Theory of Many-Boson Systems: Pair Theory*

M. GIRARDEAU†‡ AND R. ARNOWITT
Department of Physics, Syracuse University, Syracuse, New York
(Received September 11, 1958)

The many-boson system with repulsive interactions is treated by a variational method based on a variational trial state of an exponential pair-excitation type obtained by a generalization of that of Bogoliubov; the treatment is closely related to an intermediate-coupling approximation with respect to pairs. The nonlinear integral equation which determines the variational ground state is derived, and various properties of this ground state and the associated excited states are examined. The resultant low-lying spectrum lies below that of Bogoliubov by an amount proportional to the total number of particles. The variational principle is shown to produce rigorous energy eigenvalue differences for the pair part of the Hamiltonian. The variational states, however, still exhibit unphysical features characteristic of pair-excitation states: The pair correlation function does not go to zero at zero particle separation and the phonon spectrum exhibits a gap above the ground state. It is suggested that these features can be removed by using states which take into account excitation of momentum-conserving groups of more than two particles.

I. INTRODUCTION

SINCE the appearance of Tisza's[1] and Landau's[2] semiphenomenological theories of superfluidity, there has been considerable progress in deriving the salient features of the low-lying spectrum of a many-boson system with repulsive interactions from first principles. The approximate low-lying states found by Bogoliubov,[3] Lee, Huang, and Yang,[4] and Brueckner and Sawada[5] are all of the "pair-excitation" form. Such a state is a linear combination of states of the type Φ_P,

$$\Phi_P=\sum_{j=0}^{[n/2]}\sum_{\mathbf{k}_1\cdots\mathbf{k}_j\neq 0}\psi_j(\mathbf{k}_1\cdots\mathbf{k}_j)\left(\prod_{l=1}^{j}a_{\mathbf{k}_l}^{\dagger}a_{-\mathbf{k}_l}^{\dagger}\right)a_0^{2j}\Phi^{(0)}, \quad (1)$$

where Φ_P differs from a particular low-lying unperturbed state, $\Phi^{(0)}$, only by excitation of pairs of particles from zero momentum to paired equal and opposite momenta. In Eq. (1), $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^{\dagger}$ are the annihilation and creation operators for free bosons of momentum $\mathbf{k}$, and n is the total number of particles.

In two extreme limits the pair form represents the rigorous structure for the eigenstates of a many-boson system. First, as shown by Bogoliubov,[3] in the limit of weak coupling the eigenstates involve only excitation of particles of equal and opposite momenta.[6] Second, Lee, Huang, and Yang[4] have shown that for a hard-sphere atomic interaction, the eigenvectors are also of the above type for systems of low density. Neither of these limits, of course, are applicable to the physical liquid He. It would seem, however, worthwhile to give a more general investigation of the pair-excitation wave function for the actual liquid in order to see if the low-lying states of the total Hamiltonian may be reasonably approximated by them.

The technique of calculation used in this paper is the variational method. The trial states assumed are of an exponential type obtained by a generalization of those of Bogoliubov and Lee, Huang, and Yang; these states are also closely related to those employed by Lee, Low, and Pines[7] in their treatment of the polaron problem. The simple trial states used suffice to give a low-lying energy spectrum lying below those of references 3–5 by an amount proportional to the number of particles, n.

In order to examine more closely the validity of the variational method, the Hamiltonian was investigated to see what part of it is rigorously diagonalized by this technique. It will be seen below that the total Hamiltonian can be divided into three parts: a part involving occupation number operators and operators that annihilate and create pairs (the "pair Hamiltonian") and two other parts dealing with interactions involving three and four particles of nonzero momentum, respectively. The latter two contributions have zero diagonal matrix elements between pair states. The energy spectrum given by the variational principle differs from the rigorous eigenvalues of the pair Hamiltonian by a constant upward shift independent of n and of the state under consideration.[8]

The properties of the variational states are discussed in Secs. III and IV. It will be seen that these states possess several unphysical characteristics. Methods of improving on the pair type states are briefly discussed in Sec. V.

* A preliminary account of this work was given by M. Girardeau and R. Arnowitt, Bull. Am. Phys. Soc. Ser. II, 3, 54 (1958).

† This work formed part of a dissertation submitted by M. G. in partial fulfillment of the requirements for the Ph.D. degree at Syracuse University.

‡ Now at The Institute for Advanced Study, Princeton, New Jersey.

[1] L. Tisza, Phys. Rev. **72**, 838 (1947), which see for earlier references.

[2] L. Landau, J. Phys. (U.S.S.R.) **5**, 71 (1941); **8**, 1 (1944); **11**, 91 (1947); Phys. Rev. **60**, 356 (1941).

[3] N. N. Bogoliubov, J. Phys. (U.S.S.R.) **11**, 23 (1947), hereafter designated by B.

[4] Lee, Huang, and Yang, Phys. Rev. **106**, 1135 (1957), hereafter designated by LHY.

[5] K. A. Brueckner and K. Sawada, Phys. Rev. **106**, 1117, 1128 (1957).

[6] The derivation of the eigenstates of the approximate Hamiltonian considered by Bogoliubov will be carried out in Sec. II.

[7] Lee, Low, and Pines, Phys. Rev. **90**, 297 (1953).

[8] In this respect the constant shift in energy is somewhat analogous to the disconnected closed loops of quantum field theory.

II. MATHEMATICAL FORMULATION

In a quantized field representation, the Hamiltonian of a system of spinless bosons takes the form[9]

$$H=\sum_{\mathbf{k}} \tfrac{1}{2}k^2 a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}} + \tfrac{1}{2}V^{-1}\sum_{\mathbf{k}\mathbf{k}'\mathbf{k}''} \nu(\mathbf{k})a_{\mathbf{k}''-\mathbf{k}}^{\dagger}a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}'-\mathbf{k}}a_{\mathbf{k}''}, \quad (2)$$

where $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^{\dagger}$ annihilate and create particles in states $V^{-\frac{1}{2}}e^{i\mathbf{k}\cdot\mathbf{r}}$ and $\nu(\mathbf{k})$ is the Fourier transform of the interparticle potential $v(\mathbf{r})$:

$$\nu(\mathbf{k})=\int v(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{r}. \quad (3)$$

The quantization has been assumed to take place in a box of large volume V with periodic boundary conditions (surface effects being neglected). Further, the potential function $v(\mathbf{r})$ is assumed to be an even function of the interparticle distance $\mathbf{r}$.

The approximate ground states found by B and LHY can be written in the pair form (1) with $\Phi^{(0)}$ equal to the unperturbed n-particle ground state

$$|n\rangle=(n!)^{-\frac{1}{2}}(a_0^{\dagger})^n|0\rangle. \quad (4)$$

In Eq. (4), $|0\rangle$ is the normalized vacuum (state of no particles). We define the pair Hamiltonian, H_P, as that part of the total Hamiltonian H which has nonzero expectation value in such a pair-excitation state. The only potential terms having this property are those which can be written (by commutation of annihilation and creation operators if necessary) as functions only of the occupation number operators $N_{\mathbf{k}}=a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$ and the pair annihilation and creation operators $\alpha_{\mathbf{k}}=a_{\mathbf{k}}a_{-\mathbf{k}}$ and $\alpha_{\mathbf{k}}^{\dagger}=a_{\mathbf{k}}^{\dagger}a_{-\mathbf{k}}^{\dagger}$. This implies that the momentum indices $\mathbf{k}$, $\mathbf{k}'$, and $\mathbf{k}''$ in Eq. (2) must obey one or more of the relationships

$$\mathbf{k}''=\mathbf{k}-\mathbf{k}', \quad \mathbf{k}''=\mathbf{k}', \quad \mathbf{k}=0. \quad (5)$$

One finds thus, with the aid of the Bose commutation relations, that

$$H_P=\tfrac{1}{2}(n-1)\rho\nu(0)+\sum_{\mathbf{k}}{}'\,[\tfrac{1}{2}k^2+(N_0/V)\nu(\mathbf{k})]N_{\mathbf{k}} + \tfrac{1}{2}V^{-1}\sum_{\mathbf{k}}{}'\,\nu(\mathbf{k})(\alpha_{\mathbf{k}}^{\dagger}\alpha_0+\alpha_0^{\dagger}\alpha_{\mathbf{k}}) + \tfrac{1}{2}V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,\nu(\mathbf{k})\alpha_{\mathbf{k}'}^{\dagger}\alpha_{\mathbf{k}'-\mathbf{k}} + \tfrac{1}{2}V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,\nu(\mathbf{k})N_{\mathbf{k}'-\mathbf{k}}N_{\mathbf{k}'}, \quad (6)$$

where $\rho=n/V$. The primes on the single summations imply the omission of the term $\mathbf{k}=0$ while those on the double summations imply the omission of $\mathbf{k}=0$, $\mathbf{k}'=0$, $\mathbf{k}=\mathbf{k}'$, and in the last term also $\mathbf{k}=2\mathbf{k}'$. In obtaining Eq. (6) we have replaced $\sum_{\mathbf{k}}N_{\mathbf{k}}$ by the c number n since we shall deal only with eigenstates of the total number of particles belonging to eigenvalue n. The remaining part of the Hamiltonian, $H-H_P$, consists of terms where three and four annihilation and creation operators have nonzero momentum and clearly possesses no diagonal matrix elements between pair states. Thus $H-H_P$ does not contribute in the variational principle calculation.

The approximate Hamiltonian used in B is obtained by replacing a_0 and $a_0^{\dagger}$ by the c number $n_0^{\frac{1}{2}}$ and dropping cubic and quartic terms in the annihilation and creation operators for particles of nonzero momenta; the result is

$$H_B=\tfrac{1}{2}(n-1)\rho\nu(0)+\sum_{\mathbf{k}}{}'\,[\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})]N_{\mathbf{k}} + \tfrac{1}{2}\rho_0\sum_{\mathbf{k}}{}'\,\nu(\mathbf{k})(\alpha_{\mathbf{k}}+\alpha_{\mathbf{k}}^{\dagger}), \quad (7)$$

where $\rho_0=n_0/V$. H_B can then be diagonalized by the canonical transformation

$$\xi_{\mathbf{k}}=(1-L_{\mathbf{k}}^2)^{-\frac{1}{2}}(a_{\mathbf{k}}-L_{\mathbf{k}}a_{-\mathbf{k}}^{\dagger}),$$
$$L_{\mathbf{k}}=[\rho_0\nu(\mathbf{k})]^{-1}[E_B(\mathbf{k})-\tfrac{1}{2}k^2-\rho_0\nu(\mathbf{k})], \quad (8)$$
$$E_B(\mathbf{k})=k[\rho_0\nu(\mathbf{k})+\tfrac{1}{4}k^2]^{\frac{1}{2}},$$

leading to the energy spectrum

$$E_B(\eta_1\eta_2\cdots)=E_0+\sum_{\mathbf{k}}{}'\,\eta_{\mathbf{k}}E_B(\mathbf{k}), \quad (9)$$

where

$$E_0=\tfrac{1}{2}(n-1)\rho\nu(0)-\tfrac{1}{2}\sum_{\mathbf{k}}{}'[\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})-E_B(\mathbf{k})]. \quad (10)$$

In Eq. (9), the non-negative integers $\eta_{\mathbf{k}}$ represent the number of phonons of momentum $\mathbf{k}$. $E_B(\mathbf{k})$ is the phonon spectrum and reduces to that of LHY if one inserts the value $\nu(\mathbf{k})=4\pi a$ appropriate for their hard sphere pseudopotential and replaces ρ_0 by ρ.[10]

In order to find the eigenstates of H_B we note that the canonical transformation (8) is the result of a unitary transformation

$$\xi_{\mathbf{k}}=U_B a_{\mathbf{k}}U_B^{-1}. \quad (11)$$

From this it follows that the normalized eigenstates of H_B belonging to the eigenvalue $E_B(\eta_1\eta_2\cdots)$ and the eigenvalue n_0 of N_0 are

$$\Phi_B(\eta_1\eta_2\cdots)=U_B[\prod_{\mathbf{k}}{}'(\eta_{\mathbf{k}}!)^{-\frac{1}{2}}(a_{\mathbf{k}}^{\dagger})^{\eta_{\mathbf{k}}}]|n_0\rangle, \quad (12)$$

where $|n_0\rangle$ is defined in Eq. (4). In Appendix A it is shown that U_B has the form

$$U_B=\exp[\tfrac{1}{2}\sum_{\mathbf{k}}{}'(\alpha_{\mathbf{k}}^{\dagger}-\alpha_{\mathbf{k}})\tanh^{-1}L_{\mathbf{k}}]. \quad (13)$$

In order to obtain variational trial states with which to approximate the eigenstates of H, we shall generalize the states of Eq. (12) of Bogoliubov's approximate Hamiltonian. Since H_B does not commute with the total number of particles, its eigenstates are not eigenstates of the total number of particles. This defect is easily remedied by replacing in U_B the operator $\alpha_{\mathbf{k}}^{\dagger}$ (which creates a pair of particles of nonzero momenta $\pm\mathbf{k}$) by the operator $\alpha_{\mathbf{k}}^{\dagger}\alpha_0$ (which excites a pair of particles from zero momenta to momenta $\pm\mathbf{k}$). For technical reasons, however, it is more convenient to use the combination $\alpha_{\mathbf{k}}^{\dagger}\beta_0$, where β_0 is a "unitary"[11]

[9] We use units such that $\hbar=m=1$, where m is the mass of the particle.

[10] ρ and ρ_0 are equal to zeroth order in $(\rho a^3)^{\frac{1}{2}}$; see reference 4.

[11] In order that β_0 be unitary over the whole Hilbert space it is necessary to delete from the space all states containing either zero or one particle with zero momentum. We can do this without difficulty, since for the low-lying states with which we shall be

operator defined by

$$\beta_0^{\frac{1}{2}}=a_0N_0^{-\frac{1}{2}},\quad \beta_0^{-\frac{1}{2}}=(\beta_0^{\frac{1}{2}})^\dagger=N_0^{-\frac{1}{2}}a_0^\dagger, \tag{14}$$

and having the properties

$$\begin{aligned}&\beta_0|n\rangle=|n-2\rangle\quad(n\geq 2),\quad \beta_0^\dagger|n\rangle=\beta_0^{-1}|n\rangle=|n+2\rangle,\\ &[\beta_0,N_0]=2\beta_0,\quad [\beta_0^{-1},N_0]=-2\beta_0^{-1},\\ &[\beta_0,a_{\mathbf{k}}]=[\beta_0,a_{\mathbf{k}}^\dagger]=0\quad(\mathbf{k}\neq 0).\end{aligned} \tag{15}$$

We therefore take as our variational ansatz with which to approximate the ground state the state Φ_0 defined by

$$\begin{aligned}&\Phi_0=U|n\rangle,\\ &U=\exp[\tfrac{1}{2}\textstyle\sum_{\mathbf{k}}{}'\psi(\mathbf{k})(\beta_0^{-1}\alpha_{\mathbf{k}}-\beta_0\alpha_{\mathbf{k}}^\dagger)],\end{aligned} \tag{16}$$

where $\psi(\mathbf{k})$ is a real, even function of $\mathbf{k}$ to be determined by the variational principle. We shall introduce the corresponding excited states in Sec. IV.

Since U commutes with the operators representing the total number of particles and the total linear momentum, the state Φ_0 is an eigenstate of these operators (with eigenvalues n and zero, respectively). Φ_0 is closely related to the variational states employed by Lee, Low, and Pines[7] in their treatment of the polaron problem, the only essential difference being that the phonon annihilation and creation operators in the polaron problem are replaced by $\beta_0^{-1}\alpha_{\mathbf{k}}$ and $\beta_0\alpha_{\mathbf{k}}^\dagger$ in Eq. (16). This change is, of course, necessary since total particle number and total linear momentum must be conserved in the many-boson problem. As in the analysis of Lee, Low, and Pines, our treatment is a straightforward generalization of Tomonaga's intermediate-coupling approximation.[12] In fact, it can be shown that Φ_0 represents a state where the probability amplitude for observing j pairs of particles with nonzero momenta $\pm\mathbf{k}_1\cdots\pm\mathbf{k}_j$ takes on the product form $\phi(\mathbf{k}_1)\cdots\phi(\mathbf{k}_j)$; this result is very similar to the meson case where the probability amplitude for observing j mesons of momenta $\mathbf{k}_1\cdots\mathbf{k}_j$ is also a product of the above type. Thus our states (16) imply strong pair correlation but no correlation between different pairs.

III. THE VARIATIONAL GROUND STATE

We now turn to the determination of the best variational approximation to the ground-state energy of H by states of type (16). The energy expectation value, E_0, is

$$E_0=(\Phi_0,H\Phi_0)=(\Phi_0,H_P\Phi_0)=\langle n|H_P'|n\rangle, \tag{17}$$

where

$$H_P'=U^{-1}H_PU, \tag{18}$$

the second equality in Eq. (17) following from the fact that Φ_0 is of the pair-excitation form (1). Hence, in order to evaluate E_0 and other relevant observables one must find the canonical transformation of the annihilation and creation operators effected by the unitary transformation U. By a derivation paralleling that in Appendix A, one can show that for $\mathbf{k}\neq 0$

$$a_{\mathbf{k}}'=U^{-1}a_{\mathbf{k}}U=[1-\phi^2(\mathbf{k})]^{-\frac{1}{2}}[a_{\mathbf{k}}-\phi(\mathbf{k})\beta_0a_{-\mathbf{k}}^\dagger], \tag{19}$$

where

$$\phi(\mathbf{k})=\tanh\psi(\mathbf{k}). \tag{20}$$

After a somewhat lengthy calculation one finds[13]

$$\begin{aligned}\frac{E_0}{n}=&\tfrac{1}{2}\rho\nu(0)+(8\pi^3\rho)^{-1}\int[\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})\\ &+\tfrac{1}{2}I_2(\mathbf{k})]\frac{\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3\mathbf{k}-(8\pi^3\rho)^{-1}\int[\rho_0\nu(\mathbf{k})\\ &-\tfrac{1}{2}I_1(\mathbf{k})]\frac{\phi(\mathbf{k})}{1-\phi^2(\mathbf{k})}d^3\mathbf{k},\end{aligned} \tag{21}$$

where

$$\begin{aligned}\rho_0=&\rho-(2\pi)^{-3}\int\frac{\phi^2(\mathbf{k}')}{1-\phi^2(\mathbf{k}')}d^3\mathbf{k}',\\ I_1(\mathbf{k})=&(2\pi)^{-3}\int\nu(\mathbf{k}-\mathbf{k}')\frac{\phi(\mathbf{k}')}{1-\phi^2(\mathbf{k}')}d^3\mathbf{k}',\\ I_2(\mathbf{k})=&(2\pi)^{-3}\int\nu(\mathbf{k}-\mathbf{k}')\frac{\phi^2(\mathbf{k}')}{1-\phi^2(\mathbf{k}')}d^3\mathbf{k}'.\end{aligned} \tag{22}$$

In deriving Eqs. (21) and (22) we have carried out the limiting process $n\to\infty$, $V\to\infty$, $n/V\to\rho$ (where ρ is a finite nonzero constant) and have neglected terms that give no contribution in these limits.

The function $\phi(\mathbf{k})$ is determined by minimizing E_0. Upon differentiating E_0 with respect to $\phi(\mathbf{k})$ [taking into account the implicit dependence of ρ_0, I_1, and I_2 on $\phi(\mathbf{k})$], one finds as the (necessary) condition that E_0 be a minimum

$$\begin{aligned}&[\rho_0\nu(\mathbf{k})-I_1(\mathbf{k})][1+\phi^2(\mathbf{k})]-2[\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})\\ &\qquad+I_2(\mathbf{k})+I_1(0)-I_2(0)]\phi(\mathbf{k})=0.\end{aligned} \tag{23}$$

An alternative form may be obtained by solving the quadratic equation for $\phi(\mathbf{k})$ [ignoring the implicit dependence in ρ_0, I_1, and I_2]. This gives the following nonlinear integral equation[14] for $\phi(\mathbf{k})$:

$$\begin{aligned}&[\rho_0\nu(\mathbf{k})-I_1(\mathbf{k})]\phi(\mathbf{k})=\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})+I_2(\mathbf{k})+I_1(0)\\ &\quad-I_2(0)-\{\tfrac{1}{4}k^4+k^2[\rho_0\nu(\mathbf{k})+I_2(\mathbf{k})+I_1(0)-I_2(0)]\\ &\quad+2I_2(\mathbf{k})[I_1(0)-I_2(0)]+2\rho_0\nu(\mathbf{k})[I_1(\mathbf{k})+I_2(\mathbf{k})\\ &\quad+I_1(0)-I_2(0)]+I_2^2(\mathbf{k})-I_1^2(\mathbf{k})\\ &\qquad+[I_1(0)-I_2(0)]^2\}^{\frac{1}{2}}.\end{aligned} \tag{24}$$

We now examine some general properties of the

concerned $\langle N_0\rangle$ is proportional to n, and moreover the fractional dispersion of N_0 vanishes as $n\to\infty$. The simplification results from the fact that β_0 and β_0^{-1} commute whereas α_0 and $\alpha_0^\dagger$ do not.

[12] S. Tomonaga, Progr. Theoret. Phys. Japan 2, 6 (1947).

[13] The details of this calculation can be found in the Ph.D. dissertation of M. G., Department of Physics, Syracuse University, 1958 (unpublished).

[14] In solving Eq. (23) for $\phi(\mathbf{k})$ we have chosen the sign of the square root such that $\phi(\mathbf{k})$ vanish as k approaches infinity (see below).

solution $\phi(\mathbf{k})$ of Eq. (24). For small k one finds

$$\phi(\mathbf{k}) \underset{k\to 0}{\longrightarrow} [1-\epsilon^{\frac{1}{2}}][1+\epsilon^{\frac{1}{2}}]^{-1}, \quad \epsilon = I_1(0)/\rho_0\nu(0). \tag{25}$$

Upon expanding the square root in Eq. (24) through terms of order k^{-6} one finds, under the assumption that $\nu(\mathbf{k})$ decreases like k^{-2} for large k,[15] that

$$\phi(\mathbf{k}) = k^{-2}[\rho_0\nu(\mathbf{k}) - I_1(\mathbf{k})] - 5k^{-6}[I_1(0) - I_2(0)][\rho_0\nu(\mathbf{k}) - I_1(\mathbf{k})]^{-1} + O(k^{-6}), \tag{26}$$

and hence $\phi(\mathbf{k})$ decreases like k^{-4} for large k. The Bogoliubov approximation arises when one neglects the integrals $I_1(\mathbf{k})$ and $I_2(\mathbf{k})$ compared to $\frac{1}{2}k^2$ and $\rho_0\nu(\mathbf{k})$ in the integrands of Eq. (21). For the physical liquid He, this is bound to be poor in general.[16] If $\nu(\mathbf{k})$ is spherically symmetric, there can exist spherically symmetric solutions of Eq. (24). There may, however, exist nonsymmetric solutions which could reflect the short-range crystalline order possessed by all real liquids. The only definite symmetry assumption, then, that one can make on $\phi(\mathbf{k})$ is that it is an even function (which follows from the fact that $\alpha_{-\mathbf{k}} = \alpha_{\mathbf{k}}$).

We conclude this section with a brief discussion of some of the physical properties of the ground state, Φ_0.[17] One of the parameters of interest in describing a liquid is the pair correlation function $D(\mathbf{r})$. This represents the relative probability that a particle be located at point $\mathbf{r}$ when one is known to be at the origin (normalized to unity for $\mathbf{r} \to \infty$). It is given by

$$\begin{aligned} D(\mathbf{r}) &= \rho^{-2}\|\Psi(0)\Psi(\mathbf{r})\Phi_0\|^2, \\ \Psi(\mathbf{r}) &= V^{-\frac{1}{2}}\textstyle\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}. \end{aligned} \tag{27}$$

By the methods used in evaluating the energy expectation value E_0 one finds

$$\begin{aligned} D(\mathbf{r}) &= 1 - 2(\rho_0/\rho)[f_1(\mathbf{r}) - f_2(\mathbf{r})] + f_1^2(\mathbf{r}) + f_2^2(\mathbf{r}), \\ f_1(\mathbf{r}) &= (8\pi^3\rho)^{-1}\int \frac{\phi(\mathbf{k})}{1-\phi^2(\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{k}, \\ f_2(\mathbf{r}) &= (8\pi^3\rho)^{-1}\int \frac{\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})} e^{i\mathbf{k}\cdot\mathbf{r}} d^3\mathbf{k}. \end{aligned} \tag{28}$$

The functions $f_1(\mathbf{r})$ and $f_2(\mathbf{r})$ are of the same form as the functions $-G(r)$ and $F(r)$ in the LHY pair correlation function. $D(\mathbf{r})$ has the following behavior for small and large r:

$$\begin{aligned} D(0) &= 2[1-(\rho_0/\rho)^2] + [(\rho_0/\rho) - f_1(0)]^2, \\ D(\mathbf{r}) &\underset{r\to\infty}{\longrightarrow} 1 + \left\{\frac{2\rho_0\phi'(0)}{\pi^2\rho^2[1+\phi(0)]^2}\right\} r^{-4} + O(r^{-6}), \end{aligned} \tag{29}$$

where $\phi'(0)$ is the radial derivative of $\phi(\mathbf{k})$ at the origin.[18] The asymptotic approach to unity for large r (absence of long-range configurational order[19]) is typical of a liquid. If $\phi(\mathbf{k})$ is nonspherically symmetric to the extent of having symmetrically distributed "bumps" near $\mathbf{k}=0$, then $D(\mathbf{r})$ will exhibit short-range crystalline order.

One can show[20] from Eq. (28) that

$$D(\mathbf{r}) \geq 1 - 2(\rho_0/\rho)^2. \tag{30}$$

Hence it is only possible for $D(\mathbf{r})$ to become small for small r (as it must for the true ground state if there is a strong short-range repulsion) if $\rho_0/\rho > 2^{-\frac{1}{2}}$. Furthermore, one sees from Eq. (29) that $D(0) > 0$ for $(\rho_0/\rho) < 1$. We conclude that for interparticle interactions such as the hard-sphere one, our wave function and pair correlation function become physically unrealistic for small particle separations unless $(\rho_0/\rho) \sim 1$. This tendency of $D(\mathbf{r})$ to increase as $r \to 0$ seems to be a general defect of pair-excitation states,[21] and can probably only be corrected by going beyond the pair-excitation ansatz (1) so as to take into account excitation of momentum-conserving groups of more than two particles.

The ground-state energy E_0 can be rewritten in a simpler and physically more appealing form than (21) with the aid of the momentum distribution function $n_{\mathbf{k}}$ and the pair correlation function $D(\mathbf{r})$. One finds with the aid of (3), (21), (22), and (28) that

$$\begin{aligned} E_0 &= E_{\text{kin}} + E_{\text{pot}}, \\ E_{\text{kin}}/n &= (8\pi^3\rho)^{-1}\int \tfrac{1}{2}k^2 n_{\mathbf{k}} d^3\mathbf{k}, \\ E_{\text{pot}}/n &= \tfrac{1}{2}\rho\int D(\mathbf{r}) v(\mathbf{r}) d^3\mathbf{r}, \end{aligned} \tag{31}$$

where

$$n_{\mathbf{k}} = \langle n | N_{\mathbf{k}}' | n\rangle = \phi^2(\mathbf{k})[1-\phi^2(\mathbf{k})]^{-1}. \tag{32}$$

IV. THE VARIATIONAL EXCITED STATES

We consider in this section the approximate excited states, $\Phi(\eta_1\eta_2\cdots)$, which are related to the variational ground state, Φ_0, in the same fashion as Bogoliubov's excited states are related to his ground state. We define $\Phi(\eta_1\eta_2\cdots)$ by

$$\begin{aligned} \Phi(\eta_1\eta_2\cdots) &= U|\eta_1\eta_2\cdots\rangle, \\ |\eta_1\eta_2\cdots\rangle &= \Big[\prod_{\mathbf{k}}{}'(\eta_{\mathbf{k}}!)^{-\frac{1}{2}}(a_{\mathbf{k}}^\dagger)^{\eta_{\mathbf{k}}}\Big]|n - \textstyle\sum_{\mathbf{k}'}\eta_{\mathbf{k}'}\rangle. \end{aligned} \tag{33}$$

[15] This is the case for Coulomb or screened Coulomb interactions or for a soft-sphere interaction.

[16] For example, the Bogoliubov approximation requires $\phi(0) = 1$. A rough numerical solution using a soft-sphere interaction of radius 1.9×10^{-8} cm and height 0.03°K shows that even for this weak potential $\phi(0) = 0.5$.

[17] A more extended analysis of Φ_0 can be found in reference 13.

[18] In obtaining the asymptotic behavior for large r use has been made of the results in C. J. Tranter, *Integral Transforms in Mathematical Physics* (John Wiley and Sons, Inc., New York, 1951), pp. 63 ff. We have also assumed that $\phi(\mathbf{k})$ is spherically symmetric here, though one expects the same qualitative behavior if $\phi(\mathbf{k})$ does not deviate seriously from spherical symmetry.

[19] This is intimately connected with the Bose-Einstein condensation; see O. Penrose and L. Onsager, Phys. Rev. **104**, 576 (1956).

[20] This follows from the fact that $D(\mathbf{r})$ can be rewritten in the form

$$D(\mathbf{r}) = 1 - 2(\rho_0/\rho)^2 + [(\rho_0/\rho) - f_1(\mathbf{r})]^2 + [(\rho_0/\rho) + f_2(\mathbf{r})]^2.$$

[21] It is exhibited by the LHY pair correlation function, which becomes positively infinite as $r \to 0$.

In Eq. (33), $\eta_{\mathbf{k}}$ are non-negative integers which will be shown to have the significance of the number of phonons of momentum $\mathbf{k}$. Since U commutes with the operators representing the total number of particles and the total linear momentum, $\Phi(\eta_1\eta_2\cdots)$ is an eigenstate of these operators belonging to the eigenvalues n and $\sum_{\mathbf{k}}\eta_{\mathbf{k}}\mathbf{k}$, respectively. We introduce the phonon creation operators $\xi_{\mathbf{k}}^{\dagger}$ in order to rewrite Eq. (33) in the more physical form

$$\Phi(\eta_1\eta_2\cdots)=[\prod_{\mathbf{k}}{}'(\eta_{\mathbf{k}}!)^{-\frac{1}{2}}(\xi_{\mathbf{k}}^{\dagger})^{\eta_{\mathbf{k}}}]\Phi_0. \tag{34}$$

Comparing Eqs. (33) and (34) we see that they are equivalent provided we take

$$\begin{aligned}\xi_{\mathbf{k}}^{\dagger}&=Ua_{\mathbf{k}}^{\dagger}U^{-1}\beta_0^{\frac{1}{2}}\\&=[1-\phi^2(\mathbf{k})]^{-\frac{1}{2}}[\beta_0^{\frac{1}{2}}a_{\mathbf{k}}^{\dagger}+\phi(\mathbf{k})\beta_0^{-\frac{1}{2}}a_{-\mathbf{k}}].\end{aligned} \tag{35}$$

The states of Eq. (34) then possess the following energy spectrum:

$$\begin{aligned}E(\eta_1\eta_2\cdots)&=\langle\eta_1\eta_2\cdots|H_P'|\eta_1\eta_2\cdots\rangle\\&=E_0+\sum_{\mathbf{k}}{}'\eta_{\mathbf{k}}E(\mathbf{k}),\end{aligned} \tag{36}$$

where E_0 is the ground-state energy of the state Φ_0 and

$$\begin{aligned}E(\mathbf{k})=[\tfrac{1}{2}k^2+\rho_0\nu(\mathbf{k})+I_2(\mathbf{k})+I_1(0)-I_2(0)]\frac{1+\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}\\-2[\rho_0\nu(\mathbf{k})-I_1(\mathbf{k})]\frac{\phi(\mathbf{k})}{1-\phi^2(\mathbf{k})}.\end{aligned} \tag{37}$$

In obtaining Eq. (36) we have dropped terms which vanish in the limit $n\rightarrow\infty$ for the low-lying states (i.e., states for which the number of phonons $\sum_{\mathbf{k}}{}'\eta_{\mathbf{k}}$ is finite in the limit $n\rightarrow\infty$). The energy spectrum (36) is thus that of a collection of elementary excitations, $E(\mathbf{k})$ being the energy of a phonon of momentum $\mathbf{k}$.

The Bogoliubov approximation to $E(\mathbf{k})$ is of course obtained by neglecting again the integrals I_1 and I_2. The rigorous limiting behavior for small and large k is, however,

$$\begin{aligned}E(\mathbf{k})&\underset{k\rightarrow 0}{\longrightarrow}2\epsilon^{\frac{1}{2}}\rho_0\nu(0)+O(k),\\E(\mathbf{k})&\underset{k\rightarrow\infty}{\longrightarrow}\tfrac{1}{2}k^2+I_1(0)-I_2(0)+O(k^{-2}),\end{aligned} \tag{38}$$

where ϵ is defined by Eq. (25) and we have again assumed $\nu(\mathbf{k})\rightarrow O(k^{-2})$ for large k. Thus the phonon energy correctly approaches that of a free particle for large k. However, since $E(0)>0$,[22] an energy gap exists separating the first excited state from the ground state.[23] This gap seems to be unphysical for the true liquid He system[24] and seems to be a general defect of the pair-excitation states[25] just as is the behavior of the pair correlation function for small r.

In order to justify the use of the term "phonon" for our elementary excitations we consider briefly the number density operator $\rho(\mathbf{r})$. In the Schrödinger representation $\rho(\mathbf{r})$ is given by

$$\rho(\mathbf{r})=\sum_{j=1}^{n}\delta(\mathbf{r}-\mathbf{r}_j)=\sum_{\mathbf{k}}\rho_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{39}$$

which becomes in the quantized-field representation

$$\rho_{\mathbf{k}}=V^{-1}\sum_{\mathbf{k}'}a_{\mathbf{k}'}^{\dagger}a_{\mathbf{k}'+\mathbf{k}}. \tag{40}$$

If $\Phi(1_{\mathbf{k}})$ represents a state of one traveling phonon, then the state for a standing wave, $\Theta_{\mathbf{k}}$, can be obtained by superimposing two traveling waves of equal and opposite momentum[26]:

$$\Theta_{\mathbf{k}}=2^{-\frac{1}{2}}[\Phi(1_{\mathbf{k}})+\Phi(1_{-\mathbf{k}})]. \tag{41}$$

In the state $\Theta_{\mathbf{k}}$ one has

$$(\Theta_{\mathbf{k}},\rho(\mathbf{r})\Theta_{\mathbf{k}})=\rho+V^{-1}\frac{1+\phi^2(\mathbf{k})}{1-\phi^2(\mathbf{k})}\cos(2\mathbf{k}\cdot\mathbf{r}). \tag{42}$$

It is clear that Eq. (42) represents the density fluctuations appropriate for a standing sound wave.

In order to obtain a clearer picture of the meaning of the approximate variational states it is of interest to examine what part of the total Hamiltonian has been diagonalized by the variational principle. This sub-Hamiltonian, H_0, will then be diagonal in the phonon representation. To find H_0 we must pick out the part of $H'=U^{-1}HU$ which is a function only of the occupation number operators $N_{\mathbf{k}}$, and call it H_0'. Since $H-H_P$ is completely off-diagonal in the phonon representation, H_0' is completely contained in H_P'. By inspection one finds then that

$$\begin{aligned}H_0'=E_0+\sum_{\mathbf{k}}{}'E(\mathbf{k})N_{\mathbf{k}}+(V^{-1}N_0-\rho)\sum_{\mathbf{k}}{}'\nu(\mathbf{k})\\\times\frac{1-\phi(\mathbf{k})}{1+\phi(\mathbf{k})}N_{\mathbf{k}}+V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'g_1(\mathbf{k}\mathbf{k}')N_{\mathbf{k}}N_{\mathbf{k}'},\end{aligned} \tag{43}$$

where g_1 is independent of n; the low-lying variational states Φ_0, $\Phi(\eta_1\eta_2\cdots)$ are rigorous eigenstates of H_0 belonging to the eigenvalues (36) in the limit as $n\rightarrow\infty$. Now, since $H-H_P$ has no diagonal matrix elements

[22] We assume that the interparticle interaction is repulsive "on the average" in the sense that $\nu(0)=\int v(\mathbf{r})d^3\mathbf{r}$ is positive.

[23] The physical origin of this gap can be seen by noting that although the excitation of a phonon of momentum $k_{\min}=2\pi V^{-\frac{1}{3}}$ changes the total kinetic energy by a negligible amount, it changes the pair correlation function $D(\mathbf{r})$ by an amount $n^{-1}\Delta(\mathbf{r})$ with Δ independent of n, and hence [according to (31)] changes the potential energy by an amount $\frac{1}{2}\rho\int\Delta(\mathbf{r})v(\mathbf{r})d^3\mathbf{r}$.

[24] The Debye T^3 specific heat at low temperatures implies a linear excitation spectrum $E(\mathbf{k})$ at low k.

[25] In this connection it should be commented that the expectation value of the total Hamiltonian between one-phonon Bogoliubov states becomes positively infinite as $k\rightarrow 0$. Thus, in a sense, these more approximate states exhibit this defect even more seriously.

[26] $\Theta_{\mathbf{k}}$ is an eigenstate of energy but not of momentum. One would expect such a state to be set up if the system were allowed to interchange momentum but not energy with its surroundings as in an ideal standing sound wave.

between pair states, the best possible variational state of the pair type would be a rigorous eigenstate of H_P itself. In Appendix B it is shown that under the assumption that the low-lying true eigenstates of H_P can be expanded in terms of the low-lying variational states, the eigenvalues of H_P, E_P, are related to those of H_0 in the limit $n \to \infty$ by the equation

$$E_P(\eta_1\eta_2\cdots)=E_0+\sum_{\mathbf{k}}{}'\,\eta_{\mathbf{k}}E(\mathbf{k})-\lambda, \quad \lambda\geq 0, \quad (44)$$

where λ is a constant independent of n and of $\eta_{\mathbf{k}}$. Thus the eigenspectrum of the best possible pair-type states differs from the spectrum already found only by a constant downward shift. Similarly, in Appendix B it is shown under the same assumptions that the pair correlation function, $D(\mathbf{r})$, for eigenstates of H_P is of the same form as that found above for H_0.

V. DISCUSSION

In the preceding sections we have shown that a variational treatment of the many-boson problem with pair-excitation states of a simple exponential type (closely related to an intermediate-coupling approximation with respect to pairs) suffices to give a low-lying energy spectrum lower than those of references 3–5 by an amount proportional to the total number of particles. More significant, perhaps, is the relation between the variational states and the best possible pair-type state. As discussed at the end of the last section the energy spectrum differs from the variational one by only a constant shift and the pair correlation functions differ only by terms of order n^{-1}. Thus as far as these physical properties of the system are concerned, the variational ansatz "essentially" diagonalizes the pair segment of the Hamiltonian. However, in spite of this, certain unphysical characteristics remain in the pair-excitation states: the pair correlation function increases as $r \to 0$ even in the presence of a short-range repulsion and the phonon energy levels possess a gap not really present in He^4. It would seem, therefore, that the physical liquid contains states somewhat more complicated than a simple pair type.

In spite of the above, the pair-excitation states may offer a convenient departure for constructing a better wave function to represent the true liquid. The remaining part of the Hamiltonian not diagonalized by a pair-type state includes terms involving three- and four-particle groups of the type $a_{\mathbf{k}'-\mathbf{k}}{}^{\dagger}a_{\mathbf{k}}{}^{\dagger}a_{\mathbf{k}'}$ and $a_{\mathbf{k}''-\mathbf{k}}{}^{\dagger}a_{\mathbf{k}'}{}^{\dagger}a_{\mathbf{k}'-\mathbf{k}}a_{\mathbf{k}''}$. Such structures, when acting on the unperturbed ground state of the kinetic energy operator, give zero and hence do not interact directly with the totally unperturbed states. When acting on a pair state, however, they produce excitations involving three and four particles, respectively. It appears, therefore, that the true wave function would contain terms involving operators acting on pair functions which produce "triad" and "quartet" excitations. One of us (M.G.) is now investigating this possibility.

APPENDIX A

In this appendix we shall derive Eq. (13) for Bogoliubov's unitary transformation. In order to find this transformation we make the ansatz

$$U_B=e^F, \quad F=\tfrac{1}{2}\sum_{\mathbf{k}}{}'\,\gamma_{\mathbf{k}}(\alpha_{\mathbf{k}}-\alpha_{\mathbf{k}}{}^{\dagger}), \quad (A.1)$$

where $\gamma_{\mathbf{k}}$ is a real, even function of $\mathbf{k}$. We determine $\gamma_{\mathbf{k}}$ such that Eq. (11) is equivalent to Eq. (8). We first define the auxiliary quantity $a_{\mathbf{k}}(\epsilon)$ to accomplish the unitary transformation

$$a_{\mathbf{k}}(\epsilon)=e^{\epsilon F}a_{\mathbf{k}}e^{-\epsilon F}. \quad (A.2)$$

The quantities of interest are of course $a_{\mathbf{k}}(1)\equiv\xi_{\mathbf{k}}$. The equations of motion for $a_{\mathbf{k}}(\epsilon)$ are

$$da_{\mathbf{k}}(\epsilon)/d\epsilon=[F(\epsilon),a_{\mathbf{k}}(\epsilon)], \quad (A.3)$$

where $F(\epsilon)$ is obtained from F by replacing $a_{\mathbf{k}}$ and $a_{\mathbf{k}}{}^{\dagger}$ by $a_{\mathbf{k}}(\epsilon)$ and $a_{\mathbf{k}}{}^{\dagger}(\epsilon)$ in the definition (A.1). One finds then that

$$da_{\mathbf{k}}(\epsilon)/d\epsilon=\gamma_{\mathbf{k}}a_{-\mathbf{k}}{}^{\dagger}(\epsilon). \quad (A.4)$$

The solution of Eqs. (A.4) subject to the boundary conditions $a_{\mathbf{k}}(0)=a_{\mathbf{k}}$, $a_{\mathbf{k}}{}^{\dagger}(0)=a_{\mathbf{k}}{}^{\dagger}$ yields

$$\xi_{\mathbf{k}}=a_{\mathbf{k}}(1)=a_{\mathbf{k}}\cosh\gamma_{\mathbf{k}}+a_{-\mathbf{k}}{}^{\dagger}\sinh\gamma_{\mathbf{k}}. \quad (A.5)$$

Comparing Eq. (A.5) with Eq. (8), we see that

$$\gamma_{\mathbf{k}}=-\tanh^{-1}L_{\mathbf{k}}. \quad (A.6)$$

APPENDIX B

In this appendix we determine the forms of the low-lying eigenstates and eigenvalues of the pair Hamiltonian H_P. We begin by exhibiting the transformed pair Hamiltonian $H_P'=U^{-1}H_PU$. With the aid of (19) and (23) one finds[13]

$$\begin{aligned}H_P'=H_0'&+\tfrac{1}{2}V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,f(\mathbf{k}\mathbf{k}')(\beta_0{}^{-2}\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}+\beta_0{}^{2}\alpha_{\mathbf{k}}{}^{\dagger}\alpha_{\mathbf{k}'}{}^{\dagger})\\&+(\rho-V^{-1}N_0)\sum_{\mathbf{k}}{}'\,g_2(\mathbf{k})(\beta_0{}^{-1}\alpha_{\mathbf{k}}+\beta_0\alpha_{\mathbf{k}}{}^{\dagger})\\&+V^{-1}\sum_{\mathbf{k}}{}'\,g_3(\mathbf{k})(\beta_0{}^{-1}\alpha_{\mathbf{k}}+\beta_0\alpha_{\mathbf{k}}{}^{\dagger})\\&+V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,g_4(\mathbf{k}\mathbf{k}')(\beta_0{}^{-1}\alpha_{\mathbf{k}}N_{\mathbf{k}'}+\beta_0N_{\mathbf{k}'}\alpha_{\mathbf{k}}{}^{\dagger})\\&+V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,g_5(\mathbf{k}\mathbf{k}')\alpha_{\mathbf{k}}{}^{\dagger}\alpha_{\mathbf{k}'}, \quad (B.1)\end{aligned}$$

where the g_j are independent of n, and

$$\begin{aligned}f(\mathbf{k}\mathbf{k}')=\frac{\phi(\mathbf{k}')}{1-\phi^2(\mathbf{k}')}\Big[&\nu(\mathbf{k})\frac{1-\phi(\mathbf{k})}{1+\phi(\mathbf{k})}\\&+(1-\delta_{\mathbf{k}\mathbf{k}'})\nu(\mathbf{k}-\mathbf{k}')\frac{1+\phi(\mathbf{k}')}{1-\phi(\mathbf{k})}\Big]. \quad (B.2)\end{aligned}$$

It is readily shown that the part of H_P involving the g_j is of order $n^{-\frac{1}{2}}$ on the manifold of low-lying[27] variational states $\Phi(\eta_1\eta_2\cdots)$, since one has by (B.1)

$$\begin{aligned}\|[H_P'-H_0'-\tfrac{1}{2}V^{-1}\sum_{\mathbf{k}\mathbf{k}'}{}'\,f(\mathbf{k}\mathbf{k}')(\beta_0{}^{-2}\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}&\\+\beta_0{}^{2}\alpha_{\mathbf{k}}{}^{\dagger}\alpha_{\mathbf{k}'}{}^{\dagger})]|\eta_1\eta_2\cdots)\|^2=O(n^{-1}).& \quad (B.3)\end{aligned}$$

[27] We require by definition of "low-lying" that the state $\Phi(\eta_1\eta_2\cdots)$ contain only a finite number $\sum_{\mathbf{k}}{}'\,\eta_k$ of phonons in the limit $n \to \infty$.

It follows that we shall make no error (in the limit $n\rightarrow\infty$) in determining the low-lying eigenstates and eigenvalues of H_P if we omit the terms involving g_j in (B.1) and take

$$H_P'=H_0'+\tfrac{1}{2}V^{-1}\sum_{\mathbf{kk}'}{}^{+}f(\mathbf{kk}')(\beta_0^{-2}\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}+\beta_0^{2}\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}'}^{\dagger})$$
$$=H_0'+2V^{-1}\sum_{\mathbf{kk}'}{}^{+}\tilde{f}(\mathbf{kk}')(\beta_0^{-2}\alpha_{\mathbf{k}}\alpha_{\mathbf{k}'}+\beta_0^{2}\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}'}^{\dagger}),\quad\text{(B.4)}$$

provided only that the rate of convergence of the expansion of the low-lying eigenstates of H_P in terms of the variational states is independent of n, so that only the low-lying $\Phi(\eta_1\eta_2\cdots)$ contribute to the expansion. In the second form of (B.4) we have replaced f by its symmetrized form

$$\tilde{f}(\mathbf{kk}')=\tfrac{1}{8}[f(\mathbf{kk}')+f(\mathbf{k}'\mathbf{k})+f(-\mathbf{k},\mathbf{k}')+f(\mathbf{k}',-\mathbf{k})$$
$$+f(\mathbf{k},-\mathbf{k}')+f(-\mathbf{k}',\mathbf{k})$$
$$+f(-\mathbf{k},-\mathbf{k}')+f(-\mathbf{k}',-\mathbf{k})]$$
$$=\tfrac{1}{4}[f(\mathbf{kk}')+f(\mathbf{k}'\mathbf{k})+f(-\mathbf{k},\mathbf{k}')+f(\mathbf{k}',-\mathbf{k})],\quad\text{(B.5)}$$

and have replaced summation over the whole $\mathbf{k}$ space by summation over half of it, since $\alpha_{\mathbf{k}}=\alpha_{-\mathbf{k}}$; in the following, the superscript "plus" on sums or integrals always implies restriction of summations or integrations to half of $\mathbf{k}$ space.

The simple form of the perturbation Hamiltonian H_P-H_0 implied by (B.4) leads to a perturbation expansion in which only the disconnected loop diagrams contribute in the limit $n\rightarrow\infty$. As a result, the low-lying spectrum of H_P differs from that of H_0 only by a constant downward shift λ,[28] as implied by Eq. (44), while the corresponding eigenstates $\Pi(\eta_1\eta_2\cdots)$ of H_P have the form

$$\Pi(\eta_1\eta_2\cdots)=U\Pi'(\eta_1\eta_2\cdots),$$

$$\Pi'(\eta_1\eta_2\cdots)=\sum_{j=0}^{\infty}[(2j)!]^{-1}V^{-j}$$
$$\times\sum_{\mathbf{q}_1\cdots\mathbf{q}_{2j}}{}^{+}\psi_j(\mathbf{q}_1\cdots\mathbf{q}_{2j})\beta_0^{2j}\alpha_{\mathbf{q}_1}^{\dagger}\cdots$$
$$\times\alpha_{\mathbf{q}_{2j}}^{\dagger}|\eta_1\eta_2\cdots\rangle.\quad\text{(B.6)}$$

It follows from Eqs. (33), (35), and (B.6) that

$$\Pi(\eta_1\eta_2\cdots)=[\prod_{\mathbf{k}}{}'(\eta_{\mathbf{k}}!)^{-\frac{1}{2}}(\xi_{\mathbf{k}}^{\dagger})^{\eta_{\mathbf{k}}}]\Pi_0,\quad\text{(B.7)}$$

where $\Pi_0=\Pi(00\cdots)$ is the ground state of H_P. Therefore the elementary excitations are the same as those of the variational states, since the corresponding creation operators $\xi_{\mathbf{k}}^{\dagger}$ in (B.7) are the same as those in (34). Nevertheless, the eigenstates of H_P have a more complicated structure than the variational states, since they contain components with zero-point phonons not present in the variational states; these zero-point phonons are described by the probability amplitudes ψ_j in (B.6). Since one can show that the pair correlation functions of the low-lying excited variational states differ from that $D(\mathbf{r})$ of the ground variational state Φ_0 only by terms of order n^{-1}, it follows that Eq. (28) gives the pair correlation function of the true low-lying eigenstates $\Pi(\eta_1\eta_2\cdots)$ of H_P.

One could obtain formal expressions for the energy shift λ and the probability amplitudes ψ_j by writing down the general terms of the perturbation expansions for the eigenvalues and eigenstates of H_P, but it is simpler to define them implicitly in terms of the coupled set of linear integral equations which follow from the eigenvalue equation $H_P'\Pi'=W\Pi'$. This procedure has the added advantage that it furnishes an independent proof of the constant shift. To derive the integral equations, we substitute (B.4) and (B.6) into the eigenvalue equation and evaluate the inner products with the states $|\eta_1'\eta_2'\cdots\rangle$. Upon converting $\mathbf{k}$-space summations into integrations one finds, apart from terms whose contribution vanishes in the limit $n\rightarrow\infty$ for low-lying states, the set of equations

$$\tfrac{1}{2}\lambda\psi_0+(2\pi)^{-6}\int\int{}^{+}d^3\mathbf{k}d^3\mathbf{k}'\,\tilde{f}(\mathbf{kk}')\psi_1(\mathbf{kk}')=0,$$

$$2\sum_{u<v}^{2j}\tilde{f}(\mathbf{q}_u\mathbf{q}_v)\psi_{j-1}(\mathbf{q}_1\cdots\mathbf{q}_{u-1}\mathbf{q}_{u+1}\cdots\mathbf{q}_{v-1}\mathbf{q}_{v+1}\cdots\mathbf{q}_{2j})$$
$$+[E(\mathbf{q}_1)+\cdots+E(\mathbf{q}_{2j})+\tfrac{1}{2}\lambda]\psi_j(\mathbf{q}_1\cdots\mathbf{q}_{2j})$$
$$+(2\pi)^{-6}\int\int{}^{+}d^3\mathbf{k}d^3\mathbf{k}'\,\tilde{f}(\mathbf{kk}')\psi_{j+1}(\mathbf{kk}'\mathbf{q}_1\cdots\mathbf{q}_{2j})$$
$$=0,\quad(j\geq 1)\quad\text{(B.8)}$$

where

$$\lambda\equiv E(\eta_1\eta_2\cdots)-W(\eta_1\eta_2\cdots),\quad\text{(B.9)}$$

with $E(\eta_1\eta_2\cdots)$ given by Eq. (36). In deriving (B.8) we have assumed, without loss of generality, that the ψ_j are symmetric functions of their arguments. Since λ plays the role of an eigenvalue parameter to be determined so that the solution of (B.8) yields a normalizable state vector $\Pi(\eta_1\eta_2\cdots)$, and the η_k appear nowhere else in (B.8), it is clear that λ is in fact independent of the η_k; this proves Eq. (44). One could construct perturbation expansions for λ and the ψ_j by applying iteration procedures to the solution of (B.8).

[28] The situation here is similar to that in the fixed-source boson theory with Hamiltonian

$$H=\Sigma_{\mathbf{k}}E(\mathbf{k})a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+V^{-\frac{1}{2}}\Sigma_{\mathbf{k}}(S_{\mathbf{k}}a_{\mathbf{k}}+S_{\mathbf{k}}^{*}a_{\mathbf{k}}^{\dagger}),$$

where the source term causes only a constant downward shift of the spectrum of H relative to that of $H_0=\Sigma_{\mathbf{k}}E(\mathbf{k})a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}$.