

# Unification of hierarchical reference theory and self-consistent Ornstein-Zernike approximation: Analysis of the critical region for fluids and lattice gases

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The hierarchical reference theory (HRT) and the self-consistent Ornstein-Zernike approximation (SCOZA) are two liquid state theories that both yield a largely satisfactory description of the critical region as well as the phase coexistence and equation of state in general. In two previous works, unification of these theories has been considered and general equations were established. Further it was shown that the solution of the mean spherical model and a generalized version of it can be obtained in this way. In the present work, analysis of the critical region for fluids and lattice gases is performed. A key result of our HRT-SCOZA approximation is that for the standard three-dimensional fluid, lattice gas, or Ising model, the critical index for the critical isotherm is  $\delta=5$  and for the curve of coexistence it is  $\beta=1/3$  provided full scaling is assumed. More generally we find  $\beta=2/(\delta+1)$ .

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## I. INTRODUCTION

Both the self-consistent Ornstein-Zernike approximation (SCOZA) [1–3] and the hierarchical reference theory (HRT) [4–6] 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 obtained by deriving 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 the SCOZA combines it with the internal energy route while the HRT, inspired by momentum-space renormalization group theory [7], uses the Helmholtz free energy route. Thus, in short, the SCOZA adds effective strength to the attractive interaction by increasing the inverse temperature  $\beta=1/k_B T$  while the HRT adds contributions to the interaction by including its Fourier components for smaller wave numbers  $Q$  until the limit of interest  $Q \rightarrow 0$  is obtained.

In a recent work thermodynamic consistency between the internal energy and free energy routes to thermodynamics was considered [8]. This work was extended to incorporate consistency with the compressibility route as well [9]. The resulting equations that unify the HRT and SCOZA were applied to an exactly solvable model, the mean spherical model (MSM) [10], and a generalization of it, the GMSM, that was introduced. The MSM is the exact solution for spins with spin dimensionality  $D \rightarrow \infty$ . (It corresponds to a Gaussian model where the average spin length is kept fixed.) The GMSM is a generalization of the MSM that turns out to have the same SCOZA and HRT equations; the difference lies in the boundary condition at  $\beta=0$  [9]. So when referring to the GMSM one needs only to have the MSM in mind in this

work. We shall refer to our unification of the HRT and SCOZA theories as the HRT-SCOZA theory.

In the present work we want to consider this unification for ordinary fluids and lattice gases or the Ising model, and we will focus upon the critical region where we are able to perform some analysis analytically. To do so we utilize known properties of the HRT and SCOZA, and we are further guided by the explicit solution of the unified GMSM problem just mentioned. Again the SCOZA and HRT equations and the resulting HRT-SCOZA equation(s) cover a rather general situation where the main difference lies in the boundary condition at  $\beta=0$  (the reference system). Also there is a difference between lattice and continuum systems that is neglected as we here will focus upon the critical region. Thus one can always have the usual Ising model in mind when performing derivations in the critical region as long as an ordinary critical point is considered.

To perform our analysis we start by establishing the partial differential equation for the unified HRT-SCOZA problem. This follows closely the derivations of Ref. [9] where details can be found. The resulting equation is essentially a sum of the HRT and SCOZA equations. In the limit of zero wave vector  $k=Q=0$  the HRT part will dominate. The  $Q$  is the wave vector inside which the Fourier transform of the attractive interaction is cut. The HRT, using a renormalization approach, has a fixed-point solution. Small deviations from this solution are described by eigenfunctions of which two of them will dominate. These are assumed to immediately give the critical indices with full scaling implied. We, however, find the situation less straightforward in this respect, and the generalized scaling found for the SCOZA will play a crucial role. Further, the interplay between HRT and SCOZA properties are important. It is as if a term is missing in the SCOZA itself. This prevents full scaling. However, this missing term may be supplied from the HRT part of the resulting equation. In this way full scaling that gives the critical index  $\beta=1/3$  can be obtained with index  $\delta=5$  for the critical isotherm. Based on a preliminary investigation this result was suggested previously [11].

In the HRT the temperature eigenvalue just mentioned turns out to be adjustable by modifying the cutoff of the

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interaction in momentum space [12]. A sharp cutoff yields  $\beta \approx 0.345 > 1/3$  [4]. However, by using a smooth cutoff, values  $\beta = 0.330$  [13] and  $0.332$  [14] have been found. Thus, from this, the value  $\beta = 1/3$  can be a possible one also for the HRT alone if a suitable cutoff is used. More generally, for the unified problem we here find

$$\beta = \frac{2}{\delta + 1}. \quad (1.1)$$

This is also consistent with the well-known solution of the two-dimensional Ising model for which  $\delta = 15$ . With scaling relations

$$\gamma + 2\beta = (\delta + 1)\beta = \nu d = 2 - \alpha \quad (1.2)$$

and  $\gamma' = \gamma$ ,  $\alpha' = \alpha$ , and  $\nu' = \nu$ , this implies ( $d$  is dimensionality)

$$\alpha = 0, \quad \gamma = \frac{\delta - 1}{\delta + 1}, \quad \nu = \frac{2}{d}, \quad 2 - \eta = d \frac{\delta - 1}{\delta + 1}. \quad (1.3)$$

Below the index  $\beta$  will be replaced with  $\beta_c$  to distinguish it from the inverse temperature  $\beta$ .

To obtain our results we are guided by previous results of SCOZA, HRT, and the HRT-SCOZA solutions of the GSM. Thus in addition to establishing the HRT-SCOZA equation we in several sections will review properties of these previous results that will form the basis for the HRT-SCOZA results for lattice gases and fluids. In view of the HRT-SCOZA results, we found reason to study the implications of the assumption that  $\delta = 5$  in three dimensions and the conditions under which this assumption might hold. Thus we have reconsidered results from previous analysis by Stell where logarithmic corrections were found for  $\delta = 5$  [15,16], and in Sec. X we conclude that  $\delta$  should be an odd number whenever the long-range decay of the direct correlation function dominates the one of the pair interaction at the critical point.

To determine the critical behavior we find that it is not sufficient to merely investigate the fixed-point solution and the two dominant eigenfunctions connected to it. It turns out that the leading correction to it is needed, and one obtains a kind of feedback loop that determines details of scaling by which we find  $\beta_c$  as given by Eq. (1.1). This brings into the picture the previous SCOZA analysis with its generalized type of scaling. But standard SCOZA alone cannot give full scaling. Because a scaling term is missing in the SCOZA, the coupling to HRT in the resulting equation can compensate for this missing term by which full scaling may be obtained.

In Sec. II we establish the general structure of the HRT-SCOZA differential equations which may determine two free parameters by combining both the SCOZA and HRT methods. The individual SCOZA and HRT equations with one free parameter are also defined there.

In Sec. III the assumed form of the Fourier-transformed correlation function with the two free parameters  $\nu$  and  $z$  embedded is established. From this form the explicit expressions for the internal energy, change in free energy due to change in the cutoff wave vector  $Q$ , and inverse compressibility follow. Thus the quantities  $X$ ,  $Y$ ,  $Z$ , and their deriva-

tives that enter the HRT-SCOZA equations are established. At the end of the section the parameter  $\nu$  is partly eliminated to obtain one partial differential equation for the parameter  $z$  with free parameters  $Q$ ,  $\beta$ , and  $m$ .

In Sec. IV the HRT-SCOZA equation for  $z$  is considered close to the critical point (i.e.,  $1 - z \rightarrow 0$ ,  $Q \rightarrow 0$ ) to sort out its leading terms expressed in powers of the magnetization  $m \rightarrow 0$ . It turns out that the HRT part dominates. However, the HRT part does not have explicit temperature dependence or a derivative with respect to  $\beta$ . Thus the subdominant SCOZA part is also needed to possibly obtain critical properties based upon analysis near the critical point. However, the latter feature has the consequence that a single dominant scaling function is not sufficient to describe critical properties; corrections to it are needed.

In Sec. V the critical isotherm with subdominant correction is evaluated for small  $m$ . This evaluation needs only the dominant HRT part of the equation for  $z$ . The result is consistent with the SCOZA critical isotherm in the next section. There and in Secs. VIII and IX the correction is crucial to determine critical properties connected to temperature dependence.

In Sec. VI the critical properties of the SCOZA equation alone are briefly reviewed, exhibiting its generalized type of scaling. In Sec. VII the HRT equation alone is considered close to the critical isotherm. Then it is noted that its temperature dependence is indeterminate due to its lack of derivative with respect to  $\beta$  or other explicit  $\beta$  dependence (away from external boundary conditions). However, the coupling to the SCOZA part of the resulting HRT-SCOZA equation may rectify this.

In Sec. VIII the possible influence of a coupling between the HRT and SCOZA parts of the HRT-SCOZA equation is considered. This coupling can be mediated via the second free parameter  $\nu$ . Its influence will be the same as adding a new term to the usual SCOZA problem. Such a term turns out to have the ability to remove the generalized scaling of SCOZA when suitably chosen. Evaluation of the curve of coexistence then leads to the critical index  $\beta_c = 2/(\delta + 1)$  for this curve provided full scaling is required.

In Sec. IX a more general investigation of the scaling behavior is performed. Then the solution of the HRT-SCOZA problem is regarded as an expansion of functions with scaled variables where the coefficients are powers of  $m$ . These powers must be consistent with both the dominant power and subdominant power of the critical isotherm. A basic assumption here is that the parameter  $\nu$  follows the same powers by which it again is sufficient to focus upon the SCOZA part of the problem. Full scaling with  $\beta_c = 2/(\delta + 1)$  is then again obtained.

In Sec. X graph expansions are considered in view of  $\gamma$  ordering [17–19]. Based upon the leading correction term by graph expansion we find that the critical index  $\delta$  should be an odd number whenever the long-range tail of the direct correlation function at the critical point dominates the long-range part of the potential. This is the case for both the two-dimensional Ising model as well as the three-dimensional one. In three dimensions this is marginal, and logarithmic corrections earlier found by Stell will be present [15,16].

## II. COMBINED SCOZA AND HRT

In this section we establish the HRT-SCOZA equations that unify the SCOZA and HRT. This follows closely the development in Ref. [9] where details are given for the GSM case. However, most of that development is valid for the present case too.

Thus, to follow Ref. [9] in the general situation, consider the function  $\Psi(\beta, Q, m)$  that represents free energy which is to be determined via two free, but unknown parameters

$$\begin{aligned} z &= z(\beta, Q, m), \\ \nu &= \nu(\beta, Q, m). \end{aligned} \quad (2.1)$$

For the determination of  $\Psi$ ,  $z$  and  $\nu$ , one needs the derivatives of  $\Psi$  that are given by known functions of  $\beta$ ,  $Q$ ,  $m$ ,  $z$ , and  $\nu$  as

$$\begin{aligned} \Psi_\beta &= X = X(\beta, Q, m, z, \nu), \\ \Psi_Q &= Y = Y(\beta, Q, m, z, \nu), \\ \Psi'' &= Z = Z(\beta, Q, m, z, \nu). \end{aligned} \quad (2.2)$$

Here and below the subscripts mean partial derivatives with respect to  $\beta$  and  $\nu$  etc. while the double prime means second derivative with respect to magnetization  $m$ . For the GSM the latter is replaced by the first derivative with respect to  $u=m^2$ . In addition to the free energy function  $\Psi$  in Eq. (2.2) the  $X$ ,  $Y$ , and  $Z$  apart from simple factors are the internal energy, the change in free energy due to change in wave vector  $Q$ , and the inverse compressibility or susceptibility. These quantities are made explicit in Sec. III. Equation (2.2) consists of three different equations with three different unknowns  $\Psi$ ,  $z$ , and  $\nu$ . The  $\Psi$  can be eliminated, and differentiation gives

$$\begin{aligned} d\Psi_\beta &= X_\beta d\beta + X_Q dQ + X_m dm + X_z dz + X_\nu d\nu, \\ d\Psi_Q &= Y_\beta d\beta + Y_Q dQ + Y_m dm + Y_z dz + Y_\nu d\nu, \\ d\Psi'' &= Z_\beta d\beta + Z_Q dQ + Z_m dm + Z_z dz + Z_\nu d\nu. \end{aligned} \quad (2.3)$$

With three unknowns  $\Psi$ ,  $z$  and  $\nu$  the set of equations (2.2) represents a rather complex problem. It is then noted as in Ref. [8] that use of the identity  $\partial\Psi_\beta/\partial Q = \partial\Psi_Q/\partial\beta$  will simplify this to obtain

$$X_Q + X_z z_Q + X_\nu \nu_Q = Y_\beta + Y_z z_\beta + Y_\nu \nu_\beta \quad (2.4)$$

by use of Eq. (2.3). Further by combining the equations in (2.2)

$$\begin{aligned} \frac{\partial\Psi''}{\partial\beta} &= Z_\beta + Z_z z_\beta + Z_\nu \nu_\beta = X'', \\ \frac{\partial\Psi''}{\partial Q} &= Z_Q + Z_z z_Q + Z_\nu \nu_Q = Y'' \end{aligned} \quad (2.5)$$

or

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

$$\nu_Q = \frac{1}{Z_\nu} (Y'' - Z_z z_Q - Z_Q). \quad (2.6)$$

With Eq. (2.6) we have obtained two HRT-SCOZA equations with two parameters  $z$  and  $\nu$  to be determined. Note that Eq. (2.4) is not independent of Eq. (2.6). For the SCOZA problem alone or the HRT problem alone only the parameter  $z$  is kept (i.e.,  $\nu$  is constant). Then the first equation of (2.6) is the SCOZA equation ( $\nu_\beta=0$ ) while the second one is the HRT equation ( $\nu_Q=0$ ). The SCOZA equation is the enforcement of thermodynamic self-consistency by using the first equation and the last one of Eq. (2.2) while the HRT equation is the similar use of its second and last equations.

To obtain explicitly the resulting HRT-SCOZA equations the  $X''$  and  $Y''$  must be evaluated. In the present case we then have

$$\begin{aligned} X' &= X_m + X_z z_m + X_\nu \nu_m, \\ X'' &= X_{mm} + 2X_{mz} z_m + 2X_{m\nu} \nu_m + X_{zz} z_m^2 \\ &\quad + 2X_{z\nu} z_m \nu_m + X_{\nu\nu} \nu_m^2 + X_{zm} z_{mm} + X_\nu \nu_{mm}, \end{aligned} \quad (2.7)$$

with similar expression for  $Y''$  with  $X$  replaced by  $Y$ . One notes that the  $\nu_{mm}$  term will cancel when this is used in Eq. (2.6) which is further inserted in Eq. (2.4). In this way one HRT-SCOZA equation is obtained. It is a second-order partial differential equation for  $z$  with coefficients that depend on  $\nu$  and its first-order derivatives. By a possible numerical treatment this may for instance be treated iteratively starting with some approximate  $\nu$ , but this will not be considered further here.

## III. TWO-PARAMETER PAIR CORRELATION FUNCTION

A simple way to introduce two parameters in the correlation function  $\Gamma(r)$  is to consider its Fourier transform as given in Ref. [9]

$$\tilde{\Gamma} = \frac{\tilde{\Sigma}(k)}{1 - \tilde{\Sigma}(k)\beta\tilde{\psi}(k)} = \frac{\nu z}{\beta[1 - z\tilde{\psi}(k)]} \quad (3.1)$$

for  $k \geq Q$  and for  $k=0$  while  $\tilde{\Gamma} = \tilde{\Sigma}(k)$  for  $0 < k < Q$ . The  $-\tilde{\psi}(k)$  is the Fourier transform of the attractive interaction which is cut inside  $k=Q$  and normalized such that  $\tilde{\psi}(0)=1$ .  $\tilde{\Sigma}(k)$  is the general hypervertex function introduced and used by Lebowitz, Stell, Baer, and Theumann in their investigations of the  $\gamma$  ordering for interactions of long range [18,19]. The parameter  $\gamma$  is the inverse range of interaction. It was further used by Høye and Stell in their initial work to obtain the general structure of the pair correlation function of polar fluids [20]. Equation (3.1) means that the ‘‘self-energy’’ function [with uncut  $\tilde{\psi}(k)$  for all  $k$ ] is

$$\tilde{\Sigma}(k) = \frac{\nu z}{\beta[1 - z(1 - \nu)\tilde{\psi}(k)]}. \quad (3.2)$$

Compared with Ref. [9] this expression is different in the way the parameter  $\nu$  enters, as the previous  $\nu$  is here replaced

with  $\nu z/\beta$ . The reason is that we find this form more convenient since the usual HRT or SCOZA with one parameter  $z$  then simply means  $\nu=1$  by which  $\nu_\beta=\nu_Q=0$ , and Eqs. (2.6) become nothing but the separate SCOZA and HRT equations. For fluids or lattice gases one can also write  $\tilde{\Gamma}=\rho/[1-\rho\tilde{c}(k)]$  where  $c(r)$  is the direct correlation function. With Eq. (3.1) one finds  $\tilde{\rho}c(k)=1-\beta\rho/(\nu z)+[(\beta\rho/\nu)\tilde{\psi}(k)]$ .

A special feature of expression (3.1) is the adjustable amplitude  $\nu$  to which the internal energy is proportional. This can influence critical properties. For the SCOZA there is a generalized kind of scaling [21]. The independence of  $\nu$  from  $z$  may change this. Note that here the  $\nu$  is not tied to a core condition which is omitted for simplicity. Such an omission is not expected to be crucial for critical properties. Anyway, at least for SCOZA itself, the core condition is not crucial in this respect [22].

With  $\tilde{\Gamma}$  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 [9]

$$X = \frac{\partial I}{\partial \beta} = C \int \tilde{\Gamma}(k) \tilde{\psi}(k) d\mathbf{k} = \frac{\nu}{\beta} J(z) + \frac{1}{2} m^2, \quad (3.3)$$

$$Y = \frac{\partial I}{\partial Q} = 4\pi C Q^2 \ln[1 - \tilde{\Sigma}(Q)\beta\tilde{\psi}(Q)] \\ = 4\pi C Q^2 \{\ln[1 - z\tilde{\psi}(Q)] - \ln[1 - z(1-\nu)\tilde{\psi}(Q)]\}, \quad (3.4)$$

$$Z = \frac{\partial^2 I}{\partial m^2} = -\frac{1}{\tilde{\Gamma}(0)} = -\beta \frac{1-z}{\nu z}, \quad (3.5)$$

with, for given  $Q$ ,

$$J = J(z) = C \int_{k>Q} \frac{z\tilde{\psi}(k)}{1-z\tilde{\psi}(k)} d\mathbf{k} \quad \text{with } C = \frac{1}{2(2\pi)^3}. \quad (3.6)$$

Here  $X=-U$  where  $U$  is the internal energy,  $Y$  represents the change in free energy due to change in  $Q$ , while  $Z$  represents the inverse compressibility or susceptibility. From this we obtain the partial derivatives

$$Y_\beta = 0, \quad Y_{mm} = 0, \\ Y_z = -L(Q, z) + (1-\nu)L(Q, \Delta z), \\ Y_\nu = -zL(Q, \Delta z), \quad (3.7)$$

where  $\Delta z = z(1-\nu)$  and

$$L = L(Q, z) = -\frac{1}{z} \frac{\partial J(z)}{\partial Q} = 4\pi C Q^2 \frac{\tilde{\psi}(Q)}{1-z\tilde{\psi}(Q)}. \quad (3.8)$$

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

$$X_Q = -\frac{\nu z}{\beta} L(Q, z),$$

$$X_z = \frac{\nu}{\beta} J'(z),$$

$$X_\nu = \frac{1}{\beta} J(z), \quad X_{mm} = 1, \quad (3.9)$$

and finally

$$Z_\beta = -\frac{1-z}{\nu z}, \quad Z_Q = 0, \\ Z_z = \frac{\beta}{\nu z^2}, \quad Z_\nu = \frac{\beta(1-z)}{\nu^2 z}. \quad (3.10)$$

Second order partial derivatives are not written down here as they will not be used below, but they follow easily from Eqs. (3.7)–(3.10). By inserting the above expressions into expressions (2.6) and (2.7), which are further used in Eq. (2.4), one resulting HRT-SCOZA equation is obtained. This equation can be written in the form

$$F_1 = F_2 + F_3 \quad (3.11)$$

with

$$F_1 = X_\nu Z_\nu \nu_Q, \quad F_2 = Y_\nu Z_\nu \nu_\beta, \\ F_3 = Z_\nu (Y_\beta + Y_z z_\beta - X_Q - X_z z_Q). \quad (3.12)$$

With  $\nu_Q$  and  $\nu_\beta$  inserted from Eqs. (2.6) and (2.7) one notes that the second derivative  $\nu_{mm}$  cancels, by which Eq. (3.11) mainly becomes an equation for  $z$ . The two basic equations for  $\nu$  and  $z$  are still Eq. (2.6), but Eqs. (2.4) and (3.11) are a related combination that via Eq. (2.7) partly eliminates  $\nu$ .

With  $\nu=1$  and (2.6) inserted, one further notes that  $F_1=0$  gives the HRT equation,  $F_2=0$  gives the SCOZA equation, while  $F_3=0$  is the consistency between free energy and internal energy considered in Ref. [8]. For the GSM case studied in Ref. [9] the value  $\nu=1$  was solution. But with (2.7) this is no longer the case.

#### IV. DIFFERENT ORDERS OF MAGNITUDE

The critical point is approached when  $z \rightarrow 1$ ,  $Q \rightarrow 0$ ,  $m \rightarrow 0$ . In this limit the HRT has the scaling relations  $1-z \sim Q^2 \sim m^4$  for fluids with interaction of finite range in three dimensions [4]. This will persist in our case too, and one can compare the magnitudes of the three quantities in (3.11). The purpose of this comparison is to show that the HRT part  $F_1$  dominates close to the critical point. This enables us to evaluate the critical isotherm as done in the next section where we obtain its subleading contribution besides its obvious leading one. However, the subleading one, according to our analysis, is crucial for the precise temperature dependence of critical properties.

From Eqs. (3.7)–(3.11) one sees that  $X_\nu \sim 1$ ,  $Z_\nu \sim 1-z \sim m^4$ ,  $Y_\nu \sim Q^2 \sim m^4$ , and  $Y_z \sim 1$ . Further, the integral (3.6) will give  $J(z) = \text{const} - \text{const} \times \sqrt{1-z}$  ( $Q \rightarrow 0$ ), which means that  $X_z \sim J'(z) \sim 1/\sqrt{1-z} \sim 1/m^2$ . In (2.6) we have the quantities

$$X'' \sim X_z z_{mm} \sim \frac{1}{m^2} \frac{1-z}{m^2} \sim 1,$$

$$Y'' \sim Y_{zmm} \sim 1 \times \frac{1-z}{m^2} \sim m^2. \quad (4.1)$$

In addition we have  $Y_\beta=0$ ,  $X_Q \sim 1$ ,  $z_Q \sim m^4/Q \sim m^2$ , and  $z_\beta \sim m^4/t \sim m^p$  where  $p$  will be 1 or something near 1.  $t$  is the deviation from the critical inverse temperature. Thus  $F_1$  contains terms of leading order

$$X_\nu Y'' \sim m^2 \quad (4.2)$$

while  $F_2$  and  $F_3$  contain terms of leading order

$$Y_\nu X'' \sim m^4. \quad (4.3)$$

From this one sees that  $F_1$  and thus the HRT part dominates when the critical point is approached. But this does not solve the full problem, as the HRT lacks the explicit temperature dependence (i.e.,  $z_\beta$ ), which is in the SCOZA part  $F_2$  and the  $F_3$ . This has the consequence that there will be some coupling between different orders, and a fixed point solution with the related dominant eigenfunctions does not seem sufficient to determine the critical behavior properly according to our analysis below.

## V. CRITICAL ISOTHERM WITH SUBLEADING CONTRIBUTION

To dominant order the critical isotherm is given by the fixed point solution of the HRT equation. However, as mentioned in the previous section, we will need the leading correction to it. To determine this correction we are guided by the HRT equation for the GSM problem which we find has the same correction and can be solved exactly. Thus we will analyze the GSM problem in a way that can be extended to the present case. To the extent we have been able to perform our analysis below, we find that the leading and subleading terms in the present case are those of the GSM. The HRT equation for the latter problem is ( $u=m^2$ ) [9]

$$\frac{\beta}{z^2} \mu_Q + 2L\mu_u = 0, \quad (5.1)$$

with a general solution that can be written as  $u = -\mu[1 + 2J(z)] + f(\mu)$ . Here  $\mu = z/\beta$ ,  $L$  and  $J$  are as given by Eqs. (3.6) and (3.8), respectively, while  $f$  is some arbitrary function. With interaction  $\tilde{\psi}(k) = 1 - \text{const} \times k^2 + \dots$ , in three dimensions one finds ( $Q \rightarrow 0$ )

$$J(z) = a - b\varepsilon + \dots, \quad \varepsilon = \sqrt{1-z} \quad (5.2)$$

where here and below in this section  $a$  and  $b$  are merely arbitrary constants.

At the critical point  $u=0$  and  $\varepsilon=0$ . Away from the critical point, but near it, one has the parabolic shape  $\varepsilon^2 = 1-z = \text{const} \times u$  ( $\propto m^2$ ). This determines the function  $f(\mu) = \text{const} \times \varepsilon^2 + \dots$ . So altogether

$$u = a\varepsilon + b\varepsilon^2. \quad (5.3)$$

Solved with respect to  $\varepsilon$  this gives

$$\varepsilon = au - b\varepsilon^2 + \dots = au - bu^2 + \dots,$$

$$\varepsilon^2 = au^2 - bu^3 + \dots = am^4 - bm^6 + \dots. \quad (5.4)$$

In the limit  $Q \rightarrow 0$  this will also be the critical isotherm of a fluid or the Ising model. To see this we first note that the solution of (5.1) gives an explicit expression for  $u$  which suggests exchanging the roles of  $u$  and  $\mu$  ( $=z/\beta$ ) as free and dependent variables. With  $y = \varepsilon^2 = 1-z$  we then find

$$y_u = 1/u_y, \quad y_Q = -u_Q/u_y. \quad (5.5)$$

Note the minus sign of the last equation of Eq. (5.5). It follows from  $dy = y_u du + y_Q dQ$  with  $dy=0$ . This inserted in Eq. (5.1) gives the equation

$$u_Q - 2L = 0. \quad (5.6)$$

Here  $\beta/z$  can be considered constant near the critical point and has been deleted for simplicity. With this the solution is  $u = -2J(z) + f(y)$ . The solution of interest is again (5.3) ( $\varepsilon = \sqrt{y}$ ).

Fluids or the Ising model have the corresponding HRT equation [ $y_Q \sim -Y'' = -\partial(Y_{zmm})/\partial m$  from Eq. (2.6) with  $\nu_Q = 0$ ]

$$y_Q + \frac{\partial}{\partial m}(Ly_m) = y_Q + L_y y_m^2 + Ly_{mm} = 0. \quad (5.7)$$

This equation differs from Eq. (5.1) with its second derivative in  $m$  that replaces the first derivative with respect to  $u = m^2$  of the latter. The reason for this difference is due to the susceptibility  $Z = (\partial^2 I / \partial m^2)$ , as given by Eq. (3.5) in the present case, while in the GSM case the transverse susceptibility is used, by which  $\partial^2 I / \partial m^2$  is replaced by  $2(\partial I / \partial u)$ . Again introducing  $u = m^2$  as dependent variable, we find

$$u_y = 2mm_y, \quad m_y = \frac{u_y}{2m},$$

$$u_{yy} = 2(m_y^2 + mm_{yy}), \quad m_{yy} = \frac{u_{yy}}{2m} - \frac{m_y^2}{m},$$

$$y_m = \frac{1}{m_y} = \frac{2m}{u_y}, \quad y_{mm} = -\frac{m_{yy}}{m_y^3} = -4m^2 \frac{u_{yy}}{u_y^3} + \frac{2}{u_y}. \quad (5.8)$$

Inserted in (5.7), this gives

$$u_Q - 2L_e = 0, \quad L_e = 2\frac{u}{u_y}L_y - 2\frac{uu_{yy}}{u_y^2}L + L = 0. \quad (5.9)$$

This equation will have a scaling or fixed point solution

$$u = 2[J_e(1) - J_e(z)], \quad J_e = - \int L_e dQ, \quad (5.10)$$

since with this and Eq. (5.9)  $L_e$ , like  $L$ , will depend only upon the scaling variable  $y/Q^2$  for small  $Q$ . In the limit  $Q \rightarrow 0$  we again will have  $u \sim \sqrt{y}$ . However, to fit the boundary condition away from the critical point the solution (5.10) must be modified. Thus we can write

$$u = 2[J_e(1) - J_e(z)] + g(Q, y)y, \quad (5.11)$$

since away from  $Q=0$  we should have mean-field behavior  $u \sim g(\infty, y)y \sim y$ . In the GSM case above the  $g(Q, y)$  was a

constant, while in the present case it will vary due to its influence upon  $L_\varepsilon$ . But this influence beyond the scaling part of the solution is of higher order and vanishes for vanishing  $y$ . Thus we will assume that  $g(Q, y)$  remains finite such that for  $Q=0$  the solution for the critical isotherm can be written

$$u = a\sqrt{y} + by \quad (5.12)$$

by which the GSM results (5.3) and (5.4) are recovered ( $\varepsilon = \sqrt{y}$ ).

## VI. SCOZA EQUATION AND ITS GENERALIZED SCALING

The purpose of this section is to reestablish basic analytic properties of the SCOZA equation. These properties play an important role in the analysis of the HRT-SCOZA problem. The SCOZA equation is the same as Eq. (2.6) with  $\nu=1$ , and for  $\varepsilon^2=1-z$  small this means  $X'' \sim z_\beta$ . Expression (5.2) for  $J(z)$  means that  $J'(z) \sim 1/\varepsilon$  such that the crucial terms of the SCOZA equation becomes [21]

$$\frac{\partial \varepsilon^2}{\partial t} = -1 + \frac{1}{2}\varepsilon''. \quad (6.1)$$

To dominant order this equation has the solution  $\varepsilon = m^2$ . (Dependence upon temperature turned out to be absent to leading order. This contrasts with the SCOZA study performed in Ref. [2], where the exponents of a tricritical point was obtained along with full scaling. Thus the SCOZA investigation of Ref. [2] was actually an investigation of SCOZA tricritical properties with  $\varepsilon < m^2$ .) Clearly, to obtain temperature dependence the leading correction to this is needed. For supercritical temperatures  $t < 0$  this is given by

$$\varepsilon = m^2 - c(3t + m^4), \quad (6.2)$$

where  $c$  is a constant. Note that the SCOZA critical isotherm ( $t=0$ ) is fully consistent with the HRT one obtained in the previous section and is given by Eq. (5.4). However, also note that SCOZA gives a definite value of the coefficient of the  $m^2$  term while HRT is flexible in this respect. The former is required to satisfy thermodynamic self-consistency. Otherwise the internal energy will have a tricritical behavior, i.e.,  $U \sim m^2$  with  $\beta_c = 1/4$ . For subcritical temperatures the situation is less transparent. However, it was found that the solution can be written as [21]

$$\varepsilon = u^2 + tg(z), \quad u = m - at^q, \quad z = u/t^{1/4}. \quad (6.3)$$

The leading correction  $g(z)$  is found by solution of an ordinary differential equation. The  $u=0$  or  $m=at^q$  determines the spinodal curve where the exponent  $q=3/4$  while  $a$  is a constant. For the critical index  $\beta_c$  of the curve of coexistence one finds  $\beta_c = (1+q)/5 = 0.35$  while the scaling variable  $z$  alone would imply  $\beta_c = 1/4$ . Thus a kind of generalized scaling was found.

## VII. HRT EQUATION NEAR THE CRITICAL ISOTHERM

The purpose of this section is to establish basic properties of the HRT equation from both analytic and numerical work

and from our extension of these results. For  $Q \ll y$  the HRT equation (5.7) reduces to  $y_Q=0$  since  $L \propto Q^2/(y+Q^2) \rightarrow 0$  as  $Q \rightarrow 0$ . Thus any  $y=y(m)$  is a solution near  $Q=0$  while the leading correction to this will be of order  $Q^3$ . However, not any solution will fit into the boundary conditions for large  $Q$ . So we have found that the critical isotherm is given by (5.4) according to the close connection with the GSM.

According to the investigations of HRT by Reatto, Parola, and Pini the behavior close to the critical isotherm or fixed point solution is determined by the eigenfunctions with the largest eigenvalues [4–6]. To perform these computations scaled quantities  $h(z, Q) = y/Q^2$  and  $z = m/\sqrt{Q}$  were introduced. More precisely the  $h(z, Q)$  is the quantity  $\partial^2 H_t / \partial z^2$  of these references. However, as will be seen below and in the following sections our analysis restricted to the critical region will differ somewhat in conclusion from some of the previous results. This difference in conclusion most likely lies in the way the problem is approached. The references base their results upon numerical solution with given outside boundary conditions for  $Q$  large. According to Eq. (55) of Ref. [4] this gives a contribution which when added to (5.4) will modify it into ( $Q \rightarrow 0$ )

$$y = \varepsilon^2 = am^4 - ctm^\lambda - bm^6 + \dots, \quad (7.1)$$

where  $t (\rightarrow 0)$  is a small deviation from the critical temperature and  $c$  is an additional constant. Numerically the exponent  $\lambda$  was found to be

$$\lambda = 2(2 - \lambda_1) = 1.098, \quad (7.2)$$

where  $\lambda_1 = 1.451$  is given by Eq. (61) of Ref. [4], and the critical index  $\beta_c$  is found from its Eqs. (57) and (58) as

$$\beta_c = \frac{\gamma}{\delta - 1} = \frac{1}{2\lambda_1} = \frac{1}{4 - \lambda} = 0.345. \quad (7.3)$$

By modifying HRT it has recently been found that  $\lambda_1$  changes somewhat. This is done by replacing the sharp cut-off  $Q$  in  $k$  space with a smooth cutoff. Then a value  $\beta_c < 1/3$  was found [12]. The special point of interest here is that  $\beta_c = 1/3$ , which means  $\lambda = 1$ , is a possible value between the two results. This variation in  $\lambda_1$  and thus  $\lambda$  may reflect the lack of explicit temperature dependence of the HRT in the critical region. Thus, when disregarding external conditions, we find that the HRT equation alone is fully flexible with respect to the value of the exponent  $\lambda$  in Eq. (7.1). This flexibility can also be realized by regarding the solution of Eq. (5.6) that was utilized to obtain the critical isotherm for the HRT equation (5.9). Its solution was  $m^2 = u = -2J(z) + f(y)$  where  $f(y)$  is the constant of integration independent of  $Q$ . Thus we can put  $f(y) = 2J(1) + b\varepsilon^2 + ct/\varepsilon^\sigma$  where  $\sigma$  is some exponent ( $y = \varepsilon^2$ ). Further  $J(z) = J(1) - a\varepsilon$  when  $Q \rightarrow 0$ , so provided  $t$  is small such that  $t/\varepsilon^\sigma \ll \varepsilon$  we find

$$u = a\varepsilon + b\varepsilon^2 + ct/\varepsilon^\sigma,$$

$$\varepsilon = au - b\varepsilon^2 - ct/\varepsilon^\sigma + \dots = au - bu^2 - ct/u^\sigma + \dots,$$

$$\varepsilon^2 = am^4 - ctm^\lambda - bm^6 + \dots, \quad (7.4)$$

where  $a$ ,  $b$ , and  $c$  are arbitrary constants and  $\lambda = 2(1 - \sigma)$ .

In the full HRT-SCOZA problem we now may expect that the flexibility of the HRT with respect to the exponent  $\lambda$  and its flexibility pointed to in the preceding section will be removed by the coupling to the SCOZA part of the full problem. This may be expected in view of the SCOZA results of that section with no flexibility on the leading term of the critical isotherm.

Further it can be noted that a shift  $m \rightarrow m - m_s$  in solution (7.1) where  $m_s$  is a constant is also a solution of the HRT equation. For small  $m_s$  this is like adding the derivative of the solution to it. So the derivative is a solution of the linearized equation, and in Ref. [5] it is considered to be one of the two relevant eigenfunctions that determines the critical exponent  $\delta$  via its eigenvalue.

### VIII. MODIFIED SCOZA WITH SCALING

In this section we will investigate how full scaling can be obtained by including a contribution related to the parameter  $\nu$  to the SCOZA part of the HRT-SCOZA equation. Here we restrict the investigation to subcritical temperatures and consider the curve of coexistence like we did in Sec. VI. For  $Q \rightarrow 0$  this inclusion will be a subdominant correction to the dominant HRT part. With this correction the investigation below, assuming full scaling, yields our main result  $\beta_c = 2/(\delta+1)$ .

As pointed out in Sec. VI the SCOZA has a generalized form of scaling. By closer investigation one sees that a crucial term is missing that prevents scaling from being obtained. Also the two terms on the right-hand side of (6.1) belongs to different orders of scaling functions. First of all the  $-1$  term that comes from the mean-field contribution to the internal energy should cancel, leaving a difference to higher order in  $m$ . The SCOZA gives a difference of order  $m^2$ . This works properly for the GSM, but for fluids, lattice gases, or the Ising model this order is too high and leads to generalized scaling. What is needed turns out to be a term of order  $m^\lambda$  where  $\lambda \approx 1$ . The unified problem may produce such a term via the second free parameter  $\nu$  that describes the amplitude of the correlation function and thus the amplitude of the internal energy  $U = -X$ . With  $X''$  given by (2.7) this gives an additional term  $X_\nu \nu'' \sim \nu''$  ( $\nu'' = \nu_{mm}$ ) as  $X_\nu \sim 1$ . This is to be included in Eq. (2.6). Further, from Eq. (3.10)  $Z_\nu \sim \varepsilon^2$  such that  $\nu_\beta Z_\nu$  can be neglected. With this Eq. (2.6) is the SCOZA equation plus the  $\nu''$  term. Equation (6.1) then changes into ( $Q=0$ )

$$\frac{\partial \varepsilon^2}{\partial t} = -1 - \nu'' + \frac{1}{2} \varepsilon'', \quad (8.1)$$

when other terms that are not crucial have been neglected. Now one can assume  $\nu \sim m^{2+\lambda}$  along the critical isotherm to get

$$\frac{\partial \varepsilon^2}{\partial t} = -m^\lambda - m^2. \quad (8.2)$$

On the left-hand side of Eq. (8.2) the  $tm^\lambda$  term from (7.1) now matches the  $m^\lambda$  term on its right-hand side. Also the coefficient  $a$ , which is flexible in the HRT, must be equal to 1 to cancel the  $-1$  in (8.1).

To see how this new term will remove the generalized scaling of the SCOZA one can consider the curve of coexistence. For subcritical temperatures one then again can make the assumption [21]

$$\varepsilon = (m - at^q)^2 + \psi,$$

$$\varepsilon^2 = (m - at^q)^4 + 2(m - at^q)^2 \psi + \psi^2. \quad (8.3)$$

In view of the HRT this expression for  $Q=0$  is not obvious as it also includes the two-phase region where the HRT gives horizontal isotherms in the limit  $Q \rightarrow 0$ . Also for  $Q > 0$  the SCOZA would give horizontal isotherms in this limit. This latter situation has some similarity to the one with SCOZA for the two-dimensional Ising model [23]. In addition HRT has infinite susceptibility at phase coexistence when approaching it from outside. So expression (8.3) assumes that for the unified problem this latter deficiency vanishes. However, recent work on HRT using a smooth cutoff of wave vector strongly indicates finite susceptibility at coexistence [12,13]. In this way a continuous transition from the HRT to the SCOZA is possible. The latter is thus an additional indication that (8.3) is valid for the unified problem too (outside phase coexistence). In this respect the HRT with a smooth cutoff may be something intermediate between the original HRT and SCOZA with properties that seem close to or may be equal to those, e.g.  $\beta_c = 1/3$ , of the unified theory considered in this work.

With (8.3) the spinodal curve is given by  $m = at^q$  where  $a$  is a constant. Without the  $m^\lambda$  term the  $\psi$  is the scaling function  $tg(z)$  in (6.3) with  $q=3/4$ . If now the  $m^\lambda$  term is inserted the  $\psi$  will incorporate the  $tm^\lambda$  term of (7.1). By that,  $\psi$  is no longer tied to or required to scale to its higher-order  $m^6$  term alone, i.e.  $m^6 \sim m^2 \psi$  is no longer required. In this way it can contribute to the leading scaling part of  $\varepsilon$  too by which the critical index  $\beta_c$  becomes  $1/(4-\lambda)$  as follows from (7.2) and (7.3).

As in SCOZA the  $t^q$  term will still be tied to the higher-order  $m^2$  term of (8.2). By inserting (8.3) in the left-hand side of (8.2) one will thus again obtain the scaling relation ( $t^q \ll m$ )

$$t^{q-1} m m^2 \sim m^2 \quad \text{or} \quad m \sim t^{1-q}. \quad (8.4)$$

But with the  $tm^\lambda$  term incorporated into  $\psi$ , the  $q$  will no longer be tied to the SCOZA value  $q=3/4$  either, and it may be possible to have full scaling. This requires that the value of  $\beta_c$  that follows from (8.4) equals the one in terms of  $\lambda$ , so

$$\beta_c = 1/(4-\lambda) = 1 - q. \quad (8.5)$$

The curve of coexistence can now be evaluated in the same way as for the SCOZA [21]. The relevant term in the internal energy  $U$  (3.3) ( $U = -X$ ) is then  $-m^2 + \varepsilon \sim t^q m$ . This term is integrated with respect to  $t$  to obtain the free energy. This integration will include an  $m^{\delta+1}$  term (so far with  $\delta=5$ ) as a constant of integration. The reason is that the second derivative of the free energy with respect to  $m$  is the susceptibility  $\sim \varepsilon^2 \sim m^{\delta-1}$ . So the free energy becomes  $\sim -t^{1+q} m + m^{\delta+1}$ . Differentiation of the free energy once with respect to  $m$  then yields the magnetic field  $\sim -t^{1+q} + m^\delta$ . Phase equilibrium in zero magnetic field thus means ( $t > 0$ )

$$t^{1+q} \sim m^\delta, \quad (8.6)$$

which implies the critical index

$$\beta_c = \frac{1+q}{\delta}. \quad (8.7)$$

Full scaling requires that (8.5) and (8.7) result in the same  $\beta_c$ . Accordingly

$$1-q = \frac{1+q}{\delta} \quad \text{or} \quad q = \frac{\delta-1}{\delta+1}, \quad (8.8)$$

from which we obtain our main result

$$\beta_c = \frac{2}{\delta+1}. \quad (8.9)$$

This is the result given in Eq. (1.1) by which other indices become those of Eq. (1.3) provided full scaling is present. For  $\delta=5$  the value for  $\lambda$  becomes  $\lambda=1$ . One can also note that scaling consistency of the internal energy term  $\sim t^q m$  [see below Eq. (8.5)] and the  $m^\lambda$  term of Eq. (8.2) requires  $t^q m \sim m^{2+\lambda}$  or  $q = \beta_c(1+\lambda)$ , consistent with Eq. (8.5) for  $\delta=5$ .

Although we here primarily have  $\delta=5$  in mind Eq. (8.2) can be extended to the more general situation considered in the next section. Then the  $\varepsilon''$  of Eq. (8.1) is replaced by  $(\varepsilon^{4/(\delta-1)})''$  as follows from Eq. (9.6) for  $J(z)$  below while  $\varepsilon^2 \sim m^{\delta-1}$  according to Eq. (9.3). With this the  $m^2$  term on the left-hand side of Eq. (8.2) and the  $m^2$  terms of Eq. (8.4) are replaced by  $m^{\delta-3}$ . There will be corresponding changes in Eq. (8.3), and the  $4-\lambda$  in Eq. (8.5) is replaced by  $\delta-1-\lambda$ . With this one finds that Eqs. (8.4)–(8.9) also hold for more general values of  $\delta$ . The exponent  $\lambda$  then obtains the value  $\lambda = (\delta-3)/2$ .

## IX. MORE DETAILED EVALUATION

The derivation in the previous section hinges on the assumption that full scaling is actually present and that the parameter  $\nu$  is consistent with this. As demonstrated the leading scaling function is closely connected to its leading correction as seen from condition (8.4) that couples terms in Eq. (8.1) of different orders in  $\varepsilon^2$ . This coupling gives a kind of feedback that led to the simple result (8.9) for  $\beta_c$ . We will now justify this in another way, which also includes supercritical temperatures, by assuming that a scaling solution with corrections to it exists. Then the solution for the free energy of the unified problem can be written in the form

$$I = m^{\delta+1}(I_0 + m^\lambda I_1 + m^{\delta-3} I_3 + \dots) \quad (9.1)$$

where  $I_i$  ( $i=0, 1, 2$ ) are functions of the scaled variables ( $d$  is dimension)

$$\frac{m}{Q^{d/(\delta+1)}} \quad \text{and} \quad \frac{t}{Q^{\lambda_1}}. \quad (9.2)$$

For  $\delta=5$  this is in accordance with the critical isotherm (5.4), but holds more generally as we will show below. (In GMSM the  $m^\lambda$  term is zero as it is not needed there.) From

expression (9.1) for  $I$  the forms of other quantities are obtained via Eqs. (3.3)–(3.10). We get

$$X = \frac{m^{\delta+1}}{t}(X_0 + m^\lambda X_1 + m^{\delta-3} X_2 + \dots),$$

$$\varepsilon^2 = 1 - z \sim Z = \frac{m^{\delta+1}}{m^2}(Z_0 + m^\lambda Z_1 + m^{\delta-3} Z_2 + \dots),$$

$$\frac{\partial \varepsilon^2}{\partial t} \sim \frac{m^{\delta+1}}{m^2 t}(Z_{0t} + m^\lambda Z_{1t} + m^{\delta-3} Z_{2t} + \dots), \quad (9.3)$$

where again  $X_i$  and  $Z_i$ , etc. ( $i=1, 2, 3$ ), are functions of the scaled variables (9.2).

The SCOZA equation is the relation  $X'' \sim \partial \varepsilon^2 / \partial t$  with  $\nu = 1$ . Via Eq. (2.7) for the unified problem the  $X$  can be related to the parameters  $\varepsilon^2$  and  $\nu$  as

$$X'' = X_{mm} + X_z z'' + X_\nu \nu'' + \dots, \quad (9.4)$$

where first-order derivatives of  $z$  and  $\nu$  have been disregarded and where

$$X_{mm} = 1, \quad X_z \sim J'(z) \sim 1/\varepsilon, \quad X_\nu \sim J(z) \sim 1 \quad (9.5)$$

with  $J(z)$  given by (3.6).

More generally, one finds (below  $a$  and  $b$  are again arbitrary constants)

$$J(z) = a - b\varepsilon^{4/(\delta-1)}. \quad (9.6)$$

This follows from integration of Eq. (3.8) when the interaction is such that

$$L \sim \frac{Q^{d-1}}{\varepsilon^2 + Q^{2-\eta}}. \quad (9.7)$$

Note that  $\eta > 0$  implies an interaction or more generally a direct correlation function of long range. So this goes beyond and is a generalization of the correlation function (3.1) where  $\eta=0$  was assumed. Thus for a general situation with  $\eta$  given by (1.3)

$$J(z) - a \sim -b \frac{Q^d}{Q^{(2-\eta)}} \sim -b \varepsilon^{2(d-2+\eta)/(2-\eta)} \sim -b \varepsilon^{4/(\delta-1)}. \quad (9.8)$$

With this, Eqs. (5.3) and (5.4) for the critical isotherm generalize to

$$u = a\varepsilon^{4/(\delta-1)} + b\varepsilon^2,$$

$$\begin{aligned} \varepsilon^{4/(\delta-1)} &= au - b\varepsilon^2 = au - bu^{(\delta-1)/2} + \dots \\ &= au(1 - bu^{(\delta-3)/2} + \dots), \end{aligned}$$

$$\varepsilon^2 = au^{(\delta-1)/2}(1 - bu^{(\delta-3)/2} + \dots) = am^{\delta-1}(1 - bm^{\delta-3} + \dots). \quad (9.9)$$

Expression (9.3) for  $\varepsilon$  is consistent with this (with  $Z_1=0$  for  $t=0$ ).

With Eqs. (9.4) and (9.5) and expression (9.8) for  $J(z)$ , we now have ( $Q \rightarrow 0$ )



$$X'' = c - a(\varepsilon^{4/(\delta-1)})'' + b\nu'' + \dots \quad (9.10)$$

At an ordinary critical point the constant  $c$  will cancel to leading order as pointed out in Sec. VI. (But this will not be the case if the critical point is a tricritical one with  $\delta=5$  and  $\beta_c=1/4$ , i.e.,  $\varepsilon^2 \sim m^4 \sim t$  and thus  $X'' \sim c$  as pointed out too.) Further we will assume that the expression for  $\nu$  will contain scaling terms with the same powers of  $m$  as the coefficients of the other terms in (9.10). This assumption about the parameter  $\nu$  is a central one as it is a key assumption behind our results. Anyway, away from the critical point  $\nu \rightarrow 1$ , so its significance will decrease as  $\nu''$  will vanish. With expression (9.3) for  $\varepsilon^2$  inserted in (9.10), we then find (as the constant  $c$  should cancel)

$$X'' = m^\lambda Z_{1x} + m^{\delta-3} Z_{2x} + \dots \quad (9.11)$$

But this expression for  $X$  should be equivalent to both the first and the last equations ( $X'' \sim \partial \varepsilon^2 / \partial t$ ) of Eq. (9.3). Thus, comparing (9.3) and (9.11), we obtain the conditions

$$\frac{m^{\delta-1}}{t} \sim m^\lambda \quad \text{and} \quad \frac{m^{\delta-1}}{t} m^\lambda \sim m^{\delta-3}. \quad (9.12)$$

The solution of these equations is

$$\lambda = \frac{\delta-3}{2} \quad \text{and} \quad t \sim m^{(\delta+1)/2}. \quad (9.13)$$

Thus the critical index  $\beta_c$  given by expression (8.9) is recovered.

The conditions expressed by Eq. (9.12) are due to the coupling of different orders of scaling functions via thermodynamic self-consistency. This coupling is directly connected to the leading correction to the critical isotherm (9.9). Thus with (9.3), (9.11), and (9.12) we have for the internal energy

$$X \sim m^{(\delta+1)/2} (X_0 + m^{(\delta-3)/2} X_1 + \dots). \quad (9.14)$$

This expression is possible due to the  $\nu''$  term of (9.4) which is present in the unified HRT-SCOZA problem. For the SCOZA alone, on the contrary, with Eq. (6.1) where this term is absent, this is not possible, and instead generalized scaling is obtained. With critical isotherm (9.9) inserted in (6.1) one then gets [with  $\varepsilon''$  replaced by  $(\varepsilon^{4/(\delta-1)})''$ , and the  $-1$  should again cancel]

$$X \sim m^{\delta-1}, \quad (9.15)$$

which corresponds only to the  $X_1$  term of Eq. (9.14). The  $X_0$  term is thus missing.

For the GSM problem, however, where  $\nu=1$ , the  $X_0$  term also vanishes. But in this case expression (9.15) is the sought result. Then the  $m^\lambda$  terms are not present either, and there is instead a direct coupling between the  $X_0$  term of (9.3) and the  $Z_{2x}$  term of (9.11) by which  $m^{\delta-1}/t \sim m^{\delta-3}$  or  $t \sim m^2$ , i.e., critical index  $\beta_c=1/2$ .

## X. LOGARITHMIC CORRECTIONS

The HRT-SCOZA analysis performed in the preceding sections is self-consistent in a way that does not rule out the

possibility that our indices are exact with a suitable choice for  $\delta$  along with our main result (8.9) for  $\beta_c$ . However, they are not consistent with known epsilon-expansion results [24,25]. A reason for our expectation of this possibility is that the pair correlation function to be used with two free parameters for its amplitude and range covers a rather general situation. And there is little or no room for further significant adjustments of leading contributions to thermodynamic quantities. But “logarithmic” type adjustments that do not change indices are at least possible. This is the situation for  $\delta=5$  by which  $\eta=0$  for  $d=3$ . Earlier, this situation was studied by Stell as part of an investigation of the pair correlation function for more general  $\delta$  and  $d$  [15,16]. He found that there would be logarithmic corrections to the decay of the pair correlation function as well as to the direct one for  $\eta=0$ . These functions are related by the scaling relation  $c(r) \sim h^\delta(r)$  at the critical point. Thus with  $\eta=0$  and  $d=3$  and expression (10.3) below, one has

$$c(r) \sim h^\delta(r) \sim \frac{e^{-\delta \kappa r}}{r^5}. \quad (10.1)$$

However, its Fourier transform  $\tilde{c}(k)$  deviates from a pure power,  $\sim k^{2-\eta}=k^2$ , by a logarithmic correction like integral (10.5) below to become  $\sim k^2 \ln k$ . This will further produce a logarithmic term  $\ln r$  in  $h(r)$  whose Fourier transform is  $\tilde{h}(k) = \tilde{c}(k) / [1 - \rho \tilde{c}(k)]$ . Thus a more detailed computation that was performed in Ref. [15], is needed to obtain the type of logarithmic correction present. For  $d=3$  and 5 the more general result obtained in Ref. [15] becomes

$$\tilde{h}(k) \sim \frac{1}{k^2 [-\ln(k/k_0)]^{1/6}} \quad \text{or} \quad h(r) \sim \frac{1}{r [\ln(k_0 r)]^{1/6}}. \quad (10.2)$$

In the Appendix we give details of the evaluation that yields this result where  $k_0$  is a constant (in the reference  $k_0=1$ ). Comparing with  $\tilde{h}(k) \sim 1/k^{2-\eta}$  expression (10.2) can be considered to effectively give a small positive value for the index  $\eta$  although strictly speaking Eq. (10.2) means that  $\eta=0$ .

Although  $\delta=5$  was studied in Refs. [15,16] it was not concluded that  $\delta$  was equal to 5 for fluids due to other evidence [24]. However, in view of the HRT-SCOZA analysis we find reason to reconsider this. If our analysis is correct the critical index  $\alpha$  as given by Eq. (1.3) is equal to zero in any case. Likewise it may be reasonable that  $\delta$  can be an odd number, i.e.  $\delta=5$  for  $d=3$  as already suggested in Refs. [15,16]. We find that we can justify this in terms of graph expansion. Then we have in mind the  $\gamma$  ordering of graph expansions for potentials of long range where  $\gamma$  is the inverse range of interaction [17–19]. There, Mayer bonds are subdivided into potential bonds that further are linked together into chains. In these chains  $\rho$  vertices are replaced by hypervertices to form the leading contribution to the correlation function  $h(r)$  or  $\Gamma(r)$  whose Fourier transform has the structure of Eq. (3.1). There will be higher-order contributions in  $\gamma$  to the correlation function. However, these contributions can be incorporated in the self-energy function  $\tilde{\Sigma}(k)$ ,

which for the HRT-SCOZA problem is approximated by the parameters  $\nu$  and  $z$  to be determined. This structure was also utilized by Høye and Stell in their work on polar fluids to obtain the basic structure of dipolar correlations [20]. By subtracting  $\tilde{\Sigma}$  from  $\tilde{\Gamma}$  and then remove both end points  $\tilde{\Sigma}$  from the remaining part one is left with a chain bond where  $\tilde{\Sigma}$  represents the hypervertices. This chain bond which has the  $r$  dependence of  $\Gamma(r)$  itself near the critical point may then replace the original chain bond of  $\gamma$  ordering. Thus these bonds will be

$$h(r) \propto \frac{e^{-\kappa r}}{r^{d-2+\eta}}, \quad \kappa \propto t^\nu, \quad (10.3)$$

where  $t$  is the deviation from critical temperature (here  $\nu$  is critical index). For the critical index  $\eta$  one has from the standard scaling relation (1.3)

$$d - (2 - \eta) = \frac{2d}{\delta + 1}. \quad (10.4)$$

Now the dominating graph to the direct correlation function is the potential bond as utilized by the SCOZA and HRT. Beyond the potential bond the leading graph in the order parameter  $\gamma$  will be the one with two bonds in parallel. These bonds meet at two three-point hypervertices, each of which has a root point. (It can be noted that the graphs for the direct correlation function are those of the free energy with two root points added.) For a general graph these bonds meet at  $n$ -point hypervertices where  $n-1$  bonds meet. If the three-point hypervertex is zero the graph with three bonds in parallel will be the leading one, and so on with 4, 5, ... bonds in parallel. Due to symmetry reasons (for lattice gases or the Ising model at least) these graphs with an even number of bonds becomes zero at critical density. Thus we find reason to conclude that the  $\delta$  is an odd number in Eq. (10.1). There are also graphs of higher order in  $\gamma$ . However, one may expect that these higher-order graphs do not have a decisive role as critical properties are not expected to depend upon  $\gamma$  as long as it is finite.

A detailed study of the correlation function at the critical point was earlier performed in Sec. 4B of Ref. [19]. There contributions from graphs to the ‘‘self-energy’’  $\Sigma(r)$  [named  $\hat{W}(r)$  in the reference] were studied in view of the  $\gamma$  ordering. The dominating graphs with respect to slow  $r$  decay for  $r \rightarrow \infty$  were considered. These graphs were those with four-point hypervertices ( $\nu_4$ ) since odd-numbered ones were found to be zero at critical density. The resulting sum of graphs was discussed, but its convergence properties remained unclear. As Ref. [19] used a different notation, it can be mentioned that its Eq. (4.3) [ $n=2\nu/(1+m)$ ] is identical to Eq. (10.4) above except for the use of symbols.

By the present study of the situation at the critical point we have come to the conclusion that retaining a nonzero four-point hypervertex may be one part of the problem. Thus we find that the  $(\delta+1)$ -point hypervertex can be the dominating one that contributes right at the critical point while those with fewer points thus must be zero. From this follows that  $\delta$  is an odd number. Further one finds that this coincides with scaling properties as can be seen from expression (10.6)

for the free energy below. The justification for our assumption or hypothesis about hypervertices at or close to the critical point is the resemblance to the basic  $\gamma$  ordering. There  $n$ -point hypervertices ( $n > 2$ ), when regarded as  $\delta$  functions, follow from derivatives of the two-point hypervertex which again follows from the equation of state of the reference system via the compressibility relation (3.5). Likewise, the renormalized hypervertices at the critical point may be corresponding derivatives of the renormalized hypervertex  $\tilde{\Sigma}(k)$ . At the critical point also the  $\Sigma(r)$  may be regarded as  $\delta$  function compared with the single  $h(r)$  bond ( $\kappa \rightarrow 0$ ), and its integral  $\tilde{\Sigma}(0)$  is determined by the equation of state via Eqs. (3.1) and (3.5).

We will also consider the leading graph correction to the free energy not included in the HRT-SCOZA analysis. This graph may account for the logarithmic singularity of the specific heat of the two-dimensional Ising model. The situation here is similar to the one for the direct correlation function considered above except that the free energy graphs have no root points. Thus the graph in question is the one with two nonzero hypervertices and a number of  $\delta+1$  bonds in parallel between these two vertices. Thus for the contribution to the free energy one finds ( $\kappa \rightarrow 0$ )

$$\Delta F \propto \int [h(r)]^{\delta+1} d\mathbf{r} \sim \int \frac{e^{-(\delta+1)\kappa r}}{r^{2d}} d\mathbf{r} \sim \kappa^d \ln \kappa. \quad (10.5)$$

[This follows from  $d$  partial integrations of (10.5), which gives the integral  $\int (e^{-\kappa r}/r) d\mathbf{r} \sim \ln \kappa$  for  $d$  integer.] Thus with (10.3) and (1.3) we get

$$\Delta F \sim t^{\nu d} \ln t \sim t^2 \ln t, \quad (10.6)$$

by which the leading contribution to the specific heat becomes  $\sim \ln t$ , i.e.,  $\alpha=0$ . For  $d=3$  this situation is less obvious due to the logarithmic terms in Eq. (10.2) and a corresponding uncertainty in the inverse correlation length  $\kappa$ ; so we will not pursue this further here.

## XI. SUMMARY

The unified HRT-SCOZA theory has been investigated in the critical region. The resulting equation is essentially a sum of the separate HRT and SCOZA equations. Close to the critical point the HRT part dominates ( $Q \rightarrow 0$ ). But this part lacks explicit temperature dependence, and there is thus via the SCOZA part a coupling to higher-order scaling terms. These terms should match the leading part of the critical isotherm and its leading correction that is found to be common to that of the GSM. In the unified theory the missing term that prevents scaling in the SCOZA may be obtained from the HRT part of the resulting equation by which full scaling is made possible. The coupling to higher-order scaling terms gives through the thermodynamic self-consistency of the SCOZA a feedback loop from which the relation  $\beta_c = 2/(\delta+1)$  for critical indices is obtained. In Sec. X, in addition, we argue in view of graph contributions that  $\delta$  should be an odd number.

So, provided our main assumption about the parameter  $\nu$  and the corresponding expansion of the scaling solution in higher-order terms holds, it is not ruled out that our evaluations may give the exact critical indices for interactions of short range for fluids, lattice gases, and Ising spin systems in three dimensions. With the standard interactions of short range this implies scaling with the critical indices  $\eta=0$ ,  $\delta=5$ ,  $\beta_c=1/3$ ,  $\gamma=4/3$ ,  $\nu=2/3$ , and  $\alpha=0$  plus corrections of logarithmic type. However, this is somewhat at variance with best estimates, which are  $\eta=0.036$ ,  $\delta=4.789$ ,  $\beta_c=0.327$ ,  $\gamma=1.237$ , and  $\alpha=0.110$  [14,25]. On the other side our results may be consistent with the numerical results of Ref. [14] for the HRT with a smooth cutoff that can be something intermediate between HRT and SCOZA. Then, as mentioned earlier, for given  $\delta=5$  the values  $\beta_c=0.330$  and  $0.332$  were found in Refs. [13,14], respectively. The other indices of the last of these two references then follow from the scaling relations (1.2) while for the first one they are not quite satisfied.

Due to the assumptions made during the derivations in this work, further analytic and numerical investigations are needed to possibly confirm the results or show inaccuracies

#### APPENDIX: CRITICAL PAIR CORRELATION FUNCTION

Below we will give an evaluation of the correlation function at the critical point for  $\delta=5$  and  $d=3$  to recover the result obtained by Stell [15]. Then consider the function  $a(r)=1/r^\alpha$ . Its Fourier transform is (three dimensions,  $0 < \alpha < 3$ )

$$\tilde{a}(k) = 4\pi k^{\alpha-3} \Gamma(2-\alpha) \sin\left(\frac{\pi}{2}\alpha\right), \quad (\text{A1})$$

where  $\Gamma$  is the  $\Gamma$  function that satisfies

$$\Gamma(u)\Gamma(1-u) = \frac{\pi}{\sin(\pi u)} \quad (\text{A2})$$

such that

$$\tilde{a}(k) = \frac{-2\pi^2 k^{\alpha-3}}{\Gamma(\alpha-1) \cos\left(\frac{\pi}{2}\alpha\right)}. \quad (\text{A3})$$

By taking the limit  $\alpha \rightarrow 1$  one finds the well-known result  $\tilde{a}(k)=4\pi/k^2$ . For  $\alpha$  close to 5, on the other hand, one finds

$$\tilde{a}(k) \approx -\frac{4\pi k^{\alpha-3}}{3!(5-\alpha)} \sim k^2 \frac{k^\tau}{\tau}, \quad \tau = \alpha - 5. \quad (\text{A4})$$

Here it is assumed that analytic continuation can be used for  $\alpha > 3$  to obtain the term of interest. At the critical point one further may assume

$$h(r) = \frac{1}{r} \int_0^\infty \frac{f(t)}{r^t} dt, \quad (\text{A5})$$

where only small values of  $t$  are assumed significant. For the direct correlation function then in accordance with Eq. (10.1) one should have (for  $\delta=5$ )

$$c(r) \sim -h^5(r) = -\frac{1}{r^5} \int \frac{d\Omega}{r^\tau}, \quad (\text{A6})$$

where

$$\tau = \sum_{i=1}^5 t_i \quad \text{and} \quad d\Omega = \prod_{i=1}^5 [f(t_i) dt_i].$$

By Fourier transform one now finds

$$\tilde{h}(k) \sim \frac{1}{k^2} I, \quad I = \int_0^\infty k^t f(t) dt \quad (\text{A7})$$

and by use of Eq. (A4)

$$\tilde{c}(k) \sim -k^2 \int \frac{k^\tau}{\tau} d\Omega. \quad (\text{A8})$$

From the relation between  $\tilde{h}$  and  $\tilde{c}$ , the Ornstein-Zernike equation, given above Eq. (10.2), one has

$$\tilde{h}(k) \sim [\tilde{c}(k)]^{-1}. \quad (\text{A9})$$

The solution of Eq. (A9) with Eqs. (A7) and (A8) inserted is then

$$k^t f(t) \sim t^{-5/6} (k/k_0)^{-t} = t^{-5/6} e^{-Lt} \quad (\text{A10})$$

with  $L = -\ln(k/k_0)$  where  $k_0$  is a constant. So from this and Eq. (A5) it follows that

$$I \sim L^{-1/6}, \quad \tilde{h}(k) = \frac{1}{k^2 L^{1/6}}, \quad h(r) \sim \frac{1}{r [\ln(k_0 r)]^{1/6}}. \quad (\text{A11})$$

As a check of this solution one has  $-d[\tilde{c}(k)/k^2]/dL \sim \int k^\tau d\Omega \sim L^{-5/6}$  by which  $-\tilde{c}(k) \sim k^2 L^{1/6}$ .

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