# New variational wave function for liquid <sup>3</sup>He

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Variational calculations, with a new wave function based on the Feynman-Cohen correlation operator, are carried out for liquid <sup>3</sup>He with a Lennard-Jones potential. The wave function contains three-body correlations and momentum-dependent two-body correlations, in addition to the Jastrow correlations commonly used in variational calculations. The Fermi hypernetted-chain summation methods are generalized to calculate energy expectation values with this wave function. The calculated equilibrium energy and density are  $-2. \pm 0.1$  °K and  $0.28 \pm 0.01 \sigma^{-3}$ , a significant improvement over the -1.25 °K and  $0.22 \sigma^{-3}$  obtained with the Jastrow wave function, and closer to the experimental -2.56 °K and  $0.28 \sigma^{-3}$ .

### I. INTRODUCTION

The Jastrow wave function,

$$\Psi_J = \prod_{i < j} f_{J,ij} \Phi \quad , \tag{1.1}$$

where  $f_{J,ij}$  is a function of the interparticle distance  $|\vec{r}_i - \vec{r}_i|$  and  $\Phi$  is the ideal Fermi-gas wave function, is commonly used for calculating upper bounds to the ground-state energy of liquid <sup>3</sup>He. The energy expectation value with  $\Psi_I$  can either be calculated with Monte Carlo integration,<sup>1</sup> or with the hierarchy of Fermi-hypernetted-chain integral equations.<sup>2</sup> Both the Monte Carlo and integral equation methods give identical results. For the Lennard-Jones (LJ) deBoer-Michaels potential, the calculated equilibrium energy and density  $E_0$  and  $\rho_0$  are, respectively, -1.25 °K and  $0.22\sigma^{-3}$ , where  $\sigma = 2.556$  Å is the length scale in the LJ potential. These results are not in satisfactory agreement with the experimental values -2.56 °K and  $0.277 \sigma^{-3}$  for  $E_0$  and  $\rho_0$ . An exact solution of the liquid <sup>4</sup>He many-body Schrödinger equation, with the same LJ potential, by the Green's-function Monte Carlo<sup>3</sup> method yields  $E_0 = -6.85$  °K,  $\rho_0 = 0.37 \sigma^{-3}$ , against the experimental values -7.15 °K and  $0.365 \sigma^{-3}$  for liquid <sup>4</sup>He. Thus, we expect the LJ potential to give a better description of the helium liquids than that obtained with the Jastrow approximation.

The correlation-function  $f_{ij}(\vec{r}_{ij}, \vec{k}_{ij})$  between two particles in a Fermi fluid can depend upon the planewave states  $e^{i\vec{k}_i\cdot\vec{r}_i}$  and  $e^{i\vec{k}_i\cdot\vec{r}_j}$ , occupied by the particles. In its simples form this dependence comes from the  $\nabla_m \prod_{i < j} f_{ij} \cdot \nabla_m \Phi$  terms in the kinetic energy.<sup>4</sup> Variational calculations with a wave function containing state-dependent correlations are difficult. Nevertheless, Pandharipande and Bethe<sup>4</sup> (PB) found that these could shift the calculated  $E_0$  and  $\rho_0$  of liquid <sup>3</sup>He to  $\sim -1.9$  °K and  $0.25\sigma^{-3}$ .

An important feature of the PB state-dependent correlation function is that it contains the "Feynman-Cohen backflow<sup>5</sup>" absent in the Jastrow wave function. In the limit  $|\vec{k}_{ij}| \rightarrow 0$  the PB correlation function reduces to an operator  $\mathfrak{F}_{ij}$ , <sup>6,7</sup>

$$\mathfrak{F}_{ij} = f_J(r_{ij}) + \eta(r_{ij}) \,\vec{\mathbf{r}}_{ij} \cdot \vec{\nabla}_{ij} \quad . \tag{1.2}$$

The second term in the above  $\mathcal{F}$  allows one to describe the backflow of <sup>4</sup>He atoms around an impurity <sup>3</sup>He atom in liquid <sup>3</sup>He, and thus calculate the enhancement of its effective mass.<sup>6</sup>

A variational wave function for Bose fluids may be constructed from a symmetrized product of  $\mathfrak{F}$ . Due to the gradient operator in  $\mathfrak{F}$  it represents arbitrarily many-body correlations, i.e.,

$$\$ \prod_{i < j} \$_{ij} = \prod_{i < j} f_{J,ij} \prod_{i < j < k} f_{3,ijk} \prod_{i < j < k < l} f_{4,ijkl} \cdots ,$$
(1.3)

where  $f_J, f_3, f_4 \cdots$  are respectively two-, three-, four-  $\cdots$  particle correlations that do not contain gradient operators. The  $\eta(r)$  is fortunately <<1, and it appears reasonable to retain only the linear term  $\eta(r_{ij})\vec{r}_{ij}\cdot\vec{\nabla}_i f_J(r_{ik})$  in  $f_3$ , and neglect  $f_{n\geq4}$ . In liquid <sup>4</sup>He the Jastrow wave function gives -5.9 °K and  $0.34\rho^{-3}$  for  $E_0$  and  $\rho_0$ . The inclusion<sup>7</sup> of this three-body correlation  $f_3$  in the wave function, shifts these to -6.7 °K nd  $0.38\sigma^{-3}$ , which are in excellent agreement with the supposedly exact Green'sfunction Monte Carlo results.

The most obvious choice of a variational wave function for Fermi fluids is

$$\Psi = \$ \prod_{i < j} \mathfrak{F}_{ij} \Phi \quad . \tag{1.4}$$

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This wave function has additional terms linear in  $\eta$  from the  $\vec{\nabla}_i$  in  $F_{ij}$  operation on the  $\Phi$ . In the present work we report variational calculations with a wave function of the form

$$\Psi_{V} = \prod_{i < J} [f_{J}(r_{ij}) + \eta \vec{r}_{ij} \cdot \vec{\nabla}_{ij}^{R}] \prod_{i < J < k} f_{3,ijk} \Phi \quad , \quad (1.5)$$

where the  $\vec{\nabla}_{ij}^{R}$  operates only on the  $\Phi$ ; the  $\eta_{ij}\vec{r}_{ij} \cdot \vec{\nabla}_{i}f_{ik}$  terms are included in  $f_3$  as in the Bose case. The calculated  $E_0$  (2. ±0.1 °K) and  $\rho_0$  (0.28 ±0.02  $\sigma^{-3}$ ) with this wave function are quite close to what we may expect from the LJ potential.

The calculation of  $\Psi_V$  and its variational parameters are discussed in Sec. II. Sections III and IV, respectively, discuss calculations of the distribution function and calculations of the energy expectation value with the FHNC technique. To some extent these sections are the generalization of the formalism developed in Ref. 7 to Fermi fluids. The results are presented in Sec. V. A casual reader uninterested in hypernetted-chain summations may wish to skip the rather technical Secs. III and IV.

### **II. VARIATIONAL WAVE FUNCTION**

The PB correlation-functions  $f(\vec{k}, \vec{r}, d)$  have a variational parameter d, and are obtained by minimizing the two-body cluster energy with the constraint that the  $f(\vec{k}, \vec{r}, d)$  go smoothly to unity at r = d. They give the exact energy in the low-density limit.<sup>8</sup> The  $f(\vec{k}, \vec{r}, d)$  is obtained from the set of equations

$$f(\vec{\mathbf{k}},\vec{\mathbf{r}},d)e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}} = \Psi(\vec{\mathbf{k}},\vec{\mathbf{r}},d) \quad , \tag{2.1}$$

$$\Psi(\vec{k},\vec{r},d) = \sum_{l=0}^{\infty} i^{l}(2l+1)f(l,k,r,d) \ j_{l}(kr)P_{l}(\cos\theta) ,$$
(2.2)

$$u_l(k,r,d) = f(l,k,r,d) j_l(k,r) r , \qquad (2.3)$$

$$-\frac{\hbar^2}{m} \left( u_l'' - \frac{l(l+1)}{r^2} u_l \right) + v u_l = \left( \frac{\hbar^2}{m} k^2 + \lambda_l(k) \right) u_l \quad .$$
(2.4)

The Schrödinger equation (2.4) is valid for r < d, and  $\lambda_l(k)$  is obtained from the boundary-condition f'(l,k,r=d) = 0.

In the limit  $k \rightarrow 0$  the  $f(\vec{k}, \vec{r}, d)$  reduces to the simple operator  $\mathcal{F}$  given by Eq. (1.2) with<sup>6</sup>

$$f_J(r,d) = f(l=0,k \to 0,r,d)$$
, (2.5)

$$\eta(r,d) = f(l=1,k \to 0,r,d) - f_J(r,d) \quad . \tag{2.6}$$

It is very difficult to calculate the many-body cluster contributions (MBCC) with the  $f(\vec{k}, \vec{r}, d)$ ; PB essentially used the  $f(l=0, k \rightarrow 0, r, d)$  to evaluate them,

and calculated only the two-body cluster energy with the  $f(\vec{k}, \vec{r})$ .

The direct two-body cluster-energy  $[C_{11}(k)]_J$  calculated with the  $f_J$  is independent of k and equals the  $[C_{11}(k \rightarrow 0)]_{\mathfrak{F}}$  calculated with the correlation operator  $\mathfrak{F}$ . The  $[C_{11}(k)]_{\mathfrak{F}}$ ,

$$C_{11}(k)]_{\mathfrak{F}} = [C_{11}(k \to 0)]_{\mathfrak{F}} + \frac{4\pi}{3\Omega}k^{2}$$

$$\times \int \eta \left( -\frac{\hbar^{2}}{m} [(f_{J}' + \eta')4r + \eta''r^{2}] + \upsilon \eta \right) r^{2} dr$$
(2.7)

has an additional attractive term proportional to  $k^2$ . The  $[C_{11}(k)]_{\mathfrak{F}}$  is very close to the  $C_{11}(k)$ , obtained from  $f(\vec{k},\vec{r})$ , up to  $k = \pi/d$  (Fig. 1); when k exceeds  $\pi/d$ , the nodes in  $j_0(kr)$  create problems in the calculation of  $f(\vec{k},\vec{r})$ . The fact that the  $C_{11}(k)$  with  $f(\vec{k},\vec{r})$  is a little above the  $[C_{11}(k)]_{\mathfrak{F}}$  is a reflection of the external constraints in the variational problem. The  $C_{11}(k)$  (Fig. 1) have both direct and exchange contributions, and at least from a variational point of view, the  $\mathfrak{F}$  seems to do well at the two-body level. Its additional advantages are: it is simpler to calculate MBCC with  $\mathfrak{F}$ ; and it can be used to generate many-body correlations  $f_3, f_4 \cdots$ 

Since  $\eta(r)$  and f'(r) are roughly proportional to each other (Fig. 2) the many-body wave function [Eq. (1.5)] is conveniently approximated by<sup>7</sup>



FIG. 1. Two-body cluster energies for parallel and antiparallel spin pairs with various correlation functions at  $d = 1.73r_0$  and  $\rho = 0.277\sigma^3$ .

$$\Psi_{v} = \prod_{i < j} f_{J}(r_{ij}) \prod_{i < j < k} (1 + \sum_{cyc} \chi_{ijk})$$
$$\times \prod_{i < j} (1 + \frac{i}{2} q_{ij} \vec{r}_{ij} \cdot [\vec{k}(i) - \vec{k}(j)] \Phi)$$
$$\equiv \prod_{i < j} f_{J}(r_{ij}) \prod_{i < l < k} f_{3,ijk} \prod_{i < l} f_{k,ij} \Phi , \qquad (2.8)$$

 $\chi_{ijk} = \xi_{ij}\xi_{ik}\vec{\mathbf{r}}_{ij}\cdot\vec{\mathbf{r}}_{ik} \quad , \tag{2.9}$ 

$$\xi_{ii} = \beta_3 \eta_{ii} / f_{ii} \quad , \tag{2.10}$$

$$q_{ij} = \beta_k \eta_{ij} / f_{ij} \quad . \tag{2.11}$$

The  $\beta_3$  and  $\beta_k$  are two extra variational parameters that, respectively, vary the magnitude of  $f_3$  and  $f_k$ . The operator  $\vec{k}(i)$  in Eq. (2.8) is defined such that when it operates on a plane-wave state with momentum  $\vec{k}_m$  occupied by the *i*th particle, it gives an eigenvalue  $\vec{k}_m$ , for example

$$\vec{\mathbf{k}}(i)e^{i(\vec{\mathbf{k}}_{m}\cdot\vec{\mathbf{r}}_{i}+\vec{\mathbf{k}}_{n}\cdot\vec{\mathbf{r}}_{j}+\cdots)} = \vec{\mathbf{k}}_{m}e^{i\vec{\mathbf{k}}_{m}\cdot\vec{\mathbf{r}}_{i}+\vec{\mathbf{k}}_{n}\cdot\vec{\mathbf{r}}_{j}+\cdots)}$$
(2.12)

It may be verified that Eq. (2.8) is antisymmetric with this definition of  $\vec{k}(i)$ . The  $(-1)^{1/2}$  in the  $q_{ij}$ term of Eq. (2.8) comes from the  $\nabla_i e^{i\vec{k}_m \cdot \vec{r}_i}$ , and does not imply that Eq. (2.8) is complex; by replacing the *i* k(i) operators by the  $\nabla_i$ , we obtain the real  $\Psi_v$ when  $\Phi$  is real.



FIG. 2. Comparison of  $f \eta r$  and ff' at  $d = 1.73r_0$  and  $\rho = 0.277 \sigma^{-3}$ .

## III. CLUSTER EXPANSION AND CHAIN SUMMATIONS

In the first part of this section we set  $\beta_k = 0$  and thus treat the simpler wave function

$$\Psi = \prod_{i < j} f_{J,ij} \prod_{i < j < k} f_{3,ijk} \alpha \prod_i \phi_i(r_i) \quad , \tag{3.1}$$

where  $\alpha$  is the antisymmetrizing operator. A diagrammatic cluster expansion of the expectation value of a symmetric two-body operator O(r),

$$\frac{\int \left(A \prod_{i} \phi_{i}^{*}(r_{i})\right) \prod_{i < j} f_{J} \prod_{i < j < k} f_{3}O_{mn}(r_{mn}) \prod_{i < j < k} f_{3} \prod_{i < j} f_{J} \prod_{i} \phi_{i}(r_{i}) d\tau}{\int \left(A \prod_{i} \phi_{i}^{*}(r_{i})\right) \prod_{i < j} f_{f}^{2} \prod_{i < j < k} f_{3}^{2} \prod_{i} \phi_{i}(r_{i}) d\tau},$$

is obtained by replacing all the  $f^2$ , except  $f_{mn}^2$  in the numerator, by 1 + F; and the  $f_3$  is replaced by  $1 + \sum_{cyc} \chi$ . The integrals in the numerator and the denominator are then represented by diagrams in which the points represent the particle coordinates,  $F_{ij}$  is a dashed line joining *i* and *j*, and solid lines *ij* and *ik*, with a marking on the angle *i* of the triangle *ijk*, denote  $\chi_{ijk}$ . Exchanges are represented by directed lines. An exchange line labeled  $\vec{k}_i$  going from *i* to *j* represents the contribution of a term in  $\Psi_v^*$ , in which particle *j* occupies the state  $\vec{k}_i$ . We antisymmetrize only the left-hand  $\Psi^*$  and thus particles  $i, j \cdots$  respectively occupy states  $k_i, k_j \cdots$  in the right-hand  $\Psi$ . All exchange lines  $\vec{k}_i$  originate from points *i*.

This diagrammatic notation is identical to that used in Ref. 7 and PB. All numerator diagrams must contain the points m and n, and the  $f_{mn}O_{mn}f_{mn}$  is implied. The expectation value is given by the sum of all irreducible numerator diagrams. We generally need to sum over all the particles  $i, j, \ldots, m$  and n; this summation yields, apart from trivial symmetry factors, a density  $\rho$  for every point in the diagram and a Slater function  $l(k_F r_{ij})$ , i.e.,

$$l(x) = 3(\sin x - x \cos x) / x^3 , \qquad (3.3)$$

for every exchange line. Similarly the expectation value of a three-body operator  $O_{mno}$  is given by the sum of all irreducible diagrams containing a triangle mno with implicit

$$f_{mn}f_{mo}f_{no}\left|\left(1+\sum_{cyc}\chi_{mno}\right)O_{mno}\left(1+\sum_{cyc}\chi_{mno}\right)f_{mn}f_{mo}f_{no}\right.$$
(3.4)

In the hypernetted-chain approximation all diagrams containing single or multiple chains connecting two particles are summeed neglecting the coupling between the chains. In the simple FHNC<sup>9</sup> (without the three-body correlation  $\chi_{ijk}$ ) there are four types of hypernetted chains, whose contributions are denoted by  $G_{dd,ij}$ ,  $G_{de,ij}$ ,  $G_{ee,ij}$ , and  $G_{cc,ij}$ . The first

(3.2)

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two subscripts of G specify the exchanges at the two ends of the chain. The dd, de, and ee respectively represent direct-direct, direct-exchange, and exchange-exchange, while cc is for an incomplete circular exchange. The following two subscripts of G denote the end particles. Since the number of exchange lines passing through a point can either be zero or two, chains  $G_{xx',ij}$  and  $G_{yy',jk}$  cannot be linked at point j unless x'y equals dd, de, ed, or cc.

The present case, the  $\chi_{ijk}$  generate additional chains formed with elements  $C_{xx',ij}$  analogous to  $C_{2-7}$ of Ref. 7. Typical hypernetted-chains  $G_{xx',ij}$  and elements  $C_{xx',ij}$  are shown in Figs. 3 and 4. Fantoni and Rosati<sup>9</sup> (FR) derived a set of coupled equations for the G's which we generalize to include the C's. (Note that in the FR notation our subscripts dd, de, ee, and cc become ss, sh, hh, and dd.) We first generalize the Slater function *l* to include many-body circular exchanges

$$L = -l + s(G_{cc} + C_{cc}) , \qquad (3.5)$$

where s is the spin degeneracy which equals two in liquid <sup>3</sup>He, we define partial two-particle distribution functions  $g_{xx'}$ , i.e.,

$$g_{dd} = f^2 \exp(G_{dd} + C_{dd}) \quad . \tag{3.6}$$

$$g_{de} = g_{dd}(G_{de} + C_{de})$$
 , (3.7)

$$g_{ee} = g_{dd} \left[ -L^2 / s + G_{ee} + C_{ee} + (G_{de} + C_{de})^2 + D \right] , \quad (3.8)$$

$$g_{cc} = g_{dd} L/s \quad . \tag{3.9}$$

The D in Eq. (3.8) represents  $f_k$  contributions treated later. The physical two-particle distribution function g is given by

$$g = g_{dd} + 2g_{de} + g_{ee} \quad . \tag{3.10}$$

The contributions of non-nodal<sup>10</sup> diagrams of type dd, *ee*, *de*, and *cc* are respectively given by  $X_{xx'}$ , i.e.,

$$X_{dd} = g_{dd} - 1 - G_{dd} \quad , \tag{3.11}$$

$$X_{ee} = g_{ee} - G_{ee} \quad , \tag{3.12}$$

$$X_{d_0} = g_{d_0} - G_{d_0} ag{3.13}$$

$$X_{ii} = g_{ii} + \frac{1}{s} - G_{ii} \qquad (3.14)$$

We now define the following two functions which link chains at point k:

$$\Theta_{ij}(x_{ik}; y_{kj}) = \rho \int d^3 r_k \, x_{ik} y_{kj} \quad , \qquad (3.15)$$

$$\Gamma_{ij}(x_{ik};y_{kj}) = \rho \int d^3 r_k g_{dd,ik} g_{dd,kj} \\ \times \left[ \left( 1 + \sum_{\text{cyc}} \chi_{ijk} \right)^2 - 1 \right] x_{ik} y_{kj} \quad , \qquad (3.16)$$

and the FR propagator

$$P_{ij} = X_{dd,ij} + 2X_{de,ij} + \Theta_{ij}(X_{dd\ ik}; X_{ee,kj}) - \Theta_{ij}(X_{de,ik}; X_{de,kj})$$
(3.17)

used to build the chains. The chain functions are then obtained as

$$G_{dd,ij} = \Theta_{ij}((g_{dd} - 1)_{ik}; P_{kj}) , \qquad (3.18)$$

$$G_{de,ij} = \Theta_{ij}(X_{dd,ik}; X_{ee,ij}) - \Theta_{ij}(X_{de,ik}; X_{de,kj}) + \Theta(g_{de,ik}; P_{kj})$$
(3.19)

$$G_{ee,ij} = \Theta_{ij}(X_{de,ik}; X_{de,kj}) - \Theta_{ij}(X_{dd,ik}; X_{ee,kj}) + \Theta(g_{ee,ik}; P_{kj})$$
(3.20)

$$G_{cc,ij} = \Theta_{ij}(X_{cc,ik}; g_{cc,kj}) \quad , \tag{3.21}$$

$$C_{dd,ij} = \Gamma_{ij} (1 + 2(C_{de} + G_{de})_{ik}; 1_{kj}) \quad , \tag{3.22}$$

$$C_{de,ll} = \Gamma_{ll} \left( \left[ -\frac{1}{2}L^2 + C_{ee} + G_{ee} + (C_{de} + G_{de})^2 \right]_{lk}; 1_{kl} \right) + \Gamma_{ll} \left( \left( C_{de} + G_{de} \right)_{lk}; (1 + C_{de} + G_{de})_{kl} \right)$$
(3.23)

$$C_{ee,ij} = \Gamma_{ij} \left( \left[ -L^2 + 2C_{ee} + 2G_{ee} + 2(C_{de} + G_{de})^2 + C_{de} + G_{de} \right]_{ik}; (C_{de} + G_{de})_{kj} \right) , \qquad (3.24)$$

$$C_{cc,lj} = \frac{1}{4} \Gamma_{lj} (L_{lk}; L_{kj}) \quad . \tag{3.25}$$

Consistent solutions of Eq. (3.5)-(3.25) can be easily obtained by iterative schemes. The above equations sum all hypernetted chain (HNC)-type diagrams except those belonging to "group II" in the notation of Ref. 7. It is shown in Ref. 7 that these should not be summed without their HNC/4 counterparts.



FIG. 3. Typical chain diagrams.



and 6; the  $G_{dd}$  is clearly the biggest contributor. However, the large magnitude of  $G_{dd}$  does not imply that HNC is a poor aapproximation (Ref. 1). The validity of the FHNC approximation may be ascertained by FHNC/4 calculation,<sup>2</sup> in which the effect of



FIG. 5.  $G_{xx'}$  at  $d = 1.73r_0$ ,  $\beta_k = 0.7$ ,  $\beta_3 = 2.4$ , and  $\rho = 0.277 \sigma^{-3}$ .



FIG. 6.  $C_{xx'}$  at  $d = 1.73r_0$ ,  $\beta_k = 0.7$ ,  $\beta_3 = 2.4$ , and  $\rho = 0.277 \sigma^{-3}$ .

pairwise coupling between the G's and C's is calculated. FHNC/4 also includes circular-exchange diagrams of type 7.1-7.4 of Fig. 7. These cannot be trivially interpreted as a coupling of two FHNC's. At small r the FHNC/4 diagrams 7.1-7.4 are comparable to the FHNC diagrams 7.5-7.8 and thus it is not obvious that they are negligible.



FIG. 7. Some FHNC/4 elementary diagrams and their FHNC counter parts in limit  $r \rightarrow 0$ .

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We report FHNC/4 calculations in two approximations called FHNC/4B and FHNC/4C. In the FHNC/4B the coupling between two G's is calculated in the Boson approximation. The three point function

$$\zeta_{add,ijk} \equiv \rho \int (g-1)_{i1} (g-1)_{j1} (g-1)_{k1} d^3 r_1 ,$$
(3.26)

is used to calculate the elementary-diagram  $E_{dd,ij}$ , i.e.,

$$E_{dd,ij} = \frac{\rho}{2} \int \zeta_{ddd,ijk} (g-1)_{jk} d^3 r_k \quad . \tag{3.27}$$

The effect of pairwise coupling between the G's is included approximately in the FHNC equations by redefining  $g_{dd}$  (Eq. 3.6) as

$$g_{dd} = f^2 \exp(G_{dd} + C_{dd} + E_{dd}) \quad . \tag{3.28}$$

To incorporate the effect of G-C coupling we redefine  $\Gamma$  as

$$\Gamma_{ij}(x_{ik}, y_{kj}) = \rho \int d^3 r_k g_{dd, ik} g_{dd, kj} \left[ \left( 1 + \sum_{cyc} \chi_{ijk} \right)^2 - 1 \right] (1 + \zeta_{ddd, ijk}) x_{ik} y_{kj} , \qquad (3.29)$$

while the coupling between two C's is neglected. We may expect the Boson approximation to FHNC/4 to be valid when all but the  $G_{dd}$  chains give small contributions.

The approximation FHNC/4C includes the  $E_{dd}$  in Boson approximation, and the four elementary diagrams 7.1–7.4. These may be easily evaluated with the three-point function

$$\zeta_{dcc,ijk} \equiv \rho \int (g_{dd} - 1)_{i1} g_{cc,j1} g_{cc,k1} d^3 r_1 \quad .$$
(3.30)

The physical three-particle distribution function  $g_{3,ijk}$  is given by

$$g_{3,ijk} = (1 + \zeta_{ddd,ijk}) \left( 1 + \sum_{cyc} \chi_{ijk} \right)^2 \times \left( \sum_{n=1,8} u_{n1,ij} u_{n2,ik} u_{n3,jk} \right) ,$$
(3.31)

in the FHNC and FHNC/4B approximations. The  $u_{nm}$  are sums of partial  $g_{xx'}$  functions given in Table I. The products of u functions in Eq. (3.31) simply superpose  $g_{xx'}$ , ensuring a correct exchange pattern.

TABLE I. The matrix  $u_{ii}$ .

i/j	1	2	3
1	$g_{dd} + 2g_{de} + g_{ee}$	8 <sub>dd</sub> + 8 <sub>de</sub>	8 <sub>dd</sub>
2	8 <sub>dd</sub>	$g_{dd} + g_{de}$	$2g_{de} + g_{ee}$
3	$g_{dd} + g_{de}$	$g_{de} + g_{ee}$	8 <sub>dd</sub>
4	8 <sub>dd</sub>	$g_{de} + g_{ee}$	8 <sub>de</sub>
5	8 <sub>de</sub>	8 <sub>dd</sub>	$2g_{de} + g_{ee}$
6	$g_{de} + g_{ee}$	8 <sub>dd</sub>	8 <sub>de</sub>
7	$2g_{de}$	8 <sub>de</sub>	8 de
8	$-4g_{cc}$	g <sub>cc</sub>	<i>B<sub>cc</sub></i>

The  $f_k$  generate diagrams having a new element—a wiggly line, denoting  $q_{ij}r_{ij}$ . A single wiggly line connecting ij (Fig. 8.1) can come from the  $(f_{k,ij}-1)$  in either  $\Psi$  or  $\Psi^*$ . Its contribution is

$$\frac{1}{2}iq_{ij}\vec{\mathbf{r}}_{ij}\cdot(\vec{\mathbf{k}}_i-\vec{\mathbf{k}}_j-\vec{\mathbf{k}}_{i'}+\vec{\mathbf{k}}_{j'}) \quad , \qquad (3.32)$$

where  $\vec{k}_{i'}$  and  $\vec{k}_{j'}$  are the states occupied by particles *i* and *j* in  $\Psi^*$ . The  $\vec{k}_{i'}$  and  $\vec{k}_{j'}$  are given, in our diagrammatic notation, by the exchange lines that enter points *i* and *j*. When *i* is not exchanged we have



FIG. 8.  $f_k$  diagrams.

 $\vec{k}_{i'} = \vec{k}_{i}$ , thus a single wiggly line with neither end exchanged gives zero contribution.

A double wiggly line connecting *i* and *j* (Fig. 8.2) depicts terms with  $(f_{k,ij}-1)$  in both  $\Psi$  and  $\Psi^*$ . Its contribution is

$$+\frac{1}{4}q_{ij}^{2}[\vec{\mathbf{r}}_{ij}\cdot(\vec{\mathbf{k}}_{i'}-\vec{\mathbf{k}}_{j'})][\vec{\mathbf{r}}_{ij}\cdot(\vec{\mathbf{k}}_{i}-\vec{\mathbf{k}}_{j})] \quad . \tag{3.33}$$

The summation over k can be easily carried out by writing the  $\vec{k}$ 's as gradients. For example, the contribution of the element shown in Fig. 8.3 is

$$\sum_{i,j,k} \frac{i}{2} q_{ij} \vec{\mathbf{r}}_{ij} \cdot (\vec{\mathbf{k}}_{i} - \vec{\mathbf{k}}_{k}) e^{i(\vec{\mathbf{k}}_{i} \cdot \vec{\mathbf{r}}_{ik} + \vec{\mathbf{k}}_{k} \vec{\mathbf{r}}_{ki})} = \sum_{i,j,k} \frac{1}{2} q_{ij} (e^{i\vec{\mathbf{k}}_{k} \cdot \vec{\mathbf{r}}_{ki}} \vec{\mathbf{r}}_{ij} \cdot \nabla_{i} e^{i\vec{\mathbf{k}}_{i} \cdot \vec{\mathbf{r}}_{ik}} \vec{\mathbf{r}}_{ij} \cdot \nabla_{i} e^{i\vec{\mathbf{k}}_{k} \cdot \vec{\mathbf{r}}_{ki}}) = \frac{1}{2} \rho^{3} q_{ij} r_{ij} l_{ik} l_{ik}' \cos\theta_{i} \quad ,$$

$$(3.34)$$

where  $\theta_i$  is the internal angle of the triangle *ijk*.

The contribution of a wiggly line diagram that contains an articulation point, at which the diagram can be separated into two pieces is not necessarily factorizable. Let us first consider the simple case of a factorizable diagram containing only dashed  $F_{ij}$  lines, e.g., diagram (8.4) in Fig. 8. The diagram (8.4) has been discussed in PB. Its contribution is the product of the two diagrams shown in Fig. (8.5). The diagram 8.4 is thus reducible; it is required to cancel the denominator and gives no contribution to the expectation value of  $O_{mn}$ . The analogous wiggly line diagram (8.6) is however not factorizable, and its contribution is

$$\sum_{n,l,j} \rho \int d^3 r_m \, d^3 r_l \, d^3 r_l \, d^3 r_j \, (f_{J,mn} O_{mn} f_{J,mn}) F_{ml} F_{lj} \frac{1}{2} \, i q_{ln} \vec{r}_{ln} \cdot (\vec{k}_l - \vec{k}_n - \vec{k}_j + \vec{k}_l) e^{i (\vec{k}_l \cdot \vec{\tau}_{ln} + \vec{k}_n \cdot \vec{\tau}_{nj} + \vec{k}_j \cdot \vec{\tau}_{jl})} ; \qquad (3.35)$$

while that of the product of the two separated diagrams (8.7) is

$$\sum_{n,l,j} \rho \int d^3 r_m \, d^3 r_i \, d^3 r_j \, (f_{J,mn} O_{mn} f_{J,mn}) F_{mi} F_{ij} i q_{in} \vec{\tau}_{in} \cdot (\vec{k}_i - \vec{k}_n) e^{i(\vec{k}_i \cdot \vec{\tau}_{in} + \vec{k}_n \cdot \vec{\tau}_{nj} + \vec{k}_j \cdot \vec{\tau}_{ji})} .$$
(3.36)

A general cluster expansion which includes such separable but not factorizable diagrams is discussed by Wiringa and Pandharipande.<sup>11</sup> Their contribution to the expectation value is the difference between that of the unseparated diagram and the product of the two separated diagrams. Thus the contribution of diagram (8.6) in Fig. 8 is obtained by subtracting the contribution of the product of diagrams (8.7) from that of the unseparated diagram (8.6).

The wiggly line elements can be trivially linked by the  $\Theta$  only to the direct end of another element. Hence, their contribution D is added to  $g_{ee}$  [Eq. (3.8)]. It is possible to decompose D into its elementary clusters. For example, the dd chain 9.1 in Fig. 9 is made up of two dd links 12 and 34, and an elementary cluster  $D_{23}(2, 1, 1)$ . The  $D_{ii}(p, p', p'')$  depicts an elementary cluster in which *i* and *j* are connected by wiggly lines or exchange links. The minimum number of particles in the cluster is denoted by p; since the cluster can have  $G_{dd}$  hypernets, the maximum number is arbitrary. The number of wiggly lines in the smallest (*p*-body) cluster is p', while p'' is a serial number. The nonzero  $D_{ij}$  having  $p + p' \leq 4$ , are shown in Fig. 10. The  $D_{ij}(3, 1, p'')$  may contain any number of  $G_{dd,ik}$  and  $G_{dd,jk}$  chains which are not shown in the figure. The contribution of separated diagrams has to be subtracted from  $D_{ii}(3, 1, p'' = 1, 4)$ .

Algebraic expressions for the  $D_{ij}$  of Fig. 10 are given in the Appendix.



FIG. 9. Chains containing  $f_k$  correlations.

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FIG. 10. Skeletons of  $D_{ij}(p,p',p'')$  diagrams.

The exact  $D_{ij}$  is given by

$$D_{ij} = \sum_{p,p'} D_{ij}(p,p') , \qquad (3.37)$$

$$D_{ij}(p,p') = \sum_{p''} D_{ij}(p,p',p'') \quad . \tag{3.38}$$



FIG. 11.  $D_{ij}(p,p')$  at  $d = 1.73r_0$ ,  $\beta_k = 0.7$ ,  $\beta_3 = 2.4$ , and  $\rho = 0.277 \sigma^{-3}$ .

Figure 11 shows the calculated D(2, 1), D(2, 2), and D(3, 1). The D(2, 2) is much smaller than D(2, 1) in the region of interest because of the additional  $\eta$  function, while the total D(3, 1) is much smaller than D(2, 1). We hope that the D(p,p') continue their rapid decline as p + p' is increased and truncate the sum in Eq. (3.37) at p + p' = 4.

Simple examples of chains containing  $D_{ij}$  summed by a consistent solution of the FHNC (3.5-3.25) and  $D_{ij}$  (A.1-A.9) equations, are shown in Fig. 9.1-9.4. Contribution of chains 9.2 and 9.3 can respectively be of order D(3, 1) and D(2, 1), while 9.4 having two D(3, 1) and a D(2, 1) element should be much smaller. Chains 9.5 and 9.6 are not summed by these equations. They constitute the D(4, 1) and should be much smaller than D(3, 1) due to the extra exchange. Chain 9.7 is an example of the omitted D(3, 2); it should be of order  $G_{de,ij}D_{ij}(2, 2)$ , which is much less than D(2, 2).

#### **IV. CALCULATION OF ENERGY**

Since  $\Phi$  is an eigenfunction of the kinetic energy operator the contribution of terms in which the  $\nabla_m^2$ operates on  $\Phi$  is exactly given by the Fermi kinetic energy  $T_F$ 

$$T_F = \frac{3}{5} \frac{\hbar^2}{2m} k_F^2 \quad . \tag{4.1}$$

In conjunction with the PB  $f_J$ , it is convenient to combine the contributions of terms in which the  $\nabla_m^2$ and  $\nabla_n^2$  operate on the  $f_{J,mn}$  with that of  $v_{mn}$ . The sum, called W is given by

$$W = 2\pi\rho \left( \lambda_0(k \to 0) \int_0^d dr \ r^2 g(r) + \int_d^\infty dr \ r^2 g(r) v(r) \right) , \qquad (4.2)$$

where g(r) is the pair distribution function 3.9. Terms having

$$\nabla_m f_{mn} \cdot \nabla_m f_{mo}$$
,  $\nabla_m^2 f_{mno}$ ,  $\nabla_m f_{mn} \cdot \nabla_m f_{mno}$ 

and

$$\nabla_m f_{mno} \cdot \nabla_m f_{mp}$$

occur also in the Bose system and have been classified as U and  $T_{i-1,6}$  in Ref. 7. The terms  $T_{1-5}$ involve the three-particle distribution function  $g_{3,mn0}$ of Eq. (3.31). Their sum is given by

$$\sum_{i=1,5}^{\infty} T_{i} = \rho^{2} \int \frac{g_{3}(\vec{r}_{mn},\vec{r}_{mo})}{f_{3,mno}} \left[ \xi_{mo}r_{mo}\mu_{mo}C_{m} + \xi_{mn} \quad \nu_{mn} - \frac{\hbar^{2}}{2m} [(r\xi')_{mo}(\xi'r + 2\hat{f}_{J}\xi r)_{mn}C_{m}^{2} + 2\hat{f}_{J,mo} \times (\xi'r)_{mn}(\xi r)_{no}C_{m}C_{n} - 2\hat{f}_{J,mo}(\xi r)_{no}\xi_{mn}C_{o}] \right] d^{3}r_{mn} d^{3}r_{mo} ,$$

where the primes denote the derivatives with respect to 
$$r$$
, and

$$\hat{f}_J = f_J'/f_J$$
 , (4.4)

$$\mu = -\hbar^2 / m \left[ \xi'' r + 4\xi' + 2\hat{f} \left( \xi' r + \xi \right) \right] , \qquad (4.5)$$

$$\nu = -\hbar^2 / m \left( \xi' r + \frac{3}{2} \xi + \hat{f}_J \xi r \right) . \tag{4.6}$$

The  $C_m$ ,  $C_n$ , and  $C_o$ , are respectively the cosines of the internal angles  $\theta_m$ ,  $\theta_n$ , and  $\theta_o$  of the triangle *mno*.

To calculate the  $T_6$  and U we have to subdivide the functions  $\alpha_{mn}$  and  $\gamma_{mn}$  of Ref. 7 according to the exchanges of particles *m* and *n*. We define the following functions:

$$\Lambda_{mno}^{dd} = (g_{dd,mo}g_{dd,on} + g_{de,mo}g_{dd,on} + g_{dd,mo}g_{ed,on}) ,$$
(4.7)

$$\Lambda_{mno}^{de} = (g_{dd,mo}g_{de,on} + g_{dd,mo}g_{ee,on} + g_{de,mo}g_{de,on}) ,$$
(4.8)

$$\Lambda_{mno}^{ed} = (g_{ed,mo}g_{dd,on} + g_{ee,mo}g_{dd,on} + g_{ed,mo}g_{ed,on}) ,$$
(4.9)

$$\Lambda_{mno}^{ee} = (g_{ed,mo}g_{de,on} + g_{ee,mo}g_{de,on} + g_{ed,mo}g_{ee,on}) ,$$

(4.10)

$$\Lambda_{mno}^{cc} = (g_{cc,mo}g_{cc,on}) \quad , \tag{4.11}$$

in which the superscripts specify the nature of the exchange at points *m* and *n*. Let  $\Upsilon_{mno}^{xx'}$  be defined as

$$\Upsilon_{mno}^{xx'} = f_{3,mno} \Lambda_{mno}^{xx'}$$
 (4.12)

The  $\alpha_{mn}^{xx'}$  and  $\gamma_{mn}^{xx'}$  are given by<sup>14</sup>

$$\alpha_{mn}^{xx'} = \rho \int \Upsilon_{mno}^{xx'} [(\xi r)_{mo} (\xi' r)_{mn} C_m + (\xi r)_{no} (\xi' r)_{mn} C_n + \xi_{mo} (\xi r)_{mn}] (1 + \zeta_{ddd,mno}) d^3 r_o , \qquad (4.13)$$
  
$$\gamma_{mn}^{xx'} = \rho \int \{ [\Upsilon_{mno}^{xx'} (\xi' r)_{mo}] [(\xi r)_{mn} C_m^2 + (\xi r)_{no} C_m C_o] \}$$

$$+ \Upsilon_{mno}^{xx'} [2(\xi r)_{mo} \xi_{mn} C_m - \xi_{mo} (\xi r)_{no} C_n] \} (1 + \zeta_{ddd,mno}) d^3 r_o , \qquad (4.14)$$

1

and

$$\delta_{mn}^{\mathbf{x}\mathbf{x}'} = \alpha_{mn}^{\mathbf{x}\mathbf{x}'} + 2\gamma_{mn}^{\mathbf{x}\mathbf{x}'} \quad . \tag{4.15}$$

The  $T_6$  in Fermi fluids is given by

$$T_{6} = -\frac{\hbar^{2}}{2m}\rho \int \left\{ g_{dd} \left[ \alpha^{dd} (\delta^{dd} + \delta^{de} + \delta^{ed} + \delta^{ee}) + \alpha^{de} (\delta^{dd} + \delta^{ed}) + \alpha^{ed} (\delta^{dd} + \delta^{de}) + \alpha^{ee} \delta^{dd} - 4\alpha^{cc} \delta^{cc} \right] + g_{de} \left[ \alpha^{dd} (2\delta^{dd} + \delta^{de} + \delta^{ed}) + (\alpha^{de} + \alpha^{ed}) \delta^{dd} \right] + g_{ee} \alpha^{dd} \delta^{dd} - 4g_{cc} (\alpha^{cc} \delta^{dd} + \alpha^{dd} \delta^{cc}) \right\} 4\pi r^{2} dr \quad ,$$

$$(4.16)$$

which ensures a proper match of the exchange pat-  
terns in 
$$g_{xx'}$$
,  $\alpha^{xx'}$ , and  $\delta^{xx'}$ .  
The matching of exchange patterns in the calculation  $\tau^{ee} = \hat{f}g_{ee} + \alpha^{ee}g_{dd} + \alpha^{dd}g_{ee} + \alpha^{ed}g_{de} + \alpha^{de}g_{ed} - 4\alpha^{cc}g_{cc}$  (4.19)

The matching of exchange patterns in the calculation of U is facilitated by defining

$$\tau^{dd} = \hat{f}g_{dd} + \alpha^{dd}g_{dd} \tag{4.17}$$

$$\tau^{de} = \hat{f}g_{de} + \alpha^{de}g_{dd} + \alpha^{dd}g_{de} \tag{4.18}$$

$$\tau^{ee} = \hat{f}g_{ee} + \alpha^{ee}g_{dd} + \alpha^{dd}g_{ee} + \alpha^{ed}g_{de} + \alpha^{de}g_{ed} - 4\alpha^{cc}g_{cc}$$
(4.20)

$$\tau^{cc} = \hat{f}g_{cc} + \alpha^{dd}g_{cc} + \alpha^{cc}g_{dd} \quad . \tag{4.21}$$

The  $t_{i-1,5,j-1,3}$  given in Table II are linear combinations of  $\tau^{xx'}$  and  $g_{xx'}$ , and the U is obtained as

$$U = -\frac{\hbar^2}{2m} \rho^2 \int f_{3,mno}^2 (1 + \zeta_{ddd,mno}) \left( \sum_{i=1,5} t_{i1,mn} t_{i2,mo} t_{i3,no} \right) C_m d^3 r_{mn} d^3 r_{mo}$$
(4.22)

(4.3)

i/j	1	2	3
1	$\tau^{dd} + 2(\tau^{de} + \tau^{ed} + \tau^{ee})$	$ au^{dd}$	$g_{dd} + g_{de}$
2	$\tau^{dd} + 2\tau^{ed}$	$ au^{dd}$	$g_{de} + g_{ee}$
3	$2\tau^{ee} + 2\tau^{ed} + \tau^{de}$	$\tau^{de}$	8 <sub>dd</sub>
4	$2\tau^{ed}$	$\tau^{de}$	8 de
5	$-4\tau^{cc}$	$\tau^{cc}$	8 <sub>cc</sub>

TABLE II. The matrix  $t_{ij}$ .

In the Fermi fluid there are two more types of kinetic energy contributions. In the first we include the  $\nabla_m f_{J,mn} \cdot \nabla_m \Phi$  and  $\nabla_m f_{3,mnp} \cdot \nabla_m \Phi$ , terms, while

second is the kinetic energy associated with the  $f_k$ . The  $\nabla_m f_{J,mn} \cdot i \vec{k}_m$  terms give zero contribution on the summation over  $\vec{k}_m$  if particle *m* is not exchanged. The nonzero terms are divided into two categories;  $W_F$  contains those in which particle *n* occupies the state  $\vec{k}_m$  in  $\Psi^*$ , while  $U_F$  contains those in which some other particle  $0 \neq n$  occupies  $\vec{k}_m$  in  $\Psi^*$ . The essential components of  $W_F$  and  $U_F$  diagrams are shown in Fig. 12.1–12.3. In these diagrams a filled arrow along the *mn* line represents  $\nabla_m f_{J,mn}$ , and the chains are not shown for clarity. The summation over  $\vec{k}_m$  can be easily carried out; it gives a  $l_{mn}'$  in  $W_F$ diagrams and  $l_{mo}'$  in  $U_F$  diagrams, i.e.,

$$W_{f} = -\frac{\hbar^{2}}{m} \rho \int l' \hat{f}_{J} g_{cc} d^{3}r \quad , \qquad (4.23)$$

$$U_{F} = -\frac{\hbar^{2}}{m} \rho^{2} \int (1 + \zeta_{ddd,mno}) f_{3,mno}^{2} C_{m} \hat{f}_{mn} \{g_{cc,mn}[(g_{dd} - 1)l']_{mo} g_{cc,no} + (l'g_{cc})_{mo} [g_{dd,mn}(g_{dd} + g_{de})_{no} + g_{de,mn}g_{dd,no}] \} d^{3}r_{mn} d^{3}r_{mo} .$$
(4.24)

The  $\nabla_m f_{3,mno}$  has many terms which are discussed in Ref. 7. Some of the  $\nabla_m f_{3,mnp} \cdot \nabla_m \Phi$  terms in which *m* is exchanged with a particle  $0 \neq n$  or *p* form type II diagrams (Ref. 1) that cannot be calculated in the FHNC approximation. The rest are calculated by defining a  $\theta^{cc}$  as follows:

$$\theta_{mn}^{cc} = \rho \int (Y_{mnp}^{cc} g_{dd,mn} + Y_{mnp}^{dd} g_{cc,mn}) \{ (\xi'r)_{mp} [(\xi r)_{mn} C_m^2 + (\xi r)_{np} C_p C_m] + 2(\xi r)_{mp} \xi_{mn} C_m - \xi_{mp} \\ \times (\xi r)_{np} C_n \} (1 + \zeta_{ddd,mnp}) d^3 r_p , \qquad (4.25)$$

and by replacing the  $\hat{f}_{J}g_{xx'}$  in Eqs. (4.23) and (4.24) by the  $\tau^{xx'}$ . The sum of  $\nabla_m f_{J,mn} \cdot \nabla_m \Phi$  and  $\nabla_m f_{3,mnp} \cdot \nabla_m \Phi$  is given by  $W_F + U_F$ , i.e.,

$$W_{F} = -\frac{\hbar^{2}}{m} \rho \int (\tau^{cc} + \theta^{cc}) l' d^{3}r , \qquad (4.26)$$

$$U_{F} = -\frac{\hbar^{2}}{m} \rho^{2} \int f_{3,mno}^{2} (1 + \zeta_{ddd,mno}) C_{m} \{ \tau^{cc}_{mn} [(g_{dd} - 1)l']_{mo} g_{cc,no} + (l'g_{cc})_{mo} [\tau_{dd,mn} (g_{dd} + g_{de})_{no} + \tau_{de,mn} g_{dd,mo}] \} d^{3}r_{mn} d^{3}r_{mo} .$$

The kinetic energy terms associated with  $f_k$  are denoted by S. In general they have



or

$$\nabla_m f_{k,mn} \cdot \nabla_m f_{k,mo}$$

Some of the T, U,  $W_F$ , and  $U_F$  terms having an  $f_k$ between interacting particles are not summed by the expressions given above. These are also included in S. By interacting we mean the particles whose correlation or single particle-wave function is differentiated. The following diagrammatic conventions are adopted in the tabulation of kinetic energy terms associated with the  $f_k$ . Only the interacting particles are shown in the S diagrams. An open arrowhead on a wiggly line denotes  $\nabla f_k$ , while two open arrowheads on a wiggly line denote  $\nabla^2 f_k$ . Hollow and



FIG. 12. Skeletons of  $W_F$  and  $U_F$  diagrams.

(4.27)

filled arrowheads represent  $\nabla f_{3,ijk}$  and  $\nabla f_{J,ij}$ . The  $(\nabla \Phi)$  is not explicitly shown; if a diagram has only one arrowhead a  $(\nabla \Phi)$  is implicit.

Following the expansion of the elementary diagrams D (Eq. (3.37) and (3.38) we have:

$$S = \sum_{p,p'} S(p,p')$$
, (4.28)

$$S(p,p') = \sum_{p''} S(p,p',p'') , \qquad (4.29)$$

where p'' is a serial diagram number, p' is the number of wiggly lines connecting interacting particles, and p is the minimum number of particles linked by wiggly lines and exchanges.

The largest term in S is S(2, 1, 1) shown in Fig. 13. Its contribution is given by

$$S(2,1,1) = \frac{\hbar^2}{2m} \frac{k_F^2}{5} \rho \int (q'r + 3q) g_{dd} d^3r \quad (4.30)$$

and is -0.73 °K at the equilibrium point. All the results quoted in this section are at the equilibrium point:  $\rho = 0.277 \sigma^{-3}$ ,  $d = 1.73r_0$ ,  $\beta_3 = 2.4$ , and  $\beta_k = 0.7$ . It is convenient to group the terms S(2, 1, i = 2, 6), shown in Fig. 13, together. Since this combination of derivatives appears frequently we denote it by an xx over the wiggly line. Define a function s as

$$s = \frac{1}{2} (q''r + 4q') + (q'r + q)(\hat{f}_J + \alpha^{dd} + \theta^{dd} + \sigma) ,$$
(4.31)

$$\sigma_{mn} = \rho \int \Lambda_{mno}^{dd} \hat{f}_{J,mo} f_{3,mno}^2 C_m \left(1 + \zeta_{ddd,mno}\right) d^3 r_o \quad ,$$

$$(4.32)$$

$$\theta_{mn}^{dd} = \rho \int \Upsilon_{mno}^{dd} \left\{ (\xi'r)_{mno} \left[ (\xi r)_{mno} C_n^2 + (\xi r)_{mno} C_m C_n \right] \right\}$$

$$+2(\xi r)_{mo}\xi_{mn}C_{m}-\xi_{mo}(\xi r)_{no}C_{n}\}$$

$$\times (1+\zeta_{ddd,mno})d^{3}r_{o} . \qquad (4.33)$$



FIG. 13. Skeletons of S(p,p',p'') diagrams having p = 2.

The S(2, 1, 6) should be very small and we have

$$\sum_{j=2,5} S(2,1,i) = -\frac{\hbar^2}{2m} \rho \int sLl' g_{dd} d^3r \quad . \tag{4.34}$$

The  $(\alpha^{dd} + \theta^{dd})$  and  $\sigma$  terms in the above respectively sum diagrams of type S(2, 1, 4) and S(2, 1, 5). The sum (4.34) is found to be +0.44 °K at the equilibrium point.

The combination of derivatives shown in Fig. 13, S(2, 1, i = 7, 11) also occurs frequently and is denoted by a single x over the wiggly line. The diagrams S(2,1,8-11) are in fact  $W_F$  and  $U_F$  diagrams (Fig. 12) containing an additional wiggly line. However, their contributions are not summed in Eqs. (4.26) and (4.27). The S(2, 1, 11) is neglected, and the rest are given by

$$\sum_{-7,10} S(2,1,i=7,10) = -(\hbar^2/2m)\rho \frac{1}{2} \int \left[ [2qr(\hat{f}_J + \alpha^{dd} + \theta^{dd} + \sigma) + q'r + q](Ll'' - l'^2) + 2q\frac{l'L}{r} \right] g_{dd} d^3r \quad ,$$
(4.35)

and their contribution is -0.23 °K. There are no more S(2, 1) diagrams; the total is S(2, 1) = -0.52 °K.

The combinations denoted by S(2,2,1-3) in Fig. 13 have contributions, i.e.,

$$S(2,2,1) = -\frac{\hbar^2}{2m} \rho \frac{k_F^2}{5} \int sqrg_{dd} d^3r \quad , \qquad (4.36)$$

$$S(2,2,2) = -\frac{\hbar^2}{2m} \rho \frac{1}{2} \int sqr (Ll'' - l'^2) g_{dd} d^3r \quad , \quad (4.37)$$

$$S(2,2,3) = -\frac{\hbar^2}{2m}\rho \frac{1}{4} \int \left[ \left[ qr\left(\hat{f}_J + \alpha^{dd} + \theta^{dd} + \sigma\right) + q'r + q \right] qr\left(l'''L - 3l''l'\right) + 2q^2 \left[ l''L - l'^2 - \frac{l'L}{r} \right] \right] g_{dd} d^3r.$$
(4.38)

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The S(2, 2, i = 1, 3) are found to be 0.23, -0.02, and +0.01 °K respectively, giving S(2, 2) = 0.22.

The convergence between S(2, 1) and S(2, 2) is not very significant. It probably can never be at the equilibrium point becauuse S(2, 1) represents the bulk of energy terms linear in  $\beta_k$ , while S(2, 2) is most of the energy quadratic in  $\beta_k$ . Thus, S(2, 2) is always positive and roughly half in magnitude of the negative S(2, 1).

There is a large number of S(3, 1) diagrams as shown in Fig. 14. For the sake of simplicity and compactness: (i) we have not shown any chains, and  $f_J$ ,  $f_3$  correlations. Note that the third particle in diagrams (14.1-14.4) must have a correlation line linking it; (ii) separable contributions must be subtracted; (iii) the direction of exchange loop is not shown, it can go both ways; (iv) only the  $\hat{f}$  diagrams are shown; some diagrams having  $\nabla f_3$  (such as diagram 14.19) are summed by simply replacing the  $\hat{f}$  by  $\hat{f} + \alpha_{dd}$ , others (such as diagram 14.20) are neglected. The algebraic expressions giving S(3, 1) are somewhat messy though simple to calculate. The total S(3, 1) is found to be -0.18 °K which is significantly smaller than S(2, 1). We hope that S(3, 2) is also much smaller than S(2, 2), and we truncate the sum in Eq. (4.28) at p + p' = 4. This truncation probably gives the largest error in the present work.

The S(3, 1) contribution is not included when the variational parameters are determined by minimizing the  $E(d, \beta_3, \beta_k)$ . At the equilibrium density,  $\rho = 0.277 \sigma^{-3}$ , the energy including the S(3, 1) can be easily minimized, and the minimum occurs at  $d = 1.73(1.73)r_0$ ,  $\beta_3 = 2.2(2.4)$ , and  $\beta_k = 1.0(0.7)$ ; the values in parenthesis are those obtained by minimizing the energy without the S(3, 1) contribution. The FHNC/4C  $E(d = 1.73r_0, \beta_3 = 2.2, \beta_k = 1.)$  is -2.15 °K, which is slightly below the -2.08 °K calculated at the parenthetical values. However at large  $\rho$ , particularly at  $\rho = 0.337 \sigma^{-3}$ , the variation including S(3, 1) leads to large values of d and  $\beta_k$  at which the convergence of the cluster expansion becomes very doubtful. For example, at these large values the S(2, 1) and S(2, 2)cancel each other, and S becomes dominated by S(3,1). This will presumably not happen if the S(3,2) is also included in the variation. For this reason it is probably better to treat the S(3, 1) as a perturbation, and not include it in the variational calculation without S(3, 2).

The FHNC calculations have  $\zeta_{ddd}$  and  $\zeta_{dcc}$  set to zero, while in the FHNC/4B only, the  $\zeta_{dcc}$  is set to zero. The results of FHNC/4C calculation are practically identical to those of FHNC/4P indicating that the diagrams of Fig. 7, and the FH NC/4C corrections to  $g_3$  are not very important in liquid <sup>3</sup>He. With the pure Jastrow wave function Zabolitzsky obtains -1.38 °K and -0.91 °K in FHNC, and FHNC/4 approximations at  $\rho = 0.277 \sigma^{-3}$  and  $d = 2.4r_0$ . The FHNC/4B and FHNC/4C results for this case are



FIG. 14. Skeletons of some S(p=3,p'=1,p'') diagrams.

-1.20 and -1.19 °K respectively. The  $\zeta_{dcc,ijk}$  has two  $g_{cc}$  functions which are very small because L, the generalized Slater function, is small at  $r > \sigma$ , while  $g_{dd}$  is small at  $r < \sigma$ . The FHNC/4C is not very good; it merely accounts for half of the difference between FHNC and FHNC/4, but it should be a fair measure of the error in the neglect of elementary diagrams.

Table III gives the calculated energies at the experimental equilibrium density  $\rho = 0.277 \sigma^{-3}$ . The variational parameters at this density are  $d = 1.73r_0$ ,  $\beta_3 = 2.4$ , and  $\beta_k = 0.7$ ; and the calculated energies with either  $\beta_k$  or  $\beta_3$  set to zero are also listed, along with those in the FHNC/4C approximation. The  $f_{3,Uk}$  by itself can lower the energy by  $\approx 0.3$  °K; it essentially reduces the contribution of the  $\nabla_m f_{J,mn} \cdot \nabla_m f_{J,mo}$  terms which account for most of the repulsive U. The backflow correlation  $f_k$  by itself can reduce the energy by  $\approx 0.5$  °K. The main attraction comes from the  $\nabla_m f_{k,mn} \cdot \nabla_m \Phi$  term in S(2, 1). Together the  $f_3$  and  $f_k$  lower the energy by  $\sim 0.75$  °K.

The small equilibrium value of  $d/r_0$  is largely responsible in making the difference E(FHNC/4C) - E(FHNC) so small. At  $\rho = 0.337 \sigma^{-3}$ for example, the difference at the minimum  $(d = 1.85r_0, \beta_3 = 2.6, \beta_k = 0.6)$  is only 0.1 °K, indicating good convergence of the elementary diagram expansion. But at larger d this difference increases very rapidly. At  $\rho = 0.377 \sigma^{-3}$ ,  $d = 2.23r_0$ ,  $\beta_3 = 2.2$  and

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		$E(\rho=0.277\sigma^{-3}$	$, d = 1.73 r_0, \beta_3, \beta$	<i>k</i> )	FHNC/4C
β3	0.0	2.4	0.0	2.4	2.4
$\beta_k$	0.0	0.0	0.7	0.7	0.7
T <sub>F</sub>	3.00	3.00	3.00	3.00	3.00
W	-5.24	-5.23	-5.23	-5.23	-5.23
U	2.09	0.96	2.20	0.91	1.19
T	0.0	0.93	0.0	1.01	0.76
$W_F$	-2.14	-2.05	-2.15	-2.05	-2.07
$U_F$	0.93	0.72	0.93	0.73	0.78
S(2,1)	0.0	0.0	-0.58	-0.52	-0.54
S(2,2)	0.0	0.0	0.22	0.22	0.22
S(3,1)	0.0	0.0	-0.25	-0.18	-0.18
E	-1.36	-1.66	-1.85	-2.11	-2.08

TABLE III. Breakdown of the energy.

 $\beta_k = 0.7$  it is 0.6 °K. As a matter of fact, at

 $\rho > 0.3 \sigma^{-3}$  the FHNC calculations give only a local minimum in  $E(d, \beta_3, \beta_k)$  at  $d < 2r_0$ . The FHNC/4C calculations confirm that this local minimum is the true minimum.

At  $d < 2r_0$  the difference between E(FHNC/4C)and E(FHNC) is much smaller with the present  $\Psi$ than with the Jastrow  $\Psi_J$ . The change in U accounts for most of E(FHNC/4) - E(FHNC) in Zabolitzky's work, which implies that the FHNC/4 corrections to the three-body distribution function have a significant influence on the Jastrow energy. In the present case, however, the energy if approximately minimized, by varying  $\beta_3$ , with respect to changes in  $g_3$ , and thus it is probably not too sensitive to FHNC/4 corrections to  $g_3$ . As a matter of fact, the change in U due to the  $\zeta$  is almost cancelled by that in T (Table III).

## **V. CONCLUSIONS**

The calculated  $E(d, \beta_3, \beta_k)$  at  $\rho = 0.277 \sigma^{-3}$ , the experimental equilibrium density, with FHNC approximation, are given in Tables IV-VI. The  $E(\beta_k)$  at

TABLE IV.	Variation	of	energy	with	$\beta_k$ .	
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$E(d = 1.73r_0, \beta_3 = 2.4, \beta_k)$				
<i>E</i> (°K)	$(E-S(3,1))(^{\circ}K)$	$\beta_k$		
-2.025	-1.893	0.5		
-2.105	-1.932	0.7		
-2.140	-1.904	0.9		
-2.144	-1.856	1.1		
-2.110	-1.770	1.3		

the equilibrium values of  $\beta_3$  and d, (Table IV) shows a rather shallow minimum at  $\beta_k = 0.7(1.0)$  when S(3, 1) is omitted (included) in the variational calculation. From the discussion in Sec. II we should expect the minimum to occur at  $\beta_k = 1.0$ .

The  $E(\beta_3)$  at equilibrium values of  $\beta_k$  and d (Table V) shows a minimum at  $\beta_3 \approx 2.4$ ; the F operator also suggests

$$\beta_3 \approx [(f'/2\eta r)_{\rm av}]^{1/2} \approx 2.4$$
 , (5.1)

as estimated from Fig. 2. The  $E(d, \beta_3, \beta_k)$  (Table VI) at the equilibrium point hs a minimum at a rather small value of  $d = 1.73r_0$ . This is very helpful for the convergence of integral equation methods.<sup>2</sup> The  $E(d, \beta_3 = \beta_k = 0)$ , shown in Table VII, has a more shallow minimum at  $d \approx 2.6r_0$  in the FHNC approximation. Unreasonable values of variational parameters would have indicated that large contributions were neglected. In this sense the calculated equilibrum values are quite encouraging.

The  $E_J(\rho, b)$  calculated with the Jastrow correlation function, i.e.,

$$f_J(b) = e^{-(b \sigma/r)^5/2}$$
, (5.2)

TABLE V. Variation of energy with  $\beta_3$ .

	$E(d = 1.73r_0, \beta_3, \beta_k = 0.7)$	-
<i>E</i> (°K)	$(E-S(3,1))(^{\circ}K)$	$\beta_3$
-2.116	-1.914	2.1
-2.117	-1.921	2.2
-2.109	-1.930	2.3
-2.105	-1.932	2.4
-2.095	-1.928	2.5

	TABLE	VI.	Variation	of	energy	with	d.
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$E(d, \beta_3 = 2.4, \beta_k = 0.7)$				
<i>E</i> (°K)	( <i>E-S</i> (3,1))(°K)	d/r <sub>0</sub>		
-2.041	-1.900	1.63		
-2.105	-1.932	1.73		
-1.961	-1.748	1.83		

TABLE VIII. Variational parameters at different densities.

ρ	$d/r_0$	$\beta_3$	$\beta_k$
0.217	1.58	2.2	0.9
0.247	1.63	2.3	0.8
0.277	1.73	2.4	0.7
0.307	1.75	2.5	0.7
0.337	1.85	2.6	0.6

commonly used in Helium liquids, and  $E_J(\rho,d)$  with the present  $f_J$ , are shown in Fig. 15. The  $E_J(\rho, b)$  is calculated by the Monte Carlo method<sup>1</sup> and with FHNC/4,<sup>2</sup> while  $E_J(\rho, d)$  is the FHNC,<sup>2</sup> FHNC/4,<sup>2</sup> and FHNC/4C integral equations. These curves indicate the following: (i) the Jastrow part of the present F is quite reasonable; (ii) FHNC/4 is very accurate; and (iii) while FHNC/4C and FHNC are not very accurate, their difference is indicative of the error. The  $E_{\alpha}(\rho, d, \beta_3, \beta_k)$  in FHNC and FHNC/4C approximations is also shown in Fig. 15 along with the experimental data.<sup>12</sup> The  $E_{\sigma}(\rho)$  is much closer to experiment than  $E_{I}(\rho)$ , and the difference between the  $E_{\alpha}(\rho)$  and experiment could partly come from the limitations of the Lennard-Jones (LJ) model. We recall here that with the Green's function Monte Carlo method, the LJ model underestimates the binding energy by  $\approx 0.3$  °K, and overestimates the equilibrium density by  $\approx 0.01 \sigma^{-3}$  in liquid <sup>4</sup>He.<sup>3</sup> The curvature  $\partial^2 E_{\sigma}(\rho)/\partial \rho^2$  at the equilibrium density is much smaller ( $\approx$ 100) than that inferred from the experimental data ( $\approx$ 223). The values of parameters and calculated energies are listed in Table VIII at various densities.

TABLE VII. Variation of the Jastrow energy with	TA	BLE	VII.	Variation	of	the	Jastrow	energy	with	6
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	$E(d,\beta_3=0,\beta_k=0)$	•
<i>E</i> (°K)	· · · · · · · · · · · · · · · · · · ·	d/r <sub>0</sub>
-1.414		2.2
-1.427		2.4
-1.442		2.6
-1.420		2.8

The calculated g(r) and S(k) at  $\rho = 0.277 \sigma^{-3}$  are compared with the experimental data<sup>13</sup> in Figs. 16 and 17. As in liquid <sup>4</sup>He the calculated g(r) in liquid <sup>3</sup>He has a little less than observed structure. The  $f_k$ and  $f_3$  have little effect on the g(r) as can be seen from Table IX, though it is in the right direction.

TABLE IX. Pair distribution function.

r(units of $\sigma$ )	g(r)	g(r)
	$\beta_3 = \beta_k$ (equilibrium)	$\beta_3 = \beta_k = 0$
0.764	0.006	0.006
0.882	0.129	0.134
1.000	0.482	0.493
1.117	0.851	0.859
1.235	1.075	1.073
1.352	1.157	1.145
1.470	1.151	1.135
1.588	1.104	1.090
1.705	1.044	1.038
1.823	1.003	1.004
1.940	0.980	0.986
2.058	0.971	0.980
2.176	0.973	0.982
2.293	0.980	0.987
2.411	0.989	0.992
2.528	0.997	0.996
2.646	1.000	0.998
2.764	1.003	0.999
2.881	1.003	1.000
2.999	1.002	1.000
3.116	1.001	1.000
3.234	1.000	1.000



FIG. 15. Comparison of calculated and experimental  $E(\rho)$  of liquid <sup>3</sup>He. The crosses and circles respectively show FHNC/4 results<sup>2</sup> with  $f_J(d)$  and  $f_J(b)$ , the Fermi Monte Carlo result is with  $f_J(b)$ .



FIG. 16. Comparison of calculated and experimentally determined g(r) at  $\rho = 0.277 \sigma^{-3}$ .



FIG. 17. Comparison of calculted and experimental S(k) at  $\rho = 0.277 \sigma^{-3}$ .

### ACKNOWLEDGMENT

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APPENDIX: 
$$D_{ij}(p,p',p'')$$

$$\begin{split} D_{ij}(2,1,1) &= (qrl'L)_{ij} , \\ D_{ij}(2,2,1) &= (qr)_{ij}^{2}k_{F}^{2}/10 , \\ D_{ij}(2,2,2) &= (qr)_{ij}^{2}\frac{1}{4}(l'^{2} - Ll'')_{ij} , \\ D_{ij}(3,1,1) &= \frac{1}{2}(qrL)_{ij}\rho \int L_{ik}l_{jk}'C_{j}g_{dd,ik} \\ &\times (g_{dd,jk}Z_{ijk} - 1) d^{3}r_{k} , \\ D_{ij}(3,1,2) &= (qr)_{ij}\rho \int (Ll')_{ij}C_{i}g_{dd,ik} g_{dd,jk}Z_{ijk}d^{3}r_{k} , \\ D_{ij}(3,1,3) &= \frac{\rho}{4} \int \left(2L_{ij}l_{ik}'L_{kj} + L_{ij}L_{ik}l_{kj}'C_{k} \\ &+ l_{ij}'L_{ik}L_{kj}C_{i}\right) (qr)_{ik}g_{dd,ik}g_{dd,jk} \\ &\times Z_{ijk} d^{3}r_{k} , \\ D_{ij}(3,1,4) &= D_{ij}(3,1,3) \end{split}$$

$$-\frac{\rho}{2} \int \left( L_{ij} l_{ik}' L_{kj} + L_{ij} L_{ik} l_{kj}' C_k \right) g_{dd,ik} d^3 r_k$$
$$D_{ij}(3, 1, 5) = (Ll')_{ij} \rho \int (qr)_{ik} C_i g_{dd,ik} g_{dd,jk} Z_{ijk} d^3 r_k ,$$
$$D_{ij}(3, 1, 6) = \rho \int (Ll')_{ik} (qr)_{jk} C_k g_{dd,ik} g_{dd,jk} Z_{ijk} d^3 r_k ,$$

 $Z_{ijk} \equiv f_{3,ijk}^2 (1+\zeta_{ddd,ijk}) \quad .$ 

- <sup>1</sup>D. Ceperly, G. V. Chester, and M. H. Kalos, Phys. Rev. B <u>16</u>, 3081 (1977).
- <sup>2</sup>J. G. Zabolitzky, Phys. Rev. A <u>16</u>, 1258 (1977).
- <sup>3</sup>M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A <u>9</u>, 2178 (1974); M. H. Kalos, Invited talk in the Workshop on Nuclear and Dense Matter, Urbana, Illinois (1977). (unpublished).
- <sup>4</sup>V. R. Pandharipande and H. A. Bethe, Phys. Rev. C <u>7</u>, 1312 (1973).
- <sup>5</sup>R. P. Feynman and M. Cohen, Phys. Rev. <u>102</u>, 1189 (1956).
- <sup>6</sup>V. R. Pandharipande and N. Itoh, Phys. Rev. A <u>8</u>, 2564 (1973).
- <sup>7</sup>V. R. Pandharipande, Phys. Rev. B <u>18</u>, 218 (1978).

- <sup>8</sup>V. R. Pandharipande and K. E. Schmidt, Phys. Rev. A <u>15</u>, 2486 (1977).
- <sup>9</sup>S. Fantoni and S. Rosați, Nuovo Cimento <u>25</u> A, 593 (1975).
- <sup>10</sup>J. M. J. van Leewven, J. Groeneveld, and J. de Boer, Physica (Utrecht) <u>25</u>, 792 (1959).
- <sup>11</sup>R. B. Wiringa and V. R. Pandharipande, Nucl. Phys. <u>299</u>, 1 (1978).
- <sup>12</sup>J. Wilks, The Properties of Liquid and Solid Helium (Clarendon, Oxford, 1967).
- <sup>13</sup>E. K. Achter and L. Meyer, Phys. Rev. <u>188</u>, 251 (1969).
- <sup>14</sup>Note that  $\hat{f}_j$  terms are erroneously included in the definition of  $\gamma$  in Ref. 7.