GROUND-STATE PROPERTIES OF 3He↑ AND D↑ WITHIN THE METHOD OF CORRELATED BASIS FUNCTIONS

J. Clark, E. Krotscheck, R. Panoff

GROUND-STATE PROPERTIES OF $^3He\uparrow$ AND $D\uparrow$ WITHIN THE METHOD OF CORRELATED BASIS FUNCTIONS

J.W. Clark, E. Krotscheck* and R.M. Panoff

McDonnell Center for the Space Sciences and Department of Physics, Washington University St. Louis, Missouri 63130, USA.

* *Department of Physics, State University of New York, Stony Brook, New York 11794, USA.*

Résumé.- On utilise des techniques d'équations-intégrales avancées, comportant des resommations de chaînes dans la théorie HNC, pour en déduire les propriétés des modèles variationnels de Jastrow pour les états fondamentaux de $^3He\uparrow$, de ^3He non polarisé et des deux espèces de $D\uparrow$. On donne les résultats pour l'énergie en fonction de la densité, pour la fonction de structure du liquide et (dans certains cas) pour la masse effective, la susceptibilité magnétique et les éléments de matrice de formation de paires. Les résultats indiquent qu'il sera nécessaire, particulièrement pour ^3He non polarisé, d'aller plus loin que le modèle de Jastrow pour obtenir une description microscopique quantitative de ces systèmes. On décrit les efforts préliminaires qui ont été faits en vue d'incorporer des corrélations dépendant de l'impulsion et du spin (et plus généralement d'autres corrélations non incluses dans le modèle de Jastrow) à l'aide de la méthode des fonctions de base corrélées.(CBF).

Abstract.— Advanced integral-equation techniques, including Fermi hypernetted-chain resummation, are used to derive the properties of Jastrow variational models of the ground states of $^3He\uparrow$, unpolarized ^3He and two species of $D\uparrow$. Results are reported for the energy as a function of density, for the liquid structure function and (in some cases) for the effective mass, magnetic susceptibility and pairing matrix elements. The results indicate that it will be necessary, particularly for unpolarized ^3He, to go beyond the Jastrow model to achieve a quantitative microscopic account of these systems. Preliminary efforts toward the incorporation of momentum-dependent, spin-dependent and other non-Jastrow correlations by means of the method of correlated basis functions are described.

1. Introduction.— In this paper we explore the properties of a Jastrow variational model of the ground states of the following highly quantal systems: (a) ordinary, spin-saturated ^3He, (b) fully spin-polarized ^3He and (c) two analogous species of spin-polarized D. The predictions of the model for such quantities as the ground-state energy, the liquid structure function, the single-particle energies and effective mass, the magnetic susceptibility and the effective pairing matrix elements are presented as functions of density. The techniques of Fermi hypernetted-chain theory /1-8/ are applied to the evaluation of these quantities. Comparing with experimental results on real, spin-saturated liquid ^3He, it is found that for this system the Jastrow description has certain clear deficiencies, which are associated with the absence of momentum-dependent (or back-flow) and spin-dependent correlations from the Jastrow ansatz. Nevertheless, the various theoretical results indicate that the Jastrow model still contains much of the correct physics of strongly-correlated Fermi systems even at relatively high density, providing a useful vantage point from which more quantitative descriptions may be sought.

The search for more realistic and more comprehensive theories may, for example, be carried out within the framework of the method of correlated basis functions /9-11,7,8/ (CBF), either by means of (i) nonorthogonal CBF perturbation theory /11-13/ or via (ii) a more powerful scheme which implements the coupled-cluster (or exponential-S) procedure in the CBF context /14/. We report here on some features of the beginnings of a theory following path (i) (which may be looked upon as a renormalized version of an earlier approach of Woo /13/ and Tan and Feenberg /15/). As an alternative

to CBF theory, one may of course elaborate on the variational description, incorporating backflow /16/, spin-dependent /17,18/ and other non-Jastrow correlations directly into the ground-state trial function.

2. The Jastrow Model.— We focus our attention on the Jastrow model of the ground state of a Fermi fluid, which is based on a trial wave function of the form

$$\Psi_0 = F\Phi_0 \ . \qquad (1)$$

In the present applications, Φ_0 is the ground-state wave function of the noninteracting Fermi gas at density $\rho = \nu k_F^3/6\pi^2$, where ν is the single-particle level degeneracy, i.e., the number of particles allowed in a given cell of $\underline{k}$-space. Correlations due to interactions are introduced by means of the operator F, which, in the Jastrow case, is taken as the superposition

$$F = \prod_{i<j} f(r_{ij}) \qquad (2)$$

of real, state-independent two-body correlation functions. Ideally, the correlation function f(r) should be determined (optimally) by solving the variational problem

$$\delta E[f]/\delta f = 0 \ , \qquad (3)$$

where the extremum of

$$E[f] = \langle H \rangle = \langle \Psi_0 | H | \Psi_0 \rangle / \langle \Psi_0 | \Psi_0 \rangle \qquad (4)$$

is supposed to be a minimum. In practice, the Euler equation (3) and the expectation value (4) must be approximated /19,20/ (or the variational problem may be solved straightaway for a functional approximating (4) /21/). A less ambitious and more widely practiced approach involves minimization of an approximate energy functional with respect to the parameters in a suitably chosen analytic form for f(r).

The exact energy functional (4)--in particular, its kinetic energy portion--can be expressed in several different (but strictly equivalent) forms related by integral identities. The most widely used are the Pandharipande-Bethe (PB), Jackson-Feenberg (JF) and Clark-Westhaus (CW) forms. Detailed expressions may be found in /1/ or /4/. These expressions give <H> in terms of the two- and three-particle radial distribution functions $g(r_{12})$, $g_3(r_{12},r_{13},r_{23})$ and portions of them involving the Slater function $\ell(k_F r) = 3(k_F r)^{-3}(\sin k_F r - k_F r \cos k_F r)$, and of course also in terms of the assumed two-particle potential $v(r_{12})$, the correlation function $f(r_{12})$ and the particle mass m. In general, if <u>approximate</u> versions of $g(r_{12})$ and $g_3(123)$ are inserted, the three expressions $\langle H \rangle_{PB}$, $\langle H \rangle_{JF}$ and $\langle H \rangle_{CW}$ will not agree. The discrepancies give some measure of the inconsistency of the approximate evaluation of the distribution functions--in particular, a measure of the violation of the BBGKY relation between g and g_3 /22/.

Construction and analysis of approximations to the distribution functions (and therewith the energy expectation value) are facilitated by a configuration-space graphical scheme, analogous to that used widely in the statistical theory of classical fluids /23,24/. The building blocks for g (and g_3) are (sub)diagrams with two external (labeled) points, say ij. In the present case of Fermi statistics such diagrams may contain two kinds of line elements, namely dynamical correlation lines corresponding to factors $f^2(r) - 1$ and statistical correlation lines (exchange lines) corresponding to Slater factors $\ell(k_F r)$. Fermi ij diagrams are therefore classified not only according to their topological structure (nodal as opposed to non-nodal /23,1/) but also according to whether a pair of exchange lines (one entering, one leaving) is present at <u>neither</u> ("dd" diagrams), <u>one</u> ("de" diagrams) or <u>both</u> ("ee" diagrams) of the external points /1/. The sums of all contributing <u>non-nodal</u>

diagrams of the indicated exchange classes are denoted, respectively, $X_{dd}(r)$, $X_{de}(r)$ and $X_{ee}(r)$ (where $r \equiv |\underline{r}_i - \underline{r}_j|$). It is convenient also to introduce a fourth exchange class, comprised of ij (sub)diagrams in which there is a continuous exchange-line path running from i to j (or vice versa), possibly through intermediate particles, but no return path closing the exchange loop. These are called "cc" diagrams; excluding the graph consisting of a single ℓ line joining i and j, the sum of all contributing non-nodal diagrams of this category is denoted $X_{cc}(r)$.

The compound-graphical objects $X_{xy}(r)$, with $xy \in \{dd,de,ee\}$, are found to be the central ingredients of the diagrammatic analysis, in the sense that once they are known, the distribution functions (or more conveniently the corresponding static structure functions) can be calculated from exact, closed formulas /2,6,1/. For example, the structure function

$$S(k) = 1 + \rho\int[g(r)-1]e^{i\underline{k}\cdot\underline{r}}\,d\underline{r} \qquad (5)$$

can be obtained from

$$\begin{aligned}
S(k) &= [1+\tilde{X}_{ee}(k)]S_d(k)/[1-\tilde{X}_{de}(k)] \ , \\
S_d(k) &= \{1+[1+\tilde{X}_{ee}(k)]\tilde{\Gamma}_{dd}(k)\}/[1-\tilde{X}_{de}(k)] \ , \\
\tilde{\Gamma}_{dd}(k) &= \tilde{X}_{dd}(k)/\{[1-\tilde{X}_{de}(k)]^2 - \tilde{X}_{dd}(k)[1+\tilde{X}_{ee}(k)]\}, \qquad (6)
\end{aligned}$$

where we have absorbed a factor ρ in forming the (dimensionless) tilde Fourier transforms, $\tilde{X}_{xy}(k) = \rho\int X_{xy}(r)\exp(i\underline{k}\cdot\underline{r})d\underline{r}$, etc.

The Fourier transforms of the sums of allowed nodal diagrams of the various exchange classes are also simple function of the $\tilde{X}_{xy}(k)$ (and of $\tilde{\ell}(k)$):

$$\begin{aligned}
\tilde{N}_{dd}(k) &= \tilde{\Gamma}_{dd}(k) - \tilde{X}_{dd}(k) \ , \\
\tilde{N}_{de}(k) &= S_d(k) - 1 - \tilde{X}_{de}(k) - \tilde{\Gamma}_{dd}(k) \ , \\
\tilde{N}_{ee}(k) &= S(k) - 2S_d(k) + 1 - \tilde{X}_{ee}(k) + \tilde{\Gamma}_{dd}(k), \\
\tilde{N}_{cc}(k) &= \tilde{X}_{cc}(k)[\nu^{-1}\tilde{\ell}(k) - \tilde{X}_{cc}(k)]/[1-\tilde{X}_{cc}(k)] \ . \qquad (7)
\end{aligned}$$

These are the Fermi chain equations, which build the chain (nodal) functions N_{xy} by <u>series connection</u> of non-nodal diagrams.

One popular scheme for calculating the key quantities X_{xy} is the Fermi hypernetted-chain procedure of Fantoni and Rosati /3/ (FR-FHNC). The X_{xy} are in their turn represented in coordinate space as simple functions of $f^2(r)$, $\ell(k_F r)$, the nodal-diagram sums N_{xy} and the elementary-diagram sums E_{xy}:

$$\begin{aligned}
X_{dd}(r) &= \Gamma_{dd}(r) - N_{dd}(r) \ , \\
X_{de}(r) &= [1+\Gamma_{dd}(r)]E_{de}(r) + \Gamma_{dd}(r)N_{de}(r) \ , \\
X_{ee}(r) &= [1+\Gamma_{dd}(r)]\{-\nu^{-1}[\ell(k_F r) - \nu N_{cc}(r) - \nu E_{cc}(r)]^2 \\
&\quad + [N_{de}(r) + E_{de}(r)]^2 + N_{ee}(r) + E_{ee}(r)\} - N_{ee}(r), \\
X_{cc}(r) &= -\nu^{-1}\Gamma_{dd}(r)[\ell(k_F r) - \nu N_{cc}(r)] \\
&\quad + [1+\Gamma_{dd}(r)]E_{cc}(r) \ , \qquad (8)
\end{aligned}$$

wherein

$$\Gamma_{dd}(r) \equiv f^2(r)\exp[N_{dd}(r) + E_{dd}(r)] - 1 \ . \qquad (9)$$

These equations express the formation of the non-nodal X quantities by <u>parallel</u> connection of "simple" (nodal or elementary) diagrams. (An elementary diagram is a non-nodal diagram which is topologically irreducible.)

In principle, equations (6) (together with an analogous construction of the structure function S_3 corresponding to g_3), equations (8) and equations (7) suffice to determine the Jastrow distribution functions g and g_3 (or S and S_3) <u>exactly</u> for a given correlation function f(r). Indeed, solution of this set of equations would generate the necessary ingredients for exact computation of the energy expectation value in any of its forms. However, these equations do not actually supply a closed solution of the problem, because the E_{xy} are given only as infinite series. In practice, therefore, successive approximations are defined by feeding in successively more complicated sets of elementary diagrams. The simplest approximation, explored by Fantoni and Rosati /3/, Zabolitzky /4/ and others, consists of setting all the $E_{xy} = 0$. This approximation is termed FHNC/0.

In the next step, elementary diagrams with four-point basic structures are incorporated, giving the FHNC/4 approximation; then five-point basic structures are to be included (FHNC/5); and so on. (For more precise specification, see, for example, reference /1/.)

It turns out that such a scheme violates (at every stage) certain long-wavelength asymptotic properties /5/ of the quantities $\tilde{X}_{de}(k)$ and $\tilde{X}_{ee}(k)$, namely

$$\left.\begin{aligned}\tilde{X}_{de}(k) &= O(k)\\ 1 + \tilde{X}_{ee}(k) &= S_F(k) + O(k^2)\end{aligned}\right\} \quad (k \to 0^+) \ , \qquad (10)$$

where $S_F(k)$ is the two-particle structure function for the noninteracting system. These properties are reflections of the Pauli exclusion principle, i.e., the antisymmetry of the (Jastrow) wave function. They may be established rigorously for the full X_{de}, X_{ee}; they also hold in approximation schemes in which suitably chosen finite subclasses of elementary diagrams are included (for example, in the so-called KR-FHNC// approximations /1,6/).

Normally, for reasonable f, violation of (10) by the FR-FHNC/0 approximation (or higher approximations within the FHNC/ scheme) will not have any serious effect on an evaluation of the ground-state energy, since it is, predominantly, the long-range behavior of the ingredients $X_{de}(r)$, $X_{ee}(r)$ which is at issue. However, other quantities of physical interest (e.g. S(k) at small k) are more sensitive to Pauli violations. Moreover, when we turn to the variational problem (3), and the implications of its behavior for the stability of many-body states, it becomes especially desirable to take proper care of the asymptotic conditions (10). To this end, we shall make use of the FHNC/C approximation devised by one of us /6/. Let the FR-FHNC/0 approximations to $\tilde{X}_{de}$, $\tilde{X}_{ee}$, as given by equations (8), be designated $\tilde{X}^{/0}_{de}$, $\tilde{X}^{/0}_{ee}$; then the effects of the omitted elementary diagrams, required to ensure (10), are estimated by using instead the "corrected" approximations

$$\begin{aligned}\tilde{X}^{/C}_{de}(k) &= S_F(k)\tilde{X}^{/0}_{de}(k) \ ,\\ \tilde{X}^{/C}_{ee}(k) &= S^2_F(k)\tilde{X}^{/0}_{ee}(k) - [S^2_F(k)-1][S_F(k)-1] \ . \qquad (11)\end{aligned}$$

In all cases in which the relevant elementary diagrams have actually been calculated, this estimate has proven to be accurate to within a few percent /6/. The FHNC/C approximation to the construction of the distribution functions consists in modifying the FHNC/0 scheme simply by the use of (11) for $\tilde{X}_{de}$ and $\tilde{X}_{ee}$ in the chain equations (7) (and only therein).

The Euler equation (3) may be subjected to a graphical analysis which parallels that already executed for the distribution functions entering <H>. Indeed, (3) assumes the form

$$-(\hbar^2/4m)\nabla^2 g(r) + g'(r) = 0 \ , \qquad (12)$$

where g'(r) is a generalized two-particle distribution function which may be formally constructed by a process of graphical differentiation, indicated throughout by a prime, applied to the diagrammatic representation of g(r) /5/. We shall not enter into the details here, but it is important to note that the explicit definition for g'(r) depends on the expression (PB, JF, CW) adopted for the kinetic energy portion of <H>, and accordingly so do the new sorts of line elements introduced upon graphical differentiation of g. The optimizations carried out in the present study are based on the JF form for <H>. In that case, each g' diagram will contain (i) a single effective-interaction line representing $v_{JF}(r) = v(r) - (\hbar^2/2m)\nabla^2 \ell nf$, or (ii) a single differentiated exchange line representing $(\hbar^2/2m)\nabla^2 \ell(k_F r)$ or (iii) a single connected pair of differentiated exchange lines representing $(\hbar^2/2m)\nabla_i \ell(k_F r_{ij}) \cdot \nabla_i \ell(k_F r_{ik})$, plus assorted f^2-1 and ℓ lines.

It is more convenient to work in Fourier space, the Euler equation becoming

$$\omega(k) \equiv (\hbar^2k^2/4m)[S(k)-1] + S'(k) = 0 \quad , \qquad (13)$$

where $S'(k) = \rho\int g'(r)\exp(i\underset{\sim}{k}\cdot\underset{\sim}{r})d\underset{\sim}{r}$ is the generalized structure factor corresponding to the generalized distribution function $g'(r)$. By diagrammatic analysis--or formally by functional and graphical differentiation--we may establish a rigorous decomposition of $S'(k)$ analogous to (6), in terms of $S(k)$, $S_d(k)$ and the primed counterparts $\tilde{X}'_{dd}(k)$, $\tilde{X}'_{de}(k)$ and $\tilde{X}'_{ee}(k)$ of the non-nodal quantities $\tilde{X}_{dd}(k)$, $\tilde{X}_{de}(k)$ and $\tilde{X}_{ee}(k)$. Equations analogous to (7), derived in a similar manner, give $\tilde{N}'_{dd}(k)$, $\tilde{N}'_{de}(k)$, $\tilde{N}'_{ee}(k)$ and $\tilde{N}'_{cc}(k)$ in terms of the primed $\tilde{X}$'s and the various unprimed quantities already introduced. Finally, by graphical differentiation of (8), we obtain a set of <u>linear</u> equations for the key quantities X'_{xy}. (These are called the FHNC-prime equations, or simply the prime equations.) We thus arrive at an array of coupled equations, namely (6)-(9) and their primed counterparts (6')-(9'), which, in conjunction with the Euler equation (13), determine in principle the <u>optimal</u> correlation function $f(r)$ as well as the corresponding two-particle structure function $S(k)$, and thereafter the optimal Jastrow distribution functions and energy expectation value. Again, however, the problem of the elementary diagrams, appearing in the infinite series E_{xy} and E'_{xy}, must be faced in actual calculation. Schemes for the incorporation of E'_{xy} diagrams run parallel to those of ordinary FHNC theory.

Corresponding to (10), the primed E's are responsible for the maintenance of the rigorous long-wavelength properties

$$\left.\begin{aligned}\tilde{X}'_{de}(k) &= 0(k)\\ \tilde{X}'_{ee}(k) &= 0(k^2)\end{aligned}\right\} \quad (k \to 0^+) \quad . \qquad (10')$$

As indicated earlier, it is desirable to observe such properties when formulating the Euler problem. Accordingly we extend the FHNC/C prescription for correcting the FHNC/0 approximation, supplementing (11) by

$$\begin{aligned}\tilde{X}'^{/C}_{de}(k) &= S_F(k)\tilde{X}'^{/0}_{de}(k) \ ,\\ \tilde{X}'^{/C}_{ee}(k) &= S_F^2(k)\{\tilde{X}'^{/0}_{ee}(k) + (\hbar^2k^2/4m)[S_F(k) - 1]\}\\ &\quad - (\hbar^2k^2/4m)[S_F(k) - 1] \ . \qquad (11')\end{aligned}$$

Means for realizing a practical numerical treatment of the Euler equation (13) will be described in a separate article. We remark that J. Owen has already published work along similar lines /19/.

3. Beyond the Jastrow Description.— The Jastrow model is expected to describe rather well some aspects of the strong spatial correlations among particles in a quantum fluid. However, since the assumed correlation operator is state independent (meaning it involves only the r_{ij}) and contains only two-body factors, such important phenomena as backflow and spin-density fluctuations will be inaccessible to this model. One would like to have some way of incorporating state-dependent (as well as direct three-body, four-body, ...) correlations into the theory without giving up the successful aspects of the Jastrow approach. Systematic procedures for correcting the Jastrow model may be formulated within the method of correlated basis functions /9-11,7,8,14/ (CBF). Discussion of this method will be confined to the aspects needed for a general understanding of the results to be presented in the following sections.

We extend consideration from a single Jastrow-correlated wave function (1)-(2) to a basis of such functions,

$$\psi_m = I_{mm}^{-\frac{1}{2}} \prod_{i<j} f(r_{ij})\Phi_m \quad , \qquad (14)$$

normalized to unity by

$$I_{mm} \equiv \langle\Phi_m|\Pi f^2(r_{ij})|\Phi_m\rangle \quad , \qquad (15)$$

the Φ_m constituting a complete orthonormal set of

Fermi-gas energy eigenfunctions. The label m identifies the collection of plane-wave single-particle states occupied in the Fermi-gas function Φ_m, with m = o denoting the filled Fermi sea. In terms of the correlated matrix elements $H_{mn} = \langle\psi_m|H|\psi_n\rangle$ and $N_{mn} = \langle\psi_m|\psi_n\rangle$ of the Hamiltonian and unity, a perturbation expansion for the ground-state energy E may be generated,

$$E = H_{oo} - \sum_{m\neq o} \frac{|H_{mo} - H_{oo}N_{mo}|^2}{H_{mm} - H_{oo}} + \ldots \quad , \qquad (16)$$

the higher terms involving more and more factors of $H_{mn} - H_{oo}N_{mn}$ or $N_{mn}(1-\delta_{mn})$. It is seen that the leading term is just the Jastrow energy expectation value, $H_{oo} = \langle H\rangle$. Here we shall concentrate on the next term, the negative semi-definite second-order perturbation correction to H_{oo}. We further restrict attention to m labels which differ from the Fermi sea o in exactly two single-particle orbitals. (Therefore we include only the effects of "correlated two-particle-two-hole states".) The resulting correction is denoted $\delta E^{(2,2)}$.

Two of us /7/ have carried out an extensive diagrammatic analysis of the quantities N_{mn}, $H_{mn} - H_{oo}N_{mn}$ and $H_{mm} - H_{nn}$ for choices of m,n including those needed for the evaluation of $\delta E^{(2,2)}$. Denoting by m_1, m_2 and o_1, o_2 the orbitals in which m and o differ, the relevant results are conveniently expressed in the forms

$$H_{mm} - H_{oo} = \varepsilon(m_1) + \varepsilon(m_2) - \varepsilon(o_1) - \varepsilon(o_2) \ ,$$
$$H_{mo} - H_{oo}N_{mo} = \langle m_1m_2|V(12)|o_1o_2 - o_2o_1\rangle \ , \qquad (17)$$

where the ε's are interpreted as single-particle energies and $V(12)$ is a (non-local) effective interaction. The derivations of reference /7/ were based on the Clark-Westhaus (CW) form for the CBF matrix elements H_{mn}, because of the formal simplicity of that choice. In the meantime, the analysis has been extended to the Jackson-Feenberg (JF) form, which we regard as generally the most reliable (least sensitive to errors, particularly in the $g \leftrightarrow g_3$ connection /22/) among the three choices PB, JF, CW. In the CW case, the single-particle energies are found to have a very simple structure in terms of the quantities already introduced in optimal FHNC theory, namely

$$\varepsilon(k) = \frac{\hbar^2k^2}{2m} + \tilde{X}'_{cc}(k)/[1 - \tilde{X}_{cc}(k)] + U_o \ , \qquad (18)$$

where U_o is a constant, independent of k. The JF result is a bit more elaborate, containing additional terms

$$-\frac{\hbar^2k^2}{4m}\tilde{X}_{cc}(k) + \frac{\hbar^2\rho}{2mv}\{\nabla[\Gamma_{dd}(r)\nabla\ell(k_Fr)]\}^F(k) \qquad (19)$$

where $\{\ \}^F$ stands for Fourier transform, and a further (small) contribution $\varepsilon^{[3]}$ arising from the three-body part of the Jackson-Feenberg kinetic energy operator. The single-particle energy $\varepsilon(k)$ determines an effective mass at the Fermi surface via

$$\hbar^2k_F/m^* = [d\varepsilon(k)/dk]_{k_F} \ . \qquad (20)$$

We shall take m* to be the effective mass predicted by the Jastrow model.

The non-local effective-interaction operator has the structure

$$\langle m_1m_2|V(12)|o_1o_2 - o_2o_1\rangle = \langle m_1m_2|W(12)|o_1o_2 - o_2o_1\rangle + \frac{1}{2}[\varepsilon(m_1)+\varepsilon(m_2)-\varepsilon(o_1)-\varepsilon(o_2)]\cdot \langle m_1m_2|N(12)|o_1o_2 - o_2o_1\rangle \ , \qquad (21)$$

where $W(12)$ and $N(12)$ are again non-local operators. In detail, the latter operators are rather complicated; however, $W(12)$ may be determined from $N(12)$ by the graphical differentiation process. The matrix elements of $N(12)$ are found to contain factorizable diagrams, implying the structure

$$\langle m_1m_2|N(12)|o_1o_2 - o_2o_1\rangle = \frac{\langle m_1m_2|N^B(12)|o_1o_2 - o_2o_1\rangle}{\{[1-\tilde{X}_{cc}(m_1)][1-\tilde{X}_{cc}(m_2)][1-\tilde{X}_{cc}(o_1)][1-\tilde{X}_{cc}(o_2)]\}^{\frac{1}{2}}} \ , \qquad (22)$$

where $N^B(12)$ is the irreducible, basic portion of $N(12)$ as defined in reference /7/; and similarly

for the matrix elements of $W(12) = N'(12)$. The leading contributions to $N^B(12)$, $W^B(12)$ are their local parts; these are simply expressible in terms of primed and unprimed quantities already encountered. In fact, it was in the CBF context /7/ that FHNC-prime equations for the X'_{xy} were first derived (albeit for the CW kinetic energy operator). It is of course natural that the ingredients of the CBF perturbation corrections, in their detailed structure, are related to the ingredients of the Euler equation for the optimal f(r). A comparable, though much less complicated, situation prevails within the paired-phonon analysis by Feenberg, Jackson and Campbell /10,25/ for the optimal Jastrow treatment of Bose systems.

In the actual calculations of $N^B(12)$ and $W^B(12)$ we have included, along with $\Gamma_{dd}(r_{12})$ and $\Gamma'_{dd}(r_{12})$, certain tractable "elementary" contributions (see Fig. 5.4 of reference /7/), as well as the effects of separable three-body contributions. The subsequent preparation of $\delta E^{(2,2)}$ for numerical computation follows an essentially standard pattern /26,27/: partial-wave analysis, angle-averaging, quadratic approximation of hole energies $\varepsilon(k)$, $k \leq k_F$, etc. However, in contradistinction to the procedure of reference /27/, the particle energies $\varepsilon(k)$, $k > k_F$, are not taken to be simply the free energies $\hbar^2k^2/2m$ but also include the constant term U_0. (It is to be noted that above the Fermi surface the remaining terms in the $\varepsilon(k)$ formula rapidly become negligible compared to the free kinetic energy.) A more thorough discussion of these matters will be presented in another article. One qualitative fact emerging from analysis of the structure of $\delta E^{(2,2)}$ should, nevertheless, be mentioned here. When this correction is reduced for the special case of optimal f, making use of the Euler equation $\omega(k) = 0$ and introducing and subtracting out an inverse energy difference $\langle e^{-1} \rangle$ averaged over holes, one may isolate a contribution attributable to non-central (angle-dependent) correlations, a contribution apparently related to backflow.

We conclude our outline of formal methods by pointing out that the results of reference /7/ for the non-diagonal CBF quantities N_{mn}, $H_{mn}-H_{oo}N_{mn}$ and $H_{mm}-H_{nn}$ not only yield the inputs necessary for estimation of the CBF perturbation corrections to the Jastrow energy, but also provide further valuable information on the Jastrow model itself. This has already been seen in the case of the Jastrow effective mass. To cite a more elaborate example: as shown in reference /8/, one may test the stability of the Jastrow ground state against pair condensation in various partial waves, in terms of effective pairing matrix elements derived from the operator $W(12)$. In a third application (which by no means exhausts the interesting possibilities), one may determine the magnetic susceptibility χ of the Jastrow model from CBF matrix elements. If the CW form is assumed for the H_{mn}, the simple formula

$$\frac{\chi_F}{\chi} = \frac{m}{m^*}[1 - \delta(^1S_0)] \qquad (23)$$

(applicable to unpolarized ^{3}He) is obtained, where χ_F is the magnetic susceptibility of the free Fermi gas and $\delta(^1S_0)$ is the dimensionless effective pairing matrix element in the $^1S_0$ channel, derived from the CBF analysis of reference /8/. (It should be remarked that equation (23) is just a formal result among CBF quantities and does not imply a corresponding physical relationship between magnetic response and pairing.)

4. Applications to Helium Systems.— We consider ordinary, unpolarized ^{3}He (with level degeneracy $\nu = 2$), together with fully spin-polarized ^{3}He ($\nu=1$). The latter system will be denoted ^{3}He$\uparrow$; the former, simply as ^{3}He. Properties of the Jastrow model of

these systems are computed for two choices of the correlation function f(r): (a) the Schiff-Verlet form /28/

$$f_{SV}(r) = \exp[-\frac{1}{2}(\frac{b}{r})^5] \quad , \qquad (24)$$

with b = 2.888 Å independent of density and polarization and (b) an optimal f(r) determined from the JF version of the Euler equation, for each ν and each density. The usual Lennard-Jones potential is assumed, $v(r)=4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6]$ with ε = 10.22 K and σ = 2.556 Å.

Results for the ground-state energy expectation value are collected in Table I and plotted (for the optimal f) in Fig. 1. The reader should focus his attention on the results for $E_{JF} = \langle H \rangle_{JF}$, since the other forms of the energy (CW, PB) contain large terms involving aspects of the three-particle distribution function which FHNC theory may represent poorly /4,6,22/. At ρ=0.0142Å^{-3} in the case of ordinary ^{3}He, the exact expectation value for the Schiff-Verlet (SV) correlation function specified above is known by Monte Carlo (MC) calculation /29/ to lie roughly midway between the JF and PB energy functionals computed in FHNC/0 or FHNC/C approximation /4,22/. However, within these approximations the PB choice is the "most likely" among PB, JF and CW to violate the upper-bound property of the exact <H> upon variation of f around a sensible reference function. We expect that in the present applications the JF choice safely preserves this property, without erring too much in the upward direction (which is usually the case for the CW form). To avoid any possible confusion, we stress that the f_{opt} results in Table I and Fig. 1 are obtained by insertion of the JF-based optimal f into the indicated functionals. We also note that all numerical energies are of course given in K per particle.

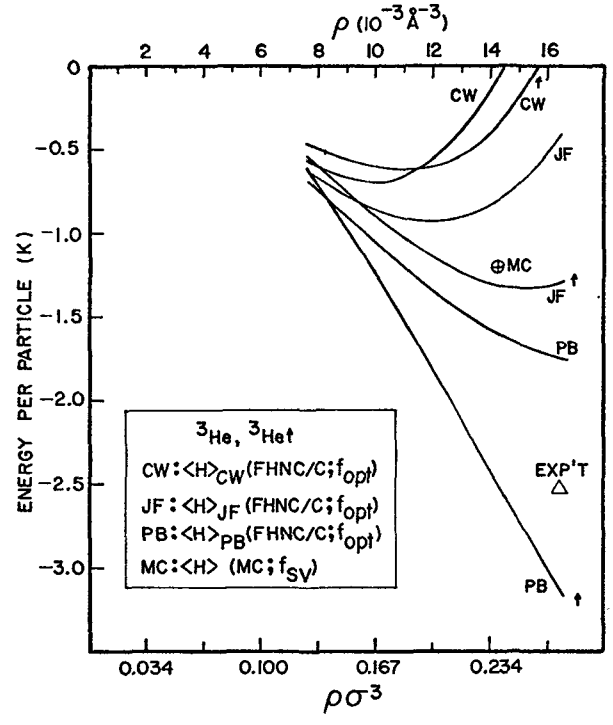

Fig. 1 : Jastrow ground-state energy versus density for unpolarized ^{3}He and for ^{3}He↑, based on the Lennard-Jones potential (σ = 2.556 Å). (Curves and points not marked with ↑ refer to unpolarized ^{3}He.)

Table I : Jastrow ground-state energies for unpolarized ^{3}He and for ^{3}He↑.

ρ (10^{-3} Å^{-3})	^{3}He, f_{SV}			^{3}He↑, f_{SV}			^{3}He, f_{opt}			^{3}He↑, f_{opt}		
	$\langle H \rangle_{CW}$	$\langle H \rangle_{JF}$	$\langle H \rangle_{PB}$	$\langle H \rangle_{CW}$	$\langle H \rangle_{JF}$	$\langle H \rangle_{PB}$	$\langle H \rangle_{CW}$	$\langle H \rangle_{JF}$	$\langle H \rangle_{PB}$	$\langle H \rangle_{CW}$	$\langle H \rangle_{JF}$	$\langle H \rangle_{PB}$
7.6	-0.43	-0.60	-0.78	-0.14	-0.23	-0.36	-0.56	-0.63	-0.69	-0.47	-0.53	-0.61
11.2	-0.46	-0.88	-1.33	-0.48	-0.83	-1.19	-0.65	-0.92	-1.24	-0.62	-1.05	-1.56
13.0	-0.23	-0.88	-1.59	-0.51	-1.05	-1.58	-0.40	-0.91	-1.47	-0.55	-1.24	-2.10
14.2	-0.03	-0.81	-1.72	-0.47	-1.19	-1.82	-0.12	-0.83	-1.61	-0.38	-1.30	-2.46
14.8	0.20	-0.76	-1.78	-0.43	-1.24	-1.94	0.07	-0.75	-1.65	-0.26	-1.33	-2.66
16.6	0.87	-0.46	-1.90	-0.22	-1.32	-2.25	0.80	-0.41	-1.75	0.25	-1.29	-3.16

One can immediately draw two interesting qualitative conclusions from this study of the ground-state energetics. First, the Jastrow model cannot reproduce the experimentally determined energy and density of unpolarized liquid ^{3}He (E_{equil} = -2.52 K, ρ_{equil} = 0.0164 $\mathring{A}^{-3}$) at zero temperature and zero external pressure. Important correlation effects (presumably associated with spin-density fluctuations and backflow) are clearly missing from the Jastrow ansatz. Indeed, the margin of failure seems especially disturbing until it is realized that the total energy E of the system results from near cancellation of relatively large kinetic and potential contributions. For these individual terms the percentage error of the Jastrow model is only of order 10%.

The second point concerns the comparison of the two polarization states of ^{3}He. It is seen that, beyond a relatively low density, the Jastrow models of ^{3}He↑ are energetically more stable than the corresponding models of the unpolarized system. This is the case even for the SV correlation function--the parameter b of which was determined for ordinary ^{3}He. We have, then, another indication that the Jastrow trial function is inadequate for unpolarized ^{3}He. On the other hand, the Jastrow model appears to be rather good for ^{3}He↑, at least so far as the energy is concerned: a reasonable interpolation between the JF and PB curves for this system would put the energy minimum somewhere in the range -1.5 K to -2 K, and the true energy surely cannot be much lower. (We assume for the sake of argument that the FHNC/C procedure is no less accurate for ^{3}He↑ than it is for ordinary ^{3}He, a supposition which has yet to be fully tested. In this connection one may observe in Fig. 1 that for ^{3}He↑, the FHNC/C approximation to the PB functional clearly violates the upper-bound property at densities exceeding ρ = 0.014 $\mathring{A}^{-3}$.)

Inspecting Table I, we notice that for ordinary ^{3}He the optimal f does not lead to much improvement over the simple SV choice, E_{JF} being especially insensitive; even for ^{3}He↑ the improvement is not dramatic. In some cases it turns out that f_{opt} raises the energy slightly, compared to the SV energy. While this might at first seem contradictory, it must be remembered that since the Euler equation (13) is derived from an exact energy functional and thereafter approximated, the solution obtained does not necessarily minimize an approximate energy functional (FHNC version of $\langle H \rangle_{JF}$, etc.).

In Fig. 2 the structure factors S(k) of the optimal Jastrow models of unpolarized and polarized systems are plotted at the same density (near ρ_{equil} of ordinary ^{3}He). The results for the two cases are very similar, the only apparent distinction being that the peak is displaced slightly inward for ^{3}He↑ compared to the normal system.

Fig. 3 exposes further shortcomings of the Jastrow description of unpolarized ^{3}He. The effective masses of optimal and SV models are far from the experimental value, which has recently been set /30/ at $(m^*/m)_{exp} = 2.12$ (for $\rho = \rho_{equil}$). An even more striking symptom is displayed by the susceptibility ratio χ_F/χ of the SV model, which dives into the negative region already at quite low density. The latter behavior corresponds to our previous finding that, within the Jastrow approach, ^{3}He↑ is energetically favored over its unpolarized counterpart, except at small ρ. (We should remark that the χ_F/χ curve drawn in Fig. 3 is not consistent through (23) with the values of m^*/m and $\delta(^1S_0)$ reported here. This curve is derived from Jastrow pairing matrix elements and effective masses /8/ based on the CW form of the H_{mn} (for which (23) applies), whereas the other

quantities in Figs. 3 and 4 are calculated using the JF form. At any rate, the χ_F/χ results given are purely illustrative, having no significance for the real system.)

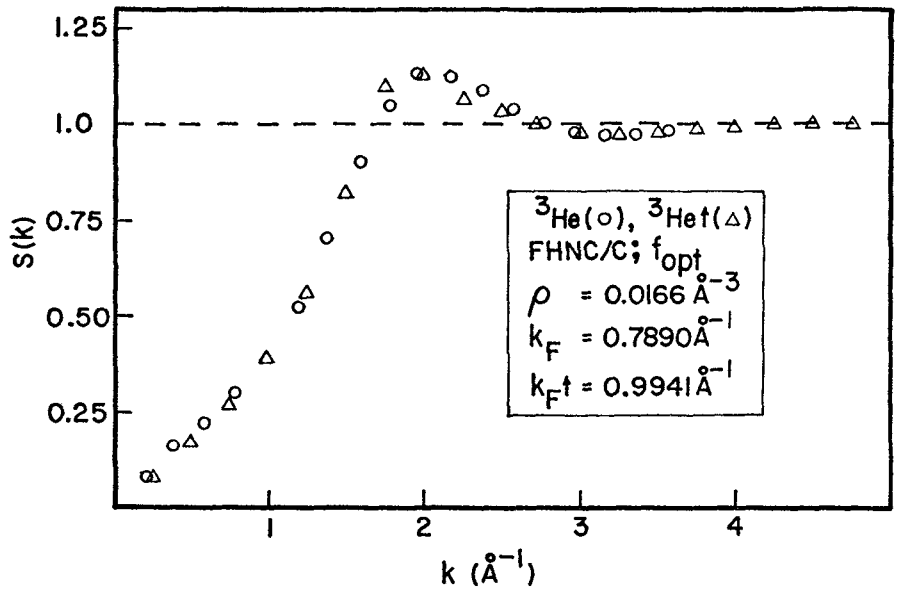

Fig. 2 : Jastrow static structure function for unpolarized ^{3}He and for ^{3}He↑.

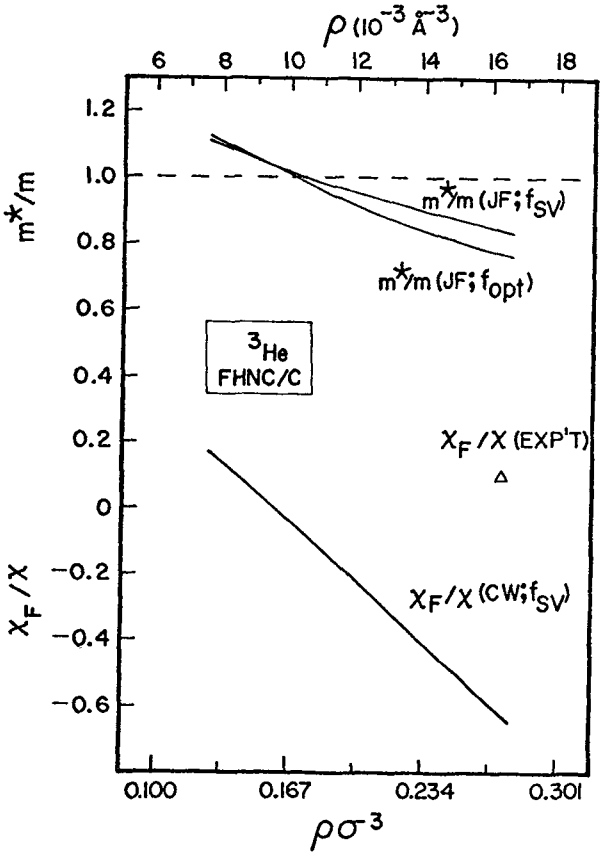

Fig. 3 : Effective mass and magnetic susceptibility of unpolarized ^{3}He, corresponding to the Jastrow models.

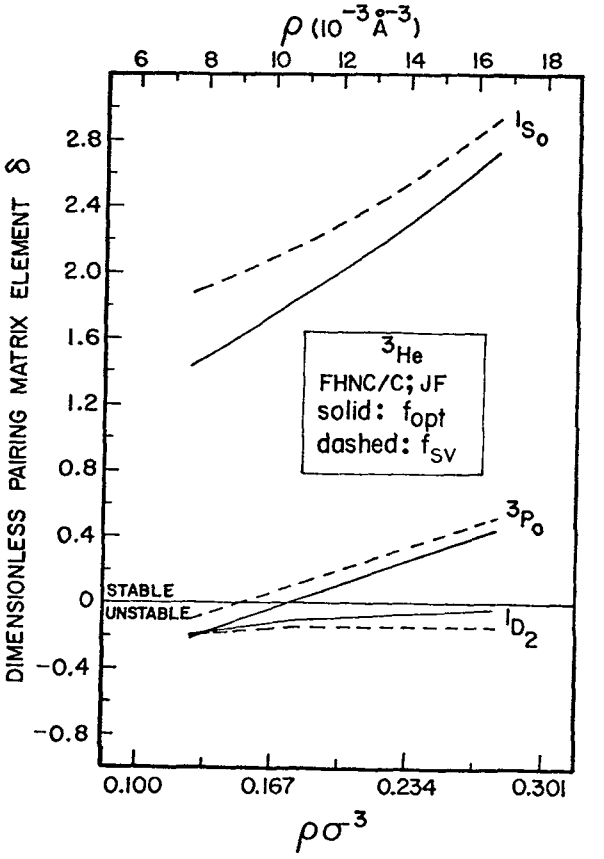

Fig. 4 : Dimensionless pairing matrix elements of unpolarized ^{3}He, corresponding to the Jastrow models, for various two-body channels.

Fig. 4 supplements the CW results of reference /8/ with plots of the (dimensionless) Jastrow pairing matrix elements δ of normal ^{3}He in $^1S_0$, $^3P_0$ and $^1D_2$ partial waves, as determined by FHNC/C-approximated CBF quantities of JF form. Negative δ values signal instability of the Jastrow state with respect to pair condensation in the given partial wave. Detailed consideration of these results (along the lines of reference /8/) leads once more to the conclusion that the Jastrow correlation operator is deficient in important respects--particularly in its lack of spin (and momentum) dependence.

Table II presents some results of an attempt to correct for the deficiencies of the Jastrow description by means of CBF perturbation theory. The required CBF matrix elements are evaluated via the FHNC/C procedure as sketched in sections 2,3. The entries for $\delta E^{(2,2)}$ represent our most complete estimate of this quantity, based on formula (22) for the $N(12)$ matrix elements and the corresponding formula for $W(12)$ derived by graphical (prime) differentiation. In the latter formula the denominator $D = \{[1-\tilde{X}_{cc}(m_1)][1-\tilde{X}_{cc}(m_2)][1-\tilde{X}_{cc}(o_1)][1-\tilde{X}_{cc}(o_2)]\}^{\frac{1}{2}}$ will also appear. As we shall document elsewhere, the correction $\delta E^{(2,2)}$ (for ^{3}He systems) is quite sensitive to the precise means used to treat this denominator. Accordingly, the results given in Table II should be regarded as illustrative rather than quantitative. It is seen that the correction is very large in magnitude and clearly overestimates the effects of the non-Jastrow correlations. The other entries in the table, labeled $\delta E_{wo}^{(2,2)}$, are the results for the perturbation correction <u>without</u> the denominator D, i.e., the factor $\{[1-\tilde{X}_{cc}]\ldots\}^{-\frac{1}{2}}$ is replaced by unity in the final formulas for $N(12)$ and $W(12)$. It may be argued that the omission of D from the present treatment simulates the effect of higher-order, RPA-type contributions to the CBF perturbation expansion. The modified second-order correction $\delta E_{wo}^{(2,2)}$ is much more reasonable in size, though larger than $\delta E^{(2,2)}$ as approximated by Woo /13/. Woo used, in effect, less highly dressed CBF matrix elements than employed herein; among other simplifications, the denominators D do not appear.

Table II : Second-order CBF perturbation corrections to Jastrow ground-state energies for unpolarized ^{3}He, using Jackson-Feenberg kinetic energy operator.

ρ	f_{SV}		f_{opt}	
(10^{-3} Å^{-3})	$\delta E^{(2,2)}$	$\delta E_{wo}^{(2,2)}$	$\delta E^{(2,2)}$	$\delta E_{wo}^{(2,2)}$
7.6	-0.84	-0.34	-0.76	-0.50
11.2	-2.57	-0.83	-2.46	-1.04
13.0	-3.26	-0.90	-3.27	-1.14
14.2	-5.18	-1.38	-5.08	-1.63
14.8	-5.74	-1.47	-5.65	-1.72
16.6	-5.73	-1.22	-5.99	-1.50

We do not report any results for the perturbation correction in the case of ^{3}He$\uparrow$, for the following reason, associated with the behavior of $\tilde{X}_{cc}(0^+)$ shown in Fig. 5. The non-nodal compound-diagrammatic quantity $\tilde{X}_{cc}(k)$ has its maximum value at $k=0$; it falls off as k increases through the Fermi sea, and displays damped oscillations about zero for $k > k_F$. From Fig. 5 we see that $\tilde{X}_{cc}(0^+)$ rises monotonically with density, reaching unity in ^{3}He$\uparrow$ at a relatively low value of ρ. Beyond that critical density, singularities appear in the expression for the CBF correction $\delta E^{(2,2)}$, because of the vanishing, at some k, of denominators $[1-\tilde{X}_{cc}(k)]^{\frac{1}{2}}$ in the W and N matrix elements and of the denominator $1-\tilde{X}_{cc}(k)$ in the single-particle energies $\varepsilon(k)$. Consequently, for densities at which $\tilde{X}_{cc}(0^+) > 1$, the CBF perturbation procedure, <u>in its present computational realization</u>, ceases

to be meaningful. Formally, it may be shown that the singularities generated by the denominator of (22) are in fact cancelled by those occuring in the $\epsilon(k)$, provided $\tilde{X}_{cc}(k)$ remains less than unity for $k > k_F$. (We are reminded of similar compensations of possible $[1-\tilde{X}_{cc}]^{-1}$ singularities within the FHNC treatment of the Jastrow spatial and momentum distributions.) However, our computational procedure, which is based on an effective-mass approximation, has yet to be reformulated to take advantage of this cancellation. The $[1-\tilde{X}_{cc}]^{-1}$ singularity in $\epsilon(k)$ (and hence in $H_{mm}-H_{oo}$) may be merely an artifact of our theory, without physical relevance. On the other hand it may actually reflect some interesting physical phenomenon; e.g., $\tilde{X}_{cc}(0^+) = 1$ may signal some imminent phase transition. Further analysis (for example, using the penetrating methods of CBF coupled-cluster theory /14/) is needed to decide between these two possibilities.

The effect of a $[1-\tilde{X}_{cc}]^{-1}$ singularity on the Jastrow values of m^*/m, the pairing matrix elements δ and the susceptibility ratio χ_F/χ will be slight unless the singularity appears near k_F. Even so, we choose not to quote any m^*/m results for ^{3}He↑ until the origin of the singularity in the single-particle energy is better understood.

That the values of $\tilde{X}_{cc}(0^+)$ in unpolarized ^{3}He are about half those in ^{3}He↑ may be attributed to the presence of a (rough) overall factor of ν^{-1} in this quantity. It is interesting to note that $\tilde{X}_{cc}(0^+)$ for ordinary ^{3}He eventually crosses unity, at a value of ρ somewhere beyond the crystallization density. Lantto /31/ has observed the vanishing of $1-\tilde{X}_{cc}(0^+)$ in the electron gas at very low density--corresponding to the strong-coupling regime of the Coulomb system.

5. Applications to Deuterium Systems.— We define D↑ as a system of deuterium atoms somehow constrained so that any pair of atoms interacts exclusively in the $b\,^3\Sigma_u^+$ state /32/. Since the latter interaction is strongly repulsive at short distances and only very weakly attractive at longer range, we have a system of fermions which is expected to display extreme quantal behavior--even more so than ^{3}He /33/.

Two species of D↑ are examined here, namely: (i) $D\uparrow_1$, with one allowed nuclear-spin state, and

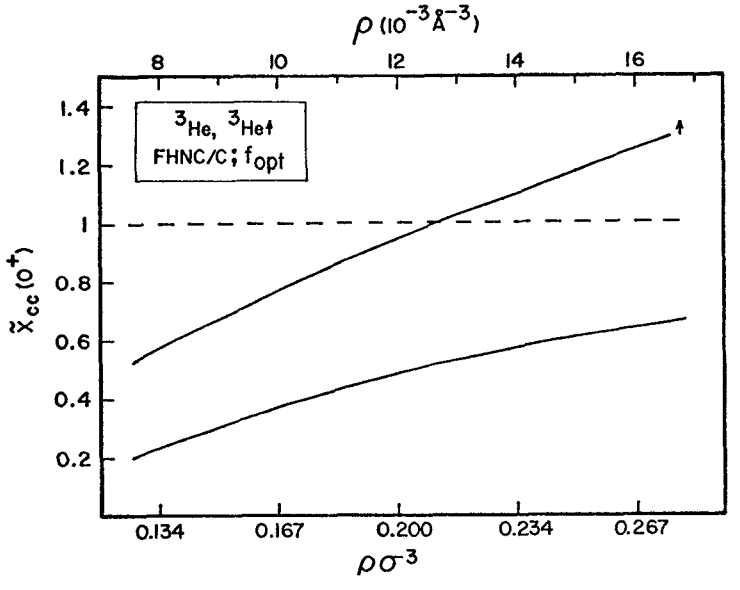

Fig. 5 : Compound-diagrammatic quantity $\tilde{X}_{cc}(0^+)$ for unpolarized ^{3}He and for ^{3}He↑, as a function of density.

(ii) $D\uparrow_2$, with <u>two</u> allowed nuclear-spin states which are assumed to be equally populated /34/. We note that $D\uparrow_1$, with one Fermi sea, has $\nu=1$ and corresponds to $^3He\uparrow$, while $D\uparrow_2$, with two equal Fermi seas and $\nu=2$, corresponds formally to ordinary ^3He. With such correspondences in mind, calculations of the type described in section 4 have been repeated for deuterium. It is found that the results preserve the stated analogies, to the extent that many of the qualitative features encountered in section 4 (as well as the associated judgments) carry over with $^3He\uparrow$ replaced by $D\uparrow_1$ and unpolarized ^3He replaced by $D\uparrow_2$. In particular, the Jastrow model shows an energetic preference for $D\uparrow_1$ over $D\uparrow_2$ (except at low density); the Jastrow trial function may again be considerably better for $\nu=1$ than for $\nu=2$.

The calculations are based on the theoretical b $^3\Sigma_u^+$ potential of Kolos and Wolniewicz /35/, as used by Miller and Nosanow /34/. We report results only for a Schiff-Verlet correlation function (24). (Optimal correlation functions for the deuterium systems will be generated in later work.) The results for energy expectation values, structure functions, effective masses, second-order perturbation corrections and $\tilde{\chi}_{cc}(0^+)$ values are presented in Tables III and IV and Figs. 6-9. Note that in these figures, $\sigma = 3.69$ Å, corresponding to a Lennard-Jones fit to the Kolos-Wolniewicz potential /34/.

Table III

Jastrow ground-state energies for two species of spin-aligned deuterium. (LO refers to lowest cluster order approximation.)

ρ (10^{-3} Å^{-3})	$D\uparrow_2$		$D\uparrow_1$	
	$\langle H\rangle_{LO}$	$\langle H\rangle_{JF}$	$\langle H\rangle_{LO}$	$\langle H\rangle_{JF}$
1.41	0.277	0.276	0.567	0.450
2.82	0.098	0.255	0.499	0.333
3.52	-0.018	0.323	0.455	0.292
4.23	-0.136	0.476	0.432	0.299
4.93	-0.256	0.741	0.412	0.374
5.63	-0.377	1.119	0.417	0.534
6.34	-0.489	1.630	0.418	0.749
7.04	-0.611	2.283	0.482	1.041

Table IV

Second-order CBF perturbation corrections to Jastrow ground-state energies for $D\uparrow_2$, using Clark-Westhaus kinetic energy operator /7/. (Six partial waves are included.)

ρ (10^{-3} Å^{-3})	$\delta E^{(2,2)}$	$\delta E^{(2,2)}_{WO}$
1.41	-0.13	-0.08
2.82	-0.51	-0.22
3.52	-0.85	-0.31
4.23	-1.34	-0.41
4.93	-2.00	-0.52
5.63	-2.86	-0.64
6.34	-4.00	-0.76
7.04	-5.48	-0.89

It is of special interest to compare the Jastrow energies obtained in FHNC/C approximation with the earlier results of Miller and Nosanow (MN). In the MN work, a hypernetted-chain (HNC) or BBGKY-KSA procedure /36/ was applied to evaluate the radial distribution function corresponding to the Jastrow factor $\Pi f(r_{ij})$, and the Wu-Feenberg (WF) antisymmetry expansion /37/, carried to three-index terms, was used to correct for the presence of the Slater determinant Φ_0 in the (Fermi) Jastrow ansatz (1)-(2). This treatment is based on the JF energy functional. The correlation function f was taken of SV form, with b determined for each ν and ρ by minimizing the Fermi-system energy in HNC-WF or BBGKY-KSA-WF approximation. We have adopted the b values corresponding to the BBGKY-KSA approximation, which were supplied by Miller. For the $D\uparrow_1$ system our JF energies agree very well with the HNC-WF results reported by Miller and Nosanow (see Fig. 6). On the other hand, in the case of $D\uparrow_2$ the JF and MN curves depart markedly from one another as the density increases past 0.003 Å^{-3} (see Fig. 7). The disagreement of our $D\uparrow_2$ results

with those of MN is even worse for their BBGKY-KSA calculation. (A calculational situation analogous to that for $D\uparrow_2$ prevails with respect to unpolarized ^{3}He: juxtapose the findings of reference /38/ against those of references /4,22/.) It must be kept in mind throughout such considerations that the net energies E of the systems under study are very small in magnitude compared to the separate kinetic and potential energies, so that relatively small errors in the evaluation of these separate parts is prominently reflected on the scale of Figs. 6 and 7.

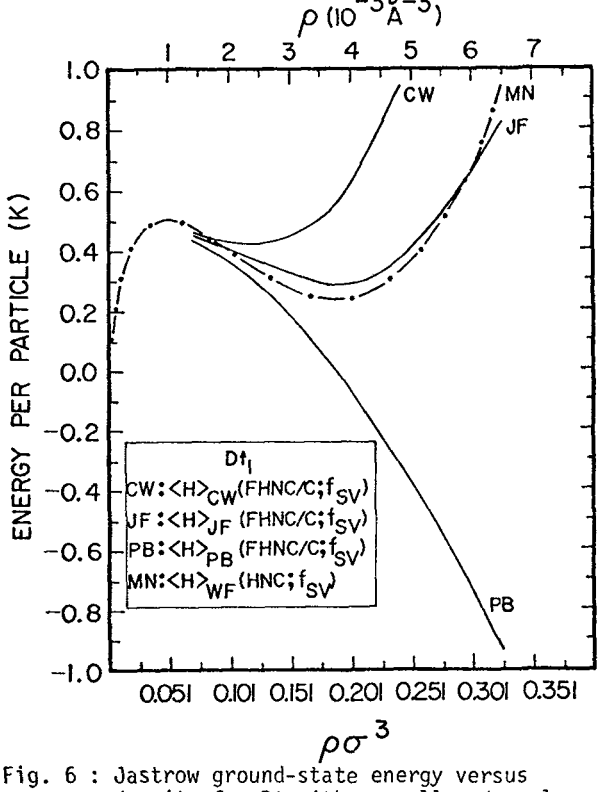

Fig. 6 : Jastrow ground-state energy versus density for D↑ with one allowed nuclear-spin state, based on the Kolos-Wolniewicz potential, (corresponding Lennard-Jones σ = 3.69 Å).

For both deuterium systems we carried out a search in the vicinity of the b values provided by Miller. It was found that these parameters are still very close to optimal for the JF energy functional as approximated here; the best parameters produce changes in the JF curves which would hardly be noticeable on the scale of Figs. 6 and 7. This is somewhat surprising for the $D\uparrow_2$ case, where the differences between our results and those of MN can exceed 1 K in the density range considered.

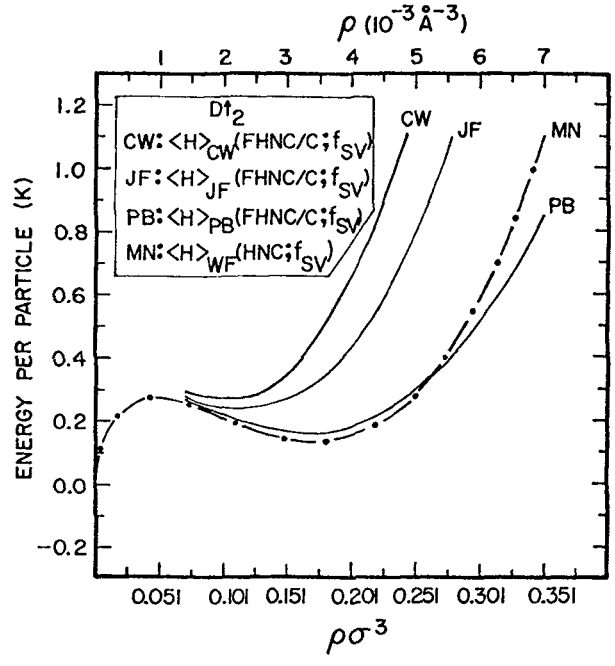

Fig. 7 : Jastrow ground-state energy versus density for D↑ with two allowed nuclear-spin states, equally populated. (Calculations based on the Kolos-Wolniewicz potential; σ = 3.69 Å.)

The present calculation still does not settle the question of whether $D\uparrow_1$ (respectively $D\uparrow_2$) is a liquid or a gas in its ground state under zero pressure. (In the former case one has a Fermi liquid like ordinary ^{3}He; in the latter, one can go from gas to liquid at T = 0 under appropriate pressure.) However, we may call attention to the very small net energies and substantial negative potential energies (e.g., $\langle V\rangle \approx -5$ K at $\rho \approx 0.004$ Å^{-3}) characterizing our Jastrow results. These features suggest that improvement of the correlation operator and/or a reliable CBF perturbation calculation may well depress the minimum theoretical ground-state energies of the deuterium systems to negative values, implying the existence of two new Fermi liquids.

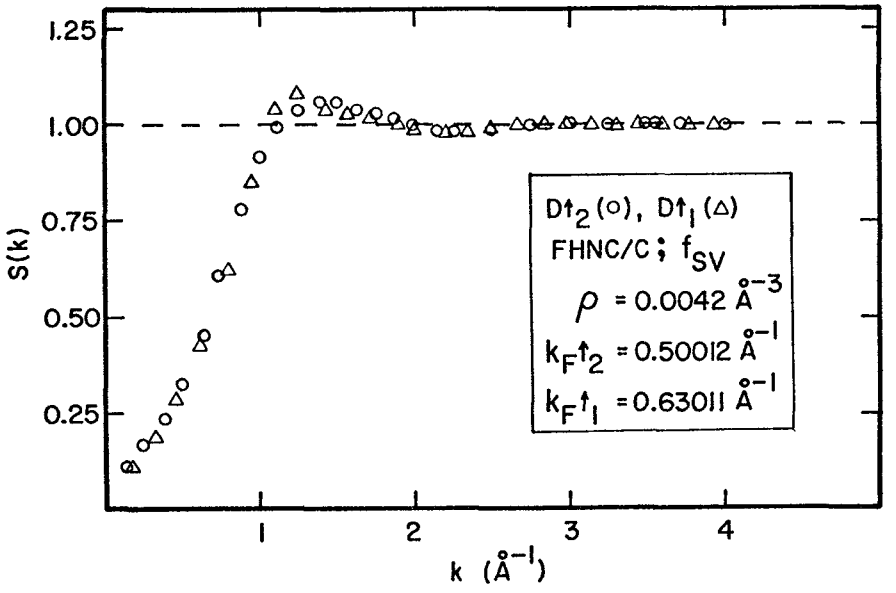

Fig. 8 :

Jastrow static structure functions for $D\uparrow_2$ and $D\uparrow_1$.

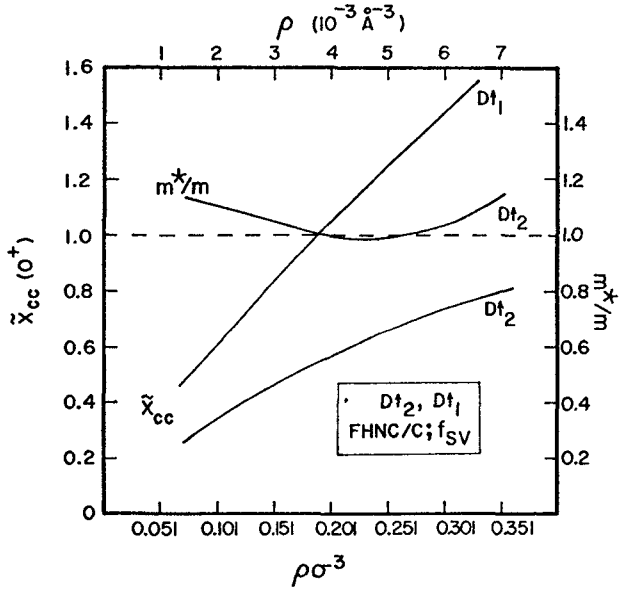

Fig. 9 : Compound-diagrammatic quantity $\tilde{X}_{cc}(0^+)$ for $D\uparrow_2$ and for $D\uparrow_1$, as a function of density. Effective mass of $D\uparrow_2$ corresponding to Jastrow model.

Acknowledgments.— This research has been supported in part by the U.S. National Science Foundation under Grant No. DMR78-08552, by the U.S. Department of Energy under Contract No. EY-76-S-3001 and by the Deutsche Forschungsgemeinschaft. E. K. acknowledges the hospitality of the Stony Brook group while on leave from I. Institut für Theoretische Physik, Universität Hamburg. We express our appreciation to M. D. Miller for informative discussions and for supplying us with potential and correlation function data. We also benefited from stimulating discussions with A. D. Jackson, L. J. Lantto and R. A. Smith.

References

/1/ Clark, J. W., in Progress in Particle and Nuclear Physics, Vol. 2, ed. Wilkinson, D. H. (Pergamon, Oxford, 1979).

/2/ Krotscheck, E. and Ristig, M. L., Nucl. Phys. A242 (1975) 389; E. Krotscheck, Phys. Lett. 54A (1975) 123.

/3/ Fantoni, S. and Rosati, S., Nuovo Cim. 25A (1975) 593.

/4/ Zabolitzky, J. G., Phys. Rev. A16 (1977) 1258.

/5/ Krotscheck, E., Phys. Rev. A15 (1977) 397.

/6/ Krotscheck, E., Nucl. Phys. A317 (1979) 149.

/7/ Krotscheck, E. and Clark, J. W., Nucl. Phys. A328 (1979) 73.

/8/ Krotscheck, E. and Clark, J. W., Nucl. Phys. A333 (1980) 77.

/9/ Clark, J. W. and Westhaus, P., Phys. Rev. 141 (1966) 833.

/10/ Feenberg, E., Theory of Quantum Fluids (Academic, N.Y., 1969).

/11/ Clark, J. W., Mead, L. R., Krotscheck, E., Kürten, K. E. and Ristig, M. L., Nucl. Phys. A328 (1979) 45.

/12/ Clark, J. W. and Feenberg, E., Phys. Rev. 113 (1959) 388.

/13/ Woo, C. W., Phys. Rev. 151 (1966) 138.

/14/ Krotscheck, E., Kümmel, H. and Zabolitzky, J. G., to be published.

/15/ Tan, H.-T. and Feenberg, E., Phys. Rev. 176 (1968) 370.

/16/ Schmidt, K. E. and Pandharipande, V. R., Phys. Rev. B19 (1979) 2504.

/17/ Pandharipande, V. R. and Wiringa, R. B., Rev. Mod. Phys. 51 (1979) 821.

/18/ Owen, J. C., Ann. of Phys. 118 (1979) 373.

/19/ Owen, J. C., Phys. Lett. 89B (1980) 303.

/20/ Krotscheck, E., to be published.

/21/ Lantto, L. J. and Siemens, P. J., Phys. Lett. 68B (1977) 308; Nucl. Phys. A317 (1979) 55.

/22/ Krotscheck, E., Z. Physik B32 (1979) 395; B33 (1979) 403.

/23/ Van Leeuwen, J. M. J., Groeneveld, J. and de Boer, J., Physica 25 (1959) 792.

/24/ Stell, G., in The Equilibrium Theory of Classical Fluids, ed. Frisch, H. L. and Lebowitz, J. L. (Benjamin, N. Y., 1964).

/25/ Campbell, C. E. and Feenberg, E., Phys. Rev. 188 (1969) 396.

/26/ MacKenzie, J. J., Phys. Rev. 179 (1969) 1002.

/27/ Clark, J. W., Lam, P. M. and Ter Louw, W. J., Nucl. Phys. A255 (1975) 1.

/28/ Schiff, D. and Verlet, L., Phys. Rev. 160 (1967) 208.

/29/ Ceperley, D., Chester, G. V. and Kalos, M. H., Phys. Rev. B16 (1977) 3081.

/30/ Alvesalo, T. A., Haavasoja, T., Main, P. C., Manninen, M. T., Ray, J. and Rehn, L. M. M., Phys. Rev. B, to be published.

/31/ Lantto, L. J.,Phys. Rev. A, to be published.

/32/ Dugan, J. V. and Etters, R. D., J. Chem. Phys. 59 (1973) 6171; Etters, R. D., Dugan, J. V. and Palmer, R. W., J. Chem. Phys. 62 (1975) 313.

/33/ Stwalley, W. C. and Nosanow, L. H., Phys. Rev. Lett. 36 (1976) 910.

/34/ Miller, M. D. and Nosanow, L. H., Phys. Rev. B15 (1977) 4376.

/35/ Kolos, W. and Wolniewicz, L., J. Chem. Phys. 43 (1965) 2429; Chem. Phys. Lett. 24 (1974) 457.

/36/ Woo, C. W., in The Physics of Liquid and Solid Helium, ed. Bennemann, K. H. and Ketterson, J. B. (Wiley, N. Y., 1976).

/37/ Wu, F. Y. and Feenberg, E., Phys. Rev. 128 (1962) 943.

/38/ Miller, M. D., Phys. Rev. B14 (1976) 3937.