which corresponds exactly to the analogous relation in the case of resonant one-photon excitation, and expresses, via Eqs. (16), dW/dt as the rate of change of internal energy $(E_1 dn_1/dt + E_0 dn_0/dt)$ of the atom plus a term representing energy loss due to collisions.

---

[1] See W. Heitler, in *The Quantum Theory of Radiation*, 3rd ed. (Oxford U. P., London, 1957), Chap. 4, for an outline of the basic (perturbation) theory of multiphoton processes.

[2] See B. R. Mollow [Phys. Rev. 175, 1555 (1968)] for a quantum-mechanical analysis of two-photon absorption which is valid for (weak) fields with arbitrary statistics. The multiphoton case has been discussed in similar terms by G. S. Agarwal, Phys. Rev. A 1, 1445 (1970).

[3] A comprehensive review of the experimental and theoretical literature on multiphoton processes is given by A. M. Bonch-Bruevich and V. A. Khodovoi, Usp. Fiz. Nauk 85, 3 (1965) [Soviet Phys. Usp. 8, 1 (1965)].

[4] A. Gold and J. P. Hernandez [Phys. Rev. 139, A2002 (1965)] have discussed the possibility of observing both one- and two-photon transitions between the same pair of levels, due to phonon-assisted parity mixing.

[5] R. Karplus and J. Schwinger, Phys. Rev. 73, 1020 (1948).

[6] The two-level problem has been discussed for the case of one-photon transitions by B. R. Mollow, Ann. Phys. (N. Y.) 52, 464 (1969); Phys. Rev. 188, 1969 (1969); and Phys. Rev. A 2, 76 (1970).

[6a] T. Oka and T. Shimizu [Phys. Rev. A 2 , 587 (1970)] have observed strong two-photon excitations in the microwave region. Their discussion of the process, which is based on pure states, leads for the simple models they consider to results similar to ours.

The analysis presented here applies equally well, with minor changes in notation, to the case of rf-induced transitions between Zeeman sublevels in a strong magnetic field (Ref. 3). In that case diagonal matrix elements in the interaction Hamiltonian will be present whenever the rf field has nonvanishing components in the direction of the constant applied field.

[8] In effect what we are requiring is that the process under consideration be a bona fide two-photon process, and not simply a succession of one-photon processes.

[8a] Time-independent perturbation theory does, on the other hand, lead to Eq. (19) for the frequency shift if the incident field is treated *quantum-mechanically*, and is represented by a single highly excited mode of oscillation.

[9] It should be noted, however, that for atomic relaxation mechanisms other than the particularly simple one under consideration here, the field may *indirectly* affect the atomic populations $\bar{n}_j$ for $j \geqslant 2$ (as well as the quantity $\bar{n}_1 + \bar{n}_0$), since altering the ratio $\bar{n}_1/\bar{n}_0$ would in general have the effect of producing a net decay rate to (or from) the other states of the atom.

PHYSICAL REVIEW A VOLUME 4, NUMBER 4 OCTOBER 1971

Ground-State Energy of a Many-Particle Boson System

Deok Kyo Lee
Department of Physics and Astronomy, University of Kansas, Lawrence, Kansas 66044

(Received 3 May 1971)

The ground state of a many-particle boson system is studied for two closely related limits: the uniform limit and the weak coupling limit. The former is defined by $\alpha = 1 - g(0) \ll 1$ and the latter by $\beta = (N - N_0)/N \ll 1$, where $g(r)$ is the radial distribution function and N_0 is the mean occupation number of the zero-momentum state. In the uniform limit the variation-perturbation approach based on (a) the method of correlated basis functions and (b) the series expansion in powers of α is found to be equivalent to the field-theoretic treatment given by Brueckner (for the charged-boson gas) in the weak coupling limit. In particular, it is shown that the variation-perturbation energy obtained for the uniform limit in the momentum representation is identical through second order to the ground-state energy evaluated for $\beta \ll 1$ by summing one- and two-ring diagrams in the Bogoliubov occupation-number representation. The charged-boson gas and the one-dimensional boson system with a δ-function interaction are considered to examine some of the interesting features of the uniform-limit procedure.

I. INTRODUCTION

In recent years, the ground state of a many-body boson system has been studied with a great variety of approximation methods. In particular, the field-theoretic techniques in conjunction with the Bogoliubov canonical transformation[1] have been widely employed in the development of exact theories for many-body boson systems—such as the hard-sphere boson gas at low density[2,3] and the charged-boson gas at high density.[4,5] These procedures are based on the Bogoliubov weak coupling limit[1] defined by the condition that the major fraction of the particles are in the zero-momentum state (i.e., nearly complete Bose-Einstein condensation into the state $k = 0$). Under this special limiting condition the Bogoliubov canonical transformation enables one to carry out the exact and complete summation of one-ring diagrams for evaluation of the leading term of the ground-state energy. Also, as pointed out by Brueckner[5] (for the charged-boson gas), the dominant correction term to the energy is obtained by summing two-ring diagrams using the perturbation theory in the Bogoliubov representation.

On the other hand, an alternative approach developed by Feenberg *et al.* has also found its extensive applications, in particular, in the problem of liquid He^4, leading to results in semiquantitative agreement with experimental observations.[6-8] The starting point of this approach is the introduction of the Bijl-Dingle-Jastrow (BDJ) trial wave function for the variational description of the ground state. Such a special form of the wave function would not, of course, be able to represent the exact eigenfunction of the many-body Hamiltonian in general. It is quite interesting that in this variational formulation one is approximating the wave function in the configuration space, whereas in the Bogoliubov representation one is approximating the Hamiltonian in the occupation-number space. Thus, the two methods seem to approach the same problem from basically different points of view.

In the variational method, the primary task is to find the optimum (BDJ) wave function which minimizes the expectation value of the Hamiltonian. Unfortunately this cannot be done exactly and analytically in general. However, if the value of the radial distribution function at the origin differs little from its asymptotic value unity (this is called the uniform limit), then the quantity representing this small difference can serve as an expansion parameter for the exact description of the variational ground state and the optimization problem becomes more amenable to solution.[9,10] Moreover, in this uniform limit the leading correction to the variational energy can be evaluated exactly by the perturbation theory which takes into account the components absent in the BDJ wave-function space.[8,11]

It is the purpose of this paper to clarify the relationship between the two substantially different methods by showing that they both lead to identical results through second order[12] in the weak coupling expansion for the ground-state energy.[13] The two methods are discussed in Secs. II and III; in Sec. IV the energy expressions resulting from these two different approaches are shown to agree exactly through second order. Section V is devoted to applications of the variation-perturbation formalism to the high-density charged-boson gas and the one-dimensional boson system with the δ-function interaction, and finally in Sec. VI some of the interesting features of the variation-perturbation method in the uniform limit are discussed.

II. OCCUPATION-NUMBER FORMALISM

We consider a system of N bosons interacting in a box of volume Ω through a two-body potential $v(r)$. The Hamiltonian in second-quantized representation is

$$H=\sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{1}{2\Omega} \sum_{\vec{k},\vec{k}',\vec{k}''} V(k) a_{\vec{k}'+\vec{k}}^\dagger a_{\vec{k}''-\vec{k}}^\dagger a_{\vec{k}''} a_{\vec{k}'} , \tag{1a}$$

where

$$V(k)=\int v(r) e^{i\vec{k}\cdot\vec{r}} d\vec{r} .$$

Under the Bogoliubov condition of weak coupling, the operators a_0 and $a_0^\dagger$ are replaced by the c number $N_0^{1/2}$, where N_0 is the number of particles in the zero-momentum state. It proves convenient to rewrite the Hamiltonian of Eq. (1a) as a sum of four different parts:

$$\begin{aligned} H &= H_0+H_1+H_2+H_3 , \\ H_0 &= \tfrac{1}{2} N\rho V(0) , \\ H_1 &= \sum_{\vec{k}}{}' \{ [\hbar^2 k^2/2m + \rho_0 V(k)] a_{\vec{k}}^\dagger a_{\vec{k}} \\ &\qquad + \tfrac{1}{2}\rho_0 V(k)(a_{\vec{k}}^\dagger a_{-\vec{k}}^\dagger + a_{\vec{k}} a_{-\vec{k}})\} , \\ H_2 &= H_{Y\lambda}+H_X , \\ H_{Y\lambda} &= (\rho_0/\Omega)^{1/2} \sum_{\vec{k},\vec{k}'}{}' V(k)(a_{\vec{k}'}^\dagger a_{\vec{k}} a_{\vec{k}'-\vec{k}} + a_{\vec{k}'-\vec{k}}^\dagger a_{\vec{k}}^\dagger a_{\vec{k}'}) , \\ H_X &= (2\Omega)^{-1} \sum_{\vec{k},\vec{k}'}{}' V(k)(a_{\vec{k}'}^\dagger a_{-\vec{k}'}^\dagger a_{\vec{k}'-\vec{k}} a_{\vec{k}-\vec{k}'} \\ &\qquad + a_{\vec{k}'}^\dagger a_{\vec{k}'} a_{\vec{k}'-\vec{k}}^\dagger a_{\vec{k}'-\vec{k}}) , \\ H_3 &= (2\Omega)^{-1} \sum_{\vec{k},\vec{k}',\vec{k}''} V(k) a_{\vec{k}'+\vec{k}}^\dagger a_{\vec{k}''-\vec{k}}^\dagger a_{\vec{k}''} a_{\vec{k}'} , \end{aligned} \tag{1b}$$

with $\rho=N/\Omega$, $\rho_0=N_0/\Omega$. The prime on the summation for H_n means that terms appearing in H_m $(m<n)$ are to be excluded.

The dominant contribution from H_n yields an nth-order term[12] for the energy in the weak coupling expansion; thus the first-order term of the energy is obtained by summing one-ring diagrams using the Bogoliubov canonical transformation, which diagonalizes the dominant part of the Hamiltonian (i.e., H_0+H_1). The results first obtained by Bogoliubov[1] can be written as

$$E(1\text{ ring}) = E_1(1\text{ ring}) + E_2(1\text{ ring}) + \cdots , \tag{2}$$

$$E_1(1\text{ ring}) = -\frac{1}{4(2\pi)^3\rho} \int \epsilon(k) \frac{[1-S(k)]^2}{S(k)} d\vec{k} , \tag{3}$$

$$E_2(1\text{ ring}) = \frac{\beta}{4(2\pi)^3\rho} \int \epsilon(k) \frac{[1-S(k)]^2[1+S(k)]}{S(k)} d\vec{k} , \tag{4}$$

$$\beta \equiv \frac{N-N_0}{N} = \frac{1}{4(2\pi)^3\rho} \int \frac{[1-S(k)]^2}{S(k)} d\vec{k} + \cdots , \tag{5}$$

where

$$S(k) = [1 + 4m\rho V(k)/\hbar^2 k^2]^{-1/2} , \tag{6}$$

$$\epsilon(k) = \hbar^2 k^2 / 2m S(k) \tag{7}$$

are, respectively, the leading term of the liquid structure function in the uniform limit[5,9] and the Bijl-Feynman energy for an elementary excitation.[14] In the weak coupling limit $\beta \ll 1$, the coupling (or expansion) parameter is ordinarily proportional to β.

The importance of two-ring diagrams as the primary contributor to the next leading term in the energy expansion was discussed in the case of the Coulomb potential by Brueckner,[5] who recognized that both terms H_X and $H_{Y\lambda}$ of the Hamiltonian contribute to the energy in second order. To evaluate the (leading) contributions from H_X and $H_{Y\lambda}$, which are not diagonalized by the Bogoliubov canonical transformation, we can follow Brueckner's procedure by applying first- and second-order perturbation theory in the Bogoliubov occupation-number space, taking the diagonalized $H_0 + H_1$ as the unperturbed Hamiltonian and H_X and $H_{Y\lambda}$ as perturbations.[5]

The contribution from the X vertex may be obtained directly from results derived in the pair theory by Girardeau and Arnowitt[15]; from Eqs. (21)–(24) of Ref. 15 one finds the leading term for the X vertex

$$E_X = \frac{N}{2(2\pi)^6 \rho} \int d\vec{k}\, d\vec{k}'\, V(k'')\, \frac{\phi(k)\phi(k')[1 + \phi(k)\phi(k')]}{[1 - \phi^2(k)][1 - \phi^2(k')]} , \tag{8}$$

where $\vec{k}'' = \vec{k} - \vec{k}'$ and the dominant part of (i.e., the Bogoliubov approximation for) the function $\phi(k)$ is related to $S(k)$ by

$$\phi(k) = [1 - S(k)]/[1 + S(k)] . \tag{9}$$

Thus, expression (8) may be rewritten as

$$E_X = \frac{N}{2[4(2\pi)^3 \rho]^2} \int \frac{d\vec{k}\, d\vec{k}'\, \epsilon(k'')}{S(k)S(k')S(k'')} [1 - S(k)][1 - S(k')][1 + S(k)S(k')][1 - S^2(k'')] . \tag{10}$$

The term arising from the $Y\lambda$ vertices is found from Eqs. (B9) and (B10) of Ref. 16 to become

$$\begin{aligned} E_{Y\lambda} &= -\frac{N}{6(2\pi)^6} \int \frac{d\vec{k}\, d\vec{k}'}{\langle \epsilon \rangle} \frac{\{V(k)[1 - \phi(k)][\phi(k') + \phi(k'')] + (\text{symm. terms})\}^2}{[1 - \phi^2(k)][1 - \phi^2(k')][1 - \phi^2(k'')]} \\ &= -\frac{N}{6[4(2\pi)^3 \rho]^2} \int \frac{d\vec{k}\, d\vec{k}'}{S(k)S(k')S(k'')\langle \epsilon \rangle} [\langle \epsilon \rangle - \langle S^2 \epsilon \rangle - S(k)S(k')S(k'')(\langle \epsilon / S \rangle - \langle S \epsilon \rangle)]^2 , \end{aligned} \tag{11}$$

where

$$\langle f \rangle = f(k) + f(k') + f(k'') ,$$

$$F(k, k', k'') + (\text{symm. terms})$$

$$= F(k, k', k'') + F(k', k'', k) + F(k'', k, k') .$$

Therefore, the exact ground-state energy to second order is

$$\begin{aligned} &E = E_0 + E_1 + E_2 , \quad E_0 = \tfrac{1}{2} N \rho V(0) , \\ &E_1 = E_1(1\text{ ring}) , \quad E_2 = E_2(1\text{ ring}) + E_X + E_{Y\lambda} . \end{aligned} \tag{12}$$

In Sec. IV this result will be compared with the variation-perturbation formula obtained in the uniform limit.[8,9,17]

III. VARIATION-PERTURBATION METHOD IN UNIFORM LIMIT

In this section we consider the uniform-limit formalism, which is mainly (but not entirely) based on the variational analysis in which the ground state is described by the BDJ trial function

$$\Psi_0 = \prod_{i<j}^{N} \exp[\tfrac{1}{2} U(r_{ij})] \left[\int \prod_{m<n}^{N} \exp U(r_{mn})\, d\vec{r}_{12\cdots N} \right]^{-1/2} ,$$

where $U(r)$ is the correlation function determined by minimizing the expectation value of the Hamiltonian. In this variational approach, however, the radial distribution function

$$g(r_{12}) = N(N-1)\rho^{-2} \int \Psi_0^2\, d\vec{r}_{34\cdots N}$$

or, equivalently, the liquid structure function

$$S(k) = 1 + \rho \int e^{i\vec{k}\cdot\vec{r}} [g(r) - 1]\, d\vec{r} ,$$

is used as an indirect variational function, and the quantity $\alpha = 1 - g(0)$ plays an important role as an expansion parameter in the development of power series for various quantities depending on the particle density and the two-body potential, such as $\beta = (N - N_0)/N$ and the ground-state energy.

The results of such a variational analysis in the uniform limit ($\alpha \ll 1$) are given in Refs. 6, 9, and 10; they include

$$E_v = E_0 + E_1 + E_{2v} + \cdots , \tag{13}$$

$$\begin{aligned} E_{2v} = 2N[4(2\pi)^3 \rho]^{-2} \int d\vec{k}\, d\vec{k}'\, \epsilon(k) S(k)[1 - S(k)] \\ \times [1 - S(k')][1 - S(k'')] , \end{aligned} \tag{14}$$

$$\alpha \equiv 1 - g(0) = [(2\pi)^3\rho]^{-1} \int [1 - S(k)] d\vec{k} + \cdots , \quad (15)$$

with E_0, E_1, $S(k)$, and $\epsilon(k)$ as defined in Sec. II. The procedure also yields a formula for β identical to Eq. (5).

The leading correction term to the variational energy was derived (and applied to liquid He^4) by Davison and Feenberg,[8] who realized that the dominant contribution to the correction arises from the three-phonon component which is absent in the BDJ wave-function space. Their result, obtained by applying second-order perturbation theory in the phonon space, is found from Eqs. (6), (23), and (31) of Ref. 8 to reduce to

$$E_{2p} = - \frac{N}{6[4(2\pi)^3\rho]^2} \int \frac{d\vec{k}\, d\vec{k}'}{S(k)S(k')S(k'')\langle \epsilon \rangle} \times [S(k)S(k')S(k'')(2\langle \epsilon \rangle - \langle S\epsilon \rangle) - \langle S \rangle \langle S\epsilon \rangle + 2\langle S^2\epsilon \rangle]^2 . \quad (16)$$

Thus, the variation-perturbation formula derived in the uniform limit may be written as (to second order)

$$E = E_0 + E_1 + E_2 , \quad E_2 = E_{2v} + E_{2p} . \quad (17)$$

The agreement of Eqs. (12) and (17) through first order is obvious; the agreement in second order is discussed in Sec. IV.

We conclude this section with some remarks on two points. First, it must be pointed out that the variational energy formula (13) was derived by varying the indirect variational function $S(k)$ freely, i.e., without taking into account the constraints on $S(k)$. However, it has been shown that the variation with respect to the direct variational function $U(r)$ leads to identical results through third order in the uniform limit.[18] The second point is that the perturbation energy (16) was evaluated using the convolution approximation[19] for the three-particle distribution function $p^{(3)}$ (1, 2, 3), but it is easy to show that this approximation gives $p^{(3)}$ (1, 2, 3) correctly through $O(\alpha^2)$ and hence Eq. (16) is the exact expression for the leading term of the perturbation correction generated by the three-phonon vertex. These remarks appear to establish Eq. (17) as the energy formula exact through second order in the uniform limit.

IV. PROOF OF EQUIVALENCE

The relationship between the two procedures based on different limiting conditions $\alpha \ll 1$ and $\beta \ll 1$ may be easy to find if the connection between α and β is known explicitly. In the special case of the Coulomb potential in the high-density limit, the two limits are equivalent since they are related by $\alpha = 4\beta + O(\beta^2)$ [see Eq. (38)]. However, there is no such a general relation known at the present time. At least, it is clear that they are not equivalent in general. For example, in the hard-sphere boson gas, $\alpha = 1$ and $\beta \ll 1$,[2,3] while in the one-dimensional boson system with a repulsive δ-function interaction, $\alpha \ll 1$ and expression (5) for β diverges logarithmically at small momenta (Sec. V).

Therefore, in the problem of the high-density charged-boson gas the two expressions, (12) and (17), for the energy must agree exactly (if both formulas are indeed correct). On the other hand, in the general case of the weak coupling limit and/or uniform limit, it is not clear whether or not the two approaches should also lead to identical results. The remainder of this section is devoted to the proof that these two procedures do indeed lead to identical results for the energy.

First, to simplify the expression for E_2 of Eq. (12) we write Eqs. (4), (10), and (11) as

$$E_2(1\ \mathrm{ring}) = \tfrac{1}{6} N [4(2\pi)^3\rho]^{-2} \int I_2(1\ \mathrm{ring}) d\vec{k}\, d\vec{k}' , \quad (18a)$$

$$E_X = \tfrac{1}{6} N [4(2\pi)^3\rho]^{-2} \int I_X\, d\vec{k}\, d\vec{k}' , \quad (18b)$$

$$E_{Y\lambda} = \tfrac{1}{6} N [4(2\pi)^3]^{-2} \int I_{Y\lambda} d\vec{k}\, d\vec{k}' , \quad (18c)$$

where

$$I_2(1\ \mathrm{ring}) = 6[S(k)S(k')]^{-1}\epsilon(k)[1 - S(k)]^2 \times [1 - S(k')]^2 [1 + S(k)] , \quad (19a)$$

$$I_X = 3[S(k)S(k')S(k'')]^{-1}[1 - S(k)][1 - S(k')][1 - S(k'')] \times \{[1 - S(k)][1 - S(k')] + [S(k) + S(k')]\} [1 + S(k'')] \epsilon(k'') , \quad (19b)$$

$$I_{Y\lambda} = - \frac{[\langle \epsilon \rangle - \langle S^2\epsilon \rangle - S(k)S(k')S(k'')(\langle \epsilon/S \rangle - \langle S\epsilon \rangle)]^2}{S(k)S(k')S(k'')\langle \epsilon \rangle} . \quad (19c)$$

We introduce the double-arrow sign $\longleftrightarrow$ to indicate "equivalence" in integrating over variables $\vec{k}$ and $\vec{k}'$, i.e., $A(k, k', k'') \longleftrightarrow B(k, k', k'')$ means

$$\int A(k, k', k'') d\vec{k}\, d\vec{k}' = \int B(k, k', k'') d\vec{k}\, d\vec{k}' .$$

Then, rearranging terms in Eqs. (19a) and (19b) and recalling the relation $S(k)\epsilon(k) = \hbar^2 k^2/2m$, one finds

$$I_2(1\ \mathrm{ring}) \longleftrightarrow 3[S(k)S(k')]^{-1}[1 - S(k)]^2[1 - S(k')]^2 \{[S(k)\epsilon(k) + S(k')\epsilon(k')] + [\epsilon(k) + \epsilon(k')]\}$$

$$\longleftrightarrow 3[S(k)S(k')]^{-1}[1 - S(k)]^2[1 - S(k')]^2 S(k'')\epsilon(k'') + 3[S(k)S(k')]^{-1} [1 - S(k)]^2[1 - S(k')]^2 [\langle \epsilon \rangle - \epsilon(k'')] , \quad (20a)$$

$$I_X = -3[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2 S(k'')\epsilon(k'') + 3[S(k)S(k')S(k'')]^{-1}[1-S(k)]^2[1-S(k')]^2\epsilon(k'')$$

$$+3[S(k)S(k')S(k'')]^{-1}[1-S(k)][1-S(k')][1-S(k'')][S(k)+S(k')][1+S(k'')]\epsilon(k'') \,. \tag{20b}$$

Noting that $I_{Y\lambda}$ of Eq. (19c) is symmetric in k, k', and k'', we now obtain a similar symmetric expression for the sum of Eqs. (20):

$$I_2(1\text{ ring}) + I_X \longleftarrow J_1 + J_2 + J_3 \,, \tag{21a}$$

$$J_1 = 3[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2\langle\epsilon\rangle \equiv 3j_1(k,k',k'') \longleftarrow j_1(k,k',k'') + j_1(k',k'',k) + j_1(k'',k,k')$$

$$= \left[\frac{\langle S\rangle}{S(k)S(k')S(k'')} - 4\left\langle\frac{1}{S}\right\rangle + \langle S\rangle\left\langle\frac{1}{S}\right\rangle + 9 - 4\langle S\rangle + S(k)S(k')S(k'')\left\langle\frac{1}{S}\right\rangle\right]\langle\epsilon\rangle \,, \tag{21b}$$

$$J_2 = 3[S(k)S(k')S(k'')]^{-1}[1-S(k)]^2[1-S(k')]^2[1-S(k'')]\epsilon(k'')$$

$$\longleftarrow [S(k)S(k')S(k'')]^{-1}[1-\langle S\rangle + S(k)S(k')S(k'')(\langle 1/S\rangle - 1)][\langle\epsilon\rangle - \langle S\rangle\langle\epsilon\rangle + \langle S\epsilon\rangle + S(k)S(k')S(k'')\langle\epsilon/S\rangle] \,, \tag{21c}$$

$$J_3 = 3[S(k)S(k')S(k'')]^{-1}[1-S(k)][1-S(k')][1-S(k'')][S(k)+S(k')][1+S(k'')]\epsilon(k'')$$

$$\longleftarrow [S(k)S(k')S(k'')]^{-1}[1-\langle S\rangle + S(k)S(k')S(k'')(\langle 1/S\rangle - 1)][\langle S\rangle\langle\epsilon\rangle - \langle S\epsilon\rangle + \langle S\rangle\langle S\epsilon\rangle - \langle S^2\epsilon\rangle] \,. \tag{21d}$$

The results of Eqs. (21c) and (21d) follow through intermediate steps similar to those of Eq. (21b). Evaluating the sum $J_1 + J_2 + J_3$ one finds that many terms cancel each other, resulting in

$$I_2(1\text{ ring}) + I_X \longleftarrow \{[S(k)S(k')S(k'')]^{-1} - 2\langle 1/S\rangle + 8 - 4\langle S\rangle\}\langle\epsilon\rangle$$

$$+\langle 1/S\rangle[\langle S\rangle\langle S\epsilon\rangle - \langle S^2\epsilon\rangle + S(k)S(k')S(k'')\langle\epsilon/S\rangle] \,. \tag{22}$$

It proves useful to rewrite Eq. (19c) as

$$I_{Y\lambda} = [S(k)S(k')S(k'')]^{-1}[2\langle S^2\epsilon\rangle - \langle\epsilon\rangle] + 2\langle\epsilon/S\rangle - 2\langle S\epsilon\rangle$$

$$+\langle\epsilon\rangle^{-1}\{S(k)S(k')S(k'')[\langle\epsilon/S\rangle - \langle S\epsilon\rangle]^2$$

$$+2\langle S^2\epsilon\rangle[\langle S\epsilon\rangle - \langle\epsilon/S\rangle - \tfrac{1}{2}\langle S^2\epsilon\rangle/S(k)S(k')S(k'')]\} \,. \tag{23}$$

After some straightforward, but rather complicated, algebra it is found that the sum of Eqs. (22) and (23) becomes

$$I_2(1\text{ ring}) + I_X + I_{Y\lambda} \longleftarrow I_{2v} + I_{2p} + 2I_c \,, \tag{24a}$$

$$I_{2v} = 12S(k)\epsilon(k)[1-S(k)][1-S(k')][1-S(k'')] \,, \tag{24b}$$

$$I_{2p} = -[S(k)S(k')S(k'')\langle\epsilon\rangle]^{-1}[S(k)S(k')S(k'')$$

$$(2\langle\epsilon\rangle - \langle S\epsilon\rangle) - \langle S\rangle\langle S\epsilon\rangle + 2\langle S^2\epsilon\rangle]^2 \,, \tag{24c}$$

$$I_c = [4 - \langle 1/S\rangle - 2\langle S\rangle + S(k)S(k')S(k'')]\langle\epsilon\rangle$$

$$+[1/S(k)S(k')S(k'') - 2\langle 1/S\rangle + 4 - \langle S\rangle]\langle S^2\epsilon\rangle$$

$$+[\langle S\rangle\langle 1/S\rangle - 3]\langle S\epsilon\rangle + \langle\epsilon/S\rangle + \langle S^3\epsilon\rangle \,. \tag{24d}$$

Thus we now have [see Eqs. (14) and (16)]

$$\tfrac{1}{6}N[4(2\pi)^3\rho]^{-2}\int I_{2v}\,d\vec{k}\,d\vec{k}' = E_{2v} \,, \tag{25a}$$

$$\tfrac{1}{6}N[4(2\pi)^3\rho]^{-2}\int I_{2p}\,d\vec{k}\,d\vec{k}' = E_{2p} \,, \tag{25b}$$

and consequently the identification of Eqs. (12) and (17) would be established if

$$\int I_c\,d\vec{k}\,d\vec{k}' = 0 \,, \tag{26}$$

which, amazingly enough, happens to be the case, as is shown through Eqs. (27)–(30).

By employing the identities

$$\langle S\rangle\langle S\epsilon\rangle - \langle S^2\epsilon\rangle = S(k)S(k')S(k'')[\langle 1/S\rangle\langle\epsilon\rangle - \langle\epsilon/S\rangle] \,, \tag{27a}$$

$$\langle S\rangle\langle S^2\epsilon\rangle - \langle S^3\epsilon\rangle = S(k)S(k')S(k'')[\langle 1/S\rangle\langle S\epsilon\rangle - \langle\epsilon\rangle] \,, \tag{27b}$$

$$\langle S^2\rangle\langle S^2\epsilon\rangle - \langle S^4\epsilon\rangle = S(k)S(k')S(k'')[\langle S\rangle\langle 1/S\rangle\langle S\epsilon\rangle$$

$$-\langle S\rangle\langle\epsilon\rangle - \langle 1/S\rangle\langle S^2\epsilon\rangle - \langle S\epsilon\rangle] \,, \tag{28}$$

we find, after some algebraic manipulation, that Eq. (24d) can be written as

$$I_c = L_1 + L_2 \tag{29a}$$

$$L_1 = 2[S(k)S(k')S(k'')]^{-1}[(1-2\langle S\rangle+\langle S^2\rangle)\langle S^2\epsilon\rangle+2\langle S^3\epsilon\rangle-\langle S^4\epsilon\rangle]+4[\langle S^2\epsilon\rangle+\langle S\epsilon\rangle(2-\langle S\rangle)+\tfrac{1}{2}S(k)S(k')S(k'')\langle\epsilon\rangle]$$

$$\equiv l_1(k,k',k'')+l_1(k',k'',k)+l_1(k'',k,k')\longrightarrow 3l_1(k,k',k'')$$

$$=3[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2[2S(k'')\epsilon(k'')] , \tag{29b}$$

$$L_2=[\langle S\rangle/S(k)S(k')S(k'')-4\langle 1/S\rangle+\langle S\rangle\langle 1/S\rangle+9-4\langle S\rangle+S(k)S(k')S(k'')\langle 1/S\rangle]\langle S\epsilon\rangle$$

$$\longrightarrow 3[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2\langle S\epsilon\rangle , \tag{29c}$$

or finally

$$I_c\longrightarrow 3[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2[S(k'')\epsilon(k'')-S(k)\epsilon(k)-S(k')\epsilon(k')]$$

$$=-3(\hbar^2/m)[S(k)S(k')]^{-1}[1-S(k)]^2[1-S(k')]^2(\vec{k}\cdot\vec{k}') , \tag{30}$$

from which follows immediately the desired relation (26).

We now remark that the expression for E_{2p} given by Eq. (16) can be put in an alternative (and probably more useful) form. Using such a form, let us first summarize results by rewriting the variation-perturbation formula (17) in a rather complete form:

$$E=E_0+E_1+E_{2v}+E_{2p} , \tag{31a}$$

$$E_0=\tfrac{1}{2}N\rho V(0) , \tag{31b}$$

$$E_1=-\frac{N}{4(2\pi)^3\rho}\int\epsilon(k)\,\frac{[1-S(k)]^2}{S(k)}\,d\vec{k} , \tag{31c}$$

$$E_{2v}=\frac{2N}{[4(2\pi)^3\rho]^2}\int d\vec{k}\,d\vec{k}'\,\epsilon(k)S(k)[1-S(k)][1-S(k')][1-S(k'')] , \tag{31d}$$

$$E_{2p}=-\frac{N}{6[4(2\pi)^3\rho]^2}\int d\vec{k}\,d\vec{k}'\,\frac{[1-S(k)]^2[1-S(k')]^2[1-S(k'')]^2}{S(k)S(k')S(k'')\langle\epsilon\rangle}\times\left[2\left\langle\frac{S^2\epsilon}{1-S}\right\rangle-\left\langle\frac{S}{1-S}\right\rangle\langle S\epsilon\rangle\right]^2 , \tag{31e}$$

with $S(k)$ and $\epsilon(k)$ defined by Eqs. (6) and (7), respectively. The derivation of Eq. (31e) from Eq. (16) is not difficult if one employs the relation of Eq. (27a) and another relation

$$S(k)S(k')S(k'')\left[\left\langle\frac{1-S}{S}\right\rangle\langle(1-S)\epsilon\rangle-\left\langle\frac{(1-S)^2\epsilon}{S}\right\rangle\right]=[1-S(k)][1-S(k')][1-S(k'')]\left[\left\langle\frac{S}{1-S}\right\rangle\langle S\epsilon\rangle-\left\langle\frac{S^2\epsilon}{1-S}\right\rangle\right] . \tag{32}$$

V. APPLICATIONS

Our discussion so far has been presented without assuming any particular form for the potential $v(r)$; we have only assumed (tacitly) that the Fourier transform $V(k)$ exists and that the interaction is mainly repulsive so as to give a positive value for $S^2(k)$ in Eq. (6). In this section we apply Eqs. (31) to two particular systems which allow straightforward evaluation of the ground-state energy.

A. Charged-Boson System at High Density

The calculation for the charged-boson system has already been carried out by Brueckner[5] in the occupation-number representation [Eq. (12)]. Here we present numerical results obtained using Eqs. (31). The summary on the equivalence of the two approaches in the case of the charged-boson gas has been reported in a recent letter.[20] For completeness, we may briefly outline the procedure based on Eqs. (31).

The Fourier transform of the Coulomb potential is

$$V(k)=4\pi e^2/k^2 ,\quad k\neq 0;\quad V(0)=0 , \tag{33}$$

the vanishing of $V(0)$ being due to the neutralizing positive charge background. Introducing convenient dimensionless quantities

$$r_s = (3/4\pi\rho)^{1/3}(me^2/\hbar^2)\ ,\quad t = \tfrac{1}{2}(\pi e^2 m\rho/\hbar^2)^{-1/4}k\ ,$$
$$\sigma(t) = t^2(1+t^4)^{-1/2}\ ,\quad \omega(t) = (1+t^4)^{1/2}\ , \tag{34}$$

and also

$$\eta_1(t) = \omega(t)[1-\sigma(t)]^2/\sigma(t)\ ,$$
$$\eta_{2v}(t,\ t',\ t'') = \omega(t)\sigma(t)[1-\sigma(t)][1-\sigma(t')][1-\sigma(t'')]\ , \tag{35}$$
$$\eta_{2p}(t,\ t',\ t'') = \frac{[1-\sigma(t)]^2[1-\sigma(t')]^2[1-\sigma(t'')]^2}{\sigma(t)\sigma(t')\sigma(t'')\langle\omega\rangle} \times\left[2\left\langle\frac{\sigma^2\omega}{1-\sigma}\right\rangle - \left\langle\frac{\sigma}{1-\sigma}\right\rangle\langle\sigma\omega\rangle\right]^2,$$

we find from Eqs. (5)–(7), (15), and (31) the following results for various quantities, with energies in Ry $(me^4/2\hbar^2)$:

$$\alpha = \frac{8r_s^{3/4}}{(12)^{1/4}\pi}\int_0^\infty [1-\sigma(t)]t^2dt + \cdots$$
$$= \frac{2\Gamma^2(\frac{1}{4})r_s^{3/4}}{3(12)^{1/4}\pi^{3/2}} + O(r_s^{3/2})\ , \tag{36}$$

$$\beta = \frac{2r_s^{3/4}}{(12)^{1/4}\pi}\int_0^\infty \frac{[1-\sigma(t)]^2}{\sigma(t)}t^2dt + \cdots$$
$$= \frac{\Gamma^2(\frac{1}{4})r_s^{3/4}}{6(12)^{1/4}\pi^{3/2}} + O(r_s^{3/2})\ , \tag{37}$$

$$\alpha = 4\beta + O(r_s^{3/2})\ , \tag{38}$$

$$E_1/N = -2(12)^{1/4}\pi^{-1}r_s^{3/4}\int_0^\infty \eta_1(t)t^2dt$$
$$= -0.8031r_s^{-3/4}\ , \tag{39}$$

$$E_{2v}/N = (2\pi^4)^{-1}\int \eta_{2v}(t,\ t',\ t'')\,d\vec{t}\,d\vec{t}\,'$$
$$= 0.028\,026\ , \tag{40}$$

$$E_{2p}/N = -(24\pi^4)^{-1}\int \eta_{2p}(t,\ t',\ t'')\,d\vec{t}\,d\vec{t}\,'$$
$$= -0.000\,5323\ , \tag{41}$$

$$E/N = -0.8031/r_s^{3/4} + 0.027\,49 + O(r_s^{3/4})\ . \tag{42}$$

The second-order term of Eq. (42) differs slightly from Brueckner's[5] numerical result $E_2/N = 0.0280$; the discrepancy must be due to small errors involved in the numerical integration(s). We may now remark that our analysis certainly clarifies any doubt concerning the possibility of $E_2 = E_{2v}$, which arose from the close numerical agreement between the two values.[5]

B. One-Dimensional Boson System

We consider a system of N bosons interacting in a one-dimensional space of length L through a repulsive δ-function potential

$$v(x) = 2c\delta(x)\ ,\ c>0\ \text{ or }\ V(k) = 2c\ . \tag{43}$$

The variational energy given by Eq. (13) was evaluated in Ref. 21; its derivation is briefly repeated in the following calculation. Here the dimensionless quantities are defined as (with $\rho = N/L$)

$$\gamma = (c/\rho)(2m/\hbar^2)\ ,$$
$$t = \hbar(8m\rho c)^{-1/2}k\ ,$$
$$\sigma(t) = |t|(1+t^2)^{-1/2}\ , \tag{44}$$
$$\omega(t) = |t|(1+t^2)^{1/2}\ ,$$

and definitions of Eq. (35) are also useful. Then, Eqs. (15) and (31) yield the following results, with energies in units of $\hbar^2/2m$:

$$\alpha = (2/\pi)\gamma^{1/2}\int_0^\infty [1-\sigma(t)]dt + \cdots$$
$$= (2/\pi)\gamma^{1/2} + O(\gamma)\ , \tag{45}$$

$$E_0/N = \rho^2\gamma\ , \tag{46}$$

$$E_1/N = -(2/\pi)\rho^2\gamma^{3/2}\int_0^\infty \eta_1(t)\,dt$$
$$= -0.4244\rho^2\gamma^{3/2}\ , \tag{47}$$

$$E_{2v}/N = (2\pi^2)^{-1}\rho^2\gamma^2\int_{-\infty}^\infty\int_{-\infty}^\infty \eta_{2v}(t,\ t',\ t'')\,dtdt'$$
$$= 0.065\,45\rho^2\gamma^2\ , \tag{48}$$

$$E_{2p}/N = -(24\pi^2)^{-1}\rho^2\gamma^2\int_{-\infty}^\infty\int_{-\infty}^\infty \eta_{2p}(t,\ t',\ t'')\,dtdt'$$
$$= -0.000\,1027\rho^2\gamma^2\ , \tag{49}$$

$$E/N = \rho^2\gamma^2[1 - 0.4244\gamma^{1/2} + 0.065\,35\gamma + O(\gamma^{3/2})]\ . \tag{50}$$

It is easily seen that the integral for the leading term of β [Eq. (5)] diverges logarithmically at low momenta. [Similar logarithmic singularities found in the integrals for E_2(1 ring), E_X, and $E_{Y\lambda}$ are discussed in Sec. VI.] The divergence of the integral for β presents some difficulty in arguing about the validity of the Bogoliubov theory based on the condition $\beta \ll 1$. On the other hand, the method based on $\alpha \ll 1$ does not suffer from such a disadvantage and consequently the equivalence of the two approaches seems to validate the Bogoliubov theory (at least in this respect).

VI. CONCLUDING REMARKS

In the applications of the variation-perturbation formula in Sec. V some of the elegance of the uniform-limit procedure begins to be apparent; in particular, the evaluation of the second-order term for the energy is straightforward, with no indications of any difficulty such as singular integrals. The situation is, however, somewhat different if the formula given by Eq. (12) is applied. To see this point, first we observe that the liquid structure function always vanishes at the origin [i.e., $S(0)=0$] and hence for small momenta the integrands given by Eqs. (19) become

$$I_2(1\ \text{ring}) \to 6[S(k)S(k')]^{-1}\epsilon(k)\ , \tag{51a}$$

$$I_X \to 3[S(k)S(k')S(k'')]^{-1}\epsilon(k'')[1-S(k)-S(k')]\ , \tag{51b}$$

$$I_{Y\lambda} \to -[S(k)S(k')S(k'')]^{-1}\langle\epsilon\rangle\ . \tag{51c}$$

In the one-dimensional boson system with the δ-function interaction, we have $\sigma(t)=\omega(t)\to|t|$ for $k\to 0$ and the integrals in Eqs. (18) diverge logarithmically at small momenta, the singular contributions being

$$\frac{E_2(1\ \text{ring})}{N}=\frac{\rho^2\gamma^2}{4\pi^2}\int\frac{dtdt'}{|t'|}\ , \tag{52a}$$

$$\frac{E_X}{N}=\frac{\rho^2\gamma^2}{8\pi^2}\int\frac{dtdt'}{|tt'|}-\frac{\rho^2\gamma^2}{4\pi^2}\int\frac{dtdt'}{|t'|}\ , \tag{52b}$$

$$\frac{E_{Y\lambda}}{N}=-\frac{\rho^2\gamma^2}{8\pi^2}\int\frac{dtdt'}{|tt'|}\ . \tag{52c}$$

We note that, two types of singularities appear in Eqs. (52). The more (or doubly) divergent terms cancel each other in the sum $E_X+E_{Y\lambda}$, whose (less) divergent contribution is, in turn, canceled by the contribution from E_2(1 ring), thus resulting in the finite value for E_2.

In the charged-boson gas, integrals for both E_X and $E_{Y\lambda}$ are also logarithmically divergent for small momenta, but E_2 (1 ring) and the sum $E_X+E_{Y\lambda}$ are finite[5,22]:

$$E_2\ (1\ \text{ring})/N=0.212\,207\ , \tag{53a}$$

$$(E_X+E_{Y\lambda})/N=-0.184713\ . \tag{53b}$$

It is interesting, however, to note that the major fraction (87%) of E_2 (1 ring) is still canceled by $E_X+E_{Y\lambda}$ in the sum E_2 (1 ring) + $(E_X+E_{Y\lambda})$.

On the other hand, it is easily seen that contributions to integrals for E_{2v} and E_{2p} are very small at small momenta, since the integrands become, as $k\to 0$,

$$I_{2v}\to 4\langle S\epsilon\rangle\ , \tag{54a}$$

$$I_{2p}\to -[S(k)S(k')S(k'')\langle\epsilon\rangle]^{-1}[2\langle S^2\epsilon\rangle-\langle S\rangle\langle S\epsilon\rangle]^2\ . \tag{54b}$$

Finally we remark that the perturbation correction E_{2p} generated by the three-phonon vertex appears to contribute only a very small fraction to the second-order term E_2, its contribution (in second order) being about 1.9% in the charged-boson gas and 0.16% in the one-dimensional boson system with the δ-function interaction. In the case of one-dimensional boson system, the fair agreement[21] between Lieb and Liniger's exact numerical result[23] and the variational result $E=E_0+E_1+E_{2v}$ over the range $0\le\gamma\lesssim 6$ may be partially explained by the smallness of the perturbation correction E_{2p}. In the problem of liquid He^4 the perturbation correction $E_{2p}/N=-0.76$ °K evaluated by Davison and Feenberg[8] is about 10.6% of the experimental value $E/N=-7.2$ °K determined at the equilibrium density $\rho=0.0218$ Å^{-3}; it must be remembered, however, that $\alpha=1$ in this case and that the second-order perturbation formula given by Eq. (31e) is not exact since in the derivation of the formula use has been made of the convolution approximation[19] for the three-particle distribution function $p^{(3)}$ (1, 2, 3).

---

[1] N. N. Bogoliubov, J. Phys. (USSR) 11, 23 (1947); N. N. Bologiubov and D. N. Zubarev, Zh. Eksperim. i Teor. Fiz. 28, 129 (1955) [Sov. Phys. JETP 1, 83 (1955)].

[2] T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. 106, 1135 (1957).

[3] T. T. Wu, Phys. Rev. 115, 1390 (1959).

[4] L. L. Foldy, Phys. Rev. 124, 649 (1961).

[5] K. A. Brueckner, Phys. Rev. 156, 204 (1967).

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

[7] F. Y. Wu and E. Feenberg, Phys. Rev. 122, 739 (1961); H. W. Jackson and E. Feenberg, Ann. Phys. (N.Y.) 15, 266 (1961); W. E. Massey, Phys. Rev. 151, 153 (1966); W. E. Massey and C. W. Woo, *ibid.* 164, 256 (1967); C. E. Campbell and E. Feenberg, *ibid.* 188, 396 (1969). A somewhat different but closely related approach is used in W. L. McMillan, *ibid.* 138, A442 (1965); J. C. Lee and A. A. Broyles, Phys. Rev. Letters 17, 424 (1966); D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967).

[8] T. B. Davison and E. Feenberg, Ann. Phys. (N.Y.) 53, 559 (1969).

[9] D. K. Lee and E. Feenberg, Phys. Rev. 137, A731 (1965).

[10] D. K. Lee, Phys. Rev. 187, 326 (1969).

[11] H.-K. Sim, C.-W. Woo, and J. R. Buchler, Phys. Rev. Letters 24, 1094 (1970).

[12] The use of the term "*second* order" in the present study usually proves to be proper (Sec. V), but not always. The same argument applies to other orders.

[13] It can be shown that with slight modifications the present analysis yields the same results as those obtained

in Ref. 11: D. K. Lee (unpublished).

[14] A. Bijl, Physica 7, 869 (1940); R. P. Feynman, Phys. Rev. 94, 262 (1954).

[15] M. Girardeau and R. Arnowitt, Phys. Rev. 113, 755 (1959).

[16] M. Girardeau, Phys. Rev. 115, 1090 (1959).

[17] Ref. 6, Chap. 7 and Appendix 5-C.

[18] D. K. Lee, Phys. Rev. A 4, 348 (1971).

[19] H. W. Jackson and E. Feenberg, Rev. Mod. Phys. 34, 686 (1962).

[20] D. K. Lee, Phys. Rev. Letters 26, 877 (1971).

[21] D. K. Lee, Phys. Rev. A 3, 345 (1971).

[22] The numerical value of Eq. (53b) is found from results given by Eqs. (40), (41), and (53a).

[23] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).