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Study of the mathematical approximations made in the basis-correlation method and those made in the canonical-transformation method for an interacting Bose gas

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Following up a new method for solving a many-body Bose gas proposed by Wong and Fung previously, we extend our study to summing all terms relating to the three-body correlation function in the canonical-transformation matrix representation. It was found that only a certain class of interaction potential will allow for an analytic representation of the one-to-one linear transformation matrices. However, the variational method based on construction of the basis correlations does not have such mathematical restriction.

I. INTRODUCTION

The main purpose of our method for solving a many-body Bose gas[1,2] is to provide a direct mathematical relationship between the so-called basis-correlation-functions method, a variation method, and the Bogoliubov method, a canonical-transformation method. However, to achieve this goal we must be able to express the explicit matrix representations of the linear unitary transformation in terms of the multiparticle basis-correlation functions, not just the so-called pair-particle correlation, otherwise known as the Bijl-Dingle-Jastrow (BDJ)[3] approximation. This point is very important because the Bogoliubov transformation diagonalizes a truncated Hamiltonian of the quadratic form exactly, which, therefore, includes all the different multiparticle correlations in its ground state. The two different approximation methods commonly used in solving the many-boson problem are, therefore, quite different in their assumptions of the important or dominant contributions toward the ground state of the system. In this paper, we show explicitly how to sum all terms involving the pair and three-body correlation functions in the unitary matrix representations. As a consequence, it is now feasible to answer the following questions regarding the fundamental differences between these two very distinct approximation methods:

(1) What are the differences in the approximations made by truncating the Hamiltonian into a quadratic form, or by choosing a variational ground state in the BDJ form?

(2) It is clear from the c-number approximation made with regards to the Bose condensate when we select the dominant terms in the quadratic Hamiltonian, diagonalizable by the Bogoliubov transformation. Under what mathematical conditions is this same approximation implied in the basis-correlation-functional method?

(3) The understanding of the nature of the off-diagonal long-range order (ODLRO)[4] of a physical system is of fundamental importance in describing its physical properties. Supposing that a BDJ approximated ground state does present a good approximation to the true ground state of the multiparticle system, can we learn from the BDJ approximated ground state the nature of the ODLRO in the actual physical system?

(4) It was shown by Lee and Wong[5] that a direct calculation of the amount of Bose-Einstein condensation in a multiparticle system is difficult from the knowledge of the pair correlation. Can we achieve this calculation via its relationship with the unitary matrix representations?

(5) Under what mathematical conditions would the application of either one of these approximation methods break down?

(6) Is there a limitation or restriction on the particle-particle interaction under which we can apply either method?

No specific form of the Hamiltonian has been introduced in this paper for the purpose of answering the above six questions posed. Therefore, the conclusions drawn by us are very general and should be applicable to a realistic model Hamiltonian for a bulk superfluid. A quantitative description of the superfluid excitations is, however, not possible unless a specific model Hamiltonian is chosen in a computation using our method. We feel that such a computation is not important at this point because previous calculations by various authors using some extended BDJ methods gave good quantitative results both to the ground-state energy and the elementary excitations of the fluid system. We would refer our readers to these works for quantitative results.[6] On the other hand, no good agreement with actual superfluid helium was ever obtained by methods using the Bogoliubov approximated Hamiltonian. Some reasons for the failure will be mentioned in our later discussions.

The unitary transformation method is exact in principle and has no limitation either on the density of the many-body system or on the strength of the particle-particle interaction. However, in practice it is impossible or difficult to obtain a simple representation of such a unitary transformation, thereby making this method purely academic. A simple specific form of a linear canonical transformation was proposed by Boboliubov which would diagonalize a truncated Hamiltonian of a quadratic form. Generalizing the Bogoliubov representation,[7] Wong and Fung[1] assumed a one-to-one linear mapping between the noninteracting vector states and the eigenvectors, but allowing the explicit presence of off-diagonal matrix elements in the linear unitary representations of the destruction and creation operators:

$$b_{\vec{p}} = \sum_{\vec{k}} (M_{\vec{p}\vec{k}} a_{-\vec{k}} + N_{\vec{p}\vec{k}} a_{\vec{k}}^{\dagger}) , \tag{1.1}$$

where $b_{\vec{p}}$, $b_{\vec{p}}^{\dagger}$ are the quasiparticle destruction and creation operators of momentum $\vec{p}$ and $a_{\vec{k}}$, $a_{\vec{k}}^{\dagger}$ are the destruction and creation free-particle operators of momentum $\vec{k}$, and $M_{\vec{p}\vec{k}}$, $N_{\vec{p}\vec{k}}$ are the explicit matrix elements of the linear canonical-transformation representation.

Thus, if the multiparticle system is nondegenerate in the free-field representation, then its ground state must be one that has no component of the quasiparticle state

$$b_{\vec{p}} |\phi_0\rangle = 0 . \tag{1.2}$$

As pointed out by Wong and Fung[1] from the theorems of Borel sets and completeness, any state of zero total momentum can be represented by superpositions of multiparticle correlation operators $\hat{Q}_n$ expressed as follows:

$$|\phi_0\rangle = \exp\left(\sum_n \hat{Q}_n\right) |N\rangle \quad , \tag{1.3}$$

where

$$\hat{Q}_n = \int \cdots \int \prod_i^n d^3x_i u_n(\vec{x}_1, \ldots, \vec{x}_n) \hat{\rho}(\vec{x}_1) \cdots \hat{\rho}(\vec{x}_n) . \tag{1.4}$$

The function u_n is called the multiparticle correlation function of order n when such a representation of the ground state is used. $\hat{\rho}(\vec{x})$ is the particle density operator and $|N\rangle$ is the unperturbed N-particle ground state which is the cyclic vector for the Boolean algebra.[8] We would like to point out here that for a bulk system with no external fields, Penrose and Onsager have shown that except for a constant phase factor, the ground-state wave function of a boson system is real and positive. We therefore treat all u_n as real functions, except u_1. In previous variational calculations for the bulk system,[9] we generally ignored the function u_1. Furthermore, most variation calculations, in fact, make use of the variation on the liquid-structure functions instead of the correlation functions directly.[5] By definition, the liquid-structure functions are always real. It is interesting to point out that the phase-factor function u_1, when treated as complex and position dependent in treating a noninteracting system imbedded in an external field, leads to the WKB equations for which u_1 satisfies. Therefore, this seemingly unimportant complex phase factor becomes important when we introduce external fields to the system, such as treating a liquid-gas boundary.

In order to make the key equation components of Eq. (1.2) truly independent and orthogonal, as suggested by Refs. 1 and 2, it is essential that we treat u_n as a purely algebraic function and that we use the grand canonical ensemble such that the single cyclic vector $|N\rangle$ is replaced with a thermodynamic averaging over the entire number spectrum having a high probability for finding the system with N particles. In Sec. II we repeated part of the work given in Ref. 1, showing explicitly the construction of the set of key equations derived from the assumption of orthogonality of the vector components generated from the expansion of Eq. (1.2). In Sec. III we obtained closed-form expressions for the first three coefficients associated with the first three key equations by including all two- and three-particle correlation functions. Details for summation of all diagrams involved in calculating these key equations' coefficients are given in the Appendices. It is shown clearly from the analytic closed-form expressions for these coefficients that the nondegenerate one-to-one linear mapping of the entire Hilbert space onto itself places a serious restriction on the form of the two-body correlation function u_2. This restriction also projects itself into a restriction on the short-range repulsive part of the particle-particle interaction. No such restriction is imposed on the variation method using basis correlations, since no restriction on the nondegeneracy of the Hilbert space is implied in the variational method. Indeed, many workers have applied the variational method using basis correlations to a system of interacting particles with hard-sphere-like short-range repulsion potential.[9-11] In Sec. IV we try to reexamine all the mathematical implications from this study and to answer the six questions we have posed earlier.

II. THE ORTHOGONAL VECTOR RAYS

In Refs. 1 and 2 we have already given the mathematical foundation necessary for the explicit construction of the exact interacting ground state in the form of superposition of multiparticle correlation operators $\hat{Q}_n$ and the cyclic vector $|N\rangle$. We have also stated the two postulates necessary for the transformation into a vector representation, such that the ground state is one with no quasiparticles. We should point out here that the construction of the explicit form of the ground-state vector is based purely on completeness and the theorems in Boolean algebra and is, therefore, valid even in the cases where there are multiparticle bound states or coordinate space exclusion due to the form of the particle-particle interaction. However, the simultaneous existence of a one-to-one linear mapping of the entire Hilbert space into that of itself, where the ground state can be represented by the representation of a vacuum state, is much more restrictive. Indeed, it has been shown explicitly that for a system with hard-core repulsion, the transformation necessary to project restricted Hilbert space is not a one-to-one linear transformation.[11,12] The above remarks will be more clearly explained in the following discussion. Let us restate the two mathematical postulates given in Ref. 1. (1) There exists a one-to-one linear mapping of the Hilbert space onto itself. (2) The ground state of such a representation is the vacuum state. The mathematical equations corresponding to the above two postulates are given by Eqs. (1.1) and (1.2). With the aid of the explicit representation of the ground-state vector given by Eqs. (1.3) and (1.4), Eqs. (1.2) can be represented in an infinite series as given by Eq. (5.1) in Ref. 1

$$\left[\sum_{\vec{q}} M_{\vec{p}\vec{q}}\left(a_{-\vec{q}}+\sum_{m=1}^{\infty}\frac{(-1)^m}{m!}[\hat{Q},\ldots,[\hat{Q},a_{-\vec{q}}]]_m\right)+N_{\vec{p}\vec{q}}\left(a_{\vec{q}}^{\dagger}+\sum_{m=1}^{\infty}\frac{(-1)^m}{m!}[\hat{Q},\ldots,[\hat{Q},a_{\vec{q}}^{\dagger}]]_m\right)\right]|\phi_0\rangle=0. \tag{2.1}$$

It is clear from the above equation that unless the matrices M and N are particle-operator dependent, the particle number associated with the series multiplied by M and that multiplied by N are different. Therefore, if the ground-state vector is one with exact particle number N, then the two series are orthogonal to each other and have only trivial solutions for the matrices M and N. Since we are only interested in nontrivial solutions, it is necessary for us to make M, N particle-operator dependent, thus violating postulate 1, or to employ the grand ensemble where the ground state is a superposition of different particle number states, with a sharp probability of states near the average number N. Such a mathematical necessity also exists in the Bogoliubov theory, which was clearly shown by Kromminga and Bolsterli.[13] Based on the grand-canonical ensemble and postulates 1 and 2, we have derived closed-form expressions for the coefficients C_0, C_1, and C_2 associated with the first three orthogonal vectors when only pair correlation u_2 was considered in Ref. 2.

For the first orthogonal state, where all particles remain at rest, we obtain

$$C_0=Ae^{-\alpha N}\sqrt{N}F_0M_{\vec{p}o}+Ae^{-\alpha(N-2)}(N-1)^{1/2}G_0N_{\vec{p}o}, \tag{2.2}$$

where α is the chemical potential, A is the normalization constant, and $N_{\vec{p}o}$, $M_{\vec{p}o}$ are the matrix elements of the canonical transformation associated with that vector state, where all particle momenta are zero. The analytic expressions for F_0 and G_0 were also given in Ref. 2; likewise, for the coefficients C_1 and C_2 associated with the next two orthogonal vectors,

$$C_1=Ae^{-\alpha N}\sqrt{N}F_1(q)M_{\vec{p}\vec{q}}+Ae^{-\alpha(N-2)}(N-1)^{1/2}G_1(q)N_{\vec{p}\vec{q}}, \tag{2.3}$$

and

$$C_2=Ae^{-\alpha N}\sqrt{N}M_{\vec{p}\vec{q}_1+\vec{q}_2}F_1(q_1)F_1(q_2)/F_0+Ae^{-\alpha(N-2)}(N-1)^{1/2}N_{\vec{p}\vec{q}_1+\vec{q}_2}G_1(q_1)G_1(q_2)/G_0+H_3, \tag{2.4}$$

where H_3 is a complicated function involving u_3 or its Fourier transform W_3. In order to derive the closed-form expressions for C_0, C_1, and C_2 when u_3 is included, we must reexamine our key equations and develop a summing procedure to ensure a total and complete counting of all terms involved. Without going into further explanation of symbols, for which we refer our readers to Refs. 1 and 2, we would like to go back to Eq. (2.1) expressed in the grand ensemble form

$$\sum_{N=0}^{\infty}\sum_{\vec{q}}\left[M_{\vec{p}\vec{q}}\left(a_{-\vec{q}}+\sum_{m=1}^{\infty}\frac{(-1)^m}{m!}[\hat{Q},\ldots,[\hat{Q},a_{-\vec{q}}]]_m\right)+N_{\vec{p}\vec{q}}\left(a_{\vec{q}}^{\dagger}+\sum_{m=1}^{\infty}\frac{(-1)^m}{m!}[\hat{Q},\ldots,[\hat{Q},a_{\vec{q}}^{\dagger}]]_m\right)\right]e^{-\alpha\hat{N}}|N\rangle=0, \tag{2.5}$$

where the operator $\hat{Q}$ is given by

$$\hat{Q} = \sum_{i=2}^{N} \hat{Q}_i \tag{2.6}$$

and

$$\hat{Q}_i = \prod_j^i \int d^3x_j u_i(\vec{x}_1, \ldots, \vec{x}_i)\hat{\rho}(\vec{x}_1)\cdots\hat{\rho}(\vec{x}_i). \tag{2.7}$$

To facilitate future discussions, we shall write out the explicit forms for the relevant commutators:

$$\begin{aligned}
[\hat{Q}_2, a_{-\vec{q}}] &= -\sum_{\vec{k}}{}' \hat{F}_1(k) a_{-\vec{q}+\vec{k}}, \\
[\hat{Q}_3, a_{-\vec{q}}] &= -\sum_{\vec{k}_1,\vec{k}_2}{}' \hat{F}_2(\vec{k}_1,\vec{k}_2) a_{-\vec{q}+\vec{k}_1+\vec{k}_2}, \\
&\vdots \\
[\hat{Q}_{n+1}, a_{-\vec{q}}] &= -\sum_{\vec{k}_1,\ldots,\vec{k}_n}{}' \hat{F}_n(\vec{k}_1,\ldots,\vec{k}_n) a_{-\vec{q}+\vec{k}_1+\cdots\vec{k}_n},
\end{aligned} \tag{2.8}$$

such that the mth order of the commutator between $\hat{Q}$ and $a_{-\vec{q}}$ is

$$[\hat{Q},\ldots,[\hat{Q},a_{-\vec{q}}]]_m = (-1)^m \prod_{j=1}^{m} \sum_{\vec{k}_1^j,\ldots,\vec{k}_N^j}{}' [\hat{F}_1(k_1^j)\delta_{\vec{k}_2^j,0}\cdots\delta_{\vec{k}_N^j,0} + \hat{F}_2(\vec{k}_1^j,\vec{k}_2^j)\delta_{\vec{k}_3^j,0}\cdots\delta_{\vec{k}_N^j,0} + \cdots + \hat{F}_N(\vec{k}_1^j,\ldots,\vec{k}_N^j)]\, a_{-\vec{q}+\Sigma}, \tag{2.9}$$

where

$$\Sigma = \sum_{j=1}^{m}\sum_{i=1}^{N} \vec{k}_i^j,$$

$$\hat{F}_1(k) = (1/\Omega) W_2(k)\hat{\rho}_{\vec{k}}, \quad \hat{F}_2(\vec{k}_1,\vec{k}_1) = (1/2!\,\Omega^2) W_3(\vec{k}_1,\vec{k}_2)(\hat{\rho}_{\vec{k}_1}\hat{\rho}_{\vec{k}_2} - \hat{\rho}_{\vec{k}_1+\vec{k}_2}), \tag{2.10}$$

and W_n is the Fourier transform for u_n. The operators $\hat{F}_3, \hat{F}_4, \ldots, \hat{F}_n$ are easily obtainable in the same manner.

In view of Eqs. (2.9) and (2.10), our key equation can be reexpressed neatly as

$$\sum_N \sum_{\vec{q}} (M_{\vec{p}\vec{q}}\hat{S}_M + N_{\vec{p}\vec{q}}\hat{S}_N) e^{-\alpha\hat{N}}|N\rangle = 0, \tag{2.11}$$

with the operator series $\hat{S}_M$ and $\hat{S}_N$ given by

$$\hat{S}_M = a_{-\vec{q}} + \sum_{m=1}^{\infty} \frac{1}{m!} \prod_{j=1}^{m} \sum_{\vec{k}_1^j,\ldots,\vec{k}_{N-1}^j}{}' [\hat{F}_1(k_1^j)\delta_{\vec{k}_2^j,0},\ldots,\delta_{\vec{k}_{N-1}^j,0} + \cdots + \hat{F}_{N-1}(\vec{k}_1^j,\ldots,\vec{k}_{N-1}^j)]\, a_{-\vec{q}+\Sigma}, \tag{2.12}$$

and

$$\hat{S}_N = a_{\vec{q}}^\dagger + \sum_{m=1}^{\infty} \frac{(-1)^m}{m!} \prod_{j=1}^{m} \sum_{\vec{k}_1^j,\ldots,\vec{k}_{N-1}^j}{}' a_{\vec{q}+\Sigma}^\dagger [\hat{F}_1(k_1^j)\delta_{\vec{k}_2^j,0}\cdots\delta_{\vec{k}_{N-1}^j,0} + \cdots \hat{F}_{N-1}(\vec{k}_1^j,\ldots,\vec{k}_{N-1}^j)]. \tag{2.13}$$

Equation (2.11) is quite general, since no approximation was made in the truncation of the operator series. To simplify our problem it is necessary to truncate these operator series by truncating the number of operators $\hat{F}_n$ to be included. Before proceeding, we would like to refer our readers to the expansion of the density operator product by Wick's theorem and a diagramatic technique developed in Ref. 2, with a condensed discussion given in Appendices A and B of this paper. These techniques will be used in the derivation of the coefficients C_0, C_1 and C_2 to be given in the next section.

III. CLOSED-FORM EXPRESSIONS FOR THE COEFFICIENTS C_0, C_1, AND C_2

In this section we shall study the closed-form expressions for the coefficients C_0, C_1, C_2 and the functions associated with them F_0, F_1, F_2, G_0, G_1, G_2, all derived in the Appendices. Some diagrammatic techniques used were previously discussed in Ref. 2; we shall refer our readers to it for further details. A brief summary is presented in Appendix A of this paper.

The first vector ray of the set of orthogonal vectors derived from the key equation (1.2) corresponds to one where all particles are at rest. Thus, in the grand-canonical ensemble, the coefficient C_0 is given by

$$C_0 = M_{\vec{0}0}F_0 + N_{\vec{0}0}G_0 e^{2\alpha}, \tag{3.1}$$

where F_0 and G_0 have been derived previously in Ref. 2 without summing terms involving u_3. In Appendix B, we have summed all terms involving u_2 and u_3. The results are given as follows:

$$F_0 = \exp(x), \tag{3.2}$$

where

$$x = \rho \int d^3r (e^{u_2(r)} - 1) + \frac{\rho^2}{2!} \int\int d^3r_1 d^3r_2 f_3(\vec{r}_1, \vec{r}_2)[1 + \rho(e^{u_2(r_1)} - 1) + \rho(e^{u_2(r_2)} - 1) + \rho^2(e^{u_2(r_1)} - 1)(e^{u_2(r_2)} - 1)], \tag{3.3}$$

and the function $f_3(r_1, r_2)$ is given by an infinite series

$$f_3(\vec{r}_1, \vec{r}_2) = e^{u_3(\vec{r}_1, \vec{r}_2)} - 1 + \frac{\rho^2}{(2!)^2} \int d^3r_3 (e^{u_3(\vec{r}_1, \vec{r}_3)} - 1)[1 + \rho(e^{u_2(r_3)} - 1)](e^{u_3(\vec{r}_3, \vec{r}_2)} - 1) + \cdots. \tag{3.4}$$

G_0 is given by

$$G_0 = \exp(y), \tag{3.5}$$

where the value of y is obtained simply by replacing u_2 in Eq. (3.3) with $-u_2$ and replacing f_3 with g_3. g_3 is obtained from Eq. (3.4) by replacing both u_2 and u_3 with $-u_2$ and $-u_3$. Obviously, as in the expressions for F_0 and G_0 given in Ref. 2, the present expressions are accurate only up to terms not involving the four-body correlation u_4.

From the definition of y, it is easy to see that y becomes infinite whenever the pair distribution function, which is proportional to $\exp[u_2(r) + u_2^*(r)]$, vanishes for any extended range of the relative coordinate r. In the approximation including u_3 terms, we do have some possible compensations from the terms multiplied to g_3. However, since these terms have different density factors, it is quite unlikely that they will remove the divergence of y. If y is infinite and the chemical potential α does not compensate for this infinity, then by equating $C_0 = 0$ we obtain the solution $N_{\vec{p}0} = 0$. In words, this result implies that the component for single-particle ODLRO vanishes. This can be seen from the inverse canonical transformation

$$a_{\vec{p}} = \sum_k M^*_{\vec{k}\vec{p}} b_{-\vec{k}} - N_{\vec{k}\vec{p}} b^\dagger_{\vec{k}} \tag{3.6}$$

[the indices of the matrix elements M^* and N given in Eq. (7.2) of Ref. 1 were inverted] and from the orthonormality of the matrices that the expectation of the zero momentum number operator is

$$\langle \hat{N}_0 \rangle = \sum_{\vec{k}} |N_{\vec{k}0}|^2 = \frac{|F_0|^2}{|G_0|^2 e^{4\alpha} - |F_0|^2}. \tag{3.7}$$

Let us assume here that we do have a soft-core-type particle-particle interaction such that G_0 remains finite. In this case the chemical potential α is given by the density constraint

$$\rho = \frac{|F_0|^2}{\Omega(|G_0|^2 e^{4\alpha} - |F_0|^2)} + \frac{1}{\Omega} \sum_{\vec{k}}{}' \frac{|C(k)|^2}{1 - |C(k)|^2}. \tag{3.8}$$

The function $C(k)$ has been given in Eq. (6.4) of Ref. 2:

$$C(k) = \frac{F_1(k)}{G_1(k) e^{2\alpha}}. \tag{3.9}$$

Also, from Eqs. (6.10) and (6.11) of the same reference, we can factor out a constant factor

$$C(k) = (F_0 / G_0 e^{2\alpha}) \chi(k), \tag{3.10}$$

where $\chi(k)$ is a defined function of k, except perhaps at $\vec{k} = 0$, which is actually excluded from the definition of $C(k)$. [There is a misprint in Eq. (6.11) of Ref. 2; the error is corrected in our Eqs. (3.20) and (3.22).] Because the density of the system is a finite quantity, it follows from Eq. (3.8) that we might combine the chemical potential α with the constants x and y, and that a renormalized chemical factor μ,

$$4\alpha + y + y^* - x - x^* = 4\mu\,, \tag{3.11}$$

exists where μ remains finite as we gradually increases the strength of the particle-particle repulsion. The renormalization procedure discussed above in handling realistic types of van der Waals form potentials is based on analytic continuation. For the hard-sphere case, postulate 1 for the existence of a one-to-one linear mapping between free-particle fields and hard-sphere fields is violated (see Siegert *et al.*[12] for detailed discussions); therefore, analytic continuation cannot be performed. For the present we shall confine ourselves only to cases where it is meaningful to rewrite the constant factor

$$|F_0|^2/|G_0|^2 e^{4\alpha} = e^{-4\mu}\,, \tag{3.12}$$

with the renormalized chemical potential μ satisfying

$$\rho = \frac{1}{\Omega(e^{4\mu}-1)} + \frac{1}{\Omega}\sum_{\vec{k}}{}' \frac{|\chi(k)|^2}{e^{4\mu} - |\chi(k)|^2}\,. \tag{3.13}$$

From Eqs. (1.1) and (3.8) we can now obtain an explicit representation for the matrix elements M, N. We have

$$\sum_{\vec{k}} [1 - e^{-4\mu}|\chi(k)|^2] M^*_{\vec{p}\vec{k}} M_{\vec{q}\vec{k}} = \delta_{\vec{p}\vec{q}}\,, \tag{3.14}$$

or

$$M_{\vec{p}\vec{q}} = \frac{\phi_{\vec{p}}(\vec{q})}{[1 - e^{-4\mu}|\chi(q)|^2]^{1/2}}\,, \tag{3.15}$$

where $\phi_{\vec{p}}(\vec{q})$ is a complete set of orthonormal functions

$$\sum_{\vec{q}} \phi^*_{\vec{p}}(\vec{q})\phi_{\vec{k}}(\vec{q}) = \delta_{\vec{p}\vec{k}} \tag{3.16}$$

to be determined by the Hamiltonian of the system. It is none the less interesting to point out here that if $\phi_{\vec{p}}(\vec{q})$ is the set of Kronecker deltas $\delta_{\vec{p}\vec{q}}$, then the Hamiltonian of the system is that of the Bogoliubov quadratic form. However, if $\phi_{\vec{p}}(\vec{q})$ is a set of cylindrical Bessel functions, then p can take on discrete integers, and the elementary excited states might be vortex lines. The freedom of choice of a complete set of $\phi_{\vec{p}}(\vec{q})$, with the ground state completely determined by the correlation functions, remains because the knowledge of the ground-state function does not uniquely determine an entire set of orthogonal functions. Whether the present method is useful in constructing models for superfluid helium with vortex states remains to be investigated.

To comment further on the question of Bose-Einstein condensation, let us turn our discussion to the function $\chi(k)$. Let us look at the coefficient C_1 associated with the single nonzero momentum particle-ray vector component of the key equation. By equating $C_1 = 0$, we obtain the ratio for the matrix elements $M_{\vec{p}\vec{q}}$ and $N_{\vec{p}\vec{q}}$ for the case $q \neq 0$,

$$C(q) = \frac{N_{\vec{p}\vec{q}}}{M_{\vec{p}\vec{q}}} = -e^{-2\alpha}\frac{F_1(q)}{G_1(q)}\,, \tag{3.17}$$

where the functions F_1 and G_1 are given as follows:

$$F_1(q) = \langle N-1;\vec{q}|\hat{S}_M|N+1\rangle \tag{3.18}$$

and

$$G_1(q) = \langle N-1;\vec{q}|\hat{S}_N|N-1\rangle\,, \tag{3.19}$$

such that q is the excited boson momentum.

Following a procedure similar to that presented for the calculation of F_0 and G_0, we find in Appendix C that F_1 and G_1 are given by

$$F_1(q) = F_0 f_1(q) \tag{3.20}$$

and

$$G_1(q) = G_0[1 + g_1(q)]\,, \tag{3.21}$$

where

$$f_1(q) = \rho\int d^3r\,(e^{u_2(r)} - 1)e^{i\vec{q}\cdot\vec{r}} + \rho^2\int\int d^3r_1 d^3r_2 f_3(\vec{r}_1,\vec{r}_2)[1 + (e^{u_2(r_1)} - 1) + \rho(e^{u_2(r_2)} - 1) + \rho^2(e^{u_2(r_1)} - 1)(e^{u_2(r_2)} - 1)]e^{i\vec{q}\cdot\vec{r}_1} \tag{3.22}$$

and

$$g_1(q) = \rho\int d^3r\,(e^{-u_2(r)} - 1)e^{i\vec{q}\cdot\vec{r}} + \rho^2\int\int d^3r_1 d^3r_2 g_3(\vec{r}_1,\vec{r}_2)[1 + \rho(e^{-u_2(r_1)} - 1) + \cdots]e^{i\vec{q}\cdot\vec{r}_1}\,. \tag{3.23}$$

If we assume that the pair-distribution function $e^{2u_2(r)}$ decreases as r^n for small values of r, then the function $e^{-u_2(r)}$ will diverge as $r^{-n/2}$ for small values of r. Thus, $g_1(k)$ will diverge if $n \geq 6$. Considering the expectation of the potential energy, the above restriction imposed by $g_1(k)$ implies that we cannot have a repulsive potential term of r^{-m} for small values of r, such that $m \geq 9$. This restriction on the repulsive part of the potential function is weak enough that we can include a large range of model potentials, though not the Lennard-Jones potential. We would like to point out further that the above restriction does not imply that $\chi(k)$ is necessarily analytic for all values of k. In fact $\chi(k)$ can have simple poles. Such a situation will certainly occur if the system has periodic properties of some kind. If $|\chi(0)|^2 \neq 1$, or for some values of k, $\max|\chi(k)|^2 > 1$, then it follows that the renormalized chemical potential μ cannot approach zero in the thermodynamic limit, and thus the system will not have Bose-Einstein condensation. From the above analysis we have just presented with regards to the properties of $\chi(k)$, it is now possible to deduce from experiments the analytic form of the pair correlation $u_2(r)$ for small values of r and to connect that with the possibility of the existence of single-particle ODLRO. A repulsive Bose gas without a Bose-Einstein condensation in the ground state does not necessarily violate the contention that a symmetric function with no nodes must have a finite zero Fourier component amplitude. This mathematical point can be seen more clearly from the hard-sphere Bose-field-operator algebra developed by Siegert *et al.*[12] Because of the nonlocal nature of these field operators, from their commutation rules, the zero Fourier component of the hard-sphere field operator is in fact a superposition of all momenta components of the free-field operator. We quote Siegert's field, $\psi(\vec{x}) = P(\vec{x})\psi_0(\vec{x})$, where $\psi_0(\vec{x})$ is the free-field operator and $P(\vec{x})$ is a projection operator which imposes the hard-sphere boundary conditions. The zero momentum component of $\psi(\vec{x})$ is, therefore, equal to $\sum_{\vec{k}} P_{-\vec{k}} a_{\vec{k}}$, where $P_{\vec{k}}$ and $a_{\vec{k}}$ are Fourier components of $P(\vec{x})$ and $\psi_0(\vec{x})$, respectively. It is not surprising that based on this algebra Meyer *et al.*[14] obtained a pseudopotential which replaces the nonlocal projection operator, and that the ground state obtained by them for the hard-sphere system gave no meaningful numerical value for the Bose-Einstein condensate at helium superfluid density.

As mentioned earlier, the pair-correlation function u_2 can be deduced from experimental results, such as the liquid-structure function. However, the liquid-structure function, similar to $F_1(k)$, is not a pure function of u_2; it includes contributions due to higher-order correlations such as u_3. Therefore, it is essential that we find the relationship between u_3 and u_2 so that we can deduce u_2 accurately from the experimental values for the liquid-structure function. In the past, investigators[15,16] made different conjectures to express u_3 in terms of u_2, or to express directly the three-body liquid-structure function S_3 in terms of the two-body liquid-structure function S_2. These conjectures, like the convolution approximation, are not derived from first principle; rather, they involve some mathematical guesses. In our present method, we are able to obtain the equation relating u_3 and u_2 from the two excited-particle vector ray component of the key equation. By equating C_2, the coefficient of that vector component, to zero, we obtain

$$F_2(\vec{q}_1,\vec{q}_2) = -e^{2\mu}\chi(\vec{q}_1+\vec{q}_2)G_2(\vec{q}_1,\vec{q}_2)\,, \tag{3.24}$$

where

$$F_2(\vec{q}_1,\vec{q}_2) = \langle N-2;\vec{q}_1,\vec{q}_2|\hat{S}_M|N+1\rangle \tag{3.25}$$

and

$$G_2(\vec{q}_1,\vec{q}_2) = \langle N-2;\vec{q}_1,\vec{q}_2|\hat{S}_N|N-1\rangle\,. \tag{3.26}$$

The derivation for F_2 and G_2 is given in Appendix D, and the result is

$$F_2(\vec{q}_1,\vec{q}_2) = \tfrac{1}{2}F_0[2f_1(q_1)f_1(q_2) + J(\vec{q}_1,\vec{q}_2)] \tag{3.27}$$

and

$$G_2(\vec{q}_1,\vec{q}_2) = \tfrac{1}{2}G_0[g_1(q_1)+g_1(q_2) + 2g_1(q_1)g_1(q_2) + V(\vec{q}_1,\vec{q}_2)], \tag{3.28}$$

where

$$J(\vec{q}_1,\vec{q}_2) = \int\int d^3r_1 d^3r_2 (e^{i\vec{q}_1\cdot\vec{r}_1 + i\vec{q}_2\cdot\vec{r}_2} + e^{i\vec{q}_1\cdot\vec{r}_2 + i\vec{q}_2\cdot\vec{r}_1})\cdot f_3(\vec{r}_1,\vec{r}_2) \times[1+2\rho(e^{u_2(r_1)}-1)+\rho^2(e^{u_2(r_1)}-1)(e^{u_2(r_2)}-1)]\,, \tag{3.29}$$

and

$$V(\vec{q}_1,\vec{q}_2) = \int\int d^3r_1 d^3r_2 (e^{i\vec{q}_1\cdot\vec{r}_1 + i\vec{q}_2\cdot\vec{r}_2} + e^{i\vec{q}_1\cdot\vec{r}_2 + i\vec{q}_2\cdot\vec{r}_1})\cdot g_3(\vec{r}_1,\vec{r}_2) \times[1+2\rho(e^{-u_2(r_1)}-1)+\rho^2(e^{-u_2(r_1)}-1)(e^{-u_2(r_2)}-1)]\,. \tag{3.30}$$

With the aid of Eqs. (3.27) and (3.28), we rewrite Eq. (3.24) as

$$J(\vec{q}_1,\vec{q}_2) + e^{2\mu+y-x}\chi(\vec{q}_1+\vec{q}_2)V(\vec{q}_1,\vec{q}_2) = -2f_1(q_1)f_1(q_2) - e^{2\mu+y-x}\chi(\vec{q}_1+\vec{q}_2)[g_1(q_1)+g_1(q_2)+2g_1(q_1)g_1(q_2)]\,. \tag{3.31}$$

Equation (3.31) can be approximated for both cases when G_0 is small or large in comparison to F_0. The first approximation was previously given in Ref. 1 and is not quite as interesting as the second approximation, because a realistic superfluid model usually has a short-range strong repulsive potential. Assuming G_0 much much larger than F_0, we see that Eq. (3.31) can be approximated with

$$V(\vec{q}_1, \vec{q}_2) \cong -g_1(q_1) - g_1(q_2) - 2g_1(q_1)g_1(q_2). \quad (3.32)$$

Supposing u_2 is given, it is now possible to deduce g_3 from Eqs. (3.30) and (3.32). In general the relationship between u_3 and u_2 as given by Eq. (3.31) is much more complex than that given by previous methods[15,16] because of the g_1 functions.

IV. CONCLUSION

We shall summarize what we have learned from the present investigation.

(1) Assuming the two postulates given by Wong and Fung,[1] we are able to connect the method of linear canonical transformation to that of a variation method based on constructing a set of basis-correlation functions. Postulate 1 unduly restricts the forms of the basis-correlation functions, which is not necessary in a pure variation calculation of the ground-state energy. Furthermore, the explicit representation of the linear transformation matrices obtained by these two postulates are unique only up to an arbitrary set of orthonormal functions. In order to determine the set of orthonormal functions, a specific Hamiltonian must be given. For example, by choosing the set to be that of Kronecker deltas, we limit ourselves to only Hamiltonians of the quadratic form.

(2) Both transformation matrices M and N are nonzero if and only if the short-range repulsive potential between two particles is less divergent than r^{-9}. This limitation will disallow the Lennard-Jones potential, but will still be general enough for construction of a van der Waals type of potential between particles.

(3) The existence of a finite portion of Bose-Einstein condensate is subject to the magnitude of the function $|\chi(k)|^2$, defined by Eq. (3.10). It is easy to see from Eq. (3.13) that both terms in that equation are positive definite. From the first term, which gives the amount of Bose-Einstein condensation, we see that the renormalized chemical potential μ must be given by

$$\mu = \tfrac{1}{4}\ln(1 + 1/AN), \quad (4.1)$$

where A is a positive constant less than 1. From the integrand of the second term of Eq. (3.13), if $\max|\chi(k)|^2 > 1$, A must approach zero like $1/N$, thus implying that in the thermodynamic limit, Bose-Einstein condensation for this case approaches zero as $1/\Omega$. Hence, Bose-Einstein condensation will exist, iff $\max|\chi(k)|^2 < 1$ and $|\chi(0)|^2 = 1$. If A remains finite, it implies that the single-particle ODLRO exists for

$$\lim_{x\to\infty} \langle \hat{\rho}(\vec{x})\rangle = N_0. \quad (4.2)$$

Higher orders of ODLRO in the system can easily be seen from the Fourier transforms of the general n-body liquid-structure functions

$$S_n(\vec{k}_1, \ldots, \vec{k}_n) = N^{-1}\langle \hat{\rho}\vec{k}_1\, \hat{\rho}\vec{k}_2, \ldots, \hat{\rho}\vec{k}_n\rangle, \quad (4.3)$$

with the constraints

$$\sum_{i=1}^{n} \vec{k}_i = 0, \quad (4.4)$$

$$m < n.$$

$$\sum_{i=1}^{m} \vec{p}_i \neq 0, \quad (4.5)$$

(4) We have derived the equation relating the three-body correlation function u_3 to the two-body correlation function u_2 from first principle. The result is given in Eq. (3.31), and the situation with strong short-range repulsive potential was given in an approximated form in Eq. (3.32). A comparison with other works is quite difficult analytically[6,15-17] because in those works an approximation of the three-body liquid-structure function or the three-body correlation function was made. A numerical test can be performed on a model Hamiltonian using our results and those of previous authors.[6,17] We have not performed any such numerical computations in this paper. We would also like to point out one advantage of our method, i.e., that a general equation relating u_n to all the lower orders of u_i can be obtained from the $(n+1)$th-order vector ray component of our key equation that is quite similar to those connecting the multiparticle T-matrix equations.[18]

(5) In the event Bose-Einstein condensation N_0 is small, we cannot make the c-number approximation, which is required, in order to be able to approximate the Hamiltonian by one of the quadratic form. This point might be the reason why no good numerical fit was ever obtained by a Bogoliubov model for superfluid helium,[14,19] whereas the method of basis-correlation functions gave rather good results, particularly when some form of u_3 or S_3 was included in the calculations.[6,16,17] From Eq. (3.15), our above observation implies that nonquadratic terms in the Hamiltonian, which lead to off-diagonal matrix elements in the canonical-transformation representation, are very important in the case of

liquid-helium calculations, even if we choose a particle interaction potential satisfying the mathematical restriction imposed by the existence condition of one-to-one linear mapping.

APPENDIX A: DIAGRAMMATIC TECHNIQUES

First we, introduce the following fundamental diagrams representing the two- and three-body correlation functions:

$$●\!— \equiv N\sum_{\vec{l}} W_2(\vec{l})e^{i\vec{l}\cdot\vec{r}} = \rho u_2(\vec{r}), \tag{A1}$$

where the solid dot symbolizes the two-body correlation and the solid line represents the argument variable $\vec{r}$. If the above diagram is replaced by ●—×, we mean that the variable $\vec{r}$ is integrated out, such that

$$●\!—\!\times \equiv N\sum_{\vec{l}} W_2(\vec{l})\,\delta_{\vec{l},0} = \rho\int u_2(\vec{r})d\vec{r}. \tag{A2}$$

However, if the diagram is connected by an additive wave line after the cross, then it represents the Fourier transform of $u_2(\vec{r})$, namely,

$$●\!—\!\times\!\sim\!\sim\!\sim\ \vec{q} \equiv N\sum_{\vec{l}} W_2(\vec{l})\delta_{\vec{l}-\vec{q},0} = \rho\int u_2(\vec{r})e^{-i\vec{q}\cdot\vec{r}}d\vec{r}. \tag{A3}$$

Similarly, we can treat the three-body correlation function in the same way, with the open circle denoting three-body correlation:

$$—\!\circ\!— \equiv N^2\sum_{\vec{l}_1,\vec{l}_2} W_3(\vec{l}_1,\vec{l}_2)e^{-i(\vec{l}_1\cdot\vec{r}_1+\vec{l}_2\cdot\vec{r}_2)} = \rho^2 u_3(\vec{r}_1,\vec{r}_2). \tag{A4}$$

Similarly,

$$—\!\circ\!—\!\times = \rho^2\int u_3(\vec{r}_1,\vec{r}_2)d\vec{r}_2, \tag{A5}$$

$$\times\!—\!\circ\!—\!\times = \rho^2\int\int u_3(\vec{r}_1,\vec{r}_2)d\vec{r}_1\,d\vec{r}_2, \tag{A6}$$

$$—\!\circ\!—\!\times\!\sim\!\sim\!\sim\ \vec{q} = \rho^2\int u_3(\vec{r}_1,\vec{r}_2)e^{-i\vec{q}\cdot\vec{r}_2}\,d\vec{r}_2, \tag{A7}$$

$$\overset{\vec{q}_1}{\sim\!\sim\!\sim}\!\times\!—\!\circ\!—\!\times\!\overset{\vec{q}_2}{\sim\!\sim\!\sim} = \rho^2\int\int u_3(\vec{r}_1,\vec{r}_2)e^{-i(\vec{q}_1\cdot\vec{r}_1+\vec{q}_2\cdot\vec{r}_2)}d\vec{r}_1\,d\vec{r}_2. \tag{A8}$$

In the previous papers[1,2] we have chosen $W_n = 0$ if any of its arguments is equal to zero. This choice stems from the fact that terms associated with vanishing arguments are always reducible to a lower-order correlation functional form. Therefore, this choice implies that any diagram having a cross at the end of a single line will in effect be zero. Hence,

$$●\!—\!\times = 0,\quad —\!\circ\!—\!\times = 0,\quad \sim\!\sim\!\sim\!\times\!—\!\circ\!—\!\times = 0.$$

However, the diagram ●—×—○— ≠0, because the cross appears at the end of two solid lines.

From the above definitions, it is clear that the correlation diagrams can either be expressed in momenta variables or in coordinate variables form. In many cases it is easier to express them in momentum form.

Some typical diagrams are chosen to illustrate the counting of the momentum-transferring process. The first representative diagram we now discuss is

$$\frac{1}{2!}\frac{1}{2!}\frac{1}{2!}\ \begin{matrix}●\!\times\!●\\ \text{◇}\end{matrix} = \frac{1}{2!}\frac{1}{2!}\frac{1}{2!}\sum_{\vec{k}_1^1,\vec{k}_1^2,\vec{k}_1^3,\vec{k}_1^4,\vec{k}_2^3,\vec{k}_2^4}{}' N^3W_2(\vec{k}_1^1)W_2(\vec{k}_1^2)\delta_{\vec{k}_1^1+\vec{k}_1^2,0} \times W_3(\vec{k}_1^3,\vec{k}_2^3)W_3(\vec{k}_1^4,\vec{k}_2^4)\delta_{\vec{k}_1^3+\vec{k}_1^4,0}\,\delta_{\vec{k}_2^3+\vec{k}_2^4,0}. \tag{A9}$$

In order to explain the numerical factor 1/2!2!2!, we note the following:

(1) Since there are four correlation functions, this diagram belongs to the 4th order commutator in (2.5). The coefficient associated to this order is 1/4!.

(2) The expansion coefficient for $2W_2$'s and $2W_3$'s in $\prod_{i=1}^4(\hat{F}_1^i+\hat{F}_2^i)$ of (2.9) is 6, following the binomial expansion.

(3) The number of possibly distinctive momentum-transfer configurations is 1×2, i.e., 1 for ●×● and 2 for ◇.

The counting coefficient for the diagram in (A9), as a result, would be

$$\frac{1}{4!}\times 6\times 1\times 2\times\left(\frac{1}{1!}\frac{1}{1!}\frac{1}{2!}\frac{1}{2!}\right) = \frac{1}{2!}\frac{1}{2!}\frac{1}{2!},$$

where the factor 1/(1!1!2!2!) accounts for the weighting for $W_2W_2W_3W_3$. Since the coefficient written before the diagram has included all counting statistics, only a single diagrammatic term representing one of the possible arrangements is necessary.

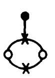
To simplify the counting process, we formulate some shortcuts:

(1) If a permutation of two correlation functions, associated with different momenta, changes the momentum-transfer configuration, the counting coefficient is simply 1/1!, implying that there is no redundant counting. For example, in the diagram

$\frac{1}{1!}$, $\frac{1}{1!}$

a permutation of $2W_3$'s though retaining the same form of the diagram, alters the momentum-transfer configuration. Hence, the counting coefficient is 1/1!.

(2) If two correlation functions are permutated, resulting in no change in the momentum-transfer configuration, the counting coefficient is 1/2! (i.e., with redundant counting). For example, in the diagram

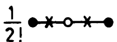
$\frac{1}{2!}$  ,

a permutation of $2W_3$'s gives the same momentum-transfer configuration. Thus, the factor 1/2! is provided to take care of the redundant counting.

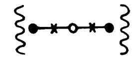
(3) Permutation of two similar groups of more than two correlation functions follows the same counting statistics.

This counting process allows the coefficients associated with other complicated diagrams to be calculated easily.

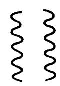
In transforming the momentum-transfer diagrams into integral forms (with real coordinates), if a permutation of two variables $\vec{r}_1, \vec{r}_2$ changes the real coordinate configurations, a factor of 2! should be incorporated. A similar argument applies for more than two variables. For instance, in the diagram

$\frac{1}{2!}$ 

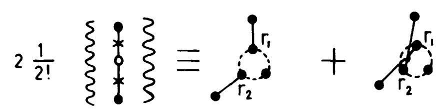
in integral form, we have two distinctive configurations

$2\,\frac{1}{2!}$  ,

where

 ,

the wiggled bracket, indicates the diagram to be represented in real space. As presented in a previous paper,[1] we have

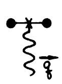


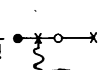
(A10)

where the symbol • represents one real particle, •—• two-particle correlation, and  three-particle correlation, on the right side of the identity. Therefore,

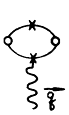
$\frac{1}{2!}$ 
$$\equiv (2)\,\frac{1}{2!}\iint \rho^4 u_2(\vec{r}_1)u_3(\vec{r}_1,\vec{r}_2)u_2(\vec{r}_2)\,d\vec{r}_1\,d\vec{r}_2 \equiv \rho^4 \iint u_2(\vec{r}_1)u_3(\vec{r}_1,\vec{r}_2)u_2(\vec{r}_2)\,d\vec{r}_1\,d\vec{r}_2 . \quad \text{(A11)}$$

We also present some relevant diagrams:

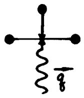
$\frac{1}{2!}$ 
$$= \frac{N}{2!}\sum_{\vec{l}_1,\vec{l}_2}{}' W_2(\vec{l}_1)W_2(\vec{l}_2)\delta_{\vec{l}_1+\vec{l}_2-\vec{q},0} = \frac{\rho}{2!}\int u_2^2(\vec{r}_1)e^{-i\vec{q}\cdot\vec{r}_1}\,d\vec{r}_1 , \quad \text{(A12)}$$

$\frac{1}{1!}$ 
$$= \frac{N^3}{1!}\sum_{\vec{l}_1,\vec{k}_1,\vec{k}_2}{}' W_2(\vec{l}_1)\,W_3(\vec{k}_1,\vec{k}_2)\delta_{\vec{l}_1+\vec{k}_1-\vec{q},0}\,\delta_{\vec{k}_2,0}$$

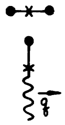
$$= \frac{\rho^3}{1!}\iint u_2(\vec{r}_1)u_3(\vec{r}_1,\vec{r}_2)e^{-i\vec{q}\cdot\vec{r}_1}\,d\vec{r}_1\,d\vec{r}_2 , \quad \text{(A13)}$$

$\frac{1}{2!}$ 
$$= \frac{N^2}{2!}\sum_{\vec{k}_1^1,\vec{k}_2^1,\vec{k}_1^2,\vec{k}_2^2}{}' W_3(\vec{k}_1^1,\vec{k}_2^1)W_3(\vec{k}_1^2,\vec{k}_2^2)\delta_{\vec{k}_1^1+\vec{k}_1^2-\vec{q},0}\,\delta_{\vec{k}_2^1+\vec{k}_2^2,0}$$

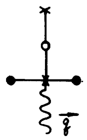
$$= \frac{\rho^2}{2!}\iint u_3^2(\vec{r}_1,\vec{r}_2)e^{-i\vec{q}\cdot\vec{r}_1}\,d\vec{r}_1\,d\vec{r}_2 , \quad \text{(A14)}$$

$\frac{1}{3!}$  $= \frac{N}{3!} \sum'_{\vec{l}_1, \vec{l}_2, \vec{l}_3} W_2(\vec{l}_1) W_2(\vec{l}_2) W_2(\vec{l}_3) \delta_{\vec{l}_1+\vec{l}_2+\vec{l}_3-\vec{q}, 0}$

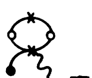
$$= \frac{\rho}{3!} \int u_2^3(\vec{r}_1) e^{-i\vec{q}\cdot\vec{r}_1} d\vec{r}_1, \qquad \text{(A15)}$$

$\frac{1}{2!}$  $= \frac{N^2}{2!} \sum'_{\vec{l}_1, \vec{l}_2, \vec{l}_3} W_2(\vec{l}_1) W_2(\vec{l}_2) W_2(\vec{l}_3) \delta_{\vec{l}_1+\vec{l}_2, 0} \delta_{\vec{l}_3-\vec{q}, 0}$

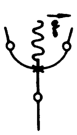
$$= \frac{\rho^2}{2!} \int u_2(\vec{r}_1) e^{-i\vec{q}\cdot\vec{r}_1} d\vec{r}_1 \int u_2^2(\vec{r}_2) d\vec{r}_2, \qquad \text{(A16)}$$

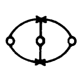
$\frac{1}{2!}$  $= \frac{N^3}{2!} \sum'_{\vec{l}_1, \vec{l}_2, \vec{k}_1, \vec{k}_2} W_2(\vec{l}_1) W_2(\vec{l}_2) W_3(\vec{k}_1, \vec{k}_2) \delta_{\vec{k}_1, 0} \delta_{\vec{k}_2+\vec{l}_1+\vec{l}_2-\vec{q}, 0}$

$$= \frac{\rho^3}{2!} \iint u_2^2(\vec{r}_1) u_3(\vec{r}_1, \vec{r}_2) e^{-i\vec{q}\cdot\vec{r}_1} d\vec{r}_1 d\vec{r}_2, \qquad \text{(A17)}$$

$\frac{1}{2!}$  $= \frac{N^3}{2!} \sum'_{\vec{l}_1, \vec{k}_1^1, \vec{k}_2^1, \vec{k}_1^2, \vec{k}_2^2} W_2(\vec{l}_1) W_3(\vec{k}_1^1, \vec{k}_2^1) W_3(\vec{k}_1^2, \vec{k}_2^2) \delta_{\vec{k}_1^1+\vec{k}_1^2, 0} \delta_{\vec{l}_1+\vec{k}_2^1+\vec{k}_2^2-\vec{q}, 0}$

$$= \frac{\rho^3}{2!} \iint u_2(\vec{r}_1) u_3^2(\vec{r}_1, \vec{r}_2) e^{-i\vec{q}\cdot\vec{r}_1} d\vec{r}_1 d\vec{r}_2, \qquad \text{(A18)}$$

$\frac{1}{3!}$  $= \frac{\rho^6}{3!} \int u_3(\vec{r}_1, \vec{r}_4) u_3(\vec{r}_2, \vec{r}_4) u_3(\vec{r}_3, \vec{r}_4) e^{-i\vec{q}\cdot\vec{r}_4} d\vec{r}_4, \qquad \text{(A19)}$

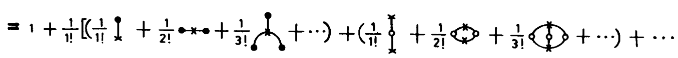
$\frac{1}{3!}$  $= \frac{\rho^2}{3!} \iint u_3^3(\vec{r}_1, \vec{r}_2) d\vec{r}_1 d\vec{r}_2. \qquad \text{(A20)}$

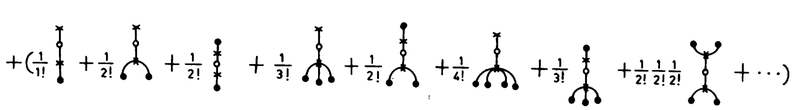
Other higher-order diagrams can be defined in a similar manner. More than one momentum exchange vector (represented by a number of wave lines) can be joined to the "joints" (represented by crosses), which are frequently present in higher orthogonal states. On the other hand, diagrams without wave lines contribute to the calculation of the coefficient C_0.

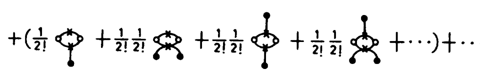
APPENDIX B: SUMMING OF F_0, G_0

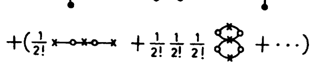
In momentum-transfer diagrams, the series of F_0 can be written as

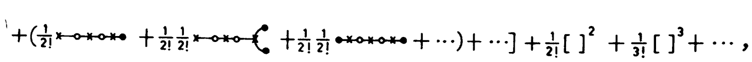
$F_0 = \langle N | \hat{S}_M | N+1 \rangle$



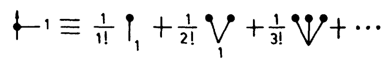






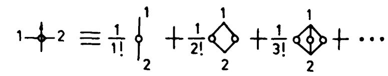
 (B1)

where the series in the square bracket [ ] is the same for all powers of expansion. In order to sum the diagrams more systemmatically, the following set of diagrams is introduced:



$$=\rho(e^{u_2(\vec{r}_1)}-1)\,, \tag{B2}$$

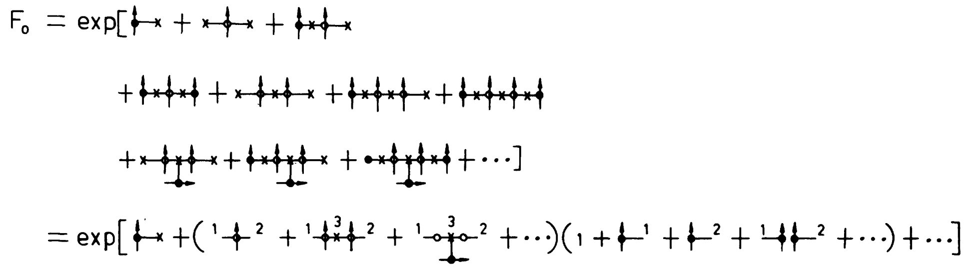
The number 1 written near a "hand" in the momentum-transfer diagrams indicates that the variable $\vec{r}_1$ is not yet integrated. This series includes all numbers of two-body correlation functions ranging from one to infinity:



$$=\rho^2(e^{u_3(\vec{r}_1,\vec{r}_2)}-1)\,. \tag{B3}$$

This series contains all number of three-body correlation functions ranging from one to infinity and is not yet integrated over variable $\vec{r}_1$, $\vec{r}_2$.

After rearrangements of the diagrams in (B1), F_0 becomes, in view of (B1) and (B2),



$$= \exp\Big(\rho\int d\vec{r}\,(e^{u_2(\vec{r})}-1)$$

$$+\frac{\rho^2}{2!}\iint d\vec{r}_1\,d\vec{r}_2 f_3(\vec{r}_1,\vec{r}_2)\,[1+\rho(e^{u_2(\vec{r}_1)}-1)+\rho(e^{u_2(\vec{r}_2)}-1)+\rho^2(e^{u_2(\vec{r}_1)}-1)(e^{u_2(\vec{r}_2)}-1)\;+\cdots\Big)\,, \tag{B4}$$

where the function $f_3(\vec{r}_1,\vec{r}_2)$ is given by an infinite series, namely,

$$f_3(\vec{r}_1,\vec{r}_2)=e^{u_3(\vec{r}_1,\vec{r}_2)}-1+\frac{\rho^2}{(2!)^2}\int d\vec{r}_3\,(e^{u_3(\vec{r}_1,\vec{r}_3)}-1)$$

$$\times[1+\rho(e^{u_2(\vec{r}_3)}-1)](e^{u_3(\vec{r}_3,\vec{r}_2)}-1)+\cdots\,. \tag{B5}$$

It should be noted that a factor of 1/2! takes care of a pair of dummy variables in the three-body correlation function. The series G_0 is summed similarly, namely,

$$G_0=\langle N|\hat{S}_N|N-1\rangle=\exp\Big(\rho\int d\vec{r}(e^{-u_2(\vec{r})}-1)$$

$$+\frac{\rho^2}{2!}\iint d\vec{r}_1\,d\vec{r}_2\,g_2(\vec{r}_1,\vec{r}_2)[1+\rho(e^{-u_2(\vec{r}_1)}-1)$$

$$+\rho(e^{-u_2(\vec{r}_2)}-1)+\rho^2(e^{-u(\vec{r}_1)}-1)(e^{-u_2(\vec{r}_2)}-1)]+\cdots\Big)\,, \tag{B6}$$

where the function $g_3(\vec{r}_1,\vec{r}_2)$ is given by

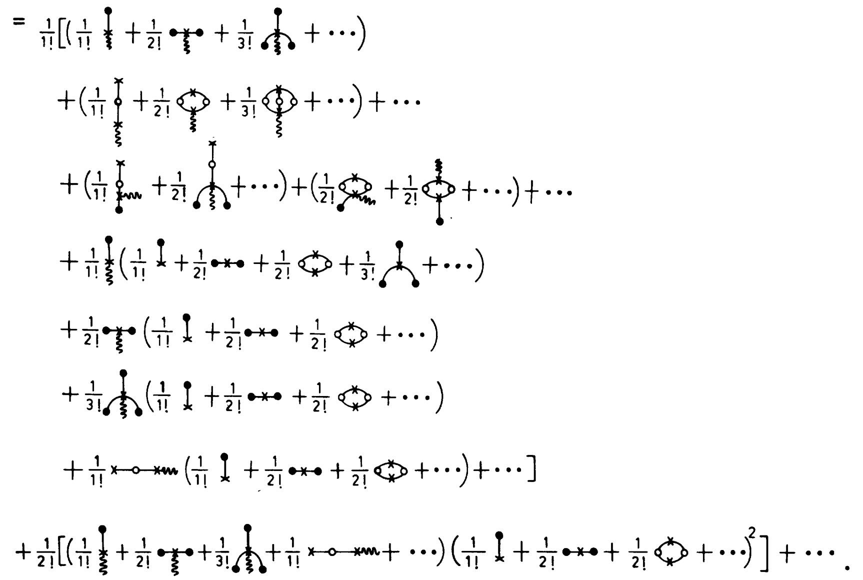
$$g_3(\vec{r}_1,\vec{r}_2)=e^{-u_3(\vec{r}_1,\vec{r}_2)}-1+\frac{\rho^2}{(2!)^2}\int d\vec{r}_3(e^{-u_3(\vec{r}_1,\vec{r}_3)}-1)[1+\rho(e^{-u_2(\vec{r}_3)}-1)](e^{-u_3(\vec{r}_3,\vec{r}_2)}-1)+\cdots\,. \tag{B7}$$

The series G_0 is obtained by simply replacing u_2 and u_3 by $-u_2$ and $-u_3$, respectively, in (B4) and (B5).

APPENDIX C: SUMMING OF $F_1(\vec{q})$, $G_1(\vec{q})$

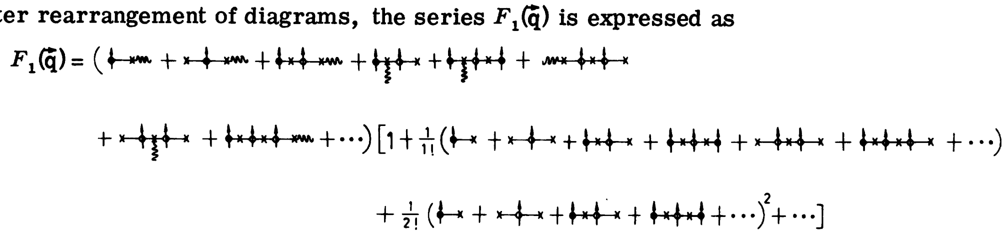
The diagrams in the series $F_1(\vec{q})$ contain a wave line indicating the nonzero momentum $\vec{q}$. With the same counting techniques, we write the summation of the series $F_1(\vec{q})$ as

$$F_1(\vec{q}) = \langle N-1; \vec{q}\,|\hat{S}_M|\,N+1\rangle$$



(C1)

After rearrangement of diagrams, the series $F_1(\vec{q})$ is expressed as



$$= f_1(\vec{q})\,F_0\,, \tag{C2}$$

where

$$f_1(\vec{q}) = \rho \int d\vec{r}\,(e^{u_2(\vec{r})}-1)e^{i\vec{q}\cdot\vec{r}} + \rho^2 \iint d\vec{r}_1\, d\vec{r}_2 f_3(\vec{r}_1,\vec{r}_2)[1+\rho(e^{u_2(\vec{r}_1)}-1) + \rho(e^{u_2(\vec{r}_2)}-1) + \rho^2(e^{u_2(\vec{r}_1)}-1)(e^{u_2(\vec{r}_2)}-1)]\, e^{i\vec{q}\cdot\vec{r}_1}\,. \tag{C3}$$

The series $G_1(\vec{q})$ is summed similarly, namely,

$$G_1(\vec{q}) = \langle N-1; \vec{q}\,|\hat{S}_N|\,N-1\rangle\,. \tag{C4}$$

However, there is an extra term where the excited particle of momentum $\vec{q}$ does not correlate with other particles which interact themselves. This term simply gives the series G_0.

As a result, we obtain

$$G_1(\vec{q}) = G_0[1+g_1(\vec{q})]\,, \tag{C5}$$

where

$$g_1(\vec{q}) = \rho \int d\vec{r}\,(e^{-u_2(\vec{r})}-1)\,e^{i\vec{q}\cdot\vec{r}} + \rho^2 \iint d\vec{r}_1\, d\vec{r}_2\, g_3(\vec{r}_1,\vec{r}_2) \times [1+\rho(e^{-u_2(\vec{r}_1)}-1)+\rho(e^{-u_2(\vec{r}_2)}-1) + \rho^2(e^{-u_2\,(\vec{r}\,)}-1)(e^{-u_2(\vec{r}_2)}-1)]\, e^{i\vec{q}\cdot\vec{r}_1}\,. \tag{C6}$$

APPENDIX D: SUMMING OF $F_2(\vec q_1, \vec q_2)$, $G_2(\vec q_1, \vec q_2)$

In the evaluation of F_0, the following result is obtained, namely

$$F_0 = \frac{1}{1!}[x] + \frac{1}{2!}[x][x] + \frac{1}{3!}[x][x][x] + \cdots , \tag{D1}$$

as stated in Eq. (3.2). The function $[x]$ is given by Eq. (3.3), which describes the effect of correlations without excitation of particles. However, for the series $F_2(\vec q_1, \vec q_2)$, two particles are excited to nonzero momenta $\vec q_1$ and $\vec q_2$, respectively. To evaluate this series, it is noted that $\vec q_1$ and $\vec q_2$ appear in the expansion of F_0 in the following patterns:

(a) $[\,{}^{\vec q_1}_{\vec q_2}]$ representing $\vec q_1, \vec q_2$ attached to one function $[x]$, but at different variables $\vec r_1, \vec r_2$;

(b) $[\,{}^{\vec q_1}][\,{}^{\vec q_2}]$ represents each $\vec q$ attached to one function $[x]$.

Moreover, the "attachments" of $\vec q_1, \vec q_2$ to the series F_0 in pattern (a) give a choice of n possibilities, while in pattern (b) there is a choice of $n(n-1)$ possibilities. Consequently, we can write F_2 as

$$\begin{aligned} F_2(\vec q_1, \vec q_2) &= \tfrac{1}{1!}(1)[\,{}^{\vec q_1}_{\vec q_2}] + \tfrac{1}{2!}(2)[\,{}^{\vec q_1}_{\vec q_2}]\,X + \tfrac{1}{3!}(3)[\,{}^{\vec q_1}_{\vec q_2}]\,X^2 + \cdots \\ &\quad + \tfrac{1}{2!}(2\cdot 1)[\,{}^{\vec q_1}][\,{}^{\vec q_2}] + \tfrac{1}{3!}(3\cdot 2)[\,{}^{\vec q_1}][\,{}^{\vec q_2}]\,X + \cdots \\ &= [\,{}^{\vec q_1}_{\vec q_2}]\,F_0 + [\,{}^{\vec q_1}][\,{}^{\vec q_2}]\,F_0 \ . \end{aligned} \tag{D2}$$

Using the diagrammatic techniques discussed in the previous Appendices, it is straightforward to write the diagrams in (D2) in integral forms:

$$\begin{aligned} [\,{}^{\vec q_1}_{\vec q_2}] &= \frac{1}{2!} J(\vec q_1, \vec q_2) \\ &= \frac{1}{2!} \iint d\vec r_1\, d\vec r_2 \left(e^{i(\vec q_1\cdot\vec r_1 + \vec q_2\cdot\vec r_2)} + e^{i(\vec q_1\cdot\vec r_2 + \vec q_2\cdot\vec r_1)}\right) \\ &\qquad \times f_3(\vec r_1, \vec r_2)[1 + 2\rho(e^{u_2(\vec r_1)} - 1) + \rho^2(e^{u_2(\vec r_1)} - 1)(e^{u_2(\vec r_2)} - 1)] , \end{aligned} \tag{D3}$$

$$[\,{}^{\vec q_1}][\,{}^{\vec q_2}] = f_1(\vec q_1) f_1(\vec q_2) , \tag{D4}$$

where $f_3(\vec r_1, \vec r_2)$ is defined by (B5) and $f_1(q)$ by (C3). Moreover, the factor $1/2!$ in (D3) accounts for the dummy variables $\vec r_1, \vec r_2$. In view of (D3) and (D4), we obtain the result

$$F_2(\vec q_1, \vec q_2) = \tfrac{1}{2} F_0 [2 f_1(q_1) f_2(q_2) + J(\vec q_1, \vec q_2)] . \tag{D5}$$

The series $G_2(\vec q_1, \vec q_2)$ can be summed in a similar manner. However, there is one extra term in the series which corresponds to $\vec q_1 + \vec q_2 = 0$. As a result, we obtain

$$\begin{aligned} G_2(\vec q_1, \vec q_2) &= \langle N-2; \vec q_1, \vec q_2 | \hat S_N | N-1 \rangle \\ &= \tfrac{1}{2} G_0 [g_1(\vec q_1) + g_1(\vec q_2) + 2 g_1(\vec q_1) g_1(\vec q_2) + \nu(\vec q_1, \vec q_2)] , \end{aligned} \tag{D6}$$

where

$$\begin{aligned} \nu(\vec q_1, \vec q_2) &= \iint d\vec r_1\, d\vec r_2 \left(e^{i(\vec q_1\cdot\vec r_1 + \vec q_2\cdot\vec r_2)} + e^{i(\vec q_1\cdot\vec r_2 + \vec q_2\cdot\vec r_1)}\right) \\ &\qquad \times g_3(\vec r_1, \vec r_2)[1 + 2\rho(e^{-u_2(\vec r_1)} - 1) + \rho^2(e^{-u_2(\vec r_1)} - 1)(e^{-u_2(\vec r_2)} - 1)] , \end{aligned} \tag{D7}$$

and $g_1(q)$ is given by (C6) and $g_3(\vec r_1, \vec r_2)$ by (B7).

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