Weak-Coupling Expansion for the Ground-State Energy of a Many-Boson System

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The pair theory of many-boson systems is used to obtain a weak-coupling expansion for the ground-state energy to third order in the coupling constant. The relationship of this expansion to the formal Rayleigh-Schrödinger perturbation expansion is discussed, with particular reference to the relationship between the divergent third-order term in the formal perturbation expansion and the terms of $\frac{5}{2}$ and third orders in the correct weak-coupling expansion. The excitation energy is discussed briefly; it is pointed out that the lowest-order "nonpair" correction to the phonon energy is of the right order of magnitude to cancel the spurious energy gap of the pair theory.

1. INTRODUCTION

THE purpose of this note is to show that the pair theory of many-boson systems[1] can be used to obtain a weak-coupling expansion for the ground-state energy correct to third order in the coupling constant; this expansion is of theoretical interest because of the well-known divergence of perturbation theory in third order which is associated with a branch point at the origin of the coupling-constant plane. The method of calculation involves analytical iteration of the basic variational integral equation of the pair theory, starting with the Bogoliubov[2] approximation; a by-product of this procedure, when supplemented by an estimate of the "triad" and "quartet" corrections by (now convergent) perturbation theory, is a determination of the domains of validity of the Bogoliubov and pair-theory approximations. Our treatment and Bogoliubov's are found to be in some respects complementary: The Bogoliubov theory gives a physically reasonable linear phonon spectrum at low momentum, but a ground-state energy incorrect in third order; the pair theory gives a rigorous upper bound for the ground-state energy which first differs from the exact energy in $\frac{7}{2}$ order, but a phonon spectrum with an unphysical energy gap at low momentum.

2. FORMULATION

The physical properties of the pair states are determined by the solution $\phi(\mathbf{k})$ of the variational integral Eq. (I.24), which approaches $\phi_0(k)\equiv -L_k$ as the interaction[3] $v(k)\to 0$; here L_k is Bogoliubov's function[2]

$$L_k=[\rho v(k)]^{-1}\{k[\tfrac{1}{4}k^2+\rho v(k)]^{\frac{1}{2}}-\tfrac{1}{2}k^2-\rho v(k)\}. \quad (1)$$

The next approximation is obtained by replacing $\phi(\mathbf{k})$ by $\phi_0(k)$ in ρ_0, I_1, and I_2 in (I.23) or (I.24); one therefore replaces ρ_0, I_1, and I_2 in these equations by $\rho_0^{(0)}$, $I_1^{(0)}$, and $I_2^{(0)}$ defined by

$$\rho-\rho_0^{(0)}\equiv(2\pi)^{-3}\int\frac{L_{k'}^2}{1-L_{k'}^2}d^3k'$$
$$=\tfrac{1}{3}\pi^{-2}\rho^{\frac{3}{2}}v^{\frac{3}{2}}(0)[1+O(\rho^{*\frac{1}{2}}\lambda^{\frac{1}{2}})], \quad (2.1)$$

$$I_1^{(0)}(k)\equiv(2\pi)^{-3}\int v(|\mathbf{k}-\mathbf{k}'|)\frac{(-L_{k'})}{1-L_{k'}^2}d^3k'$$
$$=[1+O(\rho^{*\frac{1}{2}}\lambda^{\frac{1}{2}})](2\pi)^{-3}\rho\times\int\frac{v(|\mathbf{k}-\mathbf{k}'|)v(k')}{k'^2}d^3k', \quad (2.2)$$

$$I_2^{(0)}(k)\equiv(2\pi)^{-3}\int v(|\mathbf{k}-\mathbf{k}'|)\frac{L_{k'}^2}{1-L_{k'}^2}d^3k'$$
$$=(\rho-\rho_0^{(0)})v(k)[1+O(\rho^{*\frac{1}{2}}\lambda^{\frac{1}{2}})], \quad (2.3)$$

where ρ^* and λ are, respectively, the dimensionless density and coupling constant defined, e.g., by $\rho^*=\rho a^3$ and $\lambda=a^{-1}v(0)$, where a is the range of the potential $v(\mathbf{r})$; we use units such that $\hbar=m=1$, and assume that $v(\mathbf{r})$ is repulsive "on the average" in the sense that $v(0)>0$. The results (2.1) and (2.3) were obtained by noting that the dominant contribution to these integrals comes from $0\leq k'\lesssim\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0)$, so that $v(k')$ can be replaced by $v(0)$ in $L_{k'}$ and the resulting integrals evaluated exactly; (2.2) was obtained by noting that the dominant contribution comes from $k'\gg\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0)$, where the factor $(-L_{k'})/(1-L_{k'}^2)$ can be replaced by $\rho v(k')/k'^2$. A necessary condition for validity of the Bogoliubov approximation is that the first approximation for $\phi(\mathbf{k})$ differ from $\phi_0(k)$ only by an amount $\ll 1$; putting $k=0$, one obtains from (I.25) and (2) the necessary condition

$$\epsilon\equiv I_1(0)/\rho_0 v(0)\cong[2\pi^2 v(0)]^{-1}\int_0^\infty v^2(k)dk\ll 1. \quad (3)$$

For any "reasonable" interaction, ϵ differs from the previously-defined dimensionless coupling constant λ only by a factor of order unity. We shall find that $\lambda\ll 1$ is also a sufficient condition that the Bogoliubov

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[1] M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959), hereafter referred to as I; Eq. (*n*) of this paper will be herein denoted by (I.*n*).
[2] N. N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947).
[3] We assume that $v(\mathbf{r})$, and hence $v(\mathbf{k})\equiv v(k)$, are spherically symmetric.

ground-state energy be a good approximation to the true energy.

3. GROUND-STATE ENERGY

The pair-theory expression (I.21) for the ground-state energy per particle can be rewritten in the form

$$E_0/n=\tfrac{1}{2}\rho v(0)-\frac{\rho_0}{\rho}[I_1(0)-I_2(0)]$$
$$+(8\pi^3\rho)^{-1}\Big[\int \tfrac{1}{2}k^2\frac{\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3k$$
$$+\int \tfrac{1}{2}I_1(\mathbf{k})\frac{\phi(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3k$$
$$+\int \tfrac{1}{2}I_2(\mathbf{k})\frac{\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3k\Big]. \quad (4)$$

In this section we shall calculate the approximate value of E_0/n by replacing $\phi(\mathbf{k})$ by $\phi_0(k)=-L_k$ in (4). It is shown in Appendix A that this introduces only an error of order $\lambda^{7/2}$ into E_0/n, and in Appendix B that our neglect of "nonpair" contributions also introduces only an error of order $\lambda^{7/2}$.

To obtain a result for E_0/n correct to order λ^3, it is necessary to evaluate some of the integrals (2) and (4) more accurately than was done in obtaining (2). Consider first the contribution of $I_1^{(0)}(0)$. One has by (1) and (2.2)

$$I_1^{(0)}(0)=\frac{1}{2\pi^2}\Big(\int_0^{k_c}+\int_{k_c}^{\infty}\Big)\frac{k\rho v^2(k)}{2[\frac{1}{4}k^2+\rho v(k)]^{\frac{1}{2}}}dk, \quad (5)$$

where k_c is defined by

$$\tfrac{1}{4}k_c^2=\rho v(0). \quad (6)$$

We introduce only an error $a^{-2}O(\rho^{*5/2}\lambda^{7/2})$ if we replace $v(k)$ by $v(0)$ in evaluating $\int_0^{k_c}$, which can then be evaluated exactly. To evaluate $\int_{k_c}^{\infty}$, we separate out explicitly the first two terms in the expansion of the integrand in powers of $4\rho v(k)/k^2$:

$$\frac{1}{2\pi^2}\int_{k_c}^{\infty}\frac{k\rho v^2(k)}{2[\frac{1}{4}k^2+\rho v(k)]^{\frac{1}{2}}}dk=\frac{\rho}{2\pi^2}\int_{k_c}^{\infty}v^2(k)dk$$
$$-\frac{\rho^2}{\pi^2}\int_{k_c}^{\infty}\frac{v^3(k)}{k^2}dk+\frac{1}{2\pi^2}\int_{k_c}^{\infty}\Big\{\frac{k\rho v^2(k)}{2[\frac{1}{4}k^2+\rho v(k)]^{\frac{1}{2}}}$$
$$-\rho v^2(k)+\frac{2\rho^2v^3(k)}{k^2}\Big\}dk. \quad (7)$$

Then the integrand of the last integral in (7) is of the form

$$A\frac{\rho^3v^4(k)}{k^4}-B\frac{\rho^4v^5(k)}{k^6}+\cdots,$$

where A, B, $\cdots$ are numerical coefficients of order unity, and it is easy to see that we make only an error $a^{-2}O(\rho^{*5/2}\lambda^{7/2})$ in the integral if we replace $v(k)$ by $v(0)$. The final result for $I_1^{(0)}(0)$ is of course independent of the precise value of k_c, the value (6) having been chosen only for convenience; the essential point is that $k_c\sim\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0)$. The method of evaluation of the remaining integrals in (4) is the same; the last integral is of order λ^4 and need not be considered. The final result for E_0/n is

$$E_0/n=\tfrac{1}{2}\rho v(0)-\tfrac{1}{2}(2\pi)^{-3}\int\frac{\rho v^2(k)}{k^2}d^3k+\frac{8}{15}\pi^{-2}\rho^{\frac{3}{2}}v^{\frac{5}{2}}(0)$$
$$+\tfrac{1}{2}(2\pi)^{-6}\int\int\frac{\rho v(k)v(|\mathbf{k}-\mathbf{k}'|)v(k')}{k^2k'^2}d^3kd^3k'$$
$$+(2\pi)^{-3}\,\mathrm{F}\int\frac{\rho^2v^3(k)}{k^4}d^3k+a^{-2}O(\rho^{*\frac{3}{2}}\lambda^{7/2}), \quad (8)$$

where the symbol F before the last integral means that the "finite part" of this divergent integral is to be taken according to the following prescription: One renders the integral finite by excluding from the domain of integration a small sphere of radius k_c about the origin, imagines the resulting finite integral expanded as a Laurent series in k_c, and picks out the constant term in this series.[4]

There is clearly a close correspondence between the weak-coupling expansion (8) and the lowest-order terms of the formal Rayleigh-Schrödinger perturbation expansion for E_0/n, which diverges in third order. In fact, one finds that the terms in E_0/n which are convergent when calculated by perturbation theory agree with the corresponding terms in the correct weak-coupling expansion (8), and that the lowest order in which perturbation theory diverges is the integral order immediately following the lowest nonintegral order in the correct weak-coupling expansion; the divergence is the result of trying to represent a nonanalytic function of λ (here represented by terms involving $\lambda^{5/2}$, $\lambda^{7/2}$, $\cdots$) by the perturbation series of integral powers of λ. This seems to be a rather general property of perturbation theory[5]; e.g., it also occurs in the many-electron problem, where the divergence of perturbation theory in second order[6] is associated with a nonanalytic term proportional to $\lambda^2\ln\lambda$ (λ is the square of the electron charge in dimensionless units) which is the term of next

[4] The origin of the term $\mathrm{F}\int\cdots$ is best illustrated by an example. Consider an interaction $v(k)$ that is constant for $0\leq k\leq a^{-1}$ and vanishes for $k>a^{-1}$. Then

$$\int_{k_c}^{\infty}\frac{v^3(k)}{k^2}dk=\frac{v^3(0)}{k_c}-av^3(0).$$

The term $v^3(0)/k_c$ has already been included in the term involving $v^{5/2}(0)$ in (8), while the term $-av^3(0)$ is the "finite part" $\mathrm{F}\int_0^{\infty}[v^3(k)/k^2]dk$.

[5] I am indebted to C. N. Yang for this observation.

[6] See, e.g., W. Macke, Z. Naturforsch. **5a**, 192 (1950); M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

lower order than λ^2 in the correct weak-coupling (or equivalently, high-density) expansion. A further feature of the many-boson problem that emerges from (8) is that even the third-order term, which is divergent in the formal perturbation series, can be obtained from this series provided that only the "finite part" of the divergent perturbation integral is retained.

Although the weak-coupling expansion (8) is not directly applicable to a strongly-coupled system such as the hard-sphere Bose gas, Lee, Huang, and Yang[7,8] have shown that at low density the hard-sphere interaction can be replaced by an equivalent pseudopotential of finite strength. Upon substituting the lowest-order approximation $v(k)\cong 4\pi a$ to the LHY pseudopotential into the first and third terms of (8), one obtains the LHY expression[9]

$$2\pi\rho a[1+(128/15)\pi^{-\frac{1}{2}}(\rho a^3)^{\frac{1}{2}}] \tag{9}$$

for the first two terms of the low-density expansion of the ground-state energy per particle; similarly, substitution of $v(k)\cong 4\pi a$ into (2.1) leads to the LHY expression [Eq. (40b) of reference 8] for the number $\rho_0 V$ of condensed particles. The second term of (8) does not contribute to the ground-state energy because, as shown by LHY, its omission is equivalent to replacement of the approximate pseudopotential $v(\mathbf{r})\cong 4\pi a\delta(\mathbf{r})$ in coördinate space by the correct [to the lowest few orders in $(\rho a^3)^{\frac{1}{2}}$] pseudopotential $v(\mathbf{r})=4\pi a\delta(\mathbf{r})(\partial/\partial r)r$. The fourth and fifth terms of (8) depend sensitively upon the high-momentum behavior of $v(k)$, whereas the pseudopotential $v(k)\cong 4\pi a$ is only correct for $k\ll a^{-1}$; hence these terms do not shed any light on the higher-order terms in the low-density expansion of E_0/n for the hard-sphere Bose gas.

4. EXCITATION ENERGIES

In contrast to the ground-state energy, the phonon energy $E(\mathbf{k})$ given by Eq. (I.37) is incorrect at low momentum $\mathbf{k}$ even to lowest nonvanishing order in the coupling constant λ, since there is a gap $E(0)$ which is given by (I.38), (I.25), and (2.2) as

$$E(0)=2\epsilon^{\frac{1}{2}}\rho_0 v(0)=a^{-2}O(\rho^*\lambda^{\frac{3}{2}}), \tag{10}$$

whereas one knows on physical grounds that the true phonon energy is linear in k at low k. Since the pair theory gives the best (in the sense of the variational theorem) approximation to the low-lying spectrum which can be obtained by states having a pair structure, the incorrect low-momentum behavior (10) must be due to neglect of "triad" and "quartet" effects generated by H_T and H_Q [Eqs. (B.2) and (B.3)]. It can in fact be shown that the lowest-order triad correction to $E(0)$ is given by

$$\delta_T E(0)=-\tfrac{1}{2}\rho_0(2\pi)^{-3}\int\frac{h^2(\mathbf{k})}{2E(\mathbf{k})-E(0)}d^3k, \tag{11}$$

with

$$h(\mathbf{k})=[1-\phi^2(0)]^{-\frac{1}{2}}\Big\{v(0)[3\phi(0)-2]\frac{\phi(\mathbf{k})}{1-\phi^2(\mathbf{k})} +2v(k)\frac{1+\phi(0)\phi(\mathbf{k})}{1+\phi(\mathbf{k})}\Big\}, \tag{12}$$

and the expression (11) can be shown by methods similar to those used in estimating (B.9) to be of the same order of magnitude as the gap (10) itself, so that one can hope that an adequate treatment of triad and quartet effects would exactly cancel the gap. Since the ground-state energy of the pair theory is obtained by a variational method, it is insensitive to the detailed structure of the ground-state wave function in momentum space. On the other hand, the excitation energies are intimately related to this detailed structure. It is therefore not surprising that the ground-state energy given by the pair theory is quite accurate for weak coupling, whereas the corresponding phonon energy is incorrect at low momentum. The inaccurate phonon energy is the price one pays (so long as one restricts oneself to states having a pair structure) for the more accurate ground-state energy obtained by the variational method.

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APPENDIX A

We shall show in this Appendix that the errors introduced into E_0/n by the replacement $\phi(\mathbf{k})\to\phi_0(k)$ in (4) are of order $\lambda^{7/2}$. The first approximation to the solution $\phi(\mathbf{k})$ of the variational integral equation is obtained by replacing ρ_0, I_1, and I_2 by $\rho_0^{(0)}$, $I_1^{(0)}$, and $I_2^{(0)}$ in (I.23) and solving for $\phi(\mathbf{k})$. The result is

$$\phi(\mathbf{k})=\phi_0(k)+\phi_1(k)=-L_k+\phi_1(k), \tag{A.1}$$

where $\phi_1(k)$ is found with the aid of (1) and (2) to have the following behavior for various values of k:

$$\phi_1(k)\cong-\epsilon^{\frac{1}{2}}\{[4+(\eta+\tfrac{1}{2}\epsilon^{\frac{1}{2}}\eta^2)^2]^{\frac{1}{2}}-\eta-\tfrac{1}{2}\epsilon^{\frac{1}{2}}\eta^2\}, \quad k\ll\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0), \tag{A.2}$$

$$\phi_1(k)=O(\epsilon), \quad k\sim\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0), \tag{A.3}$$

$$\phi_1(k)\cong-k^{-2}I_1^{(0)}(k), \quad k\gg\rho^{\frac{1}{2}}v^{\frac{1}{2}}(0). \tag{A.4}$$

[7] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).
[8] Lee, Huang, and Yang, Phys. Rev. **106**, 1135 (1957), hereafter denoted by LHY.
[9] The expression (9) differs from the LHY expression [Eq. (25) of reference 8] by a factor of two because they use units such that $2m=1$, whereas we require $m=1$.

The parameter ϵ is given by (3) and differs from the dimensionless coupling constant λ only by a factor of order unity; the dimensionless variable η in (A.2) is defined by

$$k=[\epsilon\rho v(0)]^{\frac{1}{2}}\eta. \tag{A.5}$$

To find the contribution of ϕ_1 to E_0/n we substitute (A.1) into the various integrals in (4). The factor

$$[1-\phi^2(\mathbf{k})]^{-1}=[1-L_k{}^2+2L_k\phi_1(k)-\phi_1{}^2(k)]^{-1} \tag{A.6}$$

which occurs in all of the integrands can be expanded in powers of

$$(1-L_k{}^2)^{-1}[2L_k\phi_1(k)-\phi_1{}^2(k)] \tag{A.7}$$

for $k>k_0$, where k_0 is defined by the requirement that the quantity (A.7) be unity for $k=k_0$; one finds $k_0\sim a^{-1}\rho^{*\frac{1}{2}}\lambda$. The contributions to E_0/n from the interval $(0,k_0)$ are all of order $\lambda^{7/2}$ or higher so that aside from such terms one has

$$E_0/n=(E_0/n)^{(0)}+\delta(E_{\rm kin}/n)+\delta(E_{\rm pot}/n), \tag{A.8}$$

where $(E_0/n)^{(0)}$ is the result (8) obtained by neglect of ϕ_1, and $\delta(E_{\rm kin}/n)$ and $\delta(E_{\rm pot}/n)$ are, respectively, the contribution of ϕ_1 to the ground-state kinetic and potential energies per particle, given by[10]

$$\delta(E_{\rm kin}/n)=-\frac{1}{2\pi^2\rho}\int_{k_0}^{\infty}\frac{L_k\phi_1(k)}{(1-L_k{}^2)^2}k^4dk + \frac{1}{2\pi^2\rho}\int_{k_0}^{\infty}\frac{(1+3L_k{}^2)\phi_1{}^2(k)}{2(1-L_k{}^2)^3}k^4dk+\cdots, \tag{A.9}$$

$$\delta(E_{\rm pot}/n)=-\frac{1}{2\pi^2}\int_{k_0}^{\infty}\frac{\nu(k)\phi_1(k)}{(1-L_k)^2}k^2dk + \frac{1}{2\pi^2}\int_{k_0}^{\infty}\frac{\nu(k)\phi_1{}^2(k)}{(1-L_k)^3}k^2dk+\cdots. \tag{A.10}$$

The contributions to all these integrals from the interval (k_0,k_c) are of order $\lambda^{7/2}$ or higher (we recall that $k_0\sim a^{-1}\rho^{*\frac{1}{2}}\lambda$ and $k_c\sim a^{-1}\rho^{*\frac{1}{2}}\lambda^{\frac{1}{2}}$) so that we need only consider the contributions from (k_c,∞). For $k\gg k_c$ one can use (A.4) for $\phi_1(k)$ and can write, according to (1),

$$L_k\cong -k^{-2}\rho v(k),\quad 1-L_k{}^2\cong 1, \tag{A.11}$$

and we introduce only errors of order $\lambda^{7/2}$ if we use these approximations even for $k\sim k_c$. One finds in this way that the integrals in (A.9) and (A.10) involving $\phi_1{}^2$ are of orders λ^4 and $\lambda^{9/2}$, respectively, while those involving ϕ_1 give

$$\delta(E_{\rm kin}/n)=-\frac{1}{2\pi^2}\int_{k_c}^{\infty}\nu(k)I_1{}^{(0)}(k)dk + a^{-2}O(\rho^{*3/2}\lambda^{7/2}), \tag{A.12}$$

$$\delta(E_{\rm pot}/n)=\frac{1}{2\pi^2}\int_{k_c}^{\infty}\nu(k)I_1{}^{(0)}(k)dk + a^{-2}O(\rho^{*3/2}\lambda^{7/2}). \tag{A.13}$$

Both of these integrals are of order λ^3 and hence of the same order of magnitude as other non-negligible terms in (8), but these contributions differ only in sign: the lowest-order contribution of ϕ_1 to E_0/n cancels between the kinetic and potential energies, leaving only a negligible term of order $\lambda^{7/2}$. This result is to be expected on the basis of the variational theorem, and hence serves as a check on the calculation.

APPENDIX B

In this Appendix we shall show that the error introduced into (8) by our neglect of "nonpair" contributions is of order $\lambda^{7/2}$. The total Hamiltonian (I.2) can be written in the form

$$H=H_P+H_T+H_Q, \tag{B.1}$$

where H_P is the pair Hamiltonian (I.6) whose ground-state energy per particle is (8), and the "triad" and "quartet" Hamiltonians H_T and H_Q are defined by

$$H_T=V^{-1}\textstyle\sum_{\mathbf{k}\mathbf{k}'}\nu(k)(a_0{}^\dagger a_{\mathbf{k}'}{}^\dagger a_{\mathbf{k}}a_{\mathbf{k}'-\mathbf{k}}+a_{\mathbf{k}'-\mathbf{k}}{}^\dagger a_{\mathbf{k}}{}^\dagger a_{\mathbf{k}'}a_0), \tag{B.2}$$

$$H_Q=\tfrac{1}{2}V^{-1}\textstyle\sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''}\nu(k)a_{\mathbf{k}''-\mathbf{k}}{}^\dagger a_{\mathbf{k}'}{}^\dagger a_{\mathbf{k}'-\mathbf{k}}a_{\mathbf{k}''}, \tag{B.3}$$

where the summation in (B.2) excludes $\mathbf{k}=0$, $\mathbf{k}'=0$, and $\mathbf{k}=\mathbf{k}'$, while that in (B.3) excludes all values of $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$ which give a term already contained in H_T or H_P [see Eq. (I.5)]. We shall estimate the "nonpair" corrections to E_0/n by perturbation theory, taking (H_T+H_Q) as the perturbation and H_P as unperturbed Hamiltonian; the "unperturbed" eigenstates and energies are then the pair eigenstates (I.B.6) and their energies (I.44). The calculations are simplified, however, by noting that matrix elements and excitation energies involving low-lying pair eigenstates (I.B.6) differ from those involving the corresponding low-lying variational states (I.33) only by terms of order n^{-1}; one has

$$E_P(\eta_1\eta_2\cdots)-E_P(00\cdots)=\textstyle\sum_{\mathbf{k}}{}'\,\eta_{\mathbf{k}}E(\mathbf{k})+O(n^{-1}), \tag{B.4}$$

$$(\Pi(\eta_1'\eta_2'\cdots),A\Pi(\eta_1\eta_2\cdots)) =(\Phi(\eta_1'\eta_2'\cdots),A\Phi(\eta_1\eta_2\cdots))[1+O(n^{-1})], \tag{B.5}$$

where A is any operator involving only a finite number of annihilation and creation operators. Equation (B.4) follows from (I.44), while (B.5) is a consequence of (I.B.6) provided that the pair eigenstates Π are normalized. Finally, it will be convenient to work in the free-particle representation; we therefore write (B.5)

[10] The kinetic energy per particle is given by

$$(8\pi^3\rho)^{-1}\int\tfrac{1}{2}k^2\frac{\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3k;$$

all other terms in (4) represent potential energy.

in the form

$$(\Pi(\eta_1'\eta_2'\cdots), A\Pi(\eta_1\eta_2\cdots)) = \langle\eta_1'\eta_2'\cdots|A'|\eta_1\eta_2\cdots\rangle[1+O(n^{-1})], \quad \text{(B.6)}$$

where the free-particle states $|\eta_1\eta_2\cdots\rangle$ and the transform A' of A are given by (I.33) and (I.19), respectively.

The transforms of the annihilation and creation operators in H_T and H_Q with nonzero momentum indices are given directly by (I.19), but a_0 and $a_0\dagger$ in H_T must be treated by an indirect method. The simplest procedure, and one that is sufficiently accurate for our purposes, is to make the replacement[11]

$$a_0 \rightarrow n_0^{\frac{1}{2}}\beta_0^{\frac{1}{2}} \quad \text{(B.7)}$$

in H_T; here n_0 is a c-number determined by the requirement

$$n_0+\sum_{\mathbf{k}}{}'\langle N_{\mathbf{k}}\rangle=n, \quad \text{(B.8)}$$

where the expectation values are evaluated in the perturbed ground state.

The simplest process generated by H_T is a three-phonon "vacuum fluctuation" process. The contribution of this process to E_0/n is found from (B.2), (B.4), (B.6), (B.7), and (I.33) to be

$$-\frac{\rho_0}{\rho}(2\pi)^{-6}\int\int{}'\frac{g^2(\mathbf{kk}')}{E(\mathbf{k})+E(\mathbf{k}')+E(\mathbf{k}+\mathbf{k}')}d^3kd^3k', \quad \text{(B.9)}$$

where

$$g(\mathbf{kk}')=\{[1-\phi^2(\mathbf{k})][1-\phi^2(\mathbf{k}')][1-\phi^2(\mathbf{k}+\mathbf{k}')]\}^{-\frac{1}{2}} \times\sum_{\mathbf{qq}'}\Delta(\mathbf{qq}'|\mathbf{kk}')\phi(\mathbf{q})[\nu(q)\phi(\mathbf{q}+\mathbf{q}')-\nu(q')], \quad \text{(B.10)}$$

and $\Delta(\mathbf{qq}'|\mathbf{kk}')$ is defined to be unity if the ordered set $\{\mathbf{q}, \mathbf{q}', -\mathbf{q}-\mathbf{q}'\}$ is any permutation of the ordered set $\{\mathbf{k}, \mathbf{k}', -\mathbf{k}-\mathbf{k}'\}$, and zero otherwise. The integral $\int\int'$ in (B.9) is restricted so that each unordered set $\{\mathbf{k}, \mathbf{k}', -\mathbf{k}-\mathbf{k}'\}$ of phonon momenta appears only once. In order to estimate its order of magnitude we note that the dominant contribution to one of the $\mathbf{k}$-space integrations comes from $0\leq k\lesssim\rho^{\frac{1}{2}}\nu^{\frac{1}{2}}(0)$; hence this integration gives a factor $[\rho\nu(0)]^{\frac{3}{2}}$. The other integration receives sizable contributions from all values of k which are not $\gg a^{-1}$; hence this integration gives a factor a^{-3}. Finally, there are dimensional factors $\nu^2(0)$ from $g^2(\mathbf{kk}')$ and a^2 from the energy denominator. One therefore concludes that the contribution (B.9) to the ground-state energy per particle is of order $a^{-2}\rho^{*3/2}\lambda^{7/2}$. By similar analysis one concludes that the contributions of all other connected diagrams generated by H_T and H_Q are of higher order than $\lambda^{7/2}$; e.g., the simplest process generated by H_Q gives a contribution of order $a^{-2}\rho^{*2}\lambda^5$.

In conclusion, a few words seem to be in order concerning the validity of the replacement (B.7) and our implicit restriction to *connected* perturbation diagrams. Although the linked-cluster form of many-body perturbation theory,[12] which has been so useful in the treatment of many-fermion systems, is not valid[13] in unmodified form for the many-boson problem due to the effects of "depletion of the ground state," there does exist a modified form[14,15] of the linked-cluster theorem which is valid for many-boson systems. The method of Pines and Hugenholtz[15] involves replacement of the Hamiltonian H of the system by the statistical operator $H-\mu N$, where N is the total particle-number operator and μ the chemical potential. The replacement $a_0\rightarrow n_0^{\frac{1}{2}}$, $a_0\dagger\rightarrow n_0^{\frac{1}{2}}$ is then made in $H-\mu N$. In the resultant "reduced" Hilbert space the unperturbed ground state is the true vacuum state $|0\rangle$ rather than the state $|n\rangle$ where all n particles have zero momentum, so that the usual linked-cluster theorem becomes applicable. Since the "nonpair" part of $H-\mu N$ is the same as the "nonpair" part of H, this furnishes a justification of our neglect of "unlinked" diagrams in estimating the ground-state energy corrections due to H_T and H_Q.

[11] This is a minor refinement of Bogoliubov's replacement $a_0\rightarrow n_0^{\frac{1}{2}}$.

[12] K. A. Brueckner, Phys. Rev. **100**, 36 (1955); J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957); N. M. Hugenholtz, Physica **23**, 481 (1957); J. Hubbard, Proc. Roy. Soc. (London) **A240**, 539 (1957); C. Bloch, Nuclear Phys. **7**, 451 (1958); F. Coester, Nuclear Phys. **7**, 421 (1958).

[13] I am indebted to D. Pines and N. M. Hugenholtz for emphasizing this fact.

[14] S. T. Beliaev, J. Exptl. Theoret. Phys. **34**, 417 (1958) [translation: Soviet Phys. JETP **34**, 289 (1958)].

[15] D. Pines and N. M. Hugenholtz (to be published).