

## Correlated pairing theory of liquid ${}^3\text{He}^\dagger$

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(Received 12 April 1977)

A variational calculation of the ground-state energy of liquid  ${}^3\text{He}$  is presented. The trial wave functions investigated are correlated pairing functions. By including pairing, we are able to investigate the possibility that the ground state of liquid  ${}^3\text{He}$  is pair condensed. The correlation permits us to apply the theory to a realistic model of the  ${}^3\text{He}$  interactions, including the strong short-range repulsion. The energy of a normal-state trial function is compared at several densities to the energy of singlet  $s$ -wave pair condensed state (BCS pairing) and the isotropic triplet pair condensed state (Balian-Werthamer pairing). Within the approximations used, the lowest-energy state from this class of trial functions is the normal state. We briefly discuss possible reasons for the failure of this calculation to exhibit the experimentally observed superfluid state.

### I. INTRODUCTION

In this paper we consider the ground state of liquid  ${}^3\text{He}$  with a view toward exhibiting the pair-condensed (i.e., superfluid) nature of the ground state. We begin with a Hamiltonian of the form

$$H = \sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i < j}^N V(r_{ij}), \quad (1)$$

where  $V(r)$  is one of the phenomenological two-body potentials obtained from gas-phase data.<sup>1</sup> To be specific, the Lennard-Jones 6-12 potential is chosen for  $V(r)$ ; we do not believe that another choice from the list of phenomenological potentials would affect the qualitative results presented here, nor do we think that the inclusion of three-body or higher-order potentials would significantly alter the results.

Our method of calculation is to consider a class of trial functions which have the possibility of either the presence or the absence of off-diagonal long-range order (ODLRO), then minimize the expectation value of the Hamiltonian in this class of functions. We are faced with the familiar problem of having to deal with the strong, short-range repulsions between the helium atoms. While this precludes the direct application of a weak-coupling, BCS type of theory to the problem, that difficulty can be overcome by introducing a factor into the trial functions which takes care of the short-range correlations in a systematic fashion (e.g., a Jastrow function). This is a correlated pairing theory, and was first introduced into condensed-matter theory by Clark and Yang, who applied it to the problem of superfluidity in neutron matter.<sup>2</sup> Here we adapt this approach to the superfluid  ${}^3\text{He}$  problem. This requires developing a new approximation scheme, which is described below. For reasons of simplicity, we limit our attention to isotropic pairing, of which there are two possi-

bilities: singlet  $s$ -wave (ordinary BCS pairing) and triplet  $p$ -wave pairing [Balian-Werthamer (BW) pairing]. The energies of these states are compared to the energy of the normal state at several densities with the same approximations throughout. We find in every case that the normal state is favored over the triplet state, which in turn is favored over the singlet state. There are several possible explanations for our failure to obtain the experimentally observed superfluid state. The most plausible reason is that we have not built into our trial functions the ability to adjust the spin-density zero-point motion. We are presently investigating that possibility more carefully.

We continue this introductory section with a brief review of previous efforts on the theories of Fermi liquids relevant to our present discussion. Section II contains the more important details of the formalism. Our comparison of the energy of the superfluid and normal-fluid trial states is given in Sec. III. Section IV contains the results of our calculation of the energy versus density for the normal system. The results of Sec. IV differ quantitatively from previous calculations of the energy of the normal state primarily because we have introduced a new approximation scheme. We conclude in Sec. V with a brief discussion of the results and prospects for improved calculations.

#### A. Pair-condensed Fermi systems

Following the success of the BCS theory of superconductivity, there were several attempts to apply the theory to other Fermi systems whose ground states might also be coherent paired states. The first work on liquid  ${}^3\text{He}$  was done by several groups at about the same time. Emery<sup>3</sup> and Thouless<sup>4</sup> related the presence of a BCS-type phase transition to the divergence of the Brueckner

$T$  matrix. Emery and Sessler<sup>5</sup> and Brueckner, Soda, Anderson, and Morel<sup>6</sup> used  $T$ -matrix theory to provide an "effective pairing interaction" at the Fermi surface; they used weak-coupling BCS theory to estimate the transition temperature and shift in specific heat. Anderson and Morel<sup>7</sup> and Balian and Werthamer<sup>8</sup> generalized previous results to paired states consisting of spin triplets with odd relative orbital angular momentum.

Throughout that work estimates of  $T_c$  ranged from below 0.2 to 1 K. In 1972 the second-order phase transition to a superfluid state was actually found at 2.5 mK, with a first-order transition to another superfluid state at somewhat lower temperature, depending on the pressure.<sup>9</sup> Those properties of the condensed phases that depend on the qualitative physical microstructure (i.e., anisotropic or isotropic triplet pairing in a relative orbital  $l=1$  state) seem to be described by the work of Anderson-Morel<sup>7</sup> and Balian-Werthamer,<sup>8</sup> respectively. But the actual transition temperature and other thermodynamic properties of the system have never been calculated from the known microscopic properties of  ${}^3\text{He}$  atoms, in part because  ${}^3\text{He}$  is a *strongly interacting system*, while the best developed theoretical approach presently available for studying the highly nonanalytical pairing correlations is the phenomenological *weak-coupling* generalized BCS formalism and strong-coupling corrections to it.<sup>10, 11</sup> The only recent microscopic theory is the sophisticated  $T$ -matrix calculations of the Daresbury group<sup>12</sup>; that theory does not appear to be any more successful than earlier work in obtaining the transition temperature or the Cooper-pair  $l$  value of the paired state for  ${}^3\text{He}$ .

### B. Correlated wave-function studies of Fermi systems

In the study of Bose systems, whose symmetric wave functions are much easier to deal with, the most successful calculations of the structure, ground-state energy, sound velocity, etc., have come from correlated wave-function theory, the central feature of which is the expression of the  $N$ -body wave function in the form<sup>13-15</sup>

$$\psi = \psi_c \phi_M. \quad (2)$$

Here  $\psi_c$  is a symmetric  $N$ -body function that vanishes very rapidly as the particle "hard cores" begin to overlap, and  $\phi_M$  is a "model function" containing special physical properties of the system such as the symmetry, pairing correlations, restriction of particles to lattice sites, etc.

Motivated by the early success of correlated Bose-system calculations, and following the work of Iwamoto and Yamada,<sup>16</sup> Feenberg and Wu laid

the theoretical groundwork for application of correlated-basis-functions (CBF) techniques to Fermi systems.<sup>17</sup> Feenberg, Woo, and Tan have applied this formalism to  ${}^3\text{He}$  and have obtained reasonable agreement with the properties of  ${}^3\text{He}$  in the normal Fermi-liquid state.<sup>18-20</sup>

To consider the possibility that the ground state of a Fermi liquid is pair condensed, Clark and Yang enlarged the class of model functions  $\phi_M$  to include pair-condensed model functions  $\phi_{\text{BCS}}$ . The reference state for the normal phase is obtained by letting  $\phi_M$  be a Slater determinant  $\phi_{\text{SD}}$ , and the estimate of the condensation energy  $\epsilon_c$  is given by

$$N\epsilon_c = \frac{\langle \psi_n | H | \psi_n \rangle}{\langle \psi_n | \psi_n \rangle} - \frac{\langle \psi_s | H | \psi_s \rangle}{\langle \psi_s | \psi_s \rangle}, \quad (3)$$

where

$$\psi_n = \psi_c \phi_{\text{SD}} \quad (4)$$

and

$$\psi_s = \psi_c \phi_{\text{BCS}}. \quad (5)$$

A positive-valued  $\epsilon_c$  for some choice of BCS parameters in  $\phi_{\text{BCS}}$  indicates that  $\psi_s$  is the lower-energy state, which is interpreted as a sign that the ground state is pair condensed.

Clark and Yang<sup>2</sup> consider the question of superfluidity in neutron matter and nuclear matter using this method. They use a Jastrow function for  $\psi_c$ :

$$\psi_c = \prod_{i < j}^N e^{u(r_{ij})/2}, \quad (6)$$

where  $e^{u/2}$  approaches zero rapidly at the hard-core radius of the nucleons. By restricting their attention to low-density nuclear matter (i.e., the hard cores are a small fraction of the total volume) they were able to use a cluster expansion of the Jastrow function to evaluate the matrix elements of the Hamiltonian. The expectation value has the same form as the usual BCS expectation value except that the local potential  $V(r_{12})$  is replaced by an effective local potential  $W(r_{12})$  given by

$$\begin{aligned} W(r_{12}) = & e^{u(r_{12})} V(r_{12}) + (\hbar^2/m) \\ & \times \left[ (\nabla_1 e^{u(r_{12})/2})^2 + \frac{1}{2} (e^{u(r_{12})} - 1) \right. \\ & \left. \times \nabla^2 \gamma(r'_{12}; r_{12}) / \gamma(r'_{12}; r_{12}) \right]_{r'_{12} = r_{12}}, \quad (7) \end{aligned}$$

where

$$\gamma(r'_{12}; r_{12}) = \sum_{\sigma_1 \sigma_2} \Gamma^{(2)}(r'_1, \sigma_1, r'_2, \sigma_2; r_1, \sigma_1, r_2, \sigma_2), \quad (8)$$

where  $\Gamma^{(2)}$  is the two-body density matrix for the model state  $\phi_{\text{BCS}}$  or  $\phi_{\text{SD}}$ .

While this is an approximation which is not valid in the density range appropriate for  ${}^3\text{He}$ , it illustrates several points which hold in general. The

first is that the effective potential reduces to the pair potential in the limit where the correlation function is turned off, since then  $e^u = 1$ . Second, this effective potential is density dependent through the density dependence of  $e^u$  and  $\gamma$ . Finally, and perhaps most importantly, the effective interaction is state dependent in that it depends on the BCS parameters through the density matrix  $\gamma$ . This is a well-known feature of so-called "strongly" interacting systems. A consequence of this is that the gap equation which is generated by maximizing  $\epsilon_c$  with respect to the BCS parameters will have extra terms.

### C. ODLRO in correlated theories

The main result of the work reported in this paper is the extension of the correlated pairing theory to include the types of triplet pairing thought to exist in superfluid  $^3\text{He}$ , and the development of an approximation scheme more suitable for the  $^3\text{He}$  than that used by Clark and Yang. Before getting on with that, there are several assumptions already made which need to be stated clearly and discussed. The most crucial assumption concerns the nature of the ordering in the trial states  $\psi_n$  and  $\psi_s$ . The premise is that the central feature of the state of a fluid which gives it the coherence which is characteristic of superfluid is the existence of ODLRO, most likely ODLRO in the lowest possible density matrix (the two-body density matrix for a fermion system). Implicit in the procedure of Clark and Yang is the assumption that the presence (or absence) of ODLRO in the model function  $\phi_M$  implies the presence (or absence) of ODLRO in  $\psi$ , i.e., the presence of the correlating factor  $\psi_c$  does not affect the order *qualitatively*. This assumption restricts the choice of  $\psi_c$ . A counter example serves to illustrate the point: consider an uncorrelated BCS wave function  $\phi_{\text{BCS}}$  written as a correlated Slater determinant

$$\psi = \phi_{\text{BCS}} = \phi_{\text{SD}} \psi_c ,$$

where

$$\psi_c = \phi_{\text{BCS}} / \phi_{\text{SD}} .$$

Then clearly  $\psi$  is more highly ordered than  $\phi_{\text{SD}}$ . We speculate that this increase in the order of  $\psi$  is due to off-diagonal long-range divergences in the density matrices of this particular choice of correlating function  $\psi_c$ .

In this paper we restrict our attention to  $\psi_c$ 's which could serve as reasonably good trial functions for the boson ground state of the Hamiltonian under consideration in this problem. An example is the Jastrow function [Eq. (6)] used by

Clark and Yang. These correlating functions, taken by themselves, have a Bose condensate and ODLRO in the higher-density matrices as well.<sup>21</sup> Since they have no off-diagonal long-range *divergences*, however, we do not expect the corresponding  $\psi_n$  for a Fermi system [see Eq. (4)] to have ODLRO in any of its density matrices.

This supposition is given further support by the recent calculations of the single-body density matrix for  $\psi_n$ . Although the single-body density matrix does not have ODLRO in a Fermi system, its detailed structure reflects the presence or absence of BCS-type ODLRO in the two-body density matrix. In particular, the single-particle occupation number  $n_k$  is the Fourier transform of the single-body density matrix. In a normal Fermi liquid,  $n_k$  has a discontinuity at the Fermi surface; when BCS ODLRO is present this discontinuity disappears. Thus it is important to note that recent calculations of  $n_k$  for correlated Slater-determinant trial functions for the ground state of liquid  $^3\text{He}$  show that there is a discontinuity in  $n_k$  at the Fermi surface.<sup>22, 23</sup> This is a strong indication that a Slater-Jastrow  $\psi_n$  does not have ODLRO in the two-body density matrix, and should therefore be a reasonable reference state for the normal phase in the correlated pairing theory. We do not at present have any calculation showing that the discontinuity in  $n_k$  is absent in a correlated-pairing function of the form  $\psi_S$  [Eq. (5)], nor do we have any direct information about the two-body density matrix for either  $\psi_n$  or  $\psi_S$ .

In summary, we are motivated to assume that  $\psi_n$  has no ODLRO while  $\psi_S$  has ODLRO in the two-body density matrix. We attempt to enforce the assumption about  $\psi_n$  by restricting the correlating function  $\psi_c$  to be a function without off-diagonal long-range divergences.

## II. CORRELATED PAIRING FORMALISM

### A. Energy of a correlated Fermi system

We start by deriving an expression for the quantity

$$E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle ,$$

when the wave function is of the form  $\psi = \psi_c f$ , with

$$\int d\tau f^* f = 1, \quad \int d\tau \psi_c^* \psi_c = 1, \quad (9)$$

and we write  $d\tau = d^3r_1, \dots, d^3r_N$ , and include spin sums in the first integral. In (1),  $\phi_M = f$  is the totally antisymmetric fermion model function, either a ground-state Slater determinant (SD) or a pair-condensed BCS state.  $\psi_c$  is a completely symmetric function of all the particle coordinates, that can be chosen to be positive definite, and thus

written in the form

$$\psi_c = e^{\Phi(\tau)/2} / \left( \int e^{\Phi} d\tau \right)^{1/2}. \quad (10)$$

Using a Hamiltonian in the form of Eq. (1), the energy expectation value is

$$E = \sum_{i=1}^N \frac{\langle \psi | -(\hbar^2/2m)\nabla_i^2 | \psi \rangle}{\langle \psi | \psi \rangle} + \sum_{i < j} \frac{\langle \psi | V(r_{ij}) | \psi \rangle}{\langle \psi | \psi \rangle} = T + V.$$

Using the Jackson-Feenberg transformation the kinetic energy becomes<sup>13</sup>

$$T = -\frac{\hbar^2}{8m} \sum_{i=1}^N \left[ \left( \int \psi^* \nabla_i^2 \psi d\tau \right) - 2 \left( \int \nabla_i \psi^* \cdot \nabla_i \psi d\tau \right) + \left( \int (\nabla_i^2 \psi^*) \psi d\tau \right) \right] / \left( \int \psi^* \psi d\tau \right). \quad (11)$$

Application of the chain rule to  $\psi = \psi_c f$  and use of (9) gives after some algebra,

$$T = -\frac{\hbar^2}{8m} \left[ \int d\tau \psi_c \left( f^* f \sum_{i=1}^N \nabla_i^2 \Phi + f^* \sum_{i=1}^N \nabla_i^2 f + f \sum_{i=1}^N \nabla_i^2 f^* - 2 \nabla_i f \cdot \nabla_i f^* \right) \psi_c \right] / \int \psi_c f^* f \psi_c d\tau, \quad (12)$$

so that, regrouping the terms

$$E = \left( \int \psi_c \left[ f^* f \left( \sum_{i=1}^N -\frac{\hbar^2}{8m} \nabla_i^2 \Phi + \sum_{i < j} V(r_{ij}) \right) \right] \psi_c d\tau \right) / \left( \int \psi_c f^* f \psi_c d\tau \right) + \left[ \int d\tau \psi_c \left( f^* \sum_{i=1}^N -\frac{\hbar^2}{8m} \nabla_i^2 f + f \sum_{i=1}^N -\frac{\hbar^2}{8m} \nabla_i^2 f^* + \frac{\hbar^2}{4m} \sum_{i=1}^N \nabla_i f^* \nabla_i f \right) \psi_c \right] / \int \psi_c f^* f \psi_c d\tau. \quad (13)$$

The first term in (13) can be dealt with using a generating function developed for Bose systems.<sup>24</sup> Define

$$\psi_c(\alpha) \equiv \psi_c e^{\alpha \bar{V}/2} / [I_c(\alpha)]^{1/2}, \quad (14)$$

where

$$\bar{V} = \sum_{i < j} V(r_{ij}) - \frac{\hbar^2}{8m} \sum_i \nabla_i^2 \Phi$$

and

$$I_c(\alpha) \equiv \int \psi_c^2 e^{\alpha \bar{V}} d\tau.$$

We can now define

$$E_c \equiv \left( \int \psi_c H \psi_c d\tau \right) / \int \psi_c^2 d\tau = \frac{d}{d\alpha} \ln I_c(\alpha) \Big|_{\alpha=0}, \quad (15)$$

where  $E_c$  is the expectation value of the Hamiltonian (1) in the symmetric state  $\psi_c$ . The first term in (13) can then be written

$$E_1 = \left( \int \psi_c f^* f \bar{V} \psi_c d\tau \right) / \int \psi_c f^* f \psi_c d\tau = \frac{d}{d\alpha} \ln \left( I_c(\alpha) \int \psi_c(\alpha) f^* f \psi_c(\alpha) d\tau \right) \Big|_{\alpha=0} = E_c + \frac{d}{d\alpha} \ln \int \psi_c(\alpha) f^* f \psi_c(\alpha) d\tau \Big|_{\alpha=0}. \quad (16)$$

Using the identity

$$\nabla_i f^* \cdot \nabla_i f = \frac{1}{2} [\nabla_i^2 (f^* f) - f^* \nabla_i^2 f - f \nabla_i^2 f^*]$$

the second term in (13) can be written

$$E_2 = \left[ \int d\tau \psi_c \left( f^* \sum_{i=1}^N -\frac{\hbar^2}{4m} \nabla_i^2 f + f \sum_{i=1}^N -\frac{\hbar^2}{4m} \nabla_i^2 f^* + \frac{\hbar^2}{8m} \sum_{i=1}^N \nabla_i^2 (f^* f) \right) \psi_c \right] / \int \psi_c f^* f \psi_c d\tau. \quad (17)$$

Combining (16) and (17), we find

$$E = E_1 + E_2 = E_c + E_f + E_a + E_b \equiv E_c + E_P, \quad (17')$$

where  $E_c$  is defined in Eq. (15),

$$E_f = \left\{ \int \psi_c^2 \left[ f^* \sum_{i=1}^N \left( -\frac{\hbar^2}{4m} \nabla_i^2 f \right) + f \sum_{i=1}^N \left( -\frac{\hbar^2}{4m} \nabla_i^2 f^* \right) \right] d\tau \right\} / \int \psi_c f^* f \psi_c d\tau, \quad (18)$$

$$E_a = \left( \frac{d}{d\alpha} \int d\tau \psi_c(\alpha) f^* f \psi_c(\alpha) \Big|_{\alpha=0} \right) / \left( \int d\tau \psi_c f^* f \psi_c \right) \\ - \left( \int \psi_c \frac{\hbar^2}{8m} \sum_{i=1}^N \nabla_i^2 (f^* f) \psi_c d\tau \right) / \int d\tau \psi_c f^* f \psi_c, \quad (19)$$

and

$$E_b = \left( 2 \int \psi_c \frac{\hbar^2}{8m} \sum_{i=1}^N \nabla_i^2 (f^* f) \psi_c d\tau \right) / \int d\tau \psi_c f^* f \psi_c. \quad (20)$$

The first term in the energy  $E_c$  is the boson expectation value of the Hamiltonian and as such contains most of the energy due to short range correlations. The second term,  $E_f$ , contains most of the energy shift due to statistics. Indeed, if  $f$  is the Slater determinant,  $E_f$  is just the energy of the Fermi sea. The remaining terms in the energy,  $E_a + E_b$ , are due to cross correlations between  $f$  and  $\psi_c$ . The reason for choosing this decomposition of the remaining terms is to take advantage of the fact that  $E_a$  vanishes for special choices of  $\psi_c$ , independent of the choice of  $f$ .<sup>15,25</sup> In particular, it vanishes if  $\psi_c$  is the boson ground-state wave function of the Hamiltonian of the problem. It also vanishes if  $\psi_c$  is the optimum Jastrow trial function for the boson ground state and the approximations introduced in Sec. IID below are used.

In summary, by decomposing the energy in a particular way we have isolated the primary dependence upon the model function  $f$  in two terms,  $E_f$  and  $E_b$ . The term  $E_c$  does not depend upon  $f$  unless we allow  $\psi_c$  to change as a function of  $f$ . For simplicity we will fix  $\psi_c$  to eliminate  $E_a$ . With this choice,  $E_c$  is no longer directly relevant to the pairing equation. We discuss the implications of this choice further below.

Having made this decomposition, we have the further advantage that  $E_c$  can be calculated using any one of many successful techniques for handling symmetric many-body wave functions. The remaining terms find the differential operator  $\nabla_i^2$  operating only on the Fermi function  $f$ , leading to expressions easier to deal with than the straightforward form  $\nabla_i^2 \psi$ . This will be shown in more detail later.

#### B. Fermi-model functions $\langle f \rangle$

The Fermi-model functions are most easily described in the language of second quantization. We use generalized BCS-type states

$$\langle f \rangle = \eta_f^{-1} \prod_{\substack{k_x > 0 \\ \sigma\sigma'}} (1 + g_{\vec{k}\sigma\sigma'} c_{\vec{k}\sigma}^\dagger c_{-\vec{k}\sigma'}) |0\rangle, \quad (21.a)$$

where  $|0\rangle$  is the vacuum and

$$\eta_f \equiv \prod_{k_x > 0} \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}\sigma\sigma'}|^2 + |h_{\vec{k}}|^2 \right)^{1/2} \quad (21.b)$$

is the normalizing factor, with  $h_{\vec{k}} \equiv g_{\vec{k}\uparrow\uparrow} g_{\vec{k}\downarrow\downarrow} - g_{\vec{k}\uparrow\downarrow} g_{\vec{k}\downarrow\uparrow}$ . Note that by definition,  $g_{-\vec{k}\sigma\sigma'} = -g_{\vec{k}\sigma'\sigma}$ . In practice, it is sometimes easier to work with (21) written

$$\langle f \rangle = \tilde{\eta}_f^{-1} \prod_{\substack{k_x > 0 \\ \sigma\sigma'}} (u_{\vec{k}\sigma\sigma'} + v_{\vec{k}\sigma\sigma'} c_{\vec{k}\sigma}^\dagger c_{-\vec{k}\sigma'}) |0\rangle, \\ g_{\vec{k}\sigma\sigma'} \equiv v_{\vec{k}\sigma\sigma'} / u_{\vec{k}\sigma\sigma'}, \quad (22)$$

where  $\tilde{\eta}_f^{-1}$  is the appropriate normalizing expression. As is well known, the choice

$$u_{\vec{k}\sigma\sigma'} = 0, \quad v_{\vec{k}\sigma\sigma'} = \delta_{\sigma,-\sigma'}, \quad k < k_F, \\ u_{\vec{k}\sigma\sigma'} = \delta_{\sigma,-\sigma'}, \quad v_{\vec{k}\sigma\sigma'} = 0, \quad k > k_F, \quad (23)$$

gives the ground-state Slater determinant for the noninteracting Fermi gas. The special cases of BCS, AM, and BW pairing are specified by choosing appropriate forms of  $u_{\vec{k}\sigma\sigma'}$ ,  $v_{\vec{k}\sigma\sigma'}$ ; or alternatively, of  $g_{\vec{k}\sigma\sigma'}$ .

These forms are chosen as follows. The "order parameter" in coordinate space is defined as

$$\chi(r_1, s_1, r_2, s_2) \equiv \langle f | \psi_{s_1}(r_1) \psi_{s_2}(r_2) | f \rangle, \quad (24)$$

where  $\psi_s(r)$  is the destruction operator for a particle at  $r$  with  $Z$  component of the spin  $s$ . For a uniform system it has Fourier transform

$$\chi_{\mathcal{B}\sigma\sigma'} = \langle f | c_{\mathcal{B}\sigma} c_{-\mathcal{B}\sigma'} | f \rangle. \quad (25)$$

The "pair wave function" is defined as

$$\psi^p(r_1, s_1, r_2, s_2) \equiv \langle 0 | \psi_{s_1}(r_1) \psi_{s_2}(r_2) | f \rangle, \quad (26)$$

and it has Fourier transform

$$\psi_{\mathcal{B}\sigma\sigma'}^p = \langle 0 | c_{\mathcal{B}\sigma} c_{-\mathcal{B}\sigma'} | f \rangle. \quad (27)$$

Both (25) and (27) are in general matrices in spin space. For a state with either BW (isotropic triplet) or BCS (isotropic singlet) pairing, the matrices (25) and (27) are proportional to one another. The AM state is more complicated because of the anisotropy. For simplicity we limit our attention in this paper to BCS and BW pairing. The coefficients  $g_{\mathbf{k}\sigma\sigma'}$  are chosen in these two cases to be proportional to the weak-coupling gap  $\Delta$  as obtained by BCS and BW, respectively.

The state (21) is not an eigenstate of the particle number operator  $\hat{N}$ . Since the correlation function  $\psi_c$  is conveniently expressed only in coordinate space, we must formally consider the component  $|N\rangle$  of the state  $|f\rangle$  which is an eigenfunction of  $\hat{N}$  with eigenvalue  $N$  ( $\langle f|\hat{N}|f\rangle = N$ ):

$$\eta_N^{-1}|N\rangle \equiv \eta_N^{-1} \left( \sum_{\mathbf{k}\sigma\sigma'} g_{\mathbf{k}\sigma\sigma'} c_{\mathbf{k}\sigma}^\dagger c_{-\mathbf{k}\sigma'}^\dagger \right)^{N/2} |0\rangle, \quad (28)$$

where  $\eta_N^{-1}$  is the normalizing expression  $\eta_N = (\langle N|N\rangle)^{1/2}$ . It can be shown that the energy calculated from (21) differs from that found using (28) by  $O(N^\delta)$ , i.e.,  $E_N = E_f [1 + O(N^\delta)]$ , where

$$-\frac{1}{2} < \delta < -\frac{1}{3},$$

so that in the thermodynamic limit (27) gives the same result as (28).<sup>26</sup>

### C. Correlating function $\psi_c$

The purpose of the correlation factor  $\psi_c$  in the many-body wave function is to take care of the strongly repulsive cores of the  ${}^3\text{He}$  particles. Thus  $\psi_c$  is chosen to vanish rapidly for interparticle distances smaller than the hard-core diameter. The two forms of  $\psi_c$  used in most previous work are<sup>13-15</sup>: (a) A Jastrow function of the form of Eq. (6), with  $u$  chosen variationally to minimize either  $E_c$  or the total energy of the fermion system; and (b) the exact  $N$ -body boson ground-state wave function of the Hamiltonian (1).

As we pointed out in Sec. II A, the simplest choice is (b), so that a major component of the energy ( $E_a$ ) vanishes. Having made this choice we are still faced with the practical task of the evaluation of integrals involving  $\psi_c$ , which means we need to know some of the distribution functions for  $\psi_c$ . While we cannot solve the boson problem exactly, we can rely on much previous theory developed for the ground state of liquid  ${}^4\text{He}$  to obtain approximate information about the necessary distribution functions. We choose to approximate  $\psi_c$  by the optimum Jastrow function for the hypothetical mass-3 boson system. The procedure we use for determining this Jastrow function, the paired-phonon analysis, is precisely the procedure which has been used for the  ${}^4\text{He}$  ground-state problem,

described in Ref. (27). The He-He potential we use is the Lennard-Jones 6-12 potential

$$V(r) = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6], \quad (29)$$

using the deBoer-Michels parameters

$$\epsilon = 10.22 \text{ }^\circ\text{K}$$

and

$$\sigma = 2.556 \text{ } \text{\AA}.$$

It should be noted, however, that explicit reference to the potential used appears only in the energy in the term  $E_c$ . The potential affects the remaining terms in the energy only through the distribution functions of  $\psi_c$ . In particular, in the approximation used in this paper (described in Sec. III) we only need the liquid structure function  $S_c(k)$  defined by

$$S_c(\vec{k}) = \langle \psi_c | \rho_{\vec{k}} \rho_{-\vec{k}} | \psi_c \rangle / N \langle \psi_c | \psi_c \rangle, \quad (30)$$

where

$$\rho_{\vec{k}} = \sum_{i=1}^N e^{i\vec{k}\cdot\vec{r}_i}$$

is the density-fluctuation operator. Thus, the potential energy enters the problem only through its boson liquid-structure function, which is a much better behaved function.

### D. Approximation for the energy

We turn now to a simplification of expression (17) for the energy. Similar expressions have been dealt with before in  ${}^3\text{He}$  in the special case that  $f$  is a Slater determinant.<sup>13,18</sup> The procedure then was to cluster expand the Slater determinant, producing an approximation for the energy in terms of low-order distribution functions for  $\psi_c$ . We cannot avail ourselves of that approximation scheme in the present context because of the more general form of  $f$  of interest here. On the other hand, while Clark and Yang included the BCS form for  $f$  in their correlated pairing theory of nuclear matter, their approximation scheme was to cluster expand the correlation function  $\psi_c$  for which they used a Jastrow function.<sup>2</sup> That is a valid procedure in low-density nuclear matter, since the hard cores take up only a small fraction of the total volume. The  ${}^3\text{He}$  core takes up a large fraction of the liquid- ${}^3\text{He}$  volume so that cluster expanding  $\psi_c$  is not appropriate.

The approximation scheme we adopt in the present work is based upon the observation that all of the terms in Eqs. (17)–(20) can be written in the general form

$$I = \int P_c(r_1, \dots, r_N) P_f(r_1, \dots, r_N) dr_1 \cdots dr_N \\ \equiv \langle P_c | P_f \rangle,$$

where  $P_c$  and  $P_f$  are both symmetric functions of their arguments. In all cases  $P_c$  is just  $|\psi_c|^2$ , but  $P_f$  is a product of  $f^*$ ,  $f$  and a symmetric operator in the several possible orders, with spins summed. A complete set of symmetric functions can now be introduced into  $I$ :

$$I = \sum_n \langle P_c | n \rangle \langle n | P_f \rangle. \quad (31)$$

Our choice for the complete set of states  $|n\rangle$  is the

$$E = E_c - \sum_{k_x > 0} \frac{\hbar^2 k^2}{2m} \frac{F_F(\vec{k}) F_c(\vec{k})}{1 - F_F(\vec{k}) F_c(\vec{k})} + 2 \operatorname{Re} \sum_{\substack{k_x > 0 \\ \sigma \sigma'}} \frac{\hbar^2 k^2}{2m} g_{k\sigma\sigma'}^* \frac{\partial}{\partial g_{k\sigma\sigma'}} \ln |\eta_F|^2 \\ + 2 \operatorname{Re} \sum_{k_x > 0} \frac{\hbar^2 k^2}{2m} g_{k\sigma\sigma'}^* \frac{\partial}{\partial g_{k\sigma\sigma'}} \ln \left( \frac{1}{\Omega^N} \prod_{k_x > 0} \frac{1}{1 - F_F(\vec{k}) F_c(\vec{k})} \right), \quad (32)$$

where

$$F_c(\vec{k}) = S_c(\vec{k}) - 1, \quad F_F(\vec{k}) = S_F(\vec{k}) - 1,$$

where

$$S_F(k) = \langle f | \rho_{\vec{k}} \rho_{-\vec{k}} | f \rangle / N \langle f | f \rangle.$$

The normalization integral  $\eta_F$  and the generalized BCS parameters  $g_{k\sigma\sigma'}$  are defined in Eq. (21). Expressions for  $F_F(k)$  for all model functions considered in this paper are given in Appendix B.

The variational equation for the BCS parameters is obtained by minimizing Eq. (32) with respect to  $g_{k\sigma\sigma'}$ . This produces the gap equation of the present work. For simplicity, we illustrate the procedure by considering isotropic singlet (i.e., BCS) pairing. Toward that end we define  $|f\rangle_{\text{BCS}}$ , the BCS model function in second quantization, by

$$\prod_{k_x > 0} (1 + g_{k\sigma-\sigma}^* c_{k\sigma}^\dagger c_{-k-\sigma}^\dagger) |0\rangle / \prod_{k_x > 0} (1 + |g_{k\uparrow\uparrow}|^2 + |g_{k\uparrow\downarrow}|^2 + |g_{k\downarrow\uparrow}|^2 + |g_{k\downarrow\downarrow}|^2)^{1/2} = \prod_{k_x > 0} (u_{k\sigma-\sigma}^* + v_{k\sigma-\sigma}^* c_{k\sigma}^\dagger c_{-k-\sigma}^\dagger) |0\rangle, \quad (33)$$

where normalization is now taken care of by requiring

$$|u_{k\sigma-\sigma}^*|^2 + |v_{k\sigma-\sigma}^*|^2 = 1. \quad (34)$$

In (33)  $u_{k\sigma-\sigma}^*$  and  $v_{k\sigma-\sigma}^*$  can both be chosen real. If we now include the chemical potential explicitly (to permit the use of the second quantized form with indeterminate particle number for  $f$ ), expression (32) becomes

$$E - \mu N = E_c + \sum_{\vec{p}\lambda} n_{\vec{p}\lambda} (\epsilon_{\vec{p}}^0 - \mu) - \sum_{\vec{p}\vec{p}'\lambda} n_{\vec{p}\lambda} n_{\vec{p}'\lambda} \left( \frac{1}{N} \frac{F_c(|\vec{p} - \vec{p}'|)}{1 - F_c(|\vec{p} - \vec{p}'|) F_F(|\vec{p} - \vec{p}'|)} \right) [\epsilon_{\vec{p}}^0 (1 - n_{\vec{p}\lambda}^*) + \epsilon_{\vec{p}'}^0 (1 - n_{\vec{p}'\lambda}^*) - \frac{1}{2} \epsilon_{|\vec{p} - \vec{p}'|}^0] \\ + \frac{1}{2} \sum_{\vec{p}\vec{p}'\lambda} \left( \frac{1}{N} \frac{F_c(|\vec{p} - \vec{p}'|)}{1 - F_c(|\vec{p} - \vec{p}'|) F_F(|\vec{p} - \vec{p}'|)} \right) [\epsilon_{\vec{p}}^0 (1 - 2n_{\vec{p}\lambda}^*) + \epsilon_{\vec{p}'}^0 (1 - 2n_{\vec{p}'\lambda}^*) - \epsilon_{|\vec{p} - \vec{p}'|}^0] u_{\vec{p}} v_{\vec{p}'} u_{\vec{p}'} v_{\vec{p}}, \quad (35)$$

where  $n_{\vec{p}\lambda}^* = v_{\vec{p}\lambda}^2$ , and  $\epsilon_{\vec{p}}^0 \equiv \hbar^2 p^2 / 2m$ . To get from (32) to (35) the expression for  $F_F(k)$  from Appendix B is used.

For the normal system described by (23), (35) becomes

$$E_F - \mu N = \sum_{\vec{p}\lambda} n_{\vec{p}\lambda} \left( \frac{\hbar^2 p^2}{2m} - \mu \right) + \frac{1}{2} \sum_{\vec{p}\vec{p}'\lambda} n_{\vec{p}\lambda} n_{\vec{p}'\lambda} \left( \frac{1}{N} \frac{F_c(\vec{p} - \vec{p}') \epsilon_{|\vec{p} - \vec{p}'|}^0}{1 - F_c(\vec{p} - \vec{p}') F_F(\vec{p} - \vec{p}')} \right), \quad (36)$$

and it is tempting to identify a quasiparticle energy (measured from the Fermi level) as

$$\xi_{\vec{p}}^0 \equiv \frac{\hbar^2 p^2}{2m} + \frac{1}{N} \sum_{\vec{p}'} n_{\vec{p}'\lambda} \left( \frac{F_c(\vec{p} - \vec{p}') \epsilon_{|\vec{p} - \vec{p}'|}^0}{1 - F_c(\vec{p} - \vec{p}') F_F(\vec{p} - \vec{p}')} \right) - \mu. \quad (37)$$

[Note that  $F_c = 0$  when  $\psi_c$  is a constant (i.e., no correlation) so that  $\xi_p^0$  takes on its usual noninteracting value in the uncorrelated theory.] Then

$$E_F - \mu N = \sum_{\vec{p}\lambda} n_{\vec{p}\lambda} \xi_{\vec{p}\lambda}^0 - \frac{1}{2} \sum_{\vec{p}\vec{p}\lambda} \frac{1}{N} \left( \frac{F_c(\vec{p} - \vec{p}') \epsilon_{\vec{p} - \vec{p}'}^0}{1 - F_c(\vec{p} - \vec{p}') F_F(\vec{p} - \vec{p}')} \right), \quad (38)$$

which is similar to the usual Hartree-Fock, or mean-field, expression. Extending this to the pair-condensed (BCS) state energy, we identify

$$\xi_{\vec{p}\lambda}^{\text{BCS}} = \frac{\hbar^2 p^2}{2m} \left( 1 - 2(1 - n_{\vec{p}\lambda}) \frac{1}{N} \sum_{\vec{p}'} \frac{F_c(\vec{p} - \vec{p}') n_{\vec{p}\lambda}}{1 - F_c(\vec{p} - \vec{p}') F_F(\vec{p} - \vec{p}')} \right) - \mu + \frac{1}{N} \sum_{\vec{p}'} \frac{\epsilon_{\vec{p} - \vec{p}'}^0 F_c(\vec{p} - \vec{p}')}{1 - F_F(\vec{p} - \vec{p}') F_c(\vec{p} - \vec{p}')}. \quad (39)$$

The effective pairing interaction is identified as the coefficient of  $u_p v_p u_{p'} v_{p'}$  in Eq. (34):

$$V_{pp'\lambda} = \frac{1}{N} \frac{F_c(\vec{p} - \vec{p}') [\epsilon_{\vec{p}}^0 (1 - 2n_{\vec{p}\lambda}) + \epsilon_{\vec{p}'}^0 (1 - 2n_{\vec{p}'\lambda}) - \epsilon_{|\vec{p} - \vec{p}'|}^0]}{1 - F_c(\vec{p} - \vec{p}') F_F(\vec{p} - \vec{p}')}. \quad (40)$$

A similar formal identification can be made with the energy of the AM and BW states, except that  $V_{pp'\lambda}$  in those two cases contains angular factors not present in (40). This effective interaction is state dependent through the function  $n_{p\lambda}$  and also through the dependence of  $F_F(k)$  on the BCS parameters. This state dependence complicates the Euler-Lagrange equation (i.e., "gap" equation), obtained by minimizing the energy with respect to  $g_{k\sigma\sigma'}$ .

Introducing the BCS angles through the usual definitions

$$u_{k\sigma\sigma'}^2 - v_{k\sigma\sigma'}^2 = \cos 2\theta_{k\sigma\sigma'},$$

$$2u_{k\sigma\sigma'} v_{k\sigma\sigma'} = \sin 2\theta_{k\sigma\sigma'},$$

the BCS "gap" equation is

$$2(\epsilon_p^0 - \mu) \sin 2\theta_{p\sigma} + \frac{1}{N} \sum_{\vec{k}} \frac{F_c(\vec{k}) [\epsilon_{\vec{k}}^0 - R_{k\sigma} F_c(\vec{k})]}{[1 - F_F(\vec{k}) F_c(\vec{k})]^2} [(1 - \cos 2\theta_{\vec{p}+\vec{k},\sigma}) \sin 2\theta_{\vec{p}\sigma} + (\cos 2\theta_{\vec{p}\sigma}) (-\sin 2\theta_{\vec{p}+\vec{k},\sigma})]$$

$$- \epsilon_p^0 \frac{1}{N} \sum_{\vec{k}} \frac{F_c(\vec{k})}{1 - F_c(\vec{k}) F_F(\vec{k})} [(1 - \cos 2\theta_{\vec{k}+\vec{p}\sigma}) (2 \sin 2\theta_{\vec{p}\sigma} \cos 2\theta_{\vec{p}\sigma}) + (\cos^2 2\theta_{\vec{p}\sigma} - \sin^2 2\theta_{\vec{p}\sigma}) (-\sin 2\theta_{\vec{p}+\vec{k},\sigma})]$$

$$- \frac{1}{N} \sum_{\vec{k}} \frac{F_c(\vec{k})}{1 - F_c(\vec{k}) F_F(\vec{k})} \epsilon_{\vec{p}+\vec{k}}^0 [\cos 2\theta_{\vec{p}\sigma} (-\cos 2\theta_{\vec{p}+\vec{k},\sigma} \sin 2\theta_{\vec{p}+\vec{k},\sigma}) + \sin 2\theta_{\vec{p}\sigma} (\sin^2 2\theta_{\vec{p}+\vec{k},\sigma})] = 0, \quad (41)$$

where

$$\epsilon_{\vec{k}}^0 = \hbar^2 k^2 / 2m$$

and

$$R_{\vec{k}\lambda} \equiv \frac{1}{N} \sum_{\vec{\Gamma}} \frac{\epsilon_{\vec{\Gamma}}^0}{2} \{ \sin 2\theta_{\vec{\Gamma}\lambda} [ \sin 2(\theta_{\vec{k}+\vec{\Gamma},\lambda} + \theta_{\vec{\Gamma}\lambda}) - \sin 2\theta_{\vec{\Gamma}\lambda} ] \}. \quad (42)$$

We discuss our attempts to solve this cumbersome set of equations in Sec. III.

### III. VARIATIONAL CALCULATIONS

The goal of the work described here is a comparison of the energy of a reference normal state with several possible pair-condensed model states, keeping everything else fixed. It is useful to have an order-of-magnitude estimate of the expected energy difference between the normal state and the

superfluid state, i.e., the condensation energy. Toward that end, recall that the condensation energy in weak-coupling BCS theory is roughly  $N(0)\Delta^2$ , where  $N(0)$  is the density of states at the Fermi level and  $\Delta$  is the gap. In superconductors,  $T_c \approx \Delta$ , and assuming the same to hold for  $^3\text{He}$ , the condensation energy is of order  $10^{-6}$  K per particle. Consequently we must resolve amongst different model states energy differences as small as  $10^{-6}$  K. A calculation of the absolute energy to that accuracy for a comparison with experiment is of course meaningless; the uncertainties in the bare two-body potential are of the order of 1 K, as are the uncertainties in our ability to calculate the energy from a given potential. All is not lost, however, since we can compare the energies of two states to a much higher precision, adequate for determining energy differences of order  $10^{-6}$  K. The sensitivity to the interaction potential is at a



TABLE I. Fermi-model structure functions for the Slater determinant, and for BCS and BW states characterized by  $T^* = 0.1$  K.

$k$	$S_F^{SD}(k)$	$S_F^{BCS}(k)$	$S_F^{BW}(k)$
0	0	0.047 106 797	0.046 893 976
0.1	0.095 291 137	0.110 351 614	0.109 691 697
0.2	0.189 810 014	0.197 154 982	0.196 428 692
0.3	0.282 784 371	0.287 514 831	0.286 775 564
0.4	0.373 441 948	0.376 864 997	0.376 121 185
0.5	0.461 010 483	0.463 649 086	0.462 903 170
0.6	0.544 717 718	0.546 833 356	0.546 086 297
0.7	0.623 791 392	0.625 533 483	0.624 785 735
0.8	0.697 459 245	0.698 921 176	0.698 172 981
0.9	0.764 949 017	0.766 193 046	0.765 444 544
1.0	0.825 488 447	0.826 558 154	0.825 809 433
1.1	0.878 305 276	0.879 232 356	0.878 483 473
1.2	0.922 627 242	0.923 435 467	0.922 686 461
1.3	0.957 682 087	0.958 389 740	0.957 640 639
1.4	0.982 697 550	0.983 318 837	0.982 569 826
1.5	0.996 901 371	0.997 427 083	0.996 699 289
1.6	1	1.000 128 808	0.999 992 368
1.7	1	1.000 000 522	1.000 000 079
1.8	1	1.000 000 001	1.000 000 005
1.9	1	1.000 000 000	1.000 000 000
2.0	1	1.000 000 000	1.000 000 000
2.1	1	1.000 000 000	1.000 000 000
2.2	1	1.000 000 000	1.000 000 000
2.3	1	1.000 000 000	1.000 000 000
2.4	1	1.000 000 000	1.000 000 000
2.5	1	1.000 000 000	1.000 000 000

comparable level, i.e., if the energy difference between two states is of order  $10^{-6}$  K based upon the Lennard-Jones potential of Eq. (29), changing the potential to another of the phenomenological He-He potentials will change the energy difference by an amount of order  $10^{-7}$  K.

Calculations for isotropic pairing are much simpler than for anisotropic pairing, so we focus our attention on BCS and BW pairing. The pairing parameters  $g_{k\sigma\sigma'}$ , for these two cases are best expressed as a matrix  $\hat{g}_k$  in spin space:

$$\hat{g}_k = B_k \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (\text{BCS}), \quad (43)$$

$$F_F(\vec{k}) = \frac{1}{8\pi^2 \rho} \frac{1}{k} \left( \int_0^\infty q dq \operatorname{sech} \frac{1}{2} \beta^* \left( \frac{\hbar^2 q^2}{2m} - \mu \right) \int_{|\alpha-k|}^{\alpha+k} l dl \operatorname{sech} \frac{1}{2} \beta^* \left( \frac{\hbar^2 l^2}{2m} - \mu \right) - \int_0^\infty q dq \left[ 1 - \tanh \frac{1}{2} \beta^* \left( \frac{\hbar^2 q^2}{2m} - \mu \right) \right] \int_{|\alpha-k|}^{\alpha+k} l dl \left[ 1 - \tanh \frac{1}{2} \beta^* \left( \frac{\hbar^2 l^2}{2m} - \mu \right) \right] \right). \quad (48)$$

The fact that the innermost integral in this expression can be done analytically allows us to make our very accurate comparison between the normal-state energy and that of the different condensed states. Since most of the energy difference comes

$$\hat{g}_k = B_k \begin{pmatrix} -\sin\Theta_k e^{-i\phi_k} & \cos\Theta_k \\ \cos\Theta_k & \sin\Theta_k e^{i\phi_k} \end{pmatrix} \quad (\text{BW}), \quad (44)$$

where  $B_k$  depends only on the magnitude of  $k$  and the angles  $\phi_k, \theta_k$  are the polar angles of the vector  $\vec{k}$ . With this notation, the expectation value of  $n_{\vec{k}}$ , the fermion number operator in the *uncorrelated* model function, is given by

$$n_{\vec{k}} = \langle \phi_M | c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma} | \phi_M \rangle / \langle \phi_M | \phi_M \rangle = B_k^2 / (1 + B_k^2) \quad (45)$$

for both BCS and BW pairing. Note also that the order-parameter matrix for the uncorrelated model state has the same form in spin space as  $\hat{g}_k$ :

$$\hat{\chi}_{k\sigma\sigma'} \equiv \langle \phi_M | c_{\vec{k}\sigma} c_{-\vec{k}\sigma'} | \phi_M \rangle / \langle \phi_M | \phi_M \rangle = (1 + B_k^2)^{-1} \hat{g}_{k\sigma\sigma'}. \quad (46)$$

Our attempts to solve the ‘‘gap’’ equation for the optimum  $B_k$  met with failure presumably for want of a good starting place in the iteration scheme. To find a good starting place we parametrized our model function in terms of two parameters,  $\beta^*$  and  $\mu$ , as follows:

$$n_{\vec{k}} = (1 + e^{\beta^*(\hbar^2 k^2 / 2m - \mu)})^{-1}. \quad (47)$$

Here  $\beta^*$  is an ‘‘effective inverse temperature’’ that allows us to vary the amount of smearing out of the Fermi surface, hence the amount of pairing. This form reproduces the general shape of the Fermi sea expected for a pair-condensed ground state. The parameter  $\mu$  is chosen so that

$$\sum_{\vec{k}\sigma} n_{\vec{k}} = N,$$

where  $N$  is the number of particles in the system. With  $\mu$  determined in this fashion,  $\beta^*$  is the single variational parameter of the calculation.

In the remainder of this section we give the formal results obtained using Eq. (46) for the singlet-pairing (BCS) case only. The BW case is treated the same way, the only changes being small modifications of one term in  $F_F^{BW}(k)$  and one in the energy.

The BCS structure factor (minus one) is given by

from a narrow region of  $k$  space about  $k_p$ , and because the integrands are varying rapidly there for large  $\beta^*$ , high accuracy is difficult with a purely numerical evaluation of the integrals. This same fact presents difficulties in solving the variational

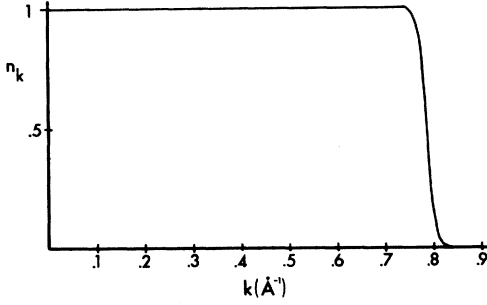


FIG. 1. Single-particle occupation number  $n_k$  as a function of  $k$  for  $T^*=0.1$  K. Here  $k_F=0.786 \text{ \AA}^{-1}$ .

equation itself numerically.

Table I lists the values of  $S_F^{\text{SD}}(k)$ ,  $S_F^{\text{BCS}}(k)$ , and  $S_F^{\text{BW}}(k)$  at  $T^*=0.1$  K for purpose of comparison. Viewed as a numerical evaluation of (48), the numbers in Table I are accurate to at least  $10^{-9}$ , and illustrate the small differences we are dealing with even in the extreme situation ( $T^*=0.1$  K) illustrated by Fig. 1. Figure 2 is a plot of  $S_F^{\text{SD}}(k)$  and  $S_F^{\text{BCS}}(k)$  as functions of  $k$ . (It should be kept in mind that the entire paper deals with  $^3\text{He}$  at  $T=0^\circ\text{K}$ , and

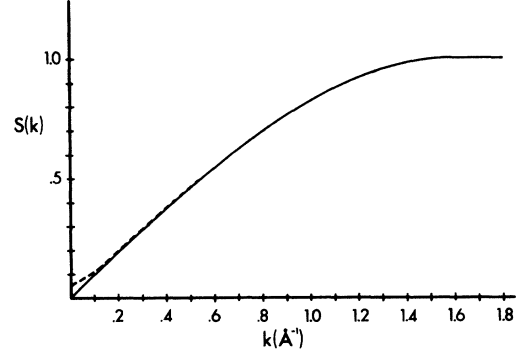


FIG. 2. Fermi-model function structure factor  $S_F(k)$  for the Slater determinant (solid line) and for a BCS-type condensed state characterized by  $T^*=0.1$  K (dashed line). On this scale the difference between  $S_F(k)$  for BCS and BW states is not visible.

that  $T^*$  is a parameter used to change the size of the region in  $k$  space over which the pairing effects are important.)

Once we have the structure factor  $S_F^{\text{BCS}}(k)$  we can find the energy. Eq. (35) in this case becomes

$$\begin{aligned}
 E^{\text{BCS}} = E_c + E_F^{\text{BCS}} = E_c + \frac{1}{8\pi^2\rho} \frac{\hbar^2}{m} \int_0^\infty k^4 dk \left[ 2[1 - \tanh y(k)] - \frac{F_c(k)F_F^{\text{BCS}}(k)}{1 - F_c(k)F_F^{\text{BCS}}(k)} \right] \\
 + \frac{1}{16\pi^4\rho^2} \int_0^\infty \frac{k dk F_c(k)}{1 - F_c(k)F_F^{\text{BCS}}(k)} \left( \int_0^\infty l dl \frac{\hbar^2 l^2}{2m} \text{sech} y(l) \tanh y(l) \int_{|l-k|}^{l+k} q dq \text{sech} y(q) \right. \\
 \left. - \int_0^\infty l dl \frac{\hbar^2 l^2}{2m} \text{sech}^2 y(l) \int_{|l-k|}^{l+k} q dq [1 - \tanh y(q)] \right), \quad (49)
 \end{aligned}$$

where  $y(x) \equiv \frac{1}{2} \beta^* (\hbar^2 x^2 / 2m - \mu)$ . All numerical integrations were done with Simpson's rule: step size was decreased until a finer mesh changed the results by  $10^{-9}$  or less. Interpolation of tabulated

functions was linear. We believe that the resulting energy shifts  $\Delta E/N$  accurately represent the predictions of our mathematical model.

Table II displays the results of this calculation

TABLE II. Fermi-sea contribution to the energy/particle at  $\rho=0.0164 \text{ \AA}^{-3}$ ,  $k_F=0.786 \text{ \AA}^{-1}$ .  $T^*$  measures the width of the region about  $\mu$  in which pairing is important. We compare singlet (BCS) and isotropic triplet (BW) states with the normal (SD) state energy at  $T=0$ .  $E_c$  must be added to get the total energy:  $E^{\text{BCS}} = E_c + E_F^{\text{BCS}}$ ,  $E^{\text{BW}} = E_c + E_F^{\text{BW}}$ , where  $E_c/N = -2.96^\circ\text{K}$  at this density.

$T^*$	$\left(\frac{E_F^{\text{SD}}}{N}\right) (^\circ\text{K})$	$\left(\frac{E_F^{\text{BCS}}}{N}\right) (^\circ\text{K})$	$\left(\frac{\Delta E_F^{\text{BCS}}}{N}\right) (^\circ\text{K})$	$\frac{E_F^{\text{BW}}}{N} (^\circ\text{K})$	$\left(\frac{\Delta E_F^{\text{BW}}}{N}\right) (^\circ\text{K})$	$\rho_{\text{cal}} (\text{\AA}^{-3})$	$\left(\frac{\Delta E^{\text{BCS}}}{N}\right) (^\circ\text{K})$
0	1.947 666 424	1.947 666 424	0	1.947 666 424	0	0.016 400 105	...
0.0001	...	1.947 788 319	0.000 121 895	1.947 788 312	0.000 121 888	0.016 400 105	...
0.0002	...	1.947 910 256	0.000 243 832	1.947 910 226	0.000 243 802	0.016 400 105	...
0.0004	...	1.948 154 230	0.000 487 805	1.948 154 110	0.000 487 686	0.016 400 106	...
0.001	...	1.948 886 968	0.001 220 544	1.948 886 219	0.001 219 795	0.016 400 106	0.000 000 067
0.002	...	1.950 111 027	0.002 444 603	1.950 108 033	0.002 441 609	0.016 400 109	...
0.004	...	1.952 569 629	0.004 903 205	1.952 557 690	0.004 891 266	0.016 400 118	...
0.01	...	1.960 028 534	0.012 336 211	1.959 954 612	0.012 288 188	0.016 400 187	...
0.1	...	2.085 490 392	0.137 823 968	2.078 983 492	0.131 317 068	0.016 408 292	0.000 006 662

TABLE III. Condensed-state energy as a function of  $T^*$  for  $\rho=0.0153 \text{ \AA}^{-3}$ ,  $k_F=0.768 \text{ \AA}^{-1}$ . Add  $E_c$  to get the total energy:  $E_c/N=-3.00^\circ\text{K}$ .

$T^*$	$E_F^{\text{BCS}}/N$	$E_F^{\text{BW}}/N$	$(E^{\text{BW}}-E^{\text{SD}})/N$	$(E^{\text{BCS}}-E^{\text{BW}})/N$
0	1.891 281 673	1.891 281 673	0	0
0.000 095	1.891 393 983	1.891 393 976	0.000 112 303	0.000 000 007
0.000 190	1.891 506 333	1.891 506 305	0.000 224 632	0.000 000 028
0.000 382	1.891 731 126	1.891 731 014	0.000 449 341	0.000 000 112
0.000 955	1.892 406 269	1.892 405 572	0.001 123 899	0.000 000 697
0.001 910	1.893 534 154	1.893 531 370	0.002 249 697	0.000 002 783
0.003 819	1.895 799 740	1.895 788 636	0.004 506 963	0.000 011 104
0.009 548	1.902 674 326	1.902 605 559	0.011 323 886	0.000 068 667
0.095 477	2.018 565 270	2.012 502 197	0.121 220 524	0.006 887 941

TABLE IV. Condensed-state energy as a function of  $T^*$  for  $\rho=0.0189 \text{ \AA}^{-3}$ ,  $k_F=0.824 \text{ \AA}^{-1}$ . Add  $E_c$  to get the total energy:  $E_c/N=-2.62^\circ\text{K}$ .

$T^*$	$E_F^{\text{BCS}}/N$	$E_F^{\text{BW}}/N$	$(E^{\text{BW}}-E^{\text{SD}})/N$	$(E^{\text{BCS}}-E^{\text{BW}})/N$
0	2.066 107 402	2.066 107 402	0	0
0.000 109	2.066 250 633	2.066 250 624	0.000 143 222	0.000 000 009
0.000 220	2.066 393 912	2.066 393 877	0.000 286 475	0.000 000 035
0.000 440	2.066 680 585	2.066 680 445	0.000 573 043	0.000 000 140
0.001 099	2.067 541 538	2.067 540 668	0.001 433 266	0.000 000 870
0.002 198	2.068 979 698	2.068 976 221	0.002 868 819	0.000 003 477
0.004 397	2.071 868 012	2.071 854 148	0.005 746 746	0.000 013 864
0.010 992	2.080 627 938	2.080 542 125	0.014 434 723	0.000 085 813
0.109 920	2.227 434 131	2.219 895 249	0.153 787 847	0.007 538 882

TABLE V. Condensed-state energy as a function of  $T^*$  for  $\rho=0.0214 \text{ \AA}^{-3}$ ,  $k_F=0.858 \text{ \AA}^{-1}$ . Add  $E_c$  to get the total energy:  $E_c/N=-1.77^\circ\text{K}$ .

$T^*$	$E_F^{\text{BCS}}/N$	$E_F^{\text{BW}}/N$	$(E^{\text{BW}}-E^{\text{SD}})/N$	$(E^{\text{BCS}}-E^{\text{BW}})/N$
0	2.174 650 223	2.174 650 223	0	0
0.000 119	2.174 814 160	2.174 814 150	0.000 163 927	0.000 000 010
0.000 239	2.174 978 151	2.174 978 112	0.000 327 889	0.000 000 039
0.000 478	2.175 306 263	2.175 306 104	0.000 655 881	0.000 000 159
0.001 194	2.176 291 650	2.176 290 658	0.001 640 435	0.000 000 992
0.002 388	2.177 937 601	2.177 933 637	0.003 283 414	0.000 003 964
0.004 776	2.181 242 987	2.181 227 180	0.006 576 957	0.000 015 807
0.011 941	2.191 265 832	2.191 168 007	0.016 517 784	0.000 097 825
0.119 411	2.358 826 778	2.350 238 035	0.175 587 812	0.008 588 743

TABLE VI. Condensed-state energy as a function of  $T^*$  for  $\rho=0.0239 \text{ \AA}^{-3}$ ,  $k_F=0.891 \text{ \AA}^{-1}$ .  $E_c$  to get the total energy:  $E_c/N=-0.35 \text{ }^\circ\text{K}$ .

$T^*$	$E_F^{\text{BCS}}/N$	$E_F^{\text{BW}}/N$	$(E^{\text{BW}}-E^{\text{SD}})/N$	$(E^{\text{BCS}}-E^{\text{BW}})/N$
0	2.274 882 890	2.274 882 890	0	0
0.000 129	2.275 067 035	2.275 067 024	0.000 184 134	0.000 000 011
0.000 257	2.275 251 240	2.275 251 195	0.000 368 305	0.000 000 045
0.000 514	2.275 619 792	2.275 619 613	0.000 736 723	0.000 000 179
0.001 285	2.276 726 616	2.276 725 500	0.001 842 61	0.000 001 116
0.002 571	2.278 575 360	2.278 570 901	0.003 638 011	0.000 004 459
0.005 142	2.282 287 801	2.282 270 024	0.007 387 134	0.000 017 777
0.012 854	2.293 543 392	2.293 433 381	0.018 550 491	0.000 110 011
0.128 539	2.481 392 779	2.471 733 401	0.196 850 511	0.009 659 378

for a range of values of  $T^*$  at the saturated vapor pressure density  $\rho=0.0164 \text{ \AA}^{-3}$  ( $k_F=0.786 \text{ \AA}^{-1}$ ). In that table we have used the definitions

$$\Delta E^{\text{BW}}/N = (E^{\text{BW}} - E^{\text{SD}})/N \quad (50)$$

and

$$\Delta E^{\text{BCS}}/N = (E^{\text{BCS}} - E^{\text{SD}})/N, \quad (51)$$

where  $E^{\text{SD}}$  is the reference normal-state energy. With these definitions, pair condensation would be signalled by a negative value of  $\Delta E$ .

The chemical potential used in these calculations is

$$\mu = \mu_0 = \hbar^2 k_F^2 / 2m, \quad (52)$$

which introduces a small error, as can be seen by the calculated density  $\rho^{\text{cal}}$  given in Table II:

$$\rho^{\text{cal}} = \frac{1}{\Omega} \sum_{\mathbf{k}} n_{\mathbf{k}}, \quad (53)$$

where  $\Omega$  is the volume of the system. We determined the effect of this approximation for  $\mu$  by including the leading correction:

$$\mu \simeq \mu_0 \left[ 1 - \frac{1}{12} \pi^2 (k_B T^* / \mu_0)^2 \right].$$

This produces an *additional* small shift in the energy given as  $\Delta E'/N$  in Table II. We see that even with the variational parameter  $T^*$  as large as 0.01 K, the additional shift  $\Delta E'/N$  is much smaller than  $\Delta E^{\text{BCS}}/N$  and  $\Delta E^{\text{BW}}/N$ .

A convenient procedure for scaling some of the Fermi quantities to other densities is given in Appendix C. Then the main results of this paper,  $\Delta E^{\text{BCS}}$  and  $\Delta E^{\text{BW}}$  as a function of the variational parameter  $T^*$  and density, are given in Tables II–VI.

It is convenient to think of  $T^*$  as the half width of the region about  $E_F$  in which pairing effects are important, i.e., where  $0 < n_{\mathbf{k}} < 1$ . Within the approximations we have made, we find no phase transition to either singlet or triplet pair-condensed state: the normal state characterized by a correlated Slater determinant is always the state of

lowest energy. This is illustrated for  $\rho=0.0164$  in Fig. 3. However, at all densities considered, the triplet-paired state has lower energy than the singlet paired state, which is a good sign that with a bit more sophisticated model function (say, the inclusion of spin-density fluctuations if possible) or perhaps a smaller number of approximations, we may soon see the condensed phases of bulk liquid  ${}^3\text{He}$  appear as a result of the atomic properties of  ${}^3\text{He}$  atoms. On the other hand, if the approximations we have made are good ones, our results might indicate that, over and beyond stabilizing the AM phase with respect to the BW phase as is now believed<sup>11,29</sup> the paramagnon fluctuations may be essential for any pairing at all to occur. We should emphasize again, however, that we have not considered anisotropic pairing. In particular we have not considered singlet *d*-wave pairing, where con-

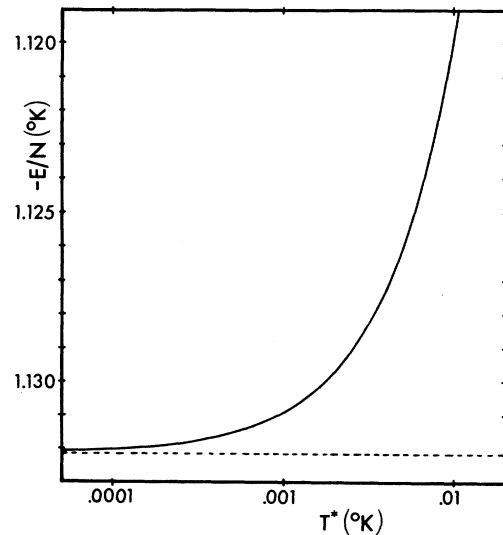


FIG. 3. Energy per particle as a function of  $T^*$  at the saturated vapor pressure density  $\rho=0.0164 \text{ \AA}^{-3}$  (solid line). The dashed line is located at the normal state (Slater determinant) energy for reference.

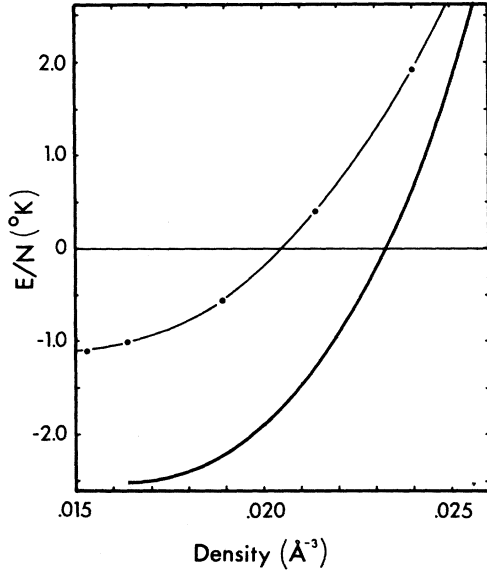


FIG. 4. Energy per particle in the normal state as a function of density. Solid circles are results of this calculation. Solid line is the experimental curve.

densation was predicted by the early *t*-matrix calculations.<sup>3-6</sup> While an extension of our calculation to *d*-wave pairing might produce a paired state of lower energy than the reference normal state, the effort required for such a calculation is not merited by this possibility.

#### IV. NORMAL-STATE RESULTS

While the focus of our calculation has been the question of superfluidity in liquid <sup>3</sup>He, we have in the process produced a new approximate expression for the normal-state energy as a function of density given by Eq. (36). This expression differs from that given by Wu and Feenberg<sup>17</sup> by the appearance of the denominator in the last term of (36).

The results of this calculation are shown in Fig. 4. Note that the experimental and theoretical results differ by a fairly constant energy ( $\approx 1.5$  °K) as a function of density, although the calculated equilibrium lies at a lower density than experiment.

#### V. DISCUSSION

The method of calculation we have introduced here gives results for the normal-state energy of <sup>3</sup>He in reasonable agreement with experiment in view of the fact that the total energy involves large cancellations between the potential energy and the kinetic

energy. We are not yet able to show the experimentally observed transition to a pair-condensed state. We hope to make refinements in the general approach described in this paper which will enable us to describe the pair-condensed ground state of liquid <sup>3</sup>He.

There are several refinements which bear mentioning here, any one of which might produce the desired result. Perhaps the first which comes to mind is to change the bare He-He interaction  $V(r)$  which appears in Eq. (1). This would affect our calculations here by changing  $\psi_c$ , which would produce a change in  $S_c(k)$ . This certainly would produce quantitative changes in our results. We believe, however, that the essential features of the <sup>3</sup>He system are well-represented by the Lennard-Jones 6-12 potential used here, namely, a strong, short-range repulsion followed by a weak attraction which goes asymptotically into the Van der Waals attraction. This potential, or any of the other phenomenological helium potentials, should produce a pair-condensed triplet phase qualitatively similar to that seen experimentally. We think the wisest course for our calculation is to stick with a single, reasonable potential and refine the many-body theory. The quantitative effects of changing the potential can be investigated after the many-body theory has been adequately developed.

There are two types of refinements of our formalism which should be considered. The first has to do with the form of the correlated pairing theory, while the second one has to do with the approximations used here. The question of the adequacy of the approximations is particularly difficult, since liquid helium seems to be a system for which there is no natural small parameter in which to expand. While we give a rationale in Appendix A for expecting the higher-order terms in our cumulant analysis to be of less import than the terms we have retained, we know of no simple way to place an estimate on these contributions.

Probably the most fertile area for modifications in the theory presented here is in the class of trial functions used in the correlated pairing theory, Eq. (2). It should be noted that all of the variations permitted in our calculation have been in the model function  $\phi_M$ . The function  $\psi_c$  has been fixed at the value determined by the <sup>3</sup>He boson problem of the same density, and  $\phi_M$  is only permitted to sample the generalized BCS functions. Thus our reference normal state (with  $\phi_M$  a Slater determinant) has no variational latitude at all. We would certainly expect some improvement in our calculated normal-state energy if we allow  $\psi_c$  to vary (being careful to let it vary only over those functions for which  $\psi = \psi_c \phi_{SD}$  does not have ODLRO). One straightforward approach to this problem is to consider a mod-

ification to  $\psi_c$ :

$$\psi_c = \psi_B \prod_{i < j} e^{u(r_{ij})/2}, \quad (54)$$

where  $\psi_B$  is the boson ground state used in this paper and  $e^{u/2}$  is a Jastrow function which can be varied to remove the over correlations due to the presence of the Slater determinant. That is,  $u$  is chosen to satisfy

$$(\delta/\delta u) \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle = 0. \quad (55)$$

With this Jastrow factor present in  $\psi_c$ , the term  $E_a$  [Eq. (19)] in the energy no longer vanishes, but it may be calculated using similar approximations to those discussed in Appendix A. The results of this calculation are reported elsewhere,<sup>30</sup> where it is noted that the resultant shift in the ground state energy per particle is rather small, (0.03 K at equilibrium density). These corrections come from throughout the Fermi sea. The significant function in the pairing question  $S_c(k)$  also undergoes small changes in the range  $0 \leq k \leq 2k_f$ , with the largest changes occurring at long wavelengths.

When the pairing model functions are used for  $\phi_M$ , Eq. (55) should be solved for each choice of BCS parameters. However since the difference in energy between the normal and pair condensed states is the primary interest here, and since the change in  $u$  has occurred for both the normal and condensed trial function, we expect the condensation energy to be changed by only a few percent. This point should be investigated further, however.

As we have pointed out several times above, the most significant omission in our calculation is a careful treatment of spin correlations (or, more suggestively, spin-density fluctuations). This is seen most clearly in the reference normal-state

trial function, where the spin coordinates enter only through the Slater determinant. It could be said that they are only treated in a mean-field fashion. The inadequacy of this trial function for spin correlations is demonstrated by the fact that the calculated magnetic susceptibility of this system is an order of magnitude larger than the experimental value<sup>31</sup> (the state is too highly paramagnetic). This problem is rectified to some extent by introducing a linear combination of excited state Slater determinants for  $\phi_M$  with coefficient determined by second order perturbation theory.<sup>18,20</sup> The result is an improvement in the ground state energy by  $-0.4$  K per particle and a magnetic susceptibility which is within 20% of the experimental value.

Thus we feel that the most promising extension of our theory is the development of a procedure for including spin density fluctuations in the formalism. We hope to make some progress in that direction in the near future.

#### APPENDIX A

To obtain Eq. (32) from (18) and (20) we express the integrands as generalized Fourier series in  $(r_1, \dots, r_N)$ . The general procedure for doing this will be given elsewhere.<sup>28</sup> To summarize it, we note first that  $\psi_c^2$  and  $f^*f$  are functions totally symmetric in the valuables  $(r_1, \dots, r_N)$  so that a good set of basis functions for a Fourier expansion is

$$\rho^{(m)}(\vec{p}_1, \dots, \vec{p}_m) \equiv \sum_{i_1 \neq i_2 \neq \dots \neq i_m} e^{i(\vec{p}_1 \cdot \vec{r}_{i_1} + \vec{p}_2 \cdot \vec{r}_{i_2} + \dots + \vec{p}_m \cdot \vec{r}_{i_m})}. \quad (A1)$$

These functions are orthogonal but not normalized. The normalized versions of (A1) are

$$q(n_1, \dots, n_r) \equiv \left\{ \left[ \left( N - \sum_{i=1}^r n_i \right)! \right]^{1/2} / \Omega^{N/2} (N!)^{1/2} \left( \prod_{i=1}^r n_i! \right)^{1/2} \right\} \rho^{(\sum_{i=1}^r n_i)}(\vec{p}_1, \dots, \vec{p}_1 \vec{p}_2, \dots, \vec{p}_2, \dots, \vec{p}_r, \dots, \vec{p}_r), \quad (A2)$$

where  $N$  is the number of particles in the system and  $\Omega$  is the system's volume; the argument  $\vec{p}_i$  appears  $n_i$  times in the set  $(\vec{p}_1, \dots, \vec{p}_r)$ . The  $\rho^{(m)}$  can be thought of as generalized density fluctuation operators, since they can be expressed as polynomials in the ordinary density fluctuation operators  $\rho_k \equiv \sum_i e^{i\vec{k} \cdot \vec{r}_i}$ ; i.e.,

$$\rho^{(1)}(\vec{k}_1) = \rho_{\vec{k}_1}, \quad (A3)$$

$$\rho^{(2)}(\vec{k}_1, \vec{k}_2) = \sum_{i \neq j} e^{i\vec{k}_1 \cdot \vec{r}_i} e^{i\vec{k}_2 \cdot \vec{r}_j} = \rho_{\vec{k}_1} \rho_{\vec{k}_2} - \rho_{\vec{k}_1 + \vec{k}_2}, \text{ etc.}$$

To use these functions in the energy expression, we assume that  $\psi_c$  is the boson ground state wave function so that  $E_a$  defined by (18) vanishes. Then

$$E = E_c + \left[ \int \psi_c \left( f^* \sum_{i=1}^N -\frac{\hbar^2}{4m} \nabla_i^2 f + f \sum_{i=1}^N -\frac{\hbar^2}{4m} \nabla_i^2 f^* \right) \psi_c d\tau \right] / \left( \int \psi_c f^* f \psi_c d\tau \right) + 2 \left( \int \psi_c \frac{\hbar^2}{8m} \sum_{i=1}^N \nabla_i^2 (f^* f) \psi_c d\tau \right) / \int \psi_c f^* f \psi_c d\tau. \quad (A4)$$

Since the second term in (A4) contains  $\nabla_{\mathbf{i}}^2$  operating on  $f$  or  $f^*$  separately, it can be evaluated only when a specific form for  $f$  has been chosen. On the other hand, the last term can be evaluated outright, and we use it to show how the density-fluctuation expansion lends itself to a simple approximation. We now evaluate

$$\left(2 \int \psi_c \frac{\hbar^2}{8m} \sum_{\mathbf{i}=1}^N \nabla_{\mathbf{i}}^2 (f^* f) \psi_c d\tau\right) / \int \psi_c f^* f \psi_c d\tau.$$

(a) Denominator. First expand

$$\begin{aligned} \int \psi_c f^* f \psi_c &= \left( \prod_{\mathbf{i}} \sum_{n_{\mathbf{i}}} \right) C(\{n_{\mathbf{i}}\}) \int \psi_c q(\{n_{\mathbf{i}}\}) \psi_c d\tau \\ &= \left( \prod_{\mathbf{i}} \sum_{n_{\mathbf{i}}} \right) \left[ \frac{(N - \sum n_{\mathbf{i}})!}{(\Omega^N N! \prod_{\mathbf{i}} n_{\mathbf{i}}!)} \right] \left( \int f^* f \rho^*(\{n_{\mathbf{i}}\}) d\tau \right) \left( \int \psi_c^2 \rho(\{n_{\mathbf{i}}\}) d\tau \right). \end{aligned} \quad (\text{A6})$$

Now define

$$\int f^* f \rho^*(\{n_{\mathbf{i}}\}) d\tau \equiv G_m^f(\{n_{\mathbf{i}}\}),$$

where

$$m \equiv \sum_{\mathbf{i}} n_{\mathbf{i}}, \quad (\text{A7})$$

and likewise

$$\int \psi_c^2 \rho(\{n_{\mathbf{i}}\}) d\tau \equiv G_m^c(\{n_{\mathbf{i}}\}).$$

These functions have cumulant expansions<sup>32</sup> defined by

$$\begin{aligned} G_1(\vec{k}_1) &\equiv F_1(\vec{k}_1), \\ G_2(\vec{k}_1, \vec{k}_2) &\equiv F_1(\vec{k}_1)F_1(\vec{k}_2) + F_2(\vec{k}_1, \vec{k}_2), \\ G_3(\vec{k}_1, \vec{k}_2, \vec{k}_3) &\equiv F_1(\vec{k}_1)F_1(\vec{k}_2)F_1(\vec{k}_3) \\ &\quad + F_1(\vec{k}_1)F_2(\vec{k}_2, \vec{k}_3) + F_1(\vec{k}_2)F_2(\vec{k}_1, \vec{k}_3) \\ &\quad + F_1(\vec{k}_3)F_2(\vec{k}_1, \vec{k}_2) + F_3(\vec{k}_1, \vec{k}_2, \vec{k}_3), \end{aligned} \quad (\text{A8})$$

etc.

Since the  $F_j(\{n_{\mathbf{i}}\})$  have the translational properties of the system, we have for a uniform system

$$F_j(\{n_{\mathbf{i}}\}) = 0 \quad \text{if} \quad \sum \vec{k} \neq 0, \quad (\text{A9})$$

The functions  $F_n$  have some very useful properties for convergence of series expressions such as (A6). The two factors on the right-hand side of (A6) are  $G_n$  functions, one  $G_n^c$  and the other  $G_n^f$ . By the definitions (A8), the right-hand side of (A6) becomes a polynomial in the  $F_n$  functions ( $F_n^c$  and  $F_n^f$ ).

$$f^* f = \left( \prod_{\mathbf{i}} \sum_{n_{\mathbf{i}}} \right) C(\{n_{\mathbf{i}}\}) q(\{n_{\mathbf{i}}\}), \quad (\text{A5})$$

where

$$C(\{n_{\mathbf{i}}\}) = \int q^*(\{n_{\mathbf{i}}\}) f^* f d\tau$$

and  $(\prod_{\mathbf{i}} \sum_{n_{\mathbf{i}}})$  means the sum over all distinct choices  $(n_1, \dots, n_r)$  such that

$$\sum_{\mathbf{i}=1}^r n_i \leq N.$$

Then the denominator is

As observed in (A9), these  $F_n$  functions either vanish or are of order  $N$ , depending on the momentum sum. Thus the different terms in (A6) are of different orders in  $N$ , and the order in  $N$  can be determined by counting the number of  $F$  factors, the number of free momentum sums, and taking account of the combinatoric factors involving  $N$ . Of course the series is not isotropic in  $N$ , but instead must exponentiate:

$$\left( \int \psi_c f^* f \psi_c d\tau \right) / \int \psi_c^2 d\tau \int f^* f d\tau = e^{O(N)}.$$

Any approximation for this series must be chosen to preserve this exponentiated dependence upon the number of particles. One such approximation scheme is to set  $F_n = 0$  for  $n$  larger than some pre-assigned value.

An approximation scheme where higher order  $F_n$ 's are zero can be given further support by considering the values these functions take on for noninteracting systems. For example, the  $F_n$  all vanish in the noninteracting Bose ground state, which follows from the fact that the  $\rho^{(n)}$  are all orthogonal to a constant. For the noninteracting Fermi gas (i.e., the ground state Slater determinant) the  $F_n$  do not vanish but they do become increasingly less important as  $n$  increases. To see this, recall the well-known result that

$$F_2(\vec{k}_1 - \vec{k}) = \frac{\langle \phi_{SD} | \rho_{\vec{k}} \rho_{-\vec{k}} - N | \phi_{SD} \rangle}{\langle \phi_{SD} | \phi_{SD} \rangle} = -2 \sum_{\substack{\vec{p} \\ p \leq k_F, |\vec{p} + \vec{k}| \leq k_F}} 1,$$

which is  $-2$  times the covolume of two Fermi spheres a distance  $k$  apart. Similarly,  $F_3(\vec{k}_1, \vec{k}_2, \vec{k}_3)$  for the Slater determinant is  $-4$  times the covol-

ume of three Fermi spheres centered at the corners of the triangle formed by the three momenta  $\vec{k}_1$ ,  $\vec{k}_2$ , and  $\vec{k}_3$ . This result generalizes so that  $F_n^f(\vec{k}_1, \dots, \vec{k}_n)$  is a measure of the covolume of  $n$  Fermi spheres centered at the vertices of the polyhedron formed by the momenta  $\vec{k}_1, \dots, \vec{k}_n$ . Thus  $F_n$  for the ground state Slater determinant is an increasingly short-ranged function of its arguments as  $n$  increases, and can be reasonably approximated by zero beyond some value of  $n$ .

It should be clear from this discussion that one systematic approximation scheme is to set  $F_n$  to zero beyond some value of  $n$  for both the Bose and Fermi factors in the correlated wave function. In this paper we have taken the simplest nontrivial approximation, which is to set  $F_n = 0$  for  $n \geq 3$  for both factors. In analogy with the analysis of products of density fluctuation operators,<sup>32,33</sup> this produces the approximate result

$$G_m(\{n_{\vec{k}}\}) = \prod_{\vec{k}} n_{\vec{k}}! [F_2(\vec{k}_i, -\vec{k}_i)]^{n_{\vec{k}_i}} \delta_{n_{\vec{k}_i}, n_{-\vec{k}_i}},$$

$$m = \sum_{\vec{k}} n_{\vec{k}} = \text{even}, \quad (\text{A10})$$

$$G_m(\{n_{\vec{k}}\}) = 0, \quad m = \text{odd}.$$

All these properties apply to both integrals

$$G_m^c(\{n_{\vec{k}}\}) = \int d\tau \psi_c^2 \rho(\{n_{\vec{k}}\}),$$

and

$$G_m^f(\{n_{\vec{k}}\}) = \int d\tau f^* f \rho^*(\{n_{\vec{k}}\}).$$

Putting them into (A6) we get

$$\int \psi_c f^* f \psi_c d\tau = \left( \prod_{\vec{k}_x > 0} \sum_{n_{\vec{k}}} \right) \left[ (N - \sum n_{\vec{k}})! / \Omega^N N! \right] \\ \times [F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k})]^{n_{\vec{k}}}. \quad (\text{A11})$$

The central assumption of all cluster expansion in many-body theory is that the series converges after a small number of terms. Thus in (A11) we set

$$(N - \sum n_{\vec{k}})! / N! \approx 1 / N^{\sum n_{\vec{k}}}, \quad (\text{A12})$$

and remove the restriction that  $m = \sum n_{\vec{k}} \leq N$ , to get

$$\int \psi_c f^* f \psi_c d\tau \approx \frac{1}{\Omega^N} \left( \prod_{\vec{k}_x > 0} \sum_{n_{\vec{k}}} \right) \left( \frac{F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k})}{N^2} \right)^{n_{\vec{k}}} \\ = \frac{1}{\Omega^N} \prod_{\vec{k}_x > 0} \frac{1}{1 - F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k}) / N^2}. \quad (\text{A13})$$

(b) Numerator. Applying (A5) to the numerator, we have

$$\int \psi_c \left[ \sum_{i=1}^N \frac{\hbar^2}{4m} \nabla_i^2 (f^* f) \right] \psi_c \\ = - \left( \prod_{\vec{k}} \sum_{n_{\vec{k}}} \right) \left( \sum_{\vec{k}} \frac{\hbar^2 k^2}{4m} n_{\vec{k}} \right) \left[ (N - \sum n_{\vec{k}})! / \Omega^N N! \prod_{\vec{k}} n_{\vec{k}}! \right] \int d\tau f^* f \rho^*(\{n_{\vec{k}}\}) \int d\tau \psi_c^2 \rho(\{n_{\vec{k}}\}), \quad (\text{A14})$$

where  $\sum_{\vec{k}}'$  means that a term characterized by  $\{n_{\vec{k}}\}$  is multiplied by  $\sum_{\vec{k}} (\hbar^2 k^2 / 4m) n_{\vec{k}}$ . Putting (A11) into the right-hand side of (A14) leads to

$$-\frac{1}{\Omega^N} \sum_{i_x > 0} \sum_{n_{\vec{k}}} \frac{\hbar^2 l^2}{4m} \times 2n_{\vec{k}} \left( \frac{F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l})}{N^2} \right)^{n_{\vec{k}}} \left[ \left( \prod_{\substack{\vec{k}_x > 0 \\ \vec{k} \neq \vec{l}, -\vec{l}}} \sum_{n_{\vec{k}}} \right) \left( \frac{F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k})}{N^2} \right)^{n_{\vec{k}}} \right] \\ = -\frac{1}{\Omega^N} \sum_{i_x > 0} \sum_{n_{\vec{k}}} \frac{\hbar^2 l^2}{2m} n_{\vec{k}} \left( \frac{F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l})}{N^2} \right)^{n_{\vec{k}}} \prod_{\substack{\vec{k}_x > 0 \\ \vec{k} \neq \vec{l}, -\vec{l}}} \left( \frac{1}{1 - F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k}) / N^2} \right) \\ = -\frac{1}{\Omega^N} \sum_{i_x > 0} \frac{\hbar^2 l^2}{2m} \frac{F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l})}{N^2} \left( \frac{1}{1 - F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l}) / N^2} \right)^2 \prod_{\substack{\vec{k}_x > 0 \\ \vec{k} \neq \vec{l}, -\vec{l}}} \left( \frac{1}{1 - F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k}) / N^2} \right) \\ = - \left( \int \psi_c f^* f \psi_c d\tau \right) \left( \sum_{i_x > 0} \frac{\hbar^2 l^2}{2m} \frac{F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l}) / N^2}{1 - F_2^f(\vec{l}, -\vec{l}) F_2^c(\vec{l}, -\vec{l}) / N^2} \right), \quad (\text{A15})$$

using (A13) to get the last line. Now we put (A15) into (A14) to get, for the last term in (A4),

$$2 \left[ \int \psi_c \left( \sum_{i=1}^N \frac{\hbar^2}{4m} \nabla_i^2 (f^* f) \right) \psi_c d\tau \right] / \int \psi_c f^* f \psi_c d\tau = -2 \sum_{\vec{k}_x > 0} \frac{\hbar^2 k^2}{2m} \frac{F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k}) / N^2}{1 - F_2^f(\vec{k}, -\vec{k}) F_2^c(\vec{k}, -\vec{k}) / N^2}. \quad (\text{A16})$$



As mentioned, the other two terms in (A4) require an explicit expression for  $f$ . Before introducing one we expand

$$\sum_{i=1}^N -\frac{\hbar^2}{4m} f^* \nabla_i^2 f = \left( \prod_{\mathbf{k}} \sum_{n_{\mathbf{k}}} \right) D(\{n_{\mathbf{k}}\}) q(\{n_{\mathbf{k}}\}), \quad (\text{A17})$$

where

$$D(\{n_{\mathbf{k}}\}) = \int q^*(\{n_{\mathbf{k}}\}) \sum_{i=1}^N -\frac{\hbar^2}{4m} f^* \nabla_i^2 f. \quad (\text{A18})$$

In second quantization (A18)

$$D(\{n_{\mathbf{k}}\}) = \langle f | q^\dagger(\{n_{\mathbf{k}}\}) \sum_{\mathbf{k}\alpha} \frac{\hbar^2 k^2}{4m} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} | f \rangle. \quad (\text{A19})$$

Now, the state corresponding to (21) but having a fixed number  $N$  of particles is

$$|f\rangle = \frac{1}{N_f} \left( \sum_{\substack{\mathbf{p}\sigma\sigma' \\ p_x > 0}} g_{\mathbf{p}\sigma\sigma'} c_{\mathbf{p}\sigma}^\dagger c_{-\mathbf{p}\sigma'}^\dagger \right)^{N/2} |0\rangle, \quad (\text{A20})$$

where  $N_f$  is a normalizing factor that will drop out at the end of the calculation. Inserting (A20) into (A19), we find with some algebra that

$$\begin{aligned} \sum_{\mathbf{k}\alpha} \frac{\hbar^2 k^2}{4m} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} \left( \sum_{\substack{\mathbf{p}\sigma\sigma' \\ p_x > 0}} g_{\mathbf{p}\sigma\sigma'} c_{\mathbf{p}\sigma}^\dagger c_{-\mathbf{p}\sigma'}^\dagger \right)^{N/2} |0\rangle &= \frac{1}{2} N \left( \sum_{\substack{\alpha\alpha' \\ k_x > 0}} \frac{\hbar^2 k^2}{4m} \cdot 2g_{\mathbf{k}\alpha\alpha'} c_{\mathbf{k}\alpha}^\dagger c_{-\mathbf{k}\alpha'}^\dagger \right) \left( \sum_{\mathbf{p}\sigma\sigma'} g_{\mathbf{p}\sigma\sigma'} c_{\mathbf{p}\sigma}^\dagger c_{-\mathbf{p}\sigma'}^\dagger \right)^{N/2-1} |0\rangle \\ &= \sum_{\substack{\alpha\alpha' \\ k_x > 0}} \frac{\hbar^2 k^2}{4m} \left( 2g_{\mathbf{k}\alpha\alpha'} \frac{\partial}{\partial g_{\mathbf{k}\alpha\alpha'}} \right) \left( \sum_{\mathbf{p}\sigma\sigma'} g_{\mathbf{p}\sigma\sigma'} c_{\mathbf{p}\sigma}^\dagger c_{-\mathbf{p}\sigma'}^\dagger \right)^{N/2} |0\rangle. \end{aligned} \quad (\text{A21})$$

So, treating the  $g_{\mathbf{k}\alpha\alpha'}$  as parameters distinct from  $g_{\mathbf{k}\alpha\alpha'}^*$ , we have

$$\langle f | q(\{n_{\mathbf{k}}\})^* \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{4m} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} | f \rangle = \frac{1}{|N_f|^2} \sum_{\substack{\mathbf{k}\sigma\sigma' \\ k_x > 0}} \frac{\hbar^2 k^2}{2m} g_{\mathbf{k}\sigma\sigma'} \frac{\partial}{\partial g_{\mathbf{k}\sigma\sigma'}} [ |N_f|^2 \langle f | q(\{n_{\mathbf{k}}\}) | f \rangle ] |_{\epsilon^*}, \quad (\text{A22})$$

where  $|_{\epsilon^*}$  means that  $g_{\mathbf{k}\sigma\sigma'}^*$  is formally held fixed.

So, putting (A23) into (A17) and using approximation (A10) gives

$$\begin{aligned} &\int \psi_c f^* \left( -\sum_i \frac{\hbar^2}{4m} \nabla_i^2 \right) f \psi_c d\tau / \int \psi_c f^* f \psi_c d\tau \\ &= \left( \prod_{\mathbf{k}} \sum_{n_{\mathbf{k}}} \right) \left\{ \left[ (N - \sum_{\mathbf{k}} n_{\mathbf{k}})! / \Omega^N N! \prod_{\mathbf{k}} n_{\mathbf{k}}! \right] \langle \psi_c | \rho(\{n_{\mathbf{k}}\}) | \psi_c \rangle \langle f | \rho(\{n_{\mathbf{k}}\})^\dagger \sum_{\mathbf{p}\sigma} \frac{\hbar^2 p^2}{4m} c_{\mathbf{p}\sigma}^\dagger c_{\mathbf{p}\sigma} | f \rangle \right\} \\ &\quad \times \left( \int \psi_c f^* f \psi_c d\tau \right)^{-1} + \text{c.c.} \\ &= \left( \prod_{\mathbf{k}} \sum_{n_{\mathbf{k}}} \right) \left\{ \left[ (N - \sum_{\mathbf{k}} n_{\mathbf{k}})! / \Omega^N N! \prod_{\mathbf{k}} n_{\mathbf{k}}! \right] \langle \psi_c | \rho(\{n_{\mathbf{k}}\}) | \psi_c \rangle \right. \\ &\quad \left. \otimes \frac{1}{|N_f|^2} \sum_{\substack{\mathbf{p}\sigma\sigma' \\ p_x > 0}} \frac{\hbar^2 p^2}{2m} g_{\mathbf{p}\sigma\sigma'} \frac{\partial}{\partial g_{\mathbf{p}\sigma\sigma'}} [ |N_f|^2 \langle f | \rho(\{n_{\mathbf{k}}\}) | f \rangle ] |_{\epsilon^*} \right\} \left( \int \psi_c f^* f \psi_c d\tau \right)^{-1} + \text{c.c.} \\ &= \left( \prod_{\mathbf{k}_x > 0} \sum_{n_{\mathbf{k}}} \right) \left\{ \left[ (N - \sum_{\mathbf{k}} n_{\mathbf{k}})! / \Omega^N N! \right] \delta_{n_{\mathbf{k}} n_{-\mathbf{k}}} [F_2^c(\mathbf{k}, -\mathbf{k}) F_2^f(\mathbf{k}, -\mathbf{k})]^{n_{\mathbf{k}}} \right\} \\ &\quad \otimes \left( \sum_{\substack{\mathbf{p}\sigma\sigma' \\ p_x > 0}} \frac{\hbar^2 p^2}{2m} g_{\mathbf{p}\sigma\sigma'} \frac{\partial}{\partial g_{\mathbf{p}\sigma\sigma'}} |N_f|^2 \right) / \left( \int \psi_c f^* f \psi_c d\tau |N_f|^2 \right) + \left( |N_f|^2 \sum_{\mathbf{p}\sigma\sigma'} \frac{\hbar^2 p^2}{2m} g_{\mathbf{p}\sigma\sigma'} \frac{\partial}{\partial g_{\mathbf{p}\sigma\sigma'}} \right) / \left( |N_f|^2 \int \psi_c f^* f \psi_c d\tau \right) \\ &\quad \times \left\{ \left( \prod_{\mathbf{k}_x > 0} \sum_{n_{\mathbf{k}}} \right) \left[ (N - \sum_{\mathbf{k}} n_{\mathbf{k}})! / \Omega^N N! \right] \delta_{n_{\mathbf{k}} n_{-\mathbf{k}}} [F_2^c(\mathbf{k}, -\mathbf{k}) F_2^f(\mathbf{k}, -\mathbf{k})]^{n_{\mathbf{k}}} \right\} + \text{c.c.}, \end{aligned} \quad (\text{A23})$$

where the first factor in large square brackets on the right-hand side cancels with  $\int \psi_c f^* f \psi_c d\tau$ . The two terms in (A23) are logarithmic derivatives, and we have

$$\begin{aligned} & \left[ \int \psi_c f^* \left( - \sum_{\mathbf{i}} \frac{\hbar^2}{4m} \nabla_{\mathbf{i}}^2 \right) f \psi_c d\tau \right] / \int \psi_c f^* f \psi_c d\tau \\ &= \sum_{\substack{p_x > 0 \\ \sigma\sigma'}} \frac{\hbar^2 p^2}{2m} g_{\vec{p}\sigma\sigma'}^- \frac{\partial}{\partial g_{\vec{p}\sigma\sigma'}^-} \ln |N_f|^2 \\ &+ \sum_{\substack{p_x > 0 \\ \sigma\sigma'}} \frac{\hbar^2 p^2}{2m} g_{\vec{v}\sigma\sigma'}^- \frac{\partial}{\partial g_{\vec{v}\sigma\sigma'}^-} \ln \\ &\quad \times \left( \prod_{k_x > 0} \frac{1}{1 - F_{(2)}^c(k, -k) F_{(2)}^F(k, -k) / N^2} \right). \quad (\text{A24}) \end{aligned}$$

This expression has been obtained from a state with fixed numbers of particles. However, (A24) depends on the Fermi-model function only through derivatives of the normalization  $|N_f|^2$ , since it is possible to express  $F_{(2)}^F(\vec{k}, -\vec{k})$  in terms of quantities like  $(\partial/\partial g_A) \ln |N_f|^2$ ,  $(\partial/\partial g_A)(\partial/\partial g_B) \ln |N_f|^2$ , etc.; and we can show that in the thermodynamic limit we can replace

$$|N_f|^2 \longrightarrow \prod_{k_x > 0} \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}\sigma\sigma'}^-|^2 + |\hbar_{\vec{k}}|^2 \right)$$

without error. That is, expression (21) and (A20) can be used interchangeably without error.

In the body of this paper we use the notation  $F_2^F(\vec{k}, -\vec{k})/N \equiv F_F(\vec{k})$ , and  $F_2^c(\vec{k}, -\vec{k})/N \equiv F_c(\vec{k})$  for con-

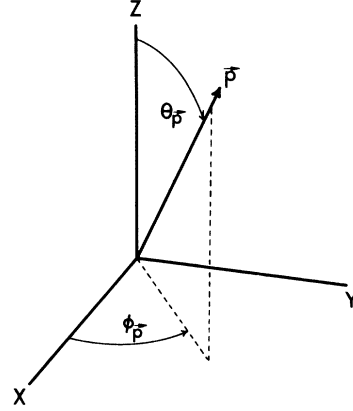


FIG. 5. Spin quantization axes.

venience. Expression (21) for the energy follows straightaway.

#### APPENDIX B

Here we give the general formulas for  $F_2^F(k, -k)$ ,  $E$ , and the variational equation, and the forms taken by these quantities in the special cases where the "pair wave function" has BCS, Anderson-Morel (AM), or BW symmetry.

(a) Structure factor. In general

$$\begin{aligned} F_{(2)}^F(\vec{k}, -\vec{k}) &\equiv \sum_{\vec{p}} F_{2\vec{p}}^F(\vec{k}, -\vec{k}) \\ &= \sum_{\vec{p}} \left\{ \sum_{\lambda\lambda'} \left[ |g_{\vec{k}+\vec{p}\lambda\lambda'}^-| - (-1)^{\delta_{\lambda\lambda'}} \hbar_{\vec{k}+\vec{p}}^* g_{\vec{k}+\vec{p}-\lambda-\lambda'}^* \right] / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}+\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{k}+\vec{p}}|^2 \right) \right. \\ &\quad \times \left[ |g_{\vec{p}\lambda\lambda'}^*| - (-1)^{\delta_{\lambda\lambda'}} \hbar_{\vec{p}}^* g_{\vec{p}-\lambda-\lambda'}^* \right] / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{p}}|^2 \right) \\ &\quad - \sum_{\gamma} \left[ \left( \sum_{\delta} |g_{\vec{k}+\vec{p}\gamma\delta}^-|^2 + |\hbar_{\vec{k}+\vec{p}}|^2 \right) / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}+\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{k}+\vec{p}}|^2 \right) \right] \\ &\quad \times \left[ \left( \sum_{\beta} |g_{\vec{p}\gamma\beta}^-|^2 + |\hbar_{\vec{p}}|^2 \right) / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{p}}|^2 \right) \right] \\ &\quad - \sum_{\gamma} \left[ \left( \sum_{\delta} g_{\vec{p}+\vec{k}\delta\gamma}^* g_{\vec{p}+\vec{k}\delta, -\gamma} \right) / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}+\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{k}+\vec{p}}|^2 \right) \right] \\ &\quad \left. \times \left[ \left( \sum_{\beta} g_{\vec{p}\delta-\gamma}^* g_{\vec{p}\delta\gamma} \right) / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{p}\sigma\sigma'}^-|^2 + |\hbar_{\vec{p}}|^2 \right) \right] \right\}. \quad (\text{B1}) \end{aligned}$$

The symmetry is given to the parameters  $g_{\vec{p}\sigma\sigma'}^-$  by requiring that the pair wave function  $\psi_{\vec{p}\sigma\sigma'}^-$  [see (26)] have the appropriate physical properties. In general

$$\psi_{\vec{p}\sigma\sigma'} = g_{\vec{p}\sigma\sigma'} \times \text{function of } |\vec{p}|. \quad (\text{B2})$$

(i) *BCS*. In this case  $(\sigma, \sigma') = (\uparrow\downarrow)$  or  $(\downarrow\uparrow)$  and the space part of the wave function is isotropic. Thus [see (21)] we can choose  $u_{\vec{k}\sigma}, v_{\vec{k}\sigma'}$  isotropic, the third term in (B1) vanishes, and we have

$$F_{(2)}^F(\vec{k}, -\vec{k}) = \sum_{\vec{p}\lambda} \left( \frac{g_{\vec{k}+\vec{p}\lambda-\lambda}}{(1+|g_{\vec{k}+\vec{p}\lambda-\lambda}|^2)} \frac{g_{\vec{p}\lambda-\lambda}}{(1+|g_{\vec{p}\lambda-\lambda}|^2)} - \frac{|g_{\vec{k}+\vec{p}\lambda-\lambda}|^2}{(1+|g_{\vec{k}+\vec{p}\lambda-\lambda}|^2)} \frac{|g_{\vec{p}\lambda-\lambda}|^2}{(1+|g_{\vec{p}\lambda-\lambda}|^2)} \right), \quad (\text{B3})$$

which reduces to

$$F_{(2)}^F(\vec{k}, -\vec{k}) = \sum_{\vec{p}\lambda} (u_{\vec{k}+\vec{p}\lambda-\lambda} v_{\vec{k}+\vec{p}\lambda-\lambda} u_{\vec{p}\lambda-\lambda} v_{\vec{p}\lambda-\lambda} - v_{\vec{k}+\vec{p}\lambda-\lambda}^2 v_{\vec{p}\lambda-\lambda}^2) \equiv 2 \sum_{\vec{p}} (u_{\vec{k}+\vec{p}} v_{\vec{k}+\vec{p}} u_{\vec{p}} v_{\vec{p}} - v_{\vec{k}+\vec{p}}^2 v_{\vec{p}}^2). \quad (\text{B4})$$

(ii) *AM*. In this case  $(\sigma, \sigma') = (\uparrow\uparrow)$  or  $(\downarrow\downarrow)$ , and (B1) simplifies to a formula like (B3) with the replacement  $(-\lambda \rightarrow \lambda)$ . In matrix notation, we now require that<sup>8</sup>

$$g_{\vec{p}\sigma\sigma'} = \begin{pmatrix} g_{\vec{p}\uparrow\uparrow} & g_{\vec{p}\uparrow\downarrow} \\ g_{\vec{p}\downarrow\uparrow} & g_{\vec{p}\downarrow\downarrow} \end{pmatrix} \sim \begin{pmatrix} Y_1^1(\hat{p}) & 0 \\ 0 & Y_1^{-1}(\hat{p}) \end{pmatrix}^*, \quad (\text{B5})$$

which leads to

$$\begin{aligned} F_{(2)}^{\text{AM}}(\vec{k}, -\vec{k}) &= 2 \sum_{\vec{p}} \left( \frac{c_{\vec{p}} \sin\theta_{\vec{p}}}{1+c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}} \frac{c_{\vec{p}+\vec{k}} \sin\theta_{\vec{p}+\vec{k}}}{1+c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}} e^{i(\phi_{\vec{p}+\vec{k}} - \phi_{\vec{p}})} - \frac{c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}}{1+c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}} \frac{c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}}{1+c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}} \right) \\ &= \sum_{\vec{p}\lambda} \left( \frac{c_{\vec{p}} \sin\theta_{\vec{p}}}{1+c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}} \frac{c_{\vec{p}+\vec{k}} \sin\theta_{\vec{p}+\vec{k}}}{1+c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}} \cos(\phi_{\vec{p}+\vec{k}} - \phi_{\vec{p}}) - \frac{c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}}{1+c_{\vec{p}}^2 \sin^2\theta_{\vec{p}}} \frac{c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}}{1+c_{\vec{p}+\vec{k}}^2 \sin^2\theta_{\vec{p}+\vec{k}}} \right), \end{aligned} \quad (\text{B6})$$

since only the real part contributes. Here the coordinates with respect to the spin-quantization axis are shown in Fig. 5. In (B6)  $c_p$  is isotropic, a function of  $|\vec{p}|$  only.

(iii) *BW*. In this case all combinations  $(\sigma, \sigma')$  appear, and we have<sup>8</sup>

$$g_{\vec{p}\sigma\sigma'} \sim \begin{pmatrix} \sqrt{2} Y_1^1(\hat{p}) & Y_1^0(\hat{p}) \\ Y_1^0(\hat{p}) & \sqrt{2} Y_1^{-1}(\hat{p}) \end{pmatrix}^*. \quad (\text{B7})$$

After some algebra we find that the third term in (B1) still vanishes, and the remaining terms reduce to

$$F_{(2)}^{\text{BW}}(\vec{k}, -\vec{k}) = 2 \sum_{\vec{p}} [u_{\vec{k}+\vec{p}} v_{\vec{k}+\vec{p}} v_{\vec{p}}^2 v_{\vec{p}} (1 - \hat{p} \cdot \hat{k}) - v_{\vec{k}+\vec{p}}^2 v_{\vec{p}}^2], \quad (\text{B8})$$

where  $u_p, v_p$  are functions of  $|\vec{p}|$  only, satisfy  $|u_p|^2 + |v_p|^2 = 1$ , and can be chosen real, i.e., (B8) uses the same notation as the second line of (B4).

(b) *Energy*. In general

$$\begin{aligned} \langle \hat{H} - \mu \hat{N} \rangle &= E - \mu N \\ &= E_c + E_F - \mu N \\ &= 2 \sum_{k_x > 0} (\epsilon_k^0 - \mu) n_k - \sum_{k_x > 0} \epsilon_k^0 \frac{[F_{(2)}^c(\vec{k}, -\vec{k})/N] F_{(2)}^F(\vec{k}, -\vec{k})/N}{1 - [F_{(2)}^c(\vec{k}, -\vec{k})/N] F_{(2)}^F(\vec{k}, -\vec{k})/N} \\ &\quad + \sum_{k_x > 0} \frac{[F_{(2)}^c(\vec{k}, -\vec{k})/N] N^{-1}}{1 - [F_{(2)}^c(\vec{k}, -\vec{k})/N] F_{(2)}^F(\vec{k}, -\vec{k})/N} \\ &\quad \times \left( 2 \sum_{\vec{p}} (1 - n_{\vec{p}}) \epsilon_{\vec{p}}^0 F_{2\vec{p}}^F(\vec{k}, -\vec{k}) + 2 \sum_{\text{all } \vec{p}} (1 - n_{\vec{p}+\vec{k}}) \epsilon_{\vec{p}+\vec{k}}^0 F_{2\vec{p}}^F(\vec{k}, -\vec{k}) - \sum_{\text{all } \vec{p}} \epsilon_{\vec{p}}^0 L_{\vec{p}}(\vec{k}, -\vec{k}) \right) + E_c, \end{aligned} \quad (\text{B9})$$

where  $\epsilon_p^0 = \hbar^2 p^2 / 2m$ ,  $n_p = v_p^2$ , and  $F_{(2)}^F(\vec{k}, -\vec{k})$  is defined by (B1), and

$$L_{\vec{p}}(\vec{k}, -\vec{k}) \equiv 4 \frac{|h_{\vec{p}}|^2 n_{\vec{k}, \vec{p}}}{1 + \sum_{\sigma\sigma'} |g_{\vec{p}\sigma\sigma'}|^2 + |h_{\vec{p}}|^2} n_{\vec{k}, \vec{p}}^* + 2 \operatorname{Re} \left\{ \sum_{\lambda\lambda'} \left[ [g_{\vec{p}\lambda\lambda'}^* + (-1)^{\delta_{\lambda\lambda'}} h_{\vec{p}}^* g_{\vec{p}-\lambda-\lambda'}] / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{p}\sigma\sigma'}|^2 + |h_{\vec{p}}|^2 \right) \right] \right. \\ \left. \times \left[ [g_{\vec{k}, \vec{p}}^* - (-1)^{\delta_{\lambda\lambda'}} h_{\vec{k}, \vec{p}}^* g_{\vec{k}, \vec{p}-\lambda-\lambda'}] / \left( 1 + \sum_{\sigma\sigma'} |g_{\vec{k}, \vec{p}\sigma\sigma'}|^2 + |h_{\vec{k}, \vec{p}}|^2 \right) \right] \right\}.$$

For future reference define

$$R_{\vec{k}} \equiv 2 \sum_{\vec{p}} [(1 - n_{\vec{p}, \vec{k}}) \epsilon_{\vec{p}, \vec{k}}^0 + (1 - n_{\vec{p}}) \epsilon_{\vec{p}}^0] F_{2\vec{p}}^F(\vec{k}, -\vec{k}) - \sum_{\vec{p}} \epsilon_{\vec{p}}^0 L_{\vec{p}}(\vec{k}, -\vec{k}). \quad (\text{B10})$$

To simplify (B9) we need only the manipulations that led to (B3), (B6), and (B8), along with a lot of patience while doing the algebra. The results are the following:

(i) BCS:

$$E - \mu N = E_c + 2 \sum_{\vec{p}} n_{\vec{p}} (\epsilon_{\vec{p}}^0 - \mu) - \sum_{k_x > 0} \epsilon_k^0 \frac{F_{\text{BCS}}(\vec{k}) F_c(\vec{k})}{1 - F_{\text{BCS}}(\vec{k}) F_c(\vec{k})} \\ + \sum_{k_x > 0} \frac{F_c(\vec{k})}{1 - F_c(\vec{k}) F_{\text{BCS}}(\vec{k})} \sum_{\vec{\lambda}} \epsilon_{\vec{p}\vec{\lambda}}^0 [-2v_{\vec{p}}^2 v_{\vec{k}-\vec{\lambda}}^2 u_{\vec{p}\vec{\lambda}}^2 + v_{\vec{p}}^2 v_{\vec{k}-\vec{\lambda}}^2 u_{\vec{p}\vec{\lambda}}^2 + v_{\vec{p}}^2 v_{\vec{k}-\vec{\lambda}}^2 u_{\vec{p}\vec{\lambda}}^2 (u_{\vec{p}\vec{\lambda}}^2 - v_{\vec{p}\vec{\lambda}}^2)], \quad (\text{B11})$$

where  $F_{\text{BCS}}(\vec{k}) \equiv F_{(2)}^F(\vec{k}, -\vec{k})/N$  for BCS symmetry. Using (B4), Eq. (B10) is easily put into the form of Eq. (24).

(ii) AM:

$$E - \mu N = E_c + 2 \sum_{\vec{p}} n_{\vec{p}} (\epsilon_{\vec{p}}^0 - \mu) - \sum_{k_x > 0} \epsilon_k^0 \frac{F_{\text{AM}}(\vec{k}) F_c(\vec{k})}{1 - F_{\text{AM}}(\vec{k}) F_c(\vec{k})} \\ + \sum_{k_x > 0} \frac{F_c(\vec{k})}{1 - F_c(\vec{k}) F_{\text{AM}}(\vec{k})} \sum_{\vec{\lambda}} \left\{ -2 \frac{C_{\vec{p}, \vec{k}}^2 \sin^2 \theta_{\vec{p}, \vec{k}}}{1 + C_{\vec{p}, \vec{k}}^2 \sin^2 \theta_{\vec{p}, \vec{k}}} \frac{C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}}{1 + C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}} \frac{1}{1 + C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}} \right. \\ \left. + \frac{C_{\vec{p}, \vec{k}} \sin \theta_{\vec{p}, \vec{k}}}{1 + C_{\vec{p}, \vec{k}}^2 \sin^2 \theta_{\vec{p}, \vec{k}}} \frac{C_{\vec{p}} \sin \theta_{\vec{p}}}{1 + C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}} \frac{1 - C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}}{1 + C_{\vec{p}}^2 \sin^2 \theta_{\vec{p}}} \cos(\phi_{\vec{p}, \vec{k}} - \phi_{\vec{p}}) \right\} \quad (\text{B12})$$

[see (B5) and (B6)].

(iii) BW:

$$E - \mu N = E_c + 2 \sum_{\vec{p}} n_{\vec{p}} (\epsilon_{\vec{p}}^0 - \mu) - \sum_{k_x > 0} \epsilon_k^0 \frac{F_{\text{BW}}(\vec{k}) F_c(\vec{k})}{1 - F_{\text{BW}}(\vec{k}) F_c(\vec{k})} \\ + \sum_{k_x > 0} \frac{F_c(\vec{k})}{1 - F_c(\vec{k}) F_{\text{BW}}(\vec{k})} 2 \sum_{\vec{p}} \epsilon_{\vec{p}}^0 [-2v_{\vec{p}, \vec{k}}^2 v_{\vec{p}}^2 u_{\vec{p}}^2 + v_{\vec{p}, \vec{k}}^2 v_{\vec{p}}^2 u_{\vec{p}}^2 + v_{\vec{p}, \vec{k}}^2 v_{\vec{p}}^2 u_{\vec{p}}^2 (u_{\vec{p}}^2 - v_{\vec{p}}^2)(1 - \hat{p} \cdot \hat{k})]. \quad (\text{B13})$$

For definitions see (B4), (B7), and (B8)

(c) "Gap equation." The general expression for the variational condition on the energy (B9) is

$$\frac{\partial}{\partial g_{\alpha\alpha\alpha'}} \left( 2 \sum_{k_x > 0} (\epsilon_k^0 - \mu) n_k \right) + \sum_{k_x > 0} \frac{F_{(2)}^c(\vec{k}, -\vec{k})/N}{1 - [F_{(2)}^c(\vec{k}, -\vec{k})/N] F_{(2)}^F(\vec{k}, -\vec{k})/N} \\ \times \frac{\partial}{\partial g_{\alpha\alpha\alpha'}} \left( 2 \sum_{\vec{p}} (1 - n_{\vec{p}}) \epsilon_{\vec{p}}^0 F_{2\vec{p}}^F(\vec{k}, -\vec{k}) + 2 \sum_{\vec{p}} (1 - n_{\vec{p}, \vec{k}}) \epsilon_{\vec{p}, \vec{k}}^0 F_{2\vec{p}}^F(\vec{k}, -\vec{k}) - \sum_{\vec{p}} \epsilon_{\vec{p}}^0 L_{\vec{p}}(\vec{k}, -\vec{k}) \right) \\ + \sum_{k_x > 0} \frac{[F_{(2)}^c(\vec{k}, -\vec{k})/N] N^{-1}}{\{1 - [F_{(2)}^F(\vec{k}, -\vec{k})/N] F_{(2)}^c(\vec{k}, -\vec{k})/N\}^2} (R_{\vec{k}}/N - \epsilon_{\vec{k}}^0) \frac{\partial}{\partial g_{\alpha\alpha\alpha'}} F_{(2)}^F(\vec{k}, -\vec{k}) = 0.$$

## APPENDIX C

Scaling Fermi quantities to other densities. In expression (47) consider two integrals characteristic of the Fermi surface.

$$F_F^{\text{BCS}}(k) \text{ [see Eq. (46)],}$$

$$C^{\text{BCS}}(k) \equiv \int_0^\infty l dl \frac{\hbar^2 l^2}{2m} \operatorname{sech} y(l) \operatorname{tanh} y(l) \int_{|l-k|}^{l+k} |q| dq \operatorname{sech} y(q)$$

$$- \int_0^\infty l dl \frac{\hbar^2 l^2}{2m} \operatorname{sech} y(l) \int_{|l-k|}^{l+k} q dq [1 - \operatorname{tanh} y(q)]. \quad (\text{C1})$$

Define dimensionless variables

$$\bar{l} \equiv l/k_F, \quad \bar{q} \equiv q/k_F, \quad \bar{k} \equiv k/k_F, \quad \bar{\beta}^* \equiv k_F^2 \beta^*; \quad (\text{C2})$$

then

$$\bar{y}(\bar{x}) = \frac{\bar{\beta}^*}{2} \left( \frac{\hbar^2 \bar{x}^2}{2m} - \mu \right) = y(x), \quad \bar{\epsilon}_{0k} \equiv \hbar^2 \bar{k}^2 / 2m;$$

and

$$F_F^{\text{BCS}}(k|\beta^*) = \frac{3}{8\bar{k}} \left( \int_0^\infty \bar{q} d\bar{q} \operatorname{sech} \bar{y}(\bar{q}) \int_{|\bar{q}-\bar{k}|}^{\bar{q}+\bar{k}} \bar{l} d\bar{l} \operatorname{sech} \bar{y}(\bar{l}) \right.$$

$$\left. - \int_0^\infty \bar{q} d\bar{q} [1 - \operatorname{tanh} \bar{y}(\bar{q})] \int_{|\bar{q}-\bar{k}|}^{\bar{q}+\bar{k}} \bar{l} d\bar{l} [1 - \operatorname{tanh} \bar{y}(\bar{l})] \right)$$

$$\equiv F_F^{\text{BCS}}(\bar{k}|\bar{\beta}^*), \quad (\text{C3})$$

and

$$C^{\text{BCS}}(k|\beta^*) = k_F^6 \left( \int_0^\infty \bar{l} d\bar{l} \frac{\hbar^2 \bar{l}^2}{2m} \operatorname{sech} \bar{y}(\bar{l}) \operatorname{tanh} \bar{y}(\bar{l}) \int_{|\bar{l}-\bar{k}|}^{\bar{l}+\bar{k}} \bar{q} d\bar{q} \operatorname{sech} \bar{y}(\bar{q}) \right.$$

$$\left. - \int_0^\infty \bar{l} d\bar{l} \frac{\hbar^2 \bar{l}^2}{2m} \operatorname{sech} \bar{y}(\bar{l}) \int_{|\bar{l}-\bar{k}|}^{\bar{l}+\bar{k}} \bar{q} d\bar{q} [1 - \operatorname{tanh} \bar{y}(\bar{q})] \right) \quad (\text{C3}')$$

so that  $F_F^{\text{BCS}}(k|\beta^*)$  and  $k_F^6 C^{\text{BCS}}(k|\beta^*)$  are functions only of the dimensionless  $\bar{k}$  and a density-scaled effective temperature  $\bar{\beta}^*$ . Arrays of numbers can thus be computed for a range of  $\beta^*$  for a given density, then scaled to other densities without repeating the entire calculation. If  $F_c(k)$  is also expressed as  $F_c(\bar{k})$  (a simple scale change), the energy (47) takes the form

$$E^{\text{BCS}} = E_c + \frac{\hbar^2 k_F^2}{2m} \left( \frac{3}{2} \int_0^\infty \bar{k}^4 d\bar{k} [1 - \operatorname{tanh} \bar{y}(\bar{k})] - \frac{3}{4} \int_0^\infty \bar{k}^4 d\bar{k} \frac{F_c(\bar{k})F(\bar{k})}{1 - F_c(\bar{k})F_F(\bar{k})} - \frac{9}{8} \int_0^\infty \bar{k} d\bar{k} \frac{F_c(\bar{k})C_F(\bar{k})}{1 - F_c(\bar{k})F_F(\bar{k})} \right).$$

The same procedure is as easily applied to the BW energy expression: however,  $C_F(\bar{k})$  and  $F_F(\bar{k})$  take on different forms in that case.

<sup>†</sup>Work supported in part by the NSF under Grant Nos. DMR74-01237 A01 and DMR76-14777 and by the Research Corporation.

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