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PHYSICAL REVIEW A VOLUME 2, NUMBER 5 NOVEMBER 1970

Diagrammatic Analysis of the Method of Correlated Basis Functions. I. Jastrow Correlating Factor for a Weakly Interacting Bose Gas[*]

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(Received 4 June 1970)

The method of correlated basis functions (CBF) is examined for the special case of a weakly interacting Bose gas. Using the Hugenholtz-Pines theory, we compute the ground-state energy exactly to fourth order in the interaction strength. The resulting expression is compared term by term with the unperturbed ground-state energy computed in the CBF using a Jastrow function as the correlating factor. We find that the three leading orders are all accounted for by the Jastrow function, while beginning in the fourth order only selected terms are included. The use of a correlated wave function in effect corresponds to summations of selected diagrams to all orders. In particular, the ring diagrams and the ladder diagrams are most susceptible to these summations. In a separate paper we shall examine effects of perturbation in the CBF.

I. INTRODUCTION

We consider a system of N particles, contained in a volume Ω and interacting pairwise via a potential $v(r)$. N and Ω both approach infinity while the number density $n \equiv N/\Omega$ remains constant. Such a system is described by the Hamiltonian

$$H=\sum_{i=1}^{N} -\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{i<j=1}^{N} v(r_{ij}) , \qquad (1)$$

and by the statistics of the particles.

A complete quantum-mechanical solution of the problem consists of determining all properly symmetrized eigenfunctions of this Hamiltonian and the corresponding spectrum of energy eigenvalues. For all realistic problems, however, we do not entertain the hope of obtaining such a complete solution; nor do we desire such a detailed description. In particular, for understanding properties of matter at low temperatures, we need only information concerning the ground state and the low-lying excitations. If the interaction $v(r)$ is weak, good approximation to these states can be found by applying low-order perturbative corrections to free-particle states.

For quantum liquids and solids, which include liquid and solid helium, Coulomb gases, and nuclear systems, the effects of $v(r)$ are far from insignificant. In fact, the interparticle correlations *dominate* the properties of these systems. Under these circumstances, the ordinary low-order perturbation theory fails. We have on our hands a many-body problem.

We distinguish in this paper two approaches toward treating the many-body problem: the independent-particle representation and the correlated representation. By the independent-particle representation we mean all field-theoretic methods which employ an independent-particle basis. When divergences arise in the matrix elements of $v(r)$, or in the perturbative expansion, one turns toward partial summation techniques – in the form of diagrammatic rearrangements or Green's functions. By the correlated representation, we mean the method of correlated basis functions (CBF), which begins with a set of basis functions containing correlating factors. With the correlating factors suitably chosen, divergences of either nature can be avoided. One recovers at once the validity and convenience of a low-order perturbation theory.

The method of CBF has by now been applied to all conceivable quantum liquids, and in each case has achieved certain degree of success. We refer the reader to a recent monograph by Feenberg,[1] and to a representative set of publications[2] and the references quoted therein. It has always appeared mysterious to many-body theorists trained in the independent-particle representation as to how and why the CBF can be so successful, particularly when it comes to numerical applications. What diagrams are being summed? To what order are they summed accurately? We begin with this paper an investigation which we hope will lead toward illuminating answers to these questions. In the remaining part of this section, we shall review briefly the method of CBF, define the specific case to be investigated here, and outline our method of attack.

A correlated basis function assumes the form of a product of two factors. One factor is known as the model function, and will be denoted by $\phi_{n_1,n_2,\ldots,n_N}(1,2,\ldots,N)$. This factor accounts for the single-particle properties of the system: The subscripts $\{n_1, n_2, \ldots, n_N\}$ specify which single-particle orbitals are occupied, and the function ϕ is simply a properly symmetrized product of these single-particle orbitals. By retaining the quantum numbers suggested by an independent-particle description, we adopt the prevailing theoretical practice of picturing low-lying states as elementary excitations. In this sense, CBF does not deviate from the mainstream of many-body concepts. The other factor is known as the correlating factor $F(1,2,\ldots,N)$, which has the responsibility of handling correlations characteristic of the interaction term in H. In the case of pairwise interactions, it is natural to select as F a product of two-particle functions:

$$F(1,2,\ldots,N)=\prod_{\substack{i<j\\=1}}^{N} f(r_{ij})\equiv\prod_{\substack{i<j\\=1}}^{N} e^{u(r_{ij})/2} \quad . \qquad (2)$$

Such a correlating factor is known as the Jastrow function. As long as the properties in which we are interested depend only on a group of states lying near one another, the state dependence of F is unimportant and is usually neglected. Whatever errors are committed by this appproximation will reveal themselves in the convergence property of the perturbation series. The crucial requirement for the success of a CBF calculation resides in an intelligent choice of $f(r)$, or equivalently $u(r)$, which leads to rapid convergence.

An ideal CBF calculation proceeds in several stages, summarized as follows.

(i) Based on a careful study of the Hamiltonian, an analysis of the properties of the system, and frequently auxiliary calculations such as a variational calculation for the ground state, a sound choice of the correlating factor $f(r)$ is made and the correlated basis constructed:

$$\psi_{n_1,n_2,\ldots,n_N}(1,2,\ldots,N)$$

$$=\prod_{\substack{i<j\\=1}}^{N} f(r_{ij})\,\phi_{n,n_2,\ldots,n_N}(1,2,\ldots,N)\ . \qquad (3)$$

(ii) Matrix elements of H and 1 are computed. Depending on the choice of F, the computation takes on various levels of difficulty. In some cases cluster expansion techniques or Monte Carlo methods are necessary.

(iii) The correlated basis is orthogonalized, i.e., the matrix of 1 is diagonalized. An effective (or quasiparticle) Hamiltonian is then constructed from the matrix elements and expressed in a second-quantized form.

(iv) A low-order perturbation theory usually suffices for extracting the ground-state and low-temperature properties. If not, with the Hamiltonian second quantized, the entire wealth of field-theoretic methods is available.

The specific problem chosen to be treated here is that of a weakly interacting Bose gas. The pairwise interaction is characterized by a strength parameter λ and by the existence of a Fourier transform:

$$v_k=\int d\vec{r}\,v(r)\,e^{i\vec{k}\cdot\vec{r}}\ . \qquad (4)$$

We compute the ground-state energy as a power series in λ using both the independent-particle and the correlated representations, and make term-by-term comparison. Results to be reported here have been summarized in a recent Letter.[3]

Section II reviews our computation of the ground-state energy to $O(\lambda^4)$ using the independent-particle representation. The prescription that we follow is due to Hugenholtz and Pines.[4] In Sec. III we carry out a zeroth-order CBF calculation of the same, using as the correlating factor a Jastrow function which corresponds to the *exact* liquid structure factor $S(k)$, the latter computed with the Hugenholtz-Pines theory. Such a Jastrow function is not the optimum choice, in the sense that it does not minimize the energy. In Sec. IV we compute the energy correction which accompanies the optimization of the Jastrow function. Finally, in Sec. V we briefly summarize our findings and speculate on the general pattern. In a second paper we formulate the perturbation theory in the CBF, and compute second-order perturbation corrections to the ground-state energy. We shall demonstrate that the simplest second-order CBF calculation sums energy exactly up to the fourth order and partially to all orders.

II. HUGENHOLTZ-PINES THEORY

For the weakly interacting Bose gas, the Hamiltonian of Eq. (1) reduces to

$$H=-\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2+\sum_{i<j=1}^{N}\lambda v(r_{ij}), \tag{5}$$

where we have extracted the strength parameter λ for explicit display and replaced $\hbar$ and $m_i\equiv m$ by 1. Second quantization converts Eq. (5) to

$$H=\sum_{\vec{k}}\tfrac{1}{2}k^2a^\dagger_{\vec{k}}\,a_{\vec{k}}+\tfrac{1}{4}\lambda\Omega\sum_{\vec{k}\vec{l}\vec{p}\vec{q}}(v_{\vec{k}-\vec{p}}+v_{\vec{k}-\vec{q}})$$
$$\times\,\delta_{\vec{k}+\vec{l},\vec{p}+\vec{q}}\,a^\dagger_{\vec{k}}\,a^\dagger_{\vec{l}}\,a_{\vec{p}}\,a_{\vec{q}}\,, \tag{6}$$

where the creation and destruction operators obey usual boson commutation relations. The obstacle to an immediate application of the diagrammatic perturbation theory comes from Bose condensation. The ground state does not form a vacuum with respect to a zero-momentum destruction operator a_0. Hugenholtz and Pine[4] (hereafter denoted by HP) replace $a_0^\dagger$ and a_0 by $(\Omega n_0)^{1/2}$, n_0 being the macroscopic condensate density, a c number. n_0 is then a free parameter, restricted only by the fact that it must not exceed the total number density n. It is to be determined by minimizing the ground-state energy E_0. The replacement of $a_0^\dagger$ and a_0 by c numbers leads to another problem: The Hamiltonian no longer conserves the number of particles. To overcome this difficulty, HP introduce a Lagrange multiplier: the chemical potential μ, to be determined by the constraint

$$\langle n'\rangle=n-n_0, \tag{7}$$

where n' is the number operator for particles outside the condensate:

$$n'=\frac{1}{\Omega}\sum_{\vec{k}\neq 0}a^\dagger_{\vec{k}}\,a_{\vec{k}}\;. \tag{8}$$

After these maneuvers, the way is clear for a valid definition of the vacuum, and the linked-cluster theorem follows.

Three kinds of Green's functions are defined, corresponding, respectively, to ground-state expectation values of time-ordered products of one creation and one destruction operator, two destruction operators, and two creation operators, denoted by G, $\tilde{G}$, and $\bar{G}$. Likewise, three types of proper self-energy parts, Σ_{11}, Σ_{02}, and Σ_{20}, are defined. Coupled Dyson-like equations are derived to relate these functions. We shall refrain from solving these equations. For the purpose of this work, it suffices to compute G, Σ_{11}, and Σ_{02} by perturbation theory. The ground-state energy is given by

$$\frac{E_0}{\Omega}=\tfrac{1}{2}n\mu+\frac{i}{(2\pi)^4}\int d\vec{k}\int_C d\epsilon\;\tfrac{1}{2}(\epsilon+\tfrac{1}{2}k^2)G(\vec{k},\epsilon), \tag{9}$$

where

$$n=n_0+\frac{i}{(2\pi)^4}\int d\vec{k}\int_C d\epsilon\;G(\vec{k},\epsilon)\,. \tag{10}$$

The contour C closes in the upper half-plane. The chemical potential μ can be determined by solving the differential equation

$$\mu=\frac{d}{dn}\left(\frac{E_0}{\Omega}\right), \tag{11}$$

or by the theorem

$$\mu=\Sigma_{11}(0,0)-\Sigma_{02}(0,0)\,. \tag{12}$$

We carry out the computation using both methods to assure accuracy.

The diagrams are constructed using free-particle propagators

$$G^{(0)}(\vec{k},\epsilon)=(\epsilon-\tfrac{1}{2}k^2+\mu+i\delta)^{-1}\,, \tag{13}$$

and the seven kinds of vertices shown in Fig. 1. The rules for evaluating contributions of diagrams are derived and stated by HP,[4] and will not be repeated here. In Fig. 2 we show schematically contributions to $G(\vec{k},\epsilon)$ up to and including all relevant fourth-order terms.

Up to this point we have ordered our diagrams by the number of vertices they contain. This assures that an mth-order diagram is at least of order m in the strength parameter λ. Actually E_0 depends on n_0 and μ, both explicitly and implicitly through $G(\vec{k},\epsilon)$, while n_0 and μ in turn possess power-series expansions in λ. We thus write

$$\frac{n_0}{n}\equiv f=\textstyle\sum_m\lambda^m f^{(m)} \tag{14}$$

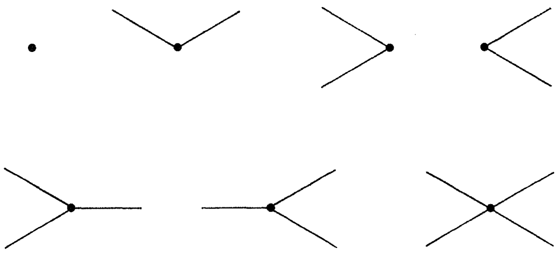

FIG. 1. Vertices in the Hugenholtz-Pines theory.

and

$$\mu = \textstyle\sum_m \lambda^m \mu^{(m)} \ . \tag{15}$$

These expansions are substituted into the expressions for G, Σ_{11}, and Σ_{02}. Comparing Eqs. (10) and (12) with Eqs. (14) and (15) and identifying order by order, we find in a zigzag fashion the following results:

$$f^{(0)} = 1 \ ,$$

$$f^{(1)} = 0 \ ,$$

$$f^{(2)} = \frac{-n}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^2}{k^4} \ , \tag{16}$$

$$f^{(3)} = \frac{4n^2}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^3}{k^6} + \frac{2n}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^2 p^4} \ ,$$

etc.,

and

$$\mu^{(0)} = 0,$$

$$\mu^{(1)} = n v_0,$$

$$\mu^{(2)} = \frac{-n}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^2}{k^2} \ ,$$

$$\mu^{(3)} = \frac{3n^2}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^3}{k^4} + \frac{n}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^2 p^2} \ , \tag{17}$$

$$\mu^{(4)} = \frac{-10n^3}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^4}{k^6} + \frac{3n^2}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p^2}{k^4 p^2}$$

$$- \frac{6n^2}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^4 p^2} - \frac{6n^2}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}} (v_p + v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}})(v_k + v_p)}{k^2 (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2 [k^2 + p^2 + (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2]}$$

$$- \frac{3n^2}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 (v_p + v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}})^2}{k^4 [k^2 + p^2 + (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2]} - \frac{n}{(2\pi)^9} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \int d\vec{\mathrm{q}} \, \frac{v_p v_q v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}} v_{\vec{\mathrm{k}}+\vec{\mathrm{q}}}}{k^2 p^2 q^2}$$

etc.

These results may now be substituted into the expressions for the ground-state energy. After rearranging in powers of λ, E_0 now reads

$$E_0 = \textstyle\sum_m \lambda^m E_0^{(m)} \ , \tag{18}$$

with

$$\frac{E_0^{(0)}}{\Omega} = 0 \ ,$$

$$\frac{E_0^{(1)}}{\Omega} = \tfrac{1}{2} n^2 v_0 \ , \tag{a}$$

$$\frac{E_0^{(2)}}{\Omega} = \frac{-n^2}{2(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^2}{k^2} \ , \tag{b}$$

$$\frac{E_0^{(3)}}{\Omega} = \frac{n^3}{(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^3}{k^4} \tag{c}$$

$$+ \frac{n^2}{2(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^2 p^2} \ , \tag{d}$$

$$\frac{E_0^{(4)}}{\Omega} = \frac{-5n^4}{2(2\pi)^3} \int d\vec{\mathrm{k}} \, \frac{v_k^4}{k^6} \tag{e}$$

$$+ \frac{n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p^2}{k^4 p^2} \tag{f}$$

$$- \frac{2n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^4 p^2} \tag{g}$$

$$- \frac{2n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^2 p^2 (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2}$$

$$- \frac{2n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}^2}{k^2 (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2 [k^2 + p^2 + (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2]} \tag{h}$$

$$- \frac{2n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_p v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}}{k^4 [k^2 + p^2 + (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2]}$$

$$- \frac{2n^3}{(2\pi)^6} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \, \frac{v_k^2 v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}}^2}{k^4 [k^2 + p^2 + (\vec{\mathrm{k}}+\vec{\mathrm{p}})^2]} \tag{i}$$

$$- \frac{n^2}{2(2\pi)^9} \int d\vec{\mathrm{k}} \int d\vec{\mathrm{p}} \int d\vec{\mathrm{q}} \, \frac{v_p v_q v_{\vec{\mathrm{k}}+\vec{\mathrm{p}}} v_{\vec{\mathrm{k}}+\vec{\mathrm{q}}}}{k^2 p^2 q^2} \ , \tag{j}$$

etc. (19)

Diagrams from which terms in E_0 arise are displayed in Figs. 3(a)–3(j). This completes our energy

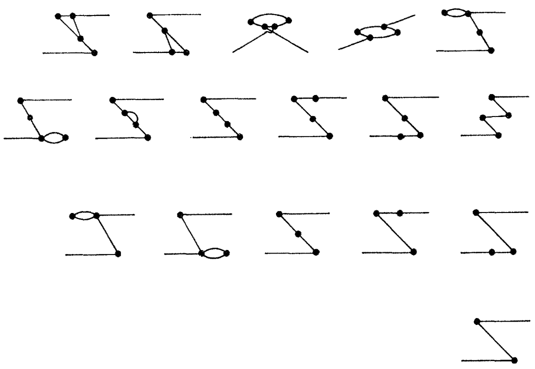

FIG. 2. Contributions to $G(\vec{k}, \epsilon)$.

calculation using the Hugenholtz-Pines theory. We next turn to a corresponding calculation using the zeroth-order CBF method.

III. ZEROTH-ORDER CBF

For a Bose gas, the model functions in a correlated basis are symmetrized products of plane waves. The momentum labels $(\vec{k}_1, \vec{k}_2, \ldots, \vec{k}_N)$ serve as the quantum numbers. For the ground state, all $\vec{k}_i = 0$. The model function is simply 1. Excited states are formed when particles evaporate out of the condensate. For example, a one-particle excited state has $\vec{k}_1 \neq 0$ and $\vec{k}_i = 0$ for $i \neq 1$. Upon symmetrization the model function becomes

$$\sum_{j=1}^{N} e^{-i\vec{k}_1 \cdot \vec{r}_j} = \rho_{\vec{k}_1} \quad . \tag{20}$$

Higher configurations can be formed in a similar way. We shall postpone this discussion to a later paper. Combining the model functions with the Jastrow correlating factor of Eq. (2), the correlated wave function for the ground state becomes

$$\psi_0(1, 2, \ldots, N) = \prod_{i<j=1}^{N} e^{u(r_{ij})/2} \quad , \tag{21}$$

which has been used often as the trial wave function for Bose systems, including liquid He^4 and charged Bose gas. For the one-particle excitation of Eq. (20), we note that the correlated wave function is given by $\rho_{\vec{k}} F$, or $\rho_{\vec{k}} \psi_0$, the phonon wave function of Feynman in his calculation of the phonon spectrum in liquid He^4.

A perturbation theory in the correlated representation requires the knowledge of all matrix elements between the correlated basis functions. The Hamiltonian matrix thus constructed is diagonalized by regarding the diagonal elements as unperturbed. Thus in zeroth order, the ground-state energy is given by the expectation value of H with respect to ψ_0. Other matrix elements do not enter the calculation until the second order. Our task reduces then to the evaluation of

$$\frac{\mathcal{E}_0}{\Omega} \equiv \frac{(\psi_0 | H | \psi_0)}{\Omega(\psi_0 | \psi_0)} \quad . \tag{22}$$

We define the m-particle distribution function $g(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_m)$ by

$$n^m g(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_m) = N(N-1) \cdots (N-m+1) \frac{\int \psi_0^2 \, d\vec{r}_{m+1, \ldots, N}}{\int \psi_0^2 \, d\vec{r}_{1,2,\ldots,N}} \quad . \tag{23}$$

In particular, the two-particle or radial distribution function is given by

$$n^2 g(r_{12}) = N(N-1) \frac{\int \psi_0^2 \, dr_{3,4,\ldots,N}}{\int \psi_0^2 \, dr_{1,2,\ldots,N}} \quad , \tag{24}$$

in terms of which

$$\mathcal{E}_0/\Omega = \tfrac{1}{8} n^2 \int g'(r) u'(r) \, d\vec{r} + \tfrac{1}{2} n^2 \int g(r) v(r) \, d\vec{r} \quad , \tag{25}$$

the prime denoting differentiation with respect to the argument. Expanding $g(r)$ and $u(r)$ in power series of λ:

$$g(r) = \textstyle\sum_m \lambda^m g^{(m)}(r) \tag{26}$$

and

$$u(r) = \textstyle\sum_m \lambda^m u^{(m)}(r) \quad , \tag{27}$$

and introducing Fourier transforms:

$$g_k^{(m)} = \int d\vec{r} \, g^{(m)}(r) e^{-i\vec{k}\cdot\vec{r}} \tag{28}$$

and

$$u_k^{(m)} = \int d\vec{r} \, u^{(m)}(r) e^{-i\vec{k}\cdot\vec{r}} \quad , \tag{29}$$

we can express $\mathcal{E}_0$ in the power series

$$\mathcal{E}_0/\Omega = \textstyle\sum_m \lambda^m \, \mathcal{E}_0^{(m)}/\Omega, \tag{30}$$

where

$$\mathcal{E}_0^{(0)}/\Omega = 0 \ ,$$

$$\mathcal{E}_0^{(1)}/\Omega = \tfrac{1}{2} n^2 v_0 \ ,$$

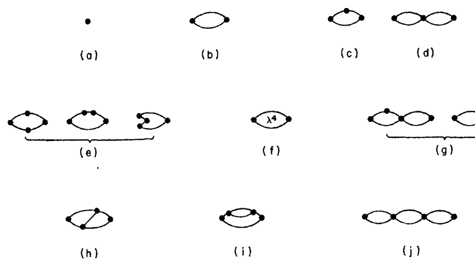

FIG. 3. Contributions to the ground-state energy E_0.

$$\mathcal{E}_0^{(2)}/\Omega = \tfrac{1}{8}n^2\sum_{\vec{k}} k^2 g_k{}^{(1)} u_k{}^{(1)} + \tfrac{1}{2}n^2 \sum_{\vec{k}} g_k{}^{(1)} v_k \,, \tag{31}$$

$$\mathcal{E}_0^{(3)}/\Omega = \tfrac{1}{8}n^2\sum_{\vec{k}} k^2 [g_k{}^{(1)} u_k{}^{(2)} + g_k{}^{(2)} u_k{}^{(1)}] + \tfrac{1}{2}n^2 \sum_{\vec{k}} g_k{}^{(2)} v_k \,,$$

$$\mathcal{E}_0^{(4)}/\Omega = \tfrac{1}{8}n^2\sum_{\vec{k}} k^2 [g_k{}^{(2)} u_k{}^{(2)} + g_k{}^{(3)} u_k{}^{(1)} + g_k{}^{(1)} u_k{}^{(3)}] + \tfrac{1}{2}n^2 \sum_{\vec{k}} g_k{}^{(3)} v_k \,,$$

etc.

We must now (i) express $u_k^{(m)}$ in terms of $g_k^{(m)}$, so that $\mathcal{E}_0/\Omega$ can be written as a functional of $g_k^{(m)}$ alone and (ii) compute $g_k^{(m)}$.

$u(r)$ and $g(r)$ are related to each other and to the three-particle distribution function $g(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ by the so-called BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) equation

$$\nabla_1 g(r_{12}) = g(r_{12})\nabla_1 u(r_{12}) + n\int g(\vec{r}_1, \vec{r}_2, \vec{r}_3) \times \nabla_1 u(r_{13})\, d\vec{r}_3 . \tag{32}$$

Since $g(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ can be expressed in terms of the radial distribution functions:

$$g(\vec{r}_1, \vec{r}_2, \vec{r}_3) = g(r_{12}) g(r_{23}) g(r_{31}) \exp A(\vec{r}_1, \vec{r}_2, \vec{r}_3) \,,$$

where

$$A(\vec{r}_1, \vec{r}_2, \vec{r}_3) = n\int [g(r_{14}) - 1][g(r_{24}) - 1] \times [g(r_{34}) - 1]\, dv_4 + O(n^2\lambda^5) + \cdots, \tag{33}$$

we have a unique relation between $u(r)$ and $g(r)$ to any desired order in λ. Going over to the Fourier transforms, we find

$$\begin{aligned} u_k{}^{(1)} &= g_k{}^{(1)} \,, \\ u_k{}^{(2)} &= g_k{}^{(2)} - \tfrac{1}{2}\sum_{\vec{p}} g_p{}^{(1)} g_{\vec{k}-\vec{p}}^{(1)} - n[g_k{}^{(1)}]^2 \,, \\ u_k{}^{(3)} &= g_k{}^{(3)} - \sum_{\vec{p}} g_p{}^{(1)} g_{\vec{k}-\vec{p}}{}^{(2)} + \tfrac{1}{3}\sum_{\vec{p}\,\vec{q}} g_p{}^{(1)} g_q{}^{(1)} g_{\vec{k}-\vec{p}-\vec{q}}{}^{(1)} - 2n g_k{}^{(1)} g_k{}^{(2)} + n^2 [g_k{}^{(1)}]^3 \,, \end{aligned} \tag{34}$$

etc.;

thus,

$$\begin{aligned} \mathcal{E}_0{}^{(0)}/\Omega &= 0 \,, \\ \mathcal{E}_0{}^{(1)}/\Omega &= \tfrac{1}{2}n^2 v_0 \,, \\ \mathcal{E}_0{}^{(2)}/\Omega &= \tfrac{1}{8}n^2 \sum_{\vec{k}} k^2 [g_k{}^{(1)}]^2 + \tfrac{1}{2}n^2\sum_{\vec{k}} g_k{}^{(1)} v_k \,, \\ \mathcal{E}_0{}^{(3)}/\Omega &= \tfrac{1}{8}n^2 \sum_{\vec{k}} k^2 \{2g_k{}^{(1)} g_k{}^{(2)} - \tfrac{1}{2}g_k{}^{(1)} \sum_{\vec{p}} g_p{}^{(1)} g_{\vec{k}-\vec{p}}{}^{(1)} - n[g_k{}^{(1)}]^3\} + \tfrac{1}{2}n^2 \sum_{\vec{k}} g_k{}^{(2)} v_k \,, \\ \mathcal{E}_0{}^{(4)}/\Omega &= \tfrac{1}{8}n^2 \sum_{\vec{k}} k^2 g_k^{(2)} \{g_k{}^{(2)} - \tfrac{1}{2}\sum_{\vec{p}} g_p{}^{(1)} g_{\vec{k}-\vec{p}}{}^{(1)} - n[g_k{}^{(1)}]^2\} + \tfrac{1}{8}n^2\sum_{\vec{k}} k^2 g_k{}^{(3)} g_k{}^{(1)} + \tfrac{1}{2}n^2 \sum_{\vec{k}} g_k{}^{(3)} v_k \\ &\quad + \tfrac{1}{8}n^2 \sum_{\vec{k}} k^2 g_k{}^{(1)} \{g_k{}^{(3)} - \sum_{\vec{p}} g_p{}^{(1)} g_{\vec{k}-\vec{p}}{}^{(2)} + \tfrac{1}{3}\sum_{\vec{p}\,\vec{q}} g_p{}^{(1)} g_q{}^{(1)} g_{\vec{k}-\vec{p}-\vec{q}}{}^{(1)} - 2n g_k{}^{(1)} g_k{}^{(2)} + n^2 [g_k{}^{(1)}]^3\} \,, \end{aligned} \tag{35}$$

etc.

To compute $g_k{}^{(m)}$, first we recognize that

$$\begin{aligned} S_k &= 1 + n\int d\vec{r}\, [g(r) - 1] e^{-i\vec{k}\cdot\vec{r}} \\ &= 1 + n\lambda g_k{}^{(1)} + n\lambda^2 g_k{}^{(2)} + \cdots \,. \end{aligned} \tag{36}$$

The quantity of interest is therefore the static structure factor S_k. In this section we compute S_k via the Hugenholtz-Pines theory. Clearly the S_k obtained is exact in every order. It corresponds to *some* Jastrow function, through Eqs. (36), (34), (29), and (27), but not the Jastrow function that minimizes $\mathcal{E}_0$. We regard the Jastrow function which corresponds to the *exact* S_k as an initial guess.

Hugenholtz and Pines[4] relate S_k to the correlation functions $F_k(\omega)$:

$$S_k = \frac{1}{n}\int_{C'} d\omega \frac{i}{2\pi} F_k(\omega) \,, \tag{37}$$

where C' closes either above or below the real axis, and

$$F_k(\omega) = \int_{-\infty}^{\infty} dt\, F_k(t) e^{i\omega t} \,, \tag{38}$$

$$F_k(t) = -i\langle 0 | T\{\rho_{\vec{k}}(t) \rho_{-\vec{k}}(0)\} | 0\rangle \,, \tag{39}$$

$$\rho_{\vec{k}}(t) = \sum_{\vec{p}} a_{\vec{p}}^{\dagger}(t)\, a_{\vec{k}+\vec{p}}(0) \,. \tag{40}$$

Setting a_0 and $a_0^\dagger$ to the c number $(\Omega n_0)^{1/2}$ gives rise to three classes of $F_k(t)$:

$$F_k(t) = F_k^a(t) + F_k^b(t) + F_k^c(t) \,, \tag{41}$$

where

$$F_k^a(t) = -i\Omega n_0 \langle 0 | T\{[a_{-\vec{k}}^\dagger(t) + a_{\vec{k}}(t)][a_{\vec{k}}^\dagger(0) + a_{-\vec{k}}(0)]\} | 0 \rangle \,, \tag{42}$$

$$\begin{aligned} F_k^b(t) &= -i(\Omega n_0)^{1/2} \langle 0 | T\{[a_{-\vec{k}}^\dagger(t) + a_{\vec{k}}(t)] \textstyle\sum_{\vec{p}} a_{\vec{k}+\vec{p}}^\dagger(0)\, a_{\vec{p}}(0) \\ &\quad + [a_{\vec{k}}^\dagger(0) + a_{-\vec{k}}(0)] \textstyle\sum_{\vec{p}} a_{\vec{p}}^\dagger(t)\, a_{\vec{k}+\vec{p}}(t)\} | 0 \rangle \,, \end{aligned} \tag{43}$$

and

$$F_k^c(t) = -i\langle 0 | T\{\textstyle\sum_{\vec{p}} a_{\vec{p}-\vec{k}}^\dagger(t)\, a_{\vec{p}}(t) \sum_{\vec{q}} a_{\vec{q}+\vec{k}}^\dagger(0)\, a_{\vec{q}}(0)\} | 0 \rangle \,. \tag{44}$$

$F_k^a(t)$ consists of diagrams possessing just two terminals, and may be related to the Green's functions, thus:

$$F_k^a(\omega) = n_0\{G_{\vec{k}}(\omega) + G_{-\vec{k}}(-\omega) + \tilde{G}_{\vec{k}}(\omega) + \bar{G}_{\vec{k}}(\omega)\} \,. \tag{45}$$

$F_k^b(t)$ are three-terminal diagrams; to order λ^2 they make no contribution toward S_k. Among the various four-terminal diagrams for $F_k^c(t)$, only one contributes in $O(\lambda^2)$. We find

$$\begin{aligned} g_k^{(0)} &= 1 \,, \\ g_k^{(1)} &= \frac{-2v_k}{k^2} \,, \\ g_k^{(2)} &= \frac{6nv_k^2}{k^4} - \frac{1}{(2\pi)^3} \int d\vec{p}\, \frac{v_p^2}{p^4} + \frac{2}{(2\pi)^3} \int d\vec{p}\, \frac{v_p v_{\vec{k}+\vec{p}}}{k^2 p^2} \\ &\quad + \frac{2}{(2\pi)^3} \int d\vec{p}\, \frac{v_p v_{\vec{k}+\vec{p}}}{p^2(\vec{k}+\vec{p})^2} \,, \end{aligned} \tag{46}$$

Substituting Eqs. (46) into Eqs. (35), we note that terms involving $g_k^{(3)}$ cancel out. This is why in computing S_k we did not bother to proceed beyond $O(\lambda^2)$. We find

$$\begin{aligned} \frac{\mathcal{E}_0^{(0)}}{\Omega} &= 0 \,, \\ \frac{\mathcal{E}_0^{(1)}}{\Omega} &= \tfrac{1}{2} n^2 v_0 \,, \\ \frac{\mathcal{E}_0^{(2)}}{\Omega} &= \frac{-n^2}{2(2\pi)^3} \int d\vec{k}\, \frac{v_k^2}{k^2} \,, \\ \frac{\mathcal{E}_0^{(3)}}{\Omega} &= \frac{n^3}{(2\pi)^3} \int d\vec{k}\, \frac{v_k^3}{k^4} + \frac{n^2}{2(2\pi)^6} \int d\vec{k} \int d\vec{p}\, \frac{v_k v_p v_{\vec{k}+\vec{p}}}{k^2 p^2} \,, \\ \frac{\mathcal{E}_0^{(4)}}{\Omega} &= -\frac{5n^4}{2(2\pi)^3} \int d\vec{k}\, \frac{v_k^4}{k^6} - \frac{3n^3}{2(2\pi)^6} \int d\vec{k} \int d\vec{p}\, \frac{v_k^2 v_p v_{\vec{k}+\vec{p}}}{k^2 p^2 (\vec{k}+\vec{p})^2} - \frac{3n^3}{(2\pi)^6} \int d\vec{k} \int d\vec{p}\, \frac{v_k^2 v_p v_{\vec{k}+\vec{p}}}{k^4 p^2} \\ &\quad - \frac{n^2}{2(2\pi)^9} \int d\vec{k} \int d\vec{p} \int d\vec{q}\, \frac{v_p v_q v_{\vec{k}+\vec{p}} v_{\vec{k}+\vec{q}}}{k^2 p^2 q^2} + \left\{ \frac{n^2}{8(2\pi)^9} \int d\vec{k} \int d\vec{p} \int d\vec{q}\, \frac{v_p^2 v_q^2}{p^4 q^4} \right. \\ &\quad \left. - \frac{n^2}{4(2\pi)^9} \int d\vec{k} \int d\vec{p} \int d\vec{q}\, \frac{p^2 v_k^2 v_q v_{\vec{p}+\vec{q}}}{k^4 q^2 (\vec{p}+\vec{q})^2} + \frac{n_2}{6(2\pi)^9} \int d\vec{k} \int d\vec{p} \int d\vec{q}\, \frac{v_p v_q v_{\vec{k}+\vec{p}} v_{\vec{k}+\vec{q}}}{p^2 q^2 (\vec{k}+\vec{q})^2} \right\} \,, \end{aligned} \tag{47}$$

etc.

In comparison to Eq. (19), we find

$$E_0^{(i)}/\Omega = \mathcal{E}_0^{(i)}/\Omega \,, \quad i \leq 3 \,. \tag{48}$$

In $O(\lambda^4)$, the ring diagram (e) of Eq. (19) is recovered, as is the ladder diagram (j). The two-ring diagram, either the ring-ladder combination (g), or the "cross-bar" diagram (h), or the "side-loop" diagram (i), is partially recovered. The λ^4 contribution of the two-vertex diagram (f) does not appear in Eq. (47). Instead, we have in $\mathcal{E}_0^{(4)}/\Omega$ a group of three terms (in curly brackets) whose structure is totally unfamiliar. We shall deal with them in Sec. IV.

IV. OPTIMIZATION OF JASTROW FUNCTION

Jackson and Feenberg[5] constructed a set of correlated basis functions, as shown in Eq. (3), where the model functions are density fluctuations.

We shall refer to these correlated basic functions as (independent) phonon wave functions. They considered the subspace spanned by the unperturbed ground state and all two-phonon wave functions, and carried out a Bogoliubov transformation in this "paired-phonon space" which resulted in an improved description of the ground state. The transformation generates an equation that maximizes the improvement:

$$\hat{S}_k = S_k[1+2w_k/e_k]^{-1/2} , \tag{49}$$

where

$$e_k = k^2/2S_k \tag{50}$$

and

$$w_k = S_k'/S_k + k^2(S_k-1)/4S_k , \tag{51}$$

with

$$\begin{aligned} S_k' = V_k^* &+ \frac{2n^3}{N}\int [g(\vec{r}_1,\vec{r}_2,\vec{r}_3) - g(r_{12})g(r_{13})]\, e^{i\vec{k}\cdot\vec{r}_{13}} \\ &\times v^*(r_{12})\, d\vec{r}_{123} + \frac{n^4}{2N}\int [g(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4) - g(r_{12}) \\ &\times g(r_{34})\,(4g(r_{13})-3)]\, e^{i\vec{k}\cdot\vec{r}_{34}} v^*(r_{12})\, d\vec{r}_{1234}, \end{aligned} \tag{52}$$

$$V_k^* = n\int e^{-i\vec{k}\cdot\vec{r}} g(r)\, v^*(r)\, d\vec{r} , \tag{53}$$

and

$$v^*(r) = v(r) - \tfrac{1}{4}\nabla^2 u(r) . \tag{54}$$

One substitutes Eqs. (50)–(54) in Eq. (49) to obtain $\hat{S}_k$, and then regards $\hat{S}_k$ as the new S_k, from which one Fourier transforms to obtain a corresponding $g(r)$ and re-solves the BBGKY equation to obtain a corresponding $u(r)$. Using the new S_k, $g(r)$, and $u(r)$, e_k and w_k may be recomputed, and the whole procedure is repeated. This iterative process stops when $\hat{S}_k = S_k$.

Clearly, in Eq. (52), $g(\vec{r}_1, \vec{r}_2, \vec{r}_3)$ and $g(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4)$ must be replaced by functionals in $g(r)$. These functionals appear as infinite series which can be truncated in various ways, forming the so-called generalized Kirkwood superposition approximation, the convolution approximation, etc. To all orders in λ of interest to us, these approximations lead to identical expressions.

Campbell and Feenberg[6] recently showed that under such a paired-phonon analysis, the improved description of the ground state remains within the Jastrow-function space. The procedure described above thus effects an optimization of the Jastrow function. We apply this procedure to the present problem, initiating with the exact S_k derived in Sec. III, Eqs. (36) and (46). We seek corrections to $g_k^{(0)}$, $g_k^{(1)}$, and $g_k^{(2)}$, i.e., corrections to S_k up to $O(\lambda^2)$.

After one iteration we find no correction to $g_k^{(0)}$ and $g_k^{(1)}$. $g_k^{(2)}$ is replaced by

$$\hat{g}_k^{(2)} = g_k^{(2)} + \Delta g_k^{(2)} , \tag{55}$$

where

$$\Delta g_k^{(2)} = \frac{1}{(2\pi)^3}\int d\vec{p}\, \frac{v_p^2}{p^4} - \frac{1}{(2\pi)^3}\int d\vec{p}\, \frac{v_p v_{\vec{k}+\vec{p}}}{p^2(\vec{k}+\vec{p})^2} . \tag{56}$$

Using Eq. (35), we find $\mathcal{E}_0^{(0)}/\Omega$ to $\mathcal{E}_0^{(3)}/\Omega$ unchanged. This is just as expected. $\mathcal{E}_0^{(4)}/\Omega$ takes on the correction

$$\begin{aligned} \frac{\Delta\mathcal{E}_0^{(4)}}{\Omega} = \frac{-n^2}{8(2\pi)^9}\int d\vec{k}\int d\vec{p}\int d\vec{q}\, k^2\, \frac{v_p^2 v_q^2}{p^4 q^4} \\ + \frac{n^2}{4(2\pi)^9}\int d\vec{k}\int d\vec{p}\int d\vec{q}\, \frac{p^2 v_k^2 v_q v_{\vec{p}+\vec{q}}}{k^4 q^2(\vec{p}+\vec{q})^2} \\ - \frac{n^2}{6(2\pi)^9}\int d\vec{k}\int d\vec{p}\int d\vec{q}\, \frac{v_p v_q v_{\vec{k}+\vec{p}} v_{\vec{k}+\vec{q}}}{p^2 q^2(\vec{k}+\vec{q})^2} , \end{aligned} \tag{57}$$

which immediately eliminates the group of three terms in the curly brackets of Eq. (47).

The second iteration makes no more modification on $g_k^{(2)}$. Corrections enter through $O(\lambda^3)$. The optimization of the Jastrow function to $O(\lambda^4)$ in the energy is thus accomplished in just one iteration.

It is possible to study also how well the Jastrow function handles the depletion effect. From Eqs. (25)–(29) we find that the kinetic energy of the system equals

$$\begin{aligned} \langle T\rangle &= \tfrac{1}{8}n^2\Omega\int g'(r)u'(r)\, d\vec{r} \\ &= \tfrac{1}{8}n^2\textstyle\sum_{\vec{k}} k^2\{\lambda^2[g_k^{(1)}u_k^{(1)}] + \lambda^3[g_k^{(1)}u_k^{(2)} + g_k^{(2)}u_k^{(1)}] \\ &\quad + \cdots\} . \end{aligned} \tag{58}$$

But

$$\langle T\rangle = \textstyle\sum_{\vec{k}} \tfrac{1}{2}k^2 n_k . \tag{59}$$

Thus

$$\begin{aligned} f = n_0/n &= 1 - \textstyle\sum_{\vec{k}} n_k/n \\ &= 1 - \textstyle\sum_{\vec{k}}\{\lambda^2[\tfrac{1}{4}ng_k^{(1)}u_k^{(1)}] + \lambda^3[\tfrac{1}{4}ng_k^{(1)}u_k^{(2)} \\ &\quad + \tfrac{1}{4}ng_k^{(2)}u_k^{(1)}] + \cdots\} . \end{aligned} \tag{60}$$

With the aid of Eqs. (14), (34), and (46), we obtain

$$f^{(0)} = 1 \quad ,$$

$$f^{(1)} = 0 \quad ,$$

$$f^{(2)} = -\tfrac{1}{4}n\sum_{\vec{k}} g_k^{(1)}u_k^{(1)} = \frac{-n}{(2\pi)^3}\int d\vec{k}\, \frac{v_k^2}{k^4} \quad ,$$

$$f^{(3)} = -\tfrac{1}{4}n\sum_{\vec{k}} [g_k^{(1)}u_k^{(2)} + g_k^{(2)}u_k^{(1)}]$$

$$=\frac{4n^2}{(2\pi)^3}\int d\vec{k}\ \frac{v_k^3}{k^6}+\frac{2n}{(2\pi)^6}\int d\vec{k}\int d\vec{p}\ \frac{v_k v_p v_{\vec{k}+\vec{p}}}{k^2 p^4}\ ,$$

etc., (61)

in complete agreement with Eq. (16), the results of Hugenholtz-Pines theory, to order λ^3.

V. SUMMARY

We have demonstrated that, in the case of a weakly interacting Bose gas, if one carries out a CBF calculation using a Jastrow correlating factor, the energy obtained corresponds to partial summations of energy diagrams in the independent-particle representation. In particular, in zeroth-order CBF, an optimized Jastrow function sums the leading three orders exactly, "most" of the fourth order, and in part all higher orders. In the fourth order, it is noted that the ring diagram and the ladder diagram are completely included. Two-ring diagrams which include the ring-ladder combination, the (vertex-renormalizing) cross-bar diagram, and the (propagator-renormalizing) side-loop diagram are summed in part. However, the λ^4 contribution of the two-vertex ring diagram is missing. Aside from this difficulty, it appears that the optimized Jastrow function is capable of summing all rings and ladders, and partially all other diagrams, to infinite orders.

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*Work supported in part by the Advanced Research Projects Agency through the Materials Research Center of Northwestern University, and in part by the National Science Foundation through Grant No. GP-11054.

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PHYSICAL REVIEW A VOLUME 2, NUMBER 5 NOVEMBER 1970

Diagrammatic Analysis of the Method of Correlated Basis Functions. II. Perturbation Theory for a Weakly Interacting Bose Gas*

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(Received 4 June 1970)

Continuing the diagrammatic analysis of the method of correlated basis functions (CBF) for the weakly interacting Bose gas, as reported in the preceding paper, we take off from the unperturbed problem, which is solved essentially by a variational method using a Jastrow correlating factor as the trial wave function. We compute low-order corrections to the unperturbed energy, using a set of correlated basis functions. It is found that the simplest second-order correction in the CBF accounts for all discrepancies (between the Hugenholtz-Pines theory and the unperturbed CBF calculation) which arise in the fourth order of the interaction strength $O(\lambda^4)$. It is also demonstrated indirectly that the Jastrow function sums rings and ladders at least up to $O(\lambda^5)$.

I. INTRODUCTION

In the preceding paper,[1] hereafter referred to as I, we discussed the role of a Jastrow correlating factor in the method of correlated basis functions (CBF). We carried out in detail the calculation of the ground-state energy, using at first a Jastrow function which corresponds to the exact liquid structure factor S_k, then proceeding to an improved calculation which optimizes the Jastrow function.

"Optimizing" in the above context refers to the minimization of the unperturbed ground-state energy. Clearly the variational principle has been invoked. The contents of I can therefore be interpreted as an