PHYSICAL REVIEW B VOLUME 30, NUMBER 3 1 AUGUST 1984

Linear integral equations and renormalization group

W. Klein*
IBM Zürich Research Laboratory, CH-8803 Rüschlikon, Switzerland

A. D. J. Haymet
Department of Chemistry, University of California, Berkeley, California 94720

(Received 16 January 1984; revised manuscript received 23 April 1984)

A formulation of the position-space renormalization-group (RG) technique is used to analyze the singular behavior of solutions to a number of integral equations used in the theory of the liquid state. In particular, we examine the truncated Kirkwood-Salsburg equation, the Ornstein-Zernike equation, and a simple nonlinear equation used in the mean-field theory of liquids. We discuss the differences in applying the position-space RG to lattice systems and to fluids, and the need for an explicit free-energy rescaling assumption in our formulation of the RG for integral equations. Our analysis provides one natural way to define a "fractal" dimension at a phase transition.

I. INTRODUCTION

The renormalization group[1] (RG) is one of the most powerful methods employed in the theoretical study of phase transitions. Recently, the RG technique has led to a deeper understanding of critical phenomena[2,3] and has contributed to our understanding of first-order transitions.[4,5] In the study of first-order transitions in lattice spin systems the position-space renormalization group (PSRG) has been particularly effective.

In the study of fluids, however, the RG techniques have not been of much utility away from the critical point. In particular, there are severe difficulties in applying PSRG techniques to fluids where, in contrast to most lattice systems, a given particle can interact with all other particles in the system. The PSRG generates a similar long-range interaction even in simple systems such as nearest-neighbor Ising models; however, the short-range interactions in the nonrenormalized Ising models make possible the various approximation schemes[3] used with the PSRG.

In a previous paper[6] a PSRG technique was presented which can be employed to obtain the singular behavior of solutions of linear integral equations. Note that the renormalization procedure is applied directly to the integral equation for the correlation function, rather than the partition function, or the free energy. This technique was applied to an integral equation used in the study of fluids,[7,8] and results were obtained that were consistent with the numerical solution.[9] In this paper we present a much more detailed analysis of this method and apply it to other linear integral equations. The RG, together with thermodynamic consistency, imposes constraints on the solution, among them being, in certain cases, a particular spatial dimension in which such consistent solutions can be obtained.

In this paper we consider two types of phase transitions from the liquid phase, to the solid in Secs. II and III, and to the gas in Secs. IV and V. In the former type we identify the singular points of the integral equation, which may correspond to the "spinodal point" or the equilibrium freezing-melting transition, depending on the integral equation and the approximations involved. In the latter type we are considering the gas-liquid critical point.

The remainder of this paper is structured as follows. In Sec. II we briefly review the linear-integral-equation renormalization group (LIRG). In Sec. III we reanalyze the LIRG and reinterpret the results. General principles for the application of the LIRG are formulated and applied to other linear equations in Sec. IV. In Sec. V we adapt this method to treat a simple nonlinear equation. Finally, in Sec. VI we summarize our results.

II. TRUNCATED KIRKWOOD-SALSBURG EQUATION

For the sake of completeness we briefly review the numerical (Ref. 9) and RG (Ref. 6) identification of a spinodal-like transition in hard-core particles from an approximate integral equation obtained by truncation[7,8] of the Kirkwood-Salsburg (KS) hierarchy.[10]

For systems with pairwise additive pair potentials, the n-particle distribution functions $\rho_n(\{x_n\})$ satisfy the Kirkwood-Salsburg equation,

$$\begin{aligned}\rho_1(\vec{x}_1)&=z\left[1+\sum_{n=1}^{N}\frac{1}{n!}\int\rho_n(\vec{x}_2,\ldots,\vec{x}_{n+1})\prod_{j=2}^{n+1}f_{1j}d\vec{x}_j\right],\\ \rho_m(\{\vec{x}_m\})&=z\prod_{j=2}^{m}(1+f_{1j})\left[\rho_{m-1}(\vec{x}_2,\ldots,\vec{x}_m)+\sum_{n=1}^{N}\frac{1}{n!}\int\rho_{m+n-1}(\vec{x}_2,\ldots,\vec{x}_{m+n})\prod_{j=m+1}^{m+n}f_{1j}d\vec{x}_j\right],\end{aligned}\tag{2.1}$$

where the Mayer function is

$$f_{ij}=\exp[-\beta u(|\vec{x}_i-\vec{x}_j|)]-1 ,$$

the activity is $z=\lambda^{-3}e^{\beta\mu_{\text{ex}}}$, $\lambda=h(2\pi mkT)^{-1/2}$, and $\beta^{-1}=kT$, and the excess chemical potential is given by

$$e^{-\beta\mu_{\text{ex}}}=1+\sum_{n=1}^{N}(1/Vn!)\int\rho_n(\vec{x}_2,\ldots,\vec{x}_{n+1})\times\prod_{j=2}^{n+1}f_{1j}d\vec{x}_j . \tag{2.2}$$

For pair potentials $u(x_{ij})$ of strictly finite range *and* with a hard core, the upper limit N of the summations is finite (approximately 13 for hard spheres in three dimensions).

Little use has been made of the KS hierarchy in numerical work. However, Chung and Espenscheid[11] found that, under the superposition approximation, the above equation for hard spheres leads to exact virial coefficients up to the fourth order, and a good approximation to the fifth order.

A truncated version of the equation, studied by Sabry,[7] Klein,[8] and Swendsen and Klein,[9] is

$$\rho_2(\vec{x}_{12})=z[1+f(x_{12})]\left[z+\int\rho_2(x_{23})f(x_{13})d\vec{x}_3\right] , \tag{2.3}$$

which correctly predicts the first three virial coefficients. An infinite series solution (in powers of the activity z) of Eq. (2.3) is obtained by iteration.

The methods of series analysis and Padé approximation[9] indicate that $\rho_2(\vec{x}_{12})$ is an analytic function of z in a neighborhood of the interval $[-1, 11.6048]$ on the real line. The physical singularity at $z=11.0468$ is characterized by a set of "critical exponents" which specify the behavior of the thermodynamic functions at the singularity. It is important to note that in this and the next section, by critical exponents we mean "spinodal" exponents which are found in mean-field theories of freezing.[12] The thermodynamic functions are obtained from the distribution function in the standard way.[2,5] One very important point, however, must be noted. In the limit $x_{12}\rightarrow\infty$, $\rho_2(x_{12})\rightarrow\rho^2$, where ρ is the density. It is easy to see that the solution of Eq. (2.3) has this property, which we will call the "product property." We can also relate $\rho_2(\vec{x}_{12})$ to the density by first obtaining[13] the pressure P from $\rho_2(\vec{x}_{12})$ using the virial equation and then the relation

$$\frac{\partial P}{\partial z}=\frac{\rho}{\beta z} . \tag{2.4}$$

If $\rho_2(\vec{x}_{12})$ were exact, these two methods for obtaining the density would give the same results. In Ref. 9 the latter method was used. As we will see below, these two methods lead, in general, to *different* exponents when approximate distribution functions are used.

With the above considerations the following "critical" exponents were obtained:

$$P-P_c\propto(1-z/z_c)^{3/2} \tag{2.5}$$

and

$$\rho-\rho_c\propto(1-z/z_c)^{1/2} , \tag{2.6}$$

where z_c, ρ_c, and P_c are the values of the activity, density, and pressure, respectively, at the singular point.

These exponents, as well as others, can also be obtained from a RG solution[6] of Eq. (2.3). The RG is generated by iteration of Eq. (2.3) to obtain

$$\rho_2(x_{12})=\psi(x_{12},z)+z^2\int\int\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4)\times\rho_2(x_{34})d\vec{x}_3d\vec{x}_4 , \tag{2.7}$$

where

$$\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4)=[1+f(x_{12})][1+f(x_{23})]f(x_{24})f(x_{13}) , \tag{2.8}$$

and $\psi(x_{12},z)$ is an analytic function of z.

If we iterate Eq. (2.7), we obtain

$$\rho_2(x_{12})=\widetilde{\psi}(x_{12},z)+z^4\int\int\int\int\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4,\vec{x}_5,\vec{x}_6)\times\rho_2(x_{34})d\vec{x}_3d\vec{x}_4d\vec{x}_5d\vec{x}_6 , \tag{2.9}$$

where $\widetilde{\psi}(x_{12},z)$ is also analytic in z. The kernel is given by

$$\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4,\vec{x}_5,\vec{x}_6)=f(x_{13})f(x_{26})f(x_{35})f(x_{46})\times[1+f(x_{25})][1+f(x_{56})]\times[1+f(x_{34})][1+f(x_{12})] . \tag{2.10}$$

If a partial trace is performed over particles 5 and 6 in Eq. (2.10), we obtain

$$\rho_2(x_{12})=\widetilde{\psi}(x_{12},z)+z^4\int\int\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4)\times\rho_2(x_{34})d\vec{x}_3d\vec{x}_4 . \tag{2.11}$$

Since $\widetilde{\psi}(x_{12},z)$ is analytic in z, the singular part of $\rho_2(x_{12})$ must satisfy

$$\rho_{2s}(x_{12})=z^4\int\int\widetilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4)\rho_{2s}(x_{34})d\vec{x}_3d\vec{x}_4 . \tag{2.12}$$

Now consider the pair distribution function constructed with a renormalized Hamiltonian by analogy with Eq. (2.7). We expect

$$\rho_2'(x_{12}')=\psi'(\vec{x}_{12}',z')+(z')^2\int\int\widetilde{k}'(\vec{x}_1',\vec{x}_2',\vec{x}_3',\vec{x}_4')\times\rho_2'(x_{34}')d\vec{x}_3'd\vec{x}_4' . \tag{2.13}$$

For the singular part,

$$\rho_{2s}'(x_{12}')=(z')^2\int\int\widetilde{k}'(\vec{x}_1',\vec{x}_2',\vec{x}_3',\vec{x}_4')\rho_{2s}'(x_{34}')d\vec{x}_3'd\vec{x}_4' . \tag{2.14}$$

In order to preserve the singular behavior, we must have

$$\rho_{2s}(x_{12})=\rho_{2s}'(x_{12}') . \tag{2.15}$$

Equations (2.7)—(2.15), together with length rescaling (i.e., $dx'=dx/b^d$), give

$$\psi'(x'_{12},z')=\psi(x_{12},z) \tag{2.16}$$

and

$$[(z')^2/b^{2d}]\tilde{k}'(\vec{x}'_1,\vec{x}'_2,\vec{x}'_3\vec{x}'_4)$$
$$=z^4\int\int d\vec{x}_5 d\vec{x}_6\tilde{k}(\vec{x}_1,\vec{x}_2,\vec{x}_3,\vec{x}_4,\vec{x}_5,\vec{x}_6)\ . \tag{2.17}$$

Equation (2.17) is our fundamental RG transformation. Note that due to the structure of the kernel in Eq. (2.1), the integration of particles 5 and 6 is restricted to a volume determined by the range of the potential and, therefore, in our RG procedure we do not integrate over all length scales. It is the range of the potential that determines the nature of the cutoff in the RG procedure. For the potentials we consider here (i.e., $\int |f(x)|\,d\vec{x}<\infty$), the cutoff is finite. The RG transformation of Eq. (2.17) generates many-body interactions[6] in an analogous way to the standard position-space RG formulations.[3] In order to avoid this complication we can investigate the RG in the limit $x_{12}\to\infty$. Since the singular behavior of the distribution function is contained in this limit, and for realistic potentials $u(x_{ij})$

$$\lim_{x_{ij}\to\infty} u(x_{ij})=0\ ,$$

we obtain significant simplification.

With the above considerations and Eqs. (2.8), (2.12), (2.14), (2.16), and (2.17), the RG transformation becomes

$$z'f'(x')/b^d=z^2\int f(|\vec{x}-\vec{y}|)f(|\vec{y}|)d\vec{y}\ . \tag{2.18}$$

Taking the Fourier transform of Eq. (2.18) and then the logarithm gives

$$\ln[z'\hat{f}'(k')]=2\ln[z\hat{f}(k)]\ . \tag{2.19}$$

The unstable fixed point of Eq. (2.19) is at $z_c\hat{f}(k_0)=1$, where k_0 is the value of k for which $\hat{f}(k)$ has a maximum. If we restrict our considerations to hard spheres in $d=3$ and choose units for which $\hat{f}(0)=-1$, we find that $z_c=11.0648\cdots$, in agreement with the numerical results.

In order to calculate "critical exponents" we must determine the rescaling length. If we fix $z=z_c$ in Eq. (2.19) and expand in k about k_0, we find

$$(k'-k_0)^2=2(k-k_0)^2\ . \tag{2.20}$$

Since k is expressed in units of inverse length, Eq. (2.20) implies that the rescaling length

$$b=\sqrt{2}\ . \tag{2.21}$$

Note also that if k is fixed at k_0, Eqs. (2.18) and (2.21) lead to

$$(z'-z_c)=b^2(z-z_c)\ . \tag{2.22}$$

Equations (2.18), (2.21), and the usual scaling relations[3,6] lead to the following critical exponents.

The correlation length ξ diverges as

$$\xi\propto(z-z_c)^{-1/2}=(z-z_c)^{-\nu}\ , \tag{2.23}$$

and the susceptibility χ_T diverges as

$$\chi_T\propto(z-z_c)^{-1/2}=(z-z_c)^{-\gamma}\ . \tag{2.24}$$

The singular parts of the pressure and density,

$$P-P_c\propto(z-z_c)^{3/2}=(z-z_c)^{2-\alpha}\ , \tag{2.25}$$

$$\rho-\rho_c\propto(z-z_c)^{1/2}=(z-z_c)^{\beta}\ , \tag{2.26}$$

are in agreement with the numerical solution.[9] The RG calculation gives the same exponents as the numerical solution and, in addition, gives values for exponents which were not calculated numerically.

As mentioned above, the numerical solution was obtained by relating the pressure to $\rho_2(x_{12})$ via the virial equation. This led to a density which was different from that obtained from using the product property. This is a common occurrence when approximate equations for distribution functions are used.[14]

The RG outlined above provides an interesting insight to this problem. We discuss this in the next section.

III. LINEAR-INTEGRAL-EQUATION RENORMALIZATION-GROUP REVISITED

The fact that the product property was not used in the analysis in the preceding section leads to thermodynamic inconsistencies. For example, the correlation exponent η is not the same when calculated from scaling laws and from the structure factor. To see this we define

$$c(x_{12})=zf(x_{12})\left[z+\int\rho_2(x_{23})f(x_{13})d\vec{x}_3\right]\ , \tag{3.1}$$

where $\rho_2(x_{23})$ is the solution of Eq. (2.3). From Eqs. (2.4) and (3.1) we obtain

$$\rho_2(x_{12})=z^2+c(x_{12})+z\int\rho_2(x_{23})f_{13}d\vec{x}_3\ . \tag{3.2}$$

If we adopt the product property, then, from Eq. (2.3),

$$\rho^2=z^2/[1-zf(0)]\ , \tag{3.3}$$

where

$$f(0)=\int f(x_{12})d\vec{x}_{12}\ . \tag{3.4}$$

Defining

$$h(x_{12})=\rho_2(x_{12})-\rho^2\ , \tag{3.5}$$

Eq. (3.2) becomes

$$h(x_{12})=c(x_{12})+z\int h(x_{13})f(x_{23})d\vec{x}_3\ . \tag{3.6}$$

Taking the Fourier transform of Eq. (3.6) with respect to the x_{12} gives

$$\hat{h}(k)=\hat{c}(k)/[1-z\hat{f}(k)]\ . \tag{3.7}$$

Since $c(x_{12})$ is the finite range for hard spheres, $\hat{c}(k)$ is an analytic function of k. For hard spheres of unit radius in $d=3$,

$$\hat{f}(k)=(4\pi/k^2)\left[\cos k-\frac{\sin k}{k}\right]\ . \tag{3.8}$$

It can easily be shown from Eqs. (3.7) and (3.8) and the analyticity of $c(k)$ that $h(k)$ will be finite for all k and positive z up to $z_0=11.6048\ldots$. At this value of z, $k=k_0\neq 0$. It can also be shown,[15] in the neighborhood of k_0, that $1-zf(k)$ is quadratic in $k-k_0$. Since the structure factor $S(k)$ is proportional to $\hat{h}(k)$, we have

$$S(k)\propto(k-k_0)^{-2}\ . \tag{3.9}$$

This implies that the critical exponent η defined by

$$S(k)\propto(k-k_0)^{-(2-\eta)} \tag{3.10}$$

is zero.

The exponent η was not calculated in either Ref. 9 or 6; however, it can be inferred from the scaling law[12]

$$\gamma/\nu=2-\eta\ . \tag{3.11}$$

With the values of γ and ν both equal to $\frac{1}{2}$, we have $\eta=1$. We justify the use of the scaling law (3.11) by noting that if scaling does not hold then we have no justification for applying a RG. We will return to this point below.

To recapitulate, different paths to thermodynamic exponents lead to different values. This is not unusual when approximate hierarchies or integral equations are used.[16]

The RG technique outlined above can be used to investigate this inconsistency. Application of the RG will lead to a necessary but insufficient condition for approximate equations to have consistent thermodynamics.

We begin the investigation with the standard relationship between the unrenormalized and renormalized free-energy density,[17]

$$f(\{u_n\})=g(\{u_n\})+b^{-d}f'(\{u_n'\})\ , \tag{3.12}$$

where f is any free-energy density, $\{u_n\}$ is the set of scaling fields, g is an analytic function of $\{u_n\}$, b is the rescaling length of the RG transformation, and primes denote renormalized quantities.

As we have seen above, the linearized scaling field for the critical phenomena associated with Eq. (2.3) is proportional to $z-z_c$. Writing $z=e^{\beta_0\mu}$, it is straightforward to see that $z-z_c$ is proportional to $\mu-\mu_c=\Delta\mu$ where μ is the chemical potential and β_0 is fixed. The RG which we used imposed the restriction that the singular part of the distribution function $\rho_{2s}(x_{12})$ remains invariant under the RG transformation. The product property would then imply that the singular part of the density also remains invariant under the RG. However,

$$\rho_s=\frac{\partial f_s}{\partial\mu}\ , \tag{3.13}$$

where f_s is the singular part of the free-energy density. From Eq. (3.12),

$$f_s(\Delta\mu)=(1/b^d)f_s'(\Delta\mu')\ . \tag{3.14}$$

We must also have

$$\rho_s'=\frac{\partial f_s'}{\partial\mu'}\ . \tag{3.15}$$

Equations (3.13)–(3.15), together with the restriction that $\rho_s=\rho_s'$, give

$$\frac{\partial f_s'}{\partial\mu'}=\frac{b^d}{b^2}\frac{\partial f_s}{\partial\mu}\ . \tag{3.16}$$

Therefore, for consistency $d=2$. We return to this point below. Since the eigenvalues and rescaling length associated with the RG transformation applied to Eq. (2.3) are independent of dimension, it is straightforward to obtain

$$\gamma=1,\ \ \nu=\tfrac{1}{2},\ \ \eta=0,\ \ \beta=0\ . \tag{3.17}$$

The exponent η is now in agreement with the exact calculation. The exponent ν can also readily be obtained from the inverse Fourier transform of Eq. (3.7) and is $\frac{1}{2}$, which is also in agreement with the value in Eq. (3.17). No one has, to our knowledge, solved Eq. (2.3) in $d=2$ with the Swendsen-Klein method. It is clear, however, that the RG calculation is now consistent with the solution employing the product property.

Another useful application of the RG is to allow us to define a fractal dimension[18] for the fluctuations at the phase transition. The fractal dimension can be defined (e.g., in percolation[19,20]) by relating a volume to a length. For example, the volume of the incipient percolation cluster N can be related to the connectedness or correlation length ξ by

$$N\propto\xi^{d_f}\ . \tag{3.18}$$

The fractal dimension, in turn, can be related to the percolation exponent ν_p and β_p by[19]

$$d_f^p=d-\beta_p/\nu_p\ . \tag{3.19}$$

Coniglio and Klein[21] have shown that a fractal dimension can also be assigned to fluctuations at the Ising critical point by first mapping the Ising transition onto a percolation problem. This results in a fractal dimension of

$$d_f=d-\beta/\nu\ , \tag{3.20}$$

where β and ν are now the order parameter and correlation length exponents, respectively, of the Ising transition. A fractal dimension can also be defined from our RG as follows.

We have seen above that $z-z_c$ is proportional to $\mu-\mu_c$. This, together with Eqs. (2.19) and (2.21), implies that

$$\Delta\mu'=b^2\Delta\mu\ . \tag{3.21}$$

Now, the singular part of the free energy F [as opposed to the free-energy density in Eq. (3.12)] is invariant under the RG, i.e.,

$$F_s(u)=F_s(u')\ . \tag{3.22}$$

Taking the derivative

$$\lim_{\Delta\mu\to 0}(\Delta F_s/\Delta\mu)=\langle N\rangle_s\ , \tag{3.23}$$

we obtain the singular part of the mean number of particles. $\langle N\rangle_s$ can be interpreted as the mean number of particles in a volume with a linear dimension of the order of the correlation length ξ. The singular part of the density is then

$$\rho_s=\langle N\rangle_s/\xi^{d_f}\ , \tag{3.24}$$

where ξ^{d_f} is the "fractal volume." From Eqs. (3.21)–(3.23) and the relation

$$\lim_{\Delta\mu'\to 0} (\Delta F_s' / \Delta\mu') = \langle N_s \rangle' , \tag{3.25}$$

we can infer that

$$\langle N_s \rangle' = \langle N_s \rangle / b^2 . \tag{3.26}$$

Since ρ_s is invariant under the RG, we must have

$$(\langle N_s \rangle / b^2)/(\xi/b)^{d_f} = \langle N_s \rangle / \xi^{d_f} , \tag{3.27}$$

which implies $d_f = 2$. For Eq. (2.3), therefore, in $d=2$, $d_f = d$.

This is consistent with $\beta = 0$ and implies that the phase transition in the system described by Eq. (2.3) is pathological in that it has features of one-dimensional (i.e., $\beta = 0$, $d_f = d$) transitions.

We will see, however, that this method of obtaining a fractal dimension readily generalizes to equations with more standard transitions and nontrivial fractal dimensions.

IV. RENORMALIZATION-GROUP ANALYSIS OF THE ORNSTEIN-ZERNIKE EQUATION

The position-space RG introduced above may be used to obtain information about the singular behavior of other (perhaps more familiar) linear integral equations. First, we derive general expressions for the critical exponents and fractal dimension from the Ornstein-Zernike (OZ) equation,[22] which for spherically symmetric potentials is

$$h(x_{12}) = c(x_{12}) + \rho \int h(x_{23}) c(x_{13}) d\vec{x}_3 , \tag{4.1}$$

where ρ is the density, $c(x_{12})$ is the direct correlation function, $h(x_{12}) = g(x_{12}) - 1$, and $g(x_{12})$ is the pair correlation function. Equation (4.1) is "exact" but devoid of content: Physical insight or other means must be used to specify another equation ("closure") that relates $c(x_{12})$ to $h(x_{12})$. For example, the assumption that $c(x_{12})$ is short ranged (i.e., $\int |c(x_{12})| d\vec{x}_{12} < \infty$) and analytic at the critical point leads to mean-field critical exponents.

The assumption made in this section is that

$$\hat{c}(k) = \int c(x_{12}) e^{-i\vec{k}\cdot\vec{x}_{12}} d\vec{x}_{12} < \infty \tag{4.2}$$

for all wave vectors $\vec{k}$. In the neighborhood of a critical point, we take the leading terms of the Fourier transform of the direct correlation function to be

$$\rho\hat{c}(k=0) = A + (\Delta\rho)^x + (\Delta T)^y , \tag{4.3}$$

where x and y can be any real numbers. In contrast to the OZ mean-field assumption of analyticity, we have taken

$$\rho_c \hat{c}(k) - 1 \approx k^{2-\eta} \tag{4.4}$$

in the vicinity of $k=0$, where ρ_c is the density at the critical point. It follows that η has its standard meaning as the correlation function exponent, since the usual definition

$$\hat{h}(k) \approx k^{-(2-\eta)} , \tag{4.5}$$

and the Fourier transform of Eq. (4.1),

$$\hat{h}(k) = \hat{c}(k)/[1 - \rho\hat{c}(k)] , \tag{4.6}$$

together, imply Eq. (4.4), given that $h(k=0) \to \infty$, but $c(k=0) < \infty$ at the critical point.

The difference in applying position-space RG to lattice systems and to integral equations is now clear. In lattice systems, the specification of the spatial dimension d and the exponents x and y, along with hyperscaling (which is implicit in the RG), uniquely determines all critical exponents. In integral equations, however, the rescaling length is not defined by the RG transformation. We will see below that, in our analysis, fixing b is equivalent to fixing η.

If *in addition to* the Ornstein-Zernike equation we *also* demand (reasonably enough) that the free energy remains invariant under the RG, we will be able to obtain all critical exponents by specifying the exponent y and *either* η or x.

As an example we return briefly to the Kirkwood-Salsburg equation. We can now see that choosing $f(x_{12})$ to be the hard-sphere Mayer function in Eq. (2.3) forces $\eta = 0$. This choice also fixes the dependence of the scaling field $z\hat{f}(k)$ on z. Since there is only *one* relevant scaling field at spinodals, this choice of $f(x_{12})$ fixes all three exponents—x, y, and η. If the standard free-energy rescaling is also invoked, as it is in Eq. (3.12), this reduces the number of free parameters in the analysis by one. However, since the spatial dimensionality d was the only remaining parameter, the effect of the free-energy rescaling condition is to fix it (to the value $d=2$).

For the OZ equation at the critical point (where there are two relevant scaling fields), the reduction by one in the number of free parameters due to the free-energy rescaling condition simply links x and y. We emphasize that this does *not* follow from the OZ equation alone.

The RG for the OZ equation is generated by iteration, just as in Eq. (2.3). Since at the critical point $h_s(x_{12})$, the singular part of $h(x_{12})$, remains invariant under the RG, we obtain

$$\rho' c'(x_{12}) = \rho^2 \int c(x_{23}) c(x_{13}) d\vec{x}_3 . \tag{4.7}$$

There are two key remarks arising from this equation.

(1) Since the asymptotic limit of $h_s(x_{12})$ is zero, rather than some function of the density [as is the limit of the distribution function $\rho_2(x_{12})$], the invariance under the RG of $h_s(x_{12})$ does not necessarily imply the invariance of ρ_s, the singular contribution to the density.

(2) In the OZ equation, $c(x_{12})$ is the inhomogeneous term as well as the kernel of the integral equation. Since $c(x_{12})$ is not assumed to be analytic, the inhomogeneous term will also be singular. However, in the following analysis we will treat $c(x_{12})$ as if it were nonsingular when it contributes to the inhomogeneous term. From Eq. (4.6), it is clear that the divergence of $h(k)$ (related to the susceptibility) is governed by the zeros of $1 - c(k)$, and has nothing to do with the nonanalyticity of $c(k)$ (which is, by assumption, finite). Consequently, to describe the long-wavelength fluctuations which cause the divergent susceptibility (isothermal compressibility), we

do not need to explicitly consider the inhomogeneous term. In other words, if $c(k)$ were replaced in the *numerator* of Eq. (4.6) by an analytic function, the critical exponents would be unchanged.

We now return to the question of how to determine the independent scaling fields, which was first mentioned in Sec. II. This discussion also leads to the evaluation of the matrix $\underline{M}$ which defines the RG transformation linearized about the singular fixed point. It is convenient to Fourier-transform Eq. (4.7) and rewrite it as

$$\ln[\rho'\hat{c}(k')]=2\ln[\rho\hat{c}(k)] \ . \tag{4.8}$$

As an illustration of the analysis we return once again to the Kirkwood-Salsburg equation and the analogous Eq. (2.9), $\ln[z'f(k')]=2\ln[zf(k)]$. Expanding $zf(k)$ about the fixed points $z=z_c$ and $k=k_c$, we obtain

$$a_1(z'-z_c)+a_2(k'-k_c)^2=2[a_1(z-z_c)+a_2(k-k_c)^2], \tag{4.9}$$

where $a_1=f(k_c)$ and $a_2=z_c$. Differentiating both sides of Eq. (4.9) with respect to z and k, we obtain

$$a_1\frac{\partial z'}{\partial z}+2a_2\frac{\partial k'}{\partial z}(k'-k_c)=2a_1 \ , \tag{4.10}$$

$$a_1\frac{\partial z'}{\partial k}+2a_2\frac{\partial k'}{\partial k}(k'-k_c)=4(k-k_c)a_2 \ . \tag{4.11}$$

We have four unknown derivatives and only two equations. However, if we assume that we have constructed a "proper" RG, then z' and k' are analytic functions[3] of z and k. This implies that $\partial k'/\partial z$ and $\partial k'/\partial k$ are finite. At the fixed point ($k'=k_c$),

$$\left.\frac{\partial z'}{\partial z}\right|_{k=k_c,z=z_c}=2 \tag{4.12}$$

and

$$\left.\frac{\partial z'}{\partial k}\right|_{k=k_c,z=z_c}=0 \ . \tag{4.13}$$

From Eqs. (4.11) and (4.13), we have

$$\left.\frac{\partial k'}{\partial k}\right|_{k=k_c,z=z_c}\lim_{k\to k_c}\left[\frac{k'-k_c}{k-k_c}\right]=2 \ , \tag{4.14}$$

and hence

$$\left[\frac{\partial k'}{\partial k}\right]^2=2 \ . \tag{4.15}$$

From Eqs. (4.12), (4.13), and (4.15), the RG matrix $\underline{M}$ evaluated at the fixed point is of the form

$$\underline{M}=\begin{bmatrix}2 & 0\\ \dfrac{\partial k'}{\partial z} & \sqrt{2}\end{bmatrix} . \tag{4.16}$$

Such a matrix, which is of the same form as simple two-parameter RG matrices at the Ising critical point, justifies the equations $\Delta k'=\sqrt{2}\,\Delta k$ and $\Delta z'=2\,\Delta z$ used in Sec. II. From the structure of Eq. (4.9), a linearized RG with $z-z_c$ and $k-k_c$ as scaling fields must have this form.

For the Ornstein-Zernike equation, the linearized RG transformation matrix may be obtained in an analogous way. Recall that near the critical point we have assumed that $c(k)$ has the form

$$\hat{c}(k)=A+B(\Delta\rho)^x+C(\Delta T)^y+D(\Delta k)^{2-\eta} \ , \tag{4.17}$$

where, from Eq. (4.8), $A=1/\rho_c$. Inserting Eq. (4.17) into Eq. (4.8) and linearizing, we obtain

$$B(\Delta\rho')^x+C(\Delta T')^y+D(\Delta k')^{2-\eta}=2[B(\Delta\rho)^x+C(\Delta T)^y+D(\Delta k)^{2-\eta}] \ . \tag{4.18}$$

We first assume that $x<y<2-\eta$ and treat the case where two or more exponents are equal below. We will also assume that all derivatives of the form $\partial T'/\partial\rho$, $\partial T'/\partial k$, etc., are finite (possibly zero). Differentiating both sides of Eq. (4.18) with respect to ρ, T, and k gives

$$xB\frac{\partial\rho'}{\partial\rho}(\Delta\rho')^{x-1}+yC\frac{\partial T'}{\partial\rho}(\Delta T')^{y-1}+(2-\eta)D\frac{\partial k'}{\partial\rho}(\Delta k')^{1-\eta}=xBb^{2-\eta}(\Delta\rho)^{x-1} \ , \tag{4.19a}$$

$$xB\frac{\partial\rho'}{\partial T}(\Delta\rho')^{x-1}+yC\frac{\partial T'}{\partial T}(\Delta T')^{y-1}+(2-\eta)D\frac{\partial k'}{\partial T}(\Delta k')^{1-\eta}=yCb^{2-\eta}(\Delta T)^{y-1} \ , \tag{4.19b}$$

$$xB\frac{\partial\rho'}{\partial k}(\Delta\rho')^{x-1}+yC\frac{\partial T'}{\partial k}(\Delta T')^{y-1}+(2-\eta)D\frac{\partial k'}{\partial k}(\Delta k')^{1-\eta}=(2-\eta)Db^{2-\eta}(\Delta k)^{1-\eta} \ , \tag{4.19c}$$

where we have defined b from the equation $b^{2-\eta}=2$. This is a natural definition in light of Eqs. (2.20) and (4.4). Dividing both sides of Eq. (4.19a) by $(\Delta\rho')^{x-1}$, we obtain

$$xB\frac{\partial\rho'}{\partial\rho}+yC\frac{\partial T'}{\partial\rho}\frac{(\Delta T')^{y-1}}{(\Delta\rho')^{x-1}}+(2-\eta)D\frac{\partial k'}{\partial\rho}\frac{(\Delta k')^{1-\eta}}{(\Delta\rho')^{x-1}}=xBb^{2-\eta}\left[\frac{\Delta\rho}{\Delta\rho'}\right]^{x-1} . \tag{4.20}$$

Since all derivatives are assumed finite and $2-\eta>y>x$, we must have

$$\frac{(\Delta T')^{y-1}}{(\Delta\rho')^{x-1}}=\frac{(\Delta k')^{1-\eta}}{(\Delta\rho')^{x-1}}=0$$

in the limit $\Delta\rho\to 0$. Since

$$\lim_{\Delta\rho\to 0}\frac{\Delta\rho'}{\Delta\rho}=\frac{\partial\rho'}{\partial\rho} \ ,$$

Eq. (4.20) implies that

$$\frac{\partial\rho'}{\partial\rho}=b^{(2-\eta)/x} \ . \tag{4.21}$$

We now divide both sides of Eq. (4.19b) by $(\Delta T')^{y-1}$ to obtain

$$xB\frac{\partial\rho'}{\partial T}\frac{(\Delta\rho')^{x-1}}{(\Delta T')^{y-1}}+yC\frac{\partial T'}{\partial T}+(2-\eta)D\frac{\partial k'}{\partial T}\frac{(\Delta k')^{1-\eta}}{(\Delta T')^{y-1}}$$
$$=yCb^{2-\eta}\left[\frac{\Delta T}{\Delta T'}\right]^{y-1} . \tag{4.22}$$

Employing the assumption that all derivitives are finite, we obtain the result that all terms except $(\Delta\rho')^{x-1}/(\Delta T')^{y-1}$ are finite. This implies that $\partial\rho'/\partial T=0$. Since $(\Delta k')^{1-\eta}/(\Delta T')^{y-1}$ approaches zero as $\Delta T'\rightarrow 0$, we obtain

$$\frac{\partial T'}{\partial T}=b^{(2-\eta)/y} \tag{4.23}$$

Application of such arguments to Eq. (4.19c) leads to the result that $\partial\rho'/\partial k=0$, $\partial T'/\partial k=0$, and

$$\frac{\partial k'}{\partial k}=b , \tag{4.24}$$

where, from above, $b=2^{1/(2-\eta)}$.

From the above discussion the matrix $\underline{M}$, which is the RG transformation linearized about the fixed point, has the form

$$\underline{M}=\begin{bmatrix} b^{(2-\eta)/x} & 0 & 0 \\ \dfrac{\partial T'}{\partial\rho} & b^{(2-\eta)/y} & 0 \\ \dfrac{\partial k'}{\partial\rho} & \dfrac{\partial k'}{\partial T} & b \end{bmatrix} . \tag{4.25}$$

This matrix applies to the case $x<y<2-\eta$. As long as no two exponents are exactly equal, changing the order of the exponents in the inequality simply permutes the nonzero off-diagonal elements of the matrix, with no change in the physics.

We now treat the case where two of the exponents x, y, and $2-\eta$ have the same value. This is exactly the situation in the truncated Kirkwood-Salsburg equation (2.3), where Δz and Δk enter with the same power (unity). The RG transformation, Eq. (2.19), for this integral equation has a fixed point whenever $z\hat{f}(k)=1$. We have already identified $z_c=11.0648$ as the singular value of z. In addition, for $z>z_c$ other special values k^* exist for which $z\hat{f}(k^*)=1$, and these values fall into two classes. For the first class, $\hat{f}(k)$ is quadratic for k in the neighborhood of k^*, and the *number* of solutions to $z\hat{f}(k)=1$ changes. For example, at the point $z=11.0648$ and $k=k_0$, the number of solutions increases from zero to one at $z=z_c$, and from zero to two for $z>z_c$.

The second class of values k^* form a continuum of solutions for which $z\hat{f}(k)=1$, but no new solutions appear, and for which $\hat{f}(k)$ is linear for k near k^*. In this region Δk and Δz enter with the same power and there is a *line* of fixed points in the RG. Such a line of fixed points has only one relevant scaling field, namely the scaling field associated with moving away from the line of fixed points. Hence, if, for example, x and y in Eq. (4.17) have the same value, then $\Delta\rho$ and ΔT are not separate scaling fields. The only scaling field is a linear combination of $(\Delta\rho)^x$ and $(\Delta T)^y$. This case is further discussed below.

We may now complete the task of relating critical exponents to the parameters x, y, and $2-\eta$.

A. Correlation-length exponent ν

From Eq. (4.25) we have

$$\Delta T'=b^{(2-\eta)/y}\Delta T . \tag{4.26}$$

From

$$\xi'=\xi/b \tag{4.27}$$

and Eq. (4.26), we have

$$\nu=y/(2-\eta) . \tag{4.28}$$

B. Order-parameter exponent β

From Eq. (4.25) we have

$$\Delta\rho'=b^{(2-\eta)/x}\Delta\rho . \tag{4.29}$$

Since $\Delta\rho'\sim(\Delta T)^{\beta}$, from Eqs. (4.26) and (4.29) we obtain

$$(b^{(2-\eta)/y}\Delta T)^{\beta}=b^{(2-\eta)/x}(\Delta T)^{\beta} , \tag{4.30}$$

which implies

$$\beta=y/x . \tag{4.31}$$

C. Specific-heat exponent α

In order to calculate the specific-heat exponent we must make use of Eq. (3.14), which we rewrite in terms of the temperature variable setting $\Delta\rho=\Delta k=0$,

$$f_s(\Delta T)=\frac{f_s'(\Delta T')}{b^d} , \tag{4.32}$$

The singular part of the specific heat c_s has the form

$$c_s\sim(\Delta T)^{1-\alpha} , \tag{4.33}$$

and is given by

$$c_s\sim\frac{\partial f_s(\Delta T)}{\partial T} . \tag{4.34}$$

From Eqs. (4.26) and (4.32)–(4.34), it is a straightforward procedure to obtain

$$(\Delta T)^{1-\alpha}=\frac{b^{(2-\eta)/y}}{b^d}(b^{(2-\eta)/y}\Delta T)^{1/\alpha} , \tag{4.35}$$

which yields

$$\alpha=2-dy/(2-\eta) . \tag{4.36}$$

With Eq. (4.28) this becomes

$$d\nu=2-\alpha , \tag{4.37}$$

as expected.

D. Compressibility exponent γ

Returning again to Eq. (3.14), but using the variables $\Delta\rho$ and ΔT, we have

$$f_s(\Delta\rho,\Delta T)=\frac{1}{b^d}f_s'(\Delta\rho',\Delta T') . \tag{4.38}$$

The compressibility χ_T is proportional to the inverse of $\partial^2 f_s/\partial\rho^2$ and diverges as

$$\chi_T \sim (\Delta T)^{-\gamma} . \tag{4.39}$$

From Eqs. (4.26), (4.29), (4.38), and (4.39) we obtain

$$(\Delta T)^{\gamma}=\frac{b^{2(2-\eta)/x}}{b^d}(b^{(2-\eta)/y}\Delta T)^{\gamma} . \tag{4.40}$$

This implies that

$$\gamma=\frac{d-(2-\eta)/x}{(2-\eta)/y} . \tag{4.41}$$

As a check it is useful to note that the exponents α, β, and γ as defined in Eqs. (4.31), (4.36), and (4.41), respectively, satisfy the equality

$$\alpha+2\beta+\gamma=2 . \tag{4.42}$$

We now turn to the question of the fractal dimension at the phase transition. At the transition the density is ρ_c. Fluctuations in the density away from this value are of a linear dimension approximately equal to the correlation length. The difference, then, between the average density ρ_c and the density ρ should be a measure of the density of a critical fluctuation. We then have

$$\Delta\rho=\rho-\rho_c=N/\xi^{d_f} , \tag{4.43}$$

where ξ is the correlation length and d_f is the "dimension" of the critical fluctuation. After renormalization,

$$\Delta\rho'=\rho'-\rho_c=N'/(\xi')^{d_f} . \tag{4.44}$$

Since $N'=N/b^{2-\eta}$ in this RG, and $\xi'=\xi/b$, we have, with Eq. (4.29),

$$\frac{N/b^{2-\eta}}{\xi^{d_f}/b^{d_f}}=b^{(2-\eta)/x}\frac{N}{\xi^{d_f}} . \tag{4.45}$$

This implies that

$$d_f=(2-\eta)/x+2-\eta . \tag{4.46}$$

Note that this implies that ΔV, the singular part of the volume, transforms as

$$\Delta V'=\Delta V/b^{d_f} . \tag{4.47}$$

From Eqs. (4.28) and (4.31), d_f becomes

$$d_f=\beta/\nu+2-\eta . \tag{4.48}$$

It is interesting to note that the expression for d_f given in Eq. (4.48) is independent of the validity of Eq. (3.14), and therefore may be a better expression for *approximate* equations. As we will see below, for exact equations, the d_f defined in Eq. (4.48) is completely equivalent to the standard definitions.

We should also mention the existence of a second fractal dimension defined through the RG. Since we demand that the correlation function remain invariant under the RG and that its Fourier transform $S(k)$ diverge as $\Delta k^{-(2-\eta)}$, this implies that the volume element $d\vec{x}$ in

$$S(k)\propto(\Delta k)^{-(2-\eta)}\propto\int e^{-i\vec{k}\cdot\vec{x}}h(x)d\vec{x}$$

must transform as

$$d\vec{x}\,'=d\vec{x}/b^{2-\eta} , \tag{4.49a}$$

which implies a fractal dimension of $2-\eta$. With the scaling relation $\gamma/\nu=2-\eta$ derived below, this fractal dimension is equivalent to the one defined by Stanley[19] in the percolation problem.

The two fractal dimensions have different physical interpretations. One can, as in percolation, interpret $d-\beta/\nu$ as the fractal dimension of the ordered phase. It is, for example, the fractal dimension of the liquid as one approaches the liquid-gas critical point. This is consistent with the mapping of the percolation problem onto the Ising critical problem.[21]

The fractal γ/ν is related through the Fourier transform of the pair correlation function minus 1 [i.e., $h(x)$] to the fluctuations about the ordered phase (that is, to the finite fluctuations). This, again, is in analogy to what is done in percolation.[19,20]

Finally, in this section we discuss the implications and validity of the free-energy scaling assumption, Eq. (3.14). In our present formulation, three parameters are necessary to specify critical exponents: x, y, and $2-\eta$. The quantity $2-\eta$ is necessary to set the rescaling length through

$$b^{2-\eta}=n , \tag{4.49b}$$

where $1/n$ is the fraction of particles decimated (in the examples in this manuscript, $n=2$), and to specify the fractal dimension. At this point in the development, $2-\eta$ is different from the other critical exponents in that it is not a function of x and y. However, after applying the free-energy rescaling condition (3.14), we shall see that $2-\eta$ is a function of x and the spatial dimension d.

We begin by determining how the singular part of the pressure p transforms under the RG transformation. Equation (3.14) is, of course, exactly the statement that the singular part of the free energy is invariant under the RG [i.e., Eq. (3.22)].[3] Since

$$p-p_c\equiv\Delta p=\frac{\partial F_s}{\partial v}=\lim_{\Delta V\to 0}\frac{\Delta F_s}{\Delta V} , \tag{4.50}$$

the singular part of the pressure transforms as

$$\Delta p'=b^{d_f}\Delta p .$$

We now rewrite Eq. (3.14) using Δp as the scaling field,

$$f_s(\Delta p)=(1/b^d)f_s'(b^{d_f}\Delta p) . \tag{4.51}$$

However, the singular part of the density is related to $f_s(\Delta p)$ by

$$\rho-\rho_s=\Delta\rho=\frac{\partial f_s(\Delta p)}{\partial p} . \tag{4.52}$$

Equations (4.51) and (4.52) imply that

$$\Delta\rho'=b^{d-d_f}\Delta\rho . \tag{4.53}$$

From Eqs. (4.29), (4.46), and (4.53) we obtain

$$d-[(2-\eta)/x]-2-\eta=(2-\eta)/x , \tag{4.54}$$

or

$$2-\eta=dx/(2+x)\ . \tag{4.55}$$

Note that this expression for $2-\eta$, together with Eqs. (4.28) and (4.41) imply the scaling law

$$\gamma/\nu=2-\eta\ . \tag{4.56}$$

This, in turn, implies that

$$d_f=(\beta+\gamma)/\nu\ . \tag{4.57}$$

From Eqs. (4.37), (4.42), and (4.57) we obtain

$$d_f=d-\beta/\nu\ . \tag{4.58}$$

The imposition of invariance of the free energy under the RG transformation, together with known thermodynamic identities, has imposed a relation between x, $2-\eta$, and d. The critical exponents are now specified by x, y, and d. As noted above, this occurs only after the imposition of relationships outside the initial integral equation.

Here, we should point out that if η is fixed independent of d, then x is fixed by the dimension. This often happens when *ad hoc* choices are made for the direct correlation function. Examples of such choices are the Ornstein-Zernike assumption of a short-ranged $c(r)$ and the truncated Kirkwood-Salsburg equation studied in Sec. II. If, as for the truncated Kirkwood-Salsburg equation, the parameter x is also fixed, then there is only one dimension in which the solution of the Ornstein-Zernike equation yields consistent thermodynamics.

We also note that if $\eta=0$ then Eq. (4.55) can be written as

$$4=(d-2)x\ . \tag{4.59}$$

If $d=2$ then $x=\infty$ and we have $\beta=0$ and $d_f=2=d$. Since $\beta=0$ usually describes a first-order transition, it would seem that $\eta=0$ and $d=2$ are mutually exclusive with critical points or, alternatively, that the standard scaling approach to such transitions must be modified. This result can, of course, be obtained from standard hyperscaling relations.[3] Again, this inconsistency cannot be seen from the integral equation alone, but requires the imposition of free-energy scaling, Eq. (3.14).

Only discussion of the volume rescaling remains. Note that in Eq. (3.14), $f(\{u_n\})$ is the free energy per unit volume. The factor b^d arises from rescaling the volume; that is, the renormalized volume V' is related to V by

$$V'=V/b^d\ . \tag{4.60}$$

Two points must be made. First, there is more than one volume to rescale. One is the critical volume, which is roughly the size of the critical fluctuation and is rescaled by a factor b^{d_f} [see Eq. (4.45)], and the other is the volume of the system which rescales with a factor b^d. Second, in standard approaches to position-space RG,[3] the factor b^d is related to the rescaling of the degrees of freedom. Thus, for example, in a lattice system such as an Ising model one decimates every other spin so that the number of lattice spins N is reduced by a factor of 2, that is

$$N'=N/2\ , \tag{4.61}$$

where N' is the renormalized number of spins. To keep the lattice invariant under the RG we must have

$$N'/V'=N/V\ , \tag{4.62}$$

which implies, from Eqs. (4.50) and (4.61), that

$$b^d=2\ . \tag{4.63}$$

In our case we have decimated every second particle and have therefore also reduced the number of particles N by a factor of 2. However, from the relation $b^{2-\eta}=2$ [see discussion after Eq. (4.19c)], we have

$$b^d=2^{d/(2-\eta)}\ . \tag{4.64}$$

Consequently, the relation between the volume rescaling and the scaling of the degrees of freedom is somewhat more complicated in this case. It is interesting to note that when $d=2-\eta$ so that $b^d=2$, this implies, from Eq. (4.55), that $x=\infty$. This, in turn, implies, from Eq. (4.31), that $\beta=0$ and, from Eq. (4.58), that $d_f=d$. It must also be noted that this rescaling is determined by how k rescales and k is a relevant variable. At the fixed point, $k=k_c$ so that $\Delta k=0$, and the k variable cannot be used to determine how lengths rescale. Consequently, at the fixed point one is free to choose, and one for consistency, must choose $b^d=2$.

Finally, we explicitly state what has been said implicitly in the above discussion and elsewhere.[6] In most RG transformations the way that lengths are rescaled is part of the definition of the transformation and is fixed by the transformation. For our analysis of integral equations for fluids this is not so: the length rescaling depends on the values of the renormalized variables. The results of this section are summarized in Table I.

As a simple example we study the *linear* integral equation of most interest, which follows from the OZ equation by assuming that $c(r)$ is short ranged and that the Fourier transform of $c(r)$ is analytic in $\Delta\rho=\rho-\rho_c$ and $\Delta T=T-T_c$, and, in fact, linear in ΔT as $T\rightarrow T_c$. In the above langauge this implies $\eta=0$ and $y=1$. From the general results, we obtain

$$x=4/(d-2)\ . \tag{4.65}$$

The critical exponents are then

$$\eta=0,\ \ \gamma=1,\ \ \nu=\tfrac{1}{2},\ \ \beta=(d-2)/4,\ \ \alpha=2-d/2\ . \tag{4.66}$$

In this form of mean-field theory, spinodal lines will be evident when there is only one relevant scaling field, which here means $x=1$. Hence the spinodal exponents are

$$\gamma=1,\ \ \nu=\tfrac{1}{2},\ \ \beta=1,\ \ \alpha=-1\ , \tag{4.67}$$

and hyperscaling holds only in $d=6$. These are, of course, the known results of the mean-field theory of spinodals (but see Ref. 23 for a discussion of the proper form of the scaling field and the exponents).

For a mean-field description of the critical point (two relevant scaling fields) we must have $x\neq y$. With the natural choice, $x=2$, we find an upper critical dimension

TABLE I. Exponents in the position-space renormalization group for fluids. $\rho_c(k,\rho,T)=A+B(\rho-\rho_c)^x+C(T-T_c)^y+Dk^{2-\eta}$, for $\rho-\rho_c$, $T-T_c$, and $k\to 0$.

Exponent	Equation	Mean-field critical point	Mean-field spinodal point
y		1	1
x		2	1
η	$2-\eta=dx/(2+x)$	0	0
d		4	6
ν	$y/(2-\eta)$	$\frac{1}{2}$	$\frac{1}{2}$
β	y/x	$\frac{1}{2}$	1[a]
α	$2-dy/(2-\eta)$	0	-1
γ	y	1	1
δ	$1+x$	4	2
d_f	$(2-\eta)(1+1/x)$	3	4

[a] At a spinodal point the correct scaling field is $(T-T_c)^2$, and hence the correct exponent is $\beta=\frac{1}{2}$ (see Ref. 23).

of $d=4$ and the correct mean-field critical exponents

$$\gamma=1,\quad \nu=\tfrac{1}{2},\quad \beta=\tfrac{1}{2},\quad \gamma=0\ . \tag{4.68}$$

The other integral equations of interest in the theory of fluids are invariably nonlinear in $c(r)$. Generalization of the position-space RG to treat such nonlinear equations is feasible but nontrivial.

V. TOWARD A RENORMALIZATION GROUP FOR NONLINEAR INTEGRAL EQUATIONS

We now extend our position-space RG method to treat a relatively simple nonlinear integral equation, which arises in the mean-field theory of metastable liquids. Grewe and Klein have shown[24] that for infinite-range, positive definite potentials of the form $\gamma^d\psi(\gamma r)$ in the limit $\gamma\to 0$, the single-particle density $\rho_1(x)$ is a solution of the equation

$$\rho_1(x)=z\exp\left[-\beta\int\rho_1(y)\psi(|\vec{x}-\vec{y}|)d\vec{y}\right], \tag{5.1}$$

where again z is the activity.

For the physically relevant region $z\geq 0$ and $\beta\geq 0$, it is easy to prove[24] that the constant function $\rho_1(x)=\rho$ is always a solution of Eq. (5.1). Furthermore, for any fixed β there is a minimum value of z where the solution of Eq. (5.1) bifurcates. This bifurcation point has been shown[24] to be related to a "spinodal" in this kind of mean-field theory, with classical spinodal exponents.[12] Here we derive these exponents very quickly using our RG procedure.

We begin by writing

$$\rho_1(x)=\rho+\phi(\vec{x})\ , \tag{5.2}$$

which is substituted into Eq. (5.1) to yield

$$\rho+\phi(x)=\rho\exp\left[-\beta\int\phi(\vec{y})\psi(|\vec{x}-\vec{y}|)d\vec{y}\right]. \tag{5.3}$$

Since the "spinodal" is associated with a true ("soft") bifurcation, Eq. (5.3) can be expanded about the bifurcation point, for small $\phi(x)$, to give

$$\phi(x)=-\beta\rho\int\phi(\vec{y})\psi(|\vec{x}-\vec{y}|)d\vec{y}\ . \tag{5.4}$$

The RG method can now be applied directly to the linearized equation (5.4). Since the kernel of the equation is now $\beta\rho\psi(x-y)$, we find, by direct comparison with the OZ equation treated in Sec. IV, that the present equation leads to $x=1$ and $y=1$. Hence we obtain the exponents

$$\beta=y/x=1,\quad \gamma=y=1\ ,$$

$$\delta=1+x=2,\quad 2-\eta=dx/(x+2)=d/3\ .$$

These exponents have also been obtained with much greater effort by other methods.[12] The exponent η depends on the dimension d. Consideration of information beyond $\rho_1(\vec{x})$, namely the structure factor,[12] leads to $\eta=0$ and $d=6$. Hence Eq. (5.1) leads to the set of mean-field "spinodal" exponents.

VI. CONCLUSIONS

We have presented a formulation of the position-space RG technique that can be used to obtain the singular behavior of the solutions to several types of integral equations. This technique is comprised of two operations, iteration and decimation. For integral equations in fluids, unlike most lattice systems, the specification of these two operations does *not* determine the rescaling length b. However, by invoking the natural free-energy rescaling condition, the RG for fluids generates sets of critical exponents.

It is important to note that *given* an ansatz for $c(r)$ in the Ornstein-Zernike equation, there may be only certain spatial dimensions where the usual scaling and hyperscaling laws hold. This behavior is found explicitly for certain examples in Sec. IV, and entirely analogous behavior occurs in the truncated Kirkwood-Salsburg equation described in Sec. III. In these examples, the choice of the kernel in the integral equation is "mean-field-like," insofar as hyperscaling holds only in one spatial dimension.

The RG also leads to one natural way to define "fractal dimensions" at a fluid phase transition, and these are shown to be intimately related to fractal dimensions which have been defined in lattice systems and percolation problems.

ACKNOWLEDGMENTS

We would like to thank C. Unger and G. Stell for stimulating discussions. One of us (W.K.) would like to thank R. Swendsen and K. A. Mueller for their hospitality at IBM Research Laboratories, Zürich. We also thank D. R. Nelson of the Lyman Laboratory of Physics, Harvard University, where part of this work was started. At Harvard University this work was supported by the (U.S.) National Science Foundation (NSF), in part through the Harvard University Materials Research Laboratory, and also through Grant No. DMR-82-07431. At Boston University this work was supported in part by NSF Grant No. DMR-82-15648.

---

[*] Present address: Department of Physics, Harvard University, Cambridge, MA 02138. Permanent address: Center for Polymer Studies and Department of Physics, Boston University, Boston, MA 02215.

[1] K. G. Wilson, Phys. Rev. B **4**, 3174 (1971); **4**, 3184 (1971).

[2] K. G. Wilson and J. Kogut, Phys. Rep. C **12**, 75 (1974).

[3] Th. Neimeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

[4] B. Nienhuis and M. Nauenberg, Phys. Rev. Lett. **35**, 477 (1975); see also M. E. Fisher and A. N. Berker, Phys. Rev. B **26**, 2507 (1982).

[5] W. Klein, D. J. Wallace, and R. K. P. Zia, Phys. Rev. Lett. **37**, 639 (1976).

[6] W. Klein, Phys. Rev. B **27**, 4475 (1983).

[7] A. Sabry, Physica (Utrecht) **54**, 60 (1971).

[8] W. Klein, J. Math. Phys. **14**, 1049 (1973).

[9] R. H. Swendsen and W. Klein, Phys. Rev. A **13**, 872 (1976).

[10] J. G. Kirkwood and Z. W. Salsburg, Discuss. Faraday Soc. **15**, 23 (1953).

[11] H. S. Chung and W. F. Espenschied, Mol. Phys. **14**, 317 (1968); see also H. S. Chung, *ibid.* **16**, 553 (1969).

[12] W. Klein and A. C. Brown, J. Chem. Phys. **74**, 6960 (1981).

[13] T. L. Hill, *Statistical Mechanics* (McGraw-Hill, London, 1956).

[14] P. T. Cummings and G. Stell, J. Chem. Phys. **78**, 1917 (1983).

[15] W. Klein, Ph.D. thesis, Temple University, 1972.

[16] P. T. Cummings and G. Stell, J. Chem. Phys. **78**, 1917 (1983).

[17] Th. Neimeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* Ref. 3, Vol. 6.

[18] B. Mandelbrot, *Fractals: Form, Chance and Dimension* (Freeman, San Francisco, 1977).

[19] Y. Gefen, A. Aharony, B. Mandelbrot, and S. Kirkpatrick, Phys. Rev. Lett. **47**, 1771 (1981).

[20] H. E. Stanley, J. Phys. A **10**, L211 (1977).

[21] A. Coniglio and W. Klein, J. Phys. A **13**, 2775 (1980).

[22] L. S. Ornstein and F. Zernike, Proc. Akad. Sci. (Amsterdam) **17**, 793 (1914), reprinted in *The Equilibrium Theory of Classical Fluids,* edited by H. L. Frisch and J. L. Lebowitz (Benjamin, New York, 1964).

[23] A. Compagner, Ph.D. thesis, Technische Hogeschool te Delft (The Netherlands), 1972.

[24] N. Grewe and W. Klein, J. Math. Phys. **18**, 1729; **18**, 1735 (1977); W. Klein and N. Grewe, J. Chem. Phys. **72**, 5456 (1980).