Towards a unification of hierarchical reference theory and self-consistent Ornstein-Zernike approximation: Analysis of exactly solvable mean-spherical and generalized mean-spherical models

J. S. Høye* and A. Reiner†
Department of Physics, Norwegian University of Science and Technology, N-7491 Trondheim, Norway
(Received 29 October 2006; published 19 April 2007)

The hierarchical reference theory (HRT) and the self-consistent Ornstein-Zernike approximation (SCOZA) are two liquid state theories that both furnish a largely satisfactory description of the critical region as well as the phase coexistence and equation of state in general. Furthermore, there are a number of similarities that suggest the possibility of a unification of both theories. Earlier in this respect we have studied consistency between the internal energy and free energy routes. As a next step toward this goal we here consider consistency with the compressibility route too, but we restrict explicit evaluations to a model whose exact solution is known showing that a unification works in that case. The model in question is the mean spherical model (MSM) which we here extend to a generalized MSM. For this case, we show that the correct solutions can be recovered from suitable boundary conditions through either SCOZA or HRT alone as well as by the combined theory. Furthermore, the relation between the HRT-SCOZA equations and those of SCOZA and HRT becomes transparent.

DOI: 10.1103/PhysRevE.75.041113 PACS number(s): 64.10.+h, 05.20.Jj, 64.70.Fx

I. INTRODUCTION

Both the self-consistent Ornstein-Zernike approximation (SCOZA) [1–3] and the hierarchical reference theory (HRT) [4] have been found to give very accurate results for fluids in thermal equilibrium. In particular, the respective nonlinear partial differential equations can be solved in the critical region, and their solution gives nonclassical, and partly Ising-like, critical indices. These equations are derived by obtaining the equation of state in two independent ways and using thermodynamic consistency to fix a free parameter in the direct correlation function.

Although both approaches appear similar in various ways, there are also marked differences. Both approaches make use of the compressibility route to thermodynamics, but SCOZA combines it with the internal energy route while HRT, inspired by momentum-space renormalization-group theory, uses the Helmholtz free-energy route. Thus, in short, the SCOZA adds effective strength to the attractive interaction by increasing inverse temperature $\beta=1/k_BT$ while HRT adds contributions to the interaction by including its Fourier components for shorter wave numbers Q until the limit of interest $Q\to 0$ is obtained.

In a recent work we considered thermodynamic consistency between the internal energy and free energy routes to thermodynamics [5]. In the present work we want to extend this to consistency with the compressibility route, too. This requires the introduction of two free parameters instead of a single one in each of the original theories. In view of the high accuracy of HRT and SCOZA, one may expect this increased freedom to give even better results both for spin systems and for fluids. Due to the complexity of the combined problem, we here limit ourselves to a simpler situation that can be analyzed explicitly and for which the exact solution can be established. This is the case for the mean spherical model (MSM). This model can be considered as the limit $D\to\infty$ for D-dimensional spins in d space dimensions where the transverse susceptibility is the relevant one for the fluctuation theorem or compressibility relation. In this connection we realize that the MSM can be extended in a straightforward way to a generalized MSM (GMSM) that yields the same HRT and SCOZA problems as the MSM; the only difference lies in the reference system boundary conditions. In the former the spin length is fixed to 1 while in the latter the spin length has some distribution of spin lengths. It should be pointed out that neither SCOZA nor HRT, nor our combined theory, are restricted to simple fluids and their lattice gas version although they are most often applied to these systems. The usual lattice gas is equivalent to the Ising model with spins $s=\pm 1$. So what we do here is to generalize and apply both of these theories to continuous spins on a lattice too.

In Sec. II we briefly consider the MSM, and in Sec. III we extend it to a GMSM whose solution is established. In Sec. IV the SCOZA problem for the GMSM model is considered while in Sec. V the corresponding HRT problem is considered. With both of these approaches one free parameter can be determined. By appropriate choice of this parameter we get partial differential equations whose solutions are those of the GMSM with the reference system as boundary condition. In Sec. VI an alternative method of solution based on a result from Ref. [5] is used. Then unification of SCOZA and HRT is considered in full generality in Sec. VII. In Sec. VIII a pair-correlation function of MSM form containing two free parameters is proposed and explicit HRT-SCOZA equations are established for the GMSM situation where transverse susceptibility replaces susceptibility. By analysis of these equations we show how the HRT-SCOZA equations work in this case and how the GMSM solution is recovered.

II. MEAN-SPHERICAL MODEL

Consider D-dimensional spins on a lattice in d space dimensions and with cells of unit volume. It is well established

*Electronic address: johan.hoye@phys.ntnu.no
†Electronic address: areiner@tph.tuwien.ac.at

that in the limit $D\to\infty$ this statistical mechanical system can be solved exactly [6,7]. Its solution is the same as that of the spherical model [8]. Here we will consider its variant, the mean-spherical model (MSM) [9]. In the MSM the Ising spins are replaced by interacting spins s_i whose length is Gaussian distributed such that $\langle s_i^2\rangle=1$. This is nothing but a Gaussian model with an adjustable one-particle harmonic potential to keep $\langle s_i^2\rangle=1$ fixed. More precisely one Laplace transforms the spherical constraint by which a Gaussian model partition function is obtained. In the thermodynamic limit (i.e., for an infinite system) the inverse transform is determined by the maximum term of the integrand. Following the evaluations by Høye and Stell the resulting Gibbs free energy g per spin becomes [10]

$$L=-\beta g=s+\frac{(\beta H)^2}{2[2s-\beta\tilde{\psi}(0)]}+\frac{1}{2}\ln\pi-\frac{1}{2}\frac{1}{(2\pi)^d}\times\int\ln[2s-\beta\tilde{\psi}(k)]d\mathbf{k}. \tag{2.1}$$

Here s is the Laplace-transform variable, H is the magnetic field, and $\tilde{\psi}(k)$ is the Fourier transform of the pair interaction normalized to $\tilde{\psi}(0)=1$. The maximum of expression (2.1) is obtained by taking $\partial L/\partial s=0$. Then the equation of state follows easily by utilizing the condition for maximum. However, in the next section we will generalize the MSM so we will come back to the equation of state there.

III. GENERALIZED MEAN-SPHERICAL MODEL

In the MSM the spherical constraint $\langle s_i^2\rangle=1$ is fixed. For D-dimensional spins ($D\to\infty$) this also corresponds to spins of fixed length. Now we can generalize this and let the D-dimensional spins have a distribution of lengths by which the spherical constraint is removed. At thermal equilibrium the average spin length squared will then change with both magnetization and temperature. This variation will depend upon the equation of state or the spin distribution specified for noninteracting spins. In the limit $D\to\infty$ this model will again be exactly solvable as the spin distribution becomes Gaussian, but the width of this distribution varies both with temperature and magnetization.

With this in mind we first generalize the MSM to $\langle s_i^2\rangle=n$ which replaces the first term of expression (2.1) by sn. Further, as n will not be fixed there must be a function $F(n)$ that accounts for the distribution of n values. In this way expression (2.1) can be generalized to

$$L=sn+\frac{(\beta H)^2}{2[2s-\beta\tilde{\psi}(0)]}+\frac{1}{2}\ln\pi-\frac{1}{2}\frac{1}{(2\pi)^d}\times\int\ln[2s-\beta\tilde{\psi}(k)]d\mathbf{k}-\frac{1}{2}F(n). \tag{3.1}$$

Again in the thermodynamic limit the free energy is determined by maximum of expression (3.1), but now with respect to both s and n. This gives the conditions

$$\frac{\partial L}{\partial s}=n-\left(\frac{\beta H}{2s-\beta}\right)^2-\frac{1}{(2\pi)^d}\int\frac{d\mathbf{k}}{2s-\beta\tilde{\psi}(k)}=0,$$

$$\frac{\partial L}{\partial n}=s-\frac{1}{2}F'(n)=0. \tag{3.2}$$

With this the magnetization becomes

$$m=\frac{\partial L}{\partial(\beta H)}=\frac{\beta H}{2s-\beta}. \tag{3.3}$$

Now we put

$$z=\frac{\beta}{2s}\quad\text{and}\quad P(z)=\frac{1}{(2\pi)^d}\int\frac{d\mathbf{k}}{1-z\tilde{\psi}(k)}, \tag{3.4}$$

and Eqs. (3.2) and (3.3) can be written

$$\beta(n-m^2)=zP(z),$$

$$\frac{z}{\beta}=f(n) \tag{3.5}$$

with $f(n)=1/F'(n)$ and

$$\beta H=m(2s-\beta)=\frac{m}{n-m^2}P(z)-\beta m=m\left(\frac{\beta}{z}-\beta\right). \tag{3.6}$$

From this we obtain the transverse susceptibility $\chi_\perp$ as (for D-dimensional spins) [10]

$$\frac{\beta}{\chi_\perp}=\frac{\partial(\beta H_\perp)}{\partial m_\perp}=\frac{\beta H}{m}=\frac{\beta}{z}-\beta, \tag{3.7}$$

where $H_\perp$ ($\to 0$) and $m_\perp$ ($\to 0$) are transverse magnetic field and transverse magnetization. The internal energy (from pair interactions) becomes

$$\begin{aligned}U&=-\left(\frac{\partial L}{\partial\beta}\right)_H-mH\\&=-\frac{1}{2}\frac{1}{(2\pi)^d}\int\frac{\tilde{\psi}(k)d\mathbf{k}}{2s-\beta\tilde{\psi}(k)}-\frac{1}{2}\left(\frac{\beta H}{2s-\beta}\right)^2\\&=-\frac{1}{2}m^2-\frac{1}{2\beta}[P(z)-1].\end{aligned} \tag{3.8}$$

In accordance with this the spin-correlation function for transverse correlations is

$$\tilde{\Gamma}_\perp(k)=\frac{z}{\beta[1-z\tilde{\psi}(k)]}. \tag{3.9}$$

Further in accordance with the fluctuation theorem $\tilde{\Gamma}_\perp(0)=\chi_\perp/\beta$ which is consistent with Eq. (3.7). By integrating this using Eqs. (3.4) and (3.5) one finds the "core" condition

$$\Gamma_{\perp}(0)=\frac{z}{\beta}P(z)=n-m^2. \tag{3.10}$$

With $n=1$ fixed one is back to the constraint of the usual MSM.

For n not fixed the function $f(n)$ must be defined by or related to the reference system at $\beta=0$ where $P(z)=1$ as then $z\to 0$. So with Eqs. (3.5)–(3.7) and (3.10) we have for the reference system

$$\mu=\mu(m^2)=\frac{\chi_{\perp}}{\beta}=n-m^2=\frac{z}{\beta}=f(n). \tag{3.11}$$

Thus

$$n=n(m^2)=\mu(m^2)+m^2. \tag{3.12}$$

For general β Eq. (3.5) then means

$$\mu=\mu(m^2)=n-m^2=\frac{z}{\beta}P(z)=f(n)P(z). \tag{3.13}$$

Now we can put

$$P(z)=1+2J \quad \text{and} \quad \mu_e=\frac{z}{\beta}=f(n)$$

by which Eq. (3.13) becomes

$$n-m^2=(1+2J)\mu_e=f(n)+2\mu_e J,$$

$$n-m_e^2=f(n)=\mu_e, \tag{3.14}$$

where

$$m_e^2=m^2+2\mu_e J. \tag{3.15}$$

Comparing Eqs. (3.14) and (3.15) with Eqs. (3.11) and (3.12) one sees that this implies

$$\mu_e=\mu_e(m^2)=n(m_e^2)-m_e^2=\mu(m_e^2). \tag{3.16}$$

IV. SCOZA FOR THE MODEL

In using the self-consistent Ornstein-Zernike approximation (SCOZA) one assumes that the direct correlation function is the same as for long-range forces outside hard cores, i.e., $-\beta\tilde{\psi}(k)$, and that there is an additional term that contains a free parameter determined from the consistency requirements of SCOZA. Traditionally this has been used to replace the temperature with an effective one, but here we will rely on the parameter z already introduced above. The SCOZA equation for D-dimensional spins ($D\to\infty$) connects transverse correlations and internal energy, i.e., with the substitution $u=m^2$,

$$\frac{\partial}{\partial\beta}\left(\frac{\beta}{\chi_{\perp}}\right)=\frac{\partial}{\partial\beta}\left(\frac{\beta H}{m}\right)=\frac{1}{m}\frac{\partial U}{\partial m}=2\frac{\partial U}{\partial u}. \tag{4.1}$$

Inserting from Eqs. (3.7) and (3.8) the SCOZA equation becomes

$$\frac{\partial}{\partial\beta}\left(\frac{\beta}{z}-\beta\right)=-1-\frac{1}{\beta}\frac{\partial}{\partial u}[P(z)-1]$$

or $[P'(z)=dP/dz]$

$$\beta\frac{\partial z}{\partial\beta}-\frac{z^2}{\beta}P'(z)\frac{\partial z}{\partial u}=z \tag{4.2}$$

whose equations for the characteristics are

$$\frac{d\beta}{\beta}=-\frac{\beta du}{z^2P'(z)}=\frac{dz}{z}. \tag{4.3}$$

One solution of these equations is

$$\mu_e=\frac{z}{\beta}=C_1. \tag{4.4}$$

The other solution follows from

$$du=-\frac{z}{\beta}P'(z)dz=-C_1P'(z)dz$$

as

$$C_1P(z)=C_2-u. \tag{4.5}$$

Comparing with the solution of the generalized mean-spherical model (GMSM) above one finds that Eqs. (4.4) and (4.5) are identical to the exact solution (3.5) and (3.13) with constants of integration

$$C_1=f(n) \quad \text{and} \quad C_2=n. \tag{4.6}$$

Thus for a given reference system the solution of the SCOZA problem will reproduce the exact result (3.16).

V. HRT FOR THE MODEL

For the HRT we will also use expression (3.9) for the correlation function where z again is the free parameter. By adding interaction at wave vector $k=Q$ for decreasing Q while keeping β constant, one obtains the equation [5]

$$\frac{\partial I}{\partial Q}=4\pi CQ^2\ln[1-z\tilde{\psi}(Q)] \quad \text{with} \quad C=\frac{1}{2}\frac{1}{(2\pi)^3} \tag{5.1}$$

for space dimensionality $d=3$. The $I=-\beta f=L-\beta Hm$ where f is Helmholtz free energy per spin while $L=-\beta g$ where g, which also appears on the left-hand side of Eq. (3.1), is the Gibbs free energy per spin. For the transverse susceptibility we then have $(u=m^2)$

$$\frac{\beta}{z}-\beta=-\frac{1}{m}\frac{\partial I}{\partial m}=-2\frac{\partial I}{\partial u}. \tag{5.2}$$

With Eq. (5.1) inserted we get the HRT self-consistency equation

$$\frac{\partial}{\partial Q}\left(\frac{\beta}{z}-\beta\right)=-2\frac{\partial}{\partial u}\left(\frac{\partial I}{\partial Q}\right),$$

$$\frac{\partial}{\partial Q}\left(\frac{\beta}{z}\right)=-\frac{\beta}{z^2}\frac{\partial z}{\partial Q}=4\pi 2CQ^2\frac{\tilde{\psi}(Q)}{1-z\tilde{\psi}(Q)}\frac{\partial z}{\partial u}. \tag{5.3}$$

Its equations for the characteristics are

$$\frac{z}{\beta}dQ = \left[4\pi 2CQ^2\left(\frac{1}{1-z\tilde{\psi}(Q)}-1\right)\right]^{-1}du = \frac{dz}{0}. \quad (5.4)$$

Again the solution is

$$\mu_e = \frac{z}{\beta} = C_1,$$

$$C_1P(z) = C_2 - u,$$

where now in the integrand in integral (3.4) for $P(z) = P(z,Q)$ the $\tilde{\psi}(k)$ is replaced by 0 for $0<k<Q$. Comparing one sees that this is nothing but Eqs. (4.4) and (4.5).

VI. ALTERNATIVE METHOD

By requiring consistency between Helmholtz free energy and internal energy when changing both β and Q Reiner and Høye obtained a more general solution beyond the one of the mean spherical approximation (MSA). They found [5]

$$I = -C\int \ln[1-\mu_e\beta\tilde{\psi}(k)]d\mathbf{k} - \sum_{n=1}^{\infty}\frac{n}{n+1}A_nK^{n+1},$$

$$\mu_e = \mu + \sum_{n=1}^{\infty}A_nK^n, \quad (6.1)$$

where $K=J/\mu_e$ and $P(z)=1+2J$. The coefficients A_n do not depend upon β and Q. Note that here the I does not contain the reference system and mean-field terms. This expression will also hold in the present case when imposing consistency with the compressibility, but now the A_n will depend upon the boundary condition at $\beta=0$. We find by use of Eq. (6.1)

$$\beta H = \beta H_0(m) - \frac{\partial I}{\partial m} = \beta H_0(m) - \sum_{n=1}^{\infty}\frac{1}{n+1}\frac{\partial A_n}{\partial m}K^{n+1} \quad (6.2)$$

where H_0 is the reference system plus the mean-field contributions. So for the transverse susceptibility (3.7) we get ($\mu_e=z/\beta$)

$$\frac{\beta H}{m} = \frac{1}{\mu_e} - \beta = \frac{1}{\mu} - \beta - 2\left(\frac{\partial\mu}{\partial u}K + \sum_{n=1}^{\infty}\frac{1}{n+1}\frac{\partial A_n}{\partial u}K^{n+1}\right). \quad (6.3)$$

This equation together with Eq. (6.1) determines μ_e, i.e., the coefficients A_n for given μ can be found by iteration by comparing equal powers of K. However, this problem can be transformed into the solution of a differential equation. So by choosing u and K as independent variables Eqs. (6.1) and (6.3) can be differentiated with respect to u and K, respectively, to obtain

$$\frac{1}{\mu_e^2}\frac{\partial\mu_e}{\partial K} = 2\frac{\partial\mu_e}{\partial u}. \quad (6.4)$$

This partial differential equation has the solution

$$\mu_e = C_1 \quad \text{and} \quad 2C_1^2K = (C_2 - C_1) - u. \quad (6.5)$$

With $C_1(1+2C_1K)=C_1P(z)$ this is again solution (4.4) and (4.5).

VII. COMBINED SCOZA AND HRT

In Ref. [5] consistency between free energy and internal energy was used to determine a single free parameter. This gave rise to first-order partial differential equations whose properties were studied more closely. Now we will require thermodynamic consistency with the compressibility route, too, so that a second free parameter can be determined.

Thus, to be general, consider a function $\Psi(\beta,Q,m)$ which is determined via two free but unknown parameters,

$$z = z(\beta,Q,m),$$

$$\nu = \nu(\beta,Q,m). \quad (7.1)$$

For the determination of Ψ, z, and ν, the derivatives of Ψ are given by known functions of β, Q, m, z, and ν as

$$\Psi_\beta = X = X(\beta,Q,m,z,\nu),$$

$$\Psi_Q = Y = Y(\beta,Q,m,z,\nu),$$

$$\Psi'' = Z = Z(\beta,Q,m,z,\nu). \quad (7.2)$$

Here and below the subscripts mean partial derivatives with respect to β and Q, etc., while the double prime means second derivative with respect to magnetization m. For the GMSM the latter is replaced by the first derivative with respect to $u=m^2$.

By differentiation with respect to β and Q we now get

$$d\Psi_\beta = X_\beta d\beta + X_Q dQ + X_m dm + X_z dz + X_\nu d\nu,$$

$$d\Psi_Q = Y_\beta d\beta + Y_Q dQ + Y_m dm + Y_z dz + Y_\nu d\nu,$$

$$d\Psi'' = Z_\beta d\beta + Z_Q dQ + Z_m dm + Z_z dz + Z_\nu d\nu, \quad (7.3)$$

where subscripts indicate partial derivatives with respect to z and ν. With three unknowns Ψ, z, and ν the set of equations (7.2) represents a rather complex problem. We then note as in Ref. [5] that use of the identity $\partial\Psi_\beta/\partial Q=\partial\Psi_Q/\partial\beta$ will simplify this, and we first obtain

$$X_Q + X_z z_Q + X_\nu\nu_Q = Y_\beta + Y_z z_\beta + Y_\nu\nu_\beta. \quad (7.4)$$

Further,

$$\frac{\partial\Psi''}{\partial\beta} = Z_\beta + Z_z z_\beta + Z_\nu\nu_\beta = X'',$$

$$\frac{\partial\Psi''}{\partial Q} = Z_Q + Z_z z_Q + Z_\nu\nu_Q = Y'' \quad (7.5)$$

or

$$\nu_\beta = \frac{1}{Z_\nu}(X'' - Z_z z_\beta - Z_\beta),$$

$$\nu_Q = \frac{1}{Z_\nu}(Y'' - Z_z z_Q - Z_Q). \tag{7.6}$$

These expressions can be used to substitute the ν_β and ν_Q in Eq. (7.4), and by some rearrangement the following equation is obtained:

$$(Z_\nu X_z - X_\nu Z_z)z_Q - (Z_\nu Y_z - Y_\nu Z_z)z_\beta + X_\nu Y'' - Y_\nu X'' + Z_\nu(X_Q - Y_\beta) - Z_Q X_\nu + Z_\beta Y_\nu = 0. \tag{7.7}$$

The previous one-parameter approximations can be recognized in Eq. (7.4) when ν is considered constant. Then with z as the free parameter and $\Psi = I = -\beta f$ where f is the free energy per particle, one finds from Eq. (7.6) that $\nu_\beta = 0$ is the SCOZA equation, $\nu_Q = 0$ is the HRT equation, while the remaining (nonzero) terms of Eq. (7.4) give the consistency between the free-energy and internal energy routes considered in Ref. [5]. But in general these various consistencies give different z so Eq. (7.4) itself will not be solved by using one of these, except for the GMSM considered in this work. Since we know the exact solution for the GMSM it should be possible to recover it directly from Eqs. (7.4) and (7.7) using a pair-correlation function containing two free parameters.

To obtain the resulting HRT-SCOZA equation the X'' and Y'' must be evaluated. In the usual case we then have

$$X' = X_m + X_z z_m + X_\nu \nu_m,$$

$$X'' = X_{mm} + 2X_{mz}z_m + 2X_{m\nu}\nu_m + X_{zz}z_m^2 + 2X_{z\nu}z_m\nu_m + X_{\nu\nu}\nu_m^2 + X_z z_{mm} + X_\nu \nu_{mm} \tag{7.8}$$

with a similar expression for Y'' with X replaced by Y. One notes that the ν_{mm} term will cancel when this is inserted in Eq. (7.7). Thus the resulting HRT-SCOZA equation becomes a second-order partial differential equation for z with coefficients that depend on ν and its first-order derivatives. This can then be treated iteratively, by starting with some approximate ν, solving for z, and updating ν according to Eq. (7.6). Note that $\nu_m = 0$ for $m = 1/2$ due to the symmetry of lattice gases if we identify ν with μ_e as we will do below. Its influence may therefore be only perturbing in the updating process and thus not crucial for the problem of performing a numerical solution. Anyway, here we will not try to pursue this question or try to analyze the properties of the general HRT-SCOZA equation any further. Instead we focus on the simplified situation with the GMSM to show how the HRT-SCOZA equation solves this problem. As mentioned earlier the susceptibility is then replaced by the transverse susceptibility. As in Secs. IV and V we then put $u = m^2$ to get

$$X'' \to 2\frac{\partial X}{\partial u} = 2(X_z z_u + X_\nu \nu_u + X_u),$$

$$Y'' \to 2\frac{\partial Y}{\partial u} = 2(Y_z z_u + Y_\nu \nu_u + Y_u). \tag{7.9}$$

For Eq. (7.7) this amounts to the substitution

$$X_\nu Y'' - Y_\nu X'' \to 2[(X_\nu Y_z - Y_\nu X_z)z_u + X_\nu Y_u - Y_\nu X_u], \tag{7.10}$$

where now the ν_u term cancels. Thus we are left with a first-order partial differential equation for z with free variables β, Q, and u. But ν, that is determined via Eq. (7.6), is still present in the coefficients of Eq. (7.7).

VIII. TWO-PARAMETER PAIR-CORRELATION FUNCTION

A simple way to introduce two parameters in the correlation function is to modify Eq. (3.9) into

$$\tilde{\Gamma}_\perp(k) = \frac{\tilde{\Sigma}(k)}{1 - \tilde{\Sigma}(k)\beta\tilde{\psi}(k)} = \frac{\nu}{1 - z\tilde{\psi}(k)} \tag{8.1}$$

for $k \geq Q$ and $k = 0$ [i.e., $\tilde{\Gamma}_\perp(k) = \tilde{\Sigma}(k)$ for $0 < k < Q$]. This means that the "self-energy" function is (for all k)

$$\tilde{\Sigma}(k) = \frac{\nu}{1 - (z - \nu\beta)\tilde{\psi}(k)}. \tag{8.2}$$

This assumed form of the correlation function for continuum spins with two free parameters ν and z can also be used for continuum fluids and their lattice gas version too. Thus various HRT-SCOZA expressions we derive in this section are also valid in the latter cases before we again specialize to the GMSA below Eq. (8.14).

An interesting feature of expression (8.1) is the adjustable amplitude ν to which the internal energy is proportional. This may influence critical properties. For SCOZA there is a generalized kind of scaling [11]. The independence of ν from z may change this. Note that here the ν is not tied to a core condition which we here omit for simplicity. Such an omission may not be crucial for qualitative properties. Anyway, at least for SCOZA itself, the core condition is not crucial in this respect [12].

With $\tilde{\Gamma}_\perp(k)$ given above we can now evaluate the quantities that enter the HRT-SCOZA equation. With $\Psi = I = -\beta f$ where f is Helmholtz free energy per particle we have [5]

$$X = \frac{\partial I}{\partial \beta} = \frac{\nu}{z}J(z) + \frac{1}{2}m^2, \tag{8.3}$$

$$Y = \frac{\partial I}{\partial Q} = 4\pi C Q^2 \ln[1 - \tilde{\Sigma}(Q)\beta\tilde{\psi}(Q)] = 4\pi C Q^2\{\ln[1 - z\tilde{\psi}(Q)] - \ln[1 - (z - \nu\beta)\tilde{\psi}(Q)]\}, \tag{8.4}$$

$$Z = 2\frac{\partial I}{\partial u} = -\frac{1}{\tilde{\Gamma}_\perp(0)} = -\frac{1 - z}{\nu} \quad (u = m^2) \tag{8.5}$$

with, for given Q,

$$J(z) = \frac{1}{2}[P(z) - 1] = C\int_{k>Q} \frac{z\tilde{\psi}(k)}{1 - z\tilde{\psi}(k)}d\mathbf{k}.$$

Here $X=-U$ is a modification of expression (3.8) for the internal energy U, the Y is a modification of expression (5.1), while Z is the corresponding modification of expression (5.2). From this we obtain the partial derivatives

$$Y_\beta = -\nu L(Q,\Delta z),$$

$$Y_z = -L(Q,z) + L(Q,\Delta z),$$

$$Y_\nu = -\beta L(Q,\Delta z), \quad Y_u = 0, \tag{8.6}$$

where $\Delta z = z - \nu\beta$ and

$$L(Q,z) = -\frac{1}{z}\frac{\partial J(z)}{\partial Q} = 4\pi C Q^2 \frac{\tilde{\psi}(Q)}{1 - z\tilde{\psi}(Q)}. \tag{8.7}$$

Further, with $J'(z) = -\partial J(z)/\partial z$

$$X_Q = -\nu L(Q,z),$$

$$X_z = \nu \frac{\partial}{\partial z}\left(\frac{J(z)}{z}\right) = -\frac{\nu}{z^2}J(z) + \frac{\nu}{z}J'(z),$$

$$X_\nu = \frac{1}{z}J(z), \quad X_u = \frac{1}{2}, \tag{8.8}$$

and finally

$$Z_\beta = 0, \quad Z_Q = 0,$$

$$Z_z = \frac{1}{\nu}, \quad Z_\nu = \frac{1-z}{\nu^2}. \tag{8.9}$$

For the GMSM case where Eq. (7.10) is used for the X'' and Y'' terms we now can evaluate the coefficients of the HRT-SCOZA equation (7.7) to obtain

$$A z_Q - B z_\beta + 2C z_u + D = 0, \tag{8.10}$$

where the coefficients are

$$A = Z_\nu X_z - X_\nu Z_z = A_1 + A_2,$$

$$A_1 = -\frac{1}{\nu z^2}J(z), \quad A_2 = \frac{1-z}{\nu z}J'(z), \tag{8.11}$$

$$B = Z_\nu Y_z - Y_\nu Z_z = B_1 + B_2,$$

$$B_1 = \frac{1-z}{\nu^2}L(Q,z), \quad B_2 = \frac{1-\Delta z}{\nu^2}L(Q,\Delta z). \tag{8.12}$$

With Eq. (7.10) we have

$$C = X_\nu Y_z - Y_\nu X_z = C_1 + C_2,$$

$$C_1 = \frac{1}{z}J(z)\left(-L(Q,z) + \frac{\Delta z}{z^2}L(Q,\Delta z)\right),$$

$$C_2 = \frac{\beta\nu}{z}J'(z)L(Q,\Delta z). \tag{8.13}$$

Finally,

$$D = Z_\nu(X_Q - Y_\beta) - Z_Q X_\nu + Z_\beta Y_\nu + 2(X_\nu Y_u - Y_\nu X_u)$$
$$= Z_\nu(X_Q - Y_\beta) - Y_\nu = D_1 + D_2,$$

$$D_1 = -\frac{1-z}{\nu}L(Q,z) = \nu B_1,$$

$$D_2 = \frac{1-\Delta z}{\nu}L(Q,\Delta z) = \nu B_2. \tag{8.14}$$

Now in the GMSM the solution to be expected yields $\nu = z/\beta$. This suggests to replace z with a new variable $\mu = z/\beta$, which simplifies the remaining analysis since then the D terms will join B terms, and Eq. (8.10) becomes

$$E_1 + E_2 + E_3 = 0 \tag{8.15}$$

with

$$E_1 = A_2\mu_Q - B_1\mu_\beta = \beta\frac{1-z}{z^2}[J'(z)\mu_Q + \beta L(Q,z)\mu_\beta],$$

$$E_2 = A_1\mu_Q + 2C_1\mu_u = -\frac{1}{z}J(z)\left(\frac{\beta}{z^2}\mu_Q + 2L(Q,z)\mu_u\right),$$

$$E_3 = -B_2\mu_\beta + 2C_2\mu_u = -\frac{1}{z^2}L(Q,\Delta z)[-\beta^2\mu_\beta + 2z^2 J'(z)\mu_u]. \tag{8.16}$$

Now one notes that $E_3=0$ is the SCOZA equation (4.2) as $P(z)=1+2J$ and $z=\beta\mu$. Likewise $E_2=0$ is the HRT equation (5.3). These equations have both the common GMSM solution given by Eqs. (4.4) and (4.5). Noting further that

$$\frac{1}{1-z}E_1 = -\frac{zJ'(z)}{J(z)}E_2 + \frac{L(Q,z)}{L(Q,\Delta z)}E_3,$$

it follows that the GMSM solution also solves $E_1=0$, and by that it solves the HRT-SCOZA equation (8.15) too. Here it can be noted that $E_1=0$ is nothing but consistency between the internal energy and free-energy routes investigated in Ref. [5]. One should expect Eq. (8.15) to have other solutions too with a third constant of integration C_3 besides the two in Eq. (4.5). But in any case the GMSM solution is sufficient here as it can be adjusted into the reference system boundary conditions (3.11) or (4.6).

Finally we have to show that $z=\beta\nu$ fulfills Eq. (7.6) too. With $\mu=\nu=z/\beta$ and Eqs. (7.9) and (8.6)–(8.9) we get

$$\mu_\beta = \frac{1}{Z_\nu}[2(X_z z_u + X_\nu \mu_u + X_u) - Z_z z_\beta - Z_\beta]$$
$$= \frac{1}{1-z}[2\mu^2 J'(z)\mu_u - z\mu_\beta],$$

$$\mu_\beta = 2\mu^2 J'(z)\mu_u \tag{8.17}$$

and

$$\mu_Q = \frac{1}{Z_\nu}[2(Y_z z_u + Y_\nu \mu_u + Y_u) - Z_z z_Q - Z_Q]$$

$$= \frac{\mu z}{1-z}\left(-2L(Q,z)\mu_u - \frac{1}{\mu}\mu_Q\right),$$

$$\mu_Q = -2\mu z L(Q,z)\mu_u. \tag{8.18}$$

And Eqs. (8.17) and (8.18) are nothing but the SCOZA and HRT equations $E_3=0$ and $E_2=0$ as given by Eq. (8.16). Thus altogether we have shown in detail how the GMSM solves the unified HRT-SCOZA equations. We have reason to believe that this demonstration of a model that can be solved exactly will be useful for the possible solution of the HRT-SCOZA problem more generally where the second derivatives of Eq. (7.8) should be used. Also other assumptions for the correlation function different from the simple expression (8.1) may then be useful or may be needed.

IX. CONCLUSIONS

In the present work general equations for the unified HRT-SCOZA problem have been established using a simple form of the pair-correlation function containing two free parameters. To analyze the problem in more detail we have considered an exactly solvable model, the MSM and its extension the GMSM that we introduce. This generalization is also natural insofar as the GMSM is merely a more general solution of the same HRT-SCOZA equations. The reference system boundary conditions determine the resulting solution. The SCOZA and HRT problems for the GMSM are first considered separately, and then they are combined. By analysis of the unified HRT-SCOZA it is shown how it can reproduce the known exact solution of the GMSM: Given correct boundary conditions and a suitable parametrization of the correlation function, HRT-SCOZA successfully traces the evolution of the free parameters. We expect the analysis of how the HRT-SCOZA works for this special case to be useful for the more general situation of possibly solving the unified HRT-SCOZA problem.

ACKNOWLEDGMENT

A.R. gratefully acknowledges financial support from Fonds zur Förderung der wissenschaftlichen Forschung (FWF) under project J2380-N08.

[1] J. S. Høye and G. Stell, Mol. Phys. **52**, 1071 (1984).
[2] J. S. Høye and G. Stell, Int. J. Thermophys. **6**, 561 (1985).
[3] J. S. Høye and G. Stell, J. Chem. Phys. **67**, 439 (1977).
[4] A. Parola and L. Reatto, Adv. Phys. **44**, 211 (1995).
[5] A. Reiner and J. S. Høye, Phys. Rev. E **72**, 061112 (2005).
[6] H. E. Stanley, Phys. Rev. Lett. **20**, 589 (1968). For a general summary of the properties of *D*-vector models, see H. E. Stanley, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1974), Vol. 3.
[7] H. E. Stanley, Phys. Rev. **176**, 718 (1968); M. Kac and C. J. Thompson, Phys. Norv. **5**, 163 (1971).
[8] T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).
[9] H. W. Levis and G. Wannier, Phys. Rev. **88**, 682 (1952); **90**, 1131 (1952).
[10] J. S. Høye and G. Stell, Physica A **244**, 176 (1997).
[11] J. S. Høye, D. Pini, and G. Stell, Physica A **279**, 213 (2000).
[12] A. Borge and J. S. Høye, J. Chem. Phys. **108**, 4516 (1998).