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1982 J. Phys. A: Math. Gen. 15 3627

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# Correlated P-wave pairing theory for Fermi systems. Application to liquid $^3\text{He}$

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Received 19 January 1982

**Abstract.** A variational theory is presented for the isotropic triplet pair-condensed state of liquid  $^3\text{He}$ . Using a correlated pairing wavefunction we express the expectation values of the required quantities in terms of the diagonal and off-diagonal matrix elements of the Hamiltonian and unit operators with respect to a correlated basis of normal wavefunctions. The correlated basis consists of Slater determinants modified by a Jastrow correlation factor which incorporates the strong short-range correlations induced by the interparticle potential. Our formalism has been developed within the weak-coupling approximation. The study of the instability of the normal state with respect to the triplet pair-condensed state is achieved via an exact criterion. This criterion has been expressed in terms of normal-state quantities which have been evaluated within the correlated basis functions scheme with the accuracy of the Fermi hypernetted chain approximation. Our numerical calculations indicate an instability of the normal ground state with respect to the  $^3\text{P}_0$  superfluid state but at too low a density.

## 1. Introduction

Since the BCS theory (Bardeen *et al* 1957) was introduced to describe pairing correlations, which lead to an isotropic superfluid state, several attempts have been made to apply the theory to strongly interacting fermion systems such as neutron and nuclear matter (Tamagaki 1970, Cooper *et al* 1959) and in particular liquid  $^3\text{He}$  (Emery and Sessler 1960, Brueckner *et al* 1960).

These early studies led to the conclusion that for liquid  $^3\text{He}$ , a condensation into higher states of the relative two-body orbital angular momentum  $L$  is more favourable than the isotropic spin-singlet S-wave state of the ordinary BCS theory. This result is a consequence of the short-range repulsive hard core of the two-body potentials, which describe the interactions of the system. The investigation of the higher spin-triplet P-wave states resulted in the BW (Balian and Werthamer 1963) and ABM (Anderson and Morel 1961, Anderson and Brinkman 1973) pairing theories which correspond to the condensed B and A phases of  $^3\text{He}$  respectively.

The main problem, which arises in the superfluid description of a strongly interacting Fermi system, is that the pair-condensed model wavefunctions do not include the short-range correlations which are necessary to renormalise the short-range repulsive hard core of the potential. Yang and Clark (1971) introduced a correlated pair-condensed state consisting of a pair-condensed model function which describes the

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$^1S_0$  pairing and a correlation operator which incorporates the correlations induced by the short-range interactions. The cluster expansion of the energy is based on the expansion of the correlation operator, assuming that in low-density nuclear matter the volume of the hard cores of the two-body potentials constitutes a small fraction of the total volume. The fact that the volume of the hard cores is a large fraction of the total volume in the case of liquid  $^3\text{He}$  led Paulick and Campbell (1977) to adopt a scheme which includes an analysis of the pair-condensed model functions, in addition to that of the correlation function, in their study for the isotropic BCS and BW pairing, which describe the pair-condensed phases of liquid  $^3\text{He}$ .

Most recently Krotscheck and Clark (KC, 1980) have developed a variational theory where the matrix elements of the desirable quantities with respect to a correlated pair-condensed model function are expressed in terms depending on diagonal and off-diagonal matrix elements of the Hamiltonian and unit operators with respect to a correlated basis of normal states. The treatment of these terms has been formulated within the correlated basis function (CBF) framework (Krotscheck and Clark 1979, hereafter referred to as KC-II) adopting the Clark-Westhaus (1966) form for the expectation value of the kinetic energy operator. For the evaluation of these CBF quantities they employ the Fermi hypernetted chain (FHNC) approximation, assuming a simple parametrised two-body Jastrow correlating function (Schiff and Verlet 1967, Iwamoto and Yamada 1957, Aviles *et al* 1958).

The advantage of this theory of pairing phenomena using pair-condensed model functions within the CBF formalism resides in the fact that for the calculation of the CBF quantities, any kind of correlation operator or cluster expansion can be used, without changing the formalism which describes the pairing effects.

The purpose of this work is the study, in the same spirit, of a variational theory for the spin-triplet P-wave pairing state incorporating a correlated pair-condensed model function. The introduction of a correlation factor into the trial wavefunction permits the application of the weak-coupling approximation in the evaluation of the superfluid energy and the derivation of the gap equation. The resulting diagonal and off-diagonal matrix elements of the Hamiltonian and unit operators are evaluated within the CBF scheme presented in Hatzikonstantinou and Irvine (1982) (HI) and KC-II respectively. We presume further that in deriving the required CBF quantities we will concentrate only on states differing in exactly two single-particle states which correspond to a single Cooper pair of particles. The evaluation of these quantities is performed via the FHNC approximately (Krotscheck and Ristig 1975, Krotscheck 1977a, b, Fantoni and Rosati 1975) which permits an infinite partial summation of cluster terms obtained from the cluster expansion of these quantities.

Finally we proceed in a numerical investigation of the instability condition of the normal phase with respect to  $^3P_0$  pairing in liquid  $^3\text{He}$ , evaluating the required quantities in conjunction with a FHNC optimisation scheme which minimises the normal ground-state energy.

## 2. Correlated model function for Cooper pairing in triplet states

Let us consider the triplet P-wave state

$$|\phi_s\rangle = \eta^{-1} \prod_{\substack{\mathbf{k} \\ \sigma\sigma'}}^{(k_x > 0)} (1 + g_{\sigma\sigma'}(\mathbf{k}) a_{\mathbf{k}\sigma}^+ a_{-\mathbf{k}\sigma'}^+) |0\rangle \quad (2.1)$$

where  $\eta$  is the normalising factor  $g_{\sigma\sigma'}(\mathbf{k}) = v_{k\sigma\sigma'}/u_{k\sigma\sigma'}$  and the operator  $a_{\mathbf{k}\sigma}^{\dagger}$  creates a particle in the orbital  $(\mathbf{k}, \sigma)$ . Adopting the appropriate forms of  $v_{k\sigma\sigma'}$  and  $u_{k\sigma\sigma'}$ , the ket (2.1) may describe the special cases of ABM and BW pairing. For the treatment of the triplet pairing we adopt a generalised form of (2.1) which is given by  $\kappa\mathcal{C}$ ,

$$|\phi_s\rangle = \prod_{\mathbf{k} (k_x > 0)} (u_{\mathbf{k}} + v_{\mathbf{k}}L_1^+(\mathbf{k}))(u_{\mathbf{k}} + v_{\mathbf{k}}L_2^+(\mathbf{k}))|0\rangle \quad (2.2)$$

where

$$L_1^+(\mathbf{k}) = \Lambda_{\uparrow\uparrow}(\mathbf{k})a_{\mathbf{k}\uparrow}^{\dagger}a_{-\mathbf{k}\uparrow}^{\dagger} + \Lambda_{\uparrow\downarrow}(\mathbf{k})a_{\mathbf{k}\uparrow}^{\dagger}a_{\mathbf{k}\downarrow}^{\dagger}, \quad L_2^+(\mathbf{k}) = \Lambda_{\downarrow\uparrow}(\mathbf{k})a_{\mathbf{k}\downarrow}^{\dagger}a_{-\mathbf{k}\uparrow}^{\dagger} + \Lambda_{\downarrow\downarrow}(\mathbf{k})a_{\mathbf{k}\downarrow}^{\dagger}a_{-\mathbf{k}\downarrow}^{\dagger} \quad (2.3)$$

and  $u_{\mathbf{k}} = \cos \Phi_{\mathbf{k}}$ ,  $v_{\mathbf{k}} = \sin \Phi_{\mathbf{k}}$  so that  $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$ . The matrix elements of the unitary matrix

$$\Lambda(\mathbf{k}) = \begin{pmatrix} \Lambda_{\uparrow\uparrow}(\mathbf{k}) & \Lambda_{\uparrow\downarrow}(\mathbf{k}) \\ \Lambda_{\downarrow\uparrow}(\mathbf{k}) & \Lambda_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} \quad (2.4)$$

are determined by the decompositions

$$\begin{aligned} \Lambda_{\sigma_1\sigma_2}(\mathbf{k}) &= \bar{\eta} \sum_{\lambda} \langle \frac{1}{2}\sigma_1, \frac{1}{2}\sigma_2 | SM_S \rangle \langle SM_S LM_L | JM_J \rangle Y_{L,M_L}(\hat{\mathbf{k}}) X_{\lambda}(k) \\ &= \bar{\eta} \sum_{\lambda} X_{\lambda}(k) \Lambda_{\sigma_1\sigma_2}^{\lambda}(\hat{\mathbf{k}}) \end{aligned} \quad (2.5)$$

where  $\bar{\eta}$  is the normalising factor,  $\hat{\mathbf{k}}$  is the unit vector along the  $\mathbf{k}$  vector and  $\lambda = JLSM_J$ . For the triplet P-state the matrix (2.4) may be defined as

$$\Lambda(\mathbf{k}) = \sum_J \Lambda_J(\mathbf{k}), \quad J = 0, 1, 2, \quad (2.6)$$

where the matrices  $\Lambda_J(\mathbf{k})$  are given in appendix 1. Considering that the triplet state corresponds to an odd  $L$  and the parity of spherical harmonics is  $(-1)^L$ , we have  $\Lambda(-\mathbf{k}) = -\Lambda(\mathbf{k})$  which, incorporated with the requirement of the time-reversed invariance of (2.2)

$$\Lambda_{\sigma_1\sigma_2}^*(-\mathbf{k}, -\sigma_1, -\sigma_2) = (-1)^{1+\sigma_1+\sigma_2} \Lambda_{\sigma_1\sigma_2}(\mathbf{k}, \sigma_1, \sigma_2), \quad (2.7)$$

is equivalent to  $X_{JLS,M_J}^*(k) = (-1)^{J+M_J} X_{JLS,-M_J}$  and yields the relation

$$\Lambda_{\sigma_1\sigma_2}^*(\mathbf{k}, -\sigma_1, -\sigma_2) = (-1)^{2+\sigma_1+\sigma_2} \Lambda_{\sigma_1\sigma_2}(\mathbf{k}, \sigma_1, \sigma_2). \quad (2.8)$$

From the unitarity of (2.4) we have the additional relation

$$|\Lambda_{\uparrow\uparrow}(\mathbf{k})|^2 + |\Lambda_{\uparrow\downarrow}(\mathbf{k})|^2 = 1. \quad (2.9)$$

The Fermi operators  $L_1^+(\mathbf{k})$ ,  $L_2^+(\mathbf{k})$  and their complex conjugate satisfy the relations

$$[L_1(\mathbf{k}), L_1^{\dagger}(\mathbf{k})]_{-}|0\rangle = |0\rangle, \quad (2.10)$$

$$[L_2(\mathbf{k}), L_2^{\dagger}(\mathbf{k})]_{-}|0\rangle = |0\rangle, \quad (2.11)$$

$$[L_1(\mathbf{k}), L_2(\mathbf{k})]_{-} = 0. \quad (2.12)$$

The subscript  $(-)$  signifies commutation relation.

The  ${}^3P_J$  model function, which describes adequately the superfluid state of a weakly interacting system, is a superposition of states with different number ordering. To

consider a variational superfluid theory appropriate for strongly interacting fermion systems we introduce the correlated pair-condensed state

$$|\psi_s\rangle = \hat{F}|\phi_s\rangle = \sum_{N, m_N} F_N |\phi_m^{(N)}\rangle \langle \phi_m^{(N)} | \phi_s\rangle \quad (2.13)$$

where  $F_N(1, 2, \dots, N)$  is an  $N$ -body translationally invariant correlation operator and  $\{|\Phi_m^{(N)}\rangle\}$  is a complete orthonormal set of  $N$ -particle Slater determinants which are labelled as  $m(N) = \{m_1, m_2, \dots, m_N\}$ . The projection of the pair state  $|\Phi_s\rangle$  on the Hilbert spaces of the  $N$  particles permits the expression of certain quantities in terms which can be evaluated in configuration space. The operator  $F_N$  satisfies the property  $F_N(1, 2, \dots, N) \rightarrow F_A(1, 2, \dots, A) F_{N-A}(A+1, \dots, N)$  setting the configuration vectors  $r_i$  of each particle of the set  $N-A$  separately to infinity. If the correlation operator  $F$  had been expressed in the occupation number representation it should obviously contain the same number of creation and annihilation operators and should commute with the number operator,

$$\hat{N} = \sum_{k\sigma} a_{k\sigma}^+ a_{k\sigma}. \quad (2.14)$$

Thus we conclude that the dispersion in the number ordering of  $F|\Phi_s\rangle$  may be attributed entirely to the superfluid state  $|\Phi_s\rangle$ .

It is evident that the  $|\Psi_s\rangle$  state includes off-diagonal long-range order (ODLRO) in the lowest two-body density matrix, which is an important characteristic of the superfluid states as has long been suggested by Paulick and Campbell.

In the occupation-number representation an  $N$ -body Slater determinant takes the form

$$|\phi_m^{(N)}\rangle = \prod_k^m L_1^+(\mathbf{k}) L_2^+(\mathbf{k}) |0\rangle = \prod_k^m \left( \frac{b_k^+}{\sqrt{2}} \right)^2 |0\rangle = \prod_k^m a_{k\uparrow}^+ a_{-k\downarrow}^+ a_{k\downarrow}^+ a_{-k\uparrow}^+ |0\rangle \quad (2.15)$$

where the pair-creation operator  $b_k^+$  is defined as

$$b_k^+ = \sum_{\sigma_1 \sigma_2} \Lambda_{\sigma_1 \sigma_2}(\mathbf{k}) a_{k\sigma_1}^+ a_{-k\sigma_2}^+ = L_1^+(\mathbf{k}) + L_2^+(\mathbf{k}) \quad (2.16)$$

with the property  $b_k b_k^{+2}/2 = b_k^+$ . The ground state  $|\Phi_0^{(N)}\rangle$  is obtained from (2.16) for  $k \leq k_F$ .

The probability for occupation of a pair of single-particle states  $k\sigma, -k\sigma'$  obtained by virtue of (2.2) is given by

$$\langle \phi_s | a_{+k\sigma}^+ a_{+k\sigma'} | \phi_s \rangle = v_k^2. \quad (2.17)$$

Hence in the uncorrelated triplet pair-condensed state of the system, the expectation value of the operator (2.14) is

$$N_0 = \langle \phi_s | \hat{N} | \phi_s \rangle = \sum_k 4v_k^2. \quad (2.18)$$

### 3. Criterion of superfluidity

One of the most important quantities which has to be evaluated is the stability criterion which expresses the stability or instability of the normal state with respect to the formation of the Cooper pairs.

In this section we review the main steps for the calculation of the stability criterion in order to fix the formalism and to define some quantities which will be used later in our work.

The stability (or instability) condition depends on the behaviour of the functional derivative with respect to the real angles  $\phi_k$ :

$$S_{kp} = \frac{\delta^2}{\delta\phi_k\delta\phi_p} \frac{\langle\phi_s|F^+(H - \mu\hat{N})F|\phi_s\rangle}{\langle\phi_s|F^+F|\phi_s\rangle} \Big|_0. \quad (3.1)$$

The notation  $|_0$  means that the parameters  $u_k$  and  $v_k$  are replaced by their expressions in the normal state  $u_{k'} = u_k$  and  $v_k = v_k \equiv \eta(k')$ , where

$$v_k^2 = \eta(k) = \begin{cases} 1, & k \leq k_F, \\ 0, & k > k_F. \end{cases} \quad (3.2)$$

In (3.1)  $\mu$  is the chemical potential, a Lagrange parameter which ensures that the expectation value of the operator  $N$  is equal to the number of particles in the system  $A$  and  $H$  is the Hamiltonian operator.

$$H = \sum_{i=1}^A -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i<j} V(ij) \quad (3.3)$$

where  $V(ij)$  is a two-body potential. In the limit  $|_0$ ,  $\mu$  becomes the chemical potential of the normal state.

The operation of the first- and second-order derivatives on the superstate  $|\Phi_s\rangle$  yields the relations

$$\frac{\delta}{\delta\phi_k} |\phi_s\rangle|_0 = \begin{cases} -b_k |\phi_0^{(A)}\rangle, & k \leq k_F, \\ b_k^+ |\phi_0^{(A)}\rangle, & k > k_F, \end{cases} \quad (3.4)$$

$$\frac{\delta^2}{\delta\phi_k \delta\phi_p} |\phi_s\rangle|_0 = \begin{cases} (-2\delta_{kp} + b_p b_k) |\phi_0^{(A)}\rangle, & k, p \leq k_F, \\ -b_k^+ b_p |\phi_0^{(A)}\rangle, & k > k_F, p \leq k_F, \\ (-2\delta_{kp} + b_k^+ b_p^+) |\phi_0^{(A)}\rangle, & k, p > k_F. \end{cases} \quad (3.5)$$

The derivatives (3.4) and (3.5) are expressed as linear combinations of 4 and 16 states respectively which corresponds to  $A + 2$ ,  $A$  or  $A - 2$  particle systems. Using (3.4) and (3.5), equation (3.1) takes the form

$$S_{kp} = \begin{cases} \langle\phi_0^{(A)}|b_k^+ F_{A-2}^+ [H_{A-2} - H_{00}^{(A-2)}] F_{A-2} b_p |\phi_0^{(A)}\rangle (I_{00}^{(A)})^{-1} + CC, & k, p \leq k_F, \\ -\langle\phi_0^{(A)}|F_A^+ [H_A - H_{00}^{(A)}] F_A b_k^+ b_p |\phi_0^{(A)}\rangle (I_{00}^{(A)})^{-1} + CC, & p \leq k_F, k > k_F, \\ \langle\phi_0^{(A)}|b_k F_{A+2}^+ [H_{A+2} - H_{00}^{(A+2)}] F_{A+2} b_p^+ |\phi_0^{(A)}\rangle (I_{00}^{(A)})^{-1} + CC, & k, p > k_F. \end{cases} \quad (3.6)$$

Taking the  $\Lambda_{\sigma\sigma'}$  factors outside the integrals in equation (3.6), we express the remaining matrix elements in terms of the quantities

$$I_{mn}^{(A)} = \langle\phi_m^{(A)}|F_A^+ F_A |\phi_n^{(A)}\rangle, \quad (3.7)$$

$$N_{mn}^{(A)} = I_{mn}^{(A)} / (I_{mm}^{(A)} I_{nn}^{(A)})^{1/2}, \quad (3.8)$$

$$H_{mn}^{(A)} = \langle\phi_m^{(A)}|F_A^+ H_A F_A |\phi_n^{(A)}\rangle / (I_{mm}^{(A)} I_{nn}^{(A)})^{1/2}, \quad (3.9)$$

which are evaluated with the following model states corresponding to the appropriate

particle number  $A$ :

$$\begin{aligned}
 N = A - 2, \quad & |\phi_m^{(N)}\rangle = a_{k\sigma_1} a_{-k\sigma_2} |\phi_0^{(A)}\rangle, \quad |\phi_n^{(N)}\rangle = a_{p\sigma_1} a_{-p\sigma_2} |\phi_0^{(A)}\rangle \quad (k, p \leq k_F), \\
 N = A, \quad & |\phi_m^{(N)}\rangle = |\phi_0^{(A)}\rangle, \quad |\phi_n^{(N)}\rangle = a_{k\sigma_1}^+ a_{-k\sigma_2}^+ a_{p\sigma_1} a_{-p\sigma_2} |\phi_0^{(A)}\rangle \quad (k > k_F, p \leq k_F), \\
 N = A + 2, \quad & |\phi_m^{(N)}\rangle = a_{k\sigma_1}^+ a_{-k\sigma_2}^+ |\phi_0^{(A)}\rangle, \quad |\phi_n^{(N)}\rangle = a_{p\sigma_1}^+ a_{-p\sigma_2}^+ |\phi_0^{(A)}\rangle \quad (k, p > k_F).
 \end{aligned}
 \tag{3.10}$$

The configurations  $m, n$ , either of which may coincide with the set of the filled Fermi sea 0, differ from one another in two single-particle states, the pairs of single-particle states  $(k \uparrow, -k \downarrow)$  and  $(p \uparrow, -p \downarrow)$  respectively. Hence the quantity  $S_{kp}$  can be written in the form

$$\begin{aligned}
 S_{kp} = 2 \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^+(\mathbf{k}) \Lambda_{\sigma_2\sigma_2'}(\mathbf{p}) Z_{m,n}^{(A)} [(H_{mm}^{(A)} - H_{00}^{(A)}) \delta_{kp} \\
 + \frac{1}{2}(H_{mn}^{(A)} - H_{00}^{(A)} N_{mn}^{(A)} + \text{cc})(1 - \delta_{kp})] (1 - 2\eta(k))(1 - 2\eta(p)), \tag{3.11} \\
 Z_{m,n}^{(A)} = [I_{mm}^{(A)} I_{nn}^{(A)} / (I_{00}^{(A)})^2]^{1/2}. \tag{3.12}
 \end{aligned}$$

Detailed studies of the diagonal and off-diagonal terms contributing to the brackets of (3.11) presented in HI indicate that in low cluster order they behave like  $A^0$  and  $A^{-1}$  respectively in the given number of particles.

Using the definition of the normalisation integrals  $I_{mn}^{(N)} = \exp G_{mn}^{(N)}$  and following the formalism of the paper KC-II, we have for  $N = A + 2$

$$G_{mm}^{(A+2)} - G_{nn}^{(A+2)} = 2(\delta G(k) - \delta G(k_F)) \tag{3.13}$$

so that

$$Z_{m,n}^{(A+2)} = \exp [\delta G(k) + \delta G(p) - 2\delta G(k_F) + 2(dG_{00}^A/dA) + O(A^{-1})]. \tag{3.14}$$

The function  $G_{mn}^{(N)}$  is of order  $A$  in the given number of particles and the differences (3.13) behave like  $O(A^0)$ . The quantity  $\delta G(k)$  is determined by the equation

$$\delta G(k) = A^{-1} \int \frac{\delta G_{00}(0)}{\delta l(k_F r_{ij})} \exp(i\mathbf{k}r_{ij}) \mathbf{d}r_i \mathbf{d}r_j. \tag{3.15}$$

Similarly considering the cases  $N = A - 2, A$  and neglecting terms  $O(A^{-1})$ , we arrive at the unified expression for the three values of  $N$

$$Z_{m,n}^{(N)} = Z(k)Z(p), \tag{3.16}$$

$$Z(k) = \exp\{(1 - 2\eta(k))[\delta G(k) - \delta G(k_F) + dG_{00}/dA]\}. \tag{3.17}$$

The factor  $Z_{m,n}^{(N)}$  in equation (3.11) may be written out of the summation over the spin states in which we keep only contributions of order  $A^{-1}$ .

The diagonal and non-diagonal contributions to  $S_{kp}$  are given by

$$\sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^+(\mathbf{k}) \Lambda_{\sigma_2\sigma_2'}(\mathbf{k}) [H_{mm}^{(A\pm 2)} - H_{00}^{(A\pm 2)}] = 2 \sum_{\sigma\sigma'} |\Lambda_{\sigma\sigma'}(\mathbf{k})|^2 |\varepsilon(k) - \mu| = 4|\varepsilon(k) - \mu| \tag{3.18}$$

and

$$P_{\mathbf{k}\mathbf{p}} = \frac{1}{2} \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^+(\mathbf{k})\Lambda_{\sigma_2\sigma_2'}(\mathbf{p})q(\mathbf{k}, \mathbf{p}), \quad (3.19)$$

$$q(\mathbf{k}, \mathbf{p}) = H_{mm}^{(N)} - H_{00}^{(N)}N_{mn}^{(N)} + \text{cc} \quad (3.20)$$

or

$$P_{\mathbf{k}\mathbf{p}} = \frac{1}{2}(\bar{W}_{mn}^{(N)} + (|\varepsilon(k) - \mu| + |\varepsilon(p) - \mu|)\bar{N}_{mn}^{(N)} + \text{cc}) \quad (3.21)$$

respectively. The single-particle (hole) energies  $\varepsilon(k)$  (Tan and Feenberg 1968), the chemical potential  $\mu$  and the quantities  $\bar{W}_{mn}$  and  $\bar{N}_{mn}$  are defined as follows:

$$2\varepsilon(k) = H_{mm}^{(A+2)} - H_{00}^{(A)}, \quad k > k_F, \quad (3.22)$$

$$2\varepsilon(k) = H_{00}^{(A)} - H_{mm}^{(A-2)}, \quad k \leq k_F, \quad (3.23)$$

$$H_{00}^{(A+2)} - 2\mu = H_{00}^{(A)} = H_{00}^{(A-2)} + 2\mu, \quad (3.24)$$

$$H_{00}^{(A\pm 2)} - H_{00}^{(A\pm 2)} = 2|\varepsilon(k) - \mu|, \quad (3.25)$$

$$\bar{W}_{mn}^{(N)} = \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^+(\mathbf{k})\Lambda_{\sigma_2\sigma_2'}(\mathbf{p})W_{mn}^{(N)}, \quad (3.26)$$

$$\bar{N}_{mn}^{(N)} = \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^+(\mathbf{k})\Lambda_{\sigma_2\sigma_2'}(\mathbf{p})N_{mn}^{(N)}, \quad (3.27)$$

$$W_{mn}^{(N)} = H_{mn}^{(N)} - \frac{1}{2}(H_{mm}^{(N)} + H_{nn}^{(N)})N_{mn}^{(N)}, \quad (3.28)$$

$$\frac{1}{2}(H_{mm}^{(N)} + H_{nn}^{(N)} - 2H_{00}^{(N)})N_{mn}^{(N)} = (|\varepsilon(k) - \mu| + |\varepsilon(p) - \mu|)N_{mn}^{(N)}. \quad (3.29)$$

The off-diagonal quantities  $W_{mn}^{(N)}$  and  $N_{mn}^{(N)}$  are the two-body matrix elements

$$W_{mn}^{(N)} = \langle k\sigma_1, -k\sigma_1' | W(12; 1'2') | p\sigma_2, -p\sigma_2' \rangle_a, \quad (3.30)$$

$$N_{mn}^{(N)} = \langle k\sigma_1, -k\sigma_1' | N(12; 1'2') | p\sigma_2, -p\sigma_2' \rangle_a, \quad (3.31)$$

of the non-local four-point operators  $W(12; 1'2')$  and  $N(12; 1'2')$ . The structure of these operators has been studied in detail in HI. The functions  $W_{mn}$  and  $N_{mn}^{(N)}$  are to be written in a more elaborate form later in this work. In the final formulae the superscript  $N$  may be dropped, because for systems with  $A$  or  $A \pm 2$  particles, where  $A$  is very large, the differences are of the order  $O(A^{-2})$ .

Finally the quantity  $S_{\mathbf{k}\mathbf{p}}$  can be written

$$S_{\mathbf{k}\mathbf{p}} = 2Z(k)Z(p)[4|\varepsilon(k) - \mu|\delta_{\mathbf{k}\mathbf{p}} + P_{\mathbf{k}\mathbf{p}}(1 - \delta_{\mathbf{k}\mathbf{p}})](1 - 2\eta(p))(1 - 2\eta(k)). \quad (3.32)$$

In the evaluation of the diagonal and non-diagonal contributions to (3.32) we keep only the leading terms which behave like  $O(A^{-1})$ . Introducing the partial-wave decomposition

$$\delta\phi_{\mathbf{k}}\Lambda_{\sigma\sigma'}(\mathbf{k}) = \sum_{\lambda} \delta X_{\lambda}(k)\Lambda_{\sigma\sigma'}^{\lambda}(\hat{\mathbf{k}}) \quad (3.33)$$

into (3.32), we obtain for the quantity within the brackets

$$\sum_{\mathbf{k}\mathbf{p}\lambda\lambda'} \delta X_{\lambda}(k)\delta X_{\lambda'}(p) \left[ 4|\varepsilon(k) - \mu|\delta_{\mathbf{k}\mathbf{p}}\delta_{\lambda\lambda'} + \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^{\lambda*}(\hat{\mathbf{k}})\Lambda_{\sigma_2\sigma_2'}^{\lambda'}(\hat{\mathbf{p}})q(\mathbf{k}, \mathbf{p}) \right]. \quad (3.34)$$



Hence the criterion for the instability of the correlated normal state against the triplet pairing state is given by the angle-averaged condition for each  $\lambda$  state.

$$\frac{1}{(4\pi)^2} \int \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^{\lambda*}(\hat{k}) \Lambda_{\sigma_2\sigma_2'}^{\lambda}(\hat{p}) q(\mathbf{k}, \mathbf{p}) d\Omega_{\mathbf{k}} d\Omega_{\mathbf{p}}|_{\mathbf{k}=\mathbf{p}=\mathbf{k}_F} \equiv P_{k_F}^{\lambda\lambda'} < 0. \quad (3.35)$$

Obviously for  $\mathbf{k} = \mathbf{p}$  we have  $S_{k_p} > 0$  which indicates the stability of the normal state. For central potentials the matrix elements  $P_{k_F}^{\lambda\lambda'}$  will be diagonal otherwise we have to consider coupling states of the form  ${}^3P_2 - {}^3P_2, {}^3P_2 - {}^3F_2$  and  ${}^3F_2 - {}^3F_2$ .

#### 4. Condensation energy

An exact treatment of the expectation values of any operator with the superstate (2.13) is not possible as in the case of the stability condition which is evaluated at the normal values of the  $v_k$  parameter. Nevertheless a suitable approximation has been suggested by some authors (κC 1980, Kennedy 1968) which consists in the evaluation of the gap function using normal-state single-particle energies. This decoupling approximation, which will be discussed further later, yields a scheme where the expectation value of an operator is approximated by a finite number of terms.

Let us consider a translationally invariant operator  $\hat{O}$  which conserves the number of particles in the system. Then we have

$$\langle \phi_s | F^+ \hat{O} F | \phi_s \rangle = \sum_{Nmn} \langle \phi_s | \phi_m^{(N)} \rangle \langle \phi_m^{(N)} | F_N^+ \hat{O} F_N | \phi_n^{(N)} \rangle \langle \phi_n^{(N)} | \phi_s \rangle. \quad (4.1)$$

For reasons explained in § 2 we restrict the series expansion of (4.1) to terms which correspond to pairs  $m, n$  differing at most in two single-particle states. Consequently in (4.1) for each configuration  $|\phi_m^{(N)}\rangle$  the sum over  $n$  is reduced to the set of configurations

$$\{ |\phi_m^{(N)}\rangle, b_k^+ b_p | \phi_m^{(N)}\rangle \} \quad (4.2)$$

where the vector  $\mathbf{p}$  belongs to the set  $m$  but  $\mathbf{k}$  does not.

The projection coefficients of the superstate  $|\Phi_s\rangle$  along the normal states of the set (4.2) are determined by the relations

$$\langle \phi_m^{(N)} | \phi_s \rangle = \prod_k^m v_k^2 \prod_{k'}^{\bar{m}} u_{k'}^2, \quad (4.3)$$

and

$$\langle \phi_m^{(N)} | b_p^+ b_k | \phi_s \rangle = 4u_p v_p u_k v_k \prod_{k' \neq p}^m v_{k'}^2 \prod_{k'' \neq k}^{\bar{m}} u_{k''}^2, \quad (4.4)$$

where  $\bar{m}$  represents the complementary set of  $m$ . That is, each vector  $\mathbf{k}$  present in  $m$  is not present in  $\bar{m}$  or vice versa. Substituting (4.3) and (4.4) into (4.1), we arrive at the relation

$$\begin{aligned} \langle \phi_s | F^+ \hat{O} F | \phi_s \rangle = & \sum_{Nmn} \left\{ \prod_{k'}^m v_{k'}^4 \prod_{k''}^{\bar{m}} u_{k''}^4 \langle \phi_m^{(N)} | F_N^+ \hat{O} F_N | \phi_m^{(N)} \rangle \right. \\ & \left. + \sum_{p,k}^{\bar{m}} 4u_p v_p^3 v_k u_k^3 \prod_{k' \neq p}^m v_{k'}^4 \prod_{k'' \neq k}^{\bar{m}} u_{k''}^4 \langle \phi_m^{(N)} | F_N^+ \hat{O} F_N b^+ b_p | \phi_m^{(N)} \rangle \right\} \quad (4.5) \end{aligned}$$

where  $\mathbf{p}$  and  $\mathbf{k}$  belong to the sets  $m$  and  $\bar{m}$  respectively.

A satisfactory approximation of the condensation energy

$$E_s - E_0 = \frac{\langle \psi_s | H | \psi_s \rangle}{\langle \psi_s | \psi_s \rangle} - \frac{\langle \psi_0 | H | \psi_0 \rangle}{\langle \psi_0 | \psi_0 \rangle} \tag{4.6}$$

may be achieved applying the equation (4.5) with the appropriate operator for the evaluation of the superfluid energy  $E_s$ . Employing the decoupling approximation and expanding the functions of (4.5), which depend on the parameters  $v_k$  and  $u_k$ , keeping only contributions up to second order in  $v_k^2 - \hat{v}_k^2$  and of first order in  $u_p v_p^3 v_k u_k^3$ , we arrive at the equation

$$\begin{aligned} E_s - E_0 = & (I_{00}^{(A)})^{-1} \left\{ \sum_{Nm} \left\{ \sum_p (v_p^2 - \hat{v}_p^2) \prod_{k \neq p} \hat{v}_k^4 \prod_{k'} \hat{u}_{k'}^4 \right. \right. \\ & + \sum_k (v_k^2 - \hat{v}_k^2)^2 \prod_{k'} \hat{v}_{k'}^4 \prod_{k'' \neq k} \hat{u}_{k''}^4 \left. \right\} \langle \phi_m^{(N)} | F_N^+ (H_N - H_{00}^{(A)}) F_N | \phi_m^{(N)} \rangle \\ & + \sum_{Nm} \sum_p \sum_k 4u_p v_p^3 v_k u_k^3 \prod_{k' \neq p} \hat{v}_{k'}^4 \prod_{k'' \neq k} \hat{u}_{k''}^4 \langle \phi_m | F_N^+ (H_N - H_{00}^{(A)}) F_N b_k^+ b_p | \phi_m^{(N)} \rangle \left. \right\} \end{aligned} \tag{4.7}$$

with  $E_0 = H_{00}$ . Carrying out the summation over the sets  $\{m\}$  for the terms which involve a single sum over  $p, k$  and a double sum over  $p$  and  $k$ , we consider the following corresponding sets of states:

- (i)  $\{ |\phi_0^{(A)}\rangle, b_p^+ | \phi_0^{(A)}\rangle \},$
- (ii)  $\{ |\phi_0^{(A)}\rangle, b_k | \phi_0^{(A)}\rangle \},$
- (iii)  $\{ |\phi_0^{(A)}\rangle, b_p^+ | \phi_0^{(A)}\rangle, b_k | \phi_0^{(A)}\rangle, b_p^+ b_k | \phi_0^{(A)}\rangle \}.$

After some manipulations similar to those performed in the derivation of the stability criterion we finally obtain

$$\begin{aligned} E_s - E_0 = & 4 \sum_k (1 - \eta(k)) v_k^4 Z^2(k) \epsilon(k) - 4 \sum_k \eta(k) u_k^4 Z^2(k) \epsilon(k) \\ & + 4 \sum_{kp} u_p v_p^3 v_k u_k^3 Z(p) \\ & \times \{ \bar{W}_{kp} + [(1 - 2\eta(k)) \epsilon(k) + (1 - 2\eta(p)) \epsilon(p)] \bar{N}_{kp} \} \end{aligned} \tag{4.9}$$

where  $\bar{W}_{kp} = \bar{W}_{mn}$  and  $\bar{N} = \bar{N}_{kp} = \bar{N}_{mn}$  are determined by the equations (3.26) and (3.27). The prime indicates that  $k \neq p$ .

The expectation value of the number operator  $\hat{N}$  with the correlated superfluid state  $|\Psi_s\rangle$  obtained with the above technique yields the formula

$$\begin{aligned} N_s - A = & 4 \sum_k (1 - \eta(k)) v_k^4 Z^2(k) - 4 \sum_k \eta(k) u_k^4 Z^2(k) \\ & + 4 \sum_{kp} u_p v_p^3 v_k u_k^3 Z(k) Z(p) [(1 - 2\eta(k)) e_k + (1 - 2\eta(p)) e_p] \bar{N}_{kp} \end{aligned} \tag{4.10}$$

where  $A$  is the number of particles in the ground state. Following the single-particle

energies (3.22), we define the single-particle function  $e_k$  via

$$2e_k = \langle \hat{N} \rangle_m^{(A+2)} - \langle \hat{N} \rangle_{00}^{(A)} = 2\theta(k - k_F), \quad k > k_F, \tag{4.11}$$

$$2e_k = \langle \hat{N} \rangle_{00}^{(A)} - \langle \hat{N} \rangle_m^{(A-2)} = 2\theta(k_F - k), \quad k \leq k_F, \tag{4.12}$$

where  $\theta$  is the Heaviside unit step function,

$$\langle \hat{N} \rangle_{mn} = \langle \phi_m | F^+ \hat{N} F | \phi_n \rangle / [I_{mm} I_{nn}]^{1/2} \tag{4.13}$$

and  $\langle \hat{N} \rangle_{00} = A$ .

In order to ensure particle number conservation during a variational minimisation of the superfluid energy, we introduce the quantity

$$\begin{aligned} E_c &= \langle \psi_s | H - \mu N | \psi_s \rangle / \langle \psi_s | \psi_s \rangle \\ &= E_0 - \mu A + 4 \sum_k (1 - \eta(k)) v_k^4 Z^2(k) [\varepsilon(k) - \mu] \\ &\quad - 4 \sum_k \eta(k) u_k^4 Z^2(k) [\varepsilon(k) - \mu] + 4 \sum_{kp}' u_p v_p^3 v_k u_k^3 Z(k) Z(p) P_{kp} \end{aligned} \tag{4.14}$$

where  $P_{kp}$  is defined by equation (3.21). The Lagrangian multiplier  $\mu$  is varied until the condition

$$N_s = A \tag{4.15}$$

is satisfied.

### 5. Gap equation

It is evident that a minimum of the superfluid energy, preserving the number of particles, is achieved varying the functional  $E_c(v_k, \{X_\lambda\}) \equiv E_c(v_k, \Lambda_{\uparrow\uparrow}(k), \Lambda_{\uparrow\downarrow}(k))$  with respect to  $v_k$  and the variables  $\Lambda_{\uparrow\uparrow}(k), \Lambda_{\uparrow\downarrow}(k)$ .

The optimal functions  $v_k$  and  $u_k$  are determined by the variational equations

$$2u_k^2 Z(k) |\varepsilon(k) - \mu| = -2 \sum_{p \neq k} u_p v_p^3 u_k v_k^{-1} (u_k^2 - v_k^2) Z(p) P_{kp}, \tag{5.1}$$

$$2v_k^2 Z(k) |\varepsilon(k) - \mu| = -2 \sum_{p \neq k} u_p^3 v_p u_k^{-1} v_k (u_k^2 - v_k^2) Z(p) P_{kp}, \tag{5.2}$$

for  $k \leq k_F$  and  $k > k_F$  respectively. Multiplying (5.1) and (5.2) by  $v_k^2$  and  $u_k^2$  respectively and dividing both equations by  $u_k v_k$ , we arrive at the unified gap equation

$$2u_k v_k Z(k) |\varepsilon(k) - \mu| = -(u_k^2 - v_k^2) \Delta(k) \tag{5.3}$$

where the 'gap function'  $\Delta(k)$  is defined as

$$\Delta(k) = 2 \sum_{p \neq k} u_p v_p [u_p^2 (1 - \eta(k)) + v_p^2 \eta(k)] Z(p) P_{kp}. \tag{5.4}$$

The functional differentiation of  $E_c$  with respect to the variables  $\Lambda_{\uparrow\uparrow}(k)$  and  $\Lambda_{\uparrow\downarrow}(k)$  yields the relations

$$\Lambda_{\uparrow\uparrow}^+(\mathbf{p}) \Lambda_{\uparrow\uparrow}(\mathbf{k}) = \Lambda_{\uparrow\uparrow}^+(\mathbf{k}) \Lambda_{\uparrow\uparrow}(\mathbf{p}), \tag{5.5}$$

$$\Lambda_{\uparrow\downarrow}^+(\mathbf{p}) \Lambda_{\uparrow\uparrow}(\mathbf{k}) = \Lambda_{\uparrow\uparrow}(\mathbf{p}) \Lambda_{\uparrow\downarrow}^+(\mathbf{k}). \tag{5.6}$$

After some manipulations by means of equation (5.3), we derive for the probability amplitudes  $v_{\mathbf{k}}^2$  and  $u_{\mathbf{k}}^2$  the expressions

$$v_{\mathbf{k}}^2 = \frac{1}{2}[1 - Z(\mathbf{k})|\varepsilon(\mathbf{k}) - \mu|/E_e(\mathbf{k})], \quad (5.7)$$

$$u_{\mathbf{k}}^2 = \frac{1}{2}[1 + Z(\mathbf{k})|\varepsilon(\mathbf{k}) - \mu|/E_e(\mathbf{k})], \quad (5.8)$$

where

$$E_e^2(\mathbf{k}) = Z^2(\mathbf{k})|\varepsilon(\mathbf{k}) - \mu|^2 + \Delta^2(\mathbf{k}). \quad (5.9)$$

The optimal angle  $\phi_{\mathbf{k}}$  is given by

$$\phi_{\mathbf{k}} = \frac{1}{2} \tan^{-1}(-\Delta(\mathbf{k})/Z(\mathbf{k})|\varepsilon(\mathbf{k}) - \mu|). \quad (5.10)$$

The derivation of an elaborate formalism for the determination of gap function is achieved as follows. We define the matrix

$$\Delta_s(\mathbf{k}) = \begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} \quad (5.11)$$

where

$$\Delta_{\sigma_1\sigma_1'}(\mathbf{k}) = \sum_{\lambda} \Delta_{\sigma_1\sigma_1'}^{\lambda}(\mathbf{k}) \quad (5.12)$$

and

$$\Delta_{\sigma_1\sigma_1'}^{\lambda}(\mathbf{k}) = 2 \sum_{\mathbf{p} \neq \mathbf{k}} u_{\mathbf{p}} v_{\mathbf{p}} [u_{\mathbf{p}}^2(1 - \eta(\mathbf{k})) + v_{\mathbf{p}}^2 \eta(\mathbf{k})] Z(\mathbf{p}) q(\mathbf{k}, \mathbf{p}) X_{\lambda}(\mathbf{p}) \Lambda_{\sigma_1\sigma_1'}^{\lambda}(\hat{\mathbf{p}}). \quad (5.13)$$

The matrices  $\Delta_s(\mathbf{k})$  and  $\Lambda(\mathbf{k})$  by means of the relations (5.5) and (5.6) satisfy the equations

$$\Delta_s(\mathbf{k})\Lambda^+(\mathbf{k}) = \Lambda(\mathbf{k})\Delta_s^+(\mathbf{k}) = D(\mathbf{k}) \times I \quad (5.14)$$

where the diagonal element  $D(\mathbf{k})$  is given by

$$D^2(\mathbf{k}) = \frac{1}{2} \text{Tr}(\Delta_s^+(\mathbf{k})\Delta_s(\mathbf{k})) = \Delta_{\uparrow\uparrow}^+(\mathbf{k})\Delta_{\uparrow\uparrow}(\mathbf{k}) + \Delta_{\uparrow\downarrow}^+(\mathbf{k})\Delta_{\uparrow\downarrow}(\mathbf{k}). \quad (5.15)$$

The relation (5.14) means that the  $\Delta_s(\mathbf{k})$  can be factorised into

$$\Delta_s(\mathbf{k}) = D(\mathbf{k})\Lambda(\mathbf{k}). \quad (5.16)$$

Then by means of (5.7), (5.8), (5.12) and (5.16) we arrive at the coupled nonlinear 'gap equations'

$$\Delta_{\sigma_1\sigma_1'}^{\lambda}(\mathbf{k}) = -2 \sum_{\mathbf{p} \neq \mathbf{k}} Z(\mathbf{p}) q(\mathbf{k}, \mathbf{p}) \left( 1 + \frac{Z(\mathbf{p})|\varepsilon(\mathbf{p}) - \mu|}{E_e(\mathbf{p})} (1 - 2\eta(\mathbf{k})) \right) \frac{\Delta_{\sigma_1\sigma_1'}^{\lambda}(\mathbf{p})}{E_e(\mathbf{p})} \quad (5.17)$$

where  $\sigma_1\sigma_1'$  corresponds to the pairs ( $\uparrow\uparrow$ ) and ( $\uparrow\downarrow$ ). The function  $E_e(\mathbf{k})$  is determined by equation (5.9) where

$$\Delta(\mathbf{k}) = \text{Tr}(\Delta_s(\mathbf{k})\Lambda^+(\mathbf{k})) = 2D(\mathbf{k}). \quad (5.18)$$

The element  $D(\mathbf{k})$  is given by (5.15) with the additional relations

$$\Delta_{\uparrow\downarrow}^+(\mathbf{k}) = \Delta_{\uparrow\downarrow}(\mathbf{k}) \quad (5.19)$$

and

$$\Delta_{\uparrow\uparrow}^+(\mathbf{k}) = - \sum_{\mathbf{p} \neq \mathbf{k}} Z(\mathbf{p}) q(\mathbf{k}, \mathbf{p}) \left( 1 + \frac{Z(\mathbf{p}) |\varepsilon(\mathbf{p}) - \mu|}{E_c(\mathbf{p})} (1 - 2\eta(\mathbf{k})) \right) \times [D^2(\mathbf{p}) - \Delta_{\uparrow\downarrow}^2(\mathbf{p})] / E_c(\mathbf{p}) \Delta_{\uparrow\uparrow}(\mathbf{p}). \quad (5.20)$$

Minimising the functional  $E_c$ , we have derived the system of coupled equations (5.17) which, together with the equations (5.9), (5.15), (5.18), (5.19) and (5.20) serving as definitions, yield the determination of the anisotropic gap-function  $\Delta(\mathbf{k})$  via (5.18). In our scheme the interactions between Cooper pairs have long been neglected as a consequence of adopting the decoupling approximation. With the derivation of the 'gap equation' we have a theory where the main ingredients are the pairing matrix elements  $q(\mathbf{k}, \mathbf{p})$ , the single-particle energies  $\varepsilon(\mathbf{k})$  and the normalisation factor  $Z(\mathbf{k})$ . The construction and evaluation of these quantities is demonstrated in the next section.

## 6. Evaluation of normal-state quantities

In the preceding sections we have derived a formalism where the off-diagonal and diagonal quantities  $W_{mn}$ ,  $N_{mn}$  and  $H_{mm} - H_{00}$  represent matrix elements with respect to a basis of correlated normal states. Considering a state-independent Jastrow correlation factor, these CBF quantities may be expressed in more elaborate forms following one of the alternative CBF techniques developed by us (HI) and Krotscheck and Clark (KC-II) within the CBF framework. These techniques, which have been developed adopting the Jackson-Feenberg and the Clark-Westhaus forms of the expectation value of the kinetic energy, respectively, express the required CBF quantities in terms of compound-diagrammatic functions which may be evaluated within the accuracy of the Fermi hypernetted chain approximation schemes (FHNC).

Within the FHNC theory the set of functions  $N_{ab}(r_{12})$  is constructed which represent the sums of nodal, non-nodal and elementary diagrams with  $ab = dd, de$  and  $ee$  in accordance with whether none, one or two exchange lines are attached to its internal points 1, 2. We also construct the sum  $\Gamma_{ab}(r_{12})$  of nodal and non-nodal diagrams. Of these functions the most prominent is the sum  $h_d(r_{12}) \equiv \Gamma_{dd}(r_{12})$  of diagrams which hereafter will play the role of the dressed correlation function (line) replacing the bare correlation function (line)  $h(r_{ij}) = f^2(r_{ij}) - 1$  in the diagrammatic representation of the cluster series of the required quantities. Following the formalism of HI, an exchange function (line) represents the factor  $-v^{-1}l(k_F r_{ij}) = -j_1(k_F r_{ij}) / (v k_F r_{ij})$  ( $v$  is the degeneracy of the system). The set of functions so constructed which are involved in the FHNC calculations may be evaluated following one of the schemes presented by Krotscheck-Ristig (1975) and Fantoni-Rosati (1975), or solving the appropriate FHNC equations in conjunction with the equations obtained variationally within an optimisation scheme for the normal ground-state energy (Owen 1979, Lantto and Siemens 1977). Another quantity involved in our formalism is the sum  $X_{cc}(r_{12})$  of all non-nodal diagrammatic contributions to  $g(r_{12})$  with a single exchange path joining the points 1, 2 including the term  $v^{-1}l(k_F r_{12})$ . The function  $X_{cc}(r)$  is evaluated by solving the appropriate set of FHNC integral equations. After the construction of the required FHNC functions we turn our attention to the evaluation of the required CHF quantities.

In accordance with our CBF scheme presented in HI the off-diagonal quantities  $N_{mn}$  and  $W_{mn}$  are given by the relations

$$N_{mn} = X_{m,n}^{-1} \langle m_1 m_2 | N^B(12; 1'2') | n_1 n_2 \rangle_a, \quad (6.1)$$

$$W_{mn} = X_{m,n}^{-1} \{ \langle m_1 m_2 | W^B(12; 1'2') | n_1 n_2 \rangle_a + J_{mn} + \frac{1}{2} [u(m_1) + u(m_2) + u(n_1) + u(n_2)] + W^{(1)}(m_1) + W^{(1)}(m_2) + W^{(1)}(n_1) + W^{(1)}(n_2) \} \langle m_1 m_2 | N^B(12; 1'2') | n_1 n_2 \rangle_a, \quad (6.2)$$

where

$$J_{mn} = (\hbar^2/8m) \int \nabla_1^2 \langle m_1 m_2 | N^B(12; 1'2') | n_1 n_2 \rangle_a \, d\mathbf{r}_2 \, d\mathbf{r}_1, \quad (6.3)$$

$$X_{m,n} = [(1 - \tilde{X}_{cc}(m_1))(1 - \tilde{X}_{cc}(m_2))(1 - \tilde{X}_{cc}(n_1))(1 - \tilde{X}_{cc}(n_2))]^{1/2}, \quad (6.4)$$

$$u(m) = \tilde{X}'_{cc}(m)/(1 - \tilde{X}_{cc}(m)). \quad (6.5)$$

Studying the diagrammatic decomposition of the four-point operators  $N^B(12; 1'2')$  and  $W^B(12; 1'2')$  which consist only of basic diagrams, it has been shown that they are constructed from local and non-local classes of diagrams. The superscript 'B' indicates the 'basic' character of these quantities. Details about the structure of these operators have been given in HI. The local parts of the operators  $N^B(12; 1'2')$  and  $W^B(12; 1'2')$  are  $N^B(12) = h_d(r_{12})$  and  $W^B(12) = h'_d(r_{12})$  respectively. The function  $h'_d(r_{12})$  is called the dressed effective potential and the prime denotes that the sum  $h'_d(r)$  is obtained from the diagrammatic contributions to the sum  $h_d(r)$  replacing, in turn, each line  $h(r)$  with a graphical element which represents the two-body effective potential

$$w_2(ij) = -(\hbar^2/4m) \nabla_i^2 \ln f^2(ij) + V(ij). \quad (6.6)$$

The function  $h'_d$  is determined by the set of integral equations

$$h'_d(r) = [h_d(r) + 1][w_2(r) + N'_{dd}(r) + E'_{dd}(r)], \quad (6.7)$$

$$\tilde{N}'_{dd}(k) = \tilde{h}'_d(k) \left[ 1 - \left( \frac{1 - \tilde{P}(k)}{1 - \tilde{X}_{de}(k)} \right)^2 \right] + \left( \frac{\tilde{X}_{dd}(k)}{1 - \tilde{X}_{de}(k)} \right) \left( 2\tilde{X}'_{de}(k) + \frac{\tilde{X}'_{ee}(k)\tilde{X}_{dd}(k)}{1 - \tilde{X}_{de}(k)} \right), \quad (6.8)$$

with

$$h_d(r) = N_{dd}(r) + X_{dd}(r) \quad (6.9)$$

$$\tilde{P}(k) = \tilde{X}_{dd}(k)(1 + \tilde{X}_{ee}(k)) + 2\tilde{X}_{de}(k) - \tilde{X}_{de}^2(k), \quad (6.10)$$

where the tilde denotes the Fourier transform multiplied by the density  $\rho$ . The quantities  $\tilde{X}_{de}(k)$ ,  $\tilde{X}'_{de}(k)$ ,  $\tilde{X}_{ee}(k)$  and  $E'_{dd}(r)$  are determined either by keeping the leading terms in suitable diagrammatic expansions or by means of additional integral equations within the FR-FHNC approximation. These functions can also be evaluated in conjunction with the appropriate equations obtained from a variational scheme.

In our method the quantities  $J_{mn}$  and  $W^{(1)}_{(m)}$  (HI) are expressed as cluster series with terms which do not include the dressed two-body effective interaction  $h'_d(r)$ . Finally the quantities  $X'_{cc}(r)$  and  $\tilde{X}'_{cc}(m)$  are determined by the set of coupled linear equations

$$X'_{cc}(r) = h'_d(r)[N_{cc}(r) + E_{cc}(r) - v^{-1}l(k_{\text{FF}})] + h_d(r)[N'_{cc}(r) + E'_{cc}(r)] + E'_{cc}(r) \quad (6.11)$$

$$\tilde{N}'_{cc}(k) = \tilde{X}'_{cc}(k)[(1 - v^{-1}l(\tilde{k}_{\text{FF}}))/(1 - \tilde{X}_{cc}(k))^2 - 1], \quad (6.12)$$

where  $v^{-1}l(k_{\text{FF}}) = \theta(k_{\text{F}} - k)$ .

Again the sum  $E_{cc}(r)$  is the 'cc' analogue of  $E_{dd}(r)$ . Using the functions  $\tilde{X}'_{cc}(k)$  and  $\tilde{X}_{cc}(k)$  so determined, we may evaluate the single-particle energies  $\varepsilon(k)$  and the

quantity  $\delta G(k)$  given by the relations

$$\varepsilon(k) = \hbar^2 k^2 / 2m + u(k) + W^{(1)}(k) + a_0, \quad (6.13)$$

$$a_0 = -\hbar^2 k_F^2 / 2m - u(k_F) - W^{(1)}(k_F) + \mu, \quad (6.14)$$

$$\delta G(k) = -\ln[1 - \hat{X}_{cc}(k)]. \quad (6.15)$$

The constant  $a_0$  can be determined in principle from the chemical potential of the normal state. The normalisation factor  $Z(k)$  is also evaluated by means of equations (3.17) and (6.15).

Finally, evaluating the required FHNC quantities, we can adopt a scheme maintaining the Fermi cancellations, which occur between the diagrammatic contributions, keeping all diagrams with the same number of dressed correlation lines but different number of particles.

## 7. Application to liquid $^3\text{He}$

Studying the condition for the existence of an instability corresponding to  $^3\text{P}_0$  pairing in liquid  $^3\text{He}$ , we performed numerical calculations for the evaluation of the diagonal matrix elements  $P_{k_F}^\lambda$  determined by (3.35) with  $S = 1$  and  $L = 1$ .

Applying the CBF-FHNC method which has been developed in the preceding sections and defining

$$W^{\lambda\lambda'}(k_F) = \frac{1}{(4\pi)^2} \int \sum_{\substack{\sigma_1\sigma_1' \\ \sigma_2\sigma_2'}} \Lambda_{\sigma_1\sigma_1'}^{\lambda*}(\hat{k}) \Lambda_{\sigma_2\sigma_2'}^\lambda(\hat{p}) \langle k\sigma_1, -k\sigma_1 | W^B(12; 1'2') | p\sigma_2, -p\sigma_2' \rangle_a \\ d\Omega_k d\Omega_p |_{k=p=k_F} = (W^B)_{k_F}^\lambda \delta_{\lambda\lambda'}, \quad (7.1)$$

as well as  $J^\lambda(k_F) = (J)_{k_F}^\lambda \delta_{\lambda\lambda'}$  and  $N(k_F) = (N)_{k_F}^\lambda \delta_{\lambda\lambda'}$ , the diagonal matrix element  $P_{k_F}^\lambda$  takes the form

$$P_{k_F}^\lambda = \frac{W(k_F)^\lambda + J^\lambda(k_F) + 2[u(k_F) + W^{(1)}(k_F)]N^\lambda(k_F)}{(1 - \hat{X}_{cc}(k_F))^2}. \quad (7.2)$$

In evaluating the quantities  $W^\lambda(k)$  and  $N^\lambda(k)$  we have considered only the local portions of  $W^B(12; 1'2')$  and  $N^B(12; 1'2')$  which are represented by the dressed effective potential  $h'_d(12)$ , defined by the set of equations (6.7) and (6.8), and the dressed correlation function  $h_d(12)$  respectively. These dressed functions have been calculated within a FHNC optimisation scheme developed by Owen (1979) for the minimisation of the ground-state energy. The function  $\hat{X}_{cc}(k)$  has been determined solving the appropriate set of coupled FHNC equations by means of an iteration scheme. The quantity  $\hat{X}'_{cc}(k)$  has been evaluated by solving the set of equations (6.11) and (6.12) using the standard matrix inversion technique in momentum space.

In our calculations we have totally ignored the sums of the elementary diagrams  $E_{dd}(r)$ ,  $E_{cc}(r)$  and  $E'_{cc}(r)$ .

Finally, evaluating the quantity  $J^\lambda(k)$ , we have considered only one diagram resulting from consideration of the local portion of the function  $N^B(12; 1'2')$  in the equation (6.3). The diagonal element  $W_{(k)}^{(1)}$  has been evaluated from all the diagrams with no more than two dressed correlation lines. The analytic form of  $W_k^{(1)}$ , expressed in the momentum space, is given in appendix 2.

In order to compare our results with those obtained by KC, it is more convenient to express our numerical results in terms of the dimensionless quantities

$$\delta_w(\lambda) = N_0 \Omega [W^\lambda(k_F) + J^\lambda(k_F)], \tag{7.3}$$

$$\delta_P(\lambda) = N_0 \Omega P_{k_F}^\lambda, \tag{7.4}$$

where  $N_0 = m^* k_F / 2\pi^2 \hbar^2$  and the effective mass  $m^*$  is defined by

$$\frac{m^*}{m} = \frac{\hbar^2 k_F}{m} \left( \frac{d\varepsilon(k)}{dk} \right)_{k=k_F}^{-1} = \left( 1 + \frac{m}{\hbar^2 k_F} \frac{d}{dk} (u(k) + W^{(1)}(k))_{k=k_F} \right)^{-1}. \tag{7.5}$$

The quantity  $\delta_P(\lambda)$  has been constructed as the analogue, in our formalism, of the quantity  $-N(0)V$  in the BCS weak-interaction theory where  $N(0) = N_0$  represents the density of states and  $V$  is the strength of the pairing interaction.

Studying the  $^3P_0$  pairing, we have performed numerical calculations using the Lennard-Jones potential with the de Boer-Michels parameters and the Frost-Musulin potential which are denoted by  $V(\text{LJ})$  and  $V(\text{FDD1})$  respectively. These potentials have the analytic forms

$$(i) \quad v(\text{LJ}) = V_0 [(\sigma/r)^{12} - (\sigma/r)^6] \tag{7.6}$$

with  $V_0 = 40.88^\circ\text{K}$  and  $\sigma = 2.556 \text{ \AA}$ .

$$(ii) \quad \begin{aligned} V(\text{FDD1}) &= -V_0 [1 + c(1 - X^{-1})] e^{c(1-x)} & (r \leq r_0), \\ &= -V_1 (C_6 r^{-6} + C_8 r^{-8}) & (r > r_0), \end{aligned} \tag{7.7}$$

with  $x = r/r_m$ ,  $V_0 = 12.54^\circ\text{K}$ ,  $c = 8.00877$ ,  $V_1 = 7250.0^\circ\text{K}$ ,  $C_6 = 1.41 \text{ \AA}$ ,  $C_8 = 3.82 \text{ \AA}$ ,  $r_m = 2.98 \text{ \AA}$  and  $r_0 = 3.51078 \text{ \AA}$ .

As we have mentioned in § 3, an instability of the normal state in favour of the  $^3P_0$  pairing is indicated when the parameter  $\delta_P(^3P_0)$  has a negative sign within the density region which is studied here. The numerical calculation of the parameters  $\delta_w(^3P_0)$  and  $\delta_P(^3P_0)$  is subject to the accuracy and the uncertainties which are involved in adopting the FHNC scheme.

Our numerical results for these parameters are shown in tables 1 and 2 for the  $V(\text{LJ})$  and  $V(\text{FDD1})$  potentials respectively. From these tables we observe that calculations with the  $V(\text{FDD1})$  potential, which has a stronger attractive part than  $V(\text{LJ})$ , show a tendency towards  $^3P_0$  pair condensation at higher density values. Our calculation is in excellent agreement with those performed by KC for the  $^3P_0$  pairing using

**Table 1.** Liquid  $^3\text{He}$  results for  $V(\text{LJ})$  potential.

$\rho \text{ (\AA}^{-3}\text{)}$	$m^*/m$	$\delta_w(^3P_0)$	$\delta_P(^3P_0)$	$u(k_F)$	$1 - \tilde{\chi}_{cc}(k_F)$
0.008	1.01	-0.005	-0.011	0.00	0.81
0.010	1.03	0.004	0.024	-0.06	0.79
0.012	1.04	0.011	0.067	-0.15	0.63
0.014	1.05	0.016	0.118	-0.25	0.57
0.016	1.05	0.022	0.193	-0.37	0.52
0.018	1.05	0.026	0.256	-0.45	0.48
0.020	1.05	0.030	0.337	-0.56	0.45



**Table 2.** Liquid  $^3\text{He}$  results for FDD1 potential.

$\rho$ ( $\text{\AA}^{-3}$ )	$m^*/m$	$\delta_W(^3\text{P}_0)$	$\delta_P(^3\text{P}_0)$	$u(k_F)$	$1 - \tilde{X}_{cc}(k_F)$
0.008	0.084	0.013	-0.032	0.04	0.87
0.010	1.023	-0.000	0.005	-0.02	0.74
0.012	1.041	0.008	0.050	-0.11	0.65
0.014	1.049	0.014	0.104	-0.26	0.50
0.016	1.052	0.021	0.183	-0.30	0.52
0.018	1.053	0.025	0.249	-0.40	0.40
0.020	1.052	0.029	0.338	-0.51	0.45

their FHNC/O, FHNC/C and FBGY/C approximations and predicts a negative  $\delta_P(^3\text{P}_0)$  only at densities smaller than  $\rho = 0.008 \text{ \AA}^{-3}$ . This result contradicts their FBGY/O method and the experimental indication that the instability of the normal state against the triplet BW pairing takes place just below the equilibrium density  $\rho_0 = 0.0164 \text{ \AA}^{-3}$ . Although our CBF-FHNC method does not give an adequately satisfactory description of the  $^3\text{P}_0$  superfluid state of liquid  $^3\text{He}$ , we believe that an improvement can be achieved within our scheme by introducing non-local contributions to  $W^\lambda(k_F)$  and  $J^\lambda(k_F)$ . In tables 1 and 2 are also shown the ratio  $m^*/m$  and the functions  $u(k_F)$  and  $1 - \tilde{X}_{cc}(k_F)$  which enter the calculation of  $P_{k_F}^\lambda$ .

The ratio  $m^*/m$  has a predicted value near to unity in comparison with the experimental value 3.08. This substantial difference is a consequence of the fact that our trial wavefunction for the normal ground state incorporates a Jastrow state-independent correlation factor.

There are several explanations of the discrepancy between our calculation and the experimental results. The most significant is that our wavefunction does not describe spin-density fluctuations, so that there is no part of our effective pairing interaction associated with exchange of spin fluctuations. On the other hand, the deficiency of using momentum-independent correlation can be rectified to some extent within a CBF perturbative formalism from the higher-order momentum-dependent correction. A substantial improvement of our calculations may be achieved using state-dependent correlation functions which incorporate three-body interactions and the dominant effects induced by the backflow behaviour of  $^3\text{He}$  atoms (Schmidt and Pandharipande 1979). We also believe that the omission of the elementary diagrams as well as the uncertainty of the interparticle potential used will not explain a substantial part of the missing effective pairing interaction.

A refinement of the present formalism is that developed by Krotscheck *et al* (1981) where perturbation corrections have been generated to the superfluid ground-state energy. In their scheme, the superfluid state is expressed in terms of correlated basis states which are related by generalised creation and annihilation operators. However their effective pairing interaction does not generate the observed P-wave pairing and yields results similar to ours mainly for the reasons given above.

A numerical estimation of the normalisation factor  $Z(k)$ , providing that the derivative  $dG_{00}^{(A)}/dA$  is given by the equation (A2.3) in appendix 2, indicates that for small densities it remains near unity. However, as the density increases the deviation of  $Z(k)$  from unity is substantial, so that an attempt to estimate the gap function  $\Delta(k)$  by solving the system of gap equations (5.17) and to calculate the condensation energy is problematic. In this case we believe that it is necessary to devise an optimisation

scheme, where the correlation function will be evaluated by minimising the superfluid energy.

**Acknowledgment**

We would like to thank Dr J C Owen for supplying us with his FHNC variational codes which were used as a starting point in the development of our programme.

**Appendix 1.**

The function  $\Lambda_{\sigma\sigma'}(\mathbf{k})$  defined by equation (2.5) which corresponds to the  ${}^3P_J$  pairing ( $S = 1, L = 1$ ) represents a decomposition over the labels  $J$  and  $M_J$ . Defining  $X_{J,M_J} = X_\lambda(k)$  and substituting the Clebsch–Gordan coefficients, we arrive at the following representation for the  $\Lambda_J(\mathbf{k})$  matrices.

(i)  ${}^3P_0$  pairing.

$$\Lambda_0 = \frac{1}{\sqrt{3}} X_{00} \begin{pmatrix} Y_{1-1} & -Y_{10}/\sqrt{2} \\ -Y_{10}/\sqrt{2} & Y_{11} \end{pmatrix}. \tag{A1.1}$$

(ii)  ${}^3P_1$  pairing.

$$\Lambda_1 = \begin{pmatrix} (X_{11}Y_{10} + X_{10}Y_{1-1})/\sqrt{2} & \frac{1}{2}(-X_{11}Y_{11} + X_{1-1}Y_{1-1}) \\ \frac{1}{2}(-X_{11}Y_{11} + X_{1-1}Y_{1-1}) & -(X_{10}Y_{11} + X_{1-1}Y_{10})/\sqrt{2} \end{pmatrix}. \tag{A1.2}$$

(iii)  ${}^3P_2$  pairing.

$$\Lambda_2 = \begin{pmatrix} X_{22}Y_{11} + \frac{1}{\sqrt{2}}X_{21}Y_{10} + \frac{1}{\sqrt{6}}X_{20}Y_{1-1} & \frac{1}{2}X_{21}Y_{11} + \frac{1}{\sqrt{3}}X_{20}Y_{10} + \frac{1}{2}X_{2-1}Y_{1-1} \\ \frac{1}{2}X_{21}Y_{11} + \frac{1}{\sqrt{3}}X_{20}Y_{10} + \frac{1}{2}X_{2-1}Y_{1-1} & X_{2-2}Y_{1-1} + \frac{1}{\sqrt{2}}X_{2-1}Y_{10} + \frac{1}{\sqrt{6}}X_{20}Y_{11} \end{pmatrix}. \tag{A1.3}$$

**Appendix 2.**

The diagrammatic contributions to the various required quantities are most easily evaluated in momentum space.

The function  $W^{(1)}(k)$  which is given by  $W^{(1)}(m)$  with  $\mathbf{k} = \mathbf{k}_m$  was evaluated from all the diagrams (HI) with no more than two dressed correlation lines and may be written as follows:

$$\begin{aligned} W^{(1)}(k) = & \frac{\hbar^2}{8m} \int \frac{d\mathbf{k}_1}{(2\pi)^3 \rho} \tilde{h}_d(k_1) \left\{ \theta(k_F - |\mathbf{k} - \mathbf{k}_1|) k_1^2 \right. \\ & - \int \frac{d\mathbf{k}_2}{(2\pi)^3 \rho} \tilde{h}_d(k_2) [\theta(k_F - |\mathbf{k} - \mathbf{k}_2 - \mathbf{k}_1|) \theta(k_F - |\mathbf{k} - \mathbf{k}_2|) (\mathbf{k}_1 + \mathbf{k}_2)^2 \\ & + \frac{1}{2} k_1^2 \theta(k_F - |\mathbf{k} + \mathbf{k}_2|) (\theta(k_F - |\mathbf{k} - \mathbf{k}_1|) \\ & \left. - 2\theta(k_F - |\mathbf{k} + \mathbf{k}_1|) \theta(k_F - |\mathbf{k} + \mathbf{k}_1 + \mathbf{k}_2|)) \right\}. \tag{A2.1} \end{aligned}$$

The quantity  $dG_{00}/dA$  was evaluated from all the diagrams contributing to  $G_{00}$  with no more than two dressed correlation lines and is given by

$$\begin{aligned} \frac{dG_{00}}{dA} = & \frac{\tilde{h}(k)}{2} - \frac{1}{2} \int \frac{dk_1}{(2\pi)^3 \rho} \tilde{h}(k_1) Q_1(k_1) [1 + \tilde{h}(k_1) - \frac{1}{2} \tilde{h}(k_1) Q_1(k_1)] \\ & + \frac{v}{2} \int \frac{dk_1 dk_2}{(2\pi)^3 \rho^2} \tilde{h}(k_1) \tilde{h}(k_2) [Q_2(\mathbf{k}_1, \mathbf{k}_2) - \frac{1}{2} v^2 Q_3(\mathbf{k}_1, \mathbf{k}_2)] \end{aligned} \quad (\text{A2.2})$$

where

$$Q_1(k_1) = \frac{(2\pi)^3 \rho}{v} \int dk_1 \theta(k_F - k_1) \theta(k_F - |k_1 - k|) = 1 - S_F(k), \quad (\text{A2.3})$$

$$Q_2(\mathbf{k}_1, \mathbf{k}_2) = \int \frac{dk_3}{(2\pi)^3 \rho} \theta(k_F - k_3) \theta(k_F - |k_2 + k_3|) \theta(k_F - |k_1 + k_2 + k_3|), \quad (\text{A2.4})$$

$$Q_3(\mathbf{k}_1, \mathbf{k}_2) = \int \frac{dk_3}{(2\pi)^3 \rho} \theta(k_F - k_3) \theta(k_F - |k_3 + k_1|) \theta(k_F - |k_3 - k_2|) \theta(k_F - k_3 + k_1 - k_2). \quad (\text{A2.5})$$

The function  $S_F(k)$  is the static structure function of the non-interacting Fermi gas which for  $k \leq 2k_F$  has the form

$$S_F(k) = \frac{3}{4} k/k_F - \frac{1}{16} (k/k_F)^3. \quad (\text{A2.6})$$

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