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A modified version of a self-consistent Ornstein–Zernike approximation for a fluid with a one-Yukawa pair potential

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Abstract

We present a modified version of a thermodynamically self-consistent Ornstein–Zernike approximation (SCOZA) for a fluid of spherical particles with a pair potential given by a hard core repulsion and a Yukawa tail $\phi(r) = -k_B T \mathcal{K}^{(2,-1)} e^{-z_2 r}/r$. We take advantage of the known analytical properties of the solution of the Ornstein–Zernike equation for the case in which the direct correlation function outside the repulsive core is given by the multi-screened Coulomb plus power series (multi-SCPPS) tails

$$c(r) = \sum_n e^{-z_n r} \sum_{\tau=-1}^{L_n} K^{(n,\tau)} z_n^{\tau+1} r^\tau \qquad r > 1,$$

and the radial distribution function $g(r)$ satisfies the exact core condition $g(r) = 0$ for $r < 1$. The SCOZA is known to provide very good overall thermodynamics and a remarkably accurate critical point and coexistence curve. However, the SCOZA presented so far for continuum fluids has the deficiency that the solution behaves singularly at a density ρ where the screening length $z_1(\rho)$ of the hard sphere fluid nearly coincides with the Yukawa-tail screening length z_2 (>3.8). This is by no means a rare case in the studies of real fluids and colloidal suspensions. We show that the deficiency is resolved in the modified version of the SCOZA with multi-SCPPS tails. As a demonstration, we present some numerical results for $z_2 = 8.0$.

1. Introduction

The self-consistent Ornstein–Zernike approximation (SCOZA) [1–8], the generalized mean spherical approximation (GMSA) [9, 10], the modified hypernetted chain (MHNC) approximation [11], and the hierarchical reference theory (HRT) [12–14] are well known to be powerful tools in the study of fluids. These sophisticated microscopic theories are shown to produce results for systems well inside the liquid-state region that are practically indistinguishable from the Monte Carlo or molecular dynamic simulation data. However, the accuracy of these approaches begins to decrease as one leaves the liquid-state region and approaches the liquid–gas coexistence curve and/or the critical region. Some theoretical approaches even fail to converge in the critical region, so that the liquid and vapour branches of the coexistence curve remain unconnected. To overcome this highly unsatisfactory situation the SCOZA and the HRT have been developed in the past years, that cope with the problems encountered in the critical region and near the phase boundaries (see [8, 10] and references quoted therein).

The SCOZA was proposed in the 1970s by Høye and Stell [1, 2], but fast and accurate algorithms for evaluating its thermodynamic properties were developed only recently [15, 5]. Pini *et al* [4] have applied the SCOZA to a continuum fluid of spherical particles with a pair potential given by a hard core repulsion and a Yukawa attractive tail $w(r) = -\exp[-z_2(r-1)]/r$. They have considered the following direct correlation function outside the repulsive core:

$$c(r) = c_{\mathrm{HS}}(r) + R(\rho, \beta) w(r) \qquad r > 1, \tag{1}$$

where $R(\rho, \beta)$ is a function of the thermodynamic state of the system and $\beta = 1/k_{\mathrm{B}}T$, T being the absolute temperature and k_{B} the Boltzmann constant. The direct correlation function of the hard sphere fluid is given by

$$c_{\mathrm{HS}}(r) = \mathcal{K}_1 \frac{\exp[-z_1(r-1)]}{r}, \tag{2}$$

where $\mathcal{K}_1$ and z_1 are known functions of the density ρ. The thermodynamic consistency has been enforced between the internal energy and the compressibility route. Their version of the SCOZA allows one to take advantage of the known analytical properties of the solution of the Ornstein–Zernike (OZ) equation. Comparing the results from the SCOZA with Monte Carlo simulation data, they have shown that the SCOZA yields both very good overall thermodynamics and a remarkably accurate coexistence curve up to the critical point.

Stell *et al* have developed a GMSA scheme for ionic and dipolar fluids [16]. In their scheme self-consistency among the three thermodynamic routes (virial, energy and compressibility route) was enforced. However, thermodynamic consistency was achieved by fitting the available GMSA parameters to some external set of data either given by a prescribed equation of state or obtained from computer simulations. In contrast, in the SCOZA with which we will be concerned below no supplementary thermodynamic or other input is necessary. Thus this scheme is entirely self-contained.

The SCOZA has been generalized to fluids with hard-core multi-Yukawa systems [8]. This has enabled one to treat various systems with pair potentials that can be parameterized in terms of linear combinations of Yukawa tails: the Lennard-Jones potential and the Girifalco potential that describes the interaction between fullerene particles. However, the SCOZA scheme presented so far has a deficiency that the solution behaves singularly at a density ρ where the screening length $z_1(\rho)$ of the hard sphere fluid nearly coincides with one of the Yukawa-tail screening length(s). The value of $z_1(\rho)$ varies monotonically from 3.8 to 34.0 in the density range of $0 < \rho < 1$. When we apply the SCOZA to complex fluids like colloidal suspensions or globular protein solutions, or we treat various systems with pair potentials parameterized in terms of linear combinations of Yukawa tails, the value of some Yukawa screening length will be enforced to lie in the range of $z_1(\rho)$. Therefore we will encounter the singular behaviour problem when we apply the SCOZA to these fluid models.

By the way, we have recently found an analytic solution of the OZ equation for a multi-component fluid of spherical particles with screened Coulomb plus power series (multi-SCPPS) tails given by

$$c_{ij}(r) = \sum_n \mathrm{e}^{-z_n r} \sum_{\tau=-1}^{L_n} K_{ij}^{(n,\tau)} z_n^{\tau+1} r^\tau \qquad \sigma_{ij} = (\sigma_i + \sigma_j)/2 < r, \tag{3}$$

where L_n are arbitrary integers, $c_{ij}(r)$ is the direct correlation function for two spherical molecules of species i and j, σ_i is the diameter of the spherical hard core of species i, and $K_{ij}^{(n,\tau)}$ and z_n are constants to be adjusted by physical arguments. The analytic solution offers sufficient flexibility and opens access to systems with any smooth, realistic isotropic potentials where the pair potentials can be fitted by the multi-SCPPS tails [17–20]. The multi-Yukawa tails are included in the multi-SCPPS tails as a special case.

In the present paper, we will present a modified version of the SCOZA for a fluid of spherical particles with a pair potential given by a hard core repulsion and a Yukawa tail. We take advantage of the analytical properties of the solution of the OZ equation with multi-SCPPS closure. We will show that the above mentioned singular behaviour problem will be resolved in the modified version of the SCOZA considered here, presenting some numerical results for $z_2 = 8.0$.

2. Theory

We consider here a fluid of spherical particles interacting via a pair potential $\phi(r)$ which is the sum of a singular repulsive hard sphere contribution and a Yukawa tail. The expression for $\phi(r)$ is then

$$\phi(r) = \begin{cases} \infty & r < 1, \\ -k_\mathrm{B} T \mathcal{K}^{(2,-1)} \dfrac{\mathrm{e}^{-z_2 r}}{r} & r > 1, \end{cases} \tag{4}$$

where $\mathcal{K}^{(2,-1)}$ is a constant. We incorporate in the SCOZA the consistency between the compressibility and internal energy route to the thermodynamics according to the scheme of Pini *et al* (see [4, 8] and references cited therein). The requirement leads to the following equation:

$$\frac{\partial}{\partial \beta}\left(\frac{1}{\chi_\mathrm{red}}\right) = \rho \frac{\partial^2 u}{\partial \rho^2}, \tag{5}$$

where χ_red is the reduced compressibility and u is the excess internal energy per unit volume. While this relation is of course satisfied by the exact compressibility and internal energy, this is not the case with those predicted by most integral equation theories. In order to cope with this lack of thermodynamic consistency, we consider the following closure to the OZ equation:

$$\begin{cases} g(r) = 0 & r < 1, \\ c(r) = \mathcal{K}_1 \dfrac{\exp[-z_1(r-1)]}{r} + R\mathcal{K}^{(2,-1)} \dfrac{\mathrm{e}^{-z_2 r}}{r} = \displaystyle\sum_{n=1}^{2} K^{(n,-1)} \dfrac{\mathrm{e}^{-z_n r}}{r} & r > 1, \end{cases} \tag{6}$$

where R must be determined so that thermodynamic consistency condition (5) is satisfied, and $K^{(1,-1)} = \mathcal{K}^{(1,-1)} = \mathcal{K}_1 \mathrm{e}^{z_1}$, $K^{(2,-1)} = R\mathcal{K}^{(2,-1)}$. The amplitude $\mathcal{K}_1$ and the screening length z_1 of $c_\mathrm{HS}(r)$ for the hard sphere fluid are determined as a function of the density by requiring that both the compressibility and the virial route to the thermodynamics give the Carnahan–Starling equation of state [4]. It is now possible to take advantage of the fact that for the OZ equation supplemented by closure (6) extensive analytical results have been determined.

However, when we study complex fluids like colloidal suspensions and globular protein solutions we will have to set the value of z_2 equal to some value of $z_1(\rho) > 3.8$. In this case, the analytic solution of the OZ equation with closure (6) behaves singularly near the density ρ where $z_1(\rho) = z_2$ as will be seen later. In order to resolve the singular behaviour problem we expand $c(r)$ of (6) in a power series of δz $(=z_1 - z_2)$ and get the following closure:

$$\begin{cases} g(r) = 0 & r < 1, \\ c(r) = \mathrm{e}^{-z_2 r} \displaystyle\sum_{\tau=-1}^{L} K^{(2,\tau)} z_2^{\tau+1} r^{\tau} & r > 1, \end{cases} \tag{7}$$

where L is an arbitrary integer. The first three of the coefficients $K^{(2,\tau)}$ are given by

$$K^{(2,-1)} = R\mathcal{K}^{(2,-1)} + \mathcal{K}_1 \mathrm{e}^{z_1}, \qquad K^{(2,0)} = -\mathcal{K}_1 \mathrm{e}^{z_1} \frac{\delta z}{z_2}, \qquad K^{(2,1)} = \frac{\mathcal{K}_1 \mathrm{e}^{z_1}}{2} \left(\frac{\delta z}{z_2}\right)^2. \tag{8}$$

2.1. Normal case of non-small $|\delta z|$

We can take advantage of our recent analytical properties of the solution of the Baxter's factorized version of the OZ equation supplemented by closure (6) or (7). In the case where $|\delta z|$ is not so small, from equations (10) in [20] with closure (6), we obtain the following equations:

$$\mathcal{D}_1 \left[1 - \rho \widetilde{Q}^{(0)}(\mathrm{i}z_1)\right] = 1 \tag{9}$$

$$R = \mathcal{D}_2 \left[1 - \rho \widetilde{Q}^{(0)}(\mathrm{i}z_2)\right], \tag{10}$$

where $\mathcal{D}_n = z_n D^{(-1)}(z_n)/2\pi \mathcal{K}^{(n,-1)}$ and functions $\widetilde{Q}^{(0)}(\mathrm{i}z_n)$ $(n = 1, 2)$ are obtained from (B.5) in [20]. Here and hereafter we have used the same symbols as those in [17–20] otherwise speaking and we have omitted the subscripts which express the particle species.

From equations (9) in [20] we obtain for $\mathcal{D}_n$ $(n = 1, 2)$ the following linear equations:

$$\sum_{n=1}^{2} \mathcal{W}_{kn} \mathcal{D}_n = Y_k \tag{11}$$

where $\mathcal{W}_{kn}$ and Y_k $(k, n = 1, 2)$ are given in appendix A. In the normal case of non-small $|\delta z|$, the determinant of matrix $\mathcal{W}_{kn}$ has a non-zero value and $\mathcal{D}_n$ $(n = 1, 2)$ will have a normal value. On the other hand, when δz approaches zero the determinant of matrix $\mathcal{W}_{kn}$ becomes closer to zero (see figure 5) and the value of $\mathcal{D}_n$ $(n = 1, 2)$ will diverge. In order to resolve the divergence we use the closure (7) instead of (6) in the next subsection.

By the way, equation (5) can be rewritten as [4, 8]

$$\mathcal{B}(\rho, u) \frac{\partial u}{\partial \beta} = \rho \frac{\partial^2 u}{\partial \rho^2}, \tag{12}$$

where

$$\mathcal{B}(\rho, u) = \frac{A}{2\pi^2} \sum_{j=1}^{L} \frac{\partial A}{\partial \mathcal{G}_j} \frac{\partial \mathcal{G}_j}{\partial u}. \tag{13}$$

Here $L = 2$ and $\mathcal{G}_n = \mathcal{G}^{(1)}(z_n)$ $(n = 1, 2)$ in the normal case. We obtain a relation $e^{\mathcal{G}_2} = -u z_2 / 2\pi \rho^2$ from equation (33) in [20]. When u is given, the unknown variable $\mathcal{G}_1$ is obtained by solving equation (9) with equations (11). The excess internal energy u is obtained from equation (12) applying to our case straightforwardly the SCOZA scheme and boundary conditions for (12) which are described in detail in [8].

2.2. Singular case of sufficiently small $|\delta z|$

From equations (10) in [20] with closure (7) neglecting the higher order terms than $(\delta z/z_2)^2$, we obtain the following equations:

$$R\frac{\mathcal{K}^{(2,-1)}}{\mathcal{K}_1 e^{z_1}} = \mathcal{D}_1\left[1-\rho\widetilde{Q}^{(0)}(\mathrm{i}z_2)\right] - \mathcal{D}_2\left[1+z_2\rho\widetilde{Q}^{(1)}(\mathrm{i}z_2) - \rho\widetilde{Q}^{(0)}(\mathrm{i}z_2)\right] + \mathcal{D}_3 z_2\rho\left[2\widetilde{Q}^{(1)}(\mathrm{i}z_2) - z_2\widetilde{Q}^{(2)}(\mathrm{i}z_2)\right] - 1 \tag{14}$$

$$-\frac{\delta z}{z_2} = \mathcal{D}_2\left[1-\rho\widetilde{Q}^{(0)}(\mathrm{i}z_2)\right] - 2\mathcal{D}_3\left[1+z_2\rho\widetilde{Q}^{(1)}(\mathrm{i}z_2) - \rho\widetilde{Q}^{(0)}(\mathrm{i}z_2)\right] \tag{15}$$

$$\frac{1}{2}\left(\frac{\delta z}{z_2}\right)^2 = \mathcal{D}_3\left[1-\rho\widetilde{Q}^{(0)}(\mathrm{i}z_2)\right] \tag{16}$$

where $\mathcal{D}_n = z_2 D^{(n-2)}(z_2)/2\pi\mathcal{K}_1 e^{z_1}$ $(n = 1, 2, 3)$ [20]. Similarly to the previous subsection, the quantities $\mathcal{D}_n$ $(n = 1, 2, 3)$ are obtained from the following linear equations:

$$\sum_{n=1}^{3}\mathcal{W}_{kn}\mathcal{D}_n = Y_k \tag{17}$$

where $\mathcal{W}_{kn}$ and Y_k $(k, n = 1, 2, 3)$ are given in appendix B. The function $\mathcal{B}(\rho, u)$ in equation (12) is given by

$$\mathcal{B}(\rho, u) = \frac{A}{2\pi^2}\sum_{j=1}^{3}\frac{\partial A}{\partial\mathcal{G}_j}\frac{\partial\mathcal{G}_j}{\partial u}, \tag{18}$$

where $\mathcal{G}_j = \mathcal{G}^{(j)}(z_2)$ $(n = 1, 2, 3)$ and we have a relation $e^{\mathcal{G}_1} = -uz_2/2\pi\rho^2$ [20]. When u is given, the unknown variables $\mathcal{G}_2$ and $\mathcal{G}_3$ are obtained by solving equations (15) and (16) with equation (17), applying again the SCOZA scheme of [8] to the present case. Equation (14) yields R.

3. Numerical results

The numerical integration of the partial differential equation (12) with initial condition and boundary conditions given in [4, 8] has been performed on a density grid with $\Delta\rho = 10^{-4}$. At the beginning of the integration the temperature step $\Delta\beta$ was set at $\Delta\beta = 10^{-2}$. As the temperature approaches its critical value, $\Delta\beta$ can be decreased further if one wishes to get very close to the critical point ($\Delta\beta \sim 10^{-7}$), and then gradually expanded back. The inverse range parameter of the attractive tail in equation (4) has been set at $z_2 = 8.0$. The interaction strength $\varepsilon = k_B T\mathcal{K}^{(2,-1)}/\exp(z_2)$ has been set equal to one. Figures 1–3 show coexistence curves of the hard sphere Yukawa fluid in the density–temperature plane, in the internal energy–temperature plane and in the temperature–chemical potential plane, respectively (all quantities are in reduced units [4]). Critical values of the density, temperature, internal energy per particle, chemical potential and pressure are $\rho_c = 0.475$, $T_c = 0.3916$, $u_c/\rho_c = -1.297$, $\mu_c = -0.887$, and $P_c = 0.059\,16$, respectively. Figure 4 shows the results for the compressibility factor $Z = P/(\rho k_B T)$ along the critical isotherm. Figure 5 shows the determinant of the matrix $\mathcal{W}_{kn}$ in (11) as a function of the density ρ along the critical isotherm. It shows that det $\mathcal{W}$ has a value of 0 at $\rho = 0.3624$. Therefore, numerical solutions will diverge in the vicinity of that density in the methods presented so far. In the present case, to resolve the singular problem we have switched from normal case to singular case in that region where we have used the switching criterion $|z_2 - z_1(\rho)| < 0.01$. Figure 6 shows the numerical solutions of $\mathcal{G}_1$ and $\mathcal{G}_2$ for the normal case and $\mathcal{G}_1$, $\mathcal{G}_2$, and $\mathcal{G}_3$ for the singular case as a function of density ρ along the critical isotherm.

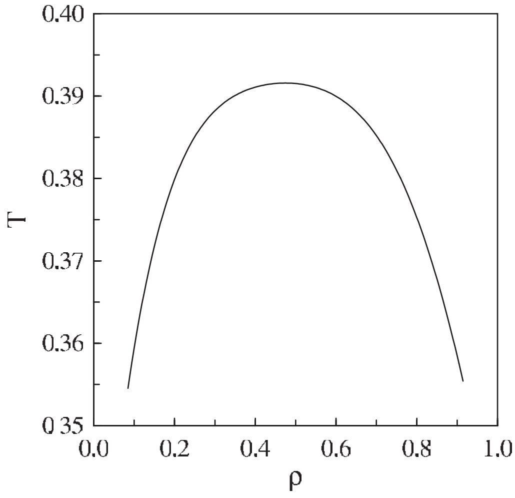

Figure 1. Coexistence curve of the hard sphere Yukawa fluid ($z_2 = 8.0$) in the density–temperature plane (density and temperature are in reduced units).

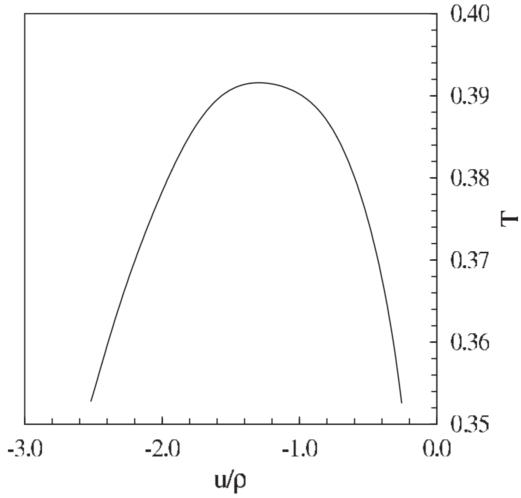

Figure 2. Coexistence curve of the hard sphere Yukawa fluid in the internal energy–temperature plane. u/ρ is the internal energy per particle in reduced units.

4. Concluding remarks

We have presented a modified version of a thermodynamically self-consistent Ornstein–Zernike approximation for a fluid of spherical particles with a pair potential given by a hard core repulsion and a Yukawa tail. The thermodynamic consistency has been enforced between the internal energy and the compressibility route. We have taken advantage of the known analytical properties of the solution of the OZ equation for the case in which the direct correlation function outside the repulsive core is given by the multi-SCPPS tails.

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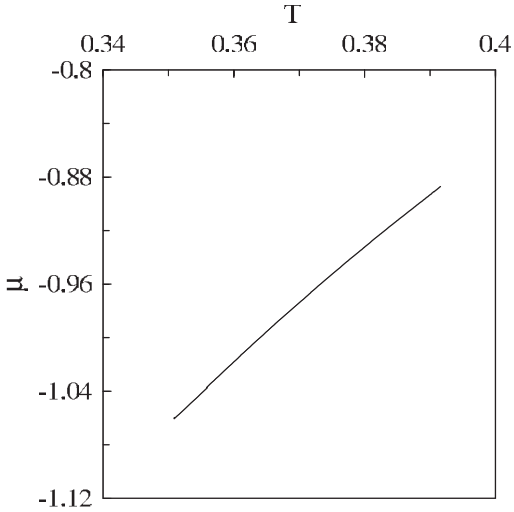

Figure 3. Coexistence curve of the hard sphere Yukawa fluid in the temperature–chemical potential plane (temperature and chemical potential are in reduced units).

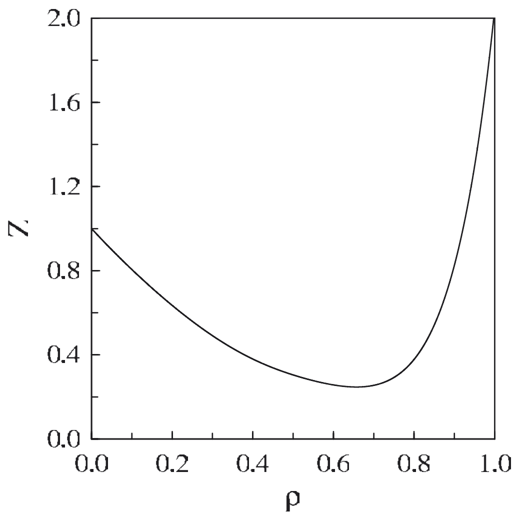

Figure 4. Compressibility factor $Z = P/(\rho k_B T)$ of the hard sphere Yukawa fluid as a function of the density ρ along the critical isotherm.

far for continuum fluids has a deficiency that the solution behaves singularly at a density where the screening length of the hard sphere fluid nearly coincides with the Yukawa-tail screening length. We will encounter the singular behaviour problem when we apply the SCOZA to real fluids or colloidal suspensions. In the present paper, we have shown that the deficiency has been resolved in the modified version of the SCOZA with multi-SCPPS tails. Though we have neglected for simplicity in the present paper the higher order terms than $(\delta z/z_2)^2$ in the closure (7), it is straightforward to include the neglected terms in the present scheme.

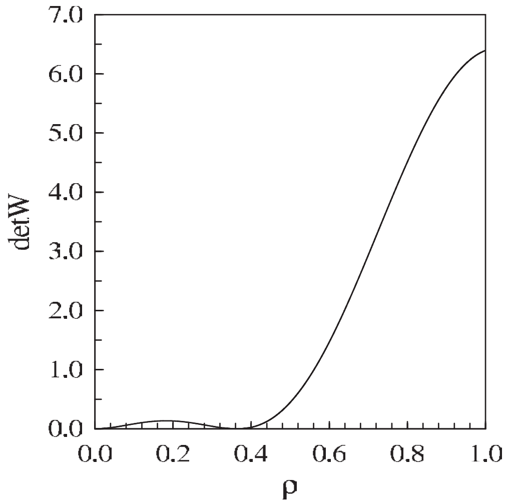

Figure 5. Determinant of the matrix $\mathcal{W}_{kn}$ in (11) as a function of the density ρ along the critical isotherm.

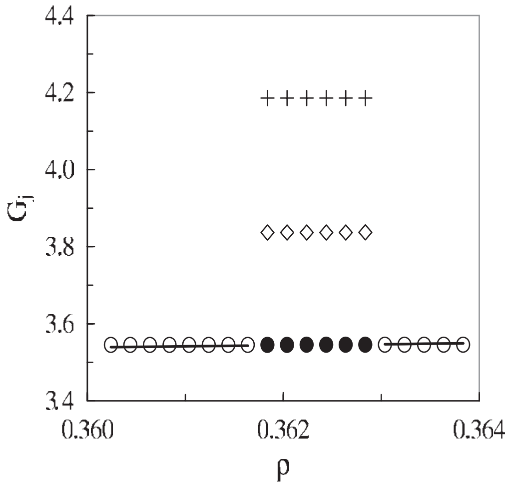

Figure 6. Solutions of $\mathcal{G}_1$ (solid lines) and $\mathcal{G}_2$ (open circles) in the normal case and $\mathcal{G}_1$ (closed circles), $\mathcal{G}_2$ (open diamonds) and $\mathcal{G}_3$ (crosses) in the singular case as a function of the density ρ along the critical isotherm in the vicinity of the region where $z_2 \sim z_1(\rho)$.

Appendix A

The quantities $\mathcal{W}_{kn}$ $(k, n = 1, 2)$ in equations (11) are

$$\frac{\mathcal{W}_{kn}}{\mathcal{K}^{(n,-1)}} = \breve{D}^{(0,-1)}(z_k, z_n) - \breve{C}^{(0,0)}(z_k, z_n) + \frac{2\pi\rho e^{-z_n}}{z_n^2}\breve{C}^{(0,0)}(z_k, z_n)e^{\mathcal{G}_n}$$
$$+ \breve{B}^{(0)}(z_k)\frac{2\pi}{z_n}\frac{2\pi}{\Delta}\rho\left[\left(1 - \frac{\pi\rho}{2\Delta}\right)H^{(-1,1)}(z_n) + \frac{\pi\rho}{4\Delta}H^{(-1,0)}(z_n)\right]$$
$$+ \frac{2\pi}{\Delta}\frac{2\pi}{z_n}\rho\breve{A}^{(0)}(z_k)\left[\frac{\pi\rho}{\Delta}H^{(-1,1)}(z_n) - \left(1 + \frac{\pi\rho}{2\Delta}\right)H^{(-1,0)}(z_n)\right]. \quad \text{(A.1)}$$

The quantities Y_k $(k = 1, 2)$ in equations (11) are given by

$$Y_k = \frac{\pi}{\Delta}\frac{\pi\rho}{2\Delta}\breve{B}^{(0)}(z_k) - \frac{\pi}{\Delta}\left(2 + \frac{\pi\rho}{\Delta}\right)\breve{A}^{(0)}(z_k) + \mathrm{e}^{\mathcal{G}_k}. \tag{A.2}$$

Appendix B

The quantities $\mathcal{W}_{kn}$ $(k, n = 1, 2, 3)$ in equations (17) are

$$\begin{aligned}\frac{\mathcal{W}_{m+1,\tau+2}}{\mathcal{K}_1\mathrm{e}^{z_1}} &= \breve{D}^{(m,\tau)}(z_2, z_2) - \breve{C}^{(m,\tau+1)}(z_2, z_2) + \breve{C}^{(m,\tau)}(z_2, z_2)(\tau + 1) \\ &\quad + \frac{2\pi\rho\mathrm{e}^{-z_2}}{z_2^2}\sum_{\beta=-1}^{\tau}\breve{C}^{(m,\beta+1)}(z_2, z_2)z_2^{\tau-\beta}C_{\tau-\beta}^{\tau+1}\mathrm{e}^{\mathcal{G}^{(\tau+1-\beta)}(z_2)} \\ &\quad + \breve{B}^{(m)}(z_2)\frac{2\pi}{z_2}\frac{2\pi}{\Delta}\rho\left[\left(1 - \frac{\pi\rho}{2\Delta}\right)H^{(\tau,1)}(z_2) + \frac{\pi\rho}{4\Delta}H^{(\tau,0)}(z_2)\right] \\ &\quad + \frac{2\pi}{\Delta}\frac{2\pi}{z_2}\rho\breve{A}^{(m)}(z_2)\left[\frac{\pi\rho}{\Delta}H^{(\tau,1)}(z_2) - \left(1 + \frac{\pi\rho}{2\Delta}\right)H^{(\tau,0)}(z_2)\right],\end{aligned} \tag{B.1}$$

where $m = 0, 1, 2$ and $\tau = -1, 0, 1$. The quantities Y_k $(k = 1, 2, 3)$ in equations (17) are given by

$$Y_{m+1} = \frac{\pi}{\Delta}\frac{\pi\rho}{2\Delta}\breve{B}^{(m)}(z_2) - \frac{\pi}{\Delta}\left(2 + \frac{\pi\rho}{\Delta}\right)\breve{A}^{(m)}(z_2) + \mathrm{e}^{\mathcal{G}^{(m+1)}(z_2)}, \tag{B.2}$$

where $m = 0, 1, 2$.

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