Abstract: Integrating seminal ideas of London, Feynman, Uhlenbeck, Bloch, Bardeen, and other illustrious antecessors, this paper continues the development of an \textit{ab initio} theory of the \(\lambda\) transition in liquid \(^4\text{He}\). The theory is based upon variational determination of a correlated density matrix suitable for description of both normal and superfluid phases, within an approach that extends to finite temperatures the very successful correlated wave-functions theory of the ground state and elementary excitations at zero temperature. We present the results of a full optimization of a correlated trial form for the density matrix that includes the effects both of temperature-dependent dynamical correlations and of statistical correlations corresponding to thermal phonon/roton and quasiparticle/hole excitations – all at the level of two-point descriptors. The optimization process involves constrained functional minimization of the associated free energy through solution of a set of Euler-Lagrange equations, consisting of a generalized paired-phonon equation for the structure function, an analogous equation for the Fourier transform of the statistical exchange function, and a Feynman equation for the dispersion law of the collective excitations.Violation of particle-hole exchange symmetry emerges as an important aspect of the transition, along with broken gauge symmetry. In conjunction with a semi-phenomenological study in which renormalized masses are introduced for quasiparticle/hole and collective excitations, the results suggest that a quantitative description of the \(\lambda\) transition and associated thermodynamic quantities can be achieved once the trial density matrix is modified – notably through the addition of three-point descriptors – to include backflow effects and allow for \textit{ab initio} treatment of important variations in effective masses.
1. INTRODUCTION

The remarkable coherent collective property of superfluidity, observable in liquid $^4$He below the famous $\lambda$ transition, was discovered by Kapitza [1] and Allen and Misener [2] in 1938. Almost immediately, Fritz London [3,4] proposed that the transition to the superfluid phase (Helium II) reflects a process that is fundamentally analogous to Bose-Einstein condensation of an ideal Bose gas:

I recently realized that ... some support could be given to the idea that the peculiar phase transition ("$\lambda$-point"), that liquid helium undergoes at 2.19 K, very probably has to be regarded as the condensation phenomenon of the Bose-Einstein statistics, distorted, of course, by the presence of molecular forces and by the fact that it manifests itself in the liquid and not in the gaseous state.

Based on this idea, Tisza [5,6] introduced a successful two-fluid model of the macroscopic behavior of Helium II; a similar model was developed independently by Landau [7] on different grounds.

Here we shall report continued progress toward a quantitative microscopic understanding of the $\lambda$ transition in liquid $^4$He in terms of Bose-Einstein condensation of strongly interacting bosons. Carried out within the semi-analytic framework of correlated density-matrix theory, this effort aims at a concrete atomistic realization of London’s hypothesis as further shaped by Feynman [8]. In developing the theory, we have encountered a number of signposts erected by great physicists, suggesting that the path being followed is the right one. As a preface to the presentation of new results, it will be instructive to re-examine some of these seminal insights.

Working in configuration space, the density matrix of a system of $N$ identical bosons can be written in the general form

$$W(R, R') = I^{-1} \Phi(R)Q(R, R')\Phi(R'),$$  \hspace{1cm} (1)

where the coherence factor $\Phi(R')$ becomes the ground-state wave function in the limit of zero temperature, $Q(R, R')$ is an incoherence factor that is non-separable in the configurations $R = (r_1, \ldots, r_N)$ and $R' = (r'_1, \ldots, r'_N)$ and describes the effects of real excitations, and $I^{-1}$ is a normalization constant. It is convenient to split the incoherence factor into two parts, $Q(R, R') = Q_{\text{coll}}(R, R')Q_{\text{qp}}(R, R')$. The factor $Q_{\text{coll}}$ embodies the effects of real, thermal collective excitations (phonons and rotons), while $Q_{\text{qp}}$ accounts for the effects of real quasiparticle excitations (or exchange correlations). In the trial density matrix currently employed, the factors $\Phi$, $Q_{\text{coll}}$, and $Q_{\text{qp}}$ are built from two-point functions. In particular, $\Phi(R)$ and $Q_{\text{coll}}(R, R')$ are taken essentially as Jastrow products of appropriate dynamical and collective-thermal correlation functions \cite{9-11} $\exp[u(|r_i - r_j|)]/2$ and $\exp[\gamma(|r_i - r_j|)]$, respectively, while $Q_{\text{qp}}(R, R')$ is expressed in terms of a permanent of appropriate statistical correlation functions \cite{12} $\Gamma_{cc}(|r_i - r_j|)$. Ultimately, the functions $u$, $\gamma$, and $\Gamma_{cc}$ are to be determined by functional minimization of the free energy. A description of backflow effects requires the inclusion of three-point functions in the coherence factor $\Phi(R)$ and the incoherence factor $Q(R, R')$.

Decomposition of the factors $\Phi(R)$, $\Phi(R')$, $Q_{\text{qp}}(R, R')$, and $Q_{\text{coll}}(R, R')$ into products of two-point functions (and, as needed, three- and higher-point functions) is
motivated by the quantitative successes of the variational wave-function theory of the ground state of a strongly interacting Bose system [13]. In this theory, the ground-state wave function is written as a Jastrow product of pair correlation functions supplemented by a product of triplet correlation functions, and so on (as needed) to higher-body products in the Feenberg representation of the exact Bose ground state [11].

The treatment of $Q_{qp}(\mathbf{R}, \mathbf{R}')$ in terms of a permanent of two-point functions (the statistical correlation functions $\Gamma_{cc}(r_i - r_j')$) exploits and extends the ideas of Feynman [8] and the formalism of Ziff, Uhlenbeck, and Kac [12]. For free bosons, which is the case studied by Ziff et al., $\Gamma_{cc}(r)$ has a Gaussian form. Feynman used this form but inserted an effective mass in place of the bare mass.

To quote Feynman’s abstract,

*It is shown from first principles that, in spite of the large interatomic forces, liquid $^4$He should exhibit a transition analogous to the transition in an ideal Bose-Einstein gas. The exact partition function is written as an integral over trajectories, using the space-time approach to quantum mechanics. It is next argued that the motion of one atom through the others is not opposed by a potential barrier because the others may move out of the way. This just increases the effective inertia of the moving atom. This permits a transition, but of the third order. It is possible that a more complete analysis would show the transition implied by the simplified partition function is actually like the experimental one.*

The strategy now being pursued within correlated density-matrix theory seeks to complete Feynman’s program using a description that is more flexible yet is rooted in the same physical picture in which exchange effects are of paramount importance. As the system goes from the normal to the superfluid state, exchange loops (or “rings” or “cycles”) of macroscopic length come to dominate the behavior of the system; this feature is revealed in the development of off-diagonal long-range order of the partial distribution function (or correlation function) $G_{cc}(r)$ that characterizes exchange processes. The path-integral Monte Carlo approach of Ceperley and Pollock [14,15] is also based on Feynman’s ideas on liquid $^4$He, played out within Feynman’s space-time approach to quantum mechanics. Quite naturally, a similar picture emerges in this work – involving a kind of percolation transition in which exchange paths can grow to macroscopic size.

The entropy corresponding to the chosen trial density matrix is determined using a replica ansatz (borrowed from the statistical physics of disordered systems), together with the so-called diagonal approximation, which implements a separability hypothesis analogous to that applied by Campbell and Feenberg [9] in the paired-phonon theory of the ground state. The work of Ziff, Uhlenbeck, and Kac [12] provides the pivotal clue for constructing a trial density matrix that is applicable in both normal and condensed phases and across the phase transition.

The presence of a *permanent* in the trial density matrix introduces complications in the evaluation of spatial distribution functions and structure functions and of the internal-energy and entropy components of the free energy. However, a powerful formalism for handling exchange correlations comes to the rescue: the technical problems created by the permanent can be solved by appealing to (and extending)
the methods of Fermi hypernetted-chain theory invented by Fantoni and Rosati [16] and Krotscheck and Ristig [17]. Fermi-hypernetted chain theory teaches us how to evaluate correlated expressions involving determinants of two-point statistical functions, and this knowledge is readily adapted to Bose statistics. Complications also arise in the evaluation of the entropy using the replica ansatz, and these can be largely overcome with the aid of methods developed by Hiroike [18] for classical fluid mixtures.

The entropy, calculated in diagonal approximation, decomposes into independent contributions from phonon-roton excitations and from two kinds of quasiparticle excitations. The internal energy also decomposes into contributions from these three excitation branches, plus a correlation-energy term that becomes the ground-state energy at zero temperature. Within the correlated density-matrix theory, as explicited using the hypernetted-chain formalism, it is natural to interpret the two particle-type excitations as quasiholes and quasiparticles. The quasihole and quasiparticle dispersion relations are identical in the normal phase, where particle-hole symmetry is maintained, but they differ markedly in the condensed phase, where the exchange symmetry is broken. The \( \lambda \) transition therefore involves two order parameters:

(i) A condensation strength parameter \( B_{cc} \) which vanishes in the normal phase and measures the breaking of gauge symmetry in the condensed phase (also occurring in the noninteracting Bose gas)

(ii) An exchange strength \( M \) which also vanishes in the normal phase and measures the violation of exchange symmetry below the \( \lambda \) point (occurring only if the interactions are strong enough)

On physical grounds, these order parameters must be coupled, the simplest reasonable connection being a straight proportionality \( M = aB_{cc} \), where the coupling parameter \( a \) is temperature dependent [19].

The interpretation of the two quasiparticle branches as quasiholes and quasiparticles modes gains support from an idea voiced by Felix Bloch to the effect that – much as in a Fermi system – there might exist quasiparticle and quasihole excitations in a system of identical bosons. Bloch’s idea (unpublished, but aired at a Stanford seminar) resonates with Pines’ phenomenological arguments [20] that strongly interacting Bose and Fermi liquids have much more in common than is normally supposed, a claim well documented by experimental findings on the properties of their elementary excitations.

The nature of the proposed exchange-symmetry-breaking phenomenon is illuminated by the existence of a striking parallel with the behavior of a diamagnetic material in a magnetic field [19]. A particle-hole exchange field may be constructed as the sum of differences between the hole energies and the corresponding free single-particle energies, weighted by normalized differences between the occupation numbers of the two types of quasiparticle excitations. Pursuing the electromagnetic analogy, a macroscopic polarization is induced by this field, which is negatively proportional to the field with a diamagnetic-susceptibility coefficient that depends on the occupations of the two quasiparticle branches. This polarization effect acts to screen the exchange field in the condensed phase. Indeed, in analogy with the Meissner effect, the condensed phase behaves like an ideal diamagnetic as \( T \) approaches zero, completely expelling the exchange field from the system. The screening leads to a
drastic reduction in the particle-hole exchange contribution to the internal energy of the system. This exchange property was considered in detail in Ref. [19], where the exchange-symmetry breaking was first proposed as an essential aspect of the $\lambda$ transition in liquid $^4$He.

The diamagnetic analogy evokes a conviction expressed by John Bardeen [21] in recounting the development of superconductivity theory:

> It seems to me that most of those who thought long and hard about superconductivity prior to the discovery of the Meissner effect in 1933 never got over an inner feeling that the really fundamental property of a superconductor is infinite conductivity or persistent currents, and this colored the way they thought about the subject in future years. While an adequate theory must explain both aspects, the diamagnetic approach has been the most fruitful in indicating the nature of the superconducting state.

This deep insight sanctions an analogous description of the superfluid state of liquid $^4$He.

In advance of a complete functional optimization of the trial density matrix, a model calculation [19] has provided strong support for the new microscopic approach and especially for the importance of exchange-symmetry breaking in the $\lambda$ transition. A standard parameterized form was assumed for the dynamical correlation function (i.e. for the pseudopotential $u(r)$), while – as in Feynman’s treatment – the statistical correlation function $\Gamma_{cc}(r)$ was determined through an effective-mass parameterization of the quasihole spectrum. The collective (or phonon-roton) incoherence factor $Q_{\text{coll}}(R, R')$, which is not expected to exert a strong influence on the transition, was set equal to unity. A simple and plausible model was introduced for the coupling parameter $a(T)$ connecting the order parameter $M$ for exchange-symmetry violation to the order parameter $B_{cc}$ for gauge-symmetry breaking. This model requires, as empirical input, the ratio of the speeds of second and first sound in the condensed phase.

Within the semi-microscopic/semi-empirical model so delineated, exchange-symmetry breaking was found to reduce the condensation temperature of liquid $^4$He from the value 3.2 K corresponding to Bose-Einstein condensation of a noninteracting Bose gas to a value 2.2 K very close to the experimentally measured $\lambda$ transition temperature. This prediction is based entirely on the extrapolated behavior of the hole chemical potential in the normal phase; it is consistent with the behavior of the model in the condensed phase but does not depend on the empirical input for the sound-speed ratio. The prediction for the specific heat shows an apparently divergent behavior at 2.2 K and qualitatively – though not quantitatively – reproduces the characteristic $\lambda$ shape of the experimental curve. The latter result contrasts with that of Feynman’s treatment, where an approximate and incomplete analysis of the geometry of exchange processes led to a continuous specific heat, as in the noninteracting Bose gas.

In this paper we continue to build upon the correlated density-matrix theory of strongly correlated Bose systems, essentially in the form designed and developed in Refs. [22-27]. The trial density matrix for liquid $^4$He and the consequent structure of the energy and entropy (the latter evaluated in diagonal approximation) are made more explicit in Sec. 2. The Euler-Lagrange equations for the optimal density
matrix without backflow, expressed in convenient form (as presented in Sec. 3), are solved numerically. The results of the full optimization are examined in detail in Sec. 4. (Additional information is furnished by Ref. [28].) Remaining obstacles to a full microscopic understanding of the $\lambda$ transition are discussed in the final section. Detailed formulas of the theory are relegated to an appendix.

2. CORRELATED TRIAL DENSITY MATRIX AND FREE ENERGY

The theory begins with suitable choices for the coherence and incoherence factors appearing in Eq. (1):
(i) A wave function of Jastrow form
\[
\Phi(R) = \exp \left\{ \frac{1}{2} \sum_{i<j}^N u(|r_i - r_j|) \right\},
\]
(ii) An incoherence factor
\[
Q = Q_{\text{coll}} Q_{\text{qp}}
\]
that takes account of real collective excitations (phonons, rotons) through
\[
Q_{\text{coll}}(R, R') = \exp \sum_{i,j}^N \left\{ \gamma (|r_i - r_j'|) - \frac{1}{2} \gamma (|r_i - r_j|) - \frac{1}{2} \gamma (|r_i' - r_j'|) \right\},
\]
and incorporates the effects of quasiparticle excitations via
\[
Q_{\text{qp}}(R, R') = \frac{1}{A^N} \frac{1}{2\pi i} \oint dz e^{A/z} \text{Perm}_{i,j} \Gamma_{cc}(|r_i - r_j'|) + B_{cc} z \right].
\]
The free-energy functional associated with the trial density matrix specified by Eqs. (2)–(4) has been constructed explicitly [19], with the following general results. The internal energy of the $N$-boson system at temperature $T$ is the sum of a correlation energy $E_c$ (which coincides with the expected ground-state energy at zero temperature) and separate contributions from collective, quasihole, and quasiparticle excitation branches,
\[
E = E_c + E_{\text{coll}} + E_{\text{qh}} + E_{\text{qp}} .
\]
rotons), quasiholes, and quasiparticles of all momenta $\hbar \mathbf{k}$,

$$E_{\text{coll}} = \sum_k \epsilon_{\text{coll}}(k)n(k),$$

$$E_{\text{qh}} = \frac{1}{2} \sum_k \epsilon_{\text{cc}}(k)n_{\text{cc}}(k),$$

$$E_{\text{qp}} = \frac{1}{2} \sum_k \epsilon_o(k)n_c(k).$$

In turn, the functions $n(k)$, $n_{\text{cc}}(k)$, and $n_c(k)$ are the respective thermally averaged occupation numbers of these three kinds of excitations, at wave vector $\mathbf{k}$. The corresponding excitation energies $\omega(k)$, $\omega_{\text{cc}}(k)$, and $\omega_c(k)$ are defined through the Bose distribution function

$$n(k) = \left[\exp \beta \omega(k) - 1\right]^{-1}$$

and through the analogous Bose distributions $n_{\text{cc}}(k)$ and $n_c(k)$.

In the diagonal approximation [24,25], the three types of excitations also contribute additively to the total entropy $S_e$,

$$S_e = S_{\text{e}}^{(\text{coll})} + S_{\text{e}}^{(\text{cc})} + S_{\text{e}}^{(c)},$$

where

$$S_{\text{e}}^{(\text{coll})} = k_B \sum_k \left\{ [1 + n(k)] \ln [1 + n(k)] - n(k) \ln n(k) \right\},$$

$$S_{\text{e}}^{(\text{cc})} = \frac{1}{2} k_B \sum_k \left\{ [1 + n_{\text{cc}}(k)] \ln [1 + n_{\text{cc}}(k)] - n_{\text{cc}}(k) \ln n_{\text{cc}}(k) \right\},$$

and $S_{\text{e}}^{(c)}$ is obtained from Eq. (11) by replacing $n_{\text{cc}}(k)$ with $n_c(k)$.

The energies $E_c$, $\epsilon_{\text{coll}}(k)$, and $\epsilon_{\text{cc}}(k)$ and the distributions $n(k)$, $n_{\text{cc}}(k)$, and $n_c(k)$ are to be regarded as functionals of the statistical function $\Gamma_{\text{cc}}(r)$ and the pseudopotentials $u(r)$ and $\gamma(r)$. In the condensed phase, they are also functions of the condensation strength $B_{\text{cc}}$. Explicit expressions for these quantities are provided in the Appendix.

The two excitation branches having Bose distribution functions $n_{\text{cc}}(k)$ and $n_c(k)$ and respective energies $\omega_{\text{cc}}(k)$ and $\omega_c(k)$ are characterized at small wave number $k$ by a quadratic dispersion law or/and an energy gap. In the normal phase where $B_{\text{cc}} \equiv 0$ these two branches merge, i.e., $n_{\text{cc}}(k) = n_c(k)$ and $\omega_{\text{cc}}(k) = \omega_c(k)$ for any $k \geq 0$. However, in the condensed phase where $B_{\text{cc}} > 0$, this degeneracy may be lifted in the presence of interactions between the boson constituents. The two branches then follow different dispersion laws. In the spirit of Felix Bloch’s conjecture as enunciated in the introduction, we view the $\text{cc}$ and $\text{c}$ branches as involving quasihole and quasiparticle excitations, respectively [19]. According to this Bloch interpretation, the symmetry between particle and hole excitations is broken in the condensed phase of a strongly interacting Bose system. Further, as sketched in the introduction, the exchange-symmetry-breaking phenomenon can be given a formal expression by developing an analogy with the behavior of a diamagnetic material in a magnetic field.
The counterpart of the Meissner effect (expulsion of the exchange field) has been studied numerically in Ref. [19] within a model in which simple parameterized forms are assumed for the dynamical correlations and for the hole spectrum that determines the statistical correlations.

To proceed beyond the model of Ref. [19] toward a systematic microscopic treatment, we now turn to the problem of full functional optimization of the Helmholtz free energy. Due to the formal complexity of this problem, the present implementation is limited to the choice (2)–(4) for the trial density matrix, implying the omission of three- and higher-body correlation functions and hence neglect of what are traditionally called “backflow” effects.

3. FUNCTIONAL OPTIMIZATION OF THE FREE ENERGY

The Delbrück–Gibbs–Moliere minimum principle for the Helmholtz free energy [23] is employed to determine the optimal density matrix (1) within the class of trial functions defined by Eqs. (2)–(4). Variation of the functional $F = E - TS\epsilon$ constructed from the results (5)–(11) is, however, constrained by a particle-number (or particle-conservation) sum rule. This sum rule takes the form [25]

$$N = B_{cc}N_o + \sum_k n_{cc}(k)$$

with

$$N_o = N + \sum_k \Gamma_{cc}(k) \left[ S_{dc}(k) + S_{cc}^{(1)}(k) \right]$$

in the condensed phase where $0 < B_{cc} \leq 1$; it of course lacks the $N_oB_{cc}$ term in the normal phase. The functions $S_{dc}(k)$ and $S_{cc}^{(1)}(k)$ are components of the structure function $S(k)$ and the exchange function $S_{cc}(k)$, respectively [19]. Coupling the condition (12) to the free energy expression with a Lagrange parameter $\lambda$, the modified functional $F_{\lambda}$ is varied with respect to the input functions $u(r)$, $\Gamma_{cc}(r)$, and $\gamma(r)$ (or their Fourier transforms $u(k)$, $\Gamma_{cc}(k)$, and $\gamma(k)$). The Euler-Lagrange equations

$$\frac{\delta F_{\lambda}}{\delta u(k)} = 0, \quad \frac{\delta F_{\lambda}}{\delta \Gamma_{cc}(k)} = 0, \quad \frac{\delta F_{\lambda}}{\delta \gamma(k)} = 0$$

then determine the optimal pseudopotential, quasihole/quasiparticle spectra, and phonon/roton spectrum.

Explicit expressions for the variational derivatives in Eqs. (14) (again, in the absence of backflow) may be found in Ref. [28]. The results can be recast in the form of a generalized paired-phonon equation [9,10]

$$\bullet S(k) + \frac{1}{2}\epsilon_0(k) [S(k) - 1] = D(k)$$

for the radial distribution function or the associated static structure function $S(k)$, an analogous equation

$$\bullet S_{cc}(k) + \frac{1}{2}\epsilon_0(k)S_{cc}(k) = D_{cc}(k)$$
for the statistical exchange function \( G_{cc}(r) \) or the corresponding Fourier transform \( S_{cc}(k) \), and a Feynman equation \([29,22]\)

\[
\omega(k) = \frac{\epsilon_0(k)}{S(k)} \coth \left[ \frac{\beta}{2} \omega(k) \right]
\]

(17)

for the collective excitations with the dispersion law \( \omega = \omega(k) \) at temperature \( T = (k_B \beta)^{-1} \). Equations (15) and (16) involve the generalized structure functions \( \hat{S}(k) \) and \( \hat{S}_{cc}(k) \) along with the functions \( D(k) \) and \( D_{cc}(k) \). The Appendix and Ref. \([28]\) furnish detailed formulas and relations for these quantities.

To solve the paired-phonon equation (15), one customarily expresses it – equivalently – as a generalized Bogoliubov equation

\[
\omega^2(k) = \epsilon_0(k) \left[ \epsilon_0(k) + 2v_{p-h}(k) - 2v^*_{\text{coll}}(k) \right],
\]

(18)

where the collective potential is given by \( v^*_{\text{coll}}(k) = -2\epsilon_0(k)n(k)(n(k)+1)/S^2(k) \) and the particle-hole potential \( v_{p-h}(k) \) is taken from Ref. \([28]\).

It is instructive to note that the correlated density-matrix theory may be fruitfully viewed as a pair-density energy-functional approach \([30]\). The theory provides for systematic construction of a universal energy functional \( E = E[G(r), G_{cc}(r), B_{cc}, \rho] \) which depends on one-body quantities (particle density \( \rho \) and condensation strength \( B_{cc} \)) and on two-body densities (the radial distribution function \( G(r) \) and the statistical exchange function \( G_{cc}(r) \)). Similarly, the internal energy, the entropy, and the Helmholtz free energy are all functionals of these one- and two-body quantities. Correlated density-matrix theory may be therefore interpreted as a generalization of the Kohn-Sham approach \([31]\) that explicitly acknowledges the role played by the dynamical and statistical correlations present in the many-body system.

We further observe that the generalized paired-phonon equation (15) may be transformed into a non-linear Schrödinger equation \([28,30]\). This equation has the form \([28]\)

\[
\left\{ -\frac{\hbar^2}{m} \Delta + v(r) + w(r) + w_{\text{coll}}(r) + w_{\text{qp}}(r) \right\} \sqrt{g(r)} = 0,
\]

(19)

where \( v(r) \) is the bare \(^4\text{He}^−^4\text{He} \) interaction and the induced potentials \( w(r), w_{\text{coll}}(r), \) and \( w_{\text{qp}}(r) \) are functionals of \( G(r) \) and \( G_{cc}(r) \) and functions of particle density \( \rho \) and temperature \( T \).

4. NUMERICAL RESULTS AND DISCUSSION

Evaluation of the various components of the structure functions \( S(k) \) and \( \hat{S}(k) \) and the statistical functions \( S_{cc}(k) \) and \( \hat{S}_{cc}(k) \) is carried out with the hypernetted-chain techniques \([25,32]\), neglecting elementary diagrams. The Bogoliubov equation (18) is employed to solve the Euler-Lagrange equations efficiently by means of a suitable iteration procedure. In the normal phase, the sum rule (12) serves to determine the chemical potential \( \mu_{cc} = -\omega_{cc}(0) \) of the quasiholes (and quasiparticles). The condensation strength characterizing the condensed phase is obtained from relation (12)
in conjunction with the assumed optimization condition $\partial F/\partial B_{cc} = 0$. It must be noted, however, that the latter prescription is not entirely adequate; in future work it should be replaced by a more appropriate renormalized Hartree equation. The HFDHE2 Aziz potential [33] is adopted for the interaction between the $^4$He atoms. The $^4$He atomic bosons are confined in a cubic box at a uniform density given by the experimental saturation density $\rho(T)$ of the liquid at temperature $T$, starting with the value $\rho = 0.02185 \text{ Å}^{-3}$ at zero temperature. Reference [28] contains further information on the numerical procedures applied. Optimal versions of the various quantities have been calculated in the temperature range $T = [0 \text{ K}, 5.5 \text{ K}]$. Figures 1–7 display a selection of the numerical results.

![Figure 1](image)

**Figure 1.** The optimal structure function $S(k)$ at various temperatures and at the experimental saturation density.

Figure 1 presents the results for the structure function at several temperatures. As expected, the calculated data look very similar to earlier results [23], demonstrating that the exchange correlations (while certainly important for other quantities) affect the spatial structure of the $^4$He liquid only in its details. The variation of the low-$k$ behavior of the structure function reflects the decrease of the velocity of first sound with increasing temperature, as has been discussed in detail in Ref. [23]. The maximum of $S(k)$ at about $k \approx 2 \text{ Å}^{-1}$ shows a monotonic decrease with increasing temperature. This predicted behavior is in accord with experimental measurements in the normal phase, but it conflicts with experiment in the condensed phase, where the maximum is found to increase with temperature. The generalized Feynman relation (17) yields theoretical results for the excitation energies of the collective phonon/roton branch. The optimal data plotted in Fig. 2 shows the familiar dependence of $\omega(k)$ on wave number $k$: the linear dispersion law for phonons at low momenta and the typical roton minimum at $k \approx 2 \text{ Å}$. However, since backflow
contributions have been sacrificed in favor of a closer examination of the effects of exchange correlations, the roton minimum is more than twice what is seen experimentally. Consequently, the number of elementary excitations increases only slowly with increasing temperature. To examine more closely the implications of this behavior, let us assume for the moment that Feynman’s treatment [34] is applicable and that the superfluid density \( \rho_s \) of the \(^4\)He liquid is approximately described by the expression

\[
\rho_s = 1 - \frac{2\beta}{3N} \sum_k \epsilon_0(k) [1 + n(k)] n(k). \tag{20}
\]

If the distribution \( n(k) \) takes small values, then the excitation energy \( \omega(k) \) is large and the sum in Eq. (20) is small; therefore the superfluid density is close to unity. Accordingly, high temperatures are needed to make \( \rho_s \) become small. This rough line of reasoning already indicates that the current realization of density-matrix theory will predict a value for the normal-to-superfluid transition temperature (i.e., the temperature \( T_\lambda \) of the \( \lambda \) transition) that is significantly higher than the experimental value.

This feature of the calculation is clearly evident in the results for the respective excitation spectra \( \omega_{cc}(k) \) and \( \omega_c(k) \) of the quasiholes and the quasiparticles. Figure 3 shows their dispersion curves for particle density \( \rho = 0.02185 ~\text{Å}^{-3} \) at three different temperatures. The excitation energies are seen to exhibit a minimum around the roton minimum for temperatures below \( T < 3.1 \) K. In contrast to the case of quasiholes, the quasiparticle spectrum \( \omega_c(k) \) is restricted to wave numbers \( k > k_0 \), excitations being forbidden at smaller wave numbers. The threshold \( k_0 \) for the onset of quasiparticle excitations decreases slowly with \( T \) at very low \( T \), but it decreases very rapidly for \( T \geq 2.8 \) K and vanishes at \( T \approx 3.4 \) K. At higher temperatures, the quasiparticle and quasihole dispersion curves coincide and show a monotonic increase with increasing wave number \( k \).

The low-temperature behavior of the excitation energies can be extracted analytically from the Euler-Lagrange equations. One readily finds

\[
\omega_{cc}(k) = 2 \left[ \epsilon_0(k) - \lambda \right], \quad k < k_0, \tag{21}
\]

\[
\omega_c(k) = \omega_{cc}(k) = \left[ \epsilon_0(k) - \lambda \right] S^{-1}(k), \quad k > k_0, \tag{22}
\]

where the threshold \( k_0 \) is determined by \( 2S(k_0) = 1 \). The chemical potential of the quasiholes is therefore \( \mu_{cc} = -\omega_{cc}(0) = 2\lambda \) in the limit \( T \to 0 \).

The numerical results for the optimal potential \( \mu_{cc} \) in the temperature range \( 0 \leq T \leq 5.5 \) K are plotted in Fig. 4. As the temperature is lowered from the “large”-\( T \) side, \( \mu_{cc}(T) \leq 0 \) increases until it vanishes at a predicted transition temperature \( T_\lambda \approx 3.4 \) K. In the temperature range \( T \geq T_\lambda \), the liquid is in the normal phase where \( B_{cc} = 0 \). For \( B_{cc} > 0 \), there is effectively a potential barrier for quasiholes, formed by the sudden decrease and subsequent slow rise of \( \mu_{cc} \) as the temperature is decreased from \( T \leq 3 \) K. As \( T \) goes to zero, the hole chemical potential vanishes again and we have \( \mu_{cc}(0) = 2\lambda = 0 \). However, this low-\( T \) behavior of \( \mu_{cc} \) is an artifact of the variational condition \( \partial F_\lambda / \partial B_{cc} = 0 \) that we have imposed on the \( B_{cc} \) parameter. We expect that an improved Hartree condition on the condensation strength will produce
Figure 2. The optimal phonon/roton excitation energy $\omega(k)$ as a function of wave number $k$ at various temperatures and at the experimental saturation density.

Figure 3. The optimal quasihole energy $\omega_{cc}(k)$ and quasiparticle energy $\omega_c(k)$ as functions of wave number $k$ at various temperatures and at the experimental saturation density.
a quasihole chemical potential that increases monotonically with temperature in the condensed phase and vanishes at the $\lambda$ transition point.

The numerical predictions for the excitation energies $\omega_{cc}(k)$ and $\omega_c(k)$ themselves are very large, implying that the associated Bose distributions $n_{cc}(k)$ and $n_c(k)$ are unrealistically small. The particle-number sum rule (12) then leads inevitably to a large critical temperature $T_\lambda \simeq 3.4$ K, even larger than for a Bose gas of non-interacting $^4$He atoms and much too high compared with the experimental $\lambda$-point, $T_\lambda = 2.18$ K. It would seem that the present ansatz for the density matrix, devoid of backflow, is not flexible enough to produce a sufficiently large effective mass of the quasiholes in the medium and a concomitant reduction of the excitation energy $\omega_{cc}(k)$. This perspective is in harmony with Feynman’s argument that the motion of one helium atom through the others in the liquid increases the effective inertia of the moving atom [8]. The parameterized model of Ref. [19] also lends support to this assessment: it involves a large quasihole effective mass $m^* \simeq 1.5m$ and yields a theoretical transition temperature $T_\lambda \simeq 2.2$ K, in quantitative agreement with results derived from the present formulation by simulating the effects of backflow (see below).

Figure 5 plots the calculated optimal data for the internal energy per particle $E/N$ as a function of temperature at the fixed density $\rho = 0.02185$ Å$^{-3}$ and at the ($T$-dependent) experimental saturation density. In the temperature range $0 \leq T \leq 2$ K, the theoretical predictions (at saturation density) lie higher than the experimental results by about 2.5 K. Numerical calculations within correlated-basis-function theory [36,37] as well as variational Monte-Carlo studies [38] at zero temperature strongly suggest that the energy excess is due in large part to the omission of triplet pseudopotentials $u(r_i, r_j, r_k)$ from ansatz (2). At zero temperature, these terms essentially account for the energetic effect of backflow. As expected, the high energy per particle obtained in the present treatment is accompanied by a large theoretical value for the transition temperature, $T_\lambda \simeq 3.4$ K.

The Bose-Einstein-condensed phase and the associated violation of gauge symmetry may be characterized by the primary order parameter $B_{cc}$, which we have termed the condensation strength, or alternatively by the non-zero condensate fraction $n_0(T)$. In the temperature interval $0 \leq T < 3$ K, the $B_{cc}$ order parameter depends rather weakly on $T$, decreasing linearly from unity at $T = 0$ to about 0.8 at $T = 3$ K. For slightly higher temperatures, a drastic reduction sets in and $B_{cc}$ vanishes at $T_\lambda \simeq 3.4$ K. In this narrow region of rapid falloff of $B_{cc}$, the behavior of the solutions of the Euler-Lagrange equations depends sensitively on the properties of the quasihole and quasiparticle excitation branches, which tends to destabilize the iteration process we have employed (for details, see Ref. [28]).

The condensate fraction $n_0(T)$ has been calculated within the hypernetted-chain formalism of Ref. [39]. The numerical results are plotted in Fig. 6, where they are compared with the path-integral Monte Carlo results of Ceperley and Pollock [14]. At zero temperature, we reproduce the value $n_0(0) \simeq 9.8\%$ obtained in an earlier application of correlated density-matrix theory and reported in Ref. [40]. This value is satisfactorily close to the estimate given by the Green’s function Monte Carlo approach [41], $n_0(0) \simeq 9.0 \pm 0.3\%$. With increasing temperature below 2 K, the optimal results for $n_0(T)$ show a gradual linear decrease similar to that suggested by the path-integral Monte-Carlo data. However, the expected precipitous decline
Figure 4. The optimized quasihole chemical potential $\mu_{cc}$ versus temperature at density $\rho = 0.02185$ Å$^{-3}$ (diamonds) and at the experimental saturation density (crosses).

Figure 5. Optimal theoretical results for the energy per particle as a function of temperature $T$ at $\rho = 0.02185$ Å$^{-3}$ (diamonds) and at saturation density (crosses). The squares mark experimental data taken from Ref. [35].
Figure 6. Optimal theoretical results for the condensate fraction $n_0$ versus temperature at density $\rho = 0.02185 \, \text{Å}^{-3}$ (diamonds) and at experimental saturation density (crosses). Shown for comparison are data from path-integral Monte Carlo [14] and Green’s function Monte Carlo [41] studies (denoted respectively by squares with error bars and by the asterisk).

toward a vanishing condensate fraction is not seen until a rather large temperature is reached, $T \simeq 3.2 \, \text{K}$. This behavior, again pointing to a normal-superfluid transition temperature that is too high, is consistent with the above findings for the excitation spectra, internal energy, and condensation strength. The results of the current treatment for other observable quantities, including the entropy and velocity of sound, are discussed in Ref. [28].

To incorporate backflow effects into the present framework, we must generalize the formulae (2)—(4) defining the choice of trial density matrix. This may be done by supplementing the pseudopotentials $u(r)$ and $\gamma(r)$ by triplet (or three-point) factors and by generalizing the permanent in expression (4). Alternatively, we may introduce higher-order correlations through the device of shadow wave functions [42,43]. Either option is both formally and computationally demanding, especially since elementary-diagram contributions should be included for consistency. In advance of such a program, it is useful to adopt a more phenomenological approach: we shall assume that “backflow” has the principal effect of renormalizing the boson mass $m$ appearing in the collective and quasiparticle and quasihole terms of the energy (5). Restricting ourselves to a treatment of the normal phase, we accordingly modify the functionals (6)—(8), derived from first principles, to read

$$
E_{\text{coll}} = \sum_k \frac{m}{m_{\ast \text{coll}}} \epsilon_{\text{coll}}(k)n(k),
$$

(23)
Figure 7. The chemical potential $\mu_{cc}(T)$ of the quasiparticles (quasiholes) in the normal phase as function of temperature $T$ at density $\rho = 0.02185 \text{Å}^{-3}$ for different values of the effective mass $m^*_\text{qp}$.

$$E_{qh} = E_{qp} = \frac{1}{4} \sum_k \frac{m}{m^*_\text{qp}} \left[ \epsilon_{cc}(k) + \epsilon_0(k) \right] n_{cc}(k).$$ (24)

In general, the effective masses $m^*_\text{coll}$ and $m^*_\text{qp}$ depend on temperature, density, and wave number and differ from each other.

As anticipated, a revised optimization based on the modified functionals (23) and (24) does indeed reveal a strong sensitivity of the theoretical transition temperature $T_\lambda$ to variations in the effective mass. Figure 7 collects numerical results for the optimal chemical potential $\mu_{cc}$ of quasiparticles/quasiholes in the normal phase at density $\rho = 0.02185 \text{Å}^{-3}$, for a selection of renormalized masses $m^*_\text{qp}$. The theoretical value for $T_\lambda$ is very close to the experimental result of 2.18 K, if the choice $m^*_\text{qp} \approx 1.6m$ is adopted. The results obtained for the connection between the predicted $T_\lambda$ and the effective quasiparticle mass are essentially independent of the value chosen for the mass parameter $m^*_\text{coll}$. We note further that a judiciously tailored temperature-dependent $m^*_\text{qp}(T)$ could be used to match the theoretical results for the specific heat to the experimental data in the normal phase.

CONCLUSIONS

In summary, we have performed a complete functional optimization of the density matrix of liquid $^4$He, based on a trial form of generalized Jastrow type involving only two-point descriptors of the dynamical correlations and the collective and single-particle thermal excitations. The Euler-Lagrange equations of this approxi-
mate description have been solved numerically in the interesting temperature range $0 \leq T \leq 5.5$ K. The ansatz for the density matrix admits a simultaneous treatment of the Bose-Einstein condensed phase and the normal phase. However, in the absence of backflow effects, the predicted lambda transition temperature of $T_\lambda \simeq 3.4$ K exceeds the experimental value of 2.18 K by some 1.2 K. We argue that this shortcoming of the theory stems from an inability of the chosen trial density matrix to accommodate important variations of effective masses – an inflexibility that results in high-lying collective excitations and quasihole and quasiparticle excitations that drive the theoretical transition temperature to unrealistically high values. This view is strengthened by the results obtained when the optimization is repeated in the normal phase with an adjustable effective mass for quasiparticles. A renormalized mass $m^*_{qp} = 1.6m$ leads to a transition temperature nearly coincident with the experimental value.

To pursue a systematic microscopic inclusion of backflow and effective mass effects, the present treatment should be generalized to allow for triplet pseudopotentials or three-point factors in the temperature-dependent wave function (2) and the incoherence factor (3). These extensions will be required to achieve quantitative accuracy for the correlation energy and the dispersion relation of phonons and rotons. Existing techniques [44,45] may be appropriated to carry through the associated analysis and computations, which should include effects of elementary diagrams. In addition, a generalization of the ansatz (4) will be needed to take proper account of the quasiparticle and quasihole effective masses. The introduction of shadow coordinates [42,43] offers an alternate route to successful microscopic extension of the current realization of density-matrix theory.

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APPENDIX

In this appendix, we collect the necessary formulae for energies, occupation numbers, generalized structure functions, and related quantities.

The ingredients $E_c$, $\epsilon_{\text{coll}}$, $\epsilon_{\text{cc}}$ of the energy functional defined by Eqs. (5)–(8) have the explicit expressions

$$E_c = N\frac{\rho}{2} \int v^*(r) g(r) \, dr$$
$$+ \frac{1}{2} \sum_k \epsilon_0(k) \left[ 1 - \Theta(\eta_c(k)) \right] \Gamma_{cc}(k) \left[ 1 + S_{cc}^{(0)}(k) + 2B_{cc}S^{(0)}(k) \right], \quad (A1)$$

where

$$v^*(r) = v(r) - \frac{\hbar^2}{4m} \Delta u(r)$$
is the Feenberg effective potential [9,10], and
\[
\epsilon_{\text{coll}}(k) = \frac{1}{2} \epsilon_o(k) \left\{ \left[ 1 + 4 \gamma(k) S(k) \right]^{1/2} + 1 \right\} S(k)^{-1}, \tag{A2}
\]
\[
\epsilon_{cc}(k) = \epsilon_o(k) \left\{ 1 - \left( 1 - X_{cc}^{(0)}(k) - \Gamma_{cc}(k) \right) \left[ S_{cc}(k) - \tilde{S}_{cc}(k) \right] \right\}. \tag{A3}
\]

The thermal occupation numbers associated with collective, quasihole, and quasiparticle excitations are given respectively by
\[
n(k) = \frac{1}{2} \left\{ \left[ 1 + 4 \gamma(k) S(k) \right]^{1/2} - 1 \right\}, \tag{A4}
\]
\[
n_{cc}(k) = \Gamma_{cc}(k) \left[ 1 + S_{cc}^{(0)}(k) \right], \tag{A5}
\]
\[
n_c(k) = \Gamma_{cc}(k) \left[ 1 + S_{cc}^{(0)}(k) + 2B_{cc}S_{cc}^{(0)}(k) \right] + 1, \tag{A6}
\]
where \([F]_+\) delivers \(F\) itself if \(F \geq 0\) and zero otherwise. The structure functions \(S(k)\) and \(S_{cc}(k)\) and their various components, as well as the corresponding Fourier inverses \(g(r) = 1 + G(r)\) and \(G_{cc}(r)\), etc., are defined in Ref. [25]. They may be evaluated by means of the hypernetted-chain equations contained therein.

The functions \(D(k)\) and \(D_{cc}(k)\) appearing in the Euler-Lagrange equations (15) and (16) are constructed as [28]
\[
D(k) = -\frac{2}{N} \sum_{k'} T(k') \cdot \frac{\delta S_D(k')}{\delta u(k)} - \lambda B_{cc} \frac{\partial}{\partial B_{cc}} S(k), \tag{A7}
\]
\[
D_{cc}(k) = -\frac{1}{N} \sum_{k'} T(k') \cdot \frac{\delta S_D(k')}{\delta \Gamma_{cc}(k)} + \left[ \frac{1}{2} \omega_{cc}(k) + \lambda \right] \left[ 1 + S_{cc}^{(0)}(k) \right] \\
+ \frac{1}{2} \omega_c(k) \left\{ 1 + S_{cc}^{(0)}(k) + 2B_{cc} \left[ S_{dd}(k) + 2S_{dc}(k) \right] \right\} \Theta(n_c(k)) \\
- \epsilon_o(k) \left[ 1 + \tilde{S}_{cc}(k) \right] \\
- \lambda B_{cc} \left\{ \frac{\partial}{\partial B_{cc}} S_{cc}^{(0)}(k) + B_{cc} \frac{\partial}{\partial B_{cc}} \left[ S_{dd}(k) + 2S_{dc}(k) + S_{cc}^{(1)}(k) \right] \right\}. \tag{A8}
\]

The quantity \(S_D(k) = (S_{dd}(k), S_{de}(k), S_{ee}(k), S_{dc}(k), S_{ec}(k), S_{cc}(k))\) is defined by the indicated sextuple of components. In Eqs. (A7) and (A8) these components form a scalar product with the six components \(T^{(i)}\) of the quantity \(T(k), i = 1, 2, 3, ..., 6.\) The component \(T^{(1)}\) is made up of two terms,
\[
T^{(1)}(k) = T_1^{(1)}(k) + T_2^{(1)}(k), \tag{A9}
\]
the first being the Fourier transform

\[ T_1^{(1)}(k) = \rho \int T_1^{(1)}(r)e^{ik \cdot r} \, dr \]  

(A10)

of

\[ T_1^{(1)}(r_{12}) = \frac{\hbar^2}{8m} \left\{ \nabla_1 \left( \tilde{N}_{cc}^{(0)}(r_{12}) + \Gamma_{cc}(r_{12}) \right) \right\}^2 
+ \nabla_1 \tilde{N}_{cd}(r_{12}) \left( 4B_{cc}^2 \nabla_1 \tilde{N}_{cd}(r_{12}) 
+ 2B_{cc} \left[ 1 + N_{dc}(r_{12}) \right] \left[ 2B_{cc} N_{dc}(r_{12}) \nabla_1 \tilde{N}_{cd}(r_{12}) 
+ \nabla_1 \left( \tilde{N}_{cc}^{(2)}(r_{12}) + \Gamma_{cc}(r_{12}) \right) \right] 
+ \nabla_1 \left( \tilde{N}_{cc}^{(2)}(r_{12}) + \Gamma_{cc}(r_{12}) \right) \left[ \left( 1 + N_{dc}(r_{12}) \right) \nabla_1 \tilde{N}_{cd}(r_{12}) 
+ \nabla_1 \left( \tilde{N}_{cc}^{(2)}(r_{12}) + \Gamma_{cc}(r_{12}) \right) \right] \right\}, \]  

(A11)

and the second being given by

\[ T_2^{(1)}(k) = \frac{1}{2} B_{cc} \epsilon_0(k) \left\{ \tilde{X}_{cd}(k) + \tilde{X}_{ce}(k) + \tilde{X}_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right\} \left\{ \begin{array}{l}
\tilde{S}_{cc}^{(2)}(k) \left[ 1 - X_{dd}(k) - X_{dc}(k) - 2B_{cc} X_{dc}(k) \right] 
- \left[ 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right] \left[ X_{dc}(k) + X_{ec}(k) + X_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right] 
+ B_{cc} \Gamma_{cc}(k) \left[ \omega_{cc}(k) - \omega_c(k) \Theta(n_c(k)) \right] 
- \frac{1}{2} B_{cc} \epsilon_0(k) \left[ \tilde{X}_{cc}^{(0)}(k) + \Gamma_{cc}(k) \right]^2.
\end{array} \right\} \]  

(A12)

For \( T^{(2)} \) and \( T^{(3)} \) we have

\[
T^{(2)}(k) = \frac{1}{2} B_{cc} \epsilon_0(k) \left\{ \begin{array}{l}
\tilde{S}_{cc}^{(2)}(k) \tilde{X}_{cd}(k) \left[ 1 - X_{dd}(k) - X_{dc}(k) - 2B_{cc} X_{dc}(k) \right] 
- \tilde{X}_{cd}(k) \left[ 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right] \left[ X_{dc}(k) + X_{ec}(k) + X_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right] 
- \left[ \tilde{S}_{cc}^{(2)}(k) X_{dd}(k) + \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right) X_{dc}(k) \right] 
\times \left( \tilde{X}_{cd}(k) + \tilde{X}_{ce}(k) + \tilde{X}_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right) \end{array} \right\} \]  

(A13)
and

\[ T^{(3)}(k) = -\frac{1}{2} B_{cc} \varepsilon_0(k) \tilde{X}_{cd}(k) \left\{ \tilde{S}_{cc}^{(2)}(k) X_{dd}(k) + \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right) X_{dc}(k) \right\}. \]  

(A14)

The component \( T^{(4)} \) again consists of two parts,

\[ T^{(4)}(k) = T^{(4)}_1(k) + T^{(4)}_2(k), \]  

(A15)

the first being the Fourier transform

\[ T^{(4)}_1(k) = \rho \int T^{(4)}_1(r) e^{ikr} \, dr \]  

(A16)

of

\[ T^{(4)}_1(r_{12}) = \frac{\hbar^2}{8m} \left( 2B_{cc} \nabla_1 \tilde{N}_{cd}(r_{12}) \right) \times \left\{ 2B_{cc} (1 + N_{cd}(r_{12})) \nabla_1 \tilde{N}_{cd}(r_{12}) + \tilde{N}_{cc}^{(2)}(r_{12}) + \Gamma_{cc}(r_{12}) \right\} \]  

(A17)

and the second having the expression

\[ T^{(4)}_2(k) = \frac{1}{2} B_{cc} \varepsilon_0(k) \left\{ \left[ \tilde{S}_{cc}^{(2)}(k) \left( 1 - X_{dd}(k) - X_{de}(k) - 2B_{cc} X_{dc}(k) \right) \right. \right. \]

\[ - \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right) \left( X_{dc}(k) + X_{ec}(k) + X_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right) \]

\[ \times \left( 2B_{cc} \tilde{X}_{cd}(k) + \tilde{X}_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right) \]

\[ + \left[ \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right) \left( 1 - 2B_{cc} X_{dc}(k) - X_{cc}^{(2)}(k) - \Gamma_{cc}(k) \right) \right. \]

\[ -2B_{cc} \tilde{S}_{cc}^{(2)}(k) \left( X_{dd}(k) + X_{dc}(k) \right) \left( \tilde{X}_{cd}(k) + \tilde{X}_{ec}(k) + \tilde{X}_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right) \] \[ \right\} \]

\[ + 2B_{cc} \left[ \Gamma_{cc}(k) \left( \omega_{cc}(k) - \omega_{c}(k) \Theta(n_c(k)) \right) \right. \]

\[ - \frac{1}{2} \varepsilon_0(k) \left( \tilde{X}_{cc}^{(0)}(k) + \Gamma_{cc}(k) \right)^2 \]. \]  

(A18)

The fifth and sixth components read

\[ T^{(5)}(k) = \frac{1}{2} B_{cc} \varepsilon_0(k) \left\{ \tilde{X}_{cd}(k) \left[ 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right] \right. \]

\[ \times \left( 1 - 2B_{cc} X_{dc}(k) - X_{cc}^{(2)}(k) - \Gamma_{cc}(k) \right) \]

\[ -2B_{cc} \tilde{S}_{cc}^{(2)}(k) \left( X_{dd}(k) + X_{dc}(k) \right) \]

\[ \left. - \left( \tilde{S}_{cc}^{(2)}(k) X_{dd}(k) + \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}_{cc}^{(2)}(k) \right) X_{dc}(k) \right) \right\] \[ \times \left( 2B_{cc} \tilde{X}_{cd}(k) + \tilde{X}_{cc}^{(2)}(k) + \Gamma_{cc}(k) \right) \] \[ . \]  

(A19)
\[ T^{(6)}(k) = \frac{1}{4} \epsilon_0(k) \left\{ \left( 2B_{cc} \tilde{S}_{cd}(k) + \tilde{S}^{(2)}_{cc}(k) \right) \right. \\
\times \left( 1 - 2B_{cc}X_{dc}(k) - X^{(2)}_{cc}(k) - \Gamma_{cc}(k) \right) \\
- 2B_{cc}\tilde{S}^{(2)}_{cc}(k) \left( X_{dd}(k) + X_{dc}(k) \right) \left( 2B_{cc}\tilde{X}_{cd}(k) + \tilde{X}^{(2)}_{cc}(k) + \Gamma_{cc}(k) \right) \\
+ \frac{1}{2} \left[ \Gamma_{cc}(k) \left( \omega_{cc}(k) - \omega_c(k) \Theta(n_c(k)) \right) \\
- \frac{1}{2} \epsilon_0(k) \left( \tilde{X}^{(0)}_{cc}(k) + \Gamma_{cc}(k) \right)^2 \right]. \] (A20)

For the normal phase \((B_{cc} \equiv 0)\), these expressions simplify considerably, since many terms vanish [28].

The generalized structure functions \(\dot{S}(k)\) and \(\dot{S}_{cc}(k)\) entering the Euler-Lagrange equations (15) and (16) may be explicated using the general prescription [28]

\[ \dot{S}_{\alpha\beta}(k) = \frac{1}{N} \sum_{k'} \left( v^*(k') + v^*_{\text{coll}}(k') \right) \frac{\delta S_{\alpha\beta}(k)}{\delta u(k')} \] \\
\[ + \frac{1}{N} \sum_{k'} \left\{ \Gamma_{cc}(k') \left( \frac{1}{2} \epsilon_0(k') - \omega_{cc}(k') - \lambda \right) \\
+ \frac{1}{2} \epsilon_0(k') \left( \tilde{X}^{(0)}_{cc}(k') + \Gamma_{cc}(k') \right)^2 \right\} \frac{\delta S_{\alpha\beta}(k)}{\delta \Gamma_{cc}(k')}, \] (A21)

where \(\alpha\beta = dd, de, ee, ec, dc, \text{ or } cc\) (see Ref. [25]). The dotted function \(\dot{S}_{\alpha\beta}\) may be analyzed and evaluated within the extended Fermi hypernetted-chain formalism [28].

REFERENCES

[1] P. Kapitza, Nature 141, 74 (1938).
[2] J. F. Allen and A. D. Misener, Nature 141, 75 (1938).
[3] F. London, Nature 141, 643 (1938).
[4] F. London, Phys. Rev. 54, 947 (1938).
[5] L. Tisza, Nature 141, 913 (1938).
[6] L. Tisza, Phys. Rev. 72, 838 (1947).
[7] L. D. Landau, Zh. Eksp. Teor. Fiz. 11, 592 (1941); J. Phys. USSR 5, 71 (1941).
[8] R. P. Feynman, Phys. Rev. 91, 1291 (1953).
[9] C. E. Campbell and E. Feenberg, Phys. Rev. 188, 396 (1969).
[10] E. Feenberg, *Theory of Quantum Fluids* (Academic Press, New York, 1969).

[11] E. Feenberg, *Ann. Phys. (NY)* **84**, 128 (1974).

[12] R. M. Ziff, G. E. Uhlenbeck, and M. Kac, *Phys. Rep.* **32**, 169 (1977).

[13] C. E. Campbell, in *Recent Progress in Many-Body Theories*, Vol. 4 edited by E. Schachinger, H. Mitter, and H. Sormann (Plenum, New York, 1995), p. 29.

[14] D. M. Ceperley and E. L. Pollock, *Phys. Rev. Lett.* **56**, 351 (1986).

[15] D. M. Ceperley, *Rev. Mod. Phys.* **67**, 279 (1995).

[16] S. Fantoni and S. Rosati, *Nuovo Cimento* **25A**, 593 (1975).

[17] E. Krotscheck and M. L. Ristig, *Nucl. Phys.* **A242**, 389 (1975).

[18] K. Hiroike, *Prog. Theor. Phys.* **24**, 317 (1960).

[19] M. L. Ristig, T. Lindenau, M. Serhan, and J. W. Clark, *J. Low Temp. Phys.* **114**, 317 (1999).

[20] D. Pines, *Recent Progress in Many-Body Theories*, Springer Lecture Notes in Physics **142**, edited by J. G. Zabolitzky, M. de Llano, M. Fortes, and J. W. Clark (Springer-Verlag, Berlin, 1981), p. 202.

[21] J. Bardeen, *Physics Today* **16**, 21 (January 1963); quoted in *Physics Today* **51**, 66 (May 1998).

[22] C. E. Campbell, K. E. Kürten, M. L. Ristig, and G. Senger, *Phys. Rev. B* **30**, 3728 (1984).

[23] G. Senger, M. L. Ristig, K. E. Kürten, and C. E. Campbell, *Phys. Rev. B* **33**, 7562 (1986).

[24] G. Senger, M. L. Ristig, C. E. Campbell, and J. W. Clark, *Ann. Phys. (N. Y.)* **218**, 116 (1992).

[25] M. L. Ristig, G. Senger, M. Serhan, and J. W. Clark, *Ann. Phys. (N. Y.)* **243**, 247 (1995).

[26] J. W. Clark, M. L. Ristig, T. Lindenau, and M. Serhan, in *Condensed Matter Theories*, Vol. 12, edited by J. W. Clark and P. V. Panat (Nova Science Publishers, Commack, NY, 1997), p. 55.

[27] M. L. Ristig, T. Lindenau, M. Serhan, and J. W. Clark, in *Condensed Matter Theories*, Vol. 13, edited by J. da Providencia and F. B. Malik (Nova Science Publishers, Commack, NY, 1998), p. 119.

[28] T. Lindenau, Doctoral thesis, Universität zu Köln (Shaker Verlag, Aachen, 1999).

[29] R. P. Feynman, *Phys. Rev.* **94**, 262 (1954).

[30] E. Krotscheck, in *150 Years of Quantum Many-Body Theory*, edited by R. F. Bishop, K. A. Gernoth, and N. R. Walet (World Scientific, Singapore, 2001).

[31] W. Kohn and L. J. Sham, *Phys. Rev.* **140**, A1133 (1965).

[32] J. W. Clark, in *Progress in Particle and Nuclear Physics*, Vol. 2, edited by D. Wilkinson (Pergamon, Oxford, 1979), p. 89.
[33] R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, *J. Chem. Phys.* 70, 4330 (1979).

[34] R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, 1972), p. 318.

[35] R. K. Crawford, in *Rare Gas Solids*, Vol. 2, edited by M. L. Klein and J. A. Venables (Academic Press, New York, 1976).

[36] C. E. Campbell, *Phys. Lett. A* 44, 471 (1973).

[37] E. Krotscheck, in *Lecture Notes in Physics*, Vol. 510, edited by J. Navarro and A. Polls (Springer, Heidelberg, 1998).

[38] K. Schmidt, M. H. Kalos, Michael A. Lee, and G. V. Chester, *Phys. Rev. Lett.* 45, 573 (1980).

[39] R. Pantfördter, T. Lindenau, and M. L. Ristig, *J. Low Temp. Phys.* 108, 245 (1997).

[40] T. Lindenau, M. L. Ristig, and J. W. Clark, in *Condensed Matter Theories*, Vol. 14, edited by D. Ernst, I. Perakis, and S. Umar (Nova Science Publishers, Huntington, New York, 1999), p.131.

[41] M. H. Kalos, M. A. Lee, P. A. Whitlock, and G. V. Chester, *Phys. Rev. B* 24, 115 (1981).

[42] S. Vitiello, K. Runge, and M. H. Kalos, *Phys. Rev. Lett.* 60, 1970 (1988).

[43] L. Reatto and G. L. Masserini, *Phys. Rev. B* 38, 4516 (1988).

[44] R. P. Feynman and M. Cohen, *Phys. Rev.* 102, 1189 (1956).

[45] B. E. Clements, E. Krotscheck, J. A. Smith, and C. E. Campbell, *Phys. Rev. B* 47, 5239 (1993).