



Analytical static structure factor for a two-component system interacting via van der Waals potential

MARWAN AL-RAEEI¹ and MOUSTAFA SAYEM EL-DAHER^{1,2,*}

¹Physics Department, Damascus University, Damascus, Syria

²Faculty of Informatics and Communications, Arab International University, Daraa, Syria

*Corresponding author. E-mail: eldaherm@scs-net.org

MS received 3 November 2016; revised 22 October 2017; accepted 15 November 2017;
published online 29 March 2018

Abstract. In this work, we derive analytical solutions for static structure factor for homogeneous and isotropic solution composed of two components interacting with each other via simple van der Waals potential which is inversely proportional to the sixth power of the distance between the two components. We assume that the first component is the solvent and the second component is the dissolved material which has low concentration or density in comparison to the concentration of the solvent, i.e. dilute solution, which is common for macromolecular fluids. The presented solution is obtained using direct and inverse Fourier transforms in solving Ornstein–Zernike equations (OZE) for multicomponent systems. We calculated isothermal compressibilities as a function of concentration and comparison with other simulation and theoretical results are presented. We believe that the presented solution can be useful in studying biomolecular fluids and other soft matter fluids.

Keywords. Ornstein–Zernike equation; Van der Waals potential; two-component fluid; macromolecular fluid; partial structure factor; isothermal compressibility; soft matter.

PACS No. 05.20.Jj

1. Introduction

Understanding simple or multicomponent fluids and their properties is very important in studying materials such as soft condensed matter and mixtures of real gases [1–8]. Thermodynamic properties of such systems are related to the radial distribution function (RDF) for the system $g(r)$. If we can find $g(r)$ we can calculate properties such as internal energy, equilibrium pressure or static pressure, heat capacity etc. Static physical properties of the systems can be expressed using static structure factor (SSF) $S(q)$ which is related to the radial distribution function via Fourier transform [1–4], but noting that RDF is a function of position while static structure factor – which can be obtained from scattering experiments – is a function of scattering vector defined as [3]

$$\vec{K}_f - \vec{K}_i = \vec{q}, \quad (1)$$

$$q = (4\pi/\lambda) \sin(\theta/2), \quad (2)$$

where \vec{K}_i represents wave vector of the incoming beam of radiation, \vec{K}_f represents the wave vector of the scattered beam of radiation while θ represents the angle of

scattering. Radial distribution function is related to the structure factor as follows [1–3,9]:

$$S_C(q) = 1 + 4\pi\rho \int_0^\infty r^2 h(r) \frac{\sin(qr)}{qr} dr, \quad (3)$$

where ρ represents the density of the fluid and $h(r)$ is the total correlation function which links to radial distribution function as [1–3]

$$h(r) \equiv g(r) - 1. \quad (4)$$

In general, we can obtain radial distribution function for definite system from integral equations describing liquid structure and the interaction potential between particle pairs in the system [2,3,8]. In the case of one-component system, we have one $g(r)$ and one $S(q)$, but in the case of multicomponent system the functions become multiple and depend on the number of components in the system. For example, radial distribution function becomes $g_{\alpha\beta}(r)$ where α, β represent components. For a system consisting of N components, there are N^2 radial distribution functions and the number becomes less in the case of homogeneous and isotropic systems. Similarly, we can write the static structure

factor and total correlation function as $S_{\alpha\beta}(q)$, $h_{\alpha\beta}(r)$ respectively.

2. Ornstein–Zernike equation for multicomponent systems

Ornstein–Zernike equation (OZE) is a basic equation used to determine radial distribution function for different fluid systems and it describes correlation between particles in the system. Ornstein–Zernike equation for one-component system is given as [2,3,10,11]

$$h(r) = c(r) + \rho \int d\vec{r}' c(|\vec{r} - \vec{r}'|) h(r'), \quad (5)$$

where $c(r)$ is the direct correlation function between pairs. The previous equation is a closed integral equation containing two functions – the direct correlation function and total correlation function. Therefore, to find the solutions we need a second equation, which we get from a number of possible approximations of the direct correlation function.

Direct correlation function can be approximated in a number of ways:

Mean spherical approximation (MSA) [2,3,12]:

$$c(r) \approx -\beta U(r); \quad r > \sigma. \quad (6)$$

Percus Yevick approximation (PYA) [2,3]:

$$c(r) \approx g(r) - y(r); \quad r > \sigma. \quad (7)$$

Hyper netted chain approximation (HNCA) [2,3]:

$$c(r) \approx h(r) - \ln y(r); \quad r > \sigma, \quad (8)$$

where σ is the diameter of the particles consisting of the system. $\beta = 1/k_B T$ is the reduced temperature, T is the absolute temperature, k_B is the Boltzman constant and $U(r)$ is the interaction potential. $y(r)$ is the cavity function which is given as

$$y(r) \equiv g(r) e^{\beta U(r)}. \quad (9)$$

As we can see, access to solutions of OZE with one of the approximation used in the theory determine direct correlation function and total correlation function and thus determine radial distribution function which enables us to calculate the properties of the system from interaction potential. We can generalise OZE to include multicomponent systems [2,3,13], situations found in soft matter, and mixtures of real gases. In this case, there is no single OZE but there is N^2 for a system consisting of N components. These equations are written as [2]

$$h_{\alpha\beta}(r) = c_{\alpha\beta}(r) + \sum_{p=1}^n \rho_p \int d\vec{r}' c_{\alpha p}(|\vec{r} - \vec{r}'|) h_{p\beta}(r'). \quad (10)$$

We can expand approximations of theory of integral equations in the case of multicomponent systems. Here we mention mean spherical approximation which we use to find solutions and is written as

$$c_{\alpha\beta}(r) \approx -\beta U_{\alpha\beta}(r), \quad r > \sigma_{\alpha\beta}. \quad (11)$$

Based on the previous equations, we can write OZE for a system composed of two components with volume density ρ_1, ρ_2 as

$$h_{11}(r) = c_{11}(r) + \rho_1 \int d\vec{r}' c_{11}(|\vec{r} - \vec{r}'|) h_{11}(r') + \rho_2 \int d\vec{r}' c_{12}(|\vec{r} - \vec{r}'|) h_{21}(r') \quad (12)$$

$$h_{12}(r) = c_{12}(r) + \rho_1 \int d\vec{r}' c_{11}(|\vec{r} - \vec{r}'|) h_{12}(r') + \rho_2 \int d\vec{r}' c_{12}(|\vec{r} - \vec{r}'|) h_{22}(r') \quad (13)$$

$$h_{21}(r) = c_{21}(r) + \rho_1 \int d\vec{r}' c_{21}(|\vec{r} - \vec{r}'|) h_{11}(r') + \rho_2 \int d\vec{r}' c_{22}(|\vec{r} - \vec{r}'|) h_{21}(r') \quad (14)$$

$$h_{22}(r) = c_{22}(r) + \rho_1 \int d\vec{r}' c_{21}(|\vec{r} - \vec{r}'|) h_{12}(r') + \rho_2 \int d\vec{r}' c_{22}(|\vec{r} - \vec{r}'|) h_{22}(r'). \quad (15)$$

These equations are four closed integral equations with eight different functions, and in homogeneous and isotropic systems, we have

$$c_{12}(r) = c_{21}(r) \quad (16)$$

$$h_{12}(r) = h_{21}(r) \quad (17)$$

Because eqs (13) and (14) are equivalent, we are left with only three closed integral equations and six different functions. Therefore, we need three additional equations to find the unknown functions. We can get these equations from approximations of theory of integral equations in multicomponent systems. In the mean spherical approximation (MSA) we can write the direct correlation functions for the two-component system as

$$c_{11}(r) \approx -\beta U_{11}(r); \quad r > \sigma_{11}, \quad (18)$$

$$c_{12}(r) \approx -\beta U_{12}(r); \quad r > \sigma_{12}, \quad (19)$$

$$c_{22}(r) \approx -\beta U_{22}(r); \quad r > \sigma_{22}, \quad (20)$$

where σ_{11} and σ_{22} are the diameters of the first and second components respectively in the system and $\sigma_{12} =$

$(\sigma_{11} + \sigma_{22})/2$. In this case, we use simple van der Waals potential which is written in the case of two-component system as [4,14]

$$U_{11}(r) = -\frac{A_{11}}{r^6} = -D_{11} \left(\frac{\sigma_{11}}{r}\right)^6, \quad (21)$$

$$U_{12}(r) = U_{21}(r) = -\frac{A_{12}}{r^6} = -D_{12} \left(\frac{\sigma_{12}}{r}\right)^6, \quad (22)$$

$$U_{22}(r) = -\frac{A_{22}}{r^6} = -D_{12} \left(\frac{\sigma_{22}}{r}\right)^6, \quad (23)$$

where D_{11} , D_{12} and D_{22} are constants with energy units.

3. Analytical solution for OZE for two-component system

We can write OZE for solution consisting of two components in the case of low-density of one of the components in the solution (let it be the second component) that is $\rho_1 \gg \rho_2$ (dilute solution). So previous OZE becomes

$$h_{11}(r) = c_{11}(r) + \rho_1 \int d\vec{r}' c_{11}(|\vec{r} - \vec{r}'|) h_{11}(r'), \quad (24)$$

$$h_{12}(r) = c_{12}(r) + \rho_1 \int d\vec{r}' c_{11}(|\vec{r} - \vec{r}'|) h_{12}(r'), \quad (25)$$

$$h_{21}(r) = c_{21}(r) + \rho_1 \int d\vec{r}' c_{21}(|\vec{r} - \vec{r}'|) h_{11}(r'), \quad (26)$$

$$h_{22}(r) = c_{22}(r) + \rho_1 \int d\vec{r}' c_{21}(|\vec{r} - \vec{r}'|) h_{12}(r'). \quad (27)$$

Equations (25) and (26) are equivalent, and this reduces the above equations to three. Replacing van der Waals potential with $U_{\alpha\beta}(r)$ in mean spherical approximation gives us

$$c_{11}(r) \approx -\beta U_{11}(r) = D_{11} \left(\frac{\sigma_{11}}{r}\right)^6; \quad r > \sigma_{11}, \quad (28)$$

$$c_{12}(r) \approx c_{21}(r) = -\beta U_{12}(r) = D_{12} \left(\frac{\sigma_{12}}{r}\right)^6; \quad r > \sigma_{12}, \quad (29)$$

$$c_{22}(r) \approx -\beta U_{22}(r) = \beta D_{12} \left(\frac{\sigma_{22}}{r}\right)^6; \quad r > \sigma_{22}. \quad (30)$$

If we take Fourier transformations for OZE and then substitute for $c_{\alpha\beta}(q)$, we can find that static structure factors for the components in the solutions are given as

$$S_{11}(q) = \frac{x_1}{1 - \rho_1 4\pi\beta D_{11}\sigma_{11}^3 M(q_{01})}, \quad (31)$$

$$S_{12}(q) = x_1 \rho_2 \frac{4\pi\beta D_{12}\sigma_{12}^3 M_{12}(q_{012})}{1 - \rho_1 4\pi\beta D_{11}\sigma_{11}^3 M(q_{01})}, \quad (32)$$

$$S_{22}(q) = x_2 + 4\pi x_2 \beta D_{22} \rho_2 \sigma_{22}^3 M(q_{02}) + x_2 \rho_2 \rho_1 \frac{[4\pi\beta D_{12}\sigma_{12}^3 M_{12}(q_{012})]^2}{1 - \rho_1 4\pi\beta D_{11}\sigma_{11}^3 M(q_{01})}, \quad (33)$$

where $q_{01} = \sigma_{11}q$, $q_{012} = \sigma_{12}q$, $q_{02} = \sigma_{22}q$ are reduced wave vectors for different components in the system and $x_1 = N_1/N$, $x_2 = N_2/N$ are the molar fractions or the concentration number for two components. $M_{\alpha\beta}(q_0)$ are functions written as

$$M_{11}(q_{01}) = \frac{\pi q_{01}^3}{48} - \frac{q_{01}^3}{24} \text{Si}(q_{01}) - \frac{1}{24q_{01}}(q_{01}^2 - 6) \sin(q_{01}) - \frac{1}{24}(\sigma_{01}^2 - 2) \cos(q_{01}) \quad (34)$$

$$M_{12}(q_{012}) = \frac{\pi q_{012}^3}{48} - \frac{q_{012}^3}{24} \text{Si}(q_{012}) - \frac{1}{24q_{012}}(q_{012}^2 - 6) \sin(q_{012}) - \frac{1}{24}(\sigma_{012}^2 - 2) \cos(q_{012}) \quad (35)$$

$$M_{22}(q_{02}) = \frac{\pi q_{02}^3}{48} - \frac{q_{02}^3}{24} \text{Si}(q_{02}) - \frac{1}{24q_{02}}(q_{02}^2 - 6) \sin(q_{02}) - \frac{1}{24}(\sigma_{02}^2 - 2) \cos(q_{02}). \quad (36)$$

We can calculate isothermal compressibility and thermodynamic fluctuations from eqs (31)–(33) by taking the limit $S_{\alpha\beta}(q \rightarrow 0)$, which gives

$$S_{11}(q \rightarrow 0) = S_{011}(x_1, x_2) = \frac{x_1}{1 - \frac{4}{3}\pi\beta D_{11}\sigma_{11}^3 \rho x_1}, \quad (37)$$

$$S_{12}(q \rightarrow 0) = S_{012}(x_1, x_2) = \frac{\frac{4}{3}\pi\beta D_{12}\sigma_{12}^3 \rho}{1 - \frac{4}{3}\pi\beta D_{11}\sigma_{11}^3 \rho x_1} x_1 x_2, \quad (38)$$

$$S_{22}(q \rightarrow 0) = S_{022}(x_1, x_2) = x_2 + \frac{4}{3}\pi\beta D_{22}\rho\sigma_{22}^3 x_2^2 + \frac{(\frac{4}{3}\pi\beta D_{12}\sigma_{12}^3 \rho)^2}{1 - \frac{4}{3}\pi\beta D_{11}\sigma_{11}^3 \rho x_1} x_1 x_2^2, \quad (39)$$

where $\rho_1 = x_1\rho$, $\rho_2 = x_2\rho$ in homogeneous systems and $\rho = N/V$ is the usual density of the system or the solution. For completeness and for the benefit of interested researchers we included formulas for higher concentration in the Appendix.

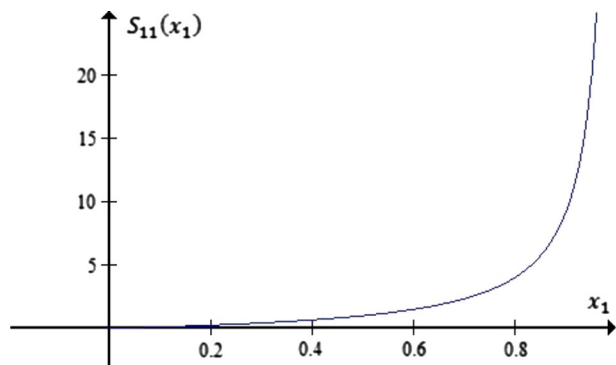


Figure 1. The static structure factor $S_{11}(q \rightarrow 0) = S_{011}(x_1)$ vs. x_1 (molar fraction for the first component) for the van der Waals potential to the first component in the system when $4\pi\sigma_{11}^3/3 = 1(\text{nm})^3$, $4\pi\sigma_{22}^3/3 = 1000(\text{nm})^3$, $\beta D_{11} = 1$, $\beta D_{12} = 0.1$, $\beta D_{22} = 0.2$ and $\rho = 10^{21}(\text{cm})^{-3}$.

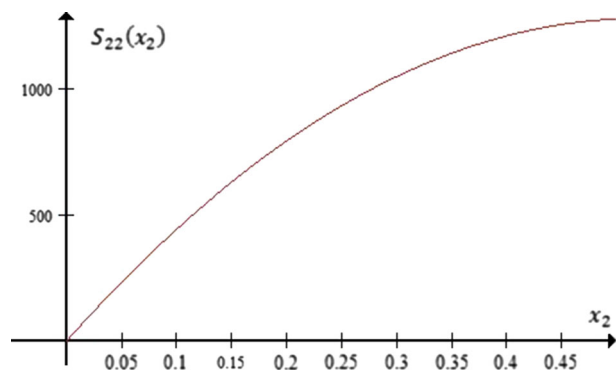


Figure 2. The static structure factor $S_{22}(q \rightarrow 0) = S_{022}(x_2)$ vs. x_2 (molar fraction for the second component) for the van der Waals potential to the second component in the system when $4\pi\sigma_{11}^3/3 = 1(\text{nm})^3$, $4\pi\sigma_{22}^3/3 = 1000(\text{nm})^3$, $\beta D_{11} = 1$, $\beta D_{12} = 0.1$, $\beta D_{22} = 0.2$ and $\rho = 10^{21}(\text{cm})^{-3}$.

4. Results and calculations

In this work, we calculated static structure factors for a dilute solution composed of two components (solvent and solution). We used eqs (31), (32) and (33).

We can represent thermodynamic fluctuations for components in our system vs. molar fractions for two components in the system as shown in figures 1 and 2.

The resulting partial static structure factor $S_{11}(q \rightarrow 0) = S_{011}(x_1)$ in this work is in agreement with the one calculated from PY hard sphere one-component solution given in ref. [3].

We can represent inverse static structure factor $S_{022}^{-1}(x_2)$ (or $S_{022}^{-1}(\phi_2)$ because $\phi_2 \propto x_2$) for the same parameter values. The results are shown in figure 3.

The resulting $S_{022}^{-1}(x_2)$ agrees qualitatively with experimental static structure factor of globular proteins in aqueous solution from the work of Fine *et al* [15].

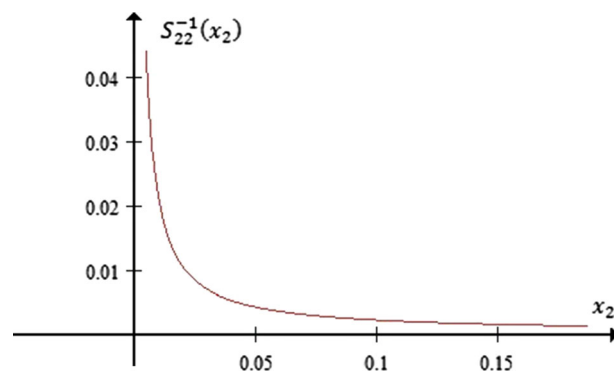


Figure 3. Inverse static structure factor $S_{022}^{-1}(x_2)$ vs. x_2 (molar fraction for the second component) for the same parameter values in figures 1 and 2.

For the purpose of quantitative comparison, partial structure factors in specific cases were calculated for a two-component system SiO_2 glass, silicon and oxygen. This system is well studied and there are many results from experiment and simulations [18]. We calculated partial structure factors for SiO_2 $S_{11}(q) = S_{\text{OO}}(q)$, $S_{22}(q) = S_{\text{SiSi}}(q)$ and $S_{12}(q) = S_{\text{SiO}}(q)$ for selected q values, $q = 0 \text{ \AA}^{-1}$, $q = 1.5 \text{ \AA}^{-1}$ and $q = 2 \text{ \AA}^{-1}$, at 2225°C where $\rho = 2.1 \times 10^{28} \text{ m}^{-3}$, using equations [31–33] and also we calculated partial structure factors for the general case from the three equations listed in Appendix, and the results are shown in table 1.

5. Conclusion

In this work, we derived analytical solutions for static structure factor for homogeneous and isotropic solution composed of two components interacting with each other via simple van der Waals potential which is inversely proportional to the sixth power of the distance between the two components. The derivation was done under the assumption that the dissolved material has low concentration in comparison to concentration of the solvent, i.e. dilute solution, which is common for macromolecular fluids. We calculated partial structure factors for the two-component systems and isothermal compressibility as a function of concentration. The results agreed qualitatively with many other studies [3,16,17]. The partial structure factors for the specific two-component system SiO_2 was calculated using the derived analytical equations and it was found that the theoretical and experimental results were in reasonable agreement [1,17]. However, the results from the generalisation listed in the Appendix are in better agreement with simulation results as shown in table 1, but

Table 1. The partial structure factors for silicon dioxide glass at 2225°C for three q values resulting from this work and the work of Vashishta *et al* [16].

q (Å ⁻¹)	$S_{Oo}(q)$			$S_{Sisi}(q)$			$S_{Sio}(q)$		
	This work	This work ^a	Ref. [16]	This work	This work ^a	Ref. [16]	This work	This work ^a	Ref. [16]
0	0.70	0.33	0.2	2.02	0.09	0.1	0.13	0.09	0.1
1.5	0.68	0.63	0.6	0.09	0.43	0.5	- 0.01	0.3	0.5
2	0.66	0.39	0.4	0.1	0.77	0.8	- 0.09	- 0.05	- 0.1

^aNumerical results calculated from general case equations are listed in Appendix.

this type of calculations is more demanding mathematically and computationally. We compared partial structure factors for protein from our results with experimental results in [15] and found that the results agreed qualitatively.

We believe that the presented analytical solution has the advantage of low computational cost and the results agree reasonably with results of other more demanding theoretical methods or simulation and it is applicable to a wide range of two-component fluids. The derived equations can be useful in studying biomolecular and

other soft matter fluids and complement simulation and other theoretical work.

Appendix

Generalisation

We can generalise our calculation to higher concentrations and in this case we use eqs (12)–(15) to derive the following formulas:

$$\begin{aligned}
 S_{11}(q) &= x_1 + x_1 \rho_1 \left(\begin{aligned} & \left[[4\pi\beta D_{11}\sigma_{11}^3 M_{11}(q_{01})][1 - 4\pi\beta D_{11}\rho_1\sigma_{11}^3 M_{11}(q_{01})]^{-1} \right] \\ & \left[\begin{aligned} & [16\pi^2 \rho_2 [\beta D_{12}\sigma_{12}^3 M_{12}(q_{012})]^2][1 - \\ & 8\pi\beta D_{11}\sigma_{11}^3 \rho_1 M_{11}(q_{01}) \\ & - 4\pi\beta D_{22}\rho_2\sigma_{22}^3 M_{22}(q_{02}) \\ & + 32\pi^2 \beta^2 \rho_1 \rho_2 D_{11}\sigma_{11}^3 M_{11}(q_{01}) D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & + 16\pi^2 \rho_1^2 [\beta D_{11}\sigma_{11}^3 M_{11}(q_{01})]^2 \\ & - 16\pi^2 \rho_1 \rho_2 [\beta D_{12}\sigma_{12}^3 M_{12}(q_{012})]^2 \\ & - 64\pi^3 \beta^3 \rho_1^2 \rho_2 [D_{11}\sigma_{11}^3 M_{11}(q_{01})]^2 D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & + 64\pi^3 \beta^3 \rho_1^2 \rho_2 D_{11}\sigma_{11}^3 M_{11}(q_{01}) [D_{12}\sigma_{12}^3 M_{12}(q_{012})]^2 \end{aligned} \right]^{-1} \end{aligned} \right) \\
 S_{12}(q) &= [4\pi x_1 \rho_2 \beta D_{12}\sigma_{22}^3 M_{22}(q_{012})] \left[\begin{aligned} & \left[\begin{aligned} & 1 - 4\pi\beta \rho_1 D_{11}\sigma_{11}^3 M_{11}(q_{01}) \\ & - 4\pi\beta \rho_2 D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & + 16\pi^2 \beta^2 \rho_1 \rho_2 D_{11}\sigma_{11}^3 M_{11}(q_{01}) D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & - 4\pi \rho_1 \rho_2 [\beta D_{12}\sigma_{22}^3 M_{22}(q_{012})]^2 \end{aligned} \right]^{-1} \end{aligned} \right) \\
 S_{22}(q) &= x_2 + \rho_2 x_2 \left(\begin{aligned} & \left[[4\pi\beta D_{22}\sigma_{22}^3 M_{22}(q_{02})][1 - 4\pi\beta \rho_2 D_{22}\sigma_{22}^3 M_{22}(q_{02})]^{-1} \right] + \\ & \left[\begin{aligned} & [16\pi^2 \rho_2 [\beta D_{12}\sigma_{22}^3 M_{22}(q_{012})]^2][1 - \\ & 8\pi\beta \rho_2 D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & - 4\pi\beta \rho_1 D_{11}\sigma_{11}^3 M_{11}(q_{01}) \\ & + 32\pi^2 \beta^2 \rho_1 \rho_2 D_{11}\sigma_{11}^3 M_{11}(q_{01}) D_{22}\sigma_{22}^3 M_{22}(q_{02}) \\ & + 16\pi^2 \rho_2^2 [\beta D_{22}\sigma_{22}^3 M_{22}(q_{02})]^2 \\ & - 16\pi^2 \rho_1 \rho_2 [\beta D_{12}\sigma_{22}^3 M_{22}(q_{012})]^2 \\ & - 64\pi^3 \beta^3 \rho_2^2 \rho_1 [\beta D_{22}\sigma_{22}^3 M_{22}(q_{02})]^2 D_{11}\sigma_{11}^3 M_{11}(q_{01}) \\ & + 64\pi^3 \beta^3 \rho_2^2 \rho_1 D_{22}\sigma_{22}^3 M_{22}(q_{02}) [D_{12}\sigma_{22}^3 M_{22}(q_{012})]^2 \end{aligned} \right]^{-1} \end{aligned} \right)
 \end{aligned}$$

and $M_{\alpha\beta}(q_0)$ are the same functions as in eqs (34)–(36).

Computational implementation

We have used Wolfram Mathematica online [18] resources to implement the computation using cloud computing. Users need to have registered software to be able to access these capabilities. To do so we did the following:

1. We defined the needed parameters like σ_{11} , σ_{22} , D_{11} etc., calculate β for specific temperature to be used in S_{ij} and in M functions.
2. We typed equations [31–33] for low densities and the general case equations as they appear in the Appendix, on Mathematica software. Note that only online Mathematica package will allow editing such long equations.
3. Then we used online Wolfram Mathematica to calculate the results S_{ij} for every q (will take from half an hour to an hour).

References

- [1] J P Hansen and I R McDonald, *Theory of simple liquids* third edn (Academic Press, 2005)
- [2] R Fantoni, *Classical liquids: Exact results, integral equations theory and Monte Carlo simulations*, Ph.D. thesis (Trieste, 2003)
- [3] G Nägele, *The physics of colloidal soft matter* (Institute of Fundamental Technological Research, Warsaw, 2004)
- [4] C N Likos, *Effective interactions in soft condensed matter physics* (DuKsseldorf, Germany, 2001)
- [5] A J Archer, *Statistical mechanics of soft core fluid mixtures*, Ph.D. thesis (University of Bristol, 2003)
- [6] E Matteoli and G A Mansoori, *J. Chem. Phys.* **4672** (1995)
- [7] W J Briels, *Theory of polymer dynamics* (Enschede, 1998)
- [8] C A Croxton, *Liquid state physics: Statistical mechanical introduction* (Cambridge University Press, 1973)
- [9] A M R de Graff and M F Thorpe, *Acta Crystallogr. A* **66**, 22 (2010)
- [10] O M Osiele, *Nigerian J. Phys.* **18(1)**, 25 (2006)
- [11] G N Chuev and M V Fedorov, *J. Chem. Phys.* **120**, 1191 (2004)
- [12] A Trokhymchuk *et al*, *Condens. Matter Phys.* **14(3)**, 33005 (2011)
- [13] J A Anta, F Bresme and S Lago, *J. Phys. Condens. Matter* **15**, 1 (2003)
- [14] P Zihlerl, *Physics of soft matter* (University of Ljubljana, Jožef Stefan Institute, Ljubljana, 2013)
- [15] B M Fine, A Lomakin, O O Ogun and G B Benedek, *J. Chem. Phys.* **104(1)**, 326 (1996)
- [16] P Vashishta, R K Kalia, J P Rino and I Ebbsjo, *Phys. Rev. B* **41**, 12197 (1990)
- [17] Q Mei *et al*, *Phys. Rev. B* **78**, 144204 (2008)
- [18] www.wolfram.com/mathematica/online/