behavior of the elements $U_{ij}(r)$ near the origin. As an illustration, a plot of $U_{12}(r)$ used in this work along with its approximate asymptotic form which was used for the resonance-distortion and B′II calculations, is shown in Fig. 1. It is interesting to note that the total cross sections calculated by the Born approximation are always smaller than those from the Bethe method B′I, and are even smaller than the B′II cross sections at energies above 20 eV. Here again replacing the interaction potential matrix elements by their asymptotic inverse-square form results in an increase of the cross sections.

Since the B′I approximation is valid for large values of l, this may be used in conjunction with the partial cross sections in Table I to calculate total inelastic cross sections. In Table II are given total cross sections calculated by means of our numerical method, resonance-distortion, B′I, and B′II approximations. Comparison of the theoretical excitation functions with the experimental data[8] is shown in Fig. 2. The results of the numerical method show better agreement with experiment than do those of the previous calculations.

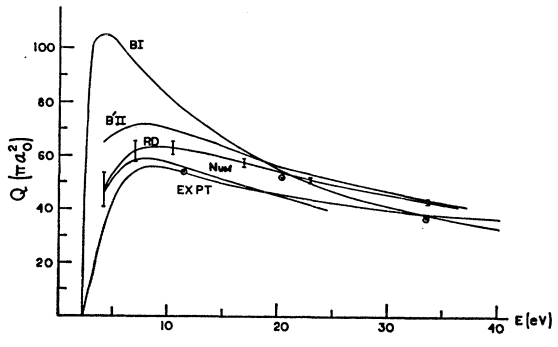

FIG. 2. Total cross sections for the $3s \rightarrow 3p$ transition in Na calculated by the methods BI, B′II, RD, and Num, and absolute measurements of Christoph, designated by the circled points, and relative measurements of Haft, represented by the curve EXPT. The Born cross section (BI) was given by Bates *et al.* (Ref. 8).

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Matrix Elements of a Fermion System in a Representation of Correlated Basis Functions*

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The ground state and low excited states of liquid He^3 (and other fermion systems) can be constructed from a set of basis functions

$$\Psi(|\mathbf{n}) = \psi_0{}^B \Phi(|\mathbf{n})$$

in which $\psi_0{}^B$ is the ground-state boson-type solution of the Schrödinger equation and the model functions $\Phi(|\mathbf{n})$ are Slater determinants suitable for describing states of the noninteracting Fermion system. Diagonal and nondiagonal matrix elements of the identity and the Hamiltonian operator are evaluated by a cluster-expansion technique. An orthonormal basis system is 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.

I. INTRODUCTION

SIMPLE correlated trial functions have proved useful in the study of nuclear matter and the He^3 and He^4 liquids.[1–8] The theory begins with a model function Φ describing a state of the N-particle system in the absence of interactions. The model is adapted to the presence of strong short-range repulsive interactions by introducing a symmetrical positive valued correlation factor $\exp\frac{1}{2}S(1,2,\cdots,N)$ which vanishes when any two particles approach closely. The resulting trial function is

$$\Psi = e^{S(1,2,\cdots,N)/2}\Phi(1,2,\cdots,N). \quad (1)$$

A linear combination of such correlated trial functions provides the possibility of a close approach to exact solutions of the many-particle problem. Construction of a suitable trial (or basis) system may start from a set of normalized orthogonal model functions Φ_n, generated by properly symmetrized products of single-particle orbitals. In the applications the functions Ψ_n are used to construct matrix elements of the identity and the Hamiltonian operator. One recognizes that the functions

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Ψ_n do not in general form a normalized, orthogonal basis.

Possible forms for the correlation factor include

$$e^{\frac{1}{2}S}=\prod_{i<j} e^{u(r_{ij})/2} \tag{2}$$

and

$$e^{\frac{1}{2}S}=\psi_0{}^B(1,2,\cdots,N). \tag{3}$$

Line (2) defines the Bijl-Dingle-Jastrow (BDJ) symmetrical product of two-particle correlation factors. Line (3) introduces $\psi_0{}^B$ (the completely symmetrical ground-state solution of a suitable Schrödinger equation) as an appropriate correlation factor. The use of $\psi_0{}^B$ as the correlation factor in theories of liquid helium gives immediate access to useful results on the excitation spectrum of the boson system[8–12] and on the properties of the ground state and of low excited states of the fermion systems.[13]

Both forms have been used to evaluate a large class of nondiagonal matrix elements occurring in the theory of the multiple excitation spectrum of the boson liquid.[7] Currently Clark and his students are evaluating nondiagonal matrix elements in nuclear problems employing the BDJ form. Clark[14] has described a procedure for computing nondiagonal matrix elements in fermion problems by an adaptation of the cluster-expansion technique.

The object of the present study is to derive matrix elements needed to extend the analysis of Wu and Feenberg[13] on liquid He^3. The problem of reducing the explicit Hamiltonian matrix to diagonal form is reserved for a later paper. In Sec. II diagonal matrix elements are constructed to serve as generating functions for nondiagonal elements. Two distinct cluster-expansion procedures for evaluating Fermion matrix elements are described in Sec. III and one (that of Iwamoto and Yamada) is shown, by critical tests, to be superior for numerical evaluation. In Sec. IV general formulas are derived for diagonal and nondiagonal matrix elements of a fermion system. A normalized orthogonal basis is introduced in Sec. V. The resulting matrix elements of the Hamiltonian operator are evaluated in Sec. VI using $\psi_0{}^B$ as the correlation factor. A quasiparticle formulation of the theory is stated in Sec. VII.

II. GENERATING FUNCTIONS

Normalized model functions $\Phi(|\mathbf{n})=\Phi(|n_1n_2\cdots n_N)$ in the form of Slater determinants are constructed from a normalized orthogonal set of single-particle orbitals $u(|n)\equiv u(\mathbf{r},m|n)$. The discrete variables (spin and isospin) are denoted by m. Where particle l is in state n, we write $u(\mathbf{r}_l,m_l|n)\equiv u(l|n)$. In particular $u(n|n)\equiv u(\mathbf{r}_n,m_n|n)$. The immediate problem is the transformation of the elements

$$(\mathbf{n}'|1|\mathbf{n})=\int\psi_0{}^{B^2}\Phi^*(|\mathbf{n}')\Phi(|\mathbf{n})d\tau_{12\cdots N},$$
$$(\mathbf{n}'|H|\mathbf{n})=\int\psi_0{}^B\Phi^*(|\mathbf{n}')H\psi_0{}^B\Phi(|\mathbf{n})d\tau_{12\cdots N}, \tag{4}$$

into a form suitable for numerical evaluation. We solve this problem in two steps:

(i) Construct a suitable diagonal matrix element to serve as a generating function for the desired nondiagonal element.

(ii) Apply a standard cluster expansion formalism to evaluate the diagonal element.

Step (i) begins with the arbitrary model function $\Phi(|\mathbf{n}^\star)$ constructed from the orbitals

$$u(|l^\star)=a_lu(|l)+b_lu(|l'),\ l'\neq 1,2,\cdots,N \text{ if } b_l\neq 0. \tag{5}$$

A proliferation of multiple indices is avoided by writing $\mathbf{n}=1,2,\cdots,N$ and $\mathbf{n}'=1',2',\cdots,N'$ without implying that either set defines the ground configuration. The use of linear combinations of single-particle states l and l' in the lth column of the model function gives the formalism for computing diagonal matrix elements the ability to generate and evaluate nondiagonal elements as well.

In the application to a uniform extended system ($N\to\infty$, $\Omega\to\infty$, $\rho=N/\Omega$ constant) the single particle orbitals are products of plane waves and spin functions:

$$e^{i\mathbf{k}\cdot\mathbf{r}}\delta(\tfrac{1}{2},m_s) \quad\text{and}\quad e^{i\mathbf{k}\cdot\mathbf{r}}\delta(-\tfrac{1}{2},m_s), \tag{6}$$

or the appropriate generalization with spin and isospin functions in the case of nuclear matter. A discrete set of wave vectors $\mathbf{k}_1$, $\mathbf{k}_2$, $\cdots$ is determined by the usual periodic boundary condition in a cube of volume Ω. The choice of orbitals implies a momentum conservation theorem $(\mathbf{n}'|A|\mathbf{n})=0$ unless $\sum\mathbf{k}_n=\sum\mathbf{k}_{n'}$ ($A=1$ or H).

In general $u(|l')$ and $u(|l)$ may differ in both wave vectors and spin states (as in the theory of static spin density waves[15]).

The following equations illustrate the way in which $(\mathbf{n}^\star|A|\mathbf{n}^\star)$ serves as a generating function ($A=1$ or H):

One Orbital Different ($a_l=1$, $b_l=0$, $l\neq 1$)

$$(1^\star2\cdots N|A|1^\star2\cdots N)=|a_1|^2(12\cdots N|A|12\cdots N)+|b_1|^2(1'2\cdots N|A|1'2\cdots N). \tag{7}$$

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[15] A. W. Overhauser, Phys. Rev. **128**, 1437 (1962).

Two Orbitals Different ($a_l=1$, $b_l=0$, $l\neq 1, 2$)

$$(1^\star 2^\star 3\cdots N|A|1^\star 2^\star 3\cdots N)=|a_1|^2|a_2|^2(123\cdots N|A|123\cdots N)+\cdots$$
$$+|b_1|^2|b_2|^2(1'2'3\cdots N|A|1'2'3\cdots N)+a_1^*a_2^*b_1b_2(123\cdots N|A|1'2'3\cdots N)+\cdots. \quad (8)$$

Three Orbitals Different ($a_l=1$, $b_l=0$, $l\neq 1, 2, 3$)

$$(1^\star 2^\star 3^\star 4\cdots N|A|1^\star 2^\star 3^\star 4\cdots N)$$
$$=|a_1|^2|a_2|^2|a_3|^2(1234\cdots N|A|1234\cdots N)+\cdots+|b_1|^2|b_2|^2|b_3|^2(1'2'3'4\cdots N|A|1'2'3'4\cdots N)$$
$$+|a_1|^2a_2^*a_3^*b_2b_3(1234\cdots N|A|12'3'4\cdots N)+\cdots+|a_2|^2a_1^*a_3^*b_1b_3(1234\cdots N|A|1'23'4\cdots N)+\cdots$$
$$+|a_3|^2a_1^*a_2^*b_1b_2(1234\cdots N|A|1'2'34\cdots N)+\cdots+a_1^*a_2^*a_3^*b_1b_2b_3(1234\cdots N|A|1'2'3'4\cdots N)+\cdots. \quad (9)$$

Momentum conservation requires that the missing coefficients of $a_1^*b_1$ and $a_1b_1^*$ in Eq. (7) vanish; also the missing coefficients of $|a_1|^2a_2^*b_2$ and of $|a_1|^2a_2b_2^*$ in Eq. (8) vanish.

General Formula

$$(\mathbf{n}^\star|A|\mathbf{n}^\star)$$
$$=\sum_{\substack{x_l=0,1\\ y_l=0,1}}\prod_{l=1}^{N}(x_la_l^*+(1-x_l)b_l^*)(y_la_l+(1-y_l)b_l)$$
$$(\cdots x_ln_l+(1-x_l)n_l'\cdots$$
$$|A|\cdots y_ln_l+(1-y_l)n_l'\cdots). \quad (10)$$

III. CLUSTER DEVELOPMENTS

We turn now to the description and critical discussion of the cluster-expansion procedures available for the evaluation of Fermion matrix elements generated by correlated basis functions. The diagonal matrix element of H with respect to $\Psi(|\mathbf{n}^\star)$ is

$$(\mathbf{n}^\star|H|\mathbf{n}^\star)$$
$$=\left[E_0^B+\frac{\hbar^2}{2M}\sum_{p=1}^{N}k_{p^\star}^2\right](\mathbf{n}^\star|1|\mathbf{n}^\star)+\frac{\hbar^2}{2M}\sum_{p=1}^{N}\int\psi_0^{B2}$$
$$\times[-\Phi^*(\Delta_p+k_{p^\star}^2)\phi+\nabla_p\cdot(\Phi^*\nabla_p\phi)]d\tau_{12\ldots N} \quad (11)$$

in which the integration includes summation over spin variables; also

$$k_{p^\star}^2=(u(|p^\star),-\Delta u(|p^\star))$$
$$=|a_p|^2k_p^2+|b_p|^2k_{p'}^2,$$
$$\phi=\prod_{p=1}^{N}u(p|p^\star), \quad (12)$$
$$\Phi=\sum_{\nu}(\pm)P_\nu\phi$$
$$=[1-\sum_{p<q}P_{qp}{}^{pq}+\cdots]\phi.$$

Next we introduce the function

$$I_N(\beta)=(\mathbf{n}^\star|1|\mathbf{n}^\star)+\beta\sum_{p=1}^{N}\int\psi_0^{B2}$$
$$\times[-\Phi^*(\Delta_p+k_{p^\star}^2)\phi+\nabla_p\cdot(\Phi^*\nabla_p\phi)]d\tau_{1\ldots N} \quad (13)$$

with the evident properties

$$(\mathbf{n}^\star|1|\mathbf{n}^\star)=I_N(0),$$
$$\left(\mathbf{n}^\star\left|H-E_0^B-\frac{\hbar^2}{2M}\sum_{p=1}^{N}k_{p^\star}^2\right|\mathbf{n}^\star\right)=\frac{\hbar^2}{2M}\left(\frac{dI(\beta)}{d\beta}\right). \quad (14)$$

To make a useful computational device out of $I(\beta)$ let

$$K(p|p^\star)=-\frac{(\Delta_p+k_{p^\star}^2)u(p|p^\star)}{u(p|p^\star)}$$
$$+\left[\nabla_p\cdot\frac{\nabla_pu(p|p^\star)}{u(p|p^\star)}\right]+\left[\frac{\nabla_pu(p|p^\star)}{u(p|p^\star)}\right]\cdot\nabla_p \quad (15)$$
$$K(12\cdots N|\mathbf{n}^\star)=\sum_{p=1}^{N}K(p|p^\star)$$

and replace Eq. (13) by

$$I_N(\beta)=\int\psi_0^{B2}\exp[\beta K(12\cdots N|\mathbf{n}^\star)]\Phi^*\phi d\tau_{12\ldots N}. \quad (16)$$

The new form gives the same constant and linear terms in β as the old and nothing more is required of it. Equation (16) defines a generalized normalization integral which serves as a mnemonic device to generate the matrix elements of H by a simple operation on the matrix elements of the identity. In Eq. (14) it is now understood that the derivative with respect to β is evaluated at $\beta=0$. A prime superscript will denote generally the derivative with respect to β at $\beta=0$.

Another form of the exponential operator in Eq. (16) is useful in generating the radial distribution function $g_F(r_{12})$. For this application Eq. (15) is replaced by

$$K(12\cdots N|\mathbf{n}^\star)=K(12\cdots N)$$
$$=\sum_{i<j}K(\mathbf{r}_{ij}) \quad (17)$$

in which $K(\mathbf{r})$ is an arbitrary function.

Two procedures for evaluating diagonal matrix elements of 1 and H have been developed in considerable detail by a number of authors. We refer to papers by

Iwamoto and Yamada,[1] Wu and Feenberg,[13] and Wu[16] for the first (IY); and to Aviles[3] and Hartogh and Tolhoek[2] for the second (AHT).

The IY development begins by introducing a sequence of approximants $I_{m\star\ldots q\star}$ and the corresponding sequence of cluster integrals $X_{m\star\ldots q\star}$:

$$
\begin{aligned}
I_{p\star} &= \int \psi_0{}^{B^2} e^{\beta K(1|p\star)} |u(1|p\star)|^2 d\tau_1 dv_{2\ldots N} \\
&= X_{p\star}, \\
I_{m\star n\star} &= \int \psi_0{}^{B^2} e^{\beta K(12|m\star n\star)} u(1|m\star)u(2|n\star)\cdot[1-P_{21}{}^{12}]u^*(1|m\star)u^*(2|n\star)d\tau_{12}dv_{3\ldots N} \\
&= X_{m\star}X_{n\star}+X_{m\star n\star}, \\
I_{m\star n\star p\star} &= \int \psi_0{}^{B^2} e^{\beta K(123|m\star n\star p\star)} u(1|m\star)u(2|n\star)u(3|p\star) \\
&\qquad \cdot[1-P_{21}{}^{12}-P_{32}{}^{23}-P_{13}{}^{31}+P_{312}{}^{123}+P_{231}{}^{123}]u^*(1|m\star)u^*(2|n\star)u^*(3|p\star)d\tau_{123}dv_{4\ldots N} \\
&= X_{m\star}X_{n\star}X_{p\star}+X_{m\star}X_{n\star p\star}+X_{n\star}X_{m\star p\star}+X_{p\star}X_{m\star n\star}+X_{m\star n\star p\star}, \\
I_{m\star n\star p\star q\star} &= \int \psi_0{}^{B^2} e^{\beta K(1234|m\star n\star p\star q\star)} u(1|m\star)u(2|n\star)u(3|p\star)u(4|q\star)\cdot[1-P_{21}{}^{12}-\cdots-P_{43}{}^{34}+P_{312}{}^{123}+\cdots \\
&\qquad +P_{342}{}^{234}+P_{21}{}^{12}P_{43}{}^{34}+\cdots+P_{41}{}^{14}P_{32}{}^{23}-P_{4123}{}^{1234}-P_{3421}{}^{1234}+\cdots-P_{2341}{}^{1234}] \\
&\qquad \cdot u^*(1|m\star)u^*(2|n\star)u^*(3|p\star)u^*(4|q\star)d\tau_{1234}dv_{5\ldots N} \\
&= X_{m\star}X_{n\star}X_{p\star}X_{q\star}+X_{m\star}X_{n\star}X_{p\star q\star}+\cdots+X_{p\star}X_{q\star}X_{m\star n\star}X_{m\star}X_{n\star p\star q\star}+\cdots+X_{q\star}X_{m\star n\star p\star} \\
&\qquad +X_{m\star n\star}X_{p\star q\star}+\cdots+X_{m\star q\star}X_{n\star p\star}+X_{m\star n\star p\star q\star},
\end{aligned}
\tag{18}
$$

and so on. (Integration over τ includes summation over spin, whereas integration over v does not.) Each approximant $I_{m\star\ldots q\star}$ is represented as well as possible by a cluster approximation formed from all the preceding cluster integrals. The difference between the approximant and the cluster approximation defines a new cluster integral $X_{m\star\ldots q\star}$. At each stage the cluster approximation is constructed so that detailed and strong cancellation occurs between the various exchange terms in $I_{m\star\ldots q\star}$ and the corresponding products of distinct cluster integrals in the cluster approximation leaving always a remainder to be represented by $X_{m\star\ldots q\star}$. Clearly the approximants and the cluster integrals do not depend on the order of the indices. Also the first few approximants are not in any sense approximations to I_N.

At the end of the chain of approximants

$$
I_N=\sum\{\cdots X_{m\star}\cdots\}\{\cdots X_{n\star p\star}\cdots\}\times\{\cdots X_{q\star r\star s\star}\cdots\}\cdots \tag{19}
$$

in which the indices on each product in the sum range over 1, 2, $\cdots$, N with no duplications and no omissions. Order of magnitude estimates of the products in Eq. (19) are based on the relations

$$
\begin{aligned}
X_{m\star} &= 1+O(\beta^2), \\
X_{m\star n\star} &= O(1/N), \\
X_{m\star n\star p\star} &= O(1/N^2),
\end{aligned}
\tag{20}
$$

and so on. The normalized cluster integrals

$$
x_{m\star\ldots q\star}=X_{m\star\ldots q\star}/X_{m\star}\cdots X_{q\star} \tag{21}
$$

are used to express I_N in the useful asymptotic ($N\to\infty$, ρ constant) exponential form

$$
I_N=\Big(\prod_{m=1}^{N} X_{m\star}\Big)\exp\mathcal{G}_{iy}(\mathbf{n}\star|\beta), \tag{22}
$$

$$
\mathcal{G}_{iy}(\mathbf{n}\star|\beta)=\sum_{m<n} x_{m\star n\star}+\sum_{m<n<p}[x_{m\star n\star p\star}-x_{m\star n\star}x_{n\star p\star}-x_{m\star p\star}x_{p\star n\star}-x_{n\star m\star}x_{m\star p\star}]+\sum_{m<n<p<q}[x_{m\star n\star p\star q\star}-\cdots]+\cdots. \tag{23}
$$

[16] F. Y. Wu, J. Math. Phys. 4, 1438 (1963).

The exponential form is useful because the exponent is proportional to N [as a consequence of the order of magnitude relations stated in Eq. (20)]. A particularly transparent justification for the exponential form and derivation of $\mathcal{G}_{iy}(\mathbf{n}^\star|\beta)$ appears in Refs. 13 and 16.

The AHT formalism is based on the theorem that the product of two determinants can be written as a single determinant:

$$\Phi^*\Phi=\det(p_{ij}),$$
$$p_{ij}=\sum_{m=1}^{N} u^*(i|m^\star)u(j|m^\star). \tag{24}$$

A cluster expansion for the radial distribution function $g_F(r_{12})$ is then generated in terms of successively larger minors of $\det(p_{ij})$. At every stage of approximation the formula for $g_F(r_{12})$ possesses the property of invariance under a unitary transformation of the single-particle orbitals contained in $\mathbf{n}^\star$ [denoted by $U(\mathbf{n}^\star)$]. Notice that the IY development for $\mathcal{G}$ lacks this property of evident invariance. At $\beta=0$ invariance fails in the 3 index addend because the product term $x_{m^\star n^\star}x_{n^\star p^\star}$ contains a repeated index. Repeated indices occur systematically for all n-index addends ($n\geq 3$) with the consequence that any truncated form for $\mathcal{G}_{iy}$ [produced by dropping all addends with $n+1$ or more indices ($n\geq 3$)] is not invariant under $U(\mathbf{n}^\star)$. The significance of a lack of evident invariance under $U(\mathbf{n}^\star)$ must be discussed. However, let us turn first to the task of generating an invariant cluster expansion for I_N.

Invariant approximants $I^{(l)}$ and cluster integrals $X^{(l)}$ are generated by averaging $I_{m^\star\cdots q^\star}$ over all possible choices of $m^\star\cdots q^\star$ within $\mathbf{n}^\star$. Thus

$$\begin{aligned}
I^{(1)}&=(1/N)\sum_p I_{p^\star}\\
&=X^{(1)},\\
I^{(2)}&=(1/N(N-1))\sum_{p,q} I_{p^\star q^\star}\\
&=X^{(1)^2}+X^{(2)},\\
I^{(3)}&=(1/N(N-1)(N-2))\sum_{n,p,q} I_{n^\star p^\star q^\star}\\
&=X^{(1)^3}+3X^{(1)}X^{(2)}+X^{(3)},\\
I^{(4)}&=(1/N(N-1)(N-2)(N-3))\sum_{m,n,p,q} I_{m^\star n^\star p^\star q^\star}\\
&=X^{(1)^4}+6X^{(1)^2}X^{(2)}+4X^{(1)}X^{(3)}+3X^{(2)^2}+X^{(4)},
\end{aligned} \tag{25}$$

and so on. The last step in this sequence is

$$I_N=\sum_{(\nu)}\frac{N!X^{(1)^{\nu_1}}X^{(2)^{\nu_2}}\cdots X^{(N)^{\nu_N}}}{\Pi l!^{\nu_l}\nu_l!} \tag{26}$$

the sum extending over all integral solutions of the equation $\sum_{l=1}^{N} l\nu_l=N$. Order of magnitude estimates of I_N are based on the general relation

$$X^{(l)}\sim O(1/N^{l-1}). \tag{27}$$

Equation (26) can be converted immediately into the useful asymptotic exponential form

$$I_N(\beta)\cong\exp\mathcal{G}_{aht}(\mathbf{n}^\star|\beta) \tag{28}$$

with

$$\begin{aligned}
\mathcal{G}_{aht}&=\tfrac{1}{2}N^2X^{(2)}+\tfrac{1}{6}N^3(X^{(3)}-3X^{(2)^2})\\
&\quad+(1/24)N^4(X^{(4)}-12X^{(2)}X^{(3)}+20X^{(2)^3})+\cdots.
\end{aligned} \tag{29}$$

Equations (28) and (29) exhibit a cluster expansion of the type developed by Aviles[3] and Hartogh and Tolhoek.[2] The circumstance that our two forms for K [Eqs. (15) and (17)] imply $X_{p^\star}=X^{(1)}=1+O(\beta^2)$ is used to simplify the statement of Eqs. (28) and (29). The same simplification can be introduced into Eqs. (21)–(23).

The averaging process exhibited in the definition of $I^{(l)}$ serves the double function of giving equal weight to all possible configurations containing l orbitals belonging to $\mathbf{n}^\star$ and, as a corollary, maintaining invariance under $U(\mathbf{n}^\star)$. Since $I_N(\beta)$ possesses the invariance property it is not unreasonable to require that a procedure for computing I_N in terms of successive approximants should also possess it at each stage of approximation. This is not however a necessary condition for a satisfactory computational method. Just the fact that a truncated form of $\mathcal{G}_{iy}$ is not invariant under $U(\mathbf{n}^\star)$ means that the series for $\mathcal{G}_{iy}$ converges most rapidly for some particular choice of orthogonal basis functions in the $\mathbf{n}^\star$ function space. In this connection simple plane waves appear well suited to utilize effectively the opportunities for detailed internal cancellation implicit in the formulas for $X_{m^\star\cdots q^\star}$ and $X'_{m^\star\cdots q^\star}$.

From the defining relations, Eqs. (18) and (25), we see that

$$\begin{aligned}
X^{(2)}&=(1/N(N-1))\sum_{m,n}{}' X_{m^\star n^\star},\\
X^{(3)}&=(1/N(N-1)(N-2))\sum_{m,n,p}{}' X_{m^\star n^\star p^\star},
\end{aligned} \tag{30}$$

the prime on the summation denoting absence of terms with two or more identical indices. However, $X^{(4)}$ is not connected with the average value of $X_{m^\star n^\star p^\star q^\star}$ in the same simple manner. The presence of $X^{(2)^2}$ in the defining equation means that

$$\begin{aligned}
X^{(4)}+3X^{(2)^2}&=\frac{1}{N(N-1)(N-2)(N-3)}\\
&\quad\times\sum_{m,n,p,q}{}' [X_{m^\star n^\star p^\star q^\star}+3X_{m^\star n^\star}X_{p^\star q^\star}].
\end{aligned} \tag{31}$$

Consequently

$$\frac{1}{4!}N^4X^{(4)}-\sum_{m<n<p<q}X_{m\star n\star p\star q\star}=\tfrac{1}{2}N^3X^{(2)2}$$
$$-\sum_{m<n<p}[X_{m\star n\star}X_{n\star p\star}+X_{n\star m\star}X_{m\star p\star}+X_{m\star p\star}X_{p\star n\star}]. \tag{32}$$

The derivation of Eq. (32) requires careful treatment of the $X_{m\star n\star}X_{p\star q\star}$ terms in Eq. (31). These terms occur multiplied by the factor

$$\frac{3}{N(N-1)(N-2)(N-3)}\rightarrow\frac{3}{N^2(N-1)^2}\left(1+\frac{4}{N}\right).$$

Equations (30) and (32) are sufficient to verify the identity of $\mathcal{G}_{iy}$ and $\mathcal{G}_{aht}$ up to and including terms in $X_{m\star n\star p\star q\star}$ and $X^{(4)}$. Here the significant point is that corresponding orders in the two developments are not identical. The superiority of the IY development is demonstrated in Sec. IV where a truncated form of $\mathcal{G}_{iy}$ meets a consistency test while $\mathcal{G}_{aht}$ to the same order fails.

A second test is provided by two formulas for the radial distribution function generated by truncated forms of $\mathcal{G}_{iy}$ and $\mathcal{G}_{aht}$ using Eq. (17). The first two addends in Eqs. (23) and (29) yield the radial functions

$$g_{iy}(r)=g_B(r)F_{iy}(r),$$
$$g_{aht}(r)=g_B(r)F_{aht}(r), \tag{33}$$

with

$$F(r)=1+F^{(2)}(r)+F^{(3)}(r),$$
$$F^{(2)}(r)=-(1/s)l^2(k_Fr),$$
$$F_{iy}{}^{(3)}(r)=-\frac{2\rho}{s}\int g_B(r')(g_B(|\mathbf{r}-\mathbf{r}'|)-1)l^2(k_Fr')dv'+\frac{2\rho}{s^2}l(k_Fr)\int g_B(r')(g_B(|\mathbf{r}-\mathbf{r}'|)-1)l(k_Fr')l(k_F|\mathbf{r}-\mathbf{r}'|)dv',$$
$$F_{aht}{}^{(3)}(r)=-\frac{2\rho}{s}\int g_B(r')(g_B(|\mathbf{r}-\mathbf{r}'|)-1)l^2(k_Fr')dv'$$
$$+\frac{2\rho}{s^2}l(k_Fr)\int g_B(r')l(k_Fr')\cdot[g_B(|\mathbf{r}-\mathbf{r}'|)l(k_F|\mathbf{r}-\mathbf{r}'|)-l(k_Fr)l(k_Fr')]dv'. \tag{34}$$

Here s denotes the number of spin (and isospin) orientations represented equally in $\mathbf{n}$ ($s=1$, ferromagnetic state of He^3; $s=2$, paramagnetic state of He^3; $s=4$, ground state of nuclear matter) and also

$$k_F=(6\pi^2\rho/s)^{1/3},$$
$$l(x)=(3/x^3)(\sin x-x\cos x). \tag{35}$$

The functions g_{iy} and g_{aht} for the paramagnetic state ($s=2$) are plotted in Fig. 1 for a particularly simple choice of $g_B(r)$. The detailed specification of $g_B(r)$ is given in Appendix C. Values of $F^{(2)}(r)$, $F_{iy}{}^{(3)}(r)$, $F_{aht}{}^{(3)}(r)$, $F_{iy}(r)$, and $F_{aht}(r)$ appear in Table I.

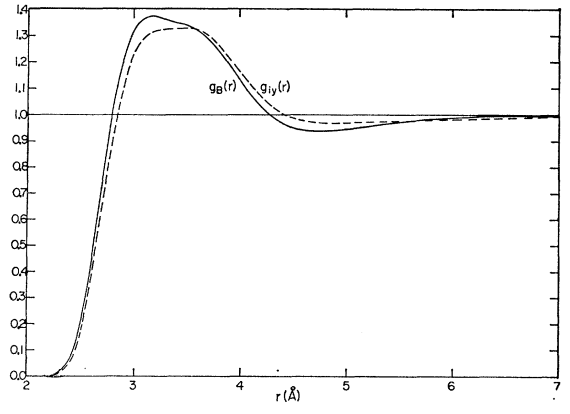

FIG. 1. The radial distribution functions $g_B(r)$ and $g_{iy}(r)$. On this plot g_{aht} and g_{iy} are indistinguishable.

TABLE I. Values of $F^{(2)}(r)$, $F_{iy}{}^{(3)}(r)$, $F_{aht}{}^{(3)}(r)$, $F_{iy}(r)$, and $F_{aht}(r)$ for $s=2$.

$r(A)$	$F^{(2)}(r)$	$F_{iy}{}^{(3)}(r)$	$F_{aht}{}^{(3)}(r)$	$F_{iy}(r)$	$F_{aht}(r)$
1.8	−0.303	0.014	0.013	0.711	0.710
2.2	−0.233	0.027	0.025	0.794	0.793
2.6	−0.167	0.037	0.035	0.870	0.868
3.0	−0.111	0.044	0.043	0.934	0.932
3.4	−0.066	0.049	0.048	0.983	0.982
3.8	−0.035	0.051	0.049	1.016	1.015
4.2	−0.015	0.047	0.046	1.032	1.032
4.6	−0.004	0.038	0.038	1.034	1.034
5.0	0.000	0.024	0.024	1.024	1.024
5.4	0.000	0.008	0.008	1.007	1.007
5.8	−0.002	−0.004	−0.004	0.994	0.994
6.2	−0.003	−0.007	−0.006	0.990	0.990
6.6	−0.004	−0.003	−0.003	0.993	0.994
7.0	−0.003	0.002	0.002	0.999	0.999
7.4	−0.003	0.005	0.005	1.003	1.003
7.8	−0.002	0.006	0.006	1.005	1.004
8.2	−0.001	0.005	0.005	1.004	1.004
8.6	0.000	0.004	0.004	1.004	1.004
9.0	0.000	0.002	0.002	1.002	1.002

TABLE II. $S_F(0)$ by Eq. (34) and Appendix C.

	IY formalism				AHT formalism			
s	1-Index contribution	2-Index contribution	3-Index contribution	$S_F(0)$	1-Index contribution	2-Index contribution	3-Index contribution	$S_F(0)$
1	1	−1.332	0.376	0.044	1	−1.332	0.373	0.041
2	1	−1.542	0.697	0.155	1	−1.542	0.692	0.150
4	1	−1.689	1.094	0.405	1	−1.689	1.093	0.404

The normalization conditions

$$\rho\int(g_B-1)dv=\rho\int(g_F-1)dv=-1 \tag{36}$$

and the equivalent statements

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

provide a criterion for testing the truncated forms. Results are shown in Table II for $s=1, 2, 4$.

These results may be evaluated as good at $s=1$, acceptable at $s=2$, and dubious at $s=4$. Consistency can be enforced on the truncated theories by incorporating an adjustable amplitude parameter into the 3-index addend in g_F. The procedure is developed in Appendix D. No conclusion can be drawn from these results on the accuracy of the formalism for nuclear matter under realistic assumptions on k_F and the hard core radius.

IV. GENERATING FUNCTIONS AND CLUSTER EXPANSIONS

To make connection between generating functions and cluster expansions the exponent $\mathcal{G}(\mathbf{n}^\star|0)$ in Eq. (22) and the derivative function $\mathcal{G}'(\mathbf{n}^\star|0)$ must both be expressed as sums of addends associated with distinct matrix elements. In the initial phase the analysis based on Eq. (5) can be simplified by requiring $|a_m|^2=|b_m|^2=\frac{1}{2}$ for some values of m and $|a_m|=1$, $b_m=0$ for all others. Results are in fact independent of this specialization of the formalism. The arbitrary phases of a_m and b_m are still available to identify components of nondiagonal elements. We consider examples in which first one, then two, and finally three orbitals involve linear combinations of simple plane-wave states. At $\beta=0$

$$\begin{aligned}&X_{p\star}=|a_p|^2X_p+|b_p|^2X_{p'}=1\\&X_{p\star'}=0,\end{aligned} \tag{38}$$

$$X_{m\star n\star}=|a_m|^2|a_n|^2X_{mn}+\cdots+|b_m|^2|b_n|^2X_{m'n'}+a_m^*a_n^*b_mb_nX_{mn;m'n'}+\cdots, \tag{39}$$

$$X_{m\star n\star p\star}=|a_m|^2|a_n|^2|a_p|^2X_{mnp}+\cdots+|b_m|^2|b_n|^2|b_p|^2X_{m'n'p'}+|a_m|^2a_n^*a_p^*b_nb_pX_{mnp;mn'p'}+\cdots+a_m^*a_n^*a_p^*b_mb_nb_pX_{mnp;m'n'p'}+\cdots, \tag{40}$$

and corresponding equations for the derivatives with respect to β evaluated at $\beta=0$ [place a prime denoting the derivative on all X's in Eqs. (39) and (40)]. The elements $X_{mn;m'n'}$, $X_{mnp;mn'p'}$, and $X_{mnp;m'n'p'}$ are defined by Eqs. (39) and (40). The element $X'_{mn;m'n'}$ is defined as the coefficient of $a_m^*a_n^*b_mb_n$ in $X'_{m\star n\star}\equiv((d/d\beta)X_{m\star n\star})_{\beta=0}$. Similar definitions yield $X'_{mnp;mn'p'}$ and $X'_{mnp;m'n'p'}$ from $X'_{m\star n\star p\star}$. The general rule is dictated by the occurrence of the linear combination orbitals in the exponential operators [Eqs. (15) and (16)]: First compute the derivative with respect to β at $\beta=0$, then expand in terms of the a, a^*, b, b^* amplitudes.

One Orbital Different ($|a_1|^2=|b_1|^2=\frac{1}{2}$)

$$\mathcal{G}(1'2\cdots N|0)=\mathcal{G}(12\cdots N|0)+\delta\mathcal{G}_{1'}(0)-\delta\mathcal{G}_1(0), \tag{41}$$

$$\mathcal{G}(\mathbf{n}^\star|0)=\tfrac{1}{2}\mathcal{G}(12\cdots N|0)+\tfrac{1}{2}\mathcal{G}(1'2\cdots N|0)+\tfrac{1}{8}[\Delta\mathcal{G}(1',1)]^2, \tag{42}$$

$$\Delta\mathcal{G}(1',1)=\sum_{m\neq1}(X_{1'm}(0)-X_{1m}(0))+\cdots. \tag{43}$$

As in Ref. 13, Appendix A, the functions $\delta\mathcal{G}_m(0)$ are defined by the statement

$$\delta\mathcal{G}_m(0)=\mathcal{G}(12\cdots m-1\ m\ m+1\cdots N|0)-\mathcal{G}(12\cdots m-1\ m+1\cdots N|0). \tag{44}$$

Equations (7) and (22) now reduce to

$$\cosh\tfrac{1}{2}(\delta\mathcal{G}_{1'}(0)-\delta\mathcal{G}_1(0))=\exp\tfrac{1}{8}[\Delta\mathcal{G}(1',1)]^2, \tag{45}$$

in agreement with the leading term for $\Delta\mathcal{G}$ given in Eq. (43) but providing the possibility of a more precise evaluation of $\Delta\mathcal{G}$ when it is not small.

Observe that the leading term for $\Delta\mathcal{G}(1',1)$ given by Eq. (43) is generated by the terms with repeated indices in the second addend of $\mathcal{G}_{iy}$ [Eq. (23)]. The truncated $\mathcal{G}_{iy}$ gives consistent results in Eq. (45) without invoking contributions from the third and higher addends. With $\mathcal{G}_{aht}$, an equal degree of consistency can be attained only by introducing terms from the third addend [Eq. (29)]. Thus the truncated IY development (two and three

index terms in $\mathcal{G}$) meets a test of internal consistency in a satisfactory manner while the corresponding truncated form of the AHT development fails.

Normalized basis functions are convenient in the following sections. Let

$$|n_1 n_2 \cdots n_N\} = \Psi_{\mathbf{n}}/(\mathbf{n}|1|\mathbf{n})^{1/2}, \qquad E^{(0)}(\mathbf{n}) = \{\mathbf{n}|H|\mathbf{n}\}. \tag{46}$$

The simple bracket $\rangle$ is reserved for an orthonormal basis system.

Two Orbitals Different ($|a_1|^2 = |a_2|^2 = |b_1|^2 = |b_2|^2 = \frac{1}{2}$)

$$\mathcal{G}(1'2'3\cdots N|0) = \mathcal{G}(123\cdots N|0) + \delta\mathcal{G}_{1'}(0) - \delta\mathcal{G}_1(0) + \delta\mathcal{G}_{2'}(0) - \delta\mathcal{G}_2(0) + O(1/N), \tag{47}$$

$$\mathcal{G}(1^\star 2^\star 3\cdots N|0) = \tfrac{1}{2}\mathcal{G}(123\cdots N|0) + \tfrac{1}{2}\mathcal{G}(1'2'3\cdots N|0) + \tfrac{1}{8}[\Delta\mathcal{G}(1',1)]^2 + \tfrac{1}{8}[\Delta\mathcal{G}(2',2)]^2 + O(1/N) + a_1^* a_2^* b_1 b_2 \mathcal{G}_{12;1'2'}(0) + \cdots, \tag{48}$$

$$\mathcal{G}_{12;1'2'}(0) = X_{12;1'2'} + \sum_{n>2} [X_{12n;1'2'n} - \tfrac{1}{2}X_{12;1'2'} \times (X_{1n} + X_{1'n} + X_{2n} + X_{2'n})] + \cdots. \tag{49}$$

Now Eq. (8) with $A=1$ and Eq. (22) with $\beta=0$ require

$$\cosh\tfrac{1}{2}(\delta\mathcal{G}_1(0) - \delta\mathcal{G}_{1'}(0))\cosh\tfrac{1}{2}(\delta\mathcal{G}_2(0) - \delta\mathcal{G}_{2'}(0)) \cong \exp\tfrac{1}{8}(\Delta\mathcal{G}(1,1'))^2 + \tfrac{1}{8}(\Delta\mathcal{G}(2,2'))^2 \tag{50}$$

in agreement with Eq. (45). This result verifies the consistency of the truncated IY form for $\mathcal{G}$ when the model function is constructed from the particular linear combination of determinantal functions generated by $u(|1^\star)$ and $u(|2^\star)$.

The fact that $\mathcal{G}_{12;1'2'}$ is of order $1/N$ means that only linear terms in $a_1^* a_2^* b_1 b_2$ need be retained when Eqs. (47)–(49) are combined with Eqs. (8) and (22). The result is

$$\{123\cdots N|1|1'2'3\cdots N\} = \mathcal{G}_{12;1'2'}(0)\cosh\tfrac{1}{2}(\delta\mathcal{G}_1(0) - \delta\mathcal{G}_{1'}(0)) \cdot \cosh\tfrac{1}{2}(\delta\mathcal{G}_2(0) - \delta\mathcal{G}_{2'}(0)). \tag{51}$$

Equation (51) is not altogether satisfactory. Observe first that $\mathcal{G}_{12;1'2'}$ is antisymmetric in 1, 2 and also in 1′, 2′. The exact matrix element $\{123\cdots N|1|1'2'3\cdots N\}$ also has this property. So fas Eq. (51) is in order. However, the remaining factor in the right hand member of Eq. (51) should be a symmetrical function of 1, 2 (and also of 1′, 2′), but it is not.

The immediate cause of the descrepancy is surely the association of states 1 and 1′ in $u(|1^\star)$ and of states 2 and 2′ in $u(|2^\star)$ so that 1 and 2 and also 1′ and 2′ enter the theory in an unsymmetrical manner. This association causes no difficulty in the expansion of Eq. (8) because the linear combination of orbitals leads directly to a linear combination of Slater determinants each with unimpaired fermion symmetry properties. On the other hand, the cluster expansion is not sufficiently flexible to reproduce in every detail the properties implied by a linear combination of determinants. We have not succeeded in resolving this difficulty. However, symmetry can be achieved in working formulas by symmetrizing the coefficient of $\mathcal{G}_{12;1'2'}$ in Eq. (51) with respect to interchange of the indices 1′ and 2′. We introduce the geometric mean coefficient and write

$$\{123\cdots N|1|1'2'3\cdots N\} \cong \mathcal{G}_{12;1'2'}(0)\Big[\prod_{i=1}^{2}\prod_{j=1}^{2}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0) - \delta\mathcal{G}_{j'}(0))\Big]^{1/2}. \tag{52}$$

Actually the factor in square brackets in Eq. (52) is replaced by 1 in the explicit working version of the theory [Eqs. (73)–(75), (86)–(96)]. The theory is most useful when the difference between Eqs. (51) and (52) is inconsequential. Numerical estimates in Appendix A verify that this is indeed the actual situation.

Three Orbitals Different
($|a_1|^2 = |a_2|^2 = |a_3|^2 = |b_1|^2 = |b_2|^2 = |b_3|^2 = \frac{1}{2}$)

$$\mathcal{G}(1'2'3'4\cdots N|0) = \mathcal{G}(1234\cdots N|0) + \delta\mathcal{G}_{1'}(0) - \delta\mathcal{G}_1(0) + \delta\mathcal{G}_{2'}(0) - \delta\mathcal{G}_2(0) + \delta\mathcal{G}_{3'}(0) - \delta\mathcal{G}_3(0) + \cdots, \tag{53}$$

$$\mathcal{G}(1^\star 2^\star 3^\star 4\cdots N|0) = \tfrac{1}{2}\mathcal{G}(1234\cdots N|0) + \tfrac{1}{2}\mathcal{G}(1'2'3'4\cdots N|0) + \tfrac{1}{8}[\Delta\mathcal{G}(1',1)]^2 + \tfrac{1}{8}[\Delta\mathcal{G}(2,2')]^2 + \tfrac{1}{8}[\Delta\mathcal{G}(3',3)]^2 + a_1^* a_2^* a_3^* b_1 b_2 b_3 \mathcal{G}_{123;1'2'3'}(0) + \cdots, \tag{54}$$

$$\mathcal{G}_{123;1'2'3'}(0) = X_{123;1'2'3'}(0) + \cdots. \tag{55}$$

Equations (47)–(49) in Eqs. (9) and (22) require

$$\prod_{i=1}^{3}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0) - \delta\mathcal{G}_{i'}(0)) = \prod_{i=1}^{3}\exp\tfrac{1}{8}[\Delta\mathcal{G}(i,i')]^2 \tag{56}$$

in agreement with Eq. (45). The nondiagonal matrix element is

$$\{1234\cdots N|1|1'2'3'4\cdots N\} = \mathcal{G}_{123;1'2'3'}(0)\prod_{i=1}^{3}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0) - \delta\mathcal{G}_{i'}(0)). \tag{57}$$

The discrepancy already noted recurs again; the matrix element is completely antisymmetric in the indices 1, 2, 3 and also in 1′, 2′, 3′; so also is $\mathcal{G}_{123;1'2'3'}(0)$. However, the coefficient of $\mathcal{G}_{123;1'2'3'}(0)$ should be invariant under permutations of 1, 2, 3 and also of 1′, 2′, 3′ and it is not. To secure correct behavior we replace the coefficient of $\mathcal{G}_{123;1'2'3'}$ by the geometric mean of the six different

coefficients generated by the permutations of 1, 2, 3:

$$\{1234\cdots N|1|1'2'3'4\cdots N\}$$
$$\cong \mathcal{G}_{123;1'2'3'}(0)\Big[\prod_{i=1}^{3}\prod_{j=1}^{3}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0)-\delta\mathcal{G}_{j'}(0))\Big]^{1/3}. \quad (58)$$

Again the factor in square brackets is replaced by 1 in the working version of the theory [Eqs. (73)–(75), (86)–(96)].

Next we develop the consequences of Eqs. (7)–(9) and (14) giving $\{\mathbf{n}^\star|H|\mathbf{n}^\star\}$ in terms of $I_N'(0)$.

One Orbital Different ($|a_1|^2=|b_1|^2=\frac{1}{2}$)

The appropriate substitutions in Eq. (14) produce a near identity:

$$\exp\tfrac{1}{2}(\delta\mathcal{G}_1(0)-\delta\mathcal{G}_{1'}(0))E^{(0)}(12\cdots N)$$
$$+\exp-\tfrac{1}{2}(\delta\mathcal{G}_1(0)-\delta\mathcal{G}_{1'}(0))E^{(0)}(1'2\cdots N)$$
$$\cong 2\cosh\tfrac{1}{2}(\delta\mathcal{G}_1(0)-\delta\mathcal{G}_{1'}(0))$$
$$\cdot\big[\tfrac{1}{2}E^{(0)}(12\cdots N)+\tfrac{1}{2}E^{(0)}(1'2\cdots N)+\delta E(1',1)\big]. \quad (59)$$

Terms proportional to N balance exactly. There are left on either side small terms independent of N. These latter may not balance exactly for the reason that terms of order $O(N^0)$ are neglected in the derivation of Eq. (22). Consequently Eqs. (14) and (22) are not exact identities with the given forms for $I_N(0)$ and $I_N'(0)$. The small cross term $\delta E(1',1)$ [also of order $O(N^0)$] is computed in Appendix B.

Two Different Orbitals ($|a_1|^2=|a_2|^2=|b_1|^2=|b_2|^2=\frac{1}{2}$)

Again employing Eq. (14) linear terms in N balance exactly. For the coefficient of $a_1^*a_2^*b_1b_2$ to vanish requires

$$\{123\cdots N|H|1'2'3\cdots N\}$$
$$=(\hbar^2/2M)\cosh\tfrac{1}{2}(\delta\mathcal{G}_1(0)-\delta\mathcal{G}_{1'}(0))$$
$$\times\cosh\tfrac{1}{2}(\delta\mathcal{G}_2(0)-\delta\mathcal{G}_{2'}(0))\mathcal{G}_{12;1'2'}$$
$$+\{123\cdots N|1|1'2'3\cdots N\}\big[\tfrac{1}{2}E^{(0)}(123\cdots N)$$
$$+\tfrac{1}{2}E^{(0)}(1'2'3\cdots N)+\delta E(1',1)+\delta E(2',2)\big]. \quad (60)$$

As in Eq. (51) the right-hand member of Eq. (60) is not exactly antisymmetrical in the indices 1, 2 or in 1', 2'. For lack of a more logical procedure we follow the precedent set in writing Eq. (52) and replace Eq. (60) by the simplest possible antisymmetric modification:

$$\{123\cdots N|H|1'2'3\cdots N\}$$
$$\cong(\hbar^2/2M)\Big[\prod_{i=1}^{2}\prod_{j=1}^{2}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0)-\delta\mathcal{G}_{j'}(0))\Big]^{1/2}\mathcal{G}_{12;1'2'}$$
$$+\{123\cdots N|1|1'2'3\cdots N\}\big[\tfrac{1}{2}E^{(0)}(123\cdots N)$$
$$+\tfrac{1}{2}E^{(0)}(1'2'3\cdots N)+\tfrac{1}{2}\delta E(1',1)+\tfrac{1}{2}\delta E(2',1)$$
$$+\tfrac{1}{2}\delta E(1',2)+\tfrac{1}{2}\delta E(2',2)\big]. \quad (61)$$

The actual numerical differences introduced by the change are quite small and consequently cannot modify the physical consequences of the formalism in any serious respect (see Appendix B).

Three Orbitals Different

($|a_1|^2=|a_2|^2=|a_3|^2=|b_1|^2=|b_2|^2=|b_3|^2=\frac{1}{2}$)

The actual form for $(1234\cdots N|H|1'2'3'4\cdots N)$ given by Eq. (14) fails to meet the test of complete antisymmetry in the indices 1, 2, 3 or in 1', 2', 3'. We write a properly symmetrized form

$$\{1234\cdots N|H|1'2'3'4\cdots N\}$$
$$=(\hbar^2/2M)\Big[\prod_{i=1}^{3}\prod_{j=1}^{3}\cosh\tfrac{1}{2}(\delta\mathcal{G}_i(0)-\delta\mathcal{G}_{j'}(0))\Big]^{1/3}\mathcal{G}_{123;1'2'3'}$$
$$+\{1234\cdots N|1|1'2'3'4\cdots N\}\big[\tfrac{1}{2}E^{(0)}(1234\cdots N)$$
$$+\tfrac{1}{2}E^{(0)}(1'2'3'4\cdots N)+\tfrac{1}{3}\sum_{i=1}^{3}\sum_{j=1}^{3}\delta E(i,j')\big] \quad (62)$$

representing the simplest possible modification of the formula computed from Eq. (14). Again the changes are small in magnitude and have little effect on the consequences of the formalism.

V. NORMALIZED-ORTHOGONAL BASIS

The matrix $\mathfrak{N}$ constructed from the elements $\{\mathbf{n}|1|\mathbf{n}'\}$ can be used to generate a normalized-orthogonal basis. Write

$$\mathfrak{N}=I+J \quad (63)$$

in which I is the unit matrix and J has only nondiagonal matrix elements. The matrices $\mathfrak{N}^{-1/2}$ and $\mathfrak{N}^{1/2}$ are defined by the binomial series

$$\mathfrak{N}^{-1/2}=I-\tfrac{1}{2}J+\tfrac{3}{8}J^2+\cdots,$$
$$\mathfrak{N}^{1/2}=I+\tfrac{1}{2}J-\tfrac{1}{8}J^2+\cdots. \quad (64)$$

With coefficients taken from Eq. (64) the Löwdin transformation[17]

$$|\mathbf{n}\rangle=\sum_{\mathbf{n}'}|\mathbf{n}'\}\{\mathbf{n}'|\mathfrak{N}^{-1/2}|\mathbf{n}\} \quad (65)$$

generates a normalized-orthogonal basis system and moreover, in this problem, produces a partial diagonalization of the Hamiltonian matrix. First

$$\langle\mathbf{n}'|1|\mathbf{n}\rangle$$
$$=\sum_{\mathbf{n}'',\mathbf{n}'''}\{\mathbf{n}''|\mathfrak{N}^{-1/2}|\mathbf{n}'\}^*\{\mathbf{n}''|1|\mathbf{n}'''\}\{\mathbf{n}'''|\mathfrak{N}^{-1/2}|\mathbf{n}\}$$
$$=\sum_{\mathbf{n}'',\mathbf{n}'''}\{\mathbf{n}'|\mathfrak{N}^{-1/2}|\mathbf{n}''\}\{\mathbf{n}''|1|\mathbf{n}'''\}\{\mathbf{n}'''|\mathfrak{N}^{-1/2}|\mathbf{n}\}$$
$$=\delta(\mathbf{n}'-\mathbf{n}). \quad (66)$$

[17] P. O. Löwdin, J. Chem. Phys. 18, 365 (1950).

Next write the matrix of H in $|\ \}$ representation in the form

$$\mathfrak{IC}=\tfrac{1}{2}(E^{(0)}\mathfrak{N}+\mathfrak{N}E^{(0)})+\mathfrak{W}, \tag{67}$$

in which $\mathfrak{W}$ has only nondiagonal matrix elements and

$$E^{(0)}=(E^{(0)}(\mathbf{n})\delta(\mathbf{n}-\mathbf{n}')), \tag{68}$$

a diagonal matrix with elements defined by Eq. (46). The transformed Hamiltonian is

$$\begin{aligned}H&=\mathfrak{N}^{-1/2}\mathfrak{IC}\mathfrak{N}^{-1/2}\\&=\tfrac{1}{2}[\mathfrak{N}^{-1/2}E^{(0)}\mathfrak{N}^{1/2}+\mathfrak{N}^{1/2}E^{(0)}\mathfrak{N}^{-1/2}]+\mathfrak{N}^{-1/2}\mathfrak{W}\mathfrak{N}^{-1/2}\\&=E^{(0)}+W^{(1)}+W^{(2)}.\end{aligned} \tag{69}$$

$$\begin{aligned}W^{(1)}&=\mathfrak{W}-\tfrac{1}{2}(J\mathfrak{W}+\mathfrak{W}J)\\W^{(2)}&=\tfrac{1}{8}[J,[J,E^{(0)}]]+\cdots\\&\quad+\tfrac{1}{4}[J\mathfrak{W}J+\tfrac{3}{2}J^2\mathfrak{W}+\tfrac{3}{2}\mathfrak{W}J^2]+\cdots.\end{aligned} \tag{70}$$

These results are particularly interesting and useful if $W^{(2)}$ is unimportant. Keeping only $W^{(1)}$, the matrix elements of H reduce to[17a]

$$\begin{aligned}\langle\mathbf{n}|H|\mathbf{n}\rangle&\equiv E^{(1)}(\mathbf{n})\\&=E^{(0)}(\mathbf{n})-\tfrac{1}{2}\sum_{\mathbf{n}''}[\{\mathbf{n}|J|\mathbf{n}''\}\{\mathbf{n}''|\mathfrak{W}|\mathbf{n}\}\\&\qquad+\{\mathbf{n}|\mathfrak{W}|\mathbf{n}''\}\{\mathbf{n}''|J|\mathbf{n}\}],\end{aligned} \tag{71}$$

$$\begin{aligned}\langle\mathbf{n}'|H|\mathbf{n}\rangle&=\{\mathbf{n}'|\mathfrak{W}|\mathbf{n}\}-\tfrac{1}{2}\sum_{\mathbf{n}''}[\{\mathbf{n}'|J|\mathbf{n}''\}\{\mathbf{n}''|\mathfrak{W}|\mathbf{n}\}\\&\qquad+\{\mathbf{n}'|\mathfrak{W}|\mathbf{n}''\}\{\mathbf{n}''|J|\mathbf{n}\}].\end{aligned} \tag{72}$$

We are interested primarily in configurations which contain only a small fraction of excited orbitals. This restriction makes possible a useful simplification in the evaluation of sums over intermediate states as in Eqs. (71) and (72). Introducing the results of Sec. II, Eq. (71) becomes

$$\begin{aligned}\langle\mathbf{n}|H|\mathbf{n}\rangle&=E^{(0)}(\mathbf{n})-\frac{\hbar}{2M}\sum_{\substack{p<q\\p'<q'}}X_{pq;p'q'}X_{p'q';pq}'+\cdots,\end{aligned} \tag{73}$$

with p, q ranging over all orbitals in $\mathbf{n}$ and p', q' over all orbitals outside of $\mathbf{n}$. However, p', q' may be taken over all orbitals outside of the ground-state configuration with negligible error. The presence or absence of a few incorrect terms in the sum over p', q' makes little difference in the value of the sum (*a few* might possibly mean a few percent).

The corresponding treatment of Eq. (72) yields

$$\begin{aligned}\langle 123\cdots N|H|1'2'3\cdots N\rangle&=(\hbar^2/2M)\mathcal{G}_{12;1'2'}-\tfrac{1}{2}(\hbar^2/2M)\sum_{p<q}[X_{12,pq}X_{pq,1'2'}'\\&\qquad+X_{12;pq}'X_{pq;1'2'}]+\cdots.\end{aligned} \tag{74}$$

Again p, q range over all orbitals not in 1, 2, $\cdots$, N, 1′, 2′. As before, negligible error is introduced by allowing p, q to range over all orbitals outside the ground-state configuration. Consequently the matrix element depends only on the orbitals in which initial and final-state functions differ. We may therefore omit all the superfluous common orbitals in labeling nondiagonal matrix elements and write

$$\langle n_1n_2n_3\cdots n_N|H|n_1'n_2'n_3\cdots n_N\rangle=\langle n_1n_2|H|n_1'n_2'\rangle,$$

$$\begin{aligned}\langle n_1n_2n_3n_4\cdots n_N|H|n_1'n_2'n_3'n_4\cdots n_N\rangle&=\langle n_1n_2n_3|H|n_1'n_2'n_3'\rangle\\&=\frac{\hbar^2}{2M}X'_{n_1n_2n_3;n_1'n_2'n_3'}+\cdots.\end{aligned} \tag{75}$$

VI. EXPLICIT FORMULAS FOR MATRIX ELEMENTS

The evaluation of the cluster integrals and their derivatives with respect to β is facilitated by writing the formulas for $X_{p^\star q^\star}(\beta)$ and $X_{n^\star p^\star q^\star}(\beta)$ as defined by Eqs. (15) and (18) in a more compact form:

$$\begin{aligned}X_{p^\star q^\star}(\beta)&=\int\left[\psi_0B^2-\frac{1}{\Omega^N}\right][\sum_{s_1}e^{\beta K(1|p^\star)}|u(1|p^\star)|^2-X_{p^\star}(\beta)][\sum_{s_2}e^{\beta K(2|q^\star)}|u(2|q^\star)|^2-X_{q^\star}(\beta)]dv_{12\ldots N}\\&\quad-\int\psi_0B^2\sum_{s_1,s_2}[e^{\beta K(1|p^\star)}u(1|p^\star)u^*(1|q^\star)][e^{\beta K(2|q^\star)}u(2|q^\star)u^*(2|p^\star)]dv_{12\ldots N},\end{aligned} \tag{76}$$

[17a] *Note added in proof.* The resolution of H into $E^{(0)}+W^{(1)}$ and $W^{(2)}$ requires care in the recognition and segregation of unlinked terms with incorrect dependence on N which occur separately in $W^{(1)}$ and $W^{(2)}$, but cancel in the sum. Such terms are not present in the approximation of Eqs. (73)–(98).

$$X_{n\star p\star q\star}(\beta)=\int\left[\psi_0{}^{B2}-\frac{1}{\Omega^N}\right][\sum_{s_1}e^{\beta K(1|n\star)}|u(1|n\star)|^2-X_{n\star}(\beta)]$$
$$\cdot[\sum_{s_2}e^{\beta K(2|p\star)}|u(2|p\star)|^2-X_{p\star}(\beta)][\sum_{s_3}e^{\beta K(3|q\star)}|u(3|q\star)|^2-X_{q\star}(\beta)]dv_{12\cdots N}$$
$$-\int\psi_0{}^{B2}[\sum_{s_1}e^{\beta K(1|n\star)}|u(1|n\star)|^2-X_{n\star}(\beta)][\sum_{s_2}e^{\beta K(2|p\star)}u(2|p\star)u^*(2|q\star)]$$
$$\cdot[\sum_{s_3}e^{\beta K(3|q\star)}u(3|q\star)u^*(3|p\star)]dv_{12\cdots N}-\cdots$$
$$+\int\psi_0{}^{B2}\sum_{s_1,s_2,s_3}[e^{\beta K(1|n\star)}u(1|n\star)u^*(1|q\star)][e^{\beta K(2|p\star)}u(2|p\star)u^*(2|n\star)]$$
$$\cdot[e^{\beta K(3|q\star)}u(3|q\star)u^*(3|p\star)]dv_{12\cdots N}$$
$$+\int\psi_0{}^{B2}\sum_{s_1,s_2,s_3}[e^{\beta K(1|n\star)}u(1|n\star)u^*(1|p\star)][e^{\beta K(2|p\star)}u(2|p\star)u^*(2|q\star)]$$
$$\cdot[e^{\beta K(3|q\star)}u(3|q\star)u^*(3|n\star)]dv_{12\cdots N}. \quad (77)$$

Here the summation over spin (spin and isospin) variables is exhibited explicitly. Note that $\psi_0{}^B$ is normalized.

Calculations closely paralleling the corresponding development in Ref. 13, Sec. II, yield

$$X_{p\star}=|a_p|^2X_p+|b_p|^2X_{p'},\qquad X_p=1+O(\beta^2),\qquad X_{p'}=1+O(\beta^2). \quad (78)$$

$$NX_{p\star q\star}(0)=-[|a_p|^2|a_q|^2\langle pq,qp\rangle(S(k_{pq})-1)+|a_p|^2|b_q|^2\langle pq',q'p\rangle(S(k_{pq'})-1)$$
$$+|b_p|^2|a_q|^2\langle p'q,qp'\rangle(S(k_{p'q})-1)+|b_p|^2|b_q|^2\langle p'q',q'p'\rangle(S(k_{p'q'})-1)]$$
$$+\delta(\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_p-\mathbf{k}_q)a_p{}^*a_q{}^*b_pb_q[\langle pq,p'q'\rangle(S(k_{pp'})-1)-\langle pq,q'p'\rangle(S(k_{p'q})-1)]+\cdots. \quad (79)$$

Here $S(k)$ is the liquid-structure function defined by the ground-state boson-type solution. The convolution form for the three-particle distribution function[12] is used in evaluating three index-cluster integrals. The spin matrix element $\langle pq,qp\rangle$ has the value 1 for parallel spins and vanishes for antiparallel spins. The general formula is

$$\langle m\cdots q,m'\cdots q'\rangle=\langle m,m'\rangle\cdots\langle q,q'\rangle.$$

$$NX_{p\star q\star'}=[|a_p|^2|a_q|^2\langle pq,qp\rangle(S(k_{pq})-1)(-2\mathbf{k}_p\cdot\mathbf{k}_q+k_{p\star}{}^2+k_{q\star}{}^2)+\cdots$$
$$+|b_p|^2|b_q|^2\langle p'q',q'p'\rangle(S(k_{p'q'})-1)(-2\mathbf{k}_{p'}\cdot\mathbf{k}_{q'}+k_{p\star}{}^2+k_{q\star}{}^2)]-\tfrac{1}{2}\delta(\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_p-\mathbf{k}_q)a_p{}^*a_q{}^*b_pb_q$$
$$\cdot[\langle pq,p'q'\rangle(S(k_{p'p})-1)(k_{pp'}{}^2+k_{qq'}{}^2)-\langle pq,q'p'\rangle(S(k_{p'q})-1)(k_{pq'}{}^2+k_{qp'}{}^2)]+\cdots. \quad (80)$$

$$N^2X_{n\star p\star q\star}(0)=[|a_n|^2|a_p|^2|a_q|^2\langle npq,qnp\rangle(nq,pn,qp)+\cdots+|b_n|^2|b_p|^2|b_q|^2\langle n'p'q',q'n'p'\rangle(n'q',p'n',q'p')]$$
$$+[|a_n|^2|a_p|^2|a_q|^2\langle npq,pqn\rangle(np,pq,qn)+\cdots+|b_n|^2|b_p|^2|b_q|^2\langle n'p'q',p'q'n'\rangle(n'p',p'q',q'n')]$$
$$+\delta(\mathbf{k}_{n'}+\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_n-\mathbf{k}_p-\mathbf{k}_q)a_n{}^*a_p{}^*a_q{}^*b_nb_pb_q[\langle npq,n'p'q'\rangle(nn',pp',qq')$$
$$-\langle npq,n'q'p'\rangle(nn',pq',qp')-\langle npq,q'p'n'\rangle(nq',pp',qn')-\langle npq,p'n'q'\rangle(np',pn',qq')$$
$$+\langle npq,q'n'p'\rangle(nq',pn',qp')+\langle npq,p'q'n'\rangle(np',pq',qn')]-\delta(\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_p-\mathbf{k}_q)a_p{}^*a_q{}^*b_pb_q$$
$$\cdot[|a_n|^2\{\langle npq,q'p'n\rangle(nq',pp',qn)+\langle npq,p'nq'\rangle(np',pn,qq')-\langle npq,q'np'\rangle(nq',pn,qp')$$
$$-\langle npq,p'q'n\rangle(np',pq',qn)\}+|b_n|^2\{\cdots\}]-\cdots. \quad (81)$$

Here we use the convenient notation

$$(np,pq,qn)\equiv(k_{np},k_{pq},k_{qn}),$$
$$(k,k',k'')=(S(k)-1)(S(k')-1)+(S(k')-1)(S(k'')-1)$$
$$+(S(k'')-1)(S(k)-1)+(S(k)-1)(S(k')-1)(S(k'')-1). \quad (82)$$

$$N^2X'_{n\star p\star q\star}=[|a_n|^2|a_p|^2|a_q|^2\{\langle npq,qnp\rangle(nq,pn,qp)(\mathbf{k}_n\cdot\mathbf{k}_q+\mathbf{k}_p\cdot\mathbf{k}_n+\mathbf{k}_q\cdot\mathbf{k}_p-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)$$
$$+\langle npq,pqn\rangle(np,pq,qn)(\mathbf{k}_n\cdot\mathbf{k}_p+\mathbf{k}_p\cdot\mathbf{k}_q+\mathbf{k}_q\cdot\mathbf{k}_n-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)\}+\cdots$$
$$+|b_n|^2|b_p|^2|b_q|^2\{\langle n'p'q',q'n'p'\rangle(n'q',p'n',q'p')(\mathbf{k}_{n'}\cdot\mathbf{k}_{q'}+\mathbf{k}_{p'}\cdot\mathbf{k}_{n'}+\mathbf{k}_{q'}\cdot\mathbf{k}_{p'}-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)$$
$$+\langle n'p'q',p'q'n'\rangle(n'p',p'q',q'n')(\mathbf{k}_{n'}\cdot\mathbf{k}_{p'}+\mathbf{k}_{p'}\cdot\mathbf{k}_{q'}+\mathbf{k}_{q'}\cdot\mathbf{k}_{n'}-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)\}]$$
$$-\delta(\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_p-\mathbf{k}_q)a_p{}^*a_q{}^*b_pb_q$$
$$\cdot[|a_n|^2\{\langle npq,q'p'n\rangle(nq',pp',qn)(\mathbf{k}_n\cdot\mathbf{k}_{q'}+\mathbf{k}_p\cdot\mathbf{k}_{p'}+\mathbf{k}_q\cdot\mathbf{k}_n-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)$$
$$+\langle npq,p'nq'\rangle(np',pn,qq')(\mathbf{k}_n\cdot\mathbf{k}_{p'}+\mathbf{k}_p\cdot\mathbf{k}_n+\mathbf{k}_q\cdot\mathbf{k}_{q'}-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)$$
$$-\langle npq,q'np'\rangle(nq',pn,qp')(\mathbf{k}_n\cdot\mathbf{k}_{q'}+\mathbf{k}_p\cdot\mathbf{k}_n+\mathbf{k}_q\cdot\mathbf{k}_{p'}-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)$$
$$-\langle npq,p'q'n\rangle(np',pq',qn)(\mathbf{k}_n\cdot\mathbf{k}_{p'}+\mathbf{k}_p\cdot\mathbf{k}_{q'}+\mathbf{k}_q\cdot\mathbf{k}_n-\tfrac{1}{2}k_{n\star}{}^2-\tfrac{1}{2}k_{p\star}{}^2-\tfrac{1}{2}k_{q\star}{}^2)\}+|b_n|^2\{\cdots\}]+\cdots$$
$$-\tfrac{1}{2}\delta(\mathbf{k}_{n'}+\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_n-\mathbf{k}_p-\mathbf{k}_q)a_n{}^*a_p{}^*a_q{}^*b_nb_pb_q[\langle npq,n'p'q'\rangle(nn',pp',qq')(k_{nn'}{}^2+k_{pp'}{}^2+k_{qq'}{}^2)$$
$$-\langle npq,n'q'p'\rangle(nn',pq',qp')(k_{nn'}{}^2+k_{pq'}{}^2+k_{qp'}{}^2)-\langle npq,q'p'n'\rangle(nq',pp',qn')(k_{nq'}{}^2+k_{pp'}{}^2+k_{qn'}{}^2)$$
$$-\langle npq,p'n'q'\rangle(np',pn',qq')(k_{np'}{}^2+k_{pn'}{}^2+k_{qq'}{}^2)+\langle npq,q'n'p'\rangle(nq',pn',qp')(k_{nq'}{}^2+k_{pn'}{}^2+k_{qp'}{}^2)$$
$$+\langle npq,p'q'n'\rangle(np',pq',qn')(k_{np'}{}^2+k_{pq'}{}^2+k_{qn'}{}^2)]+\cdots. \quad (83)$$

Equations (79)–(83) should be compared with Eqs. (39) and (40) to determine explicit forms for $X_{pq;p'q'}$, $X_{npq;n'p'q'}$ and their derivatives with respect to β.

VII. QUASIPARTICLE FORMALISM

Equation (48) of Ref. 13 is a general formula for $E^{(0)}(\mathbf{n})$ including three-index terms. An equivalent operator form, employing the discrete number operator formalism, is

$$E_{\text{operator}}{}^{(0)}=\sum_{\mathbf{k},s}\epsilon(k)a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{k}s}+\frac{1}{2N}\sum_{\mathbf{k},\mathbf{l},s}K_2(\mathbf{k}-\mathbf{l})a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{k}s}a_{\mathbf{l}s}{}^{\dagger}a_{\mathbf{l}s}+\frac{1}{2N^2}\sum_{\mathbf{k},\mathbf{l}\neq\mathbf{m};s}K_3(\mathbf{k},\mathbf{l};\mathbf{m})a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{k}s}a_{\mathbf{l}s}{}^{\dagger}a_{\mathbf{l}s}a_{\mathbf{m}s}{}^{\dagger}a_{\mathbf{m}s}, \quad (84)$$

with

$$\epsilon(k)=\hbar^2k^2/2M, \quad K_2(k)=\epsilon(k)(S(k)-1), \quad K_3(\mathbf{k},\mathbf{l};\mathbf{m})=-\epsilon(\mathbf{k}-\mathbf{l})S(\mathbf{k}-\mathbf{l})(S(\mathbf{k}-\mathbf{m})-1)(S(\mathbf{l}-\mathbf{m})-1). \quad (85)$$

The creation and destruction operators $a_{\mathbf{k}s}{}^{\dagger}$, $a_{\mathbf{k}s}$ obey the standard Fermion anticommutator relations.

To find the corresponding operator for $E^{(1)}(\mathbf{n})$, consider first the explicit statement of Eq. (73):

$$E^{(1)}(\mathbf{n})=E^{(0)}(\mathbf{n})+(\hbar^2/2MN^2)\sum_{\substack{p<q\\p'<q'}}\delta(\mathbf{k}_{p'}+\mathbf{k}_{q'}-\mathbf{k}_p-\mathbf{k}_q)\cdot[\langle pq,p'q'\rangle(S(k_{pp'})-1)^2k_{pp'}{}^2$$
$$+\langle pq,q'p'\rangle(S(k_{p'q})-1)^2k_{qp'}{}^2-\langle pq,p'q'\rangle\langle pq,q'p'\rangle(S(k_{pp'})-1)(S(k_{p'q})-1)(k_{pp'}{}^2+k_{qp'}{}^2)]+\cdots. \quad (86)$$

In Eq. (86), p and q are confined to $\mathbf{n}$ while p' and q' range over the quantum number space outside of the Fermi spheres. An equivalent statement is

$$E^{(1)}(\mathbf{n})=E^{(0)}(\mathbf{n})+\frac{1}{2N}\sum_{\mathbf{k}s,\mathbf{l}t}[\langle s,t\rangle L_p(\mathbf{k},\mathbf{l})+(1-\langle s,t\rangle)L_a(\mathbf{k},\mathbf{l})]+\cdots \quad (87)$$

in which $\mathbf{k}s$, $\mathbf{l}t$ range over $\mathbf{n}$ and

$$L_a(\mathbf{k},\mathbf{l})=(1/2N)\sum_{\substack{k'>k_F\\|\mathbf{k}+\mathbf{l}-\mathbf{k}'|>k_F}}[(S(\mathbf{k}-\mathbf{k}')-1)^2(\hbar^2(\mathbf{k}-\mathbf{k}')^2/2M)+(S(\mathbf{l}-\mathbf{k}')-1)^2(\hbar^2(\mathbf{l}-\mathbf{k}')^2/2M)],$$
$$L_p(\mathbf{k},\mathbf{l})=(1/2N)\sum_{\substack{k'>k_F\\|\mathbf{k}+\mathbf{l}-\mathbf{k}'|>k_F}}[(S(\mathbf{k}-\mathbf{k}')-1)^2(\hbar^2(\mathbf{k}-\mathbf{k}')^2/2M)+(S(\mathbf{l}-\mathbf{k}')-1)^2(\hbar^2(\mathbf{l}-\mathbf{k}')^2/2M) \quad (88)$$
$$-(S(\mathbf{k}-\mathbf{k}')-1)(S(\mathbf{l}-\mathbf{k}')-1)(\hbar^2/2M)((\mathbf{k}-\mathbf{k}')^2+(\mathbf{l}-\mathbf{k}')^2)].$$

Equation (87) yields immediately the desired operator form

$$E^{(1)}{}_{\text{operator}}=E^{(0)}{}_{\text{operator}}+(1/2N)\sum_{\mathbf{k},\mathbf{l},s}L_p(\mathbf{k},\mathbf{l})a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{k}s}a_{\mathbf{l}s}{}^{\dagger}a_{\mathbf{l}s}+(1/2N)\sum_{\mathbf{k},\mathbf{l},s}L_a(\mathbf{k},\mathbf{l})a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{k}s}a_{\mathbf{l},-s}{}^{\dagger}a_{\mathbf{l},-s}+\cdots. \quad (89)$$

Here $\mathbf{k}$, $\mathbf{l}$, s are not restricted.

The nondiagonal component of the Hamiltonian matrix can also be expressed in an equivalent operator form:

$$W^{(1)}=W_2+W_3,$$
$$W_2=\tfrac{1}{2}\sum_{\substack{\mathbf{k}s,\mathbf{l}t\\\mathbf{k}'s',\mathbf{l}'t'}}\langle\mathbf{k},\mathbf{l}|w_2|\mathbf{k}',\mathbf{l}'\rangle\langle st,s't'\rangle a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{l}t}{}^{\dagger}a_{\mathbf{l}'t'}a_{\mathbf{k}'s'}, \quad (90)$$
$$W_3=\tfrac{1}{6}\sum_{\substack{\mathbf{k}s,\mathbf{l}t,\mathbf{m}u\\\mathbf{k}'s',\mathbf{l}'t',\mathbf{m}'u'}}\langle\mathbf{k},\mathbf{l},\mathbf{m}|w_3|\mathbf{k}',\mathbf{l}',\mathbf{m}'\rangle\langle stu,s't'u'\rangle\cdot a_{\mathbf{k}s}{}^{\dagger}a_{\mathbf{l}t}{}^{\dagger}a_{\mathbf{m}u}{}^{\dagger}a_{\mathbf{m}'u'}a_{\mathbf{l}'t'}a_{\mathbf{k}'s'}.$$

Here s, t, u denote the single-particle spin states with numerical values $+\frac{1}{2}$ and $-\frac{1}{2}$. The interaction operator w_2 includes contributions from four sources: two index terms in $\mathcal{G}$, three index terms in $\mathcal{G}$, the orthogonality transformation and the δE terms from Eqs. (61) and (62) and Appendix B. To exhibit these contributions separately we write

$$W_2=W_2{}^{(2)}+W_2{}^{(3)}+W_2{}^{(\text{orth.})}+W_2{}^{(\delta E)} \quad (91)$$

and obtain

$$\langle\mathbf{k},\mathbf{l}|w_2{}^{(2)}|\mathbf{k}',\mathbf{l}'\rangle=\frac{\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})}{N}\frac{\hbar^2(\mathbf{k}-\mathbf{k}')^2}{2M}(1-S(\mathbf{k}-\mathbf{k}')). \quad (92)$$

$$\langle \mathbf{k},\mathbf{l}|w_2^{(3)}|\mathbf{k}',\mathbf{l}'\rangle=\frac{\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})}{2N^2}\sum_{q<k_F}\Big[\frac{\hbar^2(\mathbf{k}-\mathbf{q})^2}{2M}(S(\mathbf{k}'-\mathbf{q})-1)(S(\mathbf{k}-\mathbf{q})S(\mathbf{k}-\mathbf{k}')-1)$$
$$+\frac{\hbar^2(\mathbf{k}'-\mathbf{q})^2}{2M}(S(\mathbf{k}-\mathbf{q})-1)(S(\mathbf{k}'-\mathbf{q})S(\mathbf{k}-\mathbf{k}')-1)+\frac{\hbar^2(\mathbf{l}-\mathbf{q})^2}{2M}(S(\mathbf{l}'-\mathbf{q})-1)(S(\mathbf{l}-\mathbf{q})S(\mathbf{k}-\mathbf{k}')-1)$$
$$+\frac{\hbar^2(\mathbf{l}'-\mathbf{q})^2}{2M}(S(\mathbf{l}-\mathbf{q})-1)(S(\mathbf{l}'-\mathbf{q})S(\mathbf{k}-\mathbf{k}')-1)+\frac{\hbar^2(\mathbf{k}-\mathbf{k}')^2}{2M}S(\mathbf{k}-\mathbf{k}')$$
$$\cdot\{(S(\mathbf{k}-\mathbf{q})-1)(S(\mathbf{k}'-\mathbf{q})-1)+(S(\mathbf{l}-\mathbf{q})-1)(S(\mathbf{l}'-\mathbf{q})-1)\}\Big]$$
$$-\frac{\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})}{4N^2}\sum_{q<k_F}[(\hbar^2(k'^2-k^2)/2M)(S(\mathbf{k}-\mathbf{k}')-1)(S(\mathbf{k}-\mathbf{q})-S(\mathbf{k}'-\mathbf{q}))$$
$$+(\hbar^2(l'^2-l^2)/2M)(S(\mathbf{k}-\mathbf{k}')-1)(S(\mathbf{l}-\mathbf{q})-S(\mathbf{l}'-\mathbf{q}))]. \quad (93)$$

$$\langle \mathbf{k},\mathbf{l}|w_2^{(\text{orth.})}|\mathbf{k}',\mathbf{l}'\rangle$$
$$=(\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})/4N^2)\sum_{\substack{k''>k_F\\ |\mathbf{k}+\mathbf{l}-\mathbf{k}''|>k_F}}\frac{\hbar^2}{2M}[(S(\mathbf{k}-\mathbf{k}'')-1)(S(\mathbf{k}'-\mathbf{k}'')-1)((\mathbf{k}-\mathbf{k}'')^2+(\mathbf{k}'-\mathbf{k}'')^2)$$
$$+(S(\mathbf{l}-\mathbf{k}'')-1)(S(\mathbf{l}'-\mathbf{k}'')-1)((\mathbf{l}-\mathbf{k}'')^2+(\mathbf{l}'-\mathbf{k}'')^2)]. \quad (94)$$

$$\langle \mathbf{k},\mathbf{l}|w_2^{(\delta E)}|\mathbf{k}',\mathbf{l}'\rangle=(\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})/2N)(S(\mathbf{k}-\mathbf{k}')-1)\{\delta E(k',k)+\delta E(k',l)+\delta E(l',k)+\delta E(l',l)\}. \quad (95)$$

Note that cosh factors [Eqs. (52) and (58)] are neglected in Eqs. (92) and (93), and only the leading term is given in Eqs. (94) and (95). To the same order of accuracy

$$\langle \mathbf{k},\mathbf{l},\mathbf{m}|w_3|\mathbf{k}',\mathbf{l}',\mathbf{m}'\rangle=-\frac{\delta(\mathbf{k}'+\mathbf{l}'+\mathbf{m}'-\mathbf{k}-\mathbf{l}-\mathbf{m})}{2N^2}(\mathbf{k}-\mathbf{k}',\mathbf{l}-\mathbf{l}',\mathbf{m}-\mathbf{m}')\Big(\frac{\hbar^2(\mathbf{k}-\mathbf{k}')^2}{2M}+\frac{\hbar^2(\mathbf{l}-\mathbf{l}')^2}{2M}+\frac{\hbar^2(\mathbf{m}-\mathbf{m}')^2}{2M}\Big). \quad (96)$$

The summations in Eq. (90) are restricted to nonoverlapping initial and final states. This means that a given wave vector and spin orientation can occur only once in a particular product of creation and destruction operators. Otherwise no constraint (beyond those expressing conservation of momentum and z component of spin) is placed on the wave vectors and spins.

These results may be described in the language of quasiparticles.[18,19] Part of the Hamiltonian $E^{(1)}$ is diagonal in the primary set of occupation number operators $a_{\mathbf{k}s}^\dagger a_{\mathbf{k}s}$. We may say that $E^{(1)}$ is the Hamiltonian for a system of noninteracting (or free) quasiparticles. These are the carriers of momentum, spin, and statistics. The appropriate development of the Landau quasiparticle formalism has already been given in Ref. 13, but only for $E^{(0)}$.

The nondiagonal component of the Hamiltonian $W^{(1)}$ represents interactions (or collisions) involving groups of two and three quasiparticles. These collisions modify and limit the quasiparticle concept in ways that have not been investigated. Some tools, perhaps adequate ones, for evaluating the physical consequences of $E^{(1)}+W^{(1)}$ already exist in modern diagrammatic perturbation and Green's function techniques and (or) the superconducting type of canonical transformation. Problems of immediate interest in the light of current research on liquid He^3 are (1) the range of usefulness, detailed properties, and limitations of the dressed quasiparticle description generated by $E^{(1)}+W^{(1)}$ and (2) the possible existence or nonexistence of an energy gap in the excitation spectrum and the magnitude of the gap if it exists.

A brief comment is in order on the second problem. The leading term in $\langle \mathbf{k},\mathbf{l}|w_2|\mathbf{k}',\mathbf{l}'\rangle$ is

$$(\delta(\mathbf{k}'+\mathbf{l}'-\mathbf{k}-\mathbf{l})/N)(\hbar^2(\mathbf{k}-\mathbf{k}')^2/2M)(1-S(\mathbf{k}-\mathbf{k}')), \quad (97)$$

a positive quantity for mass 4 when k' is not too far from the Fermi surface [since $S(2k_F)<1$ for the He^4 boson system].

Whether or not the same statement holds at mass 3 can only be conjectured at present. Calculations by Walter Massey now in progress should soon provide information on $S(k)$ and $g_B(r)$ at mass 3. It is perhaps safe to conclude that an energy gap at mass 3, if it is actually a consequence of the theory, can only be revealed by careful detailed calculations, and must be quite small in agreement with the trend of studies on the possibility of a superfluid state of liquid He^3.[20]

The interaction matrix element of Eq. (97) defines an effective two-particle point potential in the model co-

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ordinate space:

$$v(r)=(\hbar^2/2M)\Delta g_B(r), \quad r=r_{12}. \tag{98}$$

This potential exhibits a repulsive hill on the rising slope of $g_B(r)$, reverses sign to become attractive in a region more or less centered about the nearest-neighbor peak and thereafter oscillates with rapidly decreasing amplitude and also decreasing spacing between peaks and valleys.

We are encouraged to expect that the uncertain interaction operator $W_2^{(\delta E)}$ has no important physical consequences by the fact that its matrix elements are negligible when the initial- and final-state wave vectors of the colliding quasiparticles are all close to the Fermi surface (see also Appendix B).

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APPENDIX A: ESTIMATE OF $\Delta\mathcal{G}(1',1)\cong\sum_m [X_{1'm}(0)-X_{1m}(0)]$

Equation (79) and the quadratic approximation for $S(k)$ [Ref. 6, Eq. (B1)] yield

$$X_{pq}(0)\cong-(1/N)\{B(k_{pq}/k_F)^2-1\} \tag{A1}$$

on the range $0\leq|k_{pq}|\leq 2k_F$. For He^4, $B=0.195$. In the special case $k_{1'}=k_F$, $k_1=0$:

$$\begin{aligned}\sum_m X_{1'm}(0)&\cong-\frac{s}{N}\frac{\Omega}{(2\pi)^3}\int\left\{B\frac{k_F^2+k^2}{k_F^2}-1\right\}d\mathbf{k}\\&=-3[B(\tfrac{1}{3}+\tfrac{1}{5})-\tfrac{1}{3}]\\\sum_m X_{1m}(0)&\cong-3[B\tfrac{1}{5}-\tfrac{1}{3}].\end{aligned} \tag{A2}$$

Consequently

$$\begin{aligned}\Delta\mathcal{G}(1',1)&\cong-B=-0.195\\\exp\tfrac{1}{8}(\Delta\mathcal{G}(1',1))^2&\cong1+0.005.\end{aligned} \tag{A3}$$

This result justifies the general replacement of exponential amplitude factors by unity in the explicit matrix elements of Eqs. (86)–(96).

APPENDIX B: DERIVATION OF $\delta E(k_{1'},k_1)$ AND NUMERICAL ESTIMATES

$$|a_1|^2=|b_1|^2=\tfrac{1}{2};\ a_n=1,\ b_n=0,\ n>1.$$

$$\delta E(1',1)\equiv\mathcal{G}'(\mathbf{n}^\star)-\tfrac{1}{2}[\mathcal{G}'(12\cdots N)+\mathcal{G}'(1'2\cdots N)] \tag{B1}$$

$$=\sum_{p>1}[x_{1^\star p}'-\tfrac{1}{2}x_{1p}'-\tfrac{1}{2}x_{1'p}']+\tfrac{1}{2}\sum_{p\neq q}[x_{1^\star pq}'-\tfrac{1}{2}x_{1pq}'-\tfrac{1}{2}x_{1'pq}']$$

$$-\sum_{p\neq q}[x_{1^\star p}'-\tfrac{1}{2}x_{1p}'-\tfrac{1}{2}x_{1'p}']x_{pq}-\sum_{p\neq q}[x_{p1^\star}x_{1^\star q}'-\tfrac{1}{2}x_{p1}x_{1q}'-\tfrac{1}{2}x_{p1'}x_{1'q}'] \tag{B2}$$

$$\begin{aligned}=\frac{\hbar^2(k_{1'}^2-k_1^2)}{8MN^2}&\Big[\sum_{k,l<k_F}\{S(\mathbf{k}_1-\mathbf{l})-S(\mathbf{k}_{1'}-\mathbf{l})\}S(\mathbf{k}-\mathbf{l})+\tfrac{1}{2}\{\sum_{l<k_F}S(\mathbf{k}_1-\mathbf{l})\}^2-\tfrac{1}{2}\{\sum_{l<k_F}S(\mathbf{k}_{1'}-\mathbf{l})\}^2\\&-\sum_{k,l<k_F}\{(k_1l,k_1k,lk)-(k_{1'}l,k_{1'}k,lk)\}\Big]+\frac{1}{4N^2}\sum_{k,l<k_F}\{S(\mathbf{k}_1-\mathbf{l})-S(\mathbf{k}_{1'}-\mathbf{l})\}\\&\cdot\left\{(S(\mathbf{k}_{1'}-\mathbf{k})-1)\frac{\hbar^2(\mathbf{k}_{1'}-\mathbf{k})^2}{2M}-(S(\mathbf{k}_1-\mathbf{k})-1)\frac{\hbar^2(\mathbf{k}_1-\mathbf{k})^2}{2M}\right\}.\end{aligned} \tag{B3}$$

The quadratic approximation for $S(k)$ (Appendix A) gives

$$\delta E(1',1)\cong-0.024e_F \tag{B4}$$

at the surface $k_{1'}=k_F$ and $k_1=0$. If both $k_{1'}$ and k_1 are on the Fermi surface δE vanishes.

The relative importance of terms involving δE can be estimated by evaluating the reduced formula generated by Eq. (61):

$$\{12|W|1'2'\}=(\hbar^2/2M)\mathcal{G}_{12;1'2'}+\{12|1|1'2'\}\tfrac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\delta E(i,j'). \tag{B5}$$

In the special case $k_1=k_2=0$, $\mathbf{k}_{2'}=-\mathbf{k}_{1'}$ with opposed spins in both pairs and $k_{1'}=k_{2'}=k_F$, Eq. (B4) holds for all i, j on the range 1, 2. Again using the quadratic approximation for $S(k)$,

$$\begin{aligned}(\hbar^2/2M)\mathcal{G}_{12;1'2'}&\cong((1-B)/N)e_F,\\\{12|1|1'2'\}\tfrac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\delta E(i,j')&\cong((1-B)/N)e_F\times0.048\\&\cong0.048(\hbar^2/2M)\mathcal{G}_{12;1'2'}.\end{aligned} \tag{B6}$$

APPENDIX C: APPROXIMATE ANALYTICAL FORM FOR $g_B(r)$

Theoretical formulas for $g_B(r)$ have been computed by Walter Massey using an adaptation of the Wu-Feenberg[6] procedure for computing the ground-state properties of a boson system. In our illustrative calculations we use one of Massey's forms for liquid He^4 at the equilibrium density ($\rho=0.0218$ Å^{-3}):

$$\begin{aligned} &g_B(r)=g_B{}^0(r)+\delta g_B(r),\\ &g_B{}^0(r)=e^{-(d/r)^n}[1+a(d/r)^n+b(d/r)^{2n}],\\ &\delta g_B(r)=A\exp-(1+z)(d/r)^n(d/r)^m\\ &\qquad\qquad\times[1-B(d/r)^n+C(d/r)^{2n}]. \end{aligned} \tag{C1}$$

The constants occurring in $g_B{}^0$ are subject to the constraint

$$b=\frac{n}{1-3/n}\left[\frac{1}{3}\frac{a}{n}\frac{1}{4\pi\rho d^3\Gamma(1-3/n)}\right] \tag{C2}$$

imposed by the normalization condition of Eq. (36). The correction term δg_B is constructed to leave the normalization of $g_B{}^0$ unchanged.

The curves plotted in Fig. 1 are based on the numerical values

$$\begin{aligned} &n=6, \quad m=6, \quad z=6,\\ &a=0.8, \quad b=1.737, \quad d=3.34\text{ Å},\\ &A=0.2, \quad B=100, \quad C=401.3. \end{aligned} \tag{C3}$$

APPENDIX D: CONSISTENCY CALCULATIONS ON TRUNCATED FORMS OF $\mathcal{G}(n^\star|\beta)$

We truncate the expansions for $\mathcal{G}_{iy}$ and $\mathcal{G}_{aht}$ at 3-index terms. Equations (23) and (29) are replaced by

$$\begin{aligned} \mathcal{G}_{iy}(\mathbf{n}^\star|\beta)=&\sum_{m<n} X_{m^\star n^\star}\\ &+\lambda_{iy}\sum_{m<n<p}[X_{m^\star n^\star p^\star}-X_{m^\star n^\star}X_{n^\star p^\star}\\ &-X_{m^\star p^\star}X_{p^\star n^\star}-X_{n^\star m^\star}X_{m^\star p^\star}], \end{aligned} \tag{D1}$$

$$\mathcal{G}_{aht}(\mathbf{n}^\star|\beta)=\tfrac{1}{2}N^2X^{(2)}+\tfrac{1}{6}\lambda_{aht}N^3(X^{(3)}-3X^{(2)2}). \tag{D2}$$

The adjustable parameters λ_{iy} and λ_{aht} permit a partial compensation for the omission of higher order terms.

Equation (34) is replaced by

$$F_{iy}(r)=1+F^{(2)}(r)+\lambda_{iy}F_{iy}{}^{(3)}(r), \tag{D3}$$

$$F_{aht}(r)=1+F^{(2)}(r)+\lambda_{aht}F_{aht}{}^{(3)}(r). \tag{D4}$$

To satisfy the normalization condition of Eq. (37), the amplitude parameters must assume the values listed in Table III.

The extremum property of $\{\mathbf{n}|H|\mathbf{n}\}$ may be lost when approximate procedures are used to evaluate the expectation value. Also the degree of failure may depend on density to a sufficient extent to falsify a theoretical equation of state based on the approximate procedure. These effects actually occur in a recent unpublished investigation of the cluster expansion procedure for evaluating the ground-state energy of liquid He^4.[21] Results associated with $S(0)=0$ appear reasonable; all others have doubtful significance. In the present context the use of λ to enforce the condition $S_F(0)=0$ may serve to avoid difficulties similar to those uncovered by Williams in his study of the He^4 liquid.

TABLE III. λ determined by $S_F(0)=0$ (g_B from Appendix C).

s	λ_{iy}	λ_{aht}
1	0.883	0.889
2	0.778	0.783
3	0.630	0.630

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