Density matrix of quantum fluids*

M. L. Ristig
Institut für Theoretische Physik, Universität zu Köln, 5-Köln-41, Germany

J. W. Clark
Department of Physics, Washington University, St. Louis, Missouri 63130
(Received 19 January 1976)

An elaborate cluster analysis of the single-particle occupation probability $n_{\hat{q}}$ and associated one-body density matrix $n(r)$ is performed for a Fermi system described by a Jastrow wave function. A diagrammatic formalism rooted in Ursell-Mayer theory facilitates the analysis. It is conjectured, and demonstrated to convincingly high cluster order, that $n_{\hat{q}}$ may be written as $n[N(q)+N_1(q)]$, where n is a strength factor independent of wave number q and the quantities $N(q)$ and $N_1(q)$ may be expressed as series of irreducible cluster contributions. The strength factor n has the form $n = e^Q$, where Q may also be expressed as a series of irreducible cluster contributions. Massive partial summations on the latter series yield a compact expression for Q in terms of the spatial distribution functions corresponding to the Jastrow wave function. Working with the Fourier inverse of $n_{\hat{q}}$, it is further demonstrated that $n(r)$ may be cast in the form $\rho n[N_1(r)+N_2(r)]\exp[-\mathcal{Q}(r)]$, where ρ is the particle density and the functions $N_1(r)$, $N_2(r)$, and $\mathcal{Q}(r)$ are all given by irreducible cluster series. Massive partial summations are executed in the $\mathcal{Q}(r)$ series to achieve a compact expression of this quantity in terms of the aforementioned spatial distribution functions. One has $\mathcal{Q}(0) = Q$. The leading diagrams necessary for a quantitative evaluation of the momentum distribution of liquid ^{3}He and nuclear matter are displayed. Specialization to infinite degeneracy of the single-particle levels, while shrinking the Fermi wave number to zero (Bose limit), allows liquid ^{4}He to be treated as well. In this limit off-diagonal long-range order appears, the condensate fraction $\rho^{-1}n(\infty) = n_c$ being just the strength factor n. It may also be shown (under certain reasonable assumptions) that the customary r^{-2} long-range behavior of the two-body correlations implies a singular behavior $n_q = n_c(mc/2\hbar)q^{-1}$ of the Bose momentum distribution for small q.

I. INTRODUCTION

Significant contributions have been made to the microscopic description of strongly interacting quantum fluids.[1] But despite a wealth of experimental information[2] we are still some distance from a complete theory of excitations and of the properties of the ground states of dense Bose and Fermi fluids. Indeed little is known rigorously, and approximations are often predicated upon methodological limitations rather than physical insight. For instance, theoretical estimates of the depletion of the zero-momentum single-particle state of liquid ^{4}He depend strongly on the method employed. For zero temperature the predictions range between 92% and 50%, not to mention results which give more than 100%.[3-9] Even the theoretical result which is most trusted at present[6] is in clear disagreement with experiment.[10-14]

In view of such deficiencies, it would seem imperative to gain a better understanding of the ground state of a many-body system, before thermodynamic or particle nonconserving features are brought into the picture.[15]

Advances in the theoretical description of dense quantum systems within the framework of the method of correlated basis functions[16,17] open the prospect of a quantitative understanding of the ground-state properties of Bose and Fermi fluids at medium and high densities. The total energy and related quantities, along with the spatial distribution functions and structure functions, have been the objects of detailed studies within this framework.[16] Less attention has been devoted to the one-particle density matrix, or equivalently the one-particle momentum distribution. The new experimental results for the momentum distribution of liquid ^{4}He call for a thorough theoretical examination of these quantities.[14]

In a useful first step toward a complete microscopic theory of the momentum distribution of a uniform extended Bose or Fermi system, the expectation value of the occupation number operator for orbital $\hat{q}$ may be evaluated for a correlated trial ground-state function of Jastrow form:

$$n_{\hat{q}} = \langle\Psi|a^\dagger_{\hat{q}}a_{\hat{q}}|\Psi\rangle/\langle\Psi|\Psi\rangle\,, \tag{1}$$

$$\Psi = F\Phi\,,\quad F=\prod_{i<j}^{A} f(r_{ij})\,. \tag{2}$$

Here, Φ is to be taken as the box-normalized ground-state wave function of the A-particle system with the interactions turned off, and the function F incorporates spatial correlations arising from the interactions, with $f(r)\to 1$ as $r\to\infty$.[17] For a Bose system the wave function Φ is to be set constant and the operator $a^{\dagger}_{\hat{q}}$ (respectively, $a_{\hat{q}}$) creates (destroys) a particle with momentum $\hbar\vec{q}$. For a system of fermions the wave function is the Slater determinant of the lowest A single-particle states (the "occupied" orbitals) and the operator $a^{\dagger}_{\hat{q}}$ (respectively, $a_{\hat{q}}$) creates (destroys) a particle in orbital $\hat{q}$ with momentum $\hbar\vec{q}$ and specified spin, isospin projections.

The ansatz (2) allows the straightforward development of a workable and useful method for calculating the occupation probability of orbital $\hat{q}$ in the presence of *long*-range as well as *short*-range correlations. Once the structure of the expectation value (1) is understood one can generalize to more elaborate treatments of the correlations. The quantity F may be permitted, at this next stage, to be state dependent[17] or to contain three-, four-, ..., n-body correlation factors in addition to the pair correlation factors $f(r_{ij})$.[18]

It is simple and convenient to give a unified treatment of Fermi and Bose systems. The occupation probability (1) will be studied for a normal Fermi system with *ν-fold* degeneracy. Proper specialization of the results to $\nu = A$ will lead to the density matrix and momentum distribution of the superfluid Bose system described by ansatz (2).[15]

To gain insight into what structure the expectation value (1) might have we develop it in a (factorized) Iwamoto-Yamada cluster expansion.[19,20] (The basic features of this expansion are summarized in Appendix A.) Standard procedures are available to determine any term of such a series.[17,20] In principle the evaluation of cluster contributions to the momentum distribution (1) is therefore elementary. For Bose systems this task has been attempted before.[7] However, the analytic expressions for the contributions beyond the two-body term are exceedingly cumbersome. This difficulty can be overcome by a graphical formulation.[21,22] We shall employ generalized Ursell-Mayer diagrams, which have provided a very efficient means for studying the radial distribution function[23] and the expectation value of the ground-state energy.[24,25] In this paper we use the notations and rules which have been developed in Ref. 23. (Appendix B provides an adequate summary, with examples.)

We shall present results for the two-, three-, and four-body cluster contributions to the (factorized) cluster expansion of the occupation probability $n_{\hat{q}}$. The *direct* contributions of the five-body cluster are also available. The sequence of diagrams evaluated is sufficient to reveal the structure of quantity (1) and the associated one-particle density matrix.

It is found that $n_{\hat{q}}$ contains a "strength" factor which is independent of the orbital $\hat{q}$. Specializing to bosons, this factor may be identified with the fraction of particles in the zero-momentum single-particle state (condensate fraction).[4,26,27]

The cluster expansion of the strength factor contains *reducible* diagrams among other linked graphs. On the other hand the logarithm of this quantity proves to consist of *irreducible* diagrams only. Further, its expansion may be rearranged to allow massive partial summation to all orders. This procedure results in an expansion of the logarithm of the strength factor in terms of the two-, three-, ... body spatial distribution functions.

To elucidate the further structure of quantity (1) we transform to coordinate space and deal with the one-particle density matrix, which is susceptible to a similar (but more elaborate) diagrammatic analysis, again involving partial summations which bring in the n-particle distribution functions, $n = 2, 3, 4, \ldots$.

Some formal work remains to be done on the approach described here. General proofs are needed for the various theorems and summations which are suggested by studying the cluster terms of low order. Perhaps additional higher-order terms need explicit consideration. But we feel that the present approach shows distinct promise as a practical means to quantitative evaluation of the occupation probability of single-particle states in quantum fluids at physical densities. Preliminary numerical results for liquid ^{4}He at zero temperature have already been reported.[28] Detailed numerical studies for the helium liquids and other quantum fluids are in progress. The results will be presented in a sequel to this article.

The organization of the paper is as follows: Section II contains the material basic to our structural study of the occupation probability and one-particle density matrix. The strength factor is extracted and analyzed in Sec. III. The expansion of the density matrix in terms of distribution functions is developed in Sec. IV. Section V specializes our results for a description of the density matrix and momentum distribution of interacting bosons. Two appendixes collect necessary formalism, definitions, and diagrams; a third sketches an alternative derivation of our Bose results.

II. OCCUPATION PROBABILITY

In this study we shall approximate the ground state of a large number A of strongly interacting fermions by the correlated wave function (2). To proceed, we write the occupation number operator

$a_{\hat{q}}^{\dagger}a_{\hat{q}}$ appearing in Eq. (1) as a sum of A one-body operators, $\sum_{i=1}^{A}\nu_{\hat{q}}(i)$, the action of the operator $\nu_{\hat{q}}(i)$ on the plane-wave orbital $|j(i)\rangle$ being expressed by $\nu_{\hat{q}}(i)|j(i)\rangle=\delta_{\hat{q}j}|j(i)\rangle$. The expectation value of the operator $\sum_{i=1}^{A}\nu_{\hat{q}}(i)$, i.e., the occupation probability for orbital $\hat{q}$, can then be developed in a factor-cluster expansion of Iwamoto-Yamada type[19] by applying standard procedures.[17] In the thermodynamic limit (meaning the particle number A goes to infinity with the density ρ kept constant) quantity (1) is thereby decomposed into an infinite series of terms

$$n_{\hat{q}}=(\Delta n_{\hat{q}})_1+(\Delta n_{\hat{q}})_2+\cdots+(\Delta n_{\hat{q}})_m+\cdots . \tag{3}$$

The general term $(\Delta n_{\hat{q}})_m$, the m-body part of the expectation value, is proportional to A^0, exhibiting the linked-cluster property of the expansion. Needed for this decomposition are the one-, two-, ..., m-, ... body versions of the wave function (2). The essentials of the cluster expansion procedure are presented in Appendix A, where the two-body cluster $(\Delta n_{\hat{q}})_2$ is explicitly constructed. The three-, four-, ... body cluster contributions may be obtained in the same fashion. It is advisable to evaluate them separately for momenta above and below the Fermi surface, $q=k_F$. For momenta *above* the surface we find the following structure:

$$\begin{aligned}
&(\Delta n_{\hat{q}})_1=0\,,\\
&(\Delta n_{\hat{q}})_2=[\Delta N(q)]_2\,,\\
&(\Delta n_{\hat{q}})_3=(\Delta n)_2[\Delta N(q)]_2+[\Delta N(q)]_3\,,\\
&(\Delta n_{\hat{q}})_4=(\Delta n)_3[\Delta N(q)]_2+(\Delta n)_2[\Delta N(q)]_3+[\Delta N(q)]_4\,,\\
&\quad\vdots
\end{aligned} \tag{4}$$

The various quantities $(\Delta n)_2,\ldots,[\Delta N(q)]_2,\ldots$ appearing in sequence (4) can be described most efficiently in terms of generalized Ursell-Mayer diagrams. Appendix B collects the necessary definitions and rules of diagrammatic correspondence (for more detail, see Ref. 23). The linked-cluster property of the expansion (3) ensures that the terms $(\Delta n_{\hat{q}})_2, (\Delta n_{\hat{q}})_3, \ldots$ are represented by connected (linked) graphs. However, we may (in the familiar manner) exploit the conservation of momentum to express the contribution of any reducible diagram as a product of two (or more) simpler contributions. Here, a reducible diagram is one that can be split into two disconnected parts by cutting at a single dot (vertex). This standard procedure generates the terms of sequence (4) which contain the factors $(\Delta n)_2, (\Delta n)_3, \ldots$.

An extensive analysis yields for the momentum-independent quantities $(\Delta n)_2, \ldots$ the results shown in Fig. 1. The graphs of the last bracket of Fig. 1

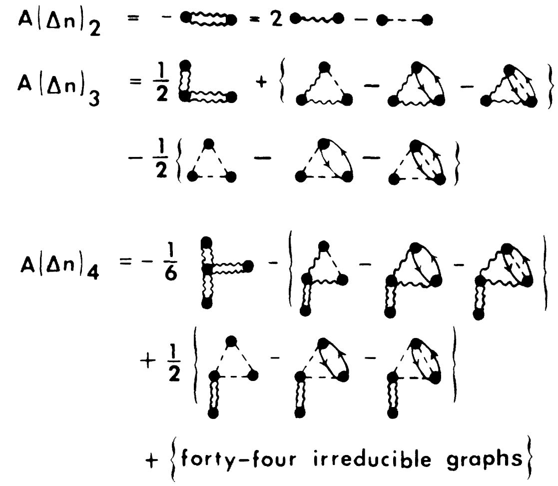

FIG. 1. Graphical representation of leading cluster contributions to the strength factor n.

are explicitly available. The wavy (dashed) line represents the function $\zeta(r)=f(r)-1$ [the function $\eta(r)=f^2(r)-1$]. The oriented line represents the exchange factor $l(k_F r)$, where

$$l(x)=3x^{-3}(\sin x - x\cos x)\,, \tag{5}$$

and is accordingly called an exchange line (see Appendix B and Fig. 11).

The momentum-dependent quantities $[\Delta N(q)]_2, \ldots$ which enter the right-hand side of Eqs. (4) can be given diagrammatic expression if we introduce an additional type of oriented line, to represent the function $A^{-1}e^{i\vec{q}\cdot\vec{r}}$ (see Appendix B and Fig. 11). In this case the arrow indicates the exchange of momentum $\hbar\vec{q}$ between the two particles involved. The two- and three-body quantities are then represented as in Fig. 2. The four-body quantity $[\Delta N(q)]_4$ is explicitly known but is not displayed because of its prohibitive length.

It is worth noting here that the diagrams gener-

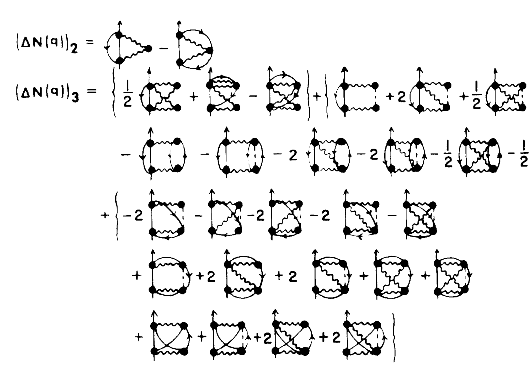

FIG. 2. Graphical representation of the two- and three-body contributions to the cluster expansion defining the function $N(q)$.

ated in this article for various quantities will be such that the oriented lines always form closed loops. Such loops will either consist entirely of exchange lines, or will consist of a chain of exchange lines closed by a directed line representing the transfer of momentum $\hbar\vec{q}$. This property, holding in any cluster order, is in concert with the conservation of particle number.

The composition of the expressions on the right-hand side in Eqs. (4) suggests the factorization theorem

$$n_{\hat{q}} = nN(q) . \tag{6}$$

The first factor is defined by the cluster series

$$n = 1 + (\Delta n)_2 + (\Delta n)_3 + (\Delta n)_4 + \cdots . \tag{7}$$

It is independent of orbital $\hat{q}$ and is an overall measure of the "strength" of the distribution (1). The second factor in relation (6) is defined by the expansion

$$N(q) = [\Delta N(q)]_2 + [\Delta N(q)]_3 + [\Delta N(q)]_4 + \cdots . \tag{8}$$

On the basis of Fig. 2 and the graphical representation of $[\Delta N(q)]_4$, it is asserted as part of the factorization theorem that the function (8) contains only *irreducible* diagrams. Detailed study of components (7) and (8) is reserved for the forthcoming sections.

Next we concentrate on the cluster contributions to expression (3) for momenta below the Fermi surface. In this case we may decompose the expectation value (1) into two parts,

$$n_{\hat{q}} = nN(q) + m_{\hat{q}} , \quad \hat{q} \in \text{Fermi sea} . \tag{9}$$

The first term is the analytic function which has been introduced in Eq. (6), but continued into the Fermi sea. The second term $m_{\hat{q}}$ takes account of the fact that orbital $\hat{q}$ is occupied, i.e., it describes the effect of the Fermi medium. Applying standard cluster techniques for this component we arrive at the expansion

$$m_{\hat{q}} = 1 + (\Delta m_{\hat{q}})_2 + (\Delta m_{\hat{q}})_3 + (\Delta m_{\hat{q}})_4 + \cdots ,$$
$$\hat{q} \in \text{Fermi sea} . \tag{10}$$

The term $(\Delta m_{\hat{q}})_2$ is explicitly displayed in Appendix A. The three-, four-, ... body contributions may be formed in the same manner. The results show a pattern which is similar to that of sequence (4), in conformity with the anticipated analog of property (6),

$$m_{\hat{q}} = nM(q) , \quad \hat{q} \in \text{Fermi sea} . \tag{11}$$

The constant n is the strength factor defined by Eq. (7). The function $M(q)$ is explicitly available through its two- and three-body terms in the defining expansion

$$M(q) = 1 + [\Delta M(q)]_2 + [\Delta M(q)]_3 + \cdots , \quad q < k_F . \tag{12}$$

See Fig. 3. The contributions to (12) are presumably all irreducible.

Insertion of result (11) into relation (9) yields for the occupation probability of occupied orbitals $\hat{q}$ the expression

$$n_{\hat{q}} = n[N(q) + M(q)] . \tag{13}$$

Comparing with formula (6) for unoccupied levels $\hat{q}$ we find a discontinuity at the Fermi surface of

$$Z_{k_F} = nM(k_F) . \tag{14}$$

This quantity measures the strength of the quasiparticle pole. The latter has been studied recently within a special model of nuclear matter.[29] According to Ref. 29 the value of the pole strength depends rather sensitively on long-range effects. Use of Fig. 3 in conjunction with the method of evaluating the strength factor n to be described in Sec. III, should permit a quantitative evaluation of Z_{k_F}, providing an independent check of the behavior claimed.

It is convenient for further considerations to introduce the discontinuous function

$$N_1(q) = \Theta(k_F - q)M(q) , \tag{15}$$

with $\Theta(x) = 1$ for $x > 0$, $\Theta(x) = 0$ otherwise. Equations (6) and (13) may then be combined as

$$n_{\hat{q}} = n[N(q) + N_1(q)] , \tag{16}$$

which applies to any orbital $\hat{q}$.

Insertion of relation (12) into definition (15) generates the cluster expansion

$$N_1(q) = [\Delta N_1(q)]_2 + [\Delta N_1(q)]_3 + [\Delta N_1(q)]_4 + \cdots . \tag{17}$$

The cluster terms may be constructed explicitly from the diagrammatic representation of Fig. 3, to obtain the results shown in Fig. 4.

III. STRENGTH FACTOR

All information about the properties of the quantities n, $N(q)$, $M(q)$, and $N_1(q)$ is stored in their respective cluster expansions (7), (8), (12), and

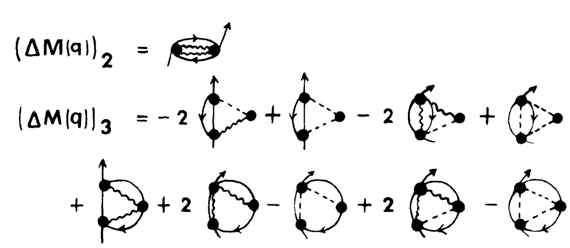

FIG. 3. Same as Fig. 2, but for $M(q)$.

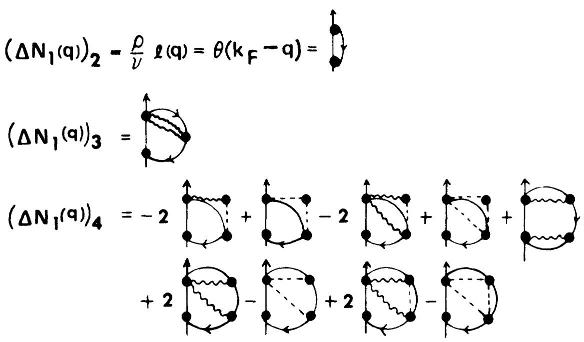

FIG. 4. Graphical representation of the two-, three-, and four-body contributions to the cluster expansion defining the function $N_1(q)$.

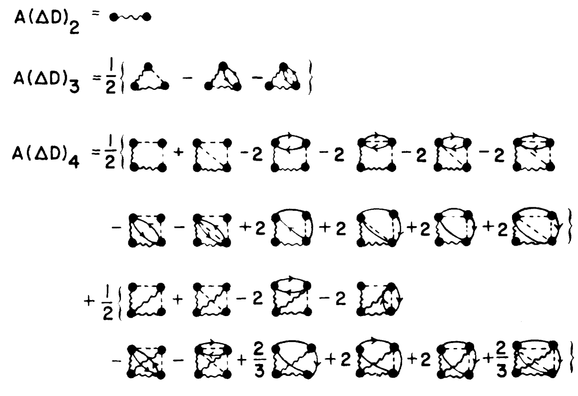

FIG. 5. Graphical representation of the two-, three-, and four-body contributions to the cluster expansion defining the functional $D[\xi]$.

(17). We begin our detailed analysis of these objects with the simplest one, namely, the strength factor n. Its study provides important clues as to the structure of the more complicated momentum-dependent quantities.

The set of graphs displayed in Fig. 1 shows that the diagrammatic expansion of the strength factor n contains both reducible and irreducible graphs. Is it possible to find a function of the quantity n which is represented by irreducible diagrams only? Apparently so: the logarithm

$$Q = \ln n \tag{18}$$

proves to have this property, at least up to four-body cluster order.

We verify this assertion by developing Q in powers of $n-1$. Then we express each term of this power series using the cluster expansion (7) and collect together the two-, three-, four-, ... body contributions. This procedure generates the expansion

$$Q = (\Delta Q)_2 + (\Delta Q)_3 + (\Delta Q)_4 + \cdots , \tag{19}$$

with

$$\begin{aligned} (\Delta Q)_2 &= (\Delta n)_2 , \\ (\Delta Q)_3 &= (\Delta n)_3 - \tfrac{1}{2}(\Delta n)_2^2 , \\ (\Delta Q)_4 &= (\Delta n)_4 - (\Delta n)_3 (\Delta n)_2 + \tfrac{1}{3}(\Delta n)_2^3 , \\ &\vdots \end{aligned} \tag{20}$$

Inserting into (20) the graphical representations of Fig. 1, it is easily confirmed that only irreducible contributions survive.

We may separate the irreducible diagrams into two distinct classes: the first consists of all diagrams containing wavy lines; the second consists of all diagrams without wavy lines. The available collection of irreducible Q diagrams yielded by the n diagrams of Fig. 1 attests to the decomposition

$$Q = 2D[\zeta(r)] - D[\eta(r)] . \tag{21}$$

The functional $D[\zeta]$ is defined by the cluster expansion

$$D[\zeta] = (\Delta D)_2 + (\Delta D)_3 + (\Delta D)_4 + \cdots . \tag{22}$$

The two-, three-, and four-body cluster terms, known explicitly, are given in graphical form in Fig. 5. To construct $D[\eta]$, replace all the wavy lines by dashed lines. We note that derivation of the four-body cluster term $(\Delta D)_4$ requires explicit knowledge of the 44 diagrams of Fig. 1 that we did not specify.

If only short-range correlations are present—short compared to the cube root of the specific volume—it should be permissible to truncate the functional $D[\zeta]$ at some low cluster order, i.e., low order in the number of bodies. If longer-range correlations are present a rearrangement of expansion (22) is indicated. A detailed study of the terms in Fig. 5 suggests the scheme depicted in Fig. 6. The second diagrammatic contribution in Fig. 6 stands for

$$\rho^3 \int \zeta(r_{13})\zeta(r_{23})[g(r_{12}) - 1] d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3 , \tag{23}$$

the function $g(r)-1$ being represented by the blob with two dots on it. Here, $g(r)$ is the radial distribution function, defined by[16]

$$g(r_{12}) = A(A-1)\frac{1}{\rho^2 N} \sum_{\sigma} \int \Psi^* \Psi\, d\vec{r}_3\, d\vec{r}_4 \cdots d\vec{r}_A , \tag{24}$$

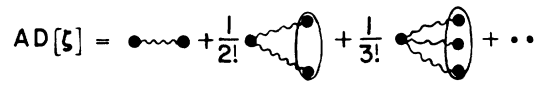

FIG. 6. Symbolic representation of the compact expansion of the functional $D[\xi]$ in terms of spatial distribution functions.

in which N is the norm of the wave function Ψ and $\sum_\sigma$ indicates summation over all spin variables.

The third diagrammatic contribution in Fig. 6 involves, in addition, the three-body distribution function

$$g(\vec{r}_1, \vec{r}_2, \vec{r}_3) = A(A-1)(A-2)\frac{1}{\rho^3 N} \times \sum_\sigma \int \Psi^*\Psi \, d\vec{r}_4 \cdots d\vec{r}_A . \tag{25}$$

In terms of the physical quantities (24) and (25), this third contribution is given analytically by

$$\rho^4 \int \zeta(r_{14})\zeta(r_{24})\zeta(r_{34})\{\cdots\}\, d\vec{r}_1\, d\vec{r}_2\, d\vec{r}_3\, d\vec{r}_4 ,$$
$$\{\cdots\} = g(\vec{r}_1, \vec{r}_2, \vec{r}_3) - g(r_{12}) - g(r_{13}) - g(r_{23}) + 2 . \tag{26}$$

The curly bracket is represented graphically by the blob with three dots on it.

A cluster development[16,22,23] within the integrals (23) and (26) generates exactly the two-, three-, and four-body terms (Fig. 5) of the expansion (22), plus higher-body terms.

Transformation of the integrals (23) and (26) into momentum space leads to a direct physical interpretation of the expansion depicted in Fig. 6, in terms of density fluctuations. The natural quantities for describing these fluctuations are the structure functions[18]

$$S_2(\vec{k}_1, \vec{k}_2) = \frac{1}{A}\frac{1}{N}\sum_\sigma \int \Psi^* \rho_{\vec{k}_1}\rho_{\vec{k}_2}\Psi \, d\vec{r}_1 \cdots d\vec{r}_A = \delta(\vec{k}_1 + \vec{k}_2) S(k) ,$$
$$S_3(\vec{k}_1, \vec{k}_2, \vec{k}_3) = \frac{1}{A}\frac{1}{N}\sum_\sigma \int \Psi^* \rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}\Psi \, d\vec{r}_1 \cdots d\vec{r}_A , \tag{27}$$

with the fluctuation operator $\rho_{\vec{k}} = \sum_1^A e^{i\vec{k}\cdot\vec{r}_j}$ as the basic ingredient. Exploiting the close relationship of the quantities (27) with the distribution functions (24), (25), we may recast (23), (26), respectively, as

$$A\rho \frac{1}{(2\pi)^3}\int \zeta^2(k)[S(k) - 1]d\vec{k} , \tag{28}$$

$$A\rho \frac{1}{(2\pi)^6}\int \zeta(k_1)\zeta(k_2)\zeta(|\vec{k}_1 + \vec{k}_2|)\{\cdots\}\, d\vec{k}_1\, d\vec{k}_2 , \tag{29}$$

where now

$$\{\cdots\} = S_3(\vec{k}_1, \vec{k}_2, -\vec{k}_1 - \vec{k}_2) - S(k_1) - S(k_2) - S(|\vec{k}_1 + \vec{k}_2|) + 2 . \tag{30}$$

The function $\zeta(k)$ is the Fourier transform of $\zeta(r)$. A reasonable estimate of the contribution (29) is obtained by replacing the curly bracket by its "convolution-approximation,"[16] i.e.,

$$\{\cdots\} \approx [S(k_1) - 1][S(k_2) - 1][S(|\vec{k}_1 + \vec{k}_2|) + 2] . \tag{31}$$

Figure 6 is seen to provide a highly compact expansion, which will serve as the basis for a quantitative evaluation of the strength factor n via

$$n = \exp(2D[\zeta] - D[\eta]) . \tag{32}$$

The factor n is manifestly non-negative. In Sec. V we shall see that upon specialization to a Bose system this quantity may be identified with the fraction of particles in the zero-momentum single-particle state.

IV. DENSITY MATRIX

The relation

$$\langle \vec{r}' | \Gamma_1 | \vec{r}'' \rangle = n(r) = \nu \frac{1}{(2\pi)^3}\int n_{\vec{q}} e^{-i\vec{q}\cdot\vec{r}} d\vec{q} , \quad r = |\vec{r}' - \vec{r}''| , \tag{33}$$

defines the one-particle density matrix of the ground state of a Fermi system. Normalization is such that the density matrix approaches the particle density ρ for vanishing relative distance r. Employing Eq. (16) for the occupation probability we may write

$$n(r) = \rho n[N_1(r) + N(r)] \tag{34}$$

upon introducing the inverse Fourier transforms

$$N_1(r) = \frac{\nu}{\rho}\frac{1}{(2\pi)^3}\int N_1(q) e^{-i\vec{q}\cdot\vec{r}} d\vec{q} , \tag{35}$$

$$N(r) = \frac{\nu}{\rho}\frac{1}{(2\pi)^3}\int N(q) e^{-i\vec{q}\cdot\vec{r}} d\vec{q} . \tag{36}$$

The cluster expansion of the function $N_1(r)$ follows from Eq. (17):

$$N_1(r) = [\Delta N_1(r)]_2 + [\Delta N_1(r)]_3 + [\Delta N_1(r)]_4 + \cdots . \tag{37}$$

Transforming the cluster contributions of Fig. 4 according to (35), one generates the diagrams shown in Fig. 7. (Note that in this process the ar-

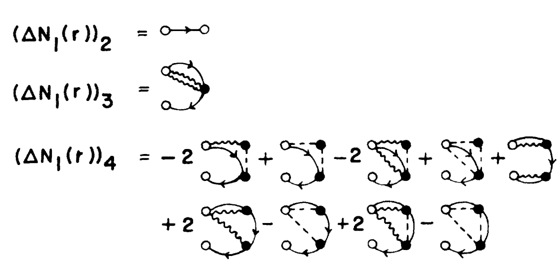

FIG. 7. Graphical representation of the two-, three-, and four-body contributions to the cluster expansion of the function $N_1(r)$.

row element corresponding to $A^{-1}e^{i\vec{q}\cdot\vec{r}_{12}}$ is stripped off and the solid dots to which this element was attached are replaced by open ones. For sample analytic expressions see Appendix B.)

The function $N(r)$ has a richer structure, which we may uncover by considerations much like those involved in Sec. III.

Insertion of the series (8) into the defining relation (36) leads to the cluster expansion

$$N(r)=[\Delta N(r)]_2+[\Delta N(r)]_3+[\Delta N(r)]_4+\cdots . \tag{38}$$

We have carried through a detailed analysis of the Fourier inverses of the cluster contributions $[\Delta N(q)]_2$ and $[\Delta N(q)]_3$ (depicted in Fig. 2) and of the contribution $[\Delta N(q)]_4$. The results show the following structural pattern:

$$\begin{aligned}
[\Delta N(r)]_2 &= -[\Delta N_1(r)]_2[\Delta\mathfrak{Q}(r)]_2+[\Delta N_2(r)]_2 ,\\
[\Delta N(r)]_3 &= \{\tfrac{1}{2}[\Delta N_1(r)]_2[\Delta\mathfrak{Q}(r)]_2^2-[\Delta N_1(r)]_3[\Delta\mathfrak{Q}(r)]_2-[\Delta N_1(r)]_2[\Delta\mathfrak{Q}(r)]_3\}+\{-[\Delta N_2(r)]_2[\Delta\mathfrak{Q}(r)]_2+[\Delta N_2(r)]_3\} ,\\
[\Delta N(r)]_4 &= \{-(1/3\,!)[\Delta N_1(r)]_2[\Delta\mathfrak{Q}(r)]_2^3+\tfrac{1}{2}[\Delta N_1(r)]_3[\Delta\mathfrak{Q}(r)]_2^2+[\Delta N_1(r)]_2[\Delta\mathfrak{Q}(r)]_3[\Delta\mathfrak{Q}(r)]_2-[\Delta N_1(r)]_3[\Delta\mathfrak{Q}(r)]_3\\
&\quad -[\Delta N_1(r)]_4[\Delta\mathfrak{Q}(r)]_2\}+\{-[\Delta N_2(r)]_2[\Delta\mathfrak{Q}(r)]_3+\tfrac{1}{2}[\Delta N_2(r)]_2[\Delta\mathfrak{Q}(r)]_2^2-[\Delta N_2(r)]_3[\Delta\mathfrak{Q}(r)]_2\}\\
&\quad +(\text{irreducible contributions}) .
\end{aligned} \tag{39}$$

New quantities have been introduced which will be defined below. Scheme (39) suggests that the function $N(r)$ may be expressed in the form

$$N(r)=N_1(r)(e^{-\mathfrak{Q}(r)}-1)+N_2(r)e^{-\mathfrak{Q}(r)} , \tag{40}$$

where the functions $N_2(r)$ and $\mathfrak{Q}(r)$, given by

$$N_2(r)=[\Delta N_2(r)]_2+[\Delta N_2(r)]_3+\cdots , \tag{41}$$

$$\mathfrak{Q}(r)=[\Delta\mathfrak{Q}(r)]_2+[\Delta\mathfrak{Q}(r)]_3+\cdots , \tag{42}$$

contain only irreducible cluster contributions. Equation (40) is an elaborate analog of Eq. (18). It regenerates expansion (38) precisely, through four-body cluster order. We are confident that expression (40) is in fact correct to all orders. [It is worthy of note that (40) has been checked to five-body cluster order in the boson limit described in Sec. V.]

Explicit diagrammatic representations of the two- and three-body contributions to the functions $\mathfrak{Q}(r)$ and $N_2(r)$ are given in Figs. 8 and 9. The diagrams appearing are all irreducible in the wider sense that none can be evaluated as the product of two simpler graphs.[22] (See also Fig. 7.)

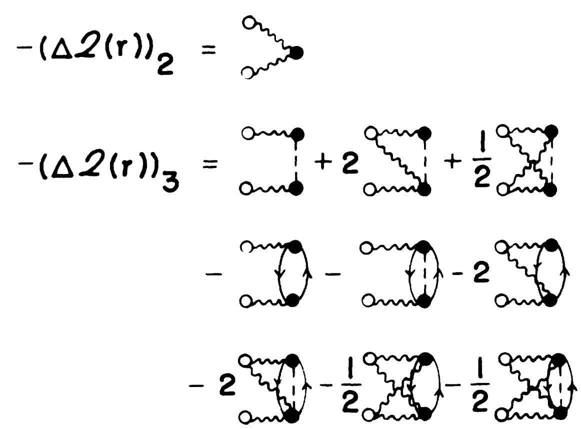

FIG. 8. Graphical representation of the two- and three-body contributions to the cluster expansion of the function $\mathfrak{Q}(r)$.

Combining Eqs. (34) and (40), the one-particle density matrix becomes

$$n(r)=\rho n[N_1(r)+N_2(r)]e^{-\mathfrak{Q}(r)} , \tag{43}$$

where the functions $N_1(r)$ and $N_2(r)$ are defined by the expansions (37) and (41), and the strength factor n is determined by Eq. (32) and Fig. 6.

We observe from Fig. 8 that the cluster diagrams contributing to $\mathfrak{Q}(r)$ bear a suggestive structural resemblance to those which make up the quantity $2D[\zeta]-D[\eta]$ (cf. Fig. 5). Guided by this resemblance, we are able to rearrange expansion (42) and perform massive partial summations which lead to a compact expansion for $\mathfrak{Q}(r)$ in terms of the spatial distribution functions, analogous to the compact expansion derived earlier for $Q=2D[\zeta]-D[\eta]$. The result is symbolized in Fig. 10 (cf. Fig. 6). As before, the blob with two solid dots on it represents $g(r_{12})-1$.

Inspection of Fig. 10 shows that the function $\mathfrak{Q}(r)$ in fact coincides with the constant Q of Eqs. (18)–(21) for vanishing relative distance r. Consider,

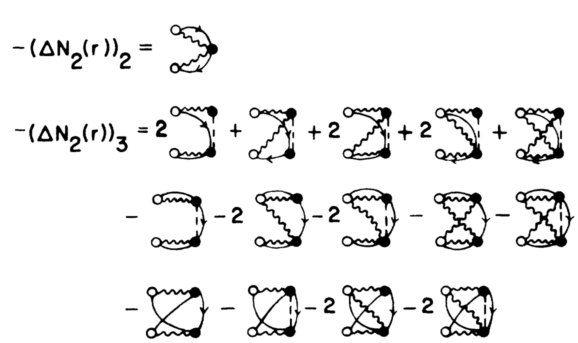

FIG. 9. Same as Fig. 8, but for $N_2(r)$.

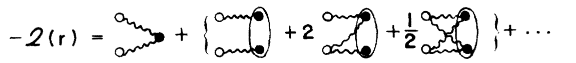

FIG. 10. Symbolic representation of the compact expansion of the function $\mathcal{Q}(r)$ in terms of spatial distribution functions.

for example, the two-body cluster contributions to both quantities. We have from Fig. 8 that

$$-[\Delta \mathcal{Q}(r=0)]_2 = \rho \int \zeta^2(r_{13}) d\vec{r}_3 = \frac{1}{A}\rho^2 \int \zeta^2(r_{13}) d\vec{r}_1\, d\vec{r}_3 = -(\Delta Q)_2 \,. \tag{44}$$

The same equality holds for the three-body, four-body, and presumably all the higher-body terms. Consequently we may write

$$n\, e^{-\mathcal{Q}(0)} = 1 \,. \tag{45}$$

Since by definition $n(0)=\rho$, the result (45), together with (43), implies the property

$$N_1(0) + N_2(0) = 1 \,. \tag{46}$$

This property can be verified independently in each cluster order through the fourth by specializing Figs. 7 and 9 to $r=0$.

According to Figs. 7 and 9 the functions $N_1(r)$ and $N_2(r)$ are represented entirely by exchange diagrams. There is only one single-exchange contribution, namely, $[\Delta N_1(r)]_2 = l(rk_F)$. All other contributions involve at least double exchange. Thus the behavior of both functions is governed predominantly by effects associated with antisymmetry of the wave function. If for actual Fermi fluids exchange correlations are not of great importance, an approximate description of $N_1(r)$ and $N_2(r)$ by low-cluster order truncations of (37), (41) should be adequate. Or better, expansions (37), (41) may be rearranged such that diagrams involving the same number of exchange lines are grouped together, and truncated at low order in the number of exchange lines (Wu-Feenberg expansion procedure[16]). This kind of treatment has in fact proved rather successful for the ground-state energy and other properties of ^{3}He (Ref. 16) and high-density neutron matter.[25] The rapid convergence of the Wu-Feenberg exchange-line expansion for the energy in these cases, might be attributable to the fact that the strong short-range repulsion discourages close approach of any two particles, partially obviating an explicit accounting of exclusion or exchange effects.

Even so, further insight into the structure of $N_1(r)$ and $N_2(r)$ is desirable. The enumeration and classification of higher-order cluster diagrams is, however, a formidable task.

The contributions explicitly available (Figs. 7, 9, and 10) are consistent with the assertion that $N_1(r)$, $N_2(r)$, and $\mathcal{Q}(r)$ all vanish as the relative distance r goes to infinity. Accordingly, the functions $N_1(r)$ and $N_2(r)$ ensure that the density matrix $n(r)$ for a system of fermions does not exhibit long-range order: we always have $n(\infty)=0$. Because of the discontinuous behavior of its Fourier transform $N_1(q)$ at the Fermi surface $q=k_F$, the function $N_1(r)$ gives rise to (presumably mild) oscillations of $n(r)$. The amplitude of these oscillations depends largely on the "damping" described by the exponential factor which appears in Eq. (43).

We conclude this section by expressing the occupation probability (1) of a system of strongly-interacting fermions in terms of our compact result for the one-particle density matrix. Fourier transformation of relation (33) yields

$$n_{\hat{q}} = \frac{1}{\nu} \int n(r) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} \,. \tag{47}$$

Insertion of (34) with (40) into (47) leads back to the formula

$$n_{\hat{q}} = n[N(q) + N_1(q)] \,, \tag{48}$$

the components now being given by

$$N(q) = \frac{\rho}{\nu} \int N_1(r)(e^{-\mathcal{Q}(r)} - 1) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} + \frac{\rho}{\nu} \int N_2(r) e^{-\mathcal{Q}(r)} e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} \,, \tag{49}$$

$$N_1(q) = \frac{\rho}{\nu} \int N_1(r) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} \,. \tag{50}$$

The integral (50) vanishes identically for values $q > k_F$. For values $q \leq k_F$ it reproduces the function $M(q)$ of Eq. (15). It is also easy to check that the formulation (48)–(50) satisfies the particle-conservation sum rule

$$\frac{1}{A} \sum_{\hat{q}} n_{\hat{q}} = 1 \tag{51}$$

[cf. discussion surrounding (45), (46)].

V. BOSE FLUIDS

With proper specialization, the procedure outlined in the preceding sections works equally well for a system of interacting bosons described by the wave function (2) with Φ set constant.

In the absence of exchange, the class of diagrams which contribute to the momentum distribution, the one-particle density matrix, and other related quantities is drastically reduced. Owing to these simplifications it becomes feasible in the Bose case to evaluate cluster contributions to the various quantities beyond the four-body term. Actually we have determined explicitly the two-, three-, four-, and five-body cluster contributions to the momentum distribution. With this raw material we have performed a study of the density matrix for bosons up to fifth cluster order, independently of the considerations of Secs. II–IV, and extrapolated the trends revealed to formulate a concise expression for $n(r)$ in terms of the spatial distribution functions.

We may, however, generate these results for the Bose one-body density matrix quite economically by specialization of the general Fermi formula (43) to the limit

$$\nu^{-1} \to 0\,, \quad k_F \to 0^+ \text{ (boson limit)}. \tag{52}$$

In this limit the function $N_1(r)$ of Eq. (37) and Fig. 7 assumes *infinite* range,

$$N_1(r) = l(rk_F) + O(\rho/\nu) \to 1\,. \tag{53}$$

We also find from inspection of Fig. 9 that the function $N_2(r)$ of Eq. (41) *vanishes* in the boson limit,

$$N_2(r) = O(\rho/\nu) \to 0\,. \tag{54}$$

Invoking (43), the Bose one-particle density matrix may then be written

$$n(r) = \rho n\, e^{-\mathfrak{Q}(r)}\,. \tag{55}$$

The function $\mathfrak{Q}(r)$ is still given by the compact expansion depicted in Fig. 10, but of course the distribution functions which enter correspond to Φ = const in Eq. (2). Similarly, the strength factor n is determined by these distribution functions via Eqs. (18) and (21) along with the compact expansion of Fig. 6. We reiterate that these results have actually been established through *fifth* cluster order. They have also been reproduced by Feenberg without the use of diagrams[30] (see Appendix C).

The infinite range of the Bose $N_1(r)$ [Eq. (53)] gives rise to the off-diagonal long-range order[26] of the corresponding density matrix (55):

$$\rho^{-1} n(\infty) = n \neq 0\,. \tag{56}$$

The quantity (56) may be identified with the fraction of bosons in the zero-momentum single-particle state, which is macroscopically occupied.[4] To see this, consider the Fourier transform of (55),

$$\begin{aligned} n_q &= \int n(r) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} \\ &= \int [n(r) - n(\infty)] e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} + n(\infty)\rho^{-1} A\delta_{q0}\,, \end{aligned} \tag{57}$$

which is of course just the momentum distribution of the Bose system described by wave function (2). Insertion of (55) into (57) produces the more explicit expression

$$n_q = \rho n \int (e^{-\mathfrak{Q}(r)} - 1) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} + nA\delta_{q0} \tag{58}$$

for the number of particles in the single-particle state with momentum $\hbar\vec{q}$. In particular

$$n_c = n \tag{59}$$

gives the fraction of particles in the zero-momentum condensate.

We may therefore employ Eq. (32) or Eqs. (18) and (21) to express the condensate fraction n_c by

$$n_c = e^{Q} = e^{2D[\zeta(r)] - D[\eta(r)]}\,. \tag{60}$$

Figure 6 then provides a recipe for practical evaluation of n_c in terms of the distribution functions of the Bose system. This procedure is the basis of a recent numerical investigation[28] of the condensate fraction in liquid ^{4}He.

The momentum distribution (58) for bosons can, of course, be considered as the appropriate limit of the quantity $\sum_\sigma n_{\hat{q}} = \nu n_{\hat{q}}$, where $n_{\hat{q}}$ is the occupation probability of orbital $\hat{q}$ in the general Fermi system studied in Secs. II–IV. In particular, it is seen from (48) and (49) that the first term of (58) represents the boson limit of the function $n\nu N(q)$ of Eq. (49); similarly, the second term of (58) derives from the function $n\nu N_1(q)$ of Eq. (50).

By virtue of the infinite range of $N_1(r)$ for bosons, the asymptotic behavior of the function $\mathfrak{Q}(r)$ can have a strong influence on the shape of the momentum distribution at small q. A rigorous discussion of this influence requires a detailed knowledge of the asymptotic behavior of the n-body distribution functions symbolized in Figs. 6 and 10. Unfortunately our knowledge of such properties is incomplete. In what follows, we assume that the asymptotic behavior of the series in Fig. 10 is governed by the long-range dependence of the pair distribution function only. This leads to the asymptotic relation

$$\mathfrak{Q}(r) \to \mathfrak{Q}_\infty(r)\,, \quad r \to \infty\,, \tag{61}$$

where $-\mathfrak{Q}_\infty(r)$ is given by the first two diagrams in Fig. 10, i.e.,

$$\begin{aligned} \mathfrak{Q}_\infty(r) = &-\rho \int \zeta(r_{13})\zeta(r_{23})\, d\vec{r}_3 \\ &-\rho^2 \int \zeta(r_{13})\zeta(r_{24})[g(r_{34}) - 1]\, d\vec{r}_3\, d\vec{r}_4\,. \end{aligned} \tag{62}$$

The Fourier transform of $\mathfrak{Q}_\infty(r)$ may be written as

$$\mathfrak{Q}_\infty(q) = \int \mathfrak{Q}_\infty(r) e^{i\vec{q}\cdot\vec{r}}\, d\vec{r} = -\rho\zeta^2(q) S(q)\,, \tag{63}$$

in terms of the structure function $S(q)$ defined by Eq. (27) for the wave function (2) with Φ = const.

It is well known from elementary sum rules that the structure function of the exact ground state of a system of interacting bosons has the behavior[16]

$$S(q) = (\hbar/2mc)q\ , \quad q \to 0\ . \tag{64}$$

This property is reproduced by the structure function which corresponds to the trial state (2) with $\Phi = \text{const}$, if we adopt the customary long-range dependence[31]

$$\zeta(r) = -(mc/2\pi^2\rho\hbar)r^{-2}\ , \quad r \to \infty \tag{65}$$

for the two-body correlations. The Fourier transform of such a $\zeta(r)$ satisfies

$$q\zeta(q) = -mc/\rho\hbar\ , \quad q \to 0\ . \tag{66}$$

Equations (63), (64), and (66) then imply the property

$$q\mathcal{Q}_\infty(q) = -mc/2\rho\hbar\ , \quad q \to 0\ . \tag{67}$$

Under assumption (61) the one-particle density matrix (55) for bosons must therefore have the asymptotic dependence

$$n(r) = n_c\rho\left(1 + \frac{1}{4\pi^2}\frac{mc}{\rho\hbar}r^{-2}\right)\ , \quad r \to \infty. \tag{68}$$

Associated with this long-range behavior is a simple singularity in the momentum distribution (58) at zero momentum,

$$n_q = n_c(mc/2\hbar)q^{-1}\ , \quad q \to 0\ . \tag{69}$$

Relation (69) agrees with earlier results of Gavoret and Nozières[32] and of Chester and Reatto.[31] The singularity is absent if the correlation function $\zeta(r)$ is taken to be of short range.

ACKNOWLEDGMENTS

Part of this work was done while M. L. Ristig was enjoying the hospitality of the Department of Physics, Washington University. We thank Professor E. Feenberg and Professor H. W. Jackson for a number of stimulating discussions.

APPENDIX A: IWAMOTO-YAMADA CLUSTER EXPANSION

The occupation probability of orbital $\hat{q}$, as defined in Eq. (1), is the expectation value of the operator $\Omega = \sum_{i=1}^{A} \nu_{\hat{q}}(i)$ with respect to the correlated wave function $|\Psi\rangle = F|\Phi\rangle$,

$$n_{\hat{q}} = \frac{\langle\Psi|\Omega|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\partial}{\partial\beta}\ln\langle\Psi|e^{\beta\Omega}|\Psi\rangle|_\beta = 0\ . \tag{A1}$$

To evaluate the generalized normalization integral $I(\beta) = \langle\Psi|e^{\beta\Omega}|\Psi\rangle$, subnormalization integrals are introduced[17]:

$$\begin{aligned} I_i &= \langle i|\exp\beta\nu_{\hat{q}}(1)|i\rangle\ , \\ I_{ij} &= \langle ij|F^\dagger(12)\{\exp\beta[\nu_{\hat{q}}(1)+\nu_{\hat{q}}(2)]\}F(12)|ij-ji\rangle\ , \\ I_{ijk} &= \langle ijk|F^\dagger(123)\{\exp\beta[\nu_{\hat{q}}(1)+\nu_{\hat{q}}(2)+\nu_{\hat{q}}(3)]\} \\ &\quad\times F(123)|ijk-jik-ikj-kji+kij+jki\rangle\ , \\ &\vdots\ , \end{aligned} \tag{A2}$$

the last, involving A occupied-orbital labels, being just $I(\beta)$. The operators 1, $F(12)$, $F(123)$, ... appearing in (A2) are the one-, two-, three-, ... body versions of the A-body correlation operator $F = F(1\cdots A)$.[17] Next, reduced cluster integrals are defined via

$$\begin{aligned} I_{ij} &= I_iI_j(1+x_{ij})\ , \\ I_{ijk} &= I_iI_jI_k(1+x_{ij}+x_{ik}+x_{jk}+x_{ijk})\ , \\ &\vdots\ . \end{aligned} \tag{A3}$$

The reduced cluster integrals $x_{ij}, x_{ijk}, \ldots$ serve to express the terms of the so-called Iwamoto-Yamada factor-cluster expansion (or factorized Iwamoto-Yamada or FIY expansion[20]) of quantity (A1).

This expansion and a renormalized version of it have been closely studied in the thermodynamic limit. The renormalized FIY expansion of the occupation probability reads

$$\begin{aligned} n_{\hat{q}} = z_{\hat{q}} &+ \frac{1}{2!}\sum_{ij} z_iz_j\left(\frac{\partial}{\partial\beta}x_{ij} + (\delta_{\hat{q}i}+\delta_{\hat{q}j})x_{ij}\right)\bigg|_{\beta=0} \\ &+ \frac{1}{3!}\sum_{ijk} z_iz_jz_k\left(\frac{\partial}{\partial\beta}x_{ijk} + (\delta_{\hat{q}i}+\delta_{\hat{q}j}+\delta_{\hat{q}k})x_{ijk}\right)\bigg|_{\beta=0} \\ &+ \cdots\ . \end{aligned} \tag{A4}$$

The weight function z_i [given as the solution of Eq. (3.4) of the second paper of Ref. 17] depends on the occupied orbital i and vanishes for unoccupied levels. The expansion (A4) is well suited to the choice $F = e^S$ of correlation operator, where S excites only n-particle–n-hole pairs, $n = 2, 3, \ldots$. (Such an F obeys the full Pauli condition in intermediate states.)

On the other hand, for the Jastrow choice (2) of correlation operator F, expansion (A4) is quite unsatisfactory if longer-range correlations are permitted. Indeed, it is meaningless for correlations which are strictly of long range, according to Eq. (65). A better starting point[23] for this case is the unrenormalized expansion, i.e., the original FIY expansion in the number of bodies. This expansion may be recaptured formally from the renormalized expansion (A4) by cluster developing the z_i [see Eq. (3.5) of the second paper of Ref. 17] and regrouping terms:

$$n_{\hat{q}} = (\Delta n_{\hat{q}})_1 + (\Delta n_{\hat{q}})_2 + (\Delta n_{\hat{q}})_3 + \cdots\ , \tag{A5}$$

with

$$
\begin{aligned}
(\Delta n_{\hat{q}})_1 &= \Theta(k_F - q)\,,\\
(\Delta n_{\hat{q}})_2 &= \frac{1}{2}\sum_{ij} \frac{\partial}{\partial\beta} x_{ij}\bigg|_{\beta=0}\,,\\
(\Delta n_{\hat{q}})_3 &= \left(\frac{1}{3!}\sum_{ijk}\frac{\partial}{\partial\beta}x_{ijk} - \sum_{ijk} x_{ij}\frac{\partial}{\partial\beta}x_{jk}\right)\bigg|_{\beta=0}\,,\\
&\vdots
\end{aligned}
\tag{A6}
$$

The general term is given in Ref. 20.

Explicit evaluation of the two-body cluster $(\Delta n_{\hat{q}})_2$ is easily accomplished; the result is

$$
\begin{aligned}
(\Delta n_{\hat{q}})_2 &= \frac{1}{2}\sum_{ij}\langle ij\,|\,\zeta(r_{12})[\nu_{\hat{q}}(1)+\nu_{\hat{q}}(2) - \delta_{\hat{q}i} - \delta_{\hat{q}j}]\zeta(r_{12})\,|\,ij - ji\rangle\\
&= \frac{1}{2}\sum_{ij}\langle ij\,|\,\zeta(r_{12})[\nu_{\hat{q}}(1)+\nu_{\hat{q}}(2)]\zeta(r_{12})\,|\,ij - ji\rangle\\
&\quad - \Theta(k_F - q)\sum_i \langle i\hat{q}\,|\,\zeta^2(r_{12})\,|\,i\hat{q} - \hat{q}i\rangle\,,
\end{aligned}
\tag{A7}
$$

or

$$
\begin{aligned}
(\Delta n_{\hat{q}})_2 &= \sum_{ij}\langle \hat{q}ji\,|\,\zeta(r_{12})\zeta(r_{23})\,|\,ij\hat{q} - ji\hat{q}\rangle\\
&\quad - \Theta(k_F - q)\sum_i\langle i\hat{q}\,|\,\zeta^2(r_{12})\,|\,i\hat{q} - \hat{q}i\rangle\,.
\end{aligned}
\tag{A8}
$$

The final form is obtained after insertion of a complete set of intermediate states just to the right of the sum of $\nu_{\hat{q}}$ operators. The second term of Eq. (A8) represents the effect of the Fermi medium in two-body cluster order:

$$
(\Delta m_{\hat{q}})_2 = \sum_i \langle i\hat{q}\,|\,\zeta^2(r_{12})\,|\,i\hat{q} - \hat{q}i\rangle\,. \tag{A9}
$$

APPENDIX B: GRAPHICAL REPRESENTATION OF FERMI CLUSTERS

The bare elements of a diagrammatic formalism based on Ursell-Mayer theory are (i) internal and external points (solid and open dots). An external point labels the coordinate $\vec{r}_i$ of particle i. An internal point indicates a factor ρ and integration over the coordinate space of the particle involved. (ii) Correlation lines (wavy and dashed lines). A wavy line represents the function $\zeta(r) = f(r) - 1$. A dashed line represents the function $\eta(r) = f^2(r) - 1$. (iii) Oriented lines. As shown in Fig. 11, these represent either an exchange function $l(x) = 3x^{-3}(\sin x - x\cos x)$ or a plane-wave factor. The graphical representation of the occupation probability (1) contains only diagrams in which the oriented lines form closed loops. With each distinct loop connecting p points is associated a factor ν^{1-p}.

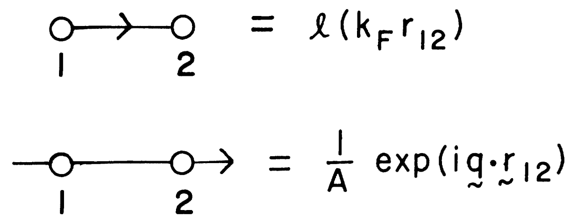

FIG. 11. Oriented lines.

The two-body cluster serves to exemplify (i)–(iii). The four contributions to $(\Delta n_{\hat{q}})_2$,

$$
\sum_i \langle i\hat{q}\,|\,\zeta^2(r_{12})\,|\,i\hat{q}\rangle = \frac{1}{A}\rho^2\int \zeta^2(r_{12})\,d\vec{r}_1\,d\vec{r}_2\,, \tag{B1}
$$

$$
\sum_i \langle i\hat{q}\,|\,\zeta^2(r_{12})\,|\,\hat{q}i\rangle = \frac{1}{A}\frac{\rho^2}{\nu}\int \zeta^2(r_{12})\,l(r_{12}k_F)\,e^{i\vec{q}\cdot\vec{r}_{12}}\,d\vec{r}_1\,d\vec{r}_2\,, \tag{B2}
$$

$$
\sum_{ij}\langle \hat{q}ji\,|\,\zeta(r_{12})\zeta(r_{23})\,|\,ij\hat{q}\rangle = \frac{1}{A}\frac{\rho^3}{\nu}\int \zeta(r_{12})\zeta(r_{23})\,l(r_{13}k_F)\,e^{i\vec{q}\cdot\vec{r}_{13}}\,d\vec{r}_1\,d\vec{r}_2\,d\vec{r}_3\,, \tag{B3}
$$

$$
\sum_{ij}\langle \hat{q}ji\,|\,\zeta(r_{12})\zeta(r_{23})\,|\,ji\hat{q}\rangle = \frac{1}{A}\frac{\rho^3}{\nu^2}\int \zeta(r_{12})\zeta(r_{23})\,l(r_{12}k_F)\,l(r_{23}k_F)\times e^{i\vec{q}\cdot\vec{r}_{13}}\,d\vec{r}_1\,d\vec{r}_2\,d\vec{r}_3\,, \tag{B4}
$$

are depicted in Fig. 12.

The diagrams introduced in Sec. IV to describe the functions $N_1(r)$ and $N(r)$ are determined by the transformations of (35), (36), applied to terms which are graphically already defined. Some of the resulting contributions to $N_1(r)$ and $\mathfrak{L}(r)$ are listed on the following page:

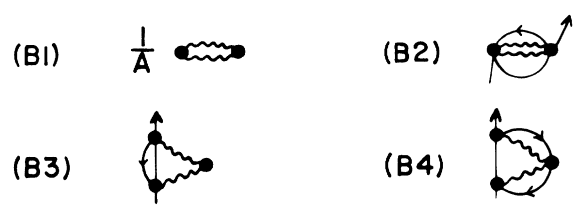

FIG. 12. Diagrams representing the four terms of the two-body cluster contribution to $n_{\hat{q}}$.

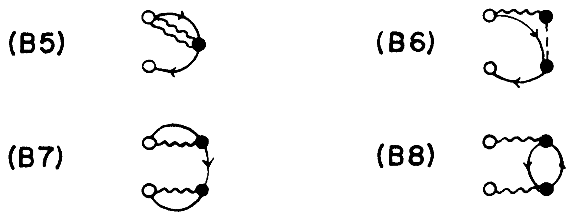

FIG. 13. Diagrams representing selected individual contributions to the functions $N_1(r)$ and $\mathcal{Q}(r)$.

$$\frac{\rho}{\nu}\int \zeta^2(r_{23})l(r_{23}k_F)l(r_{13}k_F)\,d\vec{r}_3\,, \tag{B5}$$

$$\frac{\rho^2}{\nu}\int \zeta(r_{23})\eta(r_{34})l(r_{24}k_F)l(r_{14}k_F)\,d\vec{r}_3\,d\vec{r}_4\,, \tag{B6}$$

$$\frac{\rho^2}{\nu^2}\int \zeta(r_{13})l(r_{13}k_F)l(r_{34}k_F)\zeta(r_{24})l(r_{24}k_F)\,d\vec{r}_3\,d\vec{r}_4\,, \tag{B7}$$

$$\frac{\rho^2}{\nu}\int \zeta(r_{13})l^2(r_{34}k_F)\zeta(r_{24})\,d\vec{r}_3\,d\vec{r}_4\,, \tag{B8}$$

and, as examples, represented graphically in Fig. 13.

For a more detailed presentation of the diagrammatic formalism, see Ref. 23.

APPENDIX C: FEENBERG'S ALTERNATIVE DERIVATION OF BOSE RESULTS

The multiplicative cluster expansion procedure developed by Clark and Westhaus[20] can be used to derive the Bose results (55), (59), and (60) in a very direct fashion, without the use of diagrams.[30] A brief outline of the procedure follows.

The normalized Jastrow wave function for A Bose particles is written

$$\Psi^{(A)}(1\cdots A)=\Omega^{-A/2}e^{-A\lambda/2}\prod_{i<j}f(r_{ij})\,, \tag{C1}$$

where Ω is the normalization volume. Then

$$e^{\lambda}=\int[\Psi^{(A-1)}(2\cdots A)]^2\prod_{j=2}^{A}f^2(r_{1j})\,d\vec{r}_2\cdots d\vec{r}_A\,, \tag{C2}$$

where $\Psi^{(A-1)}$ is the normalized Jastrow function for $A-1$ particles. To evaluate λ, begin with just one factor in the product:

$$\int[\Psi^{(A-1)}(2\cdots A)]^2f^2(r_{12})\,d\vec{r}_2\cdots d\vec{r}_A =1+\frac{1}{\Omega}\int[f^2(r)-1]\,d\vec{r}\,. \tag{C3}$$

Since the product contains $A-1$ factors, a first approximation for λ is given by

$$e^{\lambda^{(1)}}=\left(1+\frac{1}{\Omega}\int(f^2-1)\,d\vec{r}\right)^{A-1} \cong\exp\left(\rho\int(f^2-1)\,d\vec{r}\right). \tag{C4}$$

To generate a second approximation to λ, keep two factors in the product:

$$\int[\Psi^{(A-1)}(2\cdots A)]^2f^2(r_{12})f^2(r_{13})\,d\vec{r}_2\cdots d\vec{r}_A =\left(1+\frac{1}{\Omega}\int(f^2-1)\,d\vec{r}\right)^2\left[1+\frac{1}{\Omega^2}\int[g(r_{23})-1][f^2(r_{12})-1][f^2(r_{13})-1]\,d\vec{r}_2\,d\vec{r}_3\Big/\left(1+\frac{1}{\Omega}\int(f^2-1)\,d\vec{r}\right)^2\right]. \tag{C5}$$

Since there are $\frac{1}{2}(A-1)(A-2)$ pairs of particles in the set $\{2\cdots A\}$, we obtain

$$e^{\lambda^{(2)}}\cong e^{\lambda^{(1)}}\exp\left(\rho^2\int[g(r_{23})-1][f^2(r_{12})-1]\times[f^2(r_{13})-1]\,d\vec{r}_2\,d\vec{r}_3\right). \tag{C6}$$

The extension to third and higher orders follows the same pattern. At each step a new correction factor appears and gives rise to an additional irreducible contribution to λ.

After observing that the one-body density matrix

$$n(|\vec{r}_1'-\vec{r}_1''|) =\Omega\int\Psi^{(A)}(1',2\cdots A)\Psi^{(A)}(1'',2\cdots A)\,d\vec{r}_2\cdots d\vec{r}_A \tag{C7}$$

may be expressed as

$$n(|\vec{r}_1'-\vec{r}_1''|)=e^{-\lambda}\int[\Psi^{(A-1)}(2\cdots A)]^2 \times\prod_{j=2}^{A}f(r_{1'j})f(r_{1''j})\,d\vec{r}_2\cdots d\vec{r}_A\,, \tag{C8}$$

essentially the same procedure may be used to evaluate $n(r)$ step by step.

*Research supported by the Deutsche Forschungsgemeinschaft under Grant No. Ri 267 and by the National Science Foundation under Grant Nos. DMR72-03166 A03 and DMR76-14929.

[1]*Lectures in Theoretical Physics*, *Quantum Fluids and Nuclear Matter*, edited by K. T. Mahanthappa and W. E. Brittin (Gordon and Breach, New York, 1969), Vol. XI-B.

[2]A. D. B. Woods and R. A. Cowley, Rep. Prog. Phys. 36, 1135 (1973).

[3]E. Østgaard, J. Low Temp. Phys. 4, 239, 585 (1971).

[4]O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

[5]W. L. McMillan, Phys. Rev. 138, A442 (1965).

[6]D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967).

[7]W. E. Parry and C. R. Rathbone, Proc. Phys. Soc. Lond. 91, 273 (1967).

[8]L. Reatto and G. V. Chester, Phys. Rev. 155, 88 (1967).

[9]W. P. Francis, G. V. Chester, and L. Reatto, Phys. Rev. A 1, 86 (1970).

[10]H. W. Jackson, Phys. Rev. A 10, 278 (1974).

[11]R. A. Cowley and A. D. B. Woods, Phys. Rev. Lett. 21, 787 (1968); Can. J. Phys. 49, 177 (1971).

[12]O. K. Harling, Phys. Rev. Lett. 24, 1046 (1970); Phys. Rev. A 3, 1073 (1971).

[13]H. A. Mook, R. Scherm, and M. K. Wilkinson, Phys. Rev. A 6, 2268 (1972).

[14]H. A. Mook, Phys. Rev. Lett. 32, 1167 (1974).

[15]B. H. Brandow, Ann. Phys. 64, 21 (1971).

[16]E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969).

[17]J. W. Clark and M. L. Ristig, in *The Nuclear Many-Body Problem*, edited by F. Calogero and C. Ciofi degli Atti (Editrice Compositori, Bologna, Italy, 1973), Vol. 2, p. 273; M. L. Ristig and J. W. Clark, *ibid.*, p. 299.

[18]E. Feenberg, Ann. Phys. 84, 128 (1974).

[19]J. W. Clark and P. Westhaus, Phys. Rev. 141, 833 (1966); 149, 990 (1966).

[20]J. W. Clark and P. Westhaus, J. Math. Phys. 9, 131, 149 (1968).

[21]M. Gaudin, J. Gillespie, and G. Ripka, Nucl. Phys. A 176, 237 (1971).

[22]J. M. Van Leeuwen, J. Groeneveld, and J. de Boer, Physica 25, 792 (1959).

[23]E. Krotscheck and M. L. Ristig, Nucl. Phys. A 242, 389 (1975).

[24]S. Fantoni and S. Rosati, Nuovo Cimento Lett. 10, 545 (1974).

[25]V. R. Pandharipande and H. A. Bethe, Phys. Rev. C 7, 1312 (1973).

[26]C. N. Yang, Rev. Mod. Phys. 34, 694 (1962).

[27]E. Feenberg, Ann. Phys. 70, 133 (1972).

[28]M. L. Ristig, P. M. Lam, and J. W. Clark, Phys. Lett. 55A, 101 (1975).

[29]R. S. Poggioli and A. D. Jackson, Phys. Rev. Lett. 35, 1211 (1975); and Phys. Rev. C (to be published).

[30]E. Feenberg (private communication).

[31]G. V. Chester and L. Reatto, Phys. Lett. 22, 276 (1966).

[32]J. Gavoret and P. Nozières, Ann. Phys. 28, 349 (1964).