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# Bose quantum fluids at finite temperatures: A variational density-matrix approach

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The variational density-matrix approach introduced by Campbell, Kürten, Ristig, and Senger [Phys. Rev. B **30**, 3728 (1984)], to study finite-temperature Bose fluids is reformulated to avoid dealing directly with the entropy of the trial density matrix. We obtain exact expressions for the Euler-Lagrange equations for a finite-temperature trial statistical density matrix, which is the simplest finite-temperature generalization of a Jastrow trial ground-state wave function. A multicomponent hypernetted-chain method is developed to solve approximately these Euler-Lagrange equations at low temperatures. In leading order the results are shown to be equivalent to those obtained by Campbell *et al.* The current formalism provides a scheme to improve results of the previous approach.

## I. INTRODUCTION

Campbell, Kürten, Ristig, and Senger[1] (CKRS) developed a variational density-matrix approach to study the finite-temperature properties of Bose fluids in the liquid-gas portion of the thermodynamic phase diagram, and applied it to liquid $^4$He. Using as input the experimentally measured, temperature-dependent structure function $S(k,T)$ of Robkoff and Hallock[2] and Svensson, Sears, Woods, and Martel,[3] they calculated the isothermal sound velocity for temperatures up to 4 K. Their results agree well with the experimentally determined values of Cowley and Woods.[4]

Following this work, Senger, Ristig, Kürten, and Campbell,[5] calculated the temperature and density dependence of the Helmholtz free energy, entropy, structure function, pressure, and chemical potential. Their approach is distinguished by the fact that it is a first-principles calculation which accurately determines the liquid-gas critical point and a large portion of the spinodal line for a quantum fluid. This formalism has been extended to include binary[6] and inhomogeneous[7] Bose fluids.

On the other hand, certain approximations are introduced into their analysis which limit the applicability of their results, invalidating them when the number of thermally excited collective modes are comparable to the number of bare particles, which corresponds in the case of $^4$He to the locus of the spinodal line in the low-temperature, low-density corner of the phase diagram.[5] The approximation which causes this problem, referred to as the separabiltity approximation for the entropy, does not have an obvious means for improvement. Our present efforts are motivated in part by this difficulty, and by an interest in gaining a deeper understanding of the variational formulation of the statistical mechanics of quantum fluids.

In this paper we reformulate the CKRS derivation of the variational Euler-Lagrange equations for the trial statistical density matrix so that we might avoid dealing directly with the entropy. This enables us to focus on a set of distribution functions which are susceptible to a hypernetted-chain analysis. As the first step in this analysis we show how one recovers the results of CKRS with a simple approximation. As a consequence, this work gives some insight into their analysis, and points to a method for developing possible improvements upon the previous results. We begin by briefly reviewing the essential theory of the variational approach to quantum statistical mechanics, including a discussion of the space of trial density matrices considered in this work.

Since real quantum fluids invariably have strong short-range correlations because of the strong interparticle repulsion, quantitatively successful theories are generally formulated in coordinate space. Some important features of the coordinate-state representation of the density matrix for an $N$-body quantum fluid were established in Refs. 1 and 5. Most importantly, it may be written in the form[1]

$$\rho(\mathbf{r}_1,\ldots,\mathbf{r}_N;\mathbf{r}_1',\ldots,\mathbf{r}_N') = \psi^*(\mathbf{r}_1,\ldots,\mathbf{r}_N) \times Q(\mathbf{r}_1,\ldots,\mathbf{r}_N;\mathbf{r}_1',\ldots,\mathbf{r}_N') \times\psi(\mathbf{r}_1',\ldots,\mathbf{r}_N'), \qquad (1.1)$$

where the incoherence factor $Q$ provides a nonseparable connection between the primed and unprimed coordinates except at zero temperature, and $\psi$ and $Q$ are each temperature dependent. In boson systems, $\psi$ and $Q$ are real, non-negative functions which are symmetric under the exchange of particle coordinates (which for $Q$ means the exchange of particles within the primed set and *sep-*

*arately* within the unprimed coordinates).[1] At zero temperature $Q$ is unity and $\psi$ is the ground-state wave function. In the high-temperature limit, $\psi$ becomes a product of two-body functions (the square root of the Boltzmann factor in the infinite temperature limit), and $Q$ becomes a permanent (or determinant for a fermion system) of two-body functions $\Gamma(\mathbf{r}_i - \mathbf{r}_j')$ (Dirac $\delta$ functions at infinite temperature).[5] In the low-temperature limit in boson systems, $\psi$ becomes the ground-state wave function multiplied by a product of temperature-dependent two-body functions, $\prod_{i<j} \exp[\frac{1}{2}u_p(|\,\mathbf{r}_i - \mathbf{r}_j\,|)]$, and the incoherence factor $Q$ becomes a product of temperature-dependent one-body *off-diagonal* functions $\prod_{i,j} \exp[\frac{1}{2}\omega_p(|\,\mathbf{r}_i - \mathbf{r}_j'\,|)]$, where $u_p$ and $\omega_p$ are temperature dependent and are determined only by the velocity of sound in the fluid.[8]

To extend this theory to temperatures beyond the low-temperature limit, it was proposed by CKRS to use the Gibbs-Delbrück-Moliere minimum principle to determine $\psi$ and $Q$ variationally. This principle states that the trial Helmholtz free energy $F_t$ is bounded from below by the true free energy $F_0$ and is given by

$$F_0 \leq F_t = \mathrm{tr}(H\rho_t) + \frac{1}{\beta}\mathrm{tr}(\rho_t \ln \rho_t) \tag{1.2}$$

where $\beta = 1/k_B T$ and $\rho_t$ is a suitable trial density matrix. The first and second terms are the trial internal energy and trial entropy, respectively. The Hamiltonian, $H$, is given by

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N} \nabla_i^2 + \sum_{i<j} v(|\,\mathbf{r}_i - \mathbf{r}_j\,|). \tag{1.3}$$

Here $m$ is the bare mass of the particle and $v(r)$ is a two-body interaction potential. Thus for a trial density matrix of the form of Eq. (1.1), the formal equations for $Q$ and $\psi$ are

$$\frac{\delta F_t}{\delta Q_t} = 0, \quad \frac{\delta F_t}{\delta \psi_t} = 0, \tag{1.4}$$

subject to the constraint on $Q_t$ that $\rho_t$ is a proper density matrix. In particular, the eigenvalues of $\rho_t$ must be real and non-negative, and it must be normalized.

It was argued in CKRS that the simplest trial density matrix which is sufficiently flexible to account for both the short-range correlations, due to the repulsive cores typical of dense fluids, and the long-range correlations needed to support the phononic elementary excitations of the superfluid phase, has the coordinate space representation

$$\rho_t(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}_1', \ldots, \mathbf{r}_N') = \frac{1}{Z_t}\prod_{i<j} e^{\frac{1}{2}u(|\mathbf{r}_i - \mathbf{r}_j|)} \prod_{i,j} e^{\frac{1}{2}\omega(|\mathbf{r}_i - \mathbf{r}_j'|)} \prod_{i<j} e^{\frac{1}{2}u(|\mathbf{r}_i' - \mathbf{r}_j'|)}, \tag{1.5}$$

where $Z_t$ is the normalization integral:

$$Z_t = \int d(\mathbf{r}_1, \ldots, \mathbf{r}_N) e^{N\omega(0)} \prod_{i<j} e^{u(|\mathbf{r}_i - \mathbf{r}_j|) + 2\omega(|\mathbf{r}_i - \mathbf{r}_j|)}. \tag{1.6}$$

This density matrix has the same structure as the low-temperature density matrix derived by Reatto and Chester[8] (discussed above) if one replaces their ground-state wave function by the optimum Jastrow trial ground-state wave function:

$$\prod_{i<j} e^{\frac{1}{2}u_0(|\mathbf{r}_i - \mathbf{r}_j|)}, \tag{1.7}$$

where $u = u_0 + u_p$ is the low-temperature limit. It is also the structure of the density matrix of a set of non-interacting harmonic oscillators, derived by Penrose,[9] with complex collective coordinates $\rho_\mathbf{k}$ being identified as the density fluctuation operators[10]

$$\rho_\mathbf{k} = \sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_j}. \tag{1.8}$$

For these reasons it is appropriate that a trial density matrix of the form of Eq. (1.5) be referred to as a Penrose-Reatto-Chester-Jastrow (PRCJ) density matrix.[11,12]

With this choice of trial density matrix, the Euler-Lagrange equations [Eq. (1.4)] for $\psi$ and $Q$ become a set of coupled equations for the functions $u(r)$ and $\omega(r)$:

$$\frac{\delta F_t}{\delta u(r)} = 0, \quad \frac{\delta F_t}{\delta \omega(r)} = 0. \tag{1.9}$$

The constraint that $\rho_t$ is a density matrix is satisfied by requiring $\omega(r)$ to have a non-negative Fourier transform.[1] It should be noted that the functions $u(r)$ and $\omega(r)$ do not have an *explicit* temperature dependence, instead gaining their temperature dependence through the temperature factor multiplying the trial entropy in Eq. (1.2). At zero temperature $\omega(r)$ vanishes and $u(r)$ becomes the optimal ground-state Jastrow function, which has been widely studied and gives a reasonably good account of the ground-state properties of liquid $^4$He.[13]

It should be expected that the PRCJ density matrix will give low-temperature results with accuracy comparable to those obtained for the ground state from the Jastrow theory. However, the entropy imposes difficulties which require additional analysis. The approximations used in previous work to deal with the entropy appear to be cruder than those used for ground-state calculations, making the results somewhat more uncertain. Methods for improving the trial density matrix, similar to those which have been successful for the trial ground state,[13] are discussed in Sec. V.

An important shortcoming of the PRCJ density matrix needs to be acknowledged at the outset: it fails to evolve into the exact high-temperature limit discussed below Eq. (1.1).[5,11] Moreover, it is the fact that $\Gamma(r)$ is a short-range function of $r$ which destroys the off-diagonal long-range order (ODLRO) at high temperatures in the exact density matrix. In fact, the PCRJ density matrix has ODLRO at all temperatures in three dimensions, and quasi-ODLRO at all temperatures in two dimensions. This is closely related to the fact that, in two and three dimensions, Jastrow-type wave functions will always yield a nonzero condensate.[14] Thus the PRCJ density matrix cannot have a $\lambda$ transition. This makes the liquid-gas phase diagram obtained in Ref. 5 somewhat less interesting in the vicinity of the critical point and in the normal Bose gas region of the phase diagram, since in this trial density matrix the physics is being driven by collective modes of a superfluid and does not include single-particle modes. Nevertheless the model is applicable in the low-temperature portion of the phase diagram near the liquid densities, and, e.g., the spinodal line obtained from this theory should be described correctly in this region. Moreover, the PRCJ density matrix is the simplest imaginable density matrix for a boson system containing both short- and long-range correlations, and thus is an interesting and useful ansatz for studying the difficulties presented by the entropy in the variational statistical mechanics of quantum fluids. The high-temperature structure of the exact density matrix suggests a richer ansatz, particularly when it is realized that an infinite-range $\Gamma(r)$ will produce ODLRO.[5,11] But the entropy problem is even more severe for that ansatz; recent progress on this problem in the normal phase is reported elsewhere.[15]

In Refs. 1 and 5 an explicit form for the trial entropy was sought, thus requiring the introduction of the separability approximation, which amounts to a decoupling of the entropy due to Bijl-Feynman excitations. The Euler-Lagrange equations followed upon functional differentiation of the internal energy and the resulting approximate entropy expression. The primary difference between the analysis just summarized and the present work is that we never require a closed form expression for the entropy. Rather, we work directly with the functional derivatives of $\mathrm{tr}(\rho_t \ln \rho_t)$. In this way, we obtain formally exact expressions for the Euler-Lagrange equations in terms of derivatives of multicomponent distribution functions before it is necessary to introduce approximations. This derivation is given in Sec. II. Section III contains the hypernetted-chain (HNC) analysis of the internal energy, which can be calculated with only a slight modification of the methods used for Jastrow ground-state calculations. In Sec. IV we invoke the multicomponent hypernetted-chain equations to approximate the distribution functions, necessitated by the entropy, by an expansion in the relative density of thermally populated elementary excitations. To leading order we obtain the results of Refs. 1 and 5. The excitation spectrum is introduced by using a single-resonance approximation to describe the dynamic structure function.[1,5] We close Sec. IV by showing that the leading order expression for the entropy is that given by the Bose liquid form obtained in the separability approximation in the earlier work. In Sec. V, further discussions on this approach are given and we indicate directions for future work.

## II. EULER-LAGRANGE EQUATIONS

To obtain the Euler-Lagrange equations [Eq. (1.9)] from Eq. (1.2), we first require expressions for the trial internal energy, $U_t$, corresponding to the PRCJ density matrix. Following CKRS a closed form expression for the internal energy can be obtained from the Jackson-Feenberg form for the kinetic energy. The result is

$$U_t = \mathrm{tr}(H\rho_t) = \frac{N\rho}{2}\int d\mathbf{r}\, v^*(r) g(r) + \frac{N}{(2\pi)^3\rho}\int d\mathbf{k}\, \epsilon_0(k)\gamma(k). \tag{2.1}$$

Here, $\rho$ is the number density ($\rho = N/V$), and $v^*(r)$ is defined by

$$v^*(r) = v(r) - \frac{\hbar^2}{4m}\nabla^2[u(r) + 2\omega(r)], \tag{2.2}$$

where the $\nabla^2$ term in (2.2) and the last term in (2.1) are the kinetic energy terms, $\epsilon_0(k) = \hbar^2k^2/2m$, $g(r)$ is the radial distribution function

$$g(r) = \frac{N(N-1)}{\rho^2}\int d(\mathbf{r}_3, \ldots, \mathbf{r}_N) \times \rho_t(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}_1, \ldots, \mathbf{r}_N), \tag{2.3}$$

$S(k)$ is the liquid structure function corresponding to $g(r)$ [defined below in Eq. (2.15)], and $\gamma(k)$ is the Fourier transform of $\omega(r)$.

As discussed in the Introduction, we do not attempt to derive a closed form expression for the trial entropy, $\mathcal{S}_t$. Rather, we work directly with the functional derivatives of $\mathcal{S}_t$. This is achieved by first invoking the replica identity:

$$\mathcal{S}_t = -k_B\ \mathrm{tr}(\rho_t \ln \rho_t) \equiv -k_B \frac{d}{d\sigma} \ln \mathrm{tr}(\rho_t^\sigma)\bigg|_{\sigma=1}, \tag{2.4}$$

where $\mathrm{tr}(\rho_t^\sigma)$ is the *operator* $\rho_t$ raised to the power $\sigma$. The main challenge of the present theory is to determine the $\sigma$-dependent functional derivatives of the entropy. In principle the $\sigma$ dependence of the entropy is not very complicated, since it is equivalent to the temperature dependence of the entropy for a model Hamiltonian $H_t$ which would have $\rho_t$ for its density matrix: $\rho_t = [\exp(-\beta H_t)]/Z_t$. Then it is seen that the replica definition of the entropy is nothing more than the thermodynamic definition of the entropy for $H_t$ by the $\beta$ derivative of the free energy. Moreover, the dependence of the entropy on $\sigma$ is analytic unless the model system described by $H_t$ has a phase transition at a temperature $T/\sigma$. When one uses a model Hamiltonian to define the density matrix and varies the Hamiltonian to find the optimum density matrix, it is equivalent to replacing the Gibbs-Delbrück-Moliere minimum principle by the Gibbs-Bogoliubov minimum principle.[16]

It is a straightforward matter to deal with the $\sigma$ dependence of the quantities of interest at integer values of $\sigma$. E.g., the trace in Eq. (2.4) can be expressed as a $3\sigma N$-fold integral:

$$\mathrm{tr}(\rho_t^\sigma) = \frac{1}{Z_t^\sigma} \int \prod_{n=1}^{\sigma} \left\{ d(\mathbf{r}_{1_n}, \ldots, \mathbf{r}_{N_n}) \prod_{i_n < j_n} e^{u(|\mathbf{r}_{i_n} - \mathbf{r}_{j_n}|)} \prod_{i_n, j_{n+1}} e^{\omega(|\mathbf{r}_{i_n} - \mathbf{r}_{j_{n+1}}|)} \right\}. \tag{2.5}$$

In this equation the indices obey the cyclic condition $\mathbf{r}_{j_{n+\sigma}} = \mathbf{r}_{j_n}$ for $n \leq \sigma$. Note that, aside from the denominator $Z_t^\sigma$, this quantity is equivalent to the configuration integral of a $\sigma$-component classical fluid where the fluid components are identical to one another, and a particle in one component "interacts" only with other particles in that component [through $u(r)$] and with particles in the components on either side of it [through $\omega(r)$] in the cyclic numbering system; i.e., particles in the $n$th replica "interact" with particles in replica $n-1$ and $n+1$, where the cycle is completed by the prescription $\sigma + 1 = 1$. It is not so easy to write a coordinate space representation for $\mathrm{tr}(\rho_t^\sigma)$ for noninteger $\sigma$. Nevertheless, as we indicated above, it is a well-behaved function of $\sigma$ since $\rho_t$ is a density matrix, and thus can in principle be brought to diagonal form with eigenvalues lying between zero and one.

We make use of these observations to recast the Euler-Lagrange equations [Eq. (1.9)] by introducing two auxiliary functions $g_0(r;\sigma)$ and $g_1(r;\sigma)$ defined by

$$\frac{\delta}{\delta u(r)} \ln \mathrm{tr}(\rho_t^\sigma) = \frac{N\sigma\rho}{2}\{g_0(r;\sigma) - g(r)\}, \tag{2.6}$$

$$\frac{\delta}{\delta \omega(r)} \ln \mathrm{tr}(\rho_t^\sigma) = N\sigma\rho\{g_1(r;\sigma) - g(r)\}, \tag{2.7}$$

where $g(r)$ is the radial distribution function defined in Eq. (2.3). This notation is motivated by the fact that, for integer values of $\sigma$, $g_0(r;\sigma)$ is the intraspecies radial distribution function for the fictitious $\sigma$-component classical fluid, and similarly $g_1(r;\sigma)$ is the corresponding radial distribution function between two particles in "adjacent" replicas. To be more specific, the array of radial distribution functions for the $\sigma$-component fictitious classical fluid is defined by

$$g_{\alpha\beta}(|\,\mathbf{r}_{1_\alpha} - \mathbf{r}_{2_\beta}\,|;\sigma) = \frac{N(N-\delta_{\alpha\beta})}{\rho^2} \int \prod_{n=1}^{\sigma} \{ d(\mathbf{r}_{1_n}, \ldots, \mathbf{r}_{N_n})' \rho_t(\mathbf{r}_{1_n}, \ldots, \mathbf{r}_{N_n}; \mathbf{r}_{1_{n+1}}, \ldots, \mathbf{r}_{N_{n+1}}) \}\,, \tag{2.8}$$

where the prime on the volume elements signifies the omission of $\mathbf{r}_{1_\alpha}$ and $\mathbf{r}_{2_\beta}$ from the integration. The kronecker $\delta$ function obeys the cyclic condition that $\delta_{\alpha,\beta}(\sigma) = \delta_{\alpha,\beta+\sigma}(\sigma)$. Since $g_{\alpha\beta}$ depends only on the shortest distance between $\alpha$ and $\beta$ on the cycle $1, \ldots, \sigma$, the subscript $\alpha\beta$ is conveniently replaced by this distance, and in particular $g_0$ and $g_1$ are the first two members of this array ordered by this distance. [Note that $g_0(r;\sigma=1) = g_1(r;\sigma=1) = g(r)$, and thus the functional derivatives in Eqs. (2.6) and (2.7) vanish at $\sigma = 1$, as they must.]

With these definitions, the exact Euler-Lagrange equations for the optimal density matrix within the space of PCRJ density matrices become

$$\frac{\delta}{\delta u(r)} U_t = -\frac{\rho N k_B T}{2} \left.\frac{d}{d\sigma} g_0(r;\sigma)\right|_{\sigma=1}, \tag{2.9}$$

$$\frac{\delta}{\delta \omega(r)} U_t = \rho N k_B T \left.\frac{d}{d\sigma} g_1(r;\sigma)\right|_{\sigma=1}, \tag{2.10}$$

where the trial internal energy $U_t$ is given in Eq. (2.1), and the right-hand sides come from the entropy term under the assumption that we may interchange the functional derivatives with the $\sigma$ derivative.

The method for the evaluation of the functional derivatives of $U_t$ on the left-hand side of these two equations is well understood from the Jastrow–Euler-Lagrange theory of the optimum Jastrow ground-state wave function; the finite-temperature version needs only to take additional account of the $\omega$ dependence when it does not appear in the combination $u + 2\omega$. Equation (2.9) can then be rewritten as

$$-\frac{\hbar^2}{4m}\nabla^2 g(r) + g'(r) = k_B T \left.\frac{d}{d\sigma} g_0(r;\sigma)\right|_{\sigma=1}, \tag{2.11}$$

where

$$g'(r) \equiv \int d\mathbf{r}' v^*(r') \frac{\delta g(r')}{\delta u(r)}, \tag{2.12}$$

while Eq. (2.10) can be combined with Eq. (2.9) and Fourier transformed to give

$$\epsilon_0(k) = \frac{1}{\beta} \left.\frac{d}{d\sigma}[S_0(k;\sigma) - S_1(k;\sigma)]\right|_{\sigma=1}. \tag{2.13}$$

The Fourier transformation of Eq. (2.11) is the paired-phonon form of the Euler-Lagrange equation:[17]

$$S'(k) = \frac{\hbar^2 k^2}{4m}[1 - S(k)] - k_B T \left.\frac{d}{d\sigma} S_0(k;\sigma)\right|_{\sigma=1}, \tag{2.14}$$

where the liquid structure function $S(k)$ is given by

$$S(k) = \frac{1}{N} < |\rho_{\mathbf{k}}|^2 >= 1 + \rho \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}}[g(r) - 1], \tag{2.15}$$

and $S_0$, $S_1$, and $S'$ are defined through the Fourier transforms of the corresponding $g$ functions in the obvious generalization of Eq. (2.15). Equation (2.14) differs from the corresponding ground-state equation[13,17] by the second term on the right-hand side.

Equations (2.11)–(2.13) are the exact equations for the optimum PRCJ density matrix. The mathematical problem posed by these equations is the determination of the dependence of the radial distribution function $g(r)$ upon $u+2\omega$ and the dependence of the two auxiliary functions $g_0$ and $g_1$ upon $u$, $\omega$, and $\sigma$, which is the subject of the next section.

An equivalent form of the Euler-Lagrange equations is the finite-temperature generalization of the Siemens-Lantto form,[18] which is obtained by changing independent functional variables from $[u(r), \omega(r)]$ to $[\sqrt{g(r)}, \omega(r)]$:

$$\left\{-\frac{\hbar^2}{m}\nabla^2 + v(r) + W_0(r) + W_T(r)\right\}\sqrt{g(r)} = 0, \tag{2.16}$$

which has the form of a Schrödinger equation for the two-body amplitude $\sqrt{g(r)}$, with induced potential $W(r) = W_0(r) + W_T(r)$ given by

$$\begin{aligned} W_0(r) = {} & \frac{\hbar^2}{4m}\nabla^2[\ln g(r) - u(r) - 2\omega(r)] \\ & + \frac{\hbar^2}{4m}\int d\mathbf{r}'[\nabla^2 g(r')]\frac{\delta[\ln g(r') - u(r') - 2\omega(r')]}{\delta g(r)} \end{aligned} \tag{2.17}$$

and the new, explicitly temperature-dependent part of the induced potential

$$W_T(r) = k_B T\int d\mathbf{r}'\left.\frac{d}{d\sigma}g_0(r';\sigma)\right|_{\sigma=1}\left.\frac{\delta u(r')}{\delta g(r)}\right|_{\omega}. \tag{2.18}$$

Equation (2.16) differs from the $T = 0$ result by the presence of the term $W_T$, and by the fact that $u(r) + 2\omega(r)$ appears in place of $u(r)$ in $W_0(r)$. Moreover, Eq. (2.16) must be solved simultaneously with Eq. (2.13) or an equivalent second equation.

## III. HYPERNETTED-CHAIN ANALYSIS

Long experience with the Jastrow–Euler-Lagrange theory of the ground state of liquid $^4$He has taught us that the hypernetted-chain formulation of the relationship between the radial distribution function and the Jastrow pseudopotential is the most useful route to a manageable theory. A deeper understanding of the implications of this resummation and the reasons for its success was gained by Jackson *et al.*, who showed that the simplest approximation to the hypernetted-chain equations (the HNC/0 approximation), when used in the Jastrow–Euler-Lagrange theory of the ground-state wave function (i.e., $T = 0$), is equivalent to a self-consistent resummation of ring and ladder diagrams in diagrammatic perturbation theory, and thus includes both long-range and short-range correlations in a correct and self-consistent manner.[19]

The generalization of the HNC analysis to finite temperatures to find the $u$ and $\omega$ dependence is straightforward, and will be reviewed in the remainder of this section. The main subject of this paper is a hypernetted-chain analysis of the $\sigma$ dependence, which we deal with in the next section.

In the present case, the hypernet equation for $g(r)$ is

$$g(r) = e^{u(r)+2\omega(r)+N(r)+E(r)}, \tag{3.1}$$

where $E(r)$ is the so-called bridge or elementary function, which is a well-defined functional of $g(r)$, and the nodal function $N(r)$ is defined by the solution of the chain equation

$$N(r) = \frac{1}{(2\pi)^3\rho}\int d\mathbf{k}\, e^{-i\mathbf{k}\cdot\mathbf{r}}\frac{[S(k)-1]^2}{S(k)}. \tag{3.2}$$

These equations are exact when the exact definition of $E(r)$ is included.[20] The hypernet equation can be used to simplify the Siemens-Lantto induced potential $W(r) = W_0(r) + W_T(r)$ [Eqs. (2.17) and (2.18)] into the form

$$W_0(r) = \frac{\hbar^2}{4m}\nabla^2[N(r) + E(r)] + \frac{\hbar^2}{4m}\int d\mathbf{r}'[\nabla^2 g(r')]\frac{\delta[N(r') + E(r')]}{\delta g(r)} \tag{3.3}$$

and

$$W_T(r) = \frac{k_B T}{g(r)}\left.\frac{d}{d\sigma}g_0(r;\sigma)\right|_{\sigma=1} - k_B T\int d\mathbf{r}'\left.\frac{d}{d\sigma}g_0(r';\sigma)\right|_{\sigma=1}\left.\frac{\delta[N(r') + E(r')]}{\delta g(r)}\right|_{\omega}. \tag{3.4}$$

With regard to the paired-phonon formulation of the Euler-Lagrange equations [Eq. (2.11) or (2.14)], the HNC equations permit a simple evaluation of the functional derivative $\delta g(\mathbf{r}')/\delta \mathbf{u}(\mathbf{r})$ in Eq. (2.12).[21]

The commonly used hypernetted-chain *approximation*, often referred to as HNC/0 to distinguish it from the exact HNC equations, is obtained by setting $E(r) = 0$.[20] As noted above, it is not necessary to go beyond this approximation to obtain qualitatively and semiquantitatively correct results for $^4$He; quantitative improvements are straightforward through more elaborate approximations for $E(r)$ such as the HNC/4 approximation.

Within the HNC/0 approximation, the Euler-Lagrange equations simplify still further because of the simplicity of the dependence of $N(r)$ upon $g$ or $S$, as is seen in Eq. (3.2). E.g., the finite-temperature version of the Siemens-Lantto induced potential $W(r) = W_0(r) + W_T(r)$ is given by

$$W(r) = -\frac{1}{2(2\pi)^3\rho}\int d\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{r}}\epsilon_0(k)\left[\frac{[S(k)-1]^2[2S(k)+1]}{S(k)^2}\right] \tag{3.5}$$

and

$$W_T(r) = \frac{k_BT}{g(r)}\frac{d}{d\sigma}g_0(r;\sigma)|_{\sigma=1} - k_BT\frac{1}{(2\pi)^3\rho}\int d\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{r}}\left[\frac{S(k)^2-1}{S(k)^2}\right]\frac{d}{d\sigma}S_0(k';\sigma)\bigg|_{\sigma=1}. \tag{3.6}$$

Moreover, since *all* HNC/$n$ approximations preserve the symmetry of the functional derivative $\delta g(\mathbf{r}')/\delta \mathbf{u}(\mathbf{r})$ with respect to interchange of $\mathbf{r}'$ with $\mathbf{r}$, the equation for $S'(k)$ can be written as a linear integral equation which is trivial to solve by matrix inversion methods.[21]

In summary, in this section we have reviewed the manner in which the HNC analysis previously developed for the optimum Jastrow ground-state wave function can be applied directly to the internal energy portion of the Euler-Lagrange equations for the optimum PCRJ density matrix. In the next section we focus on the remainder of the Euler-Lagrange analysis that must be included at finite temperatures, which requires the evaluation of the $\sigma$ derivatives of $S_0$ and $S_1$ which appear on the right-hand side of Eqs. (2.13) and (2.14).

## IV. SOLUTIONS TO THE EULER-LAGRANGE EQUATIONS

In this section we determine approximate expressions for $S_0(k;\sigma)$ and $S_1(k;\sigma)$ which have analytic continuations to noninteger $\sigma$. In turn, these expressions provide formal solutions to the Euler-Lagrange equations given by Eqs. (2.11)–(2.14). We now show that the multicomponent HNC/0 equations for a $\sigma$-component system can provide suitable expressions. The multicomponent HNC/0 equations comprise the hypernet equation[22]

$$g_{\alpha\beta}(r;\sigma) = e^{\mathcal{U}_{\alpha\beta}(r;\sigma)+N_{\alpha\beta}(r;\sigma)} \tag{4.1}$$

and the chain equation

$$S_{\alpha\beta}(k;\sigma) - \delta_{\alpha\beta}(\sigma) = +\sum_{\nu=1}^{\sigma}\tilde{X}_{\alpha\nu}(k;\sigma)S_{\nu\beta}(k;\sigma), \tag{4.2}$$

where in the present analysis,

$$\mathcal{U}_{\alpha\beta}(r;\sigma) = [u(r)+2\omega(r)]\delta_{\alpha,\beta}(\sigma) + \omega_{\alpha\beta}(r;\sigma), \tag{4.3}$$

$$\omega_{\alpha\beta}(r;\sigma) = \omega(r)[\delta_{\alpha,\beta+1}(\sigma)+\delta_{\alpha+1,\beta}(\sigma)-2\delta_{\alpha,\beta}(\sigma)]. \tag{4.4}$$

The multicomponent nodal functions $N_{\alpha\beta}(r;\sigma)$ and nonnodal functions (direct correlation functions) $X_{\alpha\beta}(r;\sigma)$ are related by the second term on the right-hand side of Eq. (4.2):

$$S_{\alpha\beta}(k;\sigma) - \delta_{\alpha\beta}(\sigma) = \tilde{X}_{\alpha\beta}(k;\sigma) + \tilde{N}_{\alpha\beta}(k;\sigma). \tag{4.5}$$

The important point is that for $\sigma = 2, 3, 4, \ldots$ and $\alpha \neq \beta$ the hypernet equation couples only to $\omega(r)$ and powers of (off-diagonal) $1 - g_{\alpha\beta}(r;\sigma)$. Consequently it is useful to rewrite the hypernet equation in the form

$$X_{\alpha\beta}(r;\sigma) = \mathcal{U}_{\alpha\beta}(r;\sigma) + \sum_{n=2}^{\infty}\frac{[1-g_{\alpha\beta}(r;\sigma)]^n}{n}. \tag{4.6}$$

Equations (4.2) and (4.6) can be expressed in terms of $S_{\alpha\beta}(k;\sigma)$ and $\gamma_{\alpha\beta}(k;\sigma)$ [the Fourier transform of $\omega_{\alpha\beta}(r;\sigma)$]. The chain equation can then be used to remove the $\tilde{X}_{\alpha\alpha}(k;\sigma)$ dependence. The result is

$$\begin{aligned} S_{\alpha\beta}(k;\sigma) = {} & S_{\text{eff}}(k;\sigma)\left\{\sum_{\nu=1}^{\sigma}\gamma_{\alpha\nu}(k;\sigma)S_{\nu\beta}(k;\sigma)+\delta_{\alpha\beta}(\sigma)\right\} \\ & + \frac{1}{2(2\pi)^3\rho}S_{\text{eff}}(k;\sigma)\sum_{\nu=1}^{\sigma}\int d\mathbf{q}\; S_{\alpha\nu}(q;\sigma)S_{\alpha\nu}(|\,\mathbf{k}-\mathbf{q}\,|;\sigma)\left[S_{\nu\beta}(k;\sigma)-\frac{S_{\nu\alpha}(k;\sigma)S_{\alpha\beta}(k;\sigma)}{S_0(k;\sigma)}\right] + \cdots. \end{aligned} \tag{4.7}$$

Here, an effective structure function, $S_{\text{eff}}(k;\sigma)$, has been introduced:

$$\frac{1}{S_{\text{eff}}(k;\sigma)} = \frac{1}{S_0(k;\sigma)} - 2\gamma(k)\left\{1-\frac{S_1(k,\sigma)}{S_0(k,\sigma)}\right\}. \tag{4.8}$$

Equation (4.7) should be viewed as the expression which relates the off-diagonal $S_{\alpha\beta}(k;\sigma)$ to $S_0(k;\sigma)$ and $\gamma(k)$. In terms of the diagonal elements, Eq. (4.7) is simply an identity for $\sigma = 2, 3, 4\ldots$ . For $\sigma = 1$, the solution of Eq. (4.7) is precisely the condition that $S_1(\mathbf{k};1) = S_0(\mathbf{k};1)$. Recall that this is the condition imposed by Eq. (2.7).

The terms on the right-hand side of the equality in Eq. (4.7) have been collected in powers of $1 - g_{\alpha\beta}(r;\sigma)$, for $\alpha \neq \beta$ and $\sigma > 1$. The first and second terms arise from truncating the off-diagonal hypernet equation after the $\omega_{\alpha\beta}(r)$ and $[1-g_{\alpha\beta}(r;\sigma)]^2/2$ terms, respectively. We now assert that $[1 - g_{\alpha\beta}(r;\sigma > 1)]$ may be regarded as a smallness function. Our assertion follows directly from the HNC/0 representation of $g_{\alpha\beta}(r;\sigma > 1)$. In particular, it is evident from Eq. (4.1) that $g_{\alpha\beta}(r;\sigma > 1)$ $(\alpha \neq \beta)$ couples directly to the incoherence function, $\omega(r)$, and only weakly, through the off-diagonal nodal diagrams, to the effective hard-core function $u(r)$. It follows that $[1 - g_{\alpha\beta}(r;\sigma)]^2/2$ is of order $\omega^2$. The assertion then follows by noting that at zero temperature $\omega(r)$ is identically zero and much less than unity for low temperatures. Consequently, Eq. (4.7) represents an expansion valid at low temperatures. More specifically, it is an expansion in the off-diagonal uniform limit for $g_{\alpha\beta}$, which depends for its validity upon density and/or temperature in the present case.[23]

We now show that the leading term in Eq. (4.7) can be put into a closed form which expresses $S_\lambda(k;\sigma)$, for $\lambda > 1$, in terms of $\gamma(k)$ and $S_0(k;\sigma)$. This expression follows by diagonalizing the matrix $\gamma_{\alpha\beta}(k;\sigma)$ with the unitary transformation

$$\Gamma_{\alpha\beta} = \frac{1}{\sqrt{\sigma}}\, e^{2\pi i\alpha\beta/\sigma}. \tag{4.9}$$

The resulting equation may then be solved algebraically to yield

$$S_{\alpha\beta}(k;\sigma) = \frac{S_{\text{eff}}(k;\sigma)}{\sigma} \times \sum_{\nu=1}^{\sigma} \frac{e^{2\pi i(\alpha-\beta)\nu/\sigma}}{1 + 4\gamma(k)S_{\text{eff}}(k,\sigma)\sin^2(\frac{\pi\nu}{\sigma})}. \tag{4.10}$$

The diagonalization process couples the off-diagonal $S_{\alpha\beta}$ to the diagonal $S_{\alpha\alpha}$. Consequently, it is meaningful to evaluate the $\alpha = \beta$ case. This can be done by contour integration,[12] with the result

$$S_0(k;\sigma) = \frac{\coth\left(\frac{\sigma\phi}{2}\right)}{2\gamma(k)\sinh\phi}, \tag{4.11}$$

where $\phi = \phi(k;\sigma)$ and is defined through the relation

$$\cosh\phi = \frac{1 + 2\gamma(k)S_1(k;\sigma)}{2\gamma(k)S_0(k;\sigma)}. \tag{4.12}$$

Finally, the solution of the inhomogeneous equation $(\alpha \neq \beta)$ can be expressed in terms of hyperbolic functions:

$$S_\lambda(k;\sigma) = \frac{1}{2\gamma(k)\sinh\phi}\left\{\coth\left(\frac{\sigma\phi}{2}\right)\cosh(\phi\lambda) - \sinh(\phi\lambda)\right\}. \tag{4.13}$$

This is the desired expression which relates the off-diagonal $S_\lambda(k;\sigma)$ to $S_0(k;\sigma)$ and $\gamma(k)$.

We now make the assumption that $S_\lambda(k;\sigma)$ given in Eq. (4.13) is valid for all $\sigma$, i.e., these expressions provide the analytic continuations to noninteger $\sigma$. We may thus proceed to evaluate the $\sigma$ derivatives as required by Eqs. (2.11), (2.13), and (2.14). First, we estimate the magnitudes of those derivatives. Due to a lack of a more rigorous means, a simple finite difference argument will have to suffice. As was done above, the estimate is most easily obtained by invoking the HNC/0 representation of $g_{\alpha\beta}(r;\sigma)$ [Eq. (4.1)]. Expressing the $\sigma$ derivative of $g_0(r;\sigma)$, evaluated at $\sigma = 1$, as $g_0(r;2) - g_0(r;1)$ yields a function of order $\omega(r)$, our smallness function. Similarly, expressing the $\sigma$ derivative of $g_1(r;\sigma)$ as the finite difference $g_1(r;2) - g_1(r;1) = g_1(r;2) - g_0(r;1)$ yields a function which depends directly on the hard-core function, $u(r)$. Terms depending directly on $u(r)$ should always be retained. Thus, to leading order we set $dS_0(k;\sigma)/d\sigma|_{\sigma=1}$ identically equal to zero. From Eqs. (4.12) and (4.13), it follows that

$$\left.\frac{dS_1}{d\sigma}\right|_{\sigma=1} = -\phi(k)S(k)\tanh\left(\frac{\phi(k)}{2}\right), \tag{4.14}$$

where $\phi(k)$ is evaluated at $\sigma = 1$. Substituting this result into Eq. (2.13) yields

$$S(k) = \frac{\beta\epsilon_0(k)}{\phi(k)}\coth\left(\frac{\phi(k)}{2}\right). \tag{4.15}$$

Finally, we introduce an effective elementary excitation energy, $\epsilon(k)$, into our formalism by following the comment in Ref. 1 that a single-resonance approximation produces a temperature-dependent structure function with the same form as Eq. (4.15) but with

$$\epsilon(k) \equiv k_B T\phi(k), \tag{4.16}$$

so that

$$\epsilon(k) = \frac{\epsilon_0(k)}{S(k)}\coth\left(\frac{\beta\epsilon(k)}{2}\right). \tag{4.17}$$

The interpretation of $\epsilon(k)$ as an effective elementary excitation spectrum is given some support by examining the expression for the entropy. Defining the occupation number of the effective elementary excitation by

$$n(k) \equiv \frac{1}{e^{\beta\epsilon(k)} - 1} \tag{4.18}$$

it is easy to show that, for $\sigma = 1$, Eq. (4.12) reduces to

$$\gamma(k)S(k) = n(k)[n(k) + 1]. \tag{4.19}$$

From Eqs. (2.4), (2.7), and the approximation $dS_0(k;\sigma)/d\sigma|_{\sigma=1} = 0$, one immediately finds

$$\frac{\delta}{\delta(\gamma(k)S(k))}S_t = \frac{Nk_B}{(2\pi)^3\rho}\phi(k)\tanh\left(\frac{\phi(k)}{2}\right). \tag{4.20}$$

Equation (4.12) (with $\sigma = 1$) can now be used to remove the $\gamma S$ dependence. The resulting expression can easily be (functionally) integrated, making use of the fact that the entropy vanishes when the function $\omega$ identically vanishes, which corresponds to the vanishing of $\phi$. The result can be expressed in terms of $n(k)$ rather than $\phi(k)$ by using $\phi(k) = \ln\frac{n(k)+1}{n(k)}$. The result is

$$S_t = k_B\sum_{\mathbf{k}}\{[n(k) + 1]\ln[n(k) + 1] - n(k)\ln n(k)\}. \tag{4.21}$$

This expression can be viewed as a Bose liquid expression for the entropy, in analogy to Fermi liquid theory, since it has the form of a free Bose gas, but with a temperature-dependent excitation energy. This result was previously obtained in Ref. 1 by calculating the entropy in the separability approximation, and then using Eq. (4.19) as the definition of $n(k)$.

## V. DISCUSSION

We begin this section by clarifying the relationship between the present work and that of Refs. 1 and 5. The earlier work is appealing because it leads, in a natural way, to a Bose liquid expression for the entropy and to the corresponding temperature-dependent Bijl-Feynman excitation spectrum, while the present work, though arriving at the same results in lowest approximation, requires a somewhat more contorted analysis to do so. The primary approximation in the earlier work—the separability approximation—was used to cast the trial entropy in a closed form expression. The separability approximation stems from the so-called paired-phonon analysis, which was employed as a tool to solve the Euler-Lagrange equation for the optimum Jastrow ground-state wave function.[17] In the context of the paired-phonon analysis, the separability approximation amounts to a decoupling of elementary excitations characterized by momentum pairs $(\mathbf{k},-\mathbf{k})$ from other momenta pairs. In that analysis, it was used as an iterative tool and does not affect the final results.[13] In the context of Refs. 1 and 5, the separability approximation is equivalent to suppressing the entropy fluctuations which connect the different paired-phonon spaces. It amounts to a first iteration. However, because of the difficulties in calculating the entropy outside of this approximation, no successive iteration scheme has been realized which would rid the theory of the effects of the separability assumption, in contrast to the ground-state situation.

Since the separability approximation has been extensively studied in the paired-phonon analysis its properties are well understood. The separability approximation is reliable when the number of excitations are few relative to the particle number. In turn, this occurs in the high-density and low-temperature regime of the fluid phase, which includes the higher-density portion of the spinodal line below the $\lambda$ temperature. Shortcomings resulting from using the separability approximation at lower densities are evident in Ref. 5. There it was observed that the spinodal line for $^4$He gas extrapolated to a finite value of temperature at zero density. This same shortcoming is apparent in Ref. 6 where improper behavior is observed in the zero concentration limit of one of the components of the binary mixture.

In the previous two sections we have shown how the variational formulation proposed by Campbell *et al.*[1] can be cast into the form of an off-diagonal uniform limit expansion together with an HNC analysis of the on-diagonal correlations. We showed that the results of CKRS are consistent with the leading term of our expansion. The condition that leads to a rapid convergence of this uniform limit expansion is that the temperature be sufficiently low for a fixed density, specifically that the total number density of thermally occupied excited states be small compared to the particle density. This is the same condition for which the separability approximation is valid. Thus an approach such as the one which we have developed in the present work should have practical applications to the improvement of this low-density regime when carried out to higher order. (Of course the present analysis does not eliminate the problem that the low-density gas portion of the phase diagram is still Bose condensed in the PRCJ density matrix.)

From our analysis it is clearly possible to obtain results beyond those reported here simply by using Eq. (4.13) as an iterant in the second term of the perturbation series, Eq. (4.7). This calculation has been completed.[12] That work was focussed on the generalization of the finite-temperature elementary excitation energy in order to retain the Bose liquid formulation of the final results. Although the results are promising, the complexity of the resulting expression required very crude further approximations in order that such an excitation spectrum be incorporated by the same scheme used at the end of the previous section of the present analysis.

We close this section with a discussion of other routes to follow to remove further deficiencies of the variational approach. In particular, we mention the shortcomings of the PRCJ density matrix, and emphasize the need for a rigorous means of incorporating the excitation spectrum into this method.

The PRCJ density matrix is known to have several limitations which we review here briefly. First, we noted in the Introduction that Reatto's conclusion that Jastrow-type wave functions always have a nonzero condensate[14] can be extended to PRCJ density matrices at all temperatures. Thus, a Bose fluid described by the PRCJ density matrix will never undergo a $\lambda$ transition, in direct contradiction to experiment. A consequence of this feature is readily apparent in the temperature dependence of the static structure function, $S(k)$, calculated in CKRS. There it was observed that, in the relevant temperature regime, the first diffraction peak of $S(k)$ increases continuously with increasing temperature. The experimental $S(k)$ for $^4$He exhibits this behavior up to the $\lambda$ transition temperature, but as the temperature increases above the $\lambda$ transition, the fluid behaves as a normal fluid and the peak decreases as one expects in a classical fluid where the increasing temperature reduces the spatial order.[2,3] This evidently signifies an increase in spatial order as the off-diagonal order decreases with increasing temperature below the $\lambda$ transition, but returning to the classical fluid behavior above the $\lambda$ transition, where the increasing temperature decreases the spatial order.[24] Blendowske and Fliessbach have recently shown that this qualitative behavior of $S(k,T)$ is obtained by using, for the incoherence factor $Q$, the high-temperature form of the ideal Bose gas density matrix. For this case, $Q$ is a permanent of Gaussians suitably modified to incorporate the effects of the $\lambda$ transition.[25] (Alternatively, Gaglione *et al.* explained the decrease by roton lifetime effects,[26] which are presumably related to the appearance of single-particle modes above the $\lambda$ transition, and thus related to the explanation in terms of the density matrix.)

Secondly, it has been well established that the quantitative inaccuracy of the optimum Jastrow wave function as a trial function for the ground state of liquid $^4$He can be nearly completely removed by the inclusion of three-body factors, of the form $\prod_{i<j<k} \exp[u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)]/2$ in the ground-state trial function.[13] Similarly, it has been shown that the closely related process of one Bijl-Feynman phonon decaying to two (and the inverse process) accounts for the backflow corrections[27] to the Bijl-Feynman phonon-roton curve, gives the correct density dependence of the roton region,[28] and gives the correct transition from anomalous to normal phonon dispersion with increasing density.[29] The PRCJ density matrix also neglects the higher particle number correlation factors $\exp[\Sigma u_3(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) + \Sigma u_4(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k, \mathbf{r}_\ell) + \cdots]$ and the closely related factors in the coherence factor, e.g., the backflow factor $\exp[\omega_{1,2}(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k)]$. The importance of such factors in including backflow effects at finite temperatures has been stressed by Battaini and Reatto.[30] Backflow effects are of increasing importance at elevated temperatures ($T > 0.5$ K for $^4$He) where the roton states become increasingly populated due to their high density of states.

The inclusion of the three-body correlation factors in the ground state increases the binding energy per particle by $O(1\text{ K})$ and similarly improves the agreement between the calculated and experimental equilibrium density.[13] Since the liquid-gas critical point should roughly scale with the binding energy, a density matrix neglecting three-body correlations should lead to an underestimate of the critical temperature, $T_c$. We note that this is also consistent with the findings of Ref. 5 where a $T_c$ of 4.3 K was calculated and the experimental $T_c$ is known to be 5.2 K. Recently, three-body correlations have been incorporated into the PRCJ density matrix and will be reported elsewhere.[31]

Most of the deficiencies discussed above stem primarily from computational limitations. The final deficiency that we mention is a consequence of a lack of a rigorous means for relating the elementary excitation spectrum, $\epsilon(k)$, to the input functions $u(r)$ and $\omega(r)$. The present analysis also has this problem when one goes beyond the lowest-order approximation.[12] It would be a significant conceptual and practical contribution to the understanding of the statistical mechanics of quantum fluids if a formal procedure were established which relates the entropy to statistical excitations.

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