Theory of the (Normal) Ground State of Liquid Helium Three*

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A theory of the normal ground state of liquid He^3 is constructed using matrix elements in a representation of correlated basis functions. The Rayleigh-Schrödinger perturbation theory is adapted to our nonorthogonal basis. Several means of classifying terms are available; one of them is recognized as best suited for the study of liquid He^3. To the second order in the classification scheme, the following ground-state properties are calculated and compared with experiment and results of the Brueckner-Gammel theory: energy per particle, equilibrium density, compressibility, velocity of sound, and paramagnetic susceptibility. The radial distribution function of liquid He^3 at zero temperature is also calculated. A study of the Löwdin transformation as a procedure for orthogonalizing the correlated basis shows that the correction to the Hamiltonian involves unphysical N dependences; these arise out of high-order irreducible clusters and unlinked diagrams. It is verified that the unphysical terms cancel out completely in each of several lowest orders.

I. INTRODUCTION

A THEORY of the normal[1] ground state of liquid He^3 based on the method of correlated basis functions (CBF) is presented here. In CBF, we employ a trial basis

$$\Psi(|\mathbf{n})=\psi_0{}^B\Phi(|\mathbf{n}),$$
$$\mathbf{n}\equiv(123\cdots N)\equiv(\mathbf{k}_1\sigma_1,\mathbf{k}_2\sigma_2,\mathbf{k}_3\sigma_3,\cdots,\mathbf{k}_N\sigma_N). \quad (1)$$

$\psi_0{}^B$ is the so-called correlation factor, which in our case is taken to be the ground-state boson-type solution of the Schrödinger equation:

$$H\psi_0{}^B=E_0{}^B\psi_0{}^B,$$
$$H=\frac{-\hbar^2}{2M}\sum_{i=1}^{N}\Delta_i+\sum_{1\leqslant i<j\leqslant N}v(r_{ij}); \quad (2)$$

and the model functions $\Phi(|\mathbf{n})$ are Slater determinants suitable for describing states of a system of noninteracting fermions of mass 3. Our choice of the correlation factor is based on the belief that the correlations produced by the short-ranged repulsions depend little on the boundary conditions and type of permutation symmetry satisfied by the space part of the wave function. In a preliminary paper by Wu and Feenberg[2] (hereafter to be denoted by I), the diagonal matrix elements of the identity and the Hamiltonian operator, as well as the fermion radial distribution function, were calculated. The results were applied to establish a connection between known results for the fermion and the boson forms of a hard-sphere system at low density, and to work out properties of a hypothetical fermion He^4 system. In a second paper[3] (hereafter denoted by II), Feenberg and Woo reported the evaluation of diagonal and nondiagonal matrix elements of the interacting fermion system by a cluster-expansion technique. An orthonormal basis was constructed from $\Psi(|\mathbf{n})$ and used to express the Hamiltonian operator in quasiparticle form: a large diagonal component containing constant, linear, quadratic, and cubic terms in free-quasiparticle occupation-number operators and a nondiagonal component representing the residual interactions involved in collisions of two and three free quasiparticles. In this paper, we shall report the results of applying the method of CBF to the calculation of the ground-state properties of liquid He^3.

Section II summarizes the previous findings (Papers I and II) and recalls some results pertinent to the present application of the theory, and then discusses the convergence properties associated with the Löwdin orthogonalization procedure employed in II. In Sec. III the adaptation of the Rayleigh-Schrödinger perturbation method to a nonorthogonal basis is presented: we have, for practical reasons, chosen this procedure in preference to the more frequently used two-step procedure of successively diagonalizing 1 and H. Several means of classifying terms in this calculation are available; among them we single out one as being best suited for the study of liquid He^3. The ground-state energy and the equilibrium density are determined numerically in Sec. IV to the second order in the preferred classification scheme; so are the other ground-state properties: compressibility, velocity of sound, and paramagnetic susceptibility. Finally, these results are compared with experiment and with the Brueckner-Gammel theory.[4]

II. THE METHOD OF CORRELATED BASIS FUNCTIONS

The system of interest to us is liquid He^3 at zero temperature. The system is described as a set of N identical

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[1] By "normal" we mean that pairing effects in the Hamiltonian are not investigated. If the ground state of liquid He^3 turns out to be super, our theory should still yield a good approximate account of the properties of liquid He^3 at very low temperatures—slightly above the transition temperature which is definitely no higher than a few millidegrees.
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[3] E. Feenberg and C. W. Woo, Phys. Rev. **137**, A391 (1965).
[4] K. A. Brueckner and J. L. Gammel, Phys. Rev. **109**, 1040 (1958).

mass-3 fermions confined to a cubic volume Ω, N, and Ω approaching infinity while $\rho=N/\Omega$ remains constant. Periodic boundary conditions are prescribed so that the momentum is a discrete quantum number. Between each pair of particles, there exists a phenomenological interaction $v(r)$ which includes a strong, short-ranged repulsive component and a weak, attractive component. In fact, the form of the potential is taken to be of the Lennard-Jones 6–12 type,

$$v(r)=\epsilon^*\left[\left(\frac{r^*}{r}\right)^{12}-2\left(\frac{r^*}{r}\right)^{6}\right], \tag{3}$$

with the parameters ϵ^* and r^* determined by Massey[5] in a self-consistent calculation of the ground-state properties of liquid He^4. The problem that we are required to solve starts from the Schrödinger equation

$$H\psi^F=E\psi^F,$$
$$H=-\frac{\hbar^2}{2M}\sum_{i=1}^{N}\Delta_i+\sum_{1\leq i<j\leq N}v(r_{ij}). \tag{4}$$

ψ^F must be antisymmetric with respect to exchanging any two particles. In this paper we are interested only in the ground state $\psi_0{}^F$ corresponding to the lowest eigenvalue E_0 of Eq. (4) as a function of density and spin.

To solve Eq. (4) we choose the basis functions defined by Eqs. (1) and (2) and evaluate all matrix elements of the identity and the Hamiltonian operator in this representation. It turns out that all these matrix elements for the fermion system can be expressed in terms of the boson liquid structure function $S(k)$, which is obtainable from the Fourier transform of the boson radial distribution function $g_B(r)$:

$$S(k)=1+\rho\int e^{i\mathbf{k}\cdot\mathbf{r}}[g_B(r)-1]dv,$$
$$g_B(r_{12})=\frac{N(N-1)}{\rho^2}\int(\psi_0{}^B)^2dv_{34\cdots N}. \tag{5}$$

The essential advantage of our approach is then clear: the two-particle potential $v(r)$ is completely eliminated from the matrix elements, and all physical quantities are expressed in terms of $g_B(r)$ and $S(k)$. For further discussions on the choice of the correlation factor, see I and II and Refs. 6 and 7.

To express the fermion matrix elements in terms of $g_B(r)$ or $S(k)$, we employ a modification of the cluster-expansion technique well-known from classical statistical mechanics. Many authors[8,9] have studied such cluster expansion developments, of which two general types have emerged as useful for our purpose. In II we compared the two developments critically and decided in favor of the (noninvariant) formalism of Iwamoto and Yamada (IY) for application to the liquid He^3 problem. For the fermion radial distribution function generated by the ground-state configuration in $\Phi(|\mathbf{n})$ we found

$$g_F(r)=g_B(r)F(r),$$
$$F(r)=F^{(2)}(r)+F^{(3)}(r)+\cdots,$$
$$F^{(2)}(r)=1-\tfrac{1}{2}l^2(k_Fr),$$
$$F^{(3)}(r)=-\rho\int g_B(r')[g_B(|\mathbf{r}-\mathbf{r}'|)-1]l^2(k_Fr')dv'+\tfrac{1}{2}\rho l(k_Fr)\int g_B(r')[g_B(|\mathbf{r}-\mathbf{r}'|)-1]l(k_Fr')l(k_F|\mathbf{r}-\mathbf{r}'|)dv', \tag{6}$$

where

$$k_F=(3\pi^2\rho)^{1/3},\qquad l(x)=\frac{3}{x^3}(\sin x-x\cos x). \tag{7}$$

The asymptotic ($r\to\infty$) behavior of $F^{(2)}(r)$ and $F^{(3)}(r)$ is given by

$$F^{(2)}(r)\to 1-O\left(\frac{1}{r^4}\right),\qquad F^{(3)}(r)\to O\left(\frac{1}{r^4}\right),$$

hence $g_F(\infty)=g_B(\infty)=1$, with no term in $O(1/N)$.

Diagonal and nondiagonal matrix elements of the identity and the Hamiltonian operator are derived in I, Sec. II, and II, Secs. IV and VI. Only those equations needed in this paper are quoted here.

[5] W. E. Massey, Phys. Rev. Letters **12**, 719 (1964); Ph.D. thesis, Washington University, 1966 (unpublished).
[6] J. W. Clark and P. Westhaus, Phys. Rev. **141**, 833 (1966).
[7] C. W. Woo, Ph.D. thesis, Washington University, 1966 (unpublished).
[8] See Refs. 1–8 in II.
[9] F. Y. Wu, J. Math. Phys. 4, 1438 (1963).

Diagonal Matrix Elements

$$\{\mathbf{n}|1|\mathbf{n}\}=1, \qquad \{\mathbf{n}|H|\mathbf{n}\}\equiv E^{(0)}(\mathbf{n})=E_0{}^B+E_1{}^F+E_2{}^F+E_3{}^F+\cdots,$$

$$E_1{}^F=\frac{\hbar^2}{2M}\sum_{p=1}^{N}k_p{}^2,$$

$$E_2{}^F=\frac{\hbar^2}{2M}\sum_{m<n}X'_{mn}=\frac{\hbar^2}{2MN}\sum_{m<n}\langle mn,nm\rangle u(k_{mn})k_{mn}{}^2,$$

$$E_3{}^F=\frac{\hbar^2}{2M}\sum_{l<m<n}[X'_{lmn}-X'_{lm}X_{mn}-X_{lm}X'_{mn}-X'_{mn}X_{nl}-X_{mn}X'_{nl}-X'_{nl}X_{lm}-X_{nl}X'_{lm}]$$

$$=\frac{-3\hbar^2}{2MN^2}\sum_{l<m<n}\langle lmn,mnl\rangle S(k_{lm})u(k_{mn})u(k_{nl})k_{lm}{}^2, \tag{8}$$

where

$$\langle ab\cdots,lm\cdots\rangle=\langle a,l\rangle\langle b,m\rangle\cdots, \qquad \langle a,l\rangle=\delta(\sigma_a,\sigma_l), \qquad u(k)=S(k)-1, \tag{9}$$

and the X's and (X')'s are cluster integrals and derivatves evaluated in I and II. The notation $|\}$ carries the implication that our basis functions are normalized but not orthogonal. The simple bracket $|\rangle$ is reserved for an orthonormal basis.

Nondiagonal Matrix Elements

Given here are the working formulas for matrix elements whose initial and final states differ in 2 or 3 orbitals[10]:

$$\{123\cdots N|1|1'2'3\cdots N\}\cong\{12|1|1'2'\}$$
$$\approx X_{12;1'2'}+\sum_{n>2}[X_{12n;1'2'n}-\tfrac{1}{2}X_{12;1'2'}(X_{1n;1n}+X_{1'n;1'n}+X_{2n;2n}+X_{2'n;2'n})]+\cdots, \tag{10}$$

$$\{123\cdots N|H|1'2'3\cdots N\}\cong\{12|H|1'2'\}$$
$$\approx\frac{\hbar^2}{2M}\{X'_{12;1'2'}+\sum_{n>2}[X'_{12n;1'2'n}-\tfrac{1}{2}X'_{12;1'2'}(X_{1n;1n}+X_{1'n;1'n}+X_{2n;2n}+X_{2'n;2'n})$$
$$-\tfrac{1}{2}X_{12;1'2'}(X'_{1n;1n}+X'_{1'n;1'n}+X'_{2n;2n}+X'_{2'n;2'n})]+\cdots\}$$
$$+\{12|1|1'2'\}\{\tfrac{1}{2}E^{(0)}(123\cdots N)+\tfrac{1}{2}E^{(0)}(1'2'3\cdots N)\}, \tag{11}$$

$$\{1234\cdots N|1|1'2'3'4\cdots N\}\cong\{123|1|1'2'3'\}\approx X_{123;1'2'3'}+\cdots, \tag{12}$$

$$\{1234\cdots N|H|1'2'3'4\cdots N\}\cong\{123|H|1'2'3'\}$$
$$\approx\frac{\hbar^2}{2M}X'_{123;1'2'3'}+\cdots+\{123|1|1'2'3'\}\{\tfrac{1}{2}E^{(0)}(1234\cdots N)+\tfrac{1}{2}E^{(0)}(1'2'3'4\cdots N)\}, \tag{13}$$

$$X_{mn;mn}=\frac{-1}{N}\langle mn,nm\rangle u(k_{mn}), \tag{14}$$

$$X'_{mn;mn}=\frac{1}{N}\langle mn,nm\rangle u(k_{mn})\{k_m\star{}^2+k_n\star{}^2-2\mathbf{k}_m\cdot\mathbf{k}_n\}, \tag{15}$$

$$X_{mn;m'n'}=\frac{1}{N}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}-\mathbf{k}_m-\mathbf{k}_n)\{\langle mn,m'n'\rangle u(k_{mm'})-\langle mn,n'm'\rangle u(k_{mn'})\}, \tag{16}$$

$$X'_{mn;m'n'}=\frac{-1}{2N}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}-\mathbf{k}_m-\mathbf{k}_n)\{\langle mn,m'n'\rangle u(k_{mm'})[k_{mm'}{}^2+k_{nn'}{}^2]-\langle mn,n'm'\rangle u(k_{mn'})[k_{mn'}{}^2+k_{m'n}{}^2]\}, \tag{17}$$

[10] Note the difference between Eq. (19) here and Eq. (83) in II. The factors "$\frac{1}{2}$" associated with $k_n\star{}^2$, $k_p\star{}^2$, and $k_q\star{}^2$ in II were due to typographical errors.

$$X_{mnl;m'n'l}=\frac{-1}{N^2}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}-\mathbf{k}_m-\mathbf{k}_n)\{\langle lmn,n'm'l\rangle(ln',mm',nl)+\langle lmn,m'ln'\rangle(lm',ml,nn')$$
$$-\langle lmn,n'lm'\rangle(ln',ml,nm')-\langle lmn,m'n'l\rangle(lm',mn',nl)\}, \quad (18)$$

$$X'_{mnl;m'n'l}=\frac{1}{N^2}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}-\mathbf{k}_m-\mathbf{k}_n)$$
$$\times\{\langle lmn,n'm'l\rangle(ln',mm',nl)[k_l\star^2+k_m\star^2+k_n\star^2-\mathbf{k}_l\cdot\mathbf{k}_{n'}-\mathbf{k}_m\cdot\mathbf{k}_{m'}-\mathbf{k}_n\cdot\mathbf{k}_l]$$
$$+\langle lmn,m'ln'\rangle(lm',ml,nn')[k_l\star^2+k_m\star^2+k_n\star^2-\mathbf{k}_l\cdot\mathbf{k}_{m'}-\mathbf{k}_m\cdot\mathbf{k}_l-\mathbf{k}_n\cdot\mathbf{k}_{n'}]$$
$$-\langle lmn,n'lm'\rangle(ln',ml,nm')[k_l\star^2+k_m\star^2+k_n\star^2-\mathbf{k}_l\cdot\mathbf{k}_{n'}-\mathbf{k}_m\cdot\mathbf{k}_l-\mathbf{k}_n\cdot\mathbf{k}_{m'}]$$
$$-\langle lmn,m'n'l\rangle(lm',mn',nl)[k_l\star^2+k_m\star^2+k_n\star^2-\mathbf{k}_l\cdot\mathbf{k}_{m'}-\mathbf{k}_m\cdot\mathbf{k}_{n'}-\mathbf{k}_n\cdot\mathbf{k}_l]\}, \quad (19)$$

$$X_{mnl;m'n'l'}=\frac{1}{N^2}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}+\mathbf{k}_{l'}-\mathbf{k}_m-\mathbf{k}_n-\mathbf{k}_l)$$
$$\times\{\langle mnl,m'n'l'\rangle(mm',nn',ll')-\langle mnl,m'l'n'\rangle(mm',nl',ln')$$
$$-\langle mnl,l'n'm'\rangle(ml',nn',lm')-\langle mnl,n'm'l'\rangle(mn',nm',ll')$$
$$+\langle mnl,l'm'n'\rangle(ml',nm',ln')+\langle mnl,n'l'm'\rangle(mn',nl',lm')\}, \quad (20)$$

$$X'_{mnl;m'n'l'}=\frac{-1}{2N^2}\delta(\mathbf{k}_{m'}+\mathbf{k}_{n'}+\mathbf{k}_{l'}-\mathbf{k}_m-\mathbf{k}_n-\mathbf{k}_l)$$
$$\times\{\langle mnl,m'n'l'\rangle(mm',nn',ll')[k_{mm'}^2+k_{nn'}^2+k_{ll'}^2]-\langle mnl,m'l'n'\rangle(mm',nl',ln')[k_{mm'}^2+k_{nl'}^2+k_{ln'}^2]$$
$$-\langle mnl,l'n'm'\rangle(ml',nn',lm')[k_{ml'}^2+k_{nn'}^2+k_{lm'}^2]-\langle mnl,n'm'l'\rangle(mn',nm',ll')[k_{mn'}^2+k_{nm'}^2+k_{ll'}^2]$$
$$+\langle mnl,l'm'n'\rangle(ml',nm',ln')[k_{ml'}^2+k_{nm'}^2+k_{ln'}^2]+\langle mnl,n'l'm'\rangle(mn',nl',lm')[k_{mn'}^2+k_{nl'}^2+k_{lm'}^2]\}, \quad (21)$$

where

$$k_m\star^2\equiv\tfrac{1}{2}k_m^2+\tfrac{1}{2}k_{m'}^2, \qquad (mm',nn',ll')\equiv(k_{mm'},k_{nn'},k_{ll'}),$$
$$(k,k',k'')\equiv u(k)u(k')+u(k')u(k'')+u(k'')u(k)+u(k)u(k')u(k''). \quad (22)$$

Later in our selection of a scheme to classify terms in the perturbation calculation, some four-orbital-different elements are required. We shall introduce them when the need arises.

The diagonalization of 1 and H may follow a two-step procedure: first we transform to an orthonormal basis, and next apply a standard perturbation theory. The advantage of such a procedure is that a second-quantized or quasiparticle formalism may first be established as an intermediate stage, which then permits the employment of all modern perturbative tools. However, the choice of an orthogonalization procedure for our problem is quite limited. The only one that appears usable is the Löwdin transformation which gives rise to an explicit correction series to the Hamiltonian (Sec. V of II). We use the convenient notations

$$\{\mathbf{m}|1|\mathbf{n}\}\rightarrow\mathfrak{N}_{\mathbf{mn}}, \qquad \{\mathbf{m}|H|\mathbf{n}\}\rightarrow\mathfrak{K}_{\mathbf{mn}},$$

for matrix elements in the nonorthogonal representation and

$$\langle\mathbf{m}|1|\mathbf{n}\rangle\rightarrow N_{\mathbf{mn}}, \qquad \langle\mathbf{m}|H|\mathbf{n}\rangle\rightarrow H_{\mathbf{mn}},$$

in the orthogonal representation, and separate the matrices $\mathfrak{N}$ and $\mathfrak{K}$ each into two parts, thus:

$$\mathfrak{N}_{\mathbf{mn}}=\mathcal{G}_{\mathbf{mn}}+\mathcal{J}_{\mathbf{mn}}=\delta_{\mathbf{mn}}+\mathcal{J}_{\mathbf{mn}}, \quad (23)$$
$$\mathfrak{K}_{\mathbf{mn}}=\mathcal{W}_{\mathbf{mn}}+\tfrac{1}{2}\mathfrak{N}_{\mathbf{mn}}[E^{(0)}(\mathbf{m})+E^{(0)}(\mathbf{n})]. \quad (24)$$

Comparison of Eqs. (23)–(24) with Eqs. (8)–(13) identifies $\mathcal{G}$ and $\mathcal{W}$. It is clear that they have no nonzero diagonal elements. An extension of the work in II leads to

$$H_{\mathbf{mn}}=E^{(0)}(\mathbf{m})\delta_{\mathbf{mn}}+\mathcal{W}_{\mathbf{mn}}-\tfrac{1}{2}\sum_{\mathbf{p}}[\mathcal{W}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pn}}+\mathcal{J}_{\mathbf{mp}}\mathcal{W}_{\mathbf{pn}}]+\tfrac{1}{8}\sum_{\mathbf{p}}\mathcal{J}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pn}}[E^{(0)}(\mathbf{m})+E^{(0)}(\mathbf{n})-2E^{(0)}(\mathbf{p})]$$
$$+\tfrac{1}{8}\sum_{\mathbf{p},\mathbf{q}}[3\mathcal{W}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qn}}+2\mathcal{J}_{\mathbf{mp}}\mathcal{W}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qn}}+3\mathcal{J}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{W}_{\mathbf{qn}}]+\tfrac{1}{8}\sum_{\mathbf{p},\mathbf{q}}\mathcal{J}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qn}}[E^{(0)}(\mathbf{p})+E^{(0)}(\mathbf{q})-E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{n})]$$
$$-\tfrac{1}{16}\sum_{\mathbf{p},\mathbf{q},\mathbf{r}}[5\mathcal{W}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qr}}\mathcal{J}_{\mathbf{rn}}+3\mathcal{J}_{\mathbf{mp}}\mathcal{W}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qr}}\mathcal{J}_{\mathbf{rn}}+3\mathcal{J}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{W}_{\mathbf{qr}}\mathcal{J}_{\mathbf{rn}}+5\mathcal{J}_{\mathbf{mp}}\mathcal{J}_{\mathbf{pq}}\mathcal{J}_{\mathbf{qr}}\mathcal{W}_{\mathbf{rn}}]+\cdots. \quad (25)$$

If the nondiagonal part of H is to be considered as a perturbation, its elements must have the correct dependence on N. For example, for $|\mathbf{m}\rangle$ differing in 2 orbitals from the ground state $|\mathbf{0}\rangle$, $H_{0\mathrm{m}}$ must be proportional to N^{-1} so that the second-order correction to the energy becomes proportional to N:

$$\Delta E^{(2)}(\mathbf{0})=\sum_{\mathrm{m}\neq 0}\frac{H_{0\mathrm{m}}{}^2}{H_{00}-H_{\mathrm{mm}}}$$

$$\approx\sum_{(12|1'2')}\frac{\langle 12|H|1'2'\rangle^2}{E^{(1)}(123\cdots N)-E^{(1)}(1'2'3\cdots N)}=O(N). \tag{26}$$

In Eq. (26), $E^{(1)}(\mathbf{0})\equiv H_{00}$ denotes $E^{(0)}(\mathbf{0})$ plus the orthogonalization correction, and the symbol $(12|1'2')$ on the summation means 1, 2 ranging over the ground-state configuration and 1′, 2′ ranging outside the ground-state configuration. This requirement of a correct dependence on N constitutes the first convergence property of the Löwdin transformation that we investigated.

Upon careful term-by-term investigation of Eq. (25) by a diagrammatic technique, we noticed anomalously high N dependences coming from two sources: (1) terms with reducible vertices ($\mathcal{G}$ or $\mathcal{W}$), and (2) terms with unlinked parts. For $|\mathbf{m}\rangle$ and $|\mathbf{0}\rangle$ differing in two orbitals, we cite as an example of (1) the diagram in Fig. 1, representing the term $\sum_{\mathrm{p}}\mathcal{W}_{0\mathrm{p}}\mathcal{G}_{\mathrm{pm}}$ where $|\mathbf{p}\}$ differs from $|\mathbf{m}\}$ in 4 orbitals and from $|\mathbf{0}\}$ in two orbitals. Part of the 4-orbital-different $\mathcal{G}$ vertex is reducible into a sum of products of two 2-orbital-different $\mathcal{G}$ vertices. One of these, $\{12|\mathcal{G}|1'2'\}\{\alpha\beta|\mathcal{G}|34\}$ as indicated by the dashed line in the diagram, is responsible for the N dependence anomaly: from Eqs. (10)–(21) we obtain

$$\{12|\mathcal{G}|1'2'\}\{\alpha\beta|\mathcal{G}|34\}\{\alpha\beta|\mathcal{W}|34\}=O\left(\frac{1}{N^3}\right);$$

summation over the indices 3, 4, α, and β under the constraint

$$\mathbf{k}_\alpha+\mathbf{k}_\beta=\mathbf{k}_3+\mathbf{k}_4$$

then results in $\sum_{\mathrm{p}}\mathcal{W}_{0\mathrm{p}}\mathcal{G}_{\mathrm{pm}}=O(N^0)$, not $O(N^{-1})$ as required. As an example of (2), we cite the diagram in Fig. 2, representing the term $\sum_{\mathrm{p,q}}\mathcal{W}_{0\mathrm{p}}\mathcal{G}_{\mathrm{pq}}\mathcal{G}_{\mathrm{qm}}$. The analysis is straightforward in this case. Using the cluster-ordering scheme of Clark and Westhaus,[6] we were able to verify in several lowest orders that these anomalous N dependences cancel exactly, terms of type (2) canceling those of type (1). The crux of the verification lies in the reduction of the reducible many-orbital vertices. We are currently working on a general proof. The details of the verification will therefore be postponed till a later paper.[7] It is sufficient to remark here that there is a certain resemblance between the anomaly here and that discovered by Brueckner in the Rayleigh-Schrödinger (RS) perturbation theory. As in the latter case, the apparent anomalous N dependences in the Löwdin transformation must be spurious (complete internal cancellation of anomalous terms).

A second convergence property of the Löwdin transformation is the more practical one involving the rate of convergence of the cluster expansion. We return to

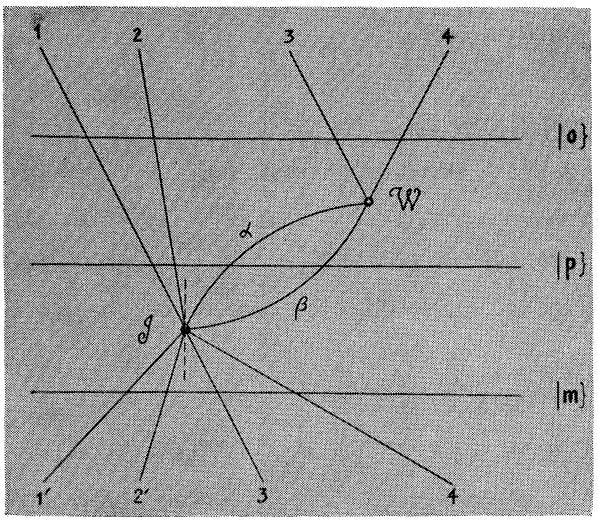

FIG. 1. A typical diagram with a reducible vertex.

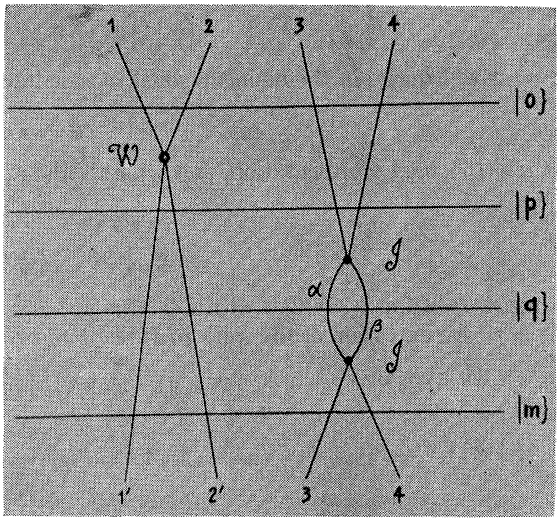

FIG. 2. A typical diagram with unlinked parts.

Eq. (25) and examine the truncated series for H_{00}.

$$E^{(1)}(\mathbf{0})\equiv H_{00}$$
$$\approx E^{(0)}(\mathbf{0})-\{\sum_{\mathbf{p}} \mathcal{W}_{0\mathbf{p}}\mathcal{G}_{\mathbf{p}0}-\tfrac{1}{4}\sum_{\mathbf{p}} \mathcal{G}_{0\mathbf{p}}{}^2[E^{(0)}(\mathbf{0})-E^{(0)}(\mathbf{p})]\}$$
$$\approx E^{(0)}(\mathbf{0})+\Delta E_{0R}(\mathbf{0}), \tag{27}$$
$$\Delta E_{0R}(\mathbf{0})=-\sum_{(12|1'2')}\left[\frac{\hbar^2}{2M}X_{12;1'2'}X'_{12;1'2'}+\frac{E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N)}{4}X_{12;1'2'}{}^2\right]. \tag{28}$$

At $\rho=0.0140$ Å^{-3} (see Appendices A and B), numerical calculations on a computer yielded

$$\frac{E^{(0)}(\mathbf{0})}{N}=\frac{1}{N}\{E_0{}^B+E_1{}^F(\mathbf{0})+E_2{}^F(\mathbf{0})+E_3{}^F(\mathbf{0})+\cdots\}$$
$$=\{-2.843+2.686-0.756-0.127+\cdots\}°\mathrm{K}\approx-1.040°\mathrm{K}, \tag{29}$$
$$\frac{\Delta E_{0R}(\mathbf{0})}{N}\approx 1.9°\mathrm{K}$$

Thus the orthogonality energy correction appears to be too large (by an order of magnitude) to form part of a sensibly convergent perturbation series. There are indications that $\Delta E_{0R}(\mathbf{0})/N$ will be lowered by the inclusion of higher order cluster integrals, but the accurate evaluation of these requires an excessive amount of computer time. This prevents a complete evaluation of the Löwdin transformation in our problem. Fortunately, the orthogonalization of the basis is not required for the study of the ground state. In the next section we return to the nonorthogonal basis and discuss an alternative, one-step procedure for computing the energy correction generated by nondiagonal elements in $\mathfrak{N}$ and $\mathfrak{IC}$.

III. RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY AND THE CLASSIFICATION OF TERMS

We have the Hamiltonian matrix and the identity matrix in a representation of nonorthogonal correlated basis functions. The matrix elements are denoted, respectively, by $\mathfrak{IC}_{\mathbf{mn}}$ and $\mathfrak{N}_{\mathbf{mn}}$. The set of basis states $|\mathbf{n}\}$ are all normalized, and each involves a Slater determinant specifying N occupied orbitals. One of these states, $|\mathbf{0}\}$, is associated with a filled Fermi sea and thus has the lowest energy expectation value (for any value of the total spin, not necessarily zero). This we identify as the unperturbed ground state (for the given total spin). Taking the diagonal part of $\mathfrak{IC}$ as the conventional unperturbed Hamiltonian, we have the unperturbed ground-state energy

$$E^{(0)}(\mathbf{0})=\mathfrak{IC}_{\mathbf{00}}\equiv\{\mathbf{0}|H|\mathbf{0}\}. \tag{30}$$

For a derivation of the Rayleigh-Schrödinger perturbation theory using a nonorthogonal basis, see for example Ref. 11. It must be emphasized that for any extended system such a derivation is purely formal. Complete justification for an extended system requires the adaptation to a nonorthogonal basis of the Goldstone-Dyson procedures in deriving the unlinked Schrödinger-type perturbation formalism. The resulting Rayleigh-Schrödinger energy series is given by

$$E-E^{(0)}(\mathbf{0})=-\mu^2\sum_{m>0}\frac{\mathcal{U}_{0\mathbf{m}}\mathcal{U}_{\mathbf{m}0}}{\mathcal{U}_{\mathbf{mm}}}+\mu^3\sum_{\substack{m,n>0\\ \mathbf{m}\neq\mathbf{n}}}\frac{\mathcal{U}_{0\mathbf{m}}\mathcal{U}_{\mathbf{mn}}\mathcal{U}_{\mathbf{n}0}}{\mathcal{U}_{\mathbf{mm}}\mathcal{U}_{\mathbf{nn}}}+\cdots, \tag{31}$$
$$\mathcal{U}_{\mathbf{mn}}=\mathfrak{IC}_{\mathbf{mn}}-E^{(0)}(\mathbf{0})\mathfrak{N}_{\mathbf{mn}}. \tag{32}$$

μ is an expansion parameter attached on to the "perturbation" $\mathcal{U}_{\mathbf{mn}}$; it is a measure of the nondiagonal matrix elements of *both* the Hamiltonian and the identity. An obvious requirement for the convergence of Eq. (31) is

$$\left|N\frac{\mathcal{U}_{\mathbf{mn}}}{\mathcal{U}_{\mathbf{mm}}}\right|\ll 1, \quad \mathbf{m}\neq\mathbf{n}. \tag{33}$$

It is, however, difficult to predict how well this condition is satisfied. We are then forced to judge the convergence of the series by numerical results.

Rewriting Eqs. (30)–(32) explicitly and letting $\mu\to 1$,

[11] J. W. Clark and E. Feenberg, Phys. Rev. **113**, 388 (1959); J. W. Clark, Ph.D. thesis, Washington University, 1959 (unpublished).

we have

$$
\begin{aligned}
&E=E^{(0)}(\mathbf{0})+\Delta E^{(1)}(\mathbf{0})+\Delta E^{(2)}(\mathbf{0})+\Delta E^{(3)}(\mathbf{0})+\cdots,\\
&E^{(0)}(\mathbf{0})=E_0{}^B+E_1{}^F(\mathbf{0})+E_2{}^F(\mathbf{0})+E_3{}^F(\mathbf{0})+\cdots,\\
&\Delta E^{(1)}(\mathbf{0})=0,\\
&\Delta E^{(2)}(\mathbf{0})=-\sum_{m>0}\frac{\mathcal{V}_{0\mathbf{m}}\mathcal{V}_{0\mathbf{m}}}{\mathcal{V}_{\mathbf{mm}}}=-\sum_{m>0}\frac{\{\mathcal{W}_{0\mathbf{m}}+\frac{1}{2}\mathcal{J}_{0\mathbf{m}}[E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{0})]\}^2}{E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{0})},\\
&\Delta E^{(3)}(\mathbf{0})=\sum_{\substack{m,n>0;\\ \mathbf{m}\neq\mathbf{n}}}\frac{\mathcal{V}_{0\mathbf{m}}\mathcal{V}_{\mathbf{mn}}\mathcal{V}_{\mathbf{n}0}}{\mathcal{V}_{\mathbf{mm}}\mathcal{V}_{\mathbf{nn}}}\\
&\qquad=\sum_{\substack{m,n>0;\\ \mathbf{m}\neq\mathbf{n}}}\left[\frac{\{\mathcal{W}_{0\mathbf{m}}+\frac{1}{2}\mathcal{J}_{0\mathbf{m}}[E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{0})]\}\{\mathcal{W}_{\mathbf{mn}}+\frac{1}{2}\mathcal{J}_{\mathbf{mn}}[E^{(0)}(\mathbf{m})+E^{(0)}(\mathbf{n})-2E^{(0)}(\mathbf{0})]\}\times\{\mathcal{W}_{\mathbf{n}0}+\frac{1}{2}\mathcal{J}_{\mathbf{n}0}[E^{(0)}(\mathbf{n})-E^{(0)}(\mathbf{0})]\}}{[E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{0})][E^{(0)}(\mathbf{n})-E^{(0)}(\mathbf{0})]}\right].
\end{aligned}
\tag{34}
$$

A scheme must be devised to classify terms in this series. It is most desirable to use a single expansion parameter, but such a parameter does not always exist. Clark and Westhaus (CW, an extension of the IY development) used the Bijl-Dingle-Jastrow form of the correlation factor $\prod_{1\leq i<j\leq N} f(r_{ij})$ and defined a cluster-ordering parameter

$$
\frac{N\omega}{\Omega}=\frac{N}{\Omega}\int\eta(r)dv,\qquad \eta(r)=f^2(r)-1. \tag{35}
$$

The order of an expression is given simply by the number of independent $\eta(r)$ factors. This results in an apparently satisfactory classification scheme for studying nuclear matter. For liquid He^3 in our development, we first tried the correspondence[12] $(N-1/N)f^2(r)\rightarrow g_B(r)$ and classified our terms by counting the number of independent $[g_B(r)-1]$ factors. Such a classification scheme is, however, unsuitable. To see this it is sufficient to investigate the convergence properties of the fermion radial distribution function $g_F(r)$ and the unperturbed ground-state energy $E^{(0)}(\mathbf{0})$.

An essential characteristic of the CW classification scheme resides in a peculiarity of the 4-orbital-different (or, more conveniently, the 4-index) contribution. Part of the 4-index contribution contains in its structure an "internal momentum conservation" condition[6,13] which restricts the orbital labels by introducing a Kronecker delta in place of a $[g_B(r)-1]$ factor. This part is then of the same ω order as the 3-index contribution and must be included with the latter in a truncated cluster expansion series. Thus, for $g_F(r)$ we have instead of Eq. (6),

$$
\begin{aligned}
F(r)&=\{F^{(2)}(r)\}+\{F^{(3)}(r)+\bar{F}^{(4)}(r)\}\\
&\quad+\{[F^{(4)}(r)-\bar{F}^{(4)}(r)]+\cdots\}+\cdots,\\
\bar{F}^{(4)}(r)&=\tfrac{1}{2}\rho\int[g_B(|\mathbf{r}-\mathbf{r}'|)-1]l^2(k_Fr')dv'.
\end{aligned}
\tag{36}
$$

In II we tested the rate of convergence by calculating the fermion liquid structure function at $k=0$: $S_F(0)$. The normalization condition for $g_F(r)$ requires

$$
S_F(0)=1+\rho\int[g_F(r)-1]dv=0. \tag{37}
$$

With Eq. (6), Eq. (37) is equivalent to requiring

$$
\begin{aligned}
&0=S_F(0)\approx S(0)+\Delta^{(2)}S_F(0)+\Delta^{(3)}S_F(0),\\
&S(0)=1+\rho\int[g_B(r)-1]dv=0,\\
&\Delta^{(2)}S_F(0)=\rho\int g_B(r)[F^{(2)}(r)-1]dv,\\
&\Delta^{(3)}S_F(0)=\rho\int g_B(r)F^{(3)}(r)dv.
\end{aligned}
\tag{38}
$$

The deviation of $S_F(0)$ from zero was computed. With the inclusion of $\bar{F}^{(4)}(r)$, Eq. (38) is replaced by

$$
\begin{aligned}
&0=S_F(0)\approx S(0)+\Delta^{(2)}S_F(0)\\
&\qquad+\{\Delta^{(3)}S_F(0)+\Delta^{(4)}\bar{S}_F(0)\},\\
&\Delta^{(4)}\bar{S}_F(0)=\rho\int g_B(r)\bar{F}^{(4)}(r)dv.
\end{aligned}
\tag{39}
$$

For a rough estimate, we continued the use of the $g_B(r)$ for a mass-4 system as specified in Appendix C of II,

[12] This correspondence can be seen from a comparison of our cluster integrals with those derived by IY or CW. It is exact for X_{mn}, X'_{mn}, X'_{lmn}, X_{klmn}, and $X'_{klmn'}$ but not for X_{lmn}.

[13] F. Iwamoto and M. Yamada, Progr. Theoret. Phys. (Kyoto) **17**, 543 (1956); **18**, 345 (1957).

where it was obtained with the truncated form of $S_F(0)$ in Eq. (38)

$$S_F(0)\approx 0-0.542+0.697=0.155. \quad (40)$$

The present, reordered Eq. (39) gave

$$S_F(0)\approx 0-0.542+(0.697-0.631)=-0.476. \quad (41)$$

While Eq. (40) does not give us a very good normalization and has little to say about the rate of convergence, Eq. (41) is certainly unacceptable. It will be seen presently that the omitted part of $\Delta^{(4)}S_F(0)$ is of the same order of magnitude as $\Delta^{(4)}{}_F\bar{S}(0)$. We believe that it is of the opposite sign, so that the two parts grouped together yield a small, negative total $\Delta^{(4)}S_F(0)$ which tends to improve Eq. (40).

Turning next to $E^{(0)}(\mathbf{0})$, the CW classification scheme replaces the truncated form

$$E^{(0)}(\mathbf{0})\approx E_0{}^B+E_1{}^F(\mathbf{0})+E_2{}^F(\mathbf{0})+E_3{}^F(\mathbf{0}) \quad (42)$$

by

$$E^{(0)}(0)\approx E_0{}^B+E_1{}^F(\mathbf{0})+E_2{}^F(\mathbf{0})+[E_3{}^F(\mathbf{0})+\bar{E}_4{}^F(\mathbf{0})], \quad (43)$$

$$\bar{E}_4{}^F(\mathbf{0})=\frac{\hbar^2}{2M}\sum_{klmn}\frac{1}{24}\bar{X}'_{klmn}$$

$$=\frac{-\hbar^2}{MN^2}\sum_{\mathbf{k}_k,\mathbf{k}_l,\mathbf{k}_m,\mathbf{k}_n}\delta(\mathbf{k}_k+\mathbf{k}_m-\mathbf{k}_l-\mathbf{k}_n)u(k_{mn})$$

$$\times\{u(k_{mn})-\tfrac{1}{2}u(k_{kn})\}k_{mn}{}^2. \quad (44)$$

Using the $g_B(r)$ for a mass-3 system as specified in Appendix A, at $\rho=0.0148$ Å^{-3}, we obtain with Eq. (42),

$$E^{(0)}(\mathbf{0})\approx N\{-2.874+2.788-0.804-0.132\}^\circ\mathrm{K}$$

$$=-(1.022^\circ\mathrm{K})N, \quad (45)$$

and with Eqs. (43) and (44),

$$E^{(0)}(\mathbf{0})\approx N\{-2.874+2.788-0.804$$

$$-[0.132+0.064]\}^\circ\mathrm{K}=-(1.086^\circ\mathrm{K})N. \quad (46)$$

Details of this calculation are given in Appendix B. In Eq. (45) the convergence is excellent; in Eq. (46) it is acceptable but obviously not as good. A more significant point is that $|\bar{E}_4{}^F(\mathbf{0})|$ is smaller than $|E_3{}^F(\mathbf{0})|$ by a factor of 2, whereas we expect $|E_4{}^F(\mathbf{0})|$ to be small compared to $|E_3{}^F(\mathbf{0})|$ by a much larger factor if the cluster expansion is convergent in a natural fashion. It is more likely that the omitted part, $[E_4{}^F(\mathbf{0})-\bar{E}_4{}^F(\mathbf{0})]$, is actually comparable in size to $\bar{E}_4{}^F(\mathbf{0})$ but of the opposite sign, so that there is a near cancellation between the two parts of $E_4{}^F(\mathbf{0})$. This conjecture could be tested by numerical evaluation of $[E_4{}^F(\mathbf{0})-\bar{E}_4{}^F(\mathbf{0})]$ which requires an extensive machine calculation that we have not attempted. *Note added in proof.* The author is grateful to Dr. F. Y. Wu for pointing out an error in the evaluation of $\bar{E}_4{}^F(\mathbf{0})$, and for providing the correct results now appearing in Eqs. (46) and (B3).

The physical reason that we distrust $N\omega/\Omega$, Eq. (35), as an ordering parameter for liquid He³ is that it is by definition a measure of the correlation volume against the specific volume, and for liquid He³ this ratio is practically unity. Thus, $[\Delta^{(4)}S_F(0)-\Delta^{(4)}\bar{S}_F(0)]$ and $[E_4{}^F(\mathbf{0})-\bar{E}_4{}^F(\mathbf{0})]$ are expected to be of the same order of magnitude as $\Delta^{(4)}\bar{S}_F(0)$ and $\bar{E}_4{}^F(\mathbf{0})$, though one order higher in ω.

A second classification scheme which we investigated next is based on the fact that

$$|u(k)|\equiv|S(k)-1|\leqslant 1. \quad (47)$$

In the range $0\leqslant k\leqslant 2k_F$, $u(k)$ averages to about -0.66. For $k\geqslant 2k_F$, $|u(k)|<0.15$. For each term to be classified, we count the number of independent $u(k)$ factors. Like the CW classification, this scheme is not always reliable. In fact there is some connection between these two schemes: compare

$$u(k)\equiv S(k)-1$$

$$=\rho\int e^{i\mathbf{k}\cdot\mathbf{r}}[g_B(r)-1)]dv$$

$$\to\frac{N}{\Omega}\int e^{i\mathbf{k}\cdot\mathbf{r}}\left[\frac{N-1}{N}f^2(r)-1\right]dv$$

$$\approx\frac{N}{\Omega}\int e^{i\mathbf{k}\cdot\mathbf{r}}[f^2(r)-1]dv$$

to $N\omega/\Omega$, Eq. (35). Numerical results similar to those discussed in connection with the ω ordering caused us to reject this scheme as well.

The classification scheme that we finally employed is the direct and natural one of using two expansion parameters. μ classifies the perturbation order and the index number subclassifies the cluster order. In the calculation of the ground-state energy, Eq. (34), the zeroth-order term is $E^{(0)}(\mathbf{0})$, which we calculate as accurately as possible, including terms up to all 3-index contributions. The first-order correction is zero. The second-order correction is given by $\Delta E^{(2)}(\mathbf{0})$. Including all 2-index contributions and no more, it reads

$$\Delta E^{(2)}(\mathbf{0})\approx-\sum_{(12|1'2')}\left\{\frac{E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N)}{4}X_{12;1'2'}{}^2+\frac{\hbar^2}{2M}X_{12;1'2'}X'_{12;1'2'}\right.$$

$$\left.+\frac{(\hbar^2/2M)^2}{E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N)}X'_{12;1'2'}{}^2\right\}, \quad (48)$$

$$E^{(0)}(\mathbf{m})-E^{(0)}(\mathbf{0})\approx\{E_0{}^B+E_1{}^F(\mathbf{m})+E_2{}^F(\mathbf{m})\}-\{E_0{}^B+E_1{}^F(\mathbf{0})+E_2{}^F(\mathbf{0})\}. \quad (49)$$

Judging from the speed at which the $E^{(0)}(\mathbf{0})$ series converges and the way $F(r)$ converges (Appendix C), we conclude that the 3-index contributions are sufficiently small so that Eqs. (48) and (49) give a good estimate of $\Delta E^{(2)}(\mathbf{0})$, which is itself small compared to $E^{(0)}(\mathbf{0})$. These 3-index contributions, as well as corrections higher than the second order, are omitted because they involve integrals too complex for actual evaluation.

This section is concluded by making the observation that the two-step procedure of diagonalizing 1 and H successively (Löwdin transformation+ordinary RS perturbation using the orthogonalized basis) would lead, at least in the second order up to 3-index contributions and in the third order up to 2-index contributions which we have checked, to precisely the same results as the one-step procedure outlined in this section. In the second order up to 2-index contributions, the corrections in the two steps are given, respectively, by

$$\Delta E_{0R}{}^{(2)}(\mathbf{0})\approx-\sum_{(12|1'2')}\left\{\frac{E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N)}{4}X_{12;1'2'}{}^2+\frac{\hbar^2}{2M}X_{12;1'2'}X'_{12;1'2'}\right\}, \tag{50}$$

and

$$\Delta E_{RS}{}^{(2)}(\mathbf{0})\approx-\sum_{(12|1'2')}\frac{(\hbar^2/2M)^2}{E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N)}X'_{12;1'2'}{}^2. \tag{51}$$

Compare Eq. (48) with Eqs. (50) and (51). It is as if we had here obtained $\Delta E^{(2)}(\mathbf{0})$, Eq. (48), by first truncating the Löwdin series long before any kind of convergence has been reached (shown numerically in Sec. II), and then turning immediately to the truncation of the (ordinary) RS series, which in all likelihood converges at an equally slow rate as the Löwdin series. In our one-step procedure such arbitrariness is avoided. The situation appears to be that the Löwdin transformation produces a strong shift in the Hamiltonian matrix away from the diagonal form. A large (unphysical) change in the diagonal matrix elements (the orthogonality correction) must then be compensated by a large change of opposite sign given by the second-order RS energy correction. That either change has been computed accurately is doubtful. On the other hand, the one-step calculation avoids the artificial resolution of a small effect into two large effects of opposite sign and yields an encouragingly small energy shift.

IV. RESULTS AND DISCUSSIONS

Figure 3 shows the fermion radial distribution function $g_F(r)$ as compared to $g_B(r)$[5] for a mass-3 system.

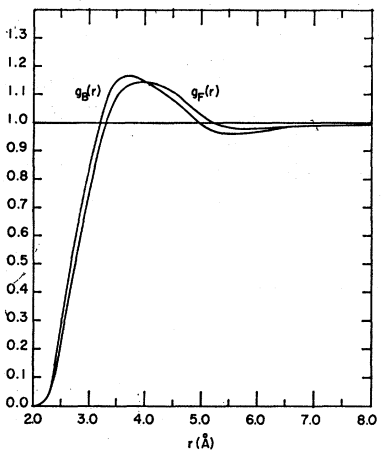

FIG. 3. The boson and fermion radial distribution functions.

There is as yet no experimental result for comparison with $g_F(r)$. Qualitatively, $g_F(r)$ shows a somewhat diminished peak and a slight shift toward larger r as compared with $g_B(r)$, consistent with the requirement of extra repulsion imposed upon a system of fermions by the Pauli principle. Quantitatively, $g_F(r)$ must be offered as a prediction. It is understood that scattering experiments measuring $S_F(k)$, thus indirectly $g_F(r)$, will soon be under way at several laboratories. Appendix C gives the essential intermediate details leading to our results.

All other ground-state properties are based on our second-order perturbative calculation using Eqs. (34) and (48). The only other device required is the so-called quadratic approximation of $S(k)$, as explained in Appendix B. The properties computed are (1) equilibrium density and ground-state energy per particle, (2) compressibility and velocity of sound, and (3) paramagnetic susceptibility. Table I gives the known experimental results, the theoretical results of Brueckner and Gammel, and our results using two different methods of analysis.

A. Equilibrium Density and Ground-State Energy per Particle

The boson energy $E_0{}^B$ and radial distribution function $g_B(r)$ for a range of densities ρ were made available to us by Massey.[5] Table II shows the fermion energy

TABLE I. Our numerical results compared with experiment and the Brueckner-Gammel calculation.

Ground-state properties[a]	Experiment	The B-G theory	Our results	Linear estimates
ρ_0	0.0164	0.0136	0.0148	fitted
$E(\mathbf{0})/N$	−2.52	−0.96	−1.35	fitted
K_0	3.8	5.3	9.9	3.6
C_0	180	169	117	184
χ/χ_F	11.1	(12)	(13.9)	···

[a] ρ_0 denotes the equilibrium density in Å^{-3}, $E(\mathbf{0})/N$ the ground-state energy per particle in °K, K_0 the compressibility in %/atm, c_0 the velocity of sound in m/sec, and χ/χ_F the paramagnetic susceptibility in terms of the ideal fermion value χ_F.

TABLE II. $E^{(0)}(\mathbf{0})$, $\Delta E^{(2)}(\mathbf{0})$, and $E(\mathbf{0})$ [energy unit: (°K)N.].

ρ(Å^{-3})	e_F	$E_0{}^B$	$E_1{}^F(\mathbf{0})$	$E_2{}^F(\mathbf{0})$	$E_3{}^F(\mathbf{0})$	$E^{(0)}(\mathbf{0})$	$\Delta E^{(2)}(\mathbf{0})$	$E(\mathbf{0})$
0.0132	4.305	−2.802	2.583	−0.702	−0.121	−1.042	−0.282	−1.324
0.0140	4.477	−2.845	2.686	−0.753	−0.127	−1.039	−0.303	−1.342
0.0148	4.647	−2.874	2.788	−0.804	−0.132	−1.022	−0.327	−1.349
0.0156	4.812	−2.885	2.887	−0.855	−0.137	−0.990	−0.351	−1.341
0.0164	4.976	−2.877	2.986	−0.905	−0.141	−0.937	−0.375	−1.312

$E(\mathbf{0})\approx E^{(0)}(\mathbf{0})+\Delta E^{(2)}(\mathbf{0})$ for several values of ρ, as calculated in our second-order theory using Eqs. (34) and (48). The calculation of $E_3{}^F(\mathbf{0})$ in $E^{(0)}(\mathbf{0})$ required the use of the quadratic approximation described in Appendix B. It is seen from Table II that the cluster-expansion leading to $E^{(0)}(\mathbf{0})$ converges quite well for all densities. The calculation of $\Delta E^{(2)}(\mathbf{0})$ made use of a geometrical construction. A detailed description appears in Appendix D. Note that $\Delta E^{(2)}(\mathbf{0})$ is smaller than $E^{(0)}(\mathbf{0})$ by a factor of about 3, indicating that the convergence is sufficiently rapid to make the second-order perturbation theory meaningful.

The results in Table II are plotted in Fig. 4, which we use as an aid to locate the minimum. The smooth curve fitted to the data shows that the minimum falls at

$$\rho_0=\text{equilibrium density}\approx 0.0148\ \text{Å}^{-3}, \tag{52}$$

$$E(\mathbf{0})/N=\text{ground-state energy per particle}\approx -1.35°\text{K}. \tag{53}$$

These values, in particular $E(\mathbf{0})/N$, do not agree too well with experiment. We suggest that the disagreement has its source in the critical nature of the boson calculation. The inadequacy results from using (1) an approximate trial function and (2) the Kirkwood superposition approximation in computing the expectation value of H. Massey believes that source (1) is by far the dominating factor, causing the energy estimate to be higher than would result from an exact calculation. All these errors are actually small, but not at all negligible since $E_0{}^B$ results from a critical balance of $\langle T\rangle$ and $\langle V\rangle$. For example, at $\rho=\rho_0=0.0148$ Å^{-3}, $\langle T\rangle/N=11.764$°K, $\langle V\rangle/N=-14.638$°K, $E_0{}^B/N=-2.874$°K. Thus a mere 7% decrease in $\langle T\rangle/N$ or $\langle V\rangle/N$ would lower $E_0{}^B/N$ by 1°K (or 35%). This critical balance is even more significant at higher densities (where $\langle T\rangle$ gradually catches up with $\langle V\rangle$ and eventually surpasses it), which means than an even smaller correction than 7% would be sufficient to account for our disagreement with experiment at the correct density 0.0164 Å^{-3}.

TABLE III. Compressibility and velocity of sound.

ρ(Å^{-3})	K(%/atom)	c(m/sec)
0.0132	27.93	74.1
0.0140	17.80	90.2
0.0148	9.94	117.4
0.0156	5.52	153.4
0.0164	3.19	196.8

Returning again to Table I, our density and energy values appear to be improved over those of Brueckner and Gammel[4] (BG), which prior to our calculation was the only first-principle theory[14] of liquid He³ in existence. This observation may however be misleading. As shown in Appendix A, the two-particle potential determined by Massey is different from that used by Brueckner and Gammel. Without an extensive recalculation it is impossible to estimate how a change of potential from that of Massey to that of BG would affect our results.

B. Compressibility and Velocity of Sound

The pressure of the liquid is given by

$$P(\rho)=\rho^2\frac{d[E(\mathbf{0};\rho)/N]}{d\rho}. \tag{54}$$

The compressibility and the velocity of sound are, respectively,

$$K(\rho)=\left(\rho\frac{dP}{d\rho}\right)^{-1}=\left\{2\rho^2\frac{d[E(\mathbf{0};\rho)/N]}{d\rho}+\rho^3\frac{d^2[E(\mathbf{0};\rho)/N]}{d\rho^2}\right\}^{-1} \tag{55}$$

and

$$c(\rho)=\left(\frac{1}{M\rho K(\rho)}\right)^{1/2}. \tag{56}$$

Table III shows $K(\rho)$ and $c(\rho)$ at various densities.

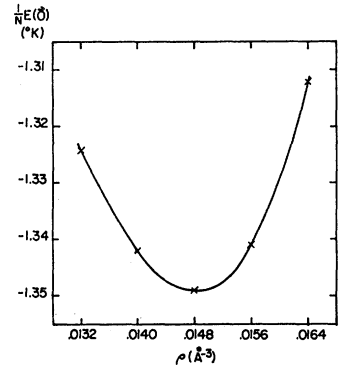

FIG 4. The energy-density curve.

[14] By a first-principle theory we mean one that starts from a Schrödinger equation with an assumed (in most cases phenomenological) interatomic potential.

At the calculated equilibrium density,

$$K_0 \approx 9.94\%/\text{atm}, \tag{57}$$

$$c_0 \approx 117.4 \text{ m/sec}. \tag{58}$$

These values have been entered into Table I.

On first sight, our results for the compressibility and the velocity of sound are disappointing. This is clearly a consequence of the very strong dependence of K on ρ. (See Table III.) With a poor determination of ρ_0, it is not unexpected that K_0, and consequently c_0, disagrees with experiment. A more reaonable way to evaluate the results of our calculation can be obtained by fitting our ρ_0 and $E(\mathbf{0})/N$ to the measured values before calculating K_0 and c_0. As discussed in an earlier paragraph, a correction for ρ_0 and $E(\mathbf{0})/N$ should begin from the boson calculation. Let us express the correction to $E_0{}^B/N$ as a power series in $(\rho-\rho_0)/\rho_0$. In the lowest order,

$$\frac{1}{N}E_{0,\text{Exact}}{}^B(\rho) \approx \frac{1}{N}E_{0,\text{M}}{}^B(\rho) + a + b\left(\frac{\rho-\rho_0}{\rho_0}\right), \tag{59}$$

where $E_{0,\text{M}}{}^B(\rho)$ is the energy computed by Massey. We can determine a and b by forcing our results to agree with experiment. Retaining $E_1{}^F$, $E_2{}^F$, $E_3{}^F$, and $\Delta E^{(2)}$ unchanged, experiment requires

$$\frac{1}{N}E_{0,\text{Exact}}{}^B(0.0164\ \text{Å}^{-3}) = \frac{1}{N}E_{0,\text{M}}{}^B(0.0164\ \text{Å}^{-3}) + \{(-2.52°\text{K}) - (-1.312°\text{K})\}, \tag{60}$$

$$\left[\frac{dE_{\text{Exact}}(\mathbf{0};\rho)}{d\rho}\right]_{\rho=0.0164\ \text{A}^{-3}} \approx \frac{E_{\text{Exact}}(\mathbf{0};\ 0.0164\ \text{Å}^{-3}) - E_{\text{Exact}}(\mathbf{0};\ 0.0156\ \text{Å}^{-3})}{(0.0164-0.0156)\ \text{Å}^{-3}} = 0, \tag{61}$$

where

$$E_{\text{Exact}}(\mathbf{0};\rho) = E_{0,\text{Exact}}{}^B(\rho) + E_1{}^F(\rho) + E_2{}^F(\rho) + E_3{}^F(\rho) + \Delta E^{(2)}(\rho). \tag{62}$$

Equations (59)–(62) then lead to

$$a = -1.15°\text{K}, \qquad b = -0.537°\text{K}. \tag{63}$$

At the experimental density $\rho = 0.0164$ Å^{-3}, we now have

$$\frac{1}{N}E_{\text{Exact}}(\mathbf{0};\ 0.0164\ \text{Å}^{-3}) = -1.312°\text{K} - 1.15°\text{K} - 0.058°\text{K} = -2.52°\text{K}.$$

The smallness of b causes the linear correction term to be small compared with the constant term a. This suggests that the linear estimate of the correction, Eq. (59), is good. In turn it means that the second derivative of $(1/N)E_{\text{Exact}}(\mathbf{0};\rho)$ with respect to ρ is unchanged from our previous value $d^2[E(\mathbf{0};\rho)/N]/d\rho^2$. At $\rho = 0.0164$ Å^{-3}, *this value is* 4.58×10^4°K/Å^{-6}. With the first derivative set to zero at equilibrium, we finally obtain

$$K(0.0164\ \text{Å}^{-3}) = 3.6\%/\text{atm}, \tag{64}$$

$$c(0.0164\ \text{Å}^{-3}) = 184\ \text{m/sec}, \tag{65}$$

in good agreement with experiment.

C. Magnetic Properties

Necessary conditions for an antiferromagnetic (total spin zero) ground state include

$$E''(\mathbf{0};\ x=0) > 0, \tag{66}$$

and

$$E(\mathbf{0};\ x=0) < E(\mathbf{0};\ x=\pm1), \tag{67}$$

where x defines the spin distribution:

$$N_\pm = N(1\pm x)/2, \tag{68}$$

and the primes on $E(\mathbf{0};x)$ refer to derivatives with respect to x. Equations (68) and (69) are also sufficient conditions provided that $E(\mathbf{0};x)$ has no minimum in the intervals between $x=0$ and $|x|=1$ excluding endpoints. If the gound state is antiferromagnetic, the paramagnetic susceptibility at $T=0$°K may be calculated by a simple formula derived in I (in a slightly different form):

$$\chi/\chi_F = \frac{1}{\frac{3}{2}[E''(\mathbf{0};\ x=0)/Ne_F]}. \tag{69}$$

A test for condition (67) was made at $\rho = 0.0140$ Å^{-3} with the result

$$E^{(0)}(\mathbf{0};\ x=0)/N \approx -1.04°\text{K}, \tag{70}$$

and

$$E^{(0)}(\mathbf{0};\ x=\pm1)/N \approx -0.66°\text{K}. \tag{71}$$

Since $\Delta E^{(2)}(\mathbf{0};\ x)$ is several times smaller than $E^{(0)}(\mathbf{0};\ x)$, and also the dependence of energy on density is not very

TABLE IV. $E_i{}^F(\mathbf{0};\ x)$ and $\Delta E^{(2)}(\mathbf{0};\ x)$ (in units of Ne_F).

$\lvert x\rvert$	0.0	0.05	0.10	0.20
$E_0{}^B$	−0.635	−0.635	−0.635	−0.635
$E_1{}^F(\mathbf{0};\ x)$	0.60000	0.60083	0.60333	0.61336[a]
$E_2{}^F(\mathbf{0};\ x)$	−0.16883	−0.16936	−0.17094	−0.17723[a]
$E_3{}^F(\mathbf{0};\ x)$	−0.02836	−0.02868	−0.02965	−0.03348[a]
$\Delta E^{(2)}(\mathbf{0};\ x)$	−0.066567	−0.066484[a]	−0.066240	−0.065382
$E(\mathbf{0};\ x)$	−0.298757	−0.298694	−0.298500	−0.297732

[a] Estimated by extrapolation or interpolation.

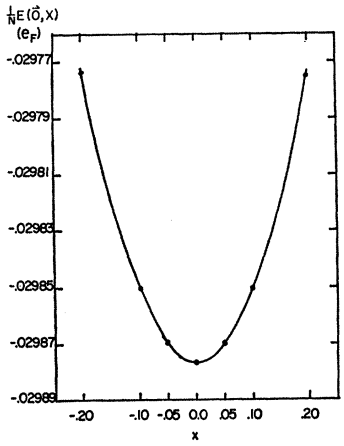

FIG. 5. $(1/N)E(\mathbf{0};x)$ at $\rho=0.0140$ Å^{-3}.

strong, Eqs. (70) and (71) indicate that condition (67) for antiferromagnetism is satisfied. This is opposite to the result found in I for a hypothetical fermion mass-4 system. The cause is traced to the more concentrated $g_B(r)$ in the latter case: a larger mass leads to smaller zero-point motions, therefore a more concentrated $g_B(r)$ and a more spread out $S(k)$; and the slower rise of $S(k)$ to its peak causes a more negative $E_2^F(\mathbf{0};x)$, which is sufficient to reverse the sign of

$$1/N\{E^{(0)}(\mathbf{0};x=0)-E^{(0)}(\mathbf{0};x=\pm1)\}.$$

To test condition (66) or calculate χ/χ_F, we need $E''(\mathbf{0};x=0)$. The proper way to calculate $E''(\mathbf{0};x=0)$ begins from the expression $\{E(\mathbf{0};x)-E(\mathbf{0};x=0)\}$. Whereas $E(\mathbf{0};x=0)$ involves integrations of momentum states over two Fermi spheres, each associated with one spin orientation and of radius k_F, $E(\mathbf{0};x)$ involves integration over two Fermi spheres of *unequal* radii k_F^+ and k_F^-. Expanding the integration limits $k_F^\pm=k_F(1\pm x)^{1/3}$ in power series of x and the integrands in Taylor series about $x=0$, $E(\mathbf{0};x)$ and $E(\mathbf{0};x=0)$ combine to yield

$$E(\mathbf{0};x)-E(\mathbf{0};x=0)=Cx^2+C'x^4+\cdots, \tag{72}$$
$$E''(\mathbf{0};x=0)=\left[\frac{d^2}{dx^2}\{E(\mathbf{0};x)-E(\mathbf{0};x=0)\}\right]_{x=0}=2C.$$

For a complete set of formulas, see Ref. 7.

In our working approximation we actually took an alternative route for convenience of numerical computation: we evaluated $E_1^F(\mathbf{0};x)$, $E_2^F(\mathbf{0};x)$, $E_3^F(\mathbf{0};x)$ and $\Delta E^{(2)}(\mathbf{0};x)$, each for a range of $|x|$: [0.0, 0.05, 0.10] for $E_i^F(\mathbf{0};x)$ and [0.0, 0.10, 0.20] for $\Delta E^{(2)}(\mathbf{0};x)$; then we fitted each set of three points to an even biquadratic in x, from which we computed the second derivative at $x=0$. The calculation of $\Delta E^{(2)}(\mathbf{0};x)$ resembled that of $\Delta E^{(2)}(\mathbf{0};x=0)$ except for a difference in integration limits. Appropriate modifications in the procedure described in Appendix D were required but will not be discussed here. Table IV and Fig. 5 show our results obtained at $\rho=0.0140$ Å^{-3}. Using these we computed

$$\begin{aligned}E''(\mathbf{0};x=0)&=\{[E_1^{F''}(\mathbf{0};x=0)+E_2^{F''}(\mathbf{0};x=0)\\&\quad+E_3^{F''}(\mathbf{0};x=0)+\cdots]+[\Delta E^{(2)''}(\mathbf{0};x=0)+\cdots]\}\\&=\{[0.667-0.424-0.262+\cdots]+[0.068+\cdots]\}Ne_F\\&=0.049Ne_F+\cdots.\end{aligned} \tag{73}$$

In our approximation, then, condition (66) for antiferromagnetism is satisfied, although it is undeniable that the almost total cancellation in Eq. (73) puts the magnetic behavior of the ground state of liquid He³ in a very critical region.

Finally, using Eq. (73),

$$\chi/\chi_F=\frac{1}{\{1-0.636-0.393+\cdots\}+\{0.101+\cdots\}}$$
$$=\frac{1}{0.072+\cdots}\approx13.9. \tag{74}$$

This is close to the (extrapolated) experimental value of 11.1 and the theoretical value of 12 given by Brueckner and Gammel, although both theoretical values are equally unreliable.

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APPENDIX A: RESULTS OF THE BOSON CALCULATION

In Fig. 6 the two-particle interaction determined by Massey[5] is compared with the Yntema-Schneider po-

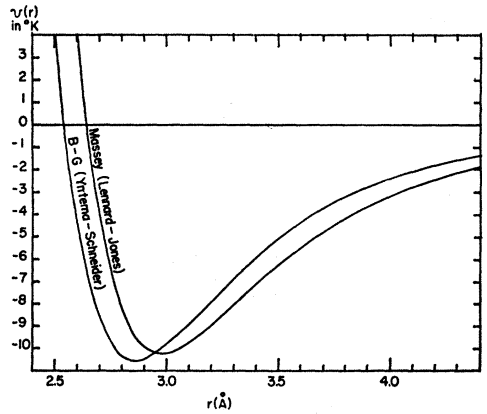

FIG. 6. Two-particle potentials assumed in the Brueckner-Gammel and the present theories.

TABLE V. Parameters used in results quoted in Appendix A.

ρ(Å^{-3})	η	A	z	y	q	$\frac{E_0^B(\rho)}{N}$(°K)
0.0132	1.43	2.24	14000	15.0	1500	−2.802
0.0140	1.505	2.29	12300	14.4	1330	−2.845
0.0148	1.58	2.34	10900	13.75	1175	−2.874
0.0156	1.655	2.39	9600	13.1	1030	−2.885
0.0164	1.73	2.42	8500	12.5	900	−2.877
0.0140[a]	1.515	2.2	9000	15.0	1200	−2.843

[a] The last line gives an earlier version of Massey's results which we used for the calculation of the magnetic susceptibility and the second-order Löwdin correction.

tential used by Brueckner and Gammel. Massey's calculation for the hypothetical boson He^3 system leads to the following results:

$$g_B(r)=(c+1)e^{-(d/r)^{10}}-ce^{-(1+z)(d/r)^{10}}$$
$$+A\left\{\left(\frac{d}{r}\right)^m e^{-(1+y)(d/r)^{10}}-B\left(\frac{d}{r}\right)^n e^{-(1+q)(d/r)^{10}}\right\},$$

$$m=6,\quad n=8,\quad d^3=\eta/2\pi\rho,$$

$$c=\{(1.155574/\eta)-1\}/\{1-(1+z)^{0.3}\},$$

$$B=\Gamma\left(\frac{m-3}{10}\right)(1+q)^{(n-3)/10}\Big/\Gamma\left(\frac{n-3}{10}\right)(1+y)^{(m-3)/10},$$

with the parameters as given in Table V.

APPENDIX B: THE UNPERTURBED GROUND-STATE ENERGY

Equation (8) giving $E^{(0)}(\mathbf{0})$ can be reduced to integrable expressions: Eq. (30) of I. The quadratic approximation

$$S(k)\approx B\left(\frac{k}{k_F}\right)^2$$

further reduces $E_2^F(\mathbf{0})$ and $E_3^F(\mathbf{0})$ to

$$E_2^F(\mathbf{0})\approx\frac{-3}{5}\left(\frac{1}{2}-\frac{6}{7}B\right)Ne_F, \tag{B1}$$

and

$$E_3^F(\mathbf{0})\approx\frac{-3}{5}\left(\frac{3}{7}B-\frac{352}{315}B^2+\frac{472}{735}B^3\right)Ne_F, \tag{B2}$$

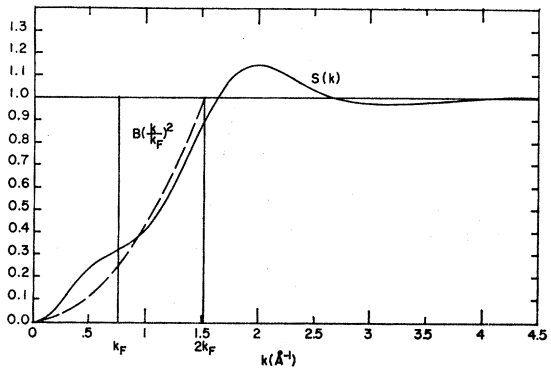

FIG. 7. The boson liquid structure function and the quadratic approximation at $\rho=0.0148$ Å^{-3}.

as given in Eqs. (B3) and (B4) of I. We determine B in the following manner: calculate $E_2^F(\mathbf{0})$ exactly through integration, using Eq. (30) of I, and then substitute into the left-hand side of Eq. (B1). Equation (B2) then gives an estimate of $E_3^F(\mathbf{0})$. For a special case, $\rho=0.0241$ Å^{-3}, the error of this approximation was found to be less than 2%.

$S(k)$ and its quadratic approximation at $\rho=0.0148$ Å^{-3} are shown in Fig. 7.

In this approximation $\bar{E}_4^F(\mathbf{0})$ reduces to

$$\bar{E}_4^F(\mathbf{0})\approx\left(\frac{-23}{770}+\frac{2164}{25025}B-\frac{2176}{25025}B^2\right)Ne_F. \tag{B3}$$

APPENDIX C: TABLE OF INTERMEDIATE RESULTS

TABLE VI. Intermediate results leading to $g_F(r)$.

r(Å)	$F^{(2)}(r)$	$F^{(2)}(r)-1$	$F^{(3)}(r)$	$F(r)$
1.8	0.660	−0.340	0.031	0.690
2.2	0.721	−0.279	0.039	0.760
2.6	0.782	−0.218	0.047	0.829
3.0	0.839	−0.161	0.053	0.891
3.4	0.888	−0.112	0.057	0.945
3.8	0.928	−0.072	0.058	0.986
4.2	0.958	−0.042	0.056	1.014
4.6	0.979	−0.021	0.051	1.029
5.0	0.991	−0.009	0.041	1.032
5.4	0.998	−0.002	0.028	1.026
5.8	1.000	0.000	0.016	1.016
6.2	1.000	0.000	0.006	1.006
6.6	0.998	−0.002	0.001	1.000
7.0	0.997	−0.003	0.000	0.997
7.4	0.996	−0.004	0.001	0.998
7.8	0.996	−0.004	0.003	0.999
8.2	0.997	−0.003	0.004	1.001
8.6	0.998	−0.002	0.005	1.003
9.0	0.999	−0.001	0.004	1.003

APPENDIX D: CALCULATION OF $\Delta E^{(2)}(0)$

Upon substitution of the explicit expressions for $X_{12;1'2'}$ and $X'_{12;1'2'}$, Eqs. (16)–(17), Eq. (53) becomes

$$\Delta E^{(2)}(0)\approx\frac{\hbar^2}{2MN^2}\sum_{(12|1'2')}\delta(\mathbf{k}_{1'}+\mathbf{k}_{2'}-\mathbf{k}_1-\mathbf{k}_2)\Big\{\langle 12,1'2'\rangle u^2(k_{11'})\Big[k_{11'}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{11'}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]$$
$$+\langle 12,2'1'\rangle u^2(k_{1'2})\Big[k_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{1'2}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]$$
$$-\langle 12,1'2'\rangle\langle 12,2'1'\rangle u(k_{11'})u(k_{1'2})\Big[k_{11'}{}^2+k_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{2}+\frac{2k_{11'}{}^2k_{1'2}{}^2}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]\Big\}$$
$$=\frac{1}{2N}\sum_{\mathbf{k}_1s_1,\mathbf{k}_2s_2}\{\langle s_1,s_2\rangle T_p(\mathbf{k}_1,\mathbf{k}_2)+(1-\langle s_1,s_2\rangle)T_a(\mathbf{k}_1,\mathbf{k}_2)\}, \tag{D1}$$

$$T_p(\mathbf{k}_1,\mathbf{k}_2)=\frac{\hbar^2}{4MN^2}\sum_{\mathbf{k}_{1'},\mathbf{k}_{2'}}\delta(\mathbf{k}_{1'}+\mathbf{k}_{2'}-\mathbf{k}_1-\mathbf{k}_2)\Big\{u^2(k_{11'})\Big[k_{11'}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{11'}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]$$
$$+u^2(k_{1'2})\Big[k_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{1'2}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]$$
$$-u(k_{11'})u(k_{1'2})\Big[k_{11'}{}^2+k_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{2}+\frac{2k_{11'}{}^2k_{1'2}{}^2}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]\Big\}, \tag{D2}$$

$$T_a(\mathbf{k}_1,\mathbf{k}_2)=\frac{\hbar^2}{4MN^2}\sum_{\mathbf{k}_{1'},\mathbf{k}_{2'}}\delta(\mathbf{k}_{1'}+\mathbf{k}_{2'}-\mathbf{k}_1-\mathbf{k}_2)$$
$$\times\Big\{u^2(k_{11'})\Big[k_{11'}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{11'}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]+u^2(k_{1'2})\Big[k_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}}{4}+\frac{k_{1'2}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}}\Big]\Big\}, \tag{D3}$$

$$\Delta^2E^{(0)}{}_{1'2';12}=E^{(0)}(1'2'3\cdots N)-E^{(0)}(123\cdots N). \tag{D4}$$

$\mathbf{k}_1$ and $\mathbf{k}_2$ range over all orbitals inside the Fermi sphere, and $\mathbf{k}_{1'}$ and $\mathbf{k}_{2'}$ range over all orbitals outside. Further, for zero total spin,

$$\Delta E^{(2)}(0)\approx\frac{1}{N}\sum_{\mathbf{k}_1,\mathbf{k}_2}\{T_p(\mathbf{k}_1,\mathbf{k}_2)+T_a(\mathbf{k}_1,\mathbf{k}_2)\}=N\Big(\frac{3}{8\pi}\Big)^2\int\{T_p(\mathbf{k}_1,\mathbf{k}_2)+T_a(\mathbf{k}_1,\mathbf{k}_2)\}d\mathbf{k}_1d\mathbf{k}_2, \tag{D5}$$

$$T_p(\mathbf{k}_1,\mathbf{k}_2)+T_a(\mathbf{k}_1,\mathbf{k}_2)=\frac{1}{2}\Big(\frac{3}{8\pi}\Big)e_F\{T_1(\mathbf{k}_1,\mathbf{k}_2)+T_2(\mathbf{k}_1,\mathbf{k}_2)-T_3(\mathbf{k}_1,\mathbf{k}_2)\}, \tag{D6}$$

$$T_1(\mathbf{k}_1,\mathbf{k}_2)=J\Big[2\Big(x_{11'}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}{4}+\frac{x_{11'}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}\Big)u^2(k_Fx_{11'})\Big], \tag{D7}$$

$$T_2(\mathbf{k}_1,\mathbf{k}_2)=J\Big[2\Big(x_{1'2}{}^2+\frac{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}{4}+\frac{x_{1'2}{}^4}{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}\Big)u^2(k_Fx_{1'2})\Big], \tag{D8}$$

$$T_3(\mathbf{k}_1,\mathbf{k}_2)=J\Big[2\Big(\frac{x_{11'}{}^2+x_{1'2}{}^2}{2}+\frac{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}{4}+\frac{x_{11'}{}^2x_{1'2}{}^2}{\Delta^2E^{(0)}{}_{1'2';12}/k_F{}^2}\Big)u(k_Fx_{11'})u(k_Fx_{1'2})\Big], \tag{D9}$$

where the functional $J[f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})]$ is defined as

$$J[f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})]=\int_{\substack{x_{1'}>1\\ x_{2'}>1(x_{2'}=|\mathbf{x}_1+\mathbf{x}_2-\mathbf{x}_{1'}|)}}f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})d\mathbf{x}_{1'}. \tag{D10}$$

The integration in Eq. (D5) reduces to a threefold one which is easy to handle. The calculation of $J[f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})]$, on the other hand, is quite complicated. The procedure is based on the following geometrical construction.

Take $\mathbf{x}_1+\mathbf{x}_2=\mathbf{x}$ along the azimuthal axis. $\mathbf{x}_{1'}$ is then defined by $\mathbf{x}_{1'}$, θ, and ϕ. The region of integration specifies that $\mathbf{x}_{1'}$ may not terminate in a unit sphere about the origin O, nor in a unit sphere about the endpoint of $\mathbf{x}$: P (see Figs. 8–9). For an arbitrary ϕ we have the construction in Fig. 8.

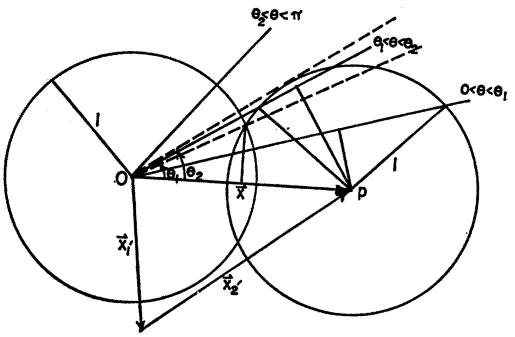

FIG. 8. Geometrical construction I.

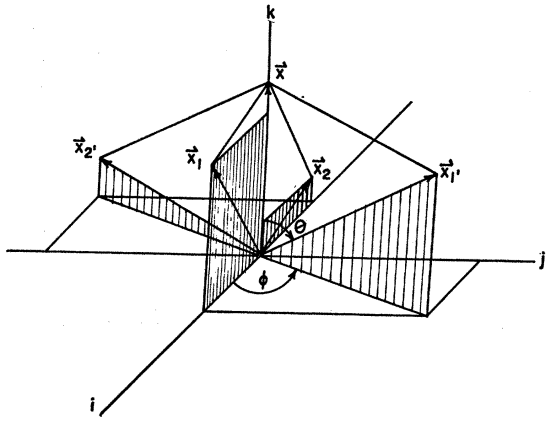

FIG. 9. Geometrical construction II.

$0\leqslant\theta\leqslant\Theta_1$, limits on $x_{1'}$ are $x\cos\theta+(1-x^2\sin^2\theta)^{1/2}$ to ∞.
$\Theta_1\leqslant\theta\leqslant\Theta_2$, limits on $x_{1'}$ are 1 to $x\cos\theta-(1-x^2\sin^2\theta)^{1/2}$, and $x\cos\theta+(1-x^2\sin^2\theta)^{1/2}$ to ∞.
$\Theta_2\leqslant\theta\leqslant\pi$, limits on $x_{1'}$ are 1 to ∞.

$$J[f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})]=\int_{\substack{x_{1'}>1\\ |\mathbf{x}_1+\mathbf{x}_2-\mathbf{x}_{1'}|>1}} f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})d\mathbf{x}_{1'}$$

$$=\int_0^{2\pi}d\phi\left\{\int_{\cos\Theta_2}^{1}dz\int_{xz+(1-x^2(1-z^2))^{1/2}}^{\infty}f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})x_{1'}{}^2dx_{1'}\right.$$

$$\left.+\int_{\cos\Theta_2}^{\cos\Theta_1}dz\int_{1}^{xz-(1-x^2(1-z^2))^{1/2}}f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})x_{1'}{}^2dx_{1'}+\int_{-1}^{\cos\Theta_2}dz\int_{1}^{\infty}f(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_{1'},\mathbf{x}_{2'})x_{1'}{}^2dx_{1'}\right\}.$$

Θ_1 and Θ_2 are defined as follows:

$$x\leqslant\sqrt{2},\qquad \cos\Theta_1=\cos\Theta_2=\frac{x}{2},$$

$$\sqrt{2}\leqslant x\leqslant 2,\qquad \cos\Theta_1=\frac{x}{2},\qquad \cos\Theta_2=\left(1-\frac{1}{x^2}\right)^{1/2},$$

$$x\geqslant 2,\qquad \cos\Theta_1=1,\qquad \cos\Theta_2=\left(1-\frac{1}{x^2}\right)^{1/2}.$$

Finally, from Fig. 9,

$$\cos(\mathbf{x}_1,\mathbf{x})=\frac{x_1{}^2+x^2-x_2{}^2}{2x_1x},$$

$$\cos(\mathbf{x}_2,\mathbf{x})=\frac{x_2{}^2+x^2-x_1{}^2}{2x_2x},$$

$$\cos(\mathbf{x}_1,\mathbf{x}_{1'})=\sin(\mathbf{x}_1,\mathbf{x})\sin\theta\cos\phi+\cos(\mathbf{x}_1,\mathbf{x})\cos\theta,$$

$$\cos(\mathbf{x}_2,\mathbf{x}_{1'})=-\sin(\mathbf{x}_2,\mathbf{x})\sin\theta\cos\phi+\cos(\mathbf{x}_2,\mathbf{x})\cos\theta.$$