasutomi M 2001 *J. Phys.: Condens. Matter* **13** L255), we obtain an analytic structure factor for a multicomponent fluid with a screened Coulomb plus power series interaction expressed as

$$c_{ij}(r) = -\frac{\phi_{ij}(r)}{k_B T} = \sum_{n=1} \sum_{\tau=-1}^{L} K_{ij}^{(n,\tau)} z_n^{\tau+1} r^{\tau} e^{-z_n r} \qquad \sigma_{ij} < r$$

where $c_{ij}(r)$ is the direct correlation function, r the interparticle separation, $\phi_{ij}(r)$ the interaction potential, k_B Boltzmann's constant, T a temperature, L an arbitrary integer, $K_{ij}^{(n,\tau)}$ and z_n constants, and σ_{ij} the distance at contact of the pair (i, j) of particles. Because almost all of the interaction potentials between particles can be well approximated by the above closure, the present results will be applicable to a large variety of colloidal fluids under the mean-spherical approximation. As an example we show a structure factor for multicomponent fluid of Lennard-Jones particles.

In the previous work (Yasutomi 2001), we have obtained analytic solutions of the Ornstein–Zernike (OZ) equation for systems of hard spheres with a screened Coulomb plus power series interaction expressed as

$$c_{ij}(r) = -\frac{\phi_{ij}(r)}{k_B T} = \sum_{n=1} \sum_{\tau=-1}^{L} K_{ij}^{(n,\tau)} z_n^{\tau+1} r^{\tau} e^{-z_n r} \qquad \sigma_{ij} = (\sigma_i + \sigma_j)/2 < r \tag{1}$$

and

$$g_{ij}(r) \equiv h_{ij}(r) + 1 = 0 \qquad r < \sigma_{ij} \tag{2}$$

where L is an arbitrary integer, $c_{ij}(r)$ and $h_{ij}(r)$ are, respectively, the direct and the total correlation functions for two spherical molecules of species i and j, r is the interparticle separation, σ_i is the diameter of the spherical hard core of species i, $K_{ij}^{(n,\tau)}$ and z_n are constants to be adjusted according to physical arguments, $\phi_{ij}(r)$ is the pair-interaction potential in the mean-spherical approximation (MSA), k_B is Boltzmann's constant, and T is a temperature. We note here that the solutions for the Yukawa-type and Sogami–Ise-type closures (Sogami and Ise (1984) and Yasutomi and Ginoza (2000)) for a multicomponent fluid are given when $L = -1$ and 0, respectively.

The physical properties of the system are obtained from the total correlation function $h_{ij}(r)$ or the distribution function $g_{ij}(r)$. So far, these functions have been obtained for neutral hard-sphere interaction (Henderson *et al* 1976, Waisman *et al* 1976, Thompson *et al* 1980, Henderson *et al* 1980, Plischke and Henderson 1986), sticky hard-sphere interaction (Baxter 1968, Perram and Smith 1975, Barboy and Tenne 1979, Ginoza and Yasutomi 1996), a Yukawa potential (Waisman 1973, Blum and Høye 1978, Blum 1980, Ginoza 1985, 1986), and sticky hard-sphere Yukawa interaction (Yasutomi and Ginoza 1996). In the previous work (Yasutomi 2002) we have applied the closure (1) to one-component fluid and obtained the structure factor. In the present letter we shall extend the work to a multicomponent fluid. The results would provide a useful model basis for studying a large variety of multicomponent fluids because the interaction potentials between particles can be well approximated by the present closure. As a demonstration, we show a structure factor for multicomponent fluid of Lennard-Jones (LJ) particles. We have closely followed the exposition of our previous work (Yasutomi 2001, 2002) and the interested reader is referred to that for details.

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

$$S(k) = \sum_{ij} (c_i c_j)^{1/2} S_{ij}(k) \tag{3}$$

and the partial structure factor $S_{ij}(k)$ is expressed as

$$S_{ij}(k) = \delta_{ij} - 2\,\mathrm{Re}[\{\hat{\Gamma}^{(1)}(\mathrm{i}k)\}_{ij}] \tag{4}$$

where

$$\{\hat{\Gamma}^{(1)}(s)\}_{ij} \equiv \frac{2\pi}{s}(c_i c_j)^{1/2} \rho \tilde{g}_{ij}^{(1)}(s) \tag{5}$$

with $k = (4\pi n/\lambda)\sin(\theta/2)$ (n is the refractive index of the medium; λ is the wavelength of light; and θ is the scattering angle) and $c_j = \rho_j/\rho$ (ρ_j is the number density of particle j and ρ the total number density).

The partial radial distribution function is calculated from

$$g_{ij}(r) = 1 + \frac{1}{2\pi^2(\rho_i\rho_j)^{1/2} r} \int_0^\infty \mathrm{d}k\, [S_{ij}(k) - \delta_{ij}]\, k \sin kr \tag{6}$$

and its contact value $g_{ij}(\sigma_{ij})$ is given by

$$2\pi\sigma_{ij} g_{ij}(\sigma_{ij}) = A_j \sigma_{ij} + B_j - \sum_{n=1} \mathrm{e}^{-z_n\sigma_{ij}} z_n \sum_{k=0}^{L+1} (z_n\sigma_{ij})^k C_{ij}^{(k)}(z_n). \tag{7}$$

The total radial distribution function is calculated from

$$g(r) = 1 + \frac{1}{2\pi^2 \rho r} \int_0^\infty \mathrm{d}k\, [S(k) - 1]\, k \sin kr. \tag{8}$$

The Laplace transforms $\tilde{g}_{il}^{(m)}(s)$ are defined as

$$2\pi\rho_l \tilde{g}_{il}^{(m)}(s) = 2\pi\rho_l \int_{\sigma_{il}}^\infty \mathrm{d}x\, \mathrm{e}^{-sx} x^m g_{il}(x) = s^{2-m} \gamma_{il}^{(m)}(s). \tag{9}$$

It satisfies the following equation:

$$\sum_l \sum_{\xi=0}^{m} 2\pi \tilde{g}_{il}^{(\xi+1)}(s)\left[\delta_{jl}\delta_{m\xi} - C_\xi^m \rho_l \tilde{Q}_{lj}^{(m-\xi)}(\mathrm{i}s)\right]$$
$$= A_j \chi^{(m+1)}(\sigma_{ij}, s) + B_j \chi^{(m)}(\sigma_{ij}, s) - \sum_n \sum_{\tau=0}^{L+1} z_n^{\tau+1} C_{ij}^{(\tau)}(z_n) \chi^{(m+\tau)}(\sigma_{ij}, z_n + s) \tag{10}$$

where $C_m^n = n!/m!(n-m)!$. The coefficients A_j, B_j, and $C_{ij}^{(\tau)}(z_n)$ and functions $\tilde{Q}_{lj}^{(m)}(\mathrm{i}s)$ and $\chi^{(m)}(\sigma_{ij}, s)$ are given in appendix A. We can write equation (10) in matrix form as

$$\sum_{\xi=0}^{m} \hat{\Gamma}^{(\xi+1)}(s) \hat{Q}^{(m,\xi)}(\mathrm{i}s) = \hat{\Lambda}^{(m)}(s) \tag{11}$$

where

$$\{\hat{\Gamma}^{(m)}(s)\}_{ij} \equiv \frac{2\pi}{s}(c_i c_j)^{1/2} \rho \tilde{g}_{ij}^{(m)}(s) \tag{12}$$

$$\{\hat{Q}^{(m,\xi)}(\mathrm{i}s)\}_{lj} \equiv \delta_{lj}\delta_{m\xi} - C_\xi^m (c_l c_j)^{1/2} \rho \tilde{Q}_{lj}^{(m-\xi)}(\mathrm{i}s) \tag{13}$$

and

$$\{\hat{\Lambda}^{(m)}(s)\}_{ij} = \frac{\rho(c_i c_j)^{1/2}}{s}\Bigg\{A_j \chi^{(m+1)}(\sigma_{ij}, s) + B_j \chi^{(m)}(\sigma_{ij}, s)$$
$$- \sum_n \sum_{\tau=0}^{L+1} z_n^{\tau+1} C_{ij}^{(\tau)}(z_n) \chi^{(m+\tau)}(\sigma_{ij}, z_n + s)\Bigg\}. \tag{14}$$

From equations (11) and (13) we obtain

$$\hat{\Gamma}^{(1)}(s) = \hat{\Lambda}^{(0)}(s) \hat{Q}^{(0,0)}(\mathrm{i}s)^{-1}. \tag{15}$$

The matrices $\hat{Q}^{(m,\xi)}(\mathrm{i}s)$ and $\hat{\Lambda}^{(m)}(s)$ in equation (11) are determined by the two sets of coefficients $[\gamma_{ij}^{(m)}(z_n), D_{ij}^{(k)}(z_n)]$ which are obtained by solving the following two sets of equations:

$$\frac{z_k^{1-m}\gamma_{ij}^{(m+1)}(z_k)}{\rho_j} = \hat{A}_{ij}^{(m)}(z_k) A_j + \hat{B}_{ij}^{(m)}(z_k) B_j + \sum_{n=1} \sum_{\tau=0}^{L+1} \sum_l \hat{C}_{ilj}^{(m,\tau)}(z_k, z_n) C_{lj}^{(\tau)}(z_n)$$
$$+ \sum_{n=1} \sum_{\tau=-1}^{L} \sum_l \hat{D}_{ilj}^{(m,\tau)}(z_k, z_n) D_{lj}^{(\tau)}(z_n) \tag{16}$$

and

$$2\pi K_{ij}^{(n,m-1)} = z_n \sum_l D_{il}^{(m-1)}(z_n)[\delta_{jl} - \rho_l \tilde{Q}_{jl}^{(0)}(\mathrm{i}z_n)]$$
$$- z_n(m+1) \sum_l D_{il}^{(m)}(z_n)[\delta_{jl} + z_n \rho_l \tilde{Q}_{jl}^{(1)}(\mathrm{i}z_n) - \rho_l \tilde{Q}_{jl}^{(0)}(\mathrm{i}z_n)]$$
$$+ \sum_{\tau=m+1}^{L} \sum_l D_{il}^{(\tau)}(z_n) \frac{z_n^{\tau+1}}{z_n^m} \rho_l [(\tau+1) C_{\tau-m}^{\tau} \tilde{Q}_{jl}^{(\tau-m)}(\mathrm{i}z_n)$$
$$- C_{\tau+1-m}^{\tau+1} z_n \tilde{Q}_{jl}^{(\tau+1-m)}(\mathrm{i}z_n)] \tag{17}$$

where coefficients $\hat{A}_{ij}^{(m)}(z_k)$, $\hat{B}_{ij}^{(m)}(z_k)$, $\hat{C}_{ilj}^{(m,\tau)}(z_k, z_n)$, and $\hat{D}_{ilj}^{(m,\tau)}(z_k, z_n)$ in equation (16) are given in appendix B. Those equations can be solved by the Newton–Raphson iteration technique. A physical branch of the solution has to be chosen from the manifold of solutions.

Table 1. Lennard-Jones parameters.

Molecule i	ϵ_i/k_B (K)	σ_i (nm)
1: Ar	119.8	0.335
2: Kr	169.04	0.3581
3: Xe	237.74	0.3790

To solve (16) and (17) for coefficients $[\gamma_{ij}^{(m)}(z_n), D_{ij}^{(k)}(z_n)]$ we first multiply $\phi_{ij}(r)$ by a factor f. We next change f from 0 to 1 through some steps. When we get solutions for f in a certain step, we can use them as approximate solutions to the next step. Then we obtain more exact solutions by the Newton–Raphson method. In this way we can finally obtain correct solutions for $f = 1$ after some steps. Thus, our problems are reduced to obtaining the solutions for $f = 0$. In this case, from (17) and (A.3) we obtain

$$D_{ij}^{(m-1)}(z_n) = C_{ij}^{(m)}(z_n) = 0 \qquad (m = 0, 1, 2, \ldots, L+1). \tag{18}$$

Substitutions of (18) into (A.1), (A.2), (A.4), (A.7), and (14) lead to

$$A_j = \frac{2\pi}{\Delta}\left(1 + \frac{\pi\zeta_2}{2\Delta}\sigma_j\right) \qquad B_j = -\frac{\zeta_2}{2}\left(\frac{\pi}{\Delta}\right)^2\sigma_j^2 \tag{19}$$

$$\{\hat{\Lambda}^{(m)}(z_k)\}_{ij} = \frac{\rho(c_i c_j)^{1/2}}{z_k}\{A_j\chi^{(m+1)}(\sigma_{ij}, z_k) + B_j\chi^{(m)}(\sigma_{ij}, z_k)\} \tag{20}$$

and

$$e^{-z_k\lambda_{lj}}\tilde{Q}_{lj}^{(m)}(iz_k) = \tfrac{1}{2}A_j\Phi_{lj}^{(m+2,m)}(z_k, 0) + B_j\Phi_{lj}^{(m+1,m)}(z_k, 0). \tag{21}$$

From equation (11) we finally obtain

$$\hat{\Gamma}^{(1)}(z_k) = \hat{\Lambda}^{(0)}(z_k)\hat{Q}^{(0,0)}(iz_k)^{-1} \tag{22}$$

and for $L + 1 \geqslant m \geqslant 1$

$$\hat{\Gamma}^{(m+1)}(z_k) = \left[\hat{\Lambda}^{(m)}(z_k) - \sum_{\xi=0}^{m-1}\hat{\Gamma}^{(\xi+1)}(z_k)\hat{Q}^{(m,\xi)}(iz_k)\right]\hat{Q}^{(0,0)}(iz_k)^{-1}. \tag{23}$$

We believe that the present results can be applied to almost all of the multicomponent fluids. As a demonstration, we show here a structure factor for a fluid of multicomponent LJ particles.

We assume that the LJ fluid is composed of argons, kryptons, and xenons and express their relevant quantities by 1, 2, and 3, respectively. The temperature is 299.5 K, the packing fraction $\pi\zeta_3/6 = 0.1$, and $c_1 = c_2 = c_3 = 1/3$. The potential between two LJ particles i and j is written as

$$\phi_{ij}(r) = 4\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right] \qquad \epsilon_{ij} = (\epsilon_i\epsilon_j)^{1/2}. \tag{24}$$

Their LJ parameters adopted are listed in table 1. We can approximate the LJ potential by equation (1) as

$$\frac{\phi_{ij}(r)}{k_B T} = -\sum_{\tau=-1}^{20} K_{ij}^{(\tau)} z^{\tau+1} r^{\tau} e^{-zr}. \tag{25}$$

Figure 1 shows that the LJ potential (solid curve) for each particle pair (i, j) is well fitted by equation (25) (filled circles) where $z\sigma_1 = 12.63001$, and parameters $a_{ij}^{(\tau)} \equiv$

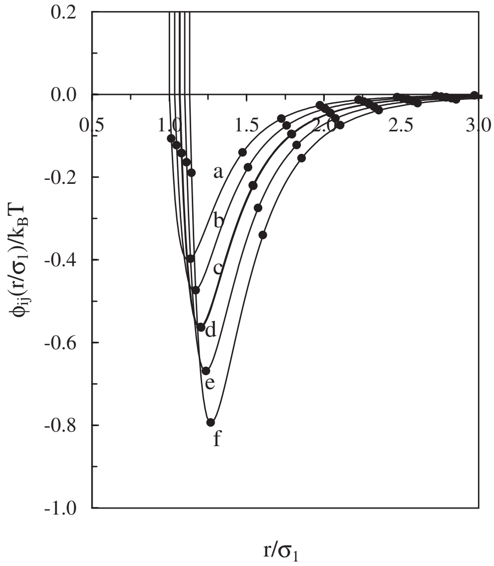

Figure 1. The LJ interaction potentials (curves) and their approximate potentials (filled circles) given by equation (25). The letters a, b, c, d, e, and f attached to the curves indicate the particle pairs (1, 1), (1, 2), (1, 3), (2, 2), (2, 3), and (3, 3), respectively, where 1, 2, and 3 indicate argon, krypton, and xenon, respectively.

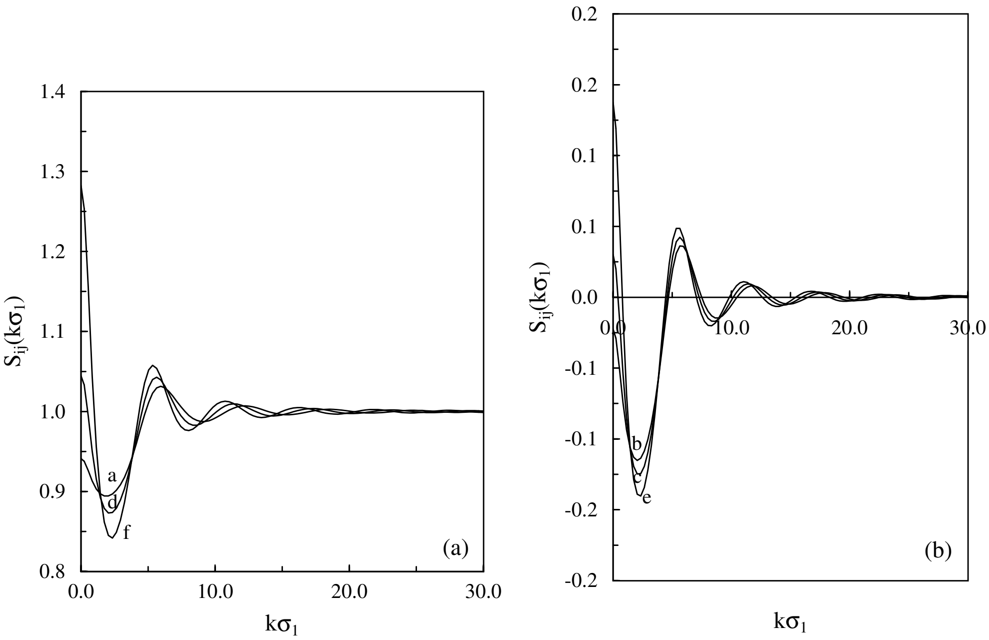

Figure 2. The partial structure factors $S_{ij}(k\sigma_1)$ for a LJ multicomponent fluid. The letters attached to the curves have the same meaning as in figure 1.

$-(k_BT/\epsilon_{ij})(K_{ij}^{(\tau)}/\sigma_1)(z\sigma_1)^{(\tau+1)}$ are listed in table 2. The partial structure factors are shown in figures 2(a) and (b) and the total structure factor is shown in figure 3. Figure 4 shows the partial

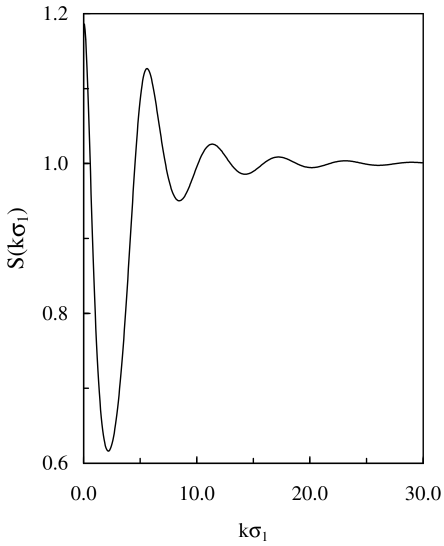

Figure 3. The total structure factor $S(k\sigma_1)$ for a LJ multicomponent fluid.

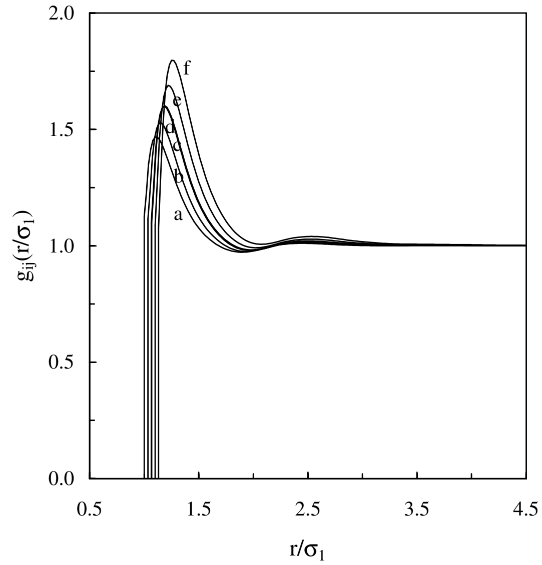

Figure 4. The partial distribution functions $g_{ij}(r/\sigma_1)$ for a LJ multicomponent fluid. The letters attached to the curves have the same meaning as for figure 1.

distribution functions and figure 5 the total distribution function. The letters a, b, c, d, e, and f attached to the lines indicate the particle pairs (1, 1), (1, 2), (1, 3), (2, 2), (2, 3), and (3, 3), respectively. We have also obtained the structure factors for the same model parameters but for ($T = 140.9$ K, $\pi\zeta_3/6 = 0.3$) and ($T = 100.0$ K, $\pi\zeta_3/6 = 0.4$), respectively, though the results are not shown here. At least in the range of model parameters considered here, it is easy to solve the equations. We will report on the stable and efficient method of computation in the near future.

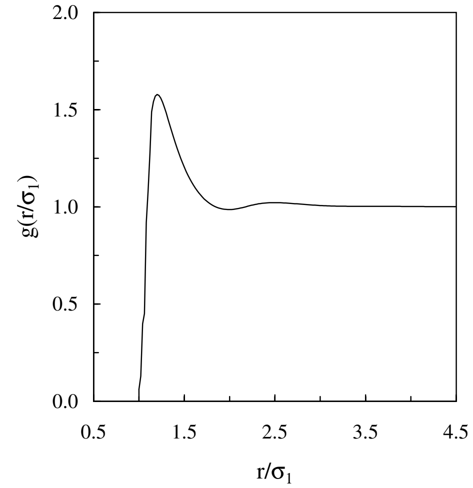

Figure 5. The total distribution function $g(r/\sigma_1)$ for a LJ multicomponent fluid.

Table 2. Fitting parameters $a_{ij}^{(\tau)}$.

τ	$a_{11}^{(\tau)}$	$a_{12}^{(\tau)}$	$a_{13}^{(\tau)}$	$a_{22}^{(\tau)}$	$a_{23}^{(\tau)}$	$a_{33}^{(\tau)}$
−1	-2.4580×10^8	2.7925×10^7	1.4034×10^9	-9.7238×10^7	8.7895×10^8	2.5382×10^8
0	1.3254×10^9	6.2335×10^8	-3.4650×10^9	1.1631×10^9	-1.6492×10^9	4.5609×10^8
1	-1.1895×10^9	-9.7238×10^8	9.3477×10^8	-1.3830×10^9	-1.6185×10^8	-1.3759×10^9
2	-2.1594×10^9	-1.7438×10^9	1.7278×10^9	-2.4892×10^9	-2.3098×10^8	-2.4409×10^9
3	1.7098×10^9	1.8875×10^9	1.2966×10^9	2.3851×10^9	2.1930×10^9	3.1115×10^9
4	3.5662×10^9	3.4187×10^9	4.2967×10^6	4.5509×10^9	2.5271×10^9	5.2852×10^9
5	-1.3846×10^9	-1.9011×10^9	-3.0507×10^9	-2.2329×10^9	-3.2613×10^9	-3.3784×10^9
6	-2.6097×10^9	-2.7084×10^9	-1.0827×10^9	-3.4988×10^9	-2.6664×10^9	-4.3465×10^9
7	-1.8915×10^9	-1.6869×10^9	6.6000×10^8	-2.3114×10^9	-8.4370×10^8	-2.5132×10^9
8	1.3062×10^9	1.6792×10^9	2.2638×10^9	2.0137×10^9	2.6199×10^9	2.9222×10^9
9	4.1340×10^9	4.3514×10^9	2.0857×10^9	5.5905×10^9	4.4800×10^9	7.0251×10^9
10	6.3916×10^7	-2.6079×10^8	-1.7115×10^9	-1.7939×10^8	-1.2311×10^9	-6.4698×10^8
11	-3.5802×10^9	-3.9785×10^9	-2.9256×10^9	-5.0116×10^9	-4.7133×10^9	-6.5674×10^9
12	-1.4981×10^9	-1.4093×10^9	1.3298×10^8	-1.8901×10^9	-9.6075×10^8	-2.1601×10^9
13	2.3349×10^9	2.6730×10^9	2.3289×10^9	3.3316×10^9	3.3846×10^9	4.4627×10^9
14	2.1255×10^9	2.2385×10^9	1.0898×10^9	2.8752×10^9	2.3128×10^9	3.6153×10^9
15	-2.1637×10^9	-2.4850×10^9	-2.2078×10^9	-3.0937×10^9	-3.1700×10^9	-4.1539×10^9
16	-1.0309×10^9	-1.0637×10^9	-4.1417×10^8	-1.3766×10^9	-1.0356×10^9	-1.7029×10^9
17	1.9768×10^9	2.2061×10^9	1.6819×10^9	2.7744×10^9	2.6440×10^9	3.6475×10^9
18	-9.9620×10^8	-1.1340×10^9	-9.6748×10^8	-1.4161×10^9	-1.4206×10^9	-1.8892×10^9
19	2.2738×10^8	2.6205×10^8	2.3826×10^8	3.2580×10^8	3.3698×10^8	4.3856×10^8
20	-2.0330×10^7	-2.3649×10^7	-2.2503×10^7	-2.9307×10^7	-3.0999×10^7	-3.9713×10^7

The present results would provide a useful model basis for studying a large variety of multicomponent fluids. We will apply the analysis to a standard problem in liquid-state physics and many other problems that could be tackled as well, including colloidal physics, and report on our work in the near future.

Appendix A

The coefficients A_j, B_j, and $C_{ij}^{(\tau)}(z_n)$ and functions $\tilde{Q}_{lj}^{(m)}(\mathrm{i}s)$ and $\chi^{(m)}(\sigma_{ij}, s)$ in equation (10) are

$$A_j = \frac{2\pi}{\Delta}\left[1 + \frac{1}{2}\zeta_2\beta_j - \sum_{n=1}\sum_{\mu=-1}^{L}\sum_{l}\rho_l D_{lj}^{(\mu)}(z_n)H_{lj}^{(\mu,0)}(z_n)\right] \tag{A.1}$$

$$B_j = \beta_j - \tfrac{1}{2}\sigma_j A_j \tag{A.2}$$

$$C_{ij}^{(k)}(z_n) = -D_{ij}^{(k-1)}(z_n) + (k+1)D_{ij}^{(k)}(z_n) + \sum_{l}\sum_{\tau=1}^{L+2-k} C_{\tau-1}^{\tau+k-1} D_{lj}^{(\tau+k-2)}(z_n)\gamma_{il}^{(\tau)}(z_n) \tag{A.3}$$

$$\begin{aligned}\mathrm{e}^{-s\lambda_{lj}}\tilde{Q}_{lj}^{(m)}(\mathrm{i}s) &= \tfrac{1}{2}A_j\Phi_{lj}^{(m+2,m)}(s,0)\\ &\quad + B_j\Phi_{lj}^{(m+1,m)}(s,0) + \sum_{n=1}\sum_{k=0}^{L+1}\sum_{\xi=0}^{k}\frac{z_n^{k-\xi}C_{lj}^{(k)}(z_n)k!}{(k-\xi)!}\Phi_{lj}^{(m+k-\xi,m)}(s,z_n)\\ &\quad + \sum_{n=1}\sum_{\tau=-1}^{L} D_{lj}^{(\tau)}(z_n)z_n^{\tau+1}\mathrm{e}^{-s\lambda_{lj}}\chi^{(m+\tau+1)}(\lambda_{jl}, z_n+s)\end{aligned} \tag{A.4}$$

and

$$\chi^{(k)}(b,a) = k!\mathrm{e}^{-ab}\sum_{\xi=0}^{k}\frac{b^{k-\xi}}{a^{\xi+1}(k-\xi)!} \qquad (b \neq 0) \tag{A.5}$$

$$\chi^{(k)}(0, x+\mathrm{i}y) = \frac{k!}{(x^2+y^2)^{(k+1)/2}}\left\{\cos\left[(k+1)\tan^{-1}\frac{y}{x}\right] - \mathrm{i}\sin\left[(k+1)\tan^{-1}\frac{y}{x}\right]\right\} \tag{A.6}$$

where

$$\beta_j = \frac{\pi}{\Delta}\sigma_j + \frac{2\pi}{\Delta}\sum_{n=1}\sum_{\mu=-1}^{L}\sum_{l}\rho_l D_{lj}^{(\mu)}(z_n)[H_{lj}^{(\mu,1)}(z_n) - \tfrac{1}{2}\sigma_j H_{lj}^{(\mu,0)}(z_n)] \tag{A.7}$$

$$\begin{aligned}\mathrm{e}^{-s\lambda_{jl}}\Phi_{lj}^{(n,m)}(s,z) &= \chi^{(n)}(\lambda_{jl}, z+s) - \chi^{(n)}(\sigma_{jl}, z+s)\\ &\quad - \sigma_{lj}^{n-m}\mathrm{e}^{-z\sigma_{lj}}[\chi^{(m)}(\lambda_{jl}, s) - \chi^{(m)}(\sigma_{jl}, s)]\end{aligned} \tag{A.8}$$

$$\begin{aligned}H_{lj}^{(\mu,m)}(z_n) &= z_n^{\mu+1}[\chi^{(m+\mu+1)}(\lambda_{jl}, z_n) - \Phi_{lj}^{(m+\mu+1,m)}(0,z_n)]\\ &\quad + \sum_{k=0}^{\mu+1}\sum_{\xi=0}^{k}\frac{z_n^{k-\xi}k!}{(k-\xi)!}\sum_{\nu}\Phi_{\nu j}^{(m+k-\xi,m)}(0,z_n)C_{\mu+1-k}^{\mu+1}\gamma_{l\nu}^{(\mu+2-k)}(z_n).\end{aligned} \tag{A.9}$$

Also, $\zeta_k = \sum_l \rho_l\sigma_l^k$, $\Delta = 1 - \pi\zeta_3/6$, and $\lambda_{ji} = (\sigma_j - \sigma_i)/2$.

Appendix B

The coefficients $\hat{A}_{ij}^{(m)}(z_k)$, $\hat{B}_{ij}^{(m)}(z_k)$, $\hat{C}_{ilj}^{(m,\tau)}(z_k, z_n)$, and $\hat{D}_{ilj}^{(m,\tau)}(z_k, z_n)$ in equation (16) are

$$\hat{A}_{ij}^{(m)}(z_k) = \chi^{(m+1)}(\sigma_{ij}, z_k) + \tfrac{1}{2}\sum_{l}\mathrm{e}^{z_k\lambda_{lj}}\sum_{\xi=0}^{m} z_k^{1-\xi}\gamma_{il}^{(\xi+1)}(z_k)C_\xi^m\Phi_{lj}^{(m-\xi+2,m-\xi)}(z_k,0) \tag{B.1}$$

$$\hat{B}_{ij}^{(m)}(z_k) = \chi^{(m)}(\sigma_{ij}, z_k) + \sum_{l}\mathrm{e}^{z_k\lambda_{lj}}\sum_{\xi=0}^{m} z_k^{1-\xi}\gamma_{il}^{(\xi+1)}(z_k)C_\xi^m\Phi_{lj}^{(m-\xi+1,m-\xi)}(z_k,0) \tag{B.2}$$

$$\hat{C}_{ilj}^{(m,\tau)}(z_k, z_n) = e^{z_k\lambda_{lj}}\tau! \sum_{\xi=0}^{m} z_k^{1-\xi}\gamma_{il}^{(\xi+1)}(z_k)C_\xi^m \sum_{\mu=0}^{\tau} \frac{z_n^{\tau-\mu}}{(\tau-\mu)!}\Phi_{lj}^{(m-\xi+\tau-\mu,m-\xi)}(z_k, z_n)$$
$$- \delta_{il}z_n^{\tau+1}\chi^{(m+\tau)}(\sigma_{lj}, z_n + z_k) \quad \text{(B.3)}$$

and

$$\hat{D}_{ilj}^{(m,\tau)}(z_k, z_n) = z_n^{\tau+1}\sum_{\xi=0}^{m} z_k^{1-\xi}\gamma_{il}^{(\xi+1)}(z_k)C_\xi^m \chi^{(m-\xi+\tau+1)}(\lambda_{jl}, z_n + z_k). \quad \text{(B.4)}$$

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