

Renormalization group and linear integral equations

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(Received 16 August 1982; revised manuscript received 13 October 1982)

We develop a position-space renormalization-group transformation which can be employed to study general linear integral equations. In this Brief Report we employ our method to study one class of such equations pertinent to the equilibrium properties of fluids. The results of applying our method are in excellent agreement with known numerical calculations where they can be compared. We also obtain information about the singular behavior of this type of equation which could not be obtained numerically.

The renormalization group¹ (RG) is one of the most useful methods employed in the theoretical investigation of phase transitions. Both momentum-space RG (MSRG) and position-space RG (PSRG) have led to deeper understanding of critical points^{2,3} and first-order^{4,5} phase transitions.

Most (though by no means all) of the progress has been restricted to lattice spin systems. Continuum systems, specifically fluids, have presented serious difficulties especially in the application of the PSRG technique. This is unfortunate, for although MSRG can be used to obtain accurate⁶ values for critical-point exponents in fluids, PSRG techniques are more useful for investigating first-order transitions such as freezing and melting. A severe difficulty in applying the PSRG technique to fluids is that unlike lattice systems a particle in a fluid can interact with all other particles in the system. The PSRG generates similar long-range forces even in simple systems such as nearest-neighbor Ising models. However, the fact that the unrenormalized system has only short-range forces makes possible the various approximation schemes developed to treat lattice models.

In this Brief Report we present a PSRG decimation procedure which can be employed to treat continuous systems. A basic step in this procedure is to employ the RG not on the Hamiltonian used in the partition function but, for example, on the kernel of one of several approximate integral equations employed in the theory of fluids. It should be stressed that although here we apply this method to an integral equation from fluid theory, it can be used to obtain information about solutions to *any* linear integral equation.

To illustrate the procedure, we consider the following equation for the pair distribution function $\rho_2(x_{12})$, where $x_{12} = |\bar{x}_1 - \bar{x}_2|$,

$$\rho_2(x_{12}) = z [1 + f(x_{12})] \left[\rho + \int \rho_2(x_{23}) f(x_{13}) d\bar{x}_3 \right]. \tag{1}$$

In Eq. (1) $z = e^{\beta\mu}$, μ is the chemical potential, $\beta = 1/k_B T$, and ρ is the density. The term

$$f(x_{ij}) = e^{-\beta\phi(x_{ij})} - 1$$

is the Mayer function, where $\phi(x_{ij})$ is the potential of interaction between particles i and j . This equation was first proposed by Sabry⁷ and derived as the first term in a perturbation expansion by Klein.⁸ A solution of Eq. (1) obtained numerically by Swendsen and Klein⁹ for hard-sphere potentials in three dimensions ($d = 3$) exhibits a singularity at $z = z_c$ ($z_c = 11.6048$) which leads to a singularity in the pressure of the form $P_s \sim (z - z_c)^{3/2}$. They also found a singularity in the density $\rho_s \sim (z - z_c)^{1/2}$. These results imply that the point z_c is a point of instability in the solution of this equation for the hard-sphere fluid. It should be stressed that the other exponents that one normally would associate¹⁰ with an instability of this kind were not obtained in Ref. 9. The RG transformation allows us to obtain a complete set of exponents for the solution of Eq. (1) as well as providing a method of obtaining singularities in a large class of equations. Although we will focus on Eq. (1) in this paper, our purpose is to introduce the RG and not to investigate the physics embodied in Eq. (1), which is discussed elsewhere.^{9,10}

In order to construct the RG we begin by iterating Eq. (1) to obtain an equation of the form

$$\rho_2(x_{12}) = \psi(x_{12}, z) + z^2 \int \int K(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4) \times \rho_2(x_{34}) d\bar{x}_3 d\bar{x}_4, \tag{2}$$

where

$$K(x_1, x_2, x_3, x_4) = [1 + f(x_{12})][1 + f(x_{23})] \times f(x_{24})f(x_{13}). \tag{3}$$

Iterating Eq. (2) we obtain

$$\rho_2(x_{12}) = \tilde{\psi}(x_{12}, z) + z^4 \int \int \int \int \bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6) \rho_2(x_{34}) d\bar{x}_3 d\bar{x}_4 d\bar{x}_5 d\bar{x}_6, \quad (4)$$

where from Eq. (3)

$$K(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6) = [1 + f(x_{25})][1 + f(x_{56})][1 + f(x_{34})][1 + f(x_{12})]f(x_{15})f(x_{26})f(x_{34})f(x_{46}). \quad (5)$$

It is important to note that both K and \bar{K} can be written as products of the kernel of Eq. (1). If a partial trace is performed on Eq. (4) that includes particles 5 and 6, Eq. (4) becomes

$$\rho_2(x_{12}) = \tilde{\psi}(x_{12}, z) + z^4 \int \int \bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4) \rho_2(x_{34}) d\bar{x}_3 d\bar{x}_4, \quad (6)$$

where

$$\bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4) = \int \int d\bar{x}_5 d\bar{x}_6 \bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6).$$

The functions $\psi(x_{12}, z)$ and $\tilde{\psi}(x_{12}, z)$ are clearly analytic in z . This implies that the singular part of $\rho_2(x_{12})$ [i.e., $\rho_{2s}(x_{12})$] must satisfy

$$\rho_{2s}(x_{12}) = z^4 \int \int \bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4) \rho_{2s}(x_{34}) d\bar{x}_3 d\bar{x}_4. \quad (7)$$

Consider now the pair distribution function constructed from a renormalized Hamiltonian. In analogy with Eq. (2) we expect

$$\rho'_2(x'_{12}) = \psi'(x'_{12}, z') + z'^2 \int \int K'(\bar{x}'_1, \bar{x}'_2, \bar{x}'_3, \bar{x}'_4) \rho'_2(x'_{34}) d\bar{x}'_3 d\bar{x}'_4, \quad (8)$$

where the primes denote renormalized quantities. For the singular part we have

$$\rho'_{2s}(x'_{12}) = z'^2 \int \int K'(\bar{x}'_1, \bar{x}'_2, \bar{x}'_3, \bar{x}'_4) \rho'_{2s}(x'_{34}) d\bar{x}'_3 d\bar{x}'_4. \quad (9)$$

In order to preserve the physics we must have

$$\rho_{2s}(x_{12}) = \rho'_{2s}(x'_{12}). \quad (10)$$

This is analogous to the requirement that the singular part of the free energy remain invariant in the standard PSRG.

Equations (2)–(10) together with the usual length rescaling (i.e., $d\bar{x}'_i = d\bar{x}_i/b^d$) gives

$$\psi'(x'_{12}, z') = \tilde{\psi}(x_{12}, z) \quad (10)$$

and

$$\frac{z'^2 K'(\bar{x}'_1, \bar{x}'_2, \bar{x}'_3, \bar{x}'_4)}{b^{2d}} = z^4 \int \int d\bar{x}_5 d\bar{x}_6 \bar{K}(\bar{x}_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6). \quad (11)$$

Equation (11) is our fundamental RG transformation. It should be noted here that even though we began this discussion by considering potentials which are pairwise additive, the RG procedure of Eq. (11) generates many-body interactions¹¹ as in the standard PSRG. This complication can be avoided by noting that the singular behavior of the distribution function $\rho_2(x_{12})$ is contained in its asymptotic form obtained as $x_{12} \rightarrow \infty$. For realistic potentials $\phi(x_{ij})$ we have

$$\lim_{x_{ij} \rightarrow \infty} \phi(x_{ij}) = 0.$$

With the above considerations and Eqs. (2), (3), (7), (9), and (10), Eq. (11) becomes

$$\frac{z' f'(x'_{12})}{b^d} \frac{z' f'(x'_{24})}{b^d} = \left[z^2 \int f(x_{15}) f(x_{35}) d\bar{x}_5 \right] \times \left[z^2 \int f(x_{26}) f(x_{16}) d\bar{x}_6 \right]. \quad (12)$$

The recursion relation is then

$$\frac{z' f'(x')}{b^d} = z^2 \int f(|\bar{x} - \bar{y}|) f(\bar{y}) d\bar{y}, \quad (13)$$

where $f(x)$ and $f'(x')$ can now be considered as Mayer functions. A more transparent form of Eq. (13) can be obtained by Fourier transforming both sides¹² and taking logarithms,

$$\ln[z' \hat{f}'(k')] = 2 \ln[z \hat{f}(k)], \quad (14)$$

where the factor b^{-d} is absorbed in the Fourier transform $\hat{f}(k)$. From Eq. (14) it follows that the solution to Eq. (1) has a singularity at that value of $z = z_c$ for which $z_c f(k_0) = 1$, where k_0 denotes the value of k for which $f(k)$ is a maximum. If we restrict ourselves to hard spheres in $d = 3$ and choose units for which $f(0) = -1$ we find that $z_c = 11.6048$ —in excellent agreement with the numerical solution.⁹

Equation (14) makes it obvious that the proper nonlinear scaling field is $\ln[z \hat{f}(k)]$ and the eigenvalue is 2. Before we can calculate exponents, how-

ever, we must specify the rescaling length b . For the standard PSRG applied to lattice systems b is determined by the requirement that the density of lattice points be invariant under the RG. In our case the density is not a fixed variable and another method for specifying the rescaling length must be found. Such a method can be based on Eq. (14).

If we restrict ourselves to potentials for which¹³

$$\int |f(x_{ij})| d\bar{x}_{ij} < \infty, \quad (15)$$

then $\hat{f}(k)$ in Eq. (14) is an analytic function of k . Since $\ln[z\hat{f}(k)]$ is the nonlinear scaling field³ $\hat{f}'(k') = \hat{f}'(k')$. If we fix $z = z_c$ and expand about k_0 , Eq. (14) becomes

$$(k' - k_0)^2 = 2(k - k_0)^2. \quad (16)$$

Since $k - k_0$ has the units of reciprocal length, Eq. (16) implies that the rescaling length $b = \sqrt{2}$. Equation (14) becomes

$$\ln[z'\hat{f}'(k')] = b^2 \ln[z\hat{f}(k)]. \quad (17)$$

The fixed points of Eq. (17) are at $z\hat{f}(k) = 0, 1, \infty$. The fixed point at $z\hat{f}(k) = 1$ is unstable. From Eq. (17) (at the unstable fixed point) and the fact that the correlation length ξ is rescaled by a factor of b we obtain

$$\xi \sim (z - z_c)^{-1/2} = (z - z_c)^{-\tilde{\nu}}.$$

Previously we have not discussed the behavior of the free energy of fluid systems under RG transformations. It should, however, be obvious that a decimation procedure constructed in any reasonable way must leave the singular part of the free-energy invariant.^{3,14} Consequently the standard scaling relation

$$F(u) = F(b^2 u)/b^d \quad (18)$$

will hold for fluid systems, where $F(u)$ is the singular part of the free energy per unit volume and u is the scaling field $\ln[z\hat{f}(k)]$.

The usual scaling arguments applied to Eq. (18) and the use of standard thermodynamic relations leads to

$$F(z\hat{f}(k_0)) \sim P_s(z) \sim (z - z_c)^{3/2} = (z - z_c)^{2-\tilde{\alpha}},$$

where $P_x(z)$ is the singular part of the pressure, and

$$\rho_s \sim (z - z_c)^{1/2} = (z - z_c)^{\tilde{\beta}},$$

where ρ_s is the singular part of the density. Finally in the same vein we have the isothermal compressibility $\chi_T \sim (z - z_c)^{-1/2} \sim (z - z_c)^{-\tilde{\gamma}}$. The exponents for the pressure and density singularities are in agreement with the numbers obtained numerically.⁹ The correlation length and susceptibility exponents were not obtained in Ref. 9; however, they can be inferred from the assumption of scaling and hyperscaling laws

and from the values of $\tilde{\nu}$ and $\tilde{\gamma}$. The values of $2 - \tilde{\alpha}$ and $\tilde{\beta}$ obtained in this way agree with the numbers obtained from the RG.

The following points should be noted:

(1) Equation (17) is the result of investigating the behavior of Eq. (11) in the limit $x_{12} \rightarrow \infty$. If in fact Eq. (11) has an unstable fixed point, then the exponents derived from Eq. (17) specify the nature of the phase transition.

(2) The rescaling length b was determined by investigating the RG in the neighborhood of the nontrivial fixed point. However if the RG is used in a different region of parameter space the rescaling length will change. This rather unusual property of our RG procedure arises because, unlike applications of the PSRG technique to lattices, the density is not a fixed parameter but a thermodynamic variable which is to be renormalized differently in different regions of parameter space.

(3) This technique is not restricted to integral equations used in the theory of fluids. The fundamental recursion relation [Eq. (11)] is obtained with no recourse to physical arguments and is valid for *any* inhomogeneous linear integral equation. Clearly the simplification exploited in this work when $x_{12} \rightarrow \infty$ will not occur for all equations; however, in such cases numerical and approximation schemes may be used. It is of course not clear that the accuracy of such a procedure would be any better than that of standard numerical techniques already available. This approach, however, allows us to adapt to the study of linear integral equations a framework or set of concepts which will be very useful in interpreting the physical significance of the solutions of the equations.

It should be pointed out that a partial solution for the critical exponents of the solution of Eq. (1) can be obtained by a Fourier transform with the assumption that the nonanalyticity of

$$\int \int e^{-i\bar{k} \cdot \bar{x}} f(\bar{x}) f(\bar{y}) \rho_2(\bar{x} - \bar{y}) d\bar{y} d\bar{x}$$

in z causes no difficulties. From this approach one can obtain $z_c f(\hat{k}_c) = 1$, $\tilde{\gamma} = 1$, and $\tilde{\nu} = \frac{1}{2}$. Exponents such as $\tilde{\beta}$, however, cannot be simply obtained using this technique. In general the RG procedure will be most useful when the kernel of the integral equation cannot be reduced to a simple displacement kernel in some limit.

(4) As far as the application to fluid systems is concerned, our approach is somewhat different from the standard lattice PSRG. In the lattice case the formally exact PSRG is intractable so approximations are developed *dictated by the RG*. In the fluid or continuum models, that approach does not seem to be tractable. We have instead employed an exact RG on approximate equations which were developed independent of any RG.

To summarize we have developed a PSRG which

involves the procedures of iteration and decimation of linear integral equations. In this Brief Report the method has been applied to an approximate integral equation for the pair distribution function in simple fluids and the results compared with a known numerical solution. Although the method introduced above was applied to an equation of interest in the study of fluids it can be used to obtain information about the singular behavior of solutions to *any* inhomogeneous linear integral equation. Application of this technique to other linear equations has been carried out and the details will be published elsewhere. We are

also attempting to generalize this method to nonlinear equations.

ACKNOWLEDGMENTS

I am especially pleased to acknowledge useful conversations with C. Unger. I would also like to acknowledge useful conversations with A. C. Brown. This Center for Polymer Studies is supported in part by Grants from the Army Research Office, the Office of Naval Research, and the National Science Foundation.

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