1965

Theory of many-boson systems

Richard David Etters
Iowa State University

This dissertation has been 65-12,472
microfilmed exactly as received

ETTERS, Richard David, 1933-
THEORY OF MANY-BOSON SYSTEMS.

Iowa State University of Science and Technology,
Ph.D., 1965
Physics, general

University Microfilms, Inc., Ann Arbor, Michigan

THEORY OF MANY-BOSON SYSTEMS

by

Richard David Etters

A Dissertation Submitted to the
Graduate Faculty in Partial Fulfillment of
The Requirements for the Degree of
DOCTOR OF PHILOSOPHY

Major Subject: Theoretical Physics

Approved:

Signature was redacted for privacy.

In Charge of Major Work

Signature was redacted for privacy.

Head of Major Department

Signature was redacted for privacy.

Dean of Graduate College

Iowa State University
Of Science and Technology
Ames, Iowa

1965

TABLE OF CONTENTS

I. INTRODUCTION

The theory of interacting many-boson systems is of fundamental interest, not only from a quantum statistical point of view but also because no single theory has been advanced that is capable of describing the curious properties of He II. These properties are thought to be principally determined by the statistical nature of the substance. For instance, the low temperature behavior of He^3 is drastically different from that of He^4, even though the only significant difference between the two isotopes, other than their mass difference, is that He^3 obeys Fermi-Dirac statistics whereas He^4 obeys Bose-Einstein statistics. It seems evident that at low temperatures, where the quantum features of the system are not masked out by thermal effects, statistics are of vital importance to a complete understanding of the problem.

For a weakly-interacting system, it is often possible to develop a basis of understanding in terms of a collection of free particles where the interaction is considered to have a small effect. However, for weakly-coupled bosons, the low-lying momentum states are highly populated and, in the limit of vanishing interaction, all particles condense to the zero-momentum state. Therefore, the kinetic energy may become small compared to the potential energy in which case the characteristics of the system depart sharply from those of a free particle model. In fact, even in the extreme weak-coupling limit, important differences occur which make it very difficult to understand the problem in terms of a non-interacting gas. Such difficulties do not generally occur for a many-fermion system since the kinetic energy is not zero, even in the limit of vanishing interactions because of the exclusion principle. Therefore, in the weak-coupling limit, the interaction may be completely dominated by the kinetic energy, in which case the properties of the system are very similar to those of a free fermion gas.

Because He II is the only known boson fluid at absolute zero, it is natural to compare its properties with those of any proposed theory. It has been found that the properties of He II are remarkably different from what would be expected on the basis of a free boson gas model. For instance, Henshaw and Woods (1) have found that the excitation spectrum is a linear function of momentum at low momenta as compared to a quadratic low momentum dependence for a free gas. Therefore, as a result, the temperature dependence of the specific heat is also quite different at low temperatures. Even less understandable are the superfluid properties of He II which cannot be predicted on the basis of a free particle model. Many attempts have been made to explain these peculiar properties from a firm theoretical basis, but without success.

The present work consists of two parts. First, an attempt is made to unify in an understandable way, several different theories that have been partially successful in describing the properties of many-boson systems and, secondly, to develop a more general theory, capable of handling problems that are outside the range of validity for the weak-coupling approximations of Bogoliubov (2), and others.

In this paper, four separate but related theories are presented, each of which views the many-boson problem in a somewhat different way. An underlying assumption in each derivation is that the momentum distribution of particles is sufficiently localized to permit the use of certain simplifying approximations. In Part 1 of Chapter III, the equation of motion for an operator related to the density fluctuation is evaluated in an approximate way, from which certain generalizations of previous theories are accomplished. In Part 2 of Chapter III, the equation of motion for a plane-wave operator is linearized and the associated quasi-particle excitation operator is then constructed, from which the properties of the system are deduced. In this development, the operator products $a_k^+ a_{-k}^+$ as well as number operators are replaced by their ground state expectation values in the interaction part of the equation of motion. In Part 3 of the same chapter, an excitation operator is generated for which the approximated equation of motion yields substantially the same results as derived in Part 2 but which does not require that the particle non-conserving products, such as $a_k^+ a_{-k}^+$, be replaced by their average values. The theory, therefore, conserves particle number, but this advantage is gained at the expense of the formal simplicity which is present in the procedure of Part 2. In Section B of Chapter III, a straightforward extension of Bogoliubov's (2) method is developed and again, the results agree with those of Part 2 and Part 3.

II. REVIEW OF EXISTING THEORIES

Among the important contributions to many-boson theory are those of Bogoliubov (2), Brueckner and Sawada (3), and Lee, Huang, and Yang (4), who have based their calculations on the assumption that a great majority of the particles are in the single-particle zero-momentum state. Because the interaction tends to deplete this state by exciting particles to states of higher momenta, these theories can be considered valid only in the extreme weak-coupling limit. Nevertheless, such derivations yield important information about the general properties of many-boson systems and, for He II, the qualitative agreement with experiment is quite good considering that, for this case, the weak-coupling theories are not even self-consistent.

Consider a collection of bosons undergoing two-body interactions which are describable by a static scalar potential. The Hamiltonian for the system is

$$H = \sum_k T_k a_k^+ a_k + \tfrac{1}{2} \sum_{p,q,k} V(k) a_{p-k}^+ a_{q+k}^+ a_q a_p \tag{1}$$

where a_k^+ and a_k are plane-wave creation and annihilation operators, $V(k)$ is the Fourier transform of the two-body interaction potential, and T_k is the kinetic energy.

$$T_k = \frac{k^2}{2m}. \tag{2}$$

The system occupies unit volume and $\hbar$ has been set equal to unity for convenience. The operators a_o and a_o^+, acting on the wave function for a system with a precise number of particles in each single-particle momentum state, give

$$a_o|N_o,--->\ =\ N_o^{\frac{1}{2}}|N_o-1,---> \tag{3}$$

$$a_o^+|N_o,--->\ =\ (N_o+1)^{\frac{1}{2}}|N_o+1,---> \tag{4}$$

where N_o is the number of particles in the zero-momentum state and, in Eqs. 3 and 4, all other occupation numbers are undisturbed.

In the Bogoliubov (2) approximation it is recognized that if $N_o>>1$ and if the fluctuation of particle number in the correct zero-momentum state of the interacting system is small compared to its average occupation value, then two things may be done;

(a) Replace $(N_o+1)^{\frac{1}{2}}$ by $N_o^{\frac{1}{2}}$

(b) Assume that the physical properties of the system are not significantly altered by adding or removing a particle from the zero-momentum state.

Under these circumstances, a_o and a_o^+ will commute with each other and, since they already commute with a_k^+, a_k for $k \neq 0$, they may simply be replaced by their c-number expectation values in the correct ground state. The Bogoliubov (2) approximation proceeds by considering only those terms in the interaction part of Eq. 1 that contain at least two operators of zero-momentum.

For N_o approximately equal to the total number of particles N, the resulting Hamiltonian is

$$H\ =\ \frac{N(N-1)V(0)}{2} + \sum_k T_k a_k^+ a_k + \frac{1}{2}\sum_{k\neq 0} NV(k)[a_k^+ a_{-k}^+ + a_k a_{-k} + 2a_k^+ a_k]. \tag{5}$$

This equation can be diagonalized by the following transformation:

$$b_k^+\ =\ u(k)a_k^+ + v(k)a_{-k} \tag{6}$$

$$b_k = u(k)a_k + v(k)a^+_{-k} \tag{7}$$

where u(k) and v(k) are real, c-number coefficients that depend only on the absolute magnitude of their arguments. If these coefficients obey the added condition

$$u^2(k) - v^2(k) = 1 \tag{8}$$

then the operators b^+_k and b_k satisfy the usual boson commutation laws. The diagonalized form of Eq. 5 is

$$H = E_o + \sum_k \omega(k) b^+_k b_k \tag{9}$$

where

$$u^2(k) = \frac{1}{2\omega(k)} [\omega(k) + T_k + NV(k)] \tag{10}$$

$$v^2(k) = \frac{1}{2\omega(k)} [T_k + NV(k) - \omega(k)] \tag{11}$$

$$E_o = \frac{N(N-1)V(0)}{2} + \frac{1}{2} \sum_{k \neq 0} [\omega(k) - T_k - NV(k)] \tag{12}$$

$$\omega(k) = [T_k{}^2 + 2T_k NV(k)]^{\frac{1}{2}}. \tag{13}$$

In Eq. 9, E_o may be interpreted as the ground state energy and $\omega(k)$ is the excitation energy for quasi-particles generated from the ground state by the excitation operator b^+_k.

The inverse of the transformation identified by Eqs. 6 and 7 is

$$\begin{pmatrix} a^+_k \\ a_{-k} \end{pmatrix} = \begin{pmatrix} u(k) & -v(k) \\ -v(k) & u(k) \end{pmatrix} \begin{pmatrix} b^+_k \\ b_{-k} \end{pmatrix}. \tag{14}$$

The expectation value of the number operator is found by using Eq. 14 along with the condition that the ground state $|0\rangle$ be a vacuum state for the generation of quasi-particles, that is

$$b_k|0\rangle = 0. \tag{15}$$

The result for the number operator is

$$N_k = \langle 0|a_k^+ a_k|0\rangle = v^2(k).$$

From Eqs. 10, 11, 14, and 15 it can be shown that the products $\langle 0|a_k^+ a_{-k}^+|0\rangle$ and $\langle 0|a_k a_{-k}|0\rangle$ have large expectation values at low momenta as do the number operators. Girardeau and Arnowitt (5) and Wentzel (6) have tried to improve the Bogoliubov (2) approximation by retaining in the Hamiltonian not only terms linear in these products but also the quadratic terms. The resulting truncated Hamiltonian is then solved in an approximate way, with limited success. A related calculation that uses the variation principle to evaluate the products N_k and $\langle 0|a_k^+ a_{-k}^+|0\rangle$, and which emphasizes the connection with techniques used in the theory of superconductivity, has been performed by Valatin and Butler (7).

For liquid He II, Feynman (8) has calculated, in a very general way, the wave functions for the low-lying excited states. It is argued that the excited states should be of the form $\sum_{x_i} f(x_i)|0\rangle$, which depends on the position of every particle and where $|0\rangle$ is the ground state wave function. By a variational calculation it is found that $\sum_{x_i} f(x_i) = \sum_{x_i} e^{ik\cdot x_i}$, which is the configuration space representation of the density. In second quantized notation the density operator is given by ρ_k,

$$\rho_k = \sum_p a_{p+k}^+ a_p. \tag{17}$$

Therefore, the Feynman excited state may be represented as

$$|k\rangle_F = \rho_k|0\rangle. \tag{18}$$

The excitation energy is then calculated from these state functions in terms of the liquid structure factor $S(k)$. The result is

$$\omega(k) = \frac{k^2}{2mS(k)}. \tag{19}$$

Using experimentally known values for $S(k)$, the excitation energy, as calculated from Eq. 19, is in good agreement with experiment at low momenta but, for momenta beyond the linear (phonon) part of the spectrum, the agreement is only qualitative at best.

To improve the calculation, Feynman and Cohen (9) proposed a more general wave function, generated from the ground state by the excitation operator $\sum_{x_i} h(x_i)e^{ik\cdot x_i}$, i.e.

$$\sum_{x_i} h(x_i)e^{ik\cdot x_i}|0\rangle = |k\rangle_{FC} \tag{20}$$

where $h(x_i)$ is a function whose purpose is to localize the excitation by forming a wave-packet. The theoretical arguments for the inclusion of $h(x_i)$ are based on the particle backflow produced when a "quasi-particle" excitation moves through the medium. By a variational calculation Feynman and Cohen (9) obtain the excitation spectrum for He II in fairly good agreement with experiment at all momenta. However, a simple closed form relation between $\omega(k)$ and $S(k)$ no longer exists, and the associated theoretical interpretations become less apparent.

III. THEORETICAL DEVELOPMENT

For a many particle system of bosons or fermions the possibility exists that the Hamiltonian may be expressed in terms of creation and annihilation operators for nearly independent quasi-particles whose action manifests the behavior of the system. If a transformation can be made to a system of weakly-interacting quasi-particles whose interaction is amenable to perturbation theory, then the problem is soluble in terms of standard techniques. The major difficulty is to uncover these composite or quasi-particle representations. It is here that the physics of the situation is vital. In this chapter, approximate procedures for determining these representations in a many-boson system are developed.

A. Equation of Motion Method

Suppose that there exists an operator b_p^+ for which

$$[H,b_p^+]|0\rangle = \omega(p)b_p^+|0\rangle \tag{21}$$

where H is the Hamiltonian for the system and $|0\rangle$ is the ground state wave function. It is very easy to show that $|p\rangle = b_p^+|0\rangle$ is an excited eigenstate of the system with an excitation energy $\omega(p)$. The momentum of the state is a constant of motion characterized by the subscript p. For an independent particle system, Eq. 21 is satisfied by the plane-wave creation operator a_p^+, and a_p^+ is a good approximation to b_p^+ for a sufficiently weakly-coupled system. In general, however, such an approximation is not adequate because of the interparticle interaction. For instance, the commutator of a_p^+ with the Hamiltonian is

$$[H,a_p^+] = T_p a_p^+ + \sum_{q,k} V(k) a_{p-k}^+ a_{q+k}^+ a_q . \qquad (22)$$

Clearly, it is the interaction part of Eq. 22 that does not conform to Eq. 21.

One procedure for studying the system is to linearize Eq. 22 by some approximate method which is valid in the domain of interest, thereby reducing it to the form of Eq. 21. The random phase approximation (RPA) is such a procedure that is valid if the interaction between the quasi-particle excitations is weak.

The equation of motion for a_p^+ can be written as[+]

$$[H,a_p^+] = [T_p + \sum_k V(k) N_{p-k}] a_p^+ + \sum_{k,q}{}' V(k) a_{p-k}^+ a_{q+k}^+ a_q$$

$$+ \sum_k V(k) [a_{p-k}^+ a_{p-k} - N_{p-k}] a_p^+ \qquad (23)$$

where N_{p-k} is now the expectation value of $a_{p-k}^+ a_{p-k}$ in the true ground state and the prime over the sum indicates that the term $\underset{\sim}{q} = \underset{\sim}{p}-\underset{\sim}{k}$ is to be omitted. The ordinary RPA (10) consists of neglecting the last two terms in Eq. 23, in which case[++]

$$[H,a_p^+]|0\rangle = [T_p + \sum_k V(p-k) N_k] a_p^+ |0\rangle . \qquad (24)$$

Thus, in the RPA, a_p^+ satisfies Eq. 21. If in addition, one replaces N_k by

---

[+]The interaction term with $\underset{\sim}{k} = 0$ in Eq. 1 only contributes a constant energy $\frac{N(N-1)V(0)}{2}$ to the N particle system and can be removed by shifting the zero of energy.

[++]An asterisk immediately preceeding an equation number will hereafter indicate that that relation is necessarily satisfied only when acting on the ground state of the system, $|0\rangle$.

its value in a non-interacting system, the result for $\omega(p)$ is

$$\omega(p) = T_p + NV(p). \tag{25}$$

At large momenta, Bogoliubov's (2) equation for $\omega(p)$ is identical with Eq. 25. The implication is that the approximate linearization of the equation of motion for a_p^+, by the ordinary RPA, is sufficient to reproduce the known weak-coupling results at large momenta but not at small momenta. This is reasonable for such a simplified treatment of the interaction because, at high momenta, it is expected that the interaction term will be of diminished importance compared to the kinetic energy. At low momenta, however, the interaction may well dominate, rendering this approximate calculation invalid. It is apparent that a more sophisticated treatment of the equation of motion is necessary if satisfactory results are to be obtained.

The most general linearization of Eq. 22, consistent with the conservation of momentum, involves the replacement of products $a_k^+a_{-k}^+$ as well as number operators by their average values in the interaction part of the equation of motion. The ground state expectation value of these opposite momentum pairs $\langle a_k^+a_{-k}^+\rangle$ is understood to mean $\langle 0;N|a_k^+a_{-k}^+|0;N-2\rangle$ where $|0;N\rangle$ is the real ground state function for an N particle system and $|0;N-2\rangle$ is the corresponding state for an N-2 particle system.

After making these replacements in the equation of motion for a_p^+, the result is

$$[H,a_p^+] = [T_p + K(p)]a_p^+ + \sum_k V(k)\langle a_{k-p}^+ a_{p-k}^+\rangle a_{-p}$$
$$+ \sum_{q,k}'' V(k)a_{p-k}^+ a_{q+k}^+ a_q + \sum_k V(k)[a_{p-k}^+ a_{p-k} - N_{p-k}]a_p^+$$

$$+ \sum_{k} V(k)[a^{+}_{k-p}a^{+}_{p-k} - \langle a^{+}_{k-p}a^{+}_{p-k}\rangle]a_{-p} \tag{26}$$

where the double prime over the sum indicates that the terms $\underset{\sim}{q} = \underset{\sim}{p}-\underset{\sim}{k}$ and $\underset{\sim}{q} = -\underset{\sim}{p}$ are to be omitted. The quantity $K(p)$ is the Hartree-Fock exchange energy.

$$K(p) = \sum_{k} V(p-k)N_{k}. \tag{27}$$

The last two terms in Eq. 26 are the fluctuation terms for operators that have been replaced by their expectation values. By neglecting the remaining non-linear terms, and provided that the fluctuation terms are negligible, the commutator $[H,a^{+}_{p}]$ acting on the ground state $|0\rangle$ is,

$$[H,a^{+}_{p}] \cong [T_{p} + K(p)]a^{+}_{p} + \sum_{k} V(k)\langle a^{+}_{p-k}a^{+}_{k-p}\rangle a_{-p}. \qquad *(28)$$

In this case, Eq. 21 is satisfied if the quasi-particle excitation operator is of the form

$$b^{+}_{p} = \alpha(p)a^{+}_{p} + \beta(p)a_{-p} \tag{29}$$

where $\alpha(p)$ and $\beta(p)$ are c-number coefficients.

It is evident that the equation of motion for a^{+}_{p}, as given by Eq. 28, exists only if the Hamiltonian itself is a particle non-conserving operator, as will be displayed in Part 2 of the present chapter. In order to consider the system represented by such a Hamiltonian, the wave function $|0\rangle$ can be interpreted as containing a mixture of states with a slight spread in particle number, which is small compared to N. In this way it is possible to consider the existence of a non-zero amplitude for the expectation value of the opposite momentum pairs $\langle a^{+}_{k}a^{+}_{-k}\rangle$ in Eqs. 26 and 28. Furthermore, for a large system, the number operator may still be an approximately good quantum number since it approximately commutes with the

Hamiltonian. Such interpretations are common in the theory of superconductivity. It is also possible to argue that, for a large boson system, the addition or removal of a few particles, particularly from heavily populated momentum states, will not significantly alter the important physical properties. This argument is completely analogous to the Bogoliubov (2) treatment of the zero-momentum state. A complete, detailed, derivation of the properties associated with such a system will be given in Part 2 of this chapter.

Another method that goes beyond the ordinary RPA for the commutator $[H,a_p^+]$, by considering not only the linearized terms in Eq. 23 but also the triple term and the fluctuation $\sum_k V(k)[a_{p-k}^+ a_{p-k} - N_{p-k}]a_p^+$, has been developed by Suhl and Werthamer (10,11). The advantage of this method is that it provides a systematic way to generate the approximate excitation operators for the system. The triple term in Eq. 23 can be included in the calculation by constructing a new excitation operator

$$b_p^+ = a_p^+ + \sum_{q,k}{}' g(q,k) a_{p-k}^+ a_{q+k}^+ a_q \tag{30}$$

where $g(q,k)$ is a c-number coefficient to be determined. The fluctuation term may also be included in an equivalent way but, as Suhl and Werthamer (10) have shown for the electron gas problem, and as we shall show in Appendix A, under certain circumstances the fluctuation term is negligibly small and, in anticipation of this result, it will hereafter be neglected. The commutator of b_p^+ with the Hamiltonian is

$$[H,b_p^+] = [H,a_p^+] + \sum_{q,k}{}' g(q,k)[H,a_{p-k}^+ a_{q+k}^+ a_q]. \tag{31}$$

The commutator $[H,a_{p-k}^+ a_{q+k}^+ a_q]$, when expanded, contains triple and quintuple products of creation and annihilation operators. These products can be contracted in a manner similar to that used in obtaining Eq. 24. All number operators, $a_k^+ a_k$, are replaced in the commutator by their expectation value in the true ground state. The quintuple terms that do not contract to singles or triples by this replacement are neglected in the second RPA. Such a procedure amounts to applying the RPA to the equation of motion for b_p^+ as defined by Eq. 30.

The uncontractable quintuple terms neglected in the second RPA can be included by constructing an operator of the form

$$b_p^+ \;=\; a_p^+ + \sum_{q,k}{}' g(q,k) a_{p-k}^+ a_{q+k}^+ a_q + \Sigma\, h a^+ a^+ a^+ aa \tag{32}$$

$[H,b_p^+]$ would then contain a commutator $[H,a^+a^+a^+aa]$ which yields, upon evaluation, quintuple and septuple terms. These can be contracted to triples and quintuples by the previously mentioned technique. The septuple terms that do not reduce to triples or quintuples are neglected in the next order of approximation. It is clear that one can continue the above procedure by generating quasi-particle creation operators of higher order than the one given by Eq. 32. In fact, Eq. 32 represents only the terms through third order in an infinite sequence of approximations designed to generate a better approximated quasi-particle excitation operator.

Werthamer and Suhl (11) point out that the solution of Eq. 21 for b_p^+ given by Eq. 32 is completely equivalent to solving the set of equations

$$[H,a_p^+]|0\rangle \;=\; \omega(p) a_p^+|0\rangle \tag*{*(33)}$$

$$[H,a_{p-k}^+ a_{q+k}^+ a_q]|0\rangle \;=\; \omega(p) a_{p-k}^+ a_{q+k}^+ a_q|0\rangle \tag*{*(34)}$$

$$[H,a^+a^+a^+aa]|0\rangle \;=\; \omega(p)a^+a^+a^+aa|0\rangle \qquad *(35)$$

Eq. 33 yields, upon contraction, singles and uncontractable triples. The uncontractable triples are evaluated using Eq. 34, which yields singles, triples, and uncontractable quintuples. The uncontractable quintuples are evaluated by using Eq. 35 which yields triples, quintuples, and uncontractable septuples. To the order of approximation indicated by Eq. 32, the uncontractable septuples are neglected. Eqs. 33, 34, and 35 then represent a set of coupled equations whose simultaneous solution will yield $\omega(p)$ and b_p^+.

Suhl and Werthamer (10,11) solve the degenerate electron gas problem by arbitrarily terminating the extended RPA procedure at the second order, which is equivalent to solving Eqs. 33 and 34. They evaluate the triple commutator, Eq. 34, approximately by utilizing the fact that the Coulomb potential is singular at the origin. Their results agree with the most sophisticated of previous calculations. It will be shown that their methods are equally successful when applied to the many-boson problem.

1. The density excitation operator

It was shown by Feynman (8) that the elementary excitations in He II at low momenta are generated by the excitation operator

$$\rho_k \;=\; \sum_p a^+_{p+k}a_p$$

which is just the Fourier transform of the density. Furthermore, it has been argued by Landau and Lifshitz (12, p. 199), and others, that any quantum fluid which obeys boson statistics displays low momentum excitations of this form. Therefore, we propose for consideration, an excitation operator that represents the most general possible linear combination of the products $a^{+}_{p+k}a_p$, and which also contains the density operator as a special case, namely

$$b^{+}_{k} = \sum_{p} c(p,k)a^{+}_{p+k}a_p \tag{36}$$

where c(p,k) are c-number coefficients to be determined. If b^{+}_{k}, acting on an energy eigenstate of the system, excites the system to an eigenstate of higher momentum, then there exists an approximate solution to the equation of motion such that

$$[H,b^{+}_{k}]|0\rangle = \omega(k)b^{+}_{k}|0\rangle. \tag{21}$$

The commutator for b^{+}_{k}, as given by Eq. 36 is

$$[H,b^{+}_{k}]|0\rangle = \sum_{p} c(p,k)[H,a^{+}_{p+k}a_p]|0\rangle \tag{37}$$

where

$$[H,a^{+}_{p+k}a_p] = [T_{p+k} - T_p]a^{+}_{p+k}a_p + \sum_{n} V(n)[\rho_n a^{+}_{p+k-n}a_p - a^{+}_{p+k}a_{p+n}\rho_n] \tag{38}$$

and $V(k) = V(-k)$. This result is considerably simplified if one makes the random phase approximation; "The motion of a pair with momentum k is determined by keeping only the terms in the interaction associated with the k^{th} momentum transfer," (Pines 13, p. 47). Eq. 38 then reduces to

$$[H,a^{+}_{p+k}a_p] = [T_{p+k} - T_p]a^{+}_{p+k}a_p + V(k)[N_p - N_{p+k}]\rho_k \tag{39}$$

where N_p is the number of particles operator for momentum p. The substitution of Eq. 39 into Eq. 37 gives

$$[H,b^{+}_{k}]|0\rangle = \sum_{p} [c(p,k)(T_{p+k} - T_p) + l(k)]a^{+}_{p+k}a_p|0\rangle \tag{40}$$

where

$$l(k) = \sum_{q} c(q,k)V(k)[N_q - N_{q+k}]. \tag{41}$$

From Eqs. 21, 36, and 40

$$\sum_p \left[c(p,k)(\omega(k) + T_p - T_{p+k}) - l(k)\right]a^+_{p+k}a_p|0\rangle = 0. \qquad *(42)$$

If the operator $l(k)$ may be replaced by its ground state expectation value, then Eq. 42 is satisfied if and only if the quantity in the square brackets vanishes. In this case $c(p,k)$ is given by the integral equation,

$$c(p,k) = V(k) \sum_q \frac{c(q,k)[N_q - N_{q+k}]}{\omega(k) + T_p - T_{p+k}} = \frac{V(k)[\rho_{-k}, b^+_k]}{\omega(k) + T_p - T_{p+k}} \qquad (43)$$

where N_q is now the ground state expectation value for the number of particles with momentum q, or simply the momentum distribution function. By multiplying both sides of Eq. 43 by $N_p - N_{p+k}$ and summing over p, we find that

$$1 = V(k) \sum_p \frac{N_p - N_{p+k}}{\omega(k) + T_p - T_{p+k}} = 2V(k)\sum_p N_p \frac{(T_{p+k} - T_p)}{\omega^2(k)-(T_{p+k}-T_p)^2}. \qquad (44)$$

It is expected that N_p will be large only for small values of p and so the major contribution to the sum over p in Eq. 44 comes from small momenta. Therefore, we approximate the square bracket in Eq. 44 by its low momentum limit.

$$\lim_{p\to 0} \frac{T_{p+k} - T_p}{\omega^2(k)-(T_{p+k}-T_p)^2} = \frac{T_k}{\omega^2(k)-T_k^2}. \qquad (45)$$

Substituting this value into Eq. 44 yields the excitation energy

$$\omega^2(k) = T_k^2 + 2T_k NV(k). \qquad (46)$$

For this approximation to be valid, it is not necessary that $N_p \approx 0$ for all states with $p>0$, as is the case in the weak-coupling approximation, but only that most of the particles lie in a narrow region $|\underset{\sim}{p}|<|\delta|$ of momentum space surrounding the origin. We require that δ be small enough to insure that the result given by Eq. 45 is a valid replacement for the square bracket in Eq. 44. Since the closely spaced, low-lying momentum states are expected to be highly degenerate for systems with weak or moderate interaction strengths, such a requirement is not unreasonable. Naturally, any precise estimate on the validity of this approximation depends on the interaction and must be tested for each individual problem. However, an investigation reveals that the approximation is valid over a fairly wide range of conditions. A rough calculation indicates that N_p remains quite local in momentum space even for interaction strengths as large as those in He II and it follows that Eq. 45 is a satisfactory replacement at all momenta, thus giving support to our discussion.

Eq. 46 is recognized to be of the form derived by Bogoliubov (2), and others, for the excitation energy. Bogoliubov (2) arrives at his result by assuming that an overwhelming portion of the particles are in the single-particle zero-momentum state with a negligibly small number at higher momenta. In our derivation, we are able to consider systems for which an arbitrary number of low-lying states contain a large number of particles, subject only to the condition that the totality of states which contain most of the particles is sufficiently localized. No undue attention is paid to the zero-momentum state, nor is an artificial separation of this state from other states of low momentum necessary. It is for this reason that we consider Eq. 46 to be more general than had previously been indicated, and possibly it is applicable to a wider class of problems.

From Eq. 36 it is seen that the excited state $|k\rangle$ is generated from the ground state in the following way:

$$|k\rangle = b_k^+|0\rangle = \sum_p c(p,k)a_{p+k}^+ a_p|0\rangle. \tag{47}$$

The plane-wave creation and annihilation operators may be transformed according to the expression

$$a_p = \sum_{x_i} \psi(x_i)e^{-ip\cdot x_i}$$

where $\psi(x_i)$ is the usual Fock space field operator. It is assumed that $c(p,k)$ is Fourier transformable as a function of both variables. Therefore, $|k\rangle$ may be written as

$$|k\rangle = \sum_{p,x_i,x_j} c(p,k)\psi^+(x_j)\psi(x_i)e^{-ip\cdot(x_i-x_j)}e^{ik\cdot x_j}|0\rangle$$

$$= \sum_{x_i,x_j,x_s} c(x_i-x_j,x_j-x_s)\psi^+(x_j)\psi(x_i)e^{ik\cdot x_s}|0\rangle. \tag{48}$$

Define

$$h(x_s) = \sum_{x_i,x_j} c(x_i-x_j,x_j-x_s)\psi^+(x_j)\psi(x_i). \tag{49}$$

The substitution of Eq. 49 into Eq. 48 gives

$$|k\rangle = \sum_{x_s} h(x_s)e^{ik\cdot x_s}|0\rangle. \tag{50}$$

This wave function has the same form as that of Feynman and Cohen (9), although their coefficients $h(x)$ are presumably different from ours, having been determined by a variational procedure.

The f-sum rule for the excitations generated by b_k^+ can be found by considering the ground state expectation value for the following commutator;

$$\langle 0|([H,b_k^+],b_{-k}^+)|0\rangle = -\sum_n \omega(k)_{no}[(b_k^+)_{on}(b_{-k}^+)_{no} + (b_{-k}^+)_{on}(b_k^+)_{no}]. \qquad (51)$$

The double commutator on the left-hand side of Eq. 51 may be evaluated exactly but, to be consistent with the approximations of this theory, it will be considered only in the limit of the RPA. The result is

$$\sum_n \omega(k)_{no}[(b_k^+)_{on}(b_{-k}^+)_{no} + (b_{-k}^+)_{on}(b_k^+)_{no}] = \sum_p c(p,k)c(p+k,-k)(T_{p+k}-T_p)(N_p-N_{p+k})$$

$$+ \sum_{p,q} c(p,k)c(q+k,-k)V(k)(N_p-N_{p+k})(N_q-N_{q+k}). \qquad (52)$$

This result can be further simplified if the momentum distribution function is sufficiently local so that the coefficients in Eq. 52 may be replaced by their mean value over the interval of integration. This, of course, is identical to the procedure used earlier to derive the excitation energy. More crudely, N_p may be replaced by its value for a non-interacting system. In either case, the result is,

$$\sum_n \omega(k)_{no}[(b_k^+)_{on}(b_{-k}^+)_{no} + (b_{-k}^+)_{on}(b_k^+)_{no}] = \frac{Nk^2}{m} c(0,k)c(k,-k)$$

$$+ N^2V(k)[c(0,k)-c(-k,k)][c(k,-k)-c(0,-k)]. \qquad (53)$$

For the special case where $b_k^+ = b_{-k}$, Eq. 53 may be further simplified. One such case, which will be shown to occur under certain circumstances, is for $c(p,k)$ independent of p, that is $c(p,k) = z(k)$. Then b_k^+ reduces to the density fluctuation, i.e.

$$b_k^+ = \sum_p z(k)a_{p+k}^+a_p = z(k)\rho_k \qquad (54)$$

and Eq. 53 becomes

$$\sum_n \omega(k)_{no}|\rho_k|_{no}^2 = \frac{Nk^2}{2m} \qquad (55)$$

which is identical to the result of Miller, Pines, and Nozieres (14).

Since Feynman (8) has shown that $|k\rangle = \rho_k|0\rangle$ is an approximate energy eigenstate for He II at low momenta and since there is every reason to believe that the same is true for any many-boson fluid, it is of considerable interest to investigate the consequences of such a proposition within the framework of our calculation. Now in the limit of small k, the excited state $|k\rangle = \sum_p c(p,k)a^+_{p+k}a_p|0\rangle$ depends only on small values of p and c(p,k) is independent of p. This follows from Eq. 43 providing $\lim_{k\to 0} NV(k) \gg T_p$, for the only p dependence on the right hand side of Eq. 43 is the kinetic energy term of the denominator, and the above inequality expresses the condition that the kinetic energy excitation is a small part of the total excitation energy. In this case the excitation operator b^+_k is of the form given by Eq. 54 and, since the following calculations are independent of the c-number coefficient z(k), it may be omitted without loss of generality. Thus, at low momenta

$$b^+_k \backsim \rho_k \tag{56}$$

and

$$[H,\rho_k] = \omega(k)\rho_k. \tag{57}$$

We may now make use of the following well-known relations (15) involving the density fluctuation ρ_k.

$$N^{-1}\langle 0|\rho^+_k\rho_k|0\rangle = S(k) \tag{58}$$

$$N^{-1}\langle 0|\rho^+_k H\rho_k|0\rangle = \frac{k^2}{2m} \tag{59}$$

$$\lim_{k\to 0} N^{-1}\langle 0|\rho^+_k H^{-1}\rho_k|0\rangle = \frac{1}{2mc^2} \tag{60}$$

where S(k) is the structure factor and c is the sound velocity. From Eqs. 57, 58, and 59 it is seen that for small k,

$$N^{-1}\langle 0|\rho_k^+ H\rho_k|0\rangle = N^{-1}\langle 0|\rho_k^+[H,\rho_k]|0\rangle = \omega(k)S(k) \tag{61}$$

where the zero of the excitation energy has been defined by $H|0\rangle = 0$. Therefore, from Eqs. 59 and 61, it is apparent that

$$\omega(k) = \frac{k^2}{2mS(k)} \tag{62}$$

which is the result originally derived by Feynman (8) using a variational calculation. Thus, Eqs. 57 and 59 reveal that, if the density fluctuation is a non-interacting elementary excitation of the system, then Eq. 62 is the correct expression for the excitation energy. This equation has been experimentally verified to be correct for He II at low momenta.

The low momentum character of S(k) may be determined from Eqs. 57 and 60. That is,

$$\lim_{k\to 0} N^{-1}\langle 0|\rho_k^+ H^{-1}\rho_k|0\rangle = \lim_{k\to 0} N^{-1}\langle 0|\rho_k^+\rho_k|0\rangle\frac{1}{\omega(k)} = \lim_{k\to 0}\frac{S(k)}{\omega(k)}. \tag{63}$$

Therefore, using Eq. 60

$$\lim_{k\to 0}\frac{S(k)}{\omega(k)} = \frac{1}{2mc^2}. \tag{64}$$

From Eq. 46

$$\lim_{k\to 0}\omega(k) = k\left[\frac{NV(0)}{m}\right]^{\frac{1}{2}} = ck \tag{65}$$

where

$$c^2 = \frac{NV(0)}{m}. \tag{66}$$

Substituting Eq. 65 into Eq. 64 gives

$$\lim_{k\to 0} S(k) = \frac{k}{2mc} \tag{67}$$

which shows that the liquid structure factor is linear in momentum at low k. This result is also found to be in very good agreement with experiment for He II. Eq. 67 may be derived directly from Eq. 62 by substituting in the expression for $\omega(k)$ as given by Eq. 46. That is,

$$\lim_{k\to 0} S(k) = \lim_{k\to 0} \frac{k}{[k^2+4mNV(k)]^{\frac{1}{2}}} = \frac{k}{2mc}$$

where we have used Eq. 66. It can be concluded that if $\rho_k|0>$ is an excited eigenstate of the system, then S(k) is correctly given by Eq. 67.

For a weakly-interacting boson system it was shown in Chapter II that the quasi-particle excitation operator is of the form

$$b_k^+ = u(k)a_k^+ + v(k)a_{-k} \tag{68}$$

where

$$u^2(k) = \frac{1}{2\omega(k)}[\omega(k) + T_k + NV(k)] \tag{69}$$

$$v^2(k) = \frac{1}{2\omega(k)}[T_k + NV(k) - \omega(k)]. \tag{70}$$

The excitation operator represented by Eq. 36 may also be given in the weak-coupling limit by retaining only those terms in the sum over p that contain at least one plane-wave operator of zero momentum, which is then replaced by the c-number

$$a_o^+ \approx a_o \approx N_o^{\frac{1}{2}} \approx N^{\frac{1}{2}}.$$

That is,

$$\begin{aligned} b_k^+ &= \sum_p c(p,k)a_{p+k}^+a_p = c(o,k)a_k^+a_o + c(-k,k)a_o^+a_{-k} \\ &= N^{\frac{1}{2}}c(o,k)a_k^+ + N^{\frac{1}{2}}c(-k,k)a_{-k}. \end{aligned} \tag{71}$$

The coefficients c(o,k) and c(-k,k) may be calculated from Eq. 43 and the normalization condition

$$\langle k|k\rangle = \sum_p c^2(p,k)[N_p - N_{p+k}] = 1. \tag{72}$$

These equations are evaluated in the weak-coupling limit by replacing the momentum distribution function by its value for a non-interacting system, in which case Eqs. 43 and 72 become,

$$Nc^2(0,k) - Nc^2(-k,k) = 1 \tag{73}$$

$$c(0,k) = \frac{-NV(k)c(-k,k)}{\omega(k) - T_k - NV(k)}. \tag{74}$$

The simultaneous solution of Eqs. 73 and 74 yield

$$Nc^2(0,k) = u^2(k) \tag{75}$$

$$Nc^2(-k,k) = v^2(k). \tag{76}$$

The substitution of these results into Eq. 71 reveals that in the limit of weak coupling, the excitation operator b_k^+, as defined by Eq. 36, is completely equivalent to the excitation operator of Bogoliubov (2). This, along with the energy spectrum already derived, establishes that, when taken to the appropriate limit, our method is entirely identical to the weak-coupling calculation of Bogoliubov (2).

2. The opposite momentum correlated pairs

Earlier in this chapter it was shown that the most general linearization of the equation of motion for the plane-wave operator a_p^+ is given by Eq. 26, where one neglects the remaining non-linear term. If the fluctuation terms are also neglected, which are shown to be negligibly small in Appendix A, the commutator $[H,a_p^+]$ acting on the ground state of the system reduces to

$$[H, a_p^+] = [T_p + K(p)]a_p^+ + \sum_k V(p-k)\langle a_k^+ a_{-k}^+ \rangle a_{-p}. \qquad *(28)$$

For such an equation, one can construct an operator b_p^+ which is a linear combination of a_p^+ and a_{-p} and satisfies Eq. 21. That is, the operator which excites the normal modes of the system is given by

$$b_p^+ = \alpha(p)a_p^+ + \beta(p)a_{-p} \qquad (29)$$

where $\alpha(p)$ and $\beta(p)$ are c-number coefficients.

The motivation for considering a linearization of the form given by Eq. 28 comes primarily from arguments based on the weak-coupling theories, where the operator products $a_k^+ a_{-k}^+$ and $a_k a_{-k}$ are known to have large expectation values at low momenta. A similar treatment occurs in the theory of superconductivity where these opposite momentum pairs are of paramount importance. In fact, Valatin and Butler (7) have demonstrated that there is a remarkable resemblence between the mathematical formulation of many-boson theory and that of superconductivity. Actually, some of the procedures of this section may be brought into formal equivalence with their work. The more complete analysis presented here will show the relationship to the weak-coupling theories in an obvious way and important generalizations are provided in a simplified form. The following approach is completely analogous to a method of Anderson and Schrieffer (16) where they calculate the excitation spectrum and the ground state energy for a superconducting system.

The most general solution to Eq. 21 for an excitation operator of the form given by Eq. 29 is found by substituting Eq. 28 and its time reversed hermitian conjugate into the following equation:

$$[H, \alpha(p)a_p^+ + \beta(p)a_{-p}]|0\rangle = \omega(p)[\alpha(p)a_p^+ + \beta(p)a_{-p}]|0\rangle. \qquad (77)$$

The result is given by a pair of coupled equations

$$\alpha(p)\,\mu(p) - \beta(p)\,\eta(p) = \alpha(p)\,\omega(p) \tag{78}$$

$$\alpha(p)\,\eta(p) - \beta(p)\,\mu(p) = \beta(p)\,\omega(p) \tag{79}$$

where

$$\mu(p) = T_p + K(p) \tag{80}$$

$$\eta(p) = \sum_k V(p-k)\langle a_k^+ a_{-k}^+\rangle . \tag{81}$$

If $\alpha(p)$ and $\beta(p)$ obey the added condition

$$\alpha^2(p) - \beta^2(p) = 1, \tag{82}$$

then the b's satisfy the usual boson commutation laws. The excitation spectrum is given by

$$\omega^2(p) = \mu^2(p) - \eta^2(p). \tag{83}$$

The inverse of the transformation, defined by Eq. 29, and its hermitian conjugate is

$$\begin{pmatrix} a_p^+ \\ a_{-p} \end{pmatrix} = \begin{pmatrix} \alpha(p) & -\beta(p) \\ -\beta(p) & \alpha(p) \end{pmatrix} \begin{pmatrix} b_p^+ \\ b_{-p} \end{pmatrix} . \tag{84}$$

This equation together with the requirement that the ground state wave function $|0\rangle$ be a vacuum state for the generation of quasi-particles, that is

$$b_p|0\rangle = 0 \tag{85}$$

is sufficient to calculate the momentum distribution function in the correct ground state.

$$N_p = \langle a_p^+ a_p\rangle = \langle[\alpha(p)b_p^+ - \beta(p)b_{-p}][\alpha(p)b_p - \beta(p)b_{-p}^+]|\rangle = \beta^2(p) \tag{86}$$

From Eqs. 78, 79, and 82

$$\beta^2(p) = \frac{1}{2}\left[\frac{\mu(p)}{\omega(p)} - 1\right] \tag{87}$$

$$\alpha^2(p) = \frac{1}{2}\left[\frac{\mu(p)}{\omega(p)} + 1\right] \tag{88}$$

The only remaining unknown quantity, $\eta(p)$, may be calculated in the following way. From Eqs. 78, 79, 85, and 86, it can be seen that the ground state expectation value of $b_p^+b_p$ is

$$\langle b_p^+b_p\rangle = 2\alpha(p)\beta(p)\langle a_p^+a_{-p}^+\rangle + 2N_p(N_p+1) = 0 \tag{89}$$

where it is assumed that $N_p = N_{-p}$. Therefore,

$$\langle a_p^+a_{-p}^+\rangle = -\frac{\alpha(p)}{\beta(p)}N_p. \tag{90}$$

Substituting this result into Eq. 81 gives

$$\eta(p) = -\sum_k V(p-k)N_k\frac{\alpha(k)}{\beta(k)}. \tag{91}$$

From Eqs. 78, 79, and 83, it can be seen that

$$\frac{-\alpha(k)}{\beta(k)} = \frac{\eta(k)}{\omega(k) - \mu(k)} = \frac{\eta(k)}{[\mu^2(k) - \eta^2(k)]^{\frac{1}{2}} - \mu(k)}. \tag{92}$$

Substituting Eq. 92 into Eq. 91 gives

$$\eta(p) = \sum_k \frac{V(p-k)N_k\eta(k)}{[\mu^2(k) - \eta^2(k)]^{\frac{1}{2}} - \mu(k)}. \tag{93}$$

Therefore, $\eta(p)$ is defined by the above integral equation.

For systems whose momentum distribution function N_k is effectively localized about the origin within a range δ, it is sufficient to evaluate $\alpha(k)/\beta(k)$ for small momenta and to work directly with Eq. 91. From Eqs. 82 and 86

$$\frac{\alpha(k)}{\beta(k)} = \pm\left[\frac{N_k+1}{N_k}\right]^{\frac{1}{2}}. \tag{94}$$

It is clear that for all $\underset{\sim}{k}$ such that

$$N_k \gg 1 \tag{95}$$

then

$$\frac{\alpha(k)}{\beta(k)} = \pm 1. \tag{96}$$

Ineq. 95 does not necessarily refer to only those single-particle states with a macroscopic particle occupation, but it also refers to all states where N_k is more than an order of magnitude greater than unity.

If the momentum distribution function is sufficiently local so that the totality of states that satisfy Ineq. 95 contain a large majority of the particles, then the substitution of Eq. 96 into Eq. 91 is quite valid. In any case, such a substitution is superior to the weak-coupling approximation since, for that result, the only term retained in Eq. 91 is the one with $\underset{\sim}{k} = 0$. The sign of Eq. 96 is of no importance provided that it does not change sign for different values of momentum in the interval $|\underset{\sim}{k}| \leq \delta$. In the weak-coupling approximation it can be seen that Eq. 90 reduces to N_o and, therefore, the negative solution of Eq. 96 must be correct. If we assume that for small momenta, $\alpha(k)/\beta(k)$ does not change discontinuously from its weak-coupling value of -1 to +1 then, wherever Eq. 96 is approximately valid, we retain its negative solution. Under these conditions, it can be seen from Eqs. 27, 91, and 96 that

$$\eta^2(p) = K^2(p). \tag{97}$$

From Eqs. 80, 83, and 97 the excitation energy is determined to be

$$\omega^2(p) = T_p^{\ 2} + 2T_pK(p). \tag{98}$$

It can be seen from Eq. 27 that Eq. 98 reduces to the weak-coupling result (2) in the appropriate limit. However, a detailed discussion of this equation and all other results in this chapter will be deferred until Chapter IV.

Naturally the validity of Eq. 96 must be tested for each individual problem and the following formulation of $\alpha(k)/\beta(k)$ is convenient for making this test. From Eqs. 87 and 88 it can be seen that

$$\frac{\alpha^2(k)}{\beta^2(k)} = 1 + \frac{2\,\omega(k)/\mu(k)}{1 - \omega(k)/\mu(k)} \tag{99}$$

so Eq. 96 is correct for small momenta if

$$\lim_{k\leq\delta} \frac{\omega(k)}{\mu(k)} = \lim_{k\leq\delta} \left[1 - \frac{K^2(k)}{[T_k + K(k)]^2}\right]^{\frac{1}{2}} \ll 1.$$

Therefore, if $T_k \ll K(k)$ for all momenta within the range of N_k, then Eq. 96 is valid and the expression for $\omega(p)$ is correctly given by Eq. 98.

At this point we consider the consequences of neglecting the triple term in Eq. 26, upon which the results of this section depend. Consider the truncated Hamiltonian generated by neglecting all but the terms $\underset{\sim}{k} = 0$, $\underset{\sim}{q} = \underset{\sim}{p}-\underset{\sim}{k}$, and $\underset{\sim}{q} = -\underset{\sim}{p}$ in the interaction part of Eq. 1. This Hamiltonian, called the "pair Hamiltonian" (5,6), has the advantage that it contains the Bogoliubov (2) Hamiltonian as well as all other possible pair terms. As previously mentioned, these opposite momentum pairs are expected to give important contributions in the many-boson problem. H_{pair} is given by

$$H_{pair} = \frac{N(N-1)V(0)}{2} + \sum_k T_k a_k^+ a_k + \frac{1}{2} \sum_{q,k\neq 0} V(k)[a^+_{q+k} a_{q+k} a^+_q a_q$$

$$+ a^+_{q-k} a^+_{k-q} a_q a_{-q}] . \qquad (100)$$

The equation of motion for a_p^+ with H_{pair} is, after neglecting only the fluctuation terms,

$$[H_{pair}, a_p^+] = [T_p + K(p)]a_p^+ + \sum_k V(p-k)\langle a_k^+ a_{-k}^+\rangle a_{-p} . \qquad *(101)$$

This result, which is identical to Eq. 28, contains no terms non-linear in the plane-wave annihilation or creation operators. The point is that Eq. 28 results only after neglecting certain non-linear terms in $[H,a_p^+]$, whereas in $[H_{pair},a_p^+]$ they do not exist. One concludes that the terms neglected by linearizing $[H,a_p^+]$ are just those neglected in the pair Hamiltonian and vice-versa.

The effective Hamiltonian which is necessary and sufficient to yield the equation of motion given by Eq. 28 and, therefore, all of the results presented here, is formed by replacing all different pairs of operators in the interaction part of Eq. 100 with their average values. This is done without neglecting any terms in H_{pair}. The result is,

$$H_{red} = \frac{N(N-1)V(0)}{2} + \sum_k T_k a_k^+ a_k + \frac{1}{2}\sum_k K(k)[a_k^+ a_{-k}^+ + a_k a_{-k} + 2a_k^+ a_k] . \tag{102}$$

Thus, it is concluded that the most general linearization of the equation of motion for an excitation operator such as given by Eq. 29 is determined from the pair Hamiltonian alone.

3. Application of the extended RPA to the many-boson problem

It has been seen that the ordinary RPA for the excitation operator a_p^+, as given by Eq. 24, is a poorer approximation than is Bogoliubov's (2) method for calculating the excitation energy. But the first extension of the RPA, as displayed by Eq. 30, not only includes all the terms retained by the Bogoliubov (2) approximation, but allows important generalizations. By neglecting the fluctuation term in Eq. 23, the commutator $[H,a_p^+]$ may be written as

$$[H,a_p^+] = [T_p + K(p)]a_p^+ + \sum_{q,k}{}' V(k) a_{p-k}^+ a_{q+k}^+ a_q . \tag{*103}$$

The extended RPA amounts to calculating the contribution to the single operator amplitude a_p^+ from the triple term in Eq. 103. This can be done by evaluating the triple commutator, Eq. 34, which is then contracted by replacing number operators with their expectation values in the correct ground state, as outlined earlier in this chapter. The solution of the contracted equation is still quite formidable, however. Suhl and Werthamer (10) get around this difficulty for a degenerate electron gas by utilizing the singular character of the Coulomb potential to extract an approximate solution. For the many-boson problem, an approximate evaluation of the triple commutator can be found by making use of the following ideas.

It has been noted, (2,5,6) that the opposite momentum pairs, $a_k^+ a_{-k}^+$ and $a_k a_{-k}$ have an unusually large weight in many-boson systems, as they do in superconductivity. These products appear in the triple term of Eq. 103 when $\underset{\sim}{q} = -\underset{\sim}{p}$. Another indication of which terms are important in the sum over the triple product comes from the result of the ordinary RPA, which is known to be a reasonable approximation at large momenta. From Eq. 24 it can be seen that only those momentum transfers within an interval δ of the momentum of the excitation contribute to the sum, where δ is the approximate range of the momentum distribution function. For small δ, the important contribution comes from momentum transfers k, in the vicinity of momentum p. There is a clear implication from this discussion that the sum over the triple product in Eq. 103 is highly weighted in the vicinity of $\{\underset{\sim}{q},\underset{\sim}{k} = -\underset{\sim}{p},\underset{\sim}{p}\}$. This conclusion is in accord with the Bogoliubov (2) approximation since, in that case, the only values that contribute to the sum over the triple product are $\underset{\sim}{q} = -\underset{\sim}{p}$ and $\underset{\sim}{k} = \underset{\sim}{p}$. The above considerations suggest that the Bogoliubov (2) approximation be generalized by extending the region of summation to include all terms in the triple product of Eq. 103 for which

$$
\begin{aligned}
&|\underset{\sim}{k}-\underset{\sim}{p}| \le \delta \\
&|\underset{\sim}{q}+\underset{\sim}{k}| \le \delta . \qquad (104)
\end{aligned}
$$

The contribution to the equation of motion from the triple term in Eq. 103 is calculated by use of Eq. 34, that is,

$$
\sum_{q,k}{}' V(k) a_{p-k}^+ a_{q+k}^+ a_q |0\rangle = \omega(p)^{-1} \sum_{q,k} V(k) [H, a_{p-k}^+ a_{q+k}^+ a_q] |0\rangle . \qquad (105)
$$

Therefore, the commutator $[H, a_{p-k}^+ a_{q+k}^+ a_q]$ is evaluated subject to the restrictions imposed by Ineqs. 104. The general result for Eq. 34 is

$$[H, a^+_{p-k} a^+_{q+k} a_q] = \omega(p) a^+_{p-k} a^+_{q+k} a_q$$

$$= [T_{p-k} + T_{q+k} - T_q] a^+_{p-k} a^+_{q+k} a_q \qquad *(106)$$

$$+ \sum_{m,n} V(n) [a^+_{m-n} a^+_{p-k+n} a^+_{q+k} a_m a_q + a^+_{m-n} a^+_{q+k+n} a^+_{p-k} a_m a_q - a^+_{m-n} a^+_{p-k} a^+_{q+k} a_{q-n} a_m]$$

$$+ \sum_n V(n) a^+_{q+k-n} a^+_{p-k+n} a_q.$$

By contracting Eq. 106 and ignoring terms of order N^{-1} compared to those that are kept, one gets

$$[\omega(p) + T_q - T_{q+k} - T_{p-k}] a^+_{p-k} a^+_{q+k} a_q = Q$$

$$+ \sum_n V(n) [N_{p+n-k} + N_{q+k+n} - N_{q-n}] a^+_{p-k} a^+_{q+k} a_q \qquad *(107)$$

$$+ \sum_n [V(q+k-p) N_q + V(n) N_q - V(q+k-p) N_{p-k} - V(n) N_{p-k}] a^+_{p-k-n} a^+_{q+k} a_{q-n}$$

$$+ \sum_n [V(k) N_q + V(n-q) N_q - V(k) N_{q+k} - V(q-n) N_{q+k}] a^+_{n+k} a^+_{p-k} a_n$$

$$+ \sum_n V(k-n) [N_{p-k} + N_{q+k}] a^+_{p-n} a^+_{q+n} a_q$$

$$+ [V(k) N_q N_{q+k} + V(q+k-p) N_q N_{q+k} + V(p-q-k) N_{p-k} N_q$$

$$+ V(k) N_q N_{p-k} - V(k) N_{p-k} N_{q+k}] a^+_p$$

where Q is the sum of the uncontractable quintuples. Under the conditions imposed by Ineqs. 104, the Q terms can be shown to yield no contribution to the equation of motion and, therefore, they are hereafter neglected. As a result, Eqs. 103 and 107 form a complete set of coupled equations which contain only single and triple operator products, and whose simultaneous solution yields the excitation spectrum and the excitation operator. Thus, the approximation represented by Ineq. 104 may be looked upon as the condition under which it is completely valid to terminate the extended RPA at second order. This point will be discussed in detail in Appendix B.

The solution of these coupled, integral equations is greatly simplified if the momentum distribution of particles is well localized so that δ is a small interval. In that case, the only term in the singlet amplitude of Eq. 107 that is not negligibly small in the interval specified by Ineq. 104 is $-V(k)N_{p-k}N_{q+k}a_p^+$. All other single terms may be neglected. Furthermore, since the triple operator products of Eq. 103 are contained in a double sum, also bounded in the momentum interval specified in Ineq. 104, the simultaneous solution of Eqs. 103 and 107 is expedited by multiplying Eq. 107 with V(k) and summing over the same interval. It has already been argued that the triple term of Eq. 103 is highly weighted for momentum transfers in the vicinity of the excitation; that is, the only terms retained are those for which $|\underset{\sim}{p}-\underset{\sim}{k}| \leq \delta$. Therefore, after summing Eq. 107 and retaining only those triple terms with momentum transfers within δ of the excitation, the result is

$$\sum_{q,k} [V(k)(\omega(p) + T_q - T_{q+k} - T_{p-k}) + K(p)V(q+k-p)]a^+_{p-k}a^+_{q+k}a_q$$

$$= -\sum_k K(k)V(k)N_{p-k}a^+_p \qquad *(108)$$

where it is understood that the summation is bounded in the interval specified by Ineq. 104. For δ sufficiently small, it is a good approximation to replace the square bracket in Eq. 108 by its mean value over the interval. That is

$$[V(k)(\omega(p) + T_q - T_{q+k} - T_{p-k}) + K(p)V(q+k-p)]$$
$$= V(k)[\omega(p) + T_p + K(p)]. \qquad (109)$$

The substitution of this result into Eq. 108 gives

$$\sum_{q,k} V(k)a^+_{p-k}a^+_{q+k}a_q = -\sum_k \frac{K(k)V(k)N_{p-k}a^+_p}{\omega(p) + T_p + K(p)}. \qquad *(110)$$

This equation, which relates the triple term appearing in the equation of motion for a^+_p to the singlet amplitude, may be further simplified for K(k) that vary smoothly over any small momentum interval δ. In this case

$$\sum_k K(k)V(k)N_{p-k} = K(p) \sum_k V(k)N_{p-k} = K^2(p). \qquad (111)$$

The substitution of Eq. 111 into Eq. 110 gives

$$\sum_{q,k} V(k)a^+_{p-k}a^+_{q+k}a_q = -\frac{K^2(p)a^+_p}{\omega(p) + T_p + K(p)}. \qquad *(112)$$

By substituting this result into Eq. 103 and with Eq. 33, the excitation energy is calculated to be

$$\omega^2(p) = T_p{}^2 + 2T_pK(p)$$

which is identical to the result derived in Part 2 of this chapter.

The operator that generates the elementary excitations of the system is given by Eq. 30. Over the limited interval of summation indicated by Ineq. 104, it is entirely sufficient for the purposes of this calculation to represent this excitation operator with

$$b^+_p = a^+_p + g(p) \sum_{q,k}{}' V(k)a^+_{p-k}a^+_{q+k}a_q. \qquad (113)$$

With the aid of Eqs. 21, 34, 103, and 110, the quantity g(p) is determined by evaluating the commutator of b^+_p with the Hamiltonian

$$[H,b_p^+] = \omega(p)[a_p^+ + g(p) \sum_{q,k}{}' V(k)a_{p-k}^+ a_{q+k}^+ a_q]$$

$$= [H,a_p^+] + g(p) \sum_{q,k}{}' V(k)[H,a_{p-k}^+ a_{q+k}^+ a_q] \qquad *(114)$$

$$= [T_p + K(p)]a_p^+ + \sum_{q,k}{}' V(k)a_{p-k}^+ a_{q+k}^+ a_q$$

$$- g(p)[T_p + K(p)] \sum_{q,k}{}' V(k)a_{p-k}^+ a_{q+k}^+ a_q - g(p)K^2(p)a_p^+.$$

By equating the coefficients of either the single or the triple terms in Eq. 114, the result for $g(p)$ is,

$$g(p) = \frac{1}{\omega(p) + T_p + K(p)}. \qquad (115)$$

The substitution of Eq. 115 into Eq. 113 gives

$$b_p^+ = a_p^+ + \sum_{q,k}{}' \frac{V(k)a_{p-k}^+ a_{q+k}^+ a_q}{\omega(p) + T_p + K(p)}. \qquad (116)$$

This excitation operator may be approximated by applying the techniques used in Part 2 of the present chapter. In Eq. 116, it is noted that the sum over q is restricted to include only the narrow interval around $\underset{\sim}{q} = -\underset{\sim}{p}$. By going to the limit of $\underset{\sim}{q} = -\underset{\sim}{p}$ and then replacing $a_{p-k}^+ a_{k-p}^+$ with its average value $\langle a_{k-p}^+ a_{p-k}^+ \rangle$, b_p^+ reduces exactly to the excitation operator defined by Eq. 29, except for a normalization coefficient which in no way affects the generality of the result. Thus, we have shown that there exists a close relationship between the particle-conserving excitations presented here and the particle non-conserving excitations generated in Part 2.

B. Extended Bogoliubov Approximation

The method developed in this section is a direct generalization of Bogoliubov's (2) technique which, however, is applicable to systems where an arbitrary number of low-lying states are occupied by a large number of particles. The zero-momentum state is not considered separately but only in conjunction with the other low-lying states. The results for the ground state energy, the excitation spectrum, and the momentum distribution function are in the form of coupled, integral equations. These equations coincide with those derived in the previous sections.

Suppose that other low-lying, single-particle states besides the zero-momentum state contain large numbers of particles. That is

$$N_k \gg 1 \qquad \text{for} \qquad |\underset{\sim}{k}| \leq \delta \tag{117}$$

and

$$N^{-1} \sum_{k>\delta} N_k \ll 1 . \tag{118}$$

A plane-wave annihilation or creation operator acting on a wave function for a many-particle system with a precise number of particles in each single-particle, plane-wave state gives

$$a_k |---N_k---\rangle \;=\; (N_k)^{\frac{1}{2}} |---N_k-1,---\rangle$$

$$a_k^+ |---N_k,---\rangle \;=\; (N_k+1)^{\frac{1}{2}} |---N_k+1,---\rangle$$

where N_k has been defined as the number of particles in the state of momentum k. If, for the correct momentum states of the interacting system, the fluctuation of particle number in each single-particle state satisfying Ineq. 117 is small compared to its mean value, then two approximations are in order:

a. Replace $(N_k+1)^{\frac{1}{2}}$ by $N_k^{\frac{1}{2}}$

b. Assume that the physical properties of the many-particle system are not significantly altered by adding or removing a particle from a state satisfying Ineq. 117.

Under these circumstances, the operators a_k and a_k^+ commute with each other as well as with all operators of different momentum and, therefore, they may be replaced by their c-number expectation values in the correct ground state of the many-particle system. These arguments are, of course, identical to those advanced by Bogoliubov (2) to justify the replacement of zero-momentum operators with their average values in the interaction part of the Hamiltonian. Here, in a completely analogous way, we extend the Bogoliubov (2) approximation by allowing operators that act on states which satisfy Ineq. 117 to be replaced by their ground state expectation values.

Consider the interaction part of the Hamiltonian

$$H_I = \frac{1}{2} \sum_{p,q,k} V(k) a^+_{p-k} a^+_{q+k} a_q a_p . \tag{119}$$

For any approximation involving the replacement of an operator or a product of operators in H_I with their expectation values, only those processes which conserve momentum are considered, since H_I is itself a momentum conserving quantity. Suppose that one replaces all four operators in Eq. 119 by their ground state expectation values, then under certain circumstances, the result might be expected to yield a reasonable estimate for the potential energy. However, all dynamical quantities such as the excitation spectrum would not be calculable from such a procedure. As a next approximation one could replace all possible products of three operators by their average values but then, providing that only momentum conserving processes are retained, the only remaining operator would be of zero momentum, a case which is also dynamically non-interesting. In fact, the very lowest order non-trivial way to consider the dynamic characteristics of a system is to replace all possible pairs of operators by their average values.

After making all possible pairwise replacements in H_I, one gets

$$H_I = \frac{N(N-1)V(0)}{2} + \frac{1}{2} \sum_{p,k\neq 0} V(k)[a^+_{p-k}a^+_{k-p}N_p + a_p a_{-p} N_{p-k} + a^+_{p-k}a_{p-k}N_p + a^+_p a_p N_{p-k}] = \frac{N(N-1)V(0)}{2} + \frac{1}{2}\sum_{p,k} V(k)[a^+_{p-k}a^+_{k-p}N_p + a_p a_{-p} N_{p-k} + a^+_{p-k}a_{p-k}N_p + a^+_p a_p N_{p-k}] - \frac{1}{2}\sum_k V(0)N_k[a^+_k a^+_{-k} + a_k a_{-k} + 2a^+_k a_k]. \tag{120}$$

By changing the indices of summation in Eq. 120 and adding to it the kinetic energy term, the total Hamiltonian is

$$H = \sum_k T_k a^+_k a_k + \frac{N(N-1)V(0)}{2} + \frac{1}{2}\sum_k K(k)[a^+_k a^+_{-k} + a_k a_{-k} + 2a^+_k a_k] \tag{121}$$

where $K(k)$ has been previously defined,

$$K(k) = \sum_p V(p)N_{p-k}. \tag{27}$$

For systems in which a large majority of the particles are in the zero-momentum, single-particle state, $K(k)$ may be evaluated by retaining only the term $\underset{\sim}{p} = \underset{\sim}{k}$ in the sum over p in Eq. 27, in which case Eq. 121 reduces to the model Hamiltonian originally derived by Bogoliubov (2). However, this a-priori assumption about the momentum distribution of particles is not required and, since $K(k)$ contains the contribution from particles in all momentum states, including the state of zero momentum, important generalizations result if $K(k)$ is calculated without making any such weak-coupling approximation. Therefore, we proceed by diagonalizing Eq. 121 directly. The result is

$$H = E_o + \sum_k \omega(k) b_k^+ b_k \tag{122}$$

where E_o is interpreted as the ground state energy and is given by

$$E_o = \frac{N(N-1)V(0)}{2} + \frac{1}{2}\sum_k \left[\omega(k) - T_k - K(k)\right]. \tag{123}$$

The equations for the excitation spectrum $\omega(k)$, the excitation operator b_k^+, and the momentum distribution function N_k, are found to be identical to the results derived in Part 2 of Chapter III. Thus, Eqs. 27, 86, 98, and 123 form a set of coupled, non-linear, integral equations whose solution yields complete knowledge about the ground state properties of the system. Finally, it can be shown that the approximate Hamiltonian, given by Eq. 121, is derivable from the pair Hamiltonian alone. This same connection was also discovered in the work of Part 2.

IV. SUMMARY AND DISCUSSION

The principal accomplishments+ of this paper are contained in the new results that have been derived for the excitation spectrum, the excitation operator, the ground state energy, and the momentum distribution function. The coupled equations for these quantities are

$$\omega(k) = [T_k{}^2 + 2T_k K(k)]^{\frac{1}{2}} \tag{124}$$

$$E_o = \frac{N(N-1)V(0)}{2} + \frac{1}{2}\sum_k [\omega(k) - T_k - K(k)] \tag{125}$$

$$N_k = \frac{1}{2\omega(k)} [-\omega(k) + T_k + K(k)] \tag{126}$$

where

$$K(k) = \sum_p V(p-k)N_p . \tag{127}$$

There are three important features of the theory that should be emphasized. They are:

(a) In the weak-coupling limit the theory reduces identically to that of Bogoliubov (2). This statement can be verified by evaluating the quantity $K(k)$ from Eq. 127, where only the term involving particles in the zero-momentum state is retained. Then $K(k) = N_oV(k)$, and to the extent that the Bogoliubov (2) approximation is known to be valid, $K(k) = NV(k)$, since $N_o = N$. By substituting this value for $K(k)$ into Eqs. 124, 125, and 126, the well known weak-coupling results are obtained. As an example, the excitation

+The separate theory presented in Part 1 of Chapter III is self-contained and will not be discussed here.

spectrum and the ground state energy become

$$\omega(k) = [T_k^{\,2} + 2T_k NV(k)]^{\frac{1}{2}} \tag{128}$$

$$E_o = \frac{N(N-1)V(0)}{2} + \frac{1}{2}\sum_k [\omega(k) - T_k - NV(k)]. \tag{129}$$

(b) The weak-coupling results are actually valid under more general circumstances than had previously been considered. For instance, it can be seen that if the Fourier transform of the interaction potential is sufficiently smooth over the approximate width of the momentum distribution function then, in the expression for $K(k)$, $V(p-k)$ may be replaced by its mean value over the interval, i.e.

$$K(k) = \sum_p V(p-k)N_p \approx V(k)\sum_p N_p \approx NV(k) \tag{130}$$

which is identical to the result obtained from the Bogoliubov (2) approximation. Again, the substitution of Eq. 130 into Eqs. 124, 125, and 126, yields the standard weak-coupling results for $\omega(k)$, E_o, and N_k. However, in this case, $K(k)$ is not sensitive to the exact momentum distribution of particles. The more local the momentum distribution function and the more regular the potential, the more accurate is Eq. 130. For instance, if an overwhelming portion of the particles are in the zero-momentum, single-particle state as is the case in the weak-coupling limit, or if N_k is so localized that it is almost a delta function, or if $V(p-k)$ is essentially constant and perhaps replaceable by its s-wave scattering length, then Eq. 130 is an excellent approximation. It is evident that the conditions required for the validity of Eq.

130 are less severe than in the Bogoliubov (2) approximation even though the results are identical. It is for this reason that we consider the weak-coupling results to be valid under more general circumstances than had previously been considered. This same conclusion was reached by the theory presented in Part 1 of Chapter III.

(c) There are conditions for which K(k) does not approximately equal NV(k) and, as a result, the weak-coupling equations are invalid. In that case, the coupled set, Eqs. 124, 125, 126, and 127 must be solved. An example of such a system is the charged boson gas. The Fourier transform of the potential changes very rapidly at low momenta and becomes infinite at the origin. Such behavior violates the conditions under which Eq. 130 can be derived and, it will be shown in Chapter V, that K(k) is much different than NV(k) at low momenta. As a result, we find an excitation spectrum which differs markedly from that obtained by the weak-coupling calculation of Foldy (17).

An important accomplishment of the general theory that has been developed in this paper is that no a-priori assumption concerning the population of any single, low-lying momentum state is required. The equations that govern the behavior of the system are explicitly dependent on the momentum distribution function which, in turn, is fully derivable from the theory. Therefore, questions concerning the depletion of particles in the zero-momentum state are not relevant because the depletion is automatically accounted for.

This conclusion is supported in a calculation recently made by

Bassichis and Foldy (18), who solve a simple boson model exactly and then compare the results with the Bogoliubov (2) solution. They found that for a system containing a large number of particles, the Bogoliubov (2) results, ignoring depletion effects, are identical to the exact solution. Based on our theory such should be the case if Eq. 130 and, therefore, Eqs. 128 and 129 are valid. The model does satisfy the conditions of Eq. 130 and, therefore, the results of Bassichis and Foldy (18) are quite reasonable.

Another case where depletion effects seem to contradict otherwise reasonable results is in He II. For instance, Brueckner and Sawada (3) have derived an excitation spectrum for He II that is in fair agreement with experiment, but the calculation ignores depletion in the zero-momentum state. When depletion is included, the agreement vanishes. However, as will be shown in Appendix C, the results for He II are probably insensitive to the precise momentum distribution of particles and, therefore, the weak-coupling equations are valid only if depletion is completely ignored.

A common practice in previous many-boson calculations has been to ignore the dynamic characteristics of the zero-momentum state by replacing certain zero-momentum operators with c-numbers and then to work separately with the particles in states of higher momentum. This procedure inevitably leads to the appearance of the expectation value N_o which, in most cases, is then replaced in the calculation by N. However, if the depletion of the zero-momentum state is too large to allow such a replacement, N_o must be retained. It is then argued that the weak-coupling equations may still be valid because the high degree of momentum correlation in the system justifies a partial neglect of particles in states of higher momenta. This is a common, and the most simple way to account for depletion. However, based on our theory, such an approach is not correct since the particles contained in the non-zero low-lying momentum states give an important contribution to the results, as can be seen by evaluating the exchange energy $K(k)$. We conclude therefore, that many attempts to generalize the weak-coupling theories, by allowing for depletion effects, are suspect and quite possibly wrong.

Finally, we draw some conclusions of great interest concerning the nature of the low-lying excitations in a many-boson system. At very low momenta the interaction is expected to be very important in determining the nature of the excitations while, at high momenta, the kinetic energy becomes large and tends to mask the effect of the interaction. From Eq. 98 it can be seen that the behavior of $\omega(k)$ at small momenta depends critically on $K(k)$. Some of the properties of $K(k)$ are,

$$K(0) = \lim_{k\to 0} K(k) = \lim_{k\to 0} \sum_{p\neq k} V(p-k)N_p = \sum_{p\neq 0} V(p)N_p. \tag{131}$$

Thus, $K(k)$ approaches a finite constant as the momentum approaches zero. Furthermore, if $K(k)$ is analytic over some non-zero interval surrounding the origin, a property which is assured if the potential $V(p-k)$ is everywhere analytic but not necessarily at the origin, then it is possible to represent $K(k)$ by a Taylor series expansion.

$$K(k) = K(0) + K'(0)k + \frac{K''(0)k^2}{2!} + ---- \tag{132}$$

where

$$K^{(n)}(0) = \sum_{p\neq 0} V^{(n)}(p)N_p$$

From Eq. 131 and with Eq. 98 for $\omega(p)$, two important facts may be established. First, it can be seen that the condition necessary for the thermodynamic stability of the quasi-particle system is

$$\sum_{p\neq 0} V(p)N_p \geq 0 \tag{133}$$

otherwise the excitation spectrum would become imaginary at sufficiently low momenta. Second, the excitation spectrum becomes zero at vanishing momentum, independent of the nature of the interaction potential. That is

$$\lim_{k \quad 0} \omega(k) = 0. \tag{134}$$

Also, since Eq. 132 converges for sufficiently small momenta, there exists a non-zero Δ such that, for $|k| \leq \Delta$, $K(k)$ becomes arbitrarily close to $K(0)$. Therefore, provided that $K(0) \neq 0$,

$$\lim_{k \leq \Delta} \omega(k) = ck \tag{135}$$

where c is a constant. Thus the lowest lying excitation energies are linear in momentum.

V. APPLICATIONS

Consider a negatively charged boson gas, where the only interaction is via a Coulomb potential. The gas is assumed to be in a uniform background of positive charge so that the entire system is electrically neutral. The Fourier transform of the potential is

$$\begin{aligned} V(p) &= \frac{4\pi e^2}{p^2} && p\neq 0 \\ &= 0 && p=0. \end{aligned} \tag{136}$$

Foldy (17) has calculated the excitation spectrum for this gas using the weak-coupling equation for $\omega(p)$, as given by Eq. 128. The result is

$$\omega(p) = [T_p{}^2 + \Omega_p{}^2]^{\frac{1}{2}} \tag{137}$$

where Ω_p is the plasma frequency.

$$\Omega_p{}^2 = \frac{4\pi Ne^2}{m} \tag{138}$$

This result clearly contradicts the conclusions reached in the last chapter which are specified by Eqs. 134 and 135. The excitation energy given by Eq. 137 becomes a constant of magnitude Ω_p as the momentum goes to zero. That is

$$\lim_{p\to 0} \omega(p) = \Omega_p .$$

The contradiction arises because the Bogoliubov (2) result for $\omega(p)$ is not sufficiently accurate at low momenta for a system interacting through a Coulomb potential. It has been shown that the weak-coupling equations are valid only if Eq. 130 is valid. This validity depends on the supposition that the Fourier transform of the potential does not vary strongly over the approximate width of the momentum distribution function, a condition which is definitely not satisfied for a Coulomb potential at small momenta. A more careful calculation of $\omega(p)$, based on Eq. 124 is necessary.

The large number of particles in single-particle states of small but not zero momentum tend to screen the Coulomb potential at low momenta, as can be seen by solving for $K(p)$ exactly. However, the coupled equations are formidable so we approximate N_p by

$$N_p = (4\pi\bar{\delta})^{3/2} N e^{-\bar{\delta}p^2} \tag{139}$$

where $\bar{\delta}$ is an adjustable parameter.

For the Coulomb potential

$$K(k) = \sum_{p\neq 0} V(p) N_{p-k} \approx \sum_{p\neq 0} \frac{4\pi e^2}{p^2} (4\pi\bar{\delta})^{3/2} N e^{-\bar{\delta}(p-k)^2}$$

$$= 8e^2 N(\pi\bar{\delta})^{\frac{1}{2}} \frac{e^{-\bar{\delta}k^2}}{k} \int_0^\infty \frac{dp}{p} e^{-\bar{\delta}p^2} \sinh 2\bar{\delta}pk. \tag{140}$$

By expanding the sinh and integrating term by term

$$K(k) = 8\pi e^2 \bar{\delta} e^{-\bar{\delta}k^2} N \sum_{n=0}^{\infty} \frac{(\bar{\delta}k^2)^n}{(2n+1)n!}$$

$$= K(0)[1 - \frac{2\bar{\delta}k^2}{3} + ---] \tag{141}$$

For sufficiently small k, Eq. 124 for $\omega(k)$ then reads

$$\omega(k) = k[\frac{K(0)}{m}]^{\frac{1}{2}} = k\Omega_p(2\bar{\delta})^{\frac{1}{2}} \tag{142}$$

which is linear in k. This contradicts Foldy's (17) result but is in accord with our general conclusions as given by Eqs. 134 and 135.

For large values of k, $K(k)$ is always equal to $NV(k)$ because of the limited range of N_p. This same result is also obtained by solving Eq. 140

for K(k) at large momenta using Laplace's method.

Fig. 1 compares Foldy's (17) result with our calculation. At low momenta our prediction is given by the solid line, which coincides with Foldy's (17) result, as given by the dotted line, only at large momenta. The slope of an excitation curve represents the velocity with which a suitable excitation would propagate through the material, and we would predict a finite velocity $(2\bar{\delta})^{\frac{1}{2}}\Omega_p$ in the limit of long wavelengths, as contrasted to Foldy's (17) zero result.

A potential such as the one given by Fig. 2 is of the form of most molecular interaction potentials including liquid He II. Its Fourier transform can be excellently described by the function

$$V(k) = Ae^{-ak^2} - Be^{-bk^2} \tag{143}$$

where A, B, a, and b are appropriate constants. For this type of potential, with Eq. 139, K(k) is found to be

$$K(k) = N[\lambda^{3/2} Ae^{-\lambda ak^2} - \mu^{3/2} Be^{-\mu bk^2}] \tag{144}$$

where

$$\lambda = \frac{\bar{\delta}}{\bar{\delta}+a}$$

$$\mu = \frac{\bar{\delta}}{\bar{\delta}+b}. \tag{145}$$

If the width of the momentum distribution function is small compared to the width of the Gaussians in Eq. 143, then

$$\bar{\delta} \gg a,b$$

and

$$\lambda \approx \mu \approx 1 \tag{146}$$

Therefore, if Eq. 146 is satisfied, it can be seen from Eqs. 143 and 144 that $K(k) \approx NV(k)$. The conditions specified by Eq. 146 represent the criteria for the system to be relatively insensitive to the precise form of the momentum distribution function.

Fig. 1. Figure 1 represents the excitation spectrum for a charged boson gas. The dashed line represents the result of Foldy and the solid line represents our prediction at low momenta. For large momenta, our prediction agrees with that of Foldy.

EXCITATION SPECTRUM

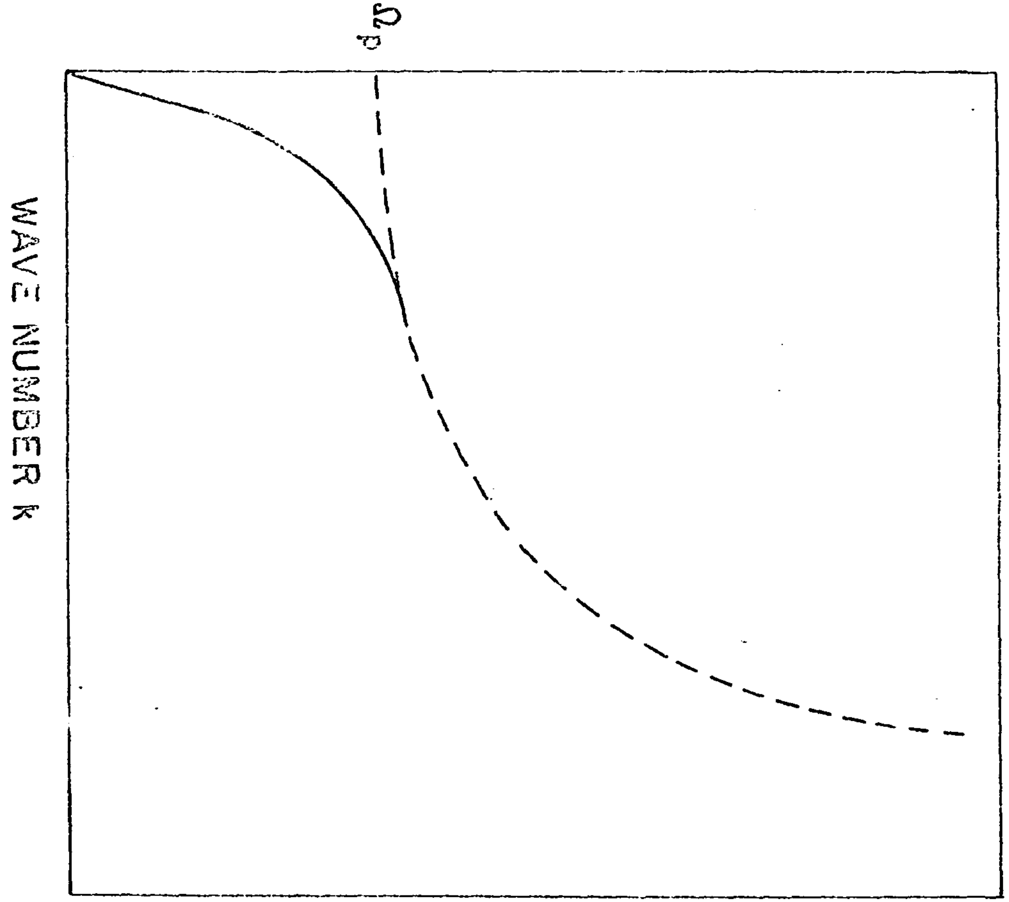
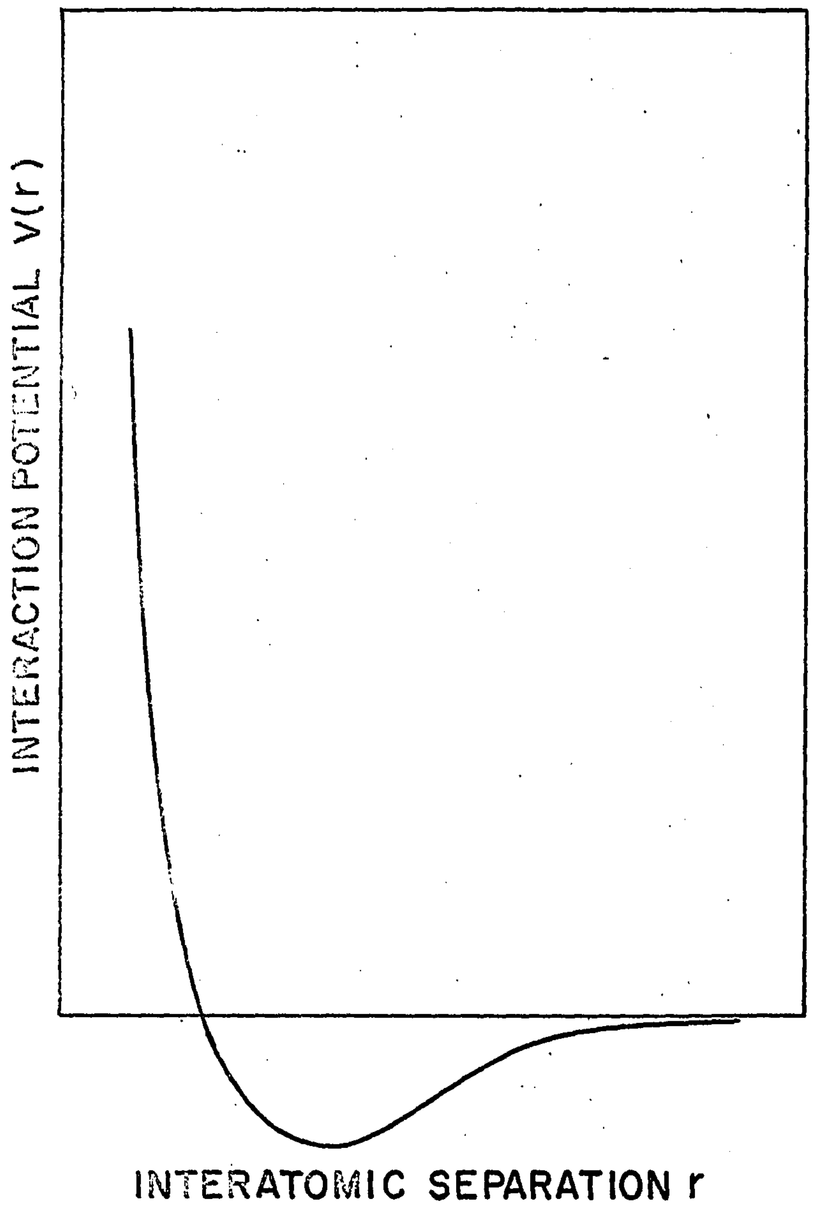


Fig. 2. Typical potential for molecular interactions


INTERACTION POTENTIAL V(r)
INTERATOMIC SEPARATION r

VI. CONCLUSIONS

An important step toward understanding the approximate procedures connected with both the equation of motion method of Part 2 in Chapter III and the extended Bogoliubov scheme is revealed by showing that all processes which contribute to the interaction are generated by the pair Hamiltonian alone, as is the case in superconductivity. Thus we know precisely which terms in the interaction part of the Hamiltonian are neglected as a result of the approximations involved. Of equal importance is that these approximations represent the most simple, non-trivial way the dynamic properties of the system may be considered. This is also true for superconductivity since analogous arguments may be constructed in that case. Perhaps it is not surprising that a very simple dynamical model is successful for both a collection of degenerate bosons and for superconductors since they are extremely correlated systems. This means that the internal degrees of freedom available to the bare particles are considerably reduced and, therefore, the dynamic behavior must be greatly simplified as compared to a normal, relatively uncorrelated system.

Lastly, it is of interest to consider the method for determining the form of the quasi-particle excitation operators. Using the method of Suhl and Werthamer (10) we proceeded by introducing as a first approximation, the correct operator in the limit of vanishing interaction, namely a_p^+. Then the equation of motion for this operator was studied which, in turn, suggested the next order of approximation. This formalism has the advantage in that it conserves particle number. Furthermore, it provides a consistent method for developing a better approximated excitation operator.

Other schemes for determining the quasi-particle excitation operator rely more on physical insight, which often provides for a considerable simplification of the formalism. However, these schemes usually lack the continuity desired in any complete theoretical development.

VII. BIBLIOGRAPHY

1. Henshaw, D. and Woods, A. Modes of Atomic Motions in Liquid Helium by Inelastic Scattering of Neutrons. Physical Review 121, 1266 (1961).

2. Bogoliubov, N. On the Theory of Superfluidity. Journal of Physics, U.S.S.R. 11, 23 (1947).

3. Brueckner, K. A. and Sawada, K. Bose-Einstein Gas with Repulsive Interactions: General Theory. Physical Review 106, 1117 (1957).

4. Lee, T. D., Huang, K., and Yang, C. N. Eigenvalues and Eigenfunctions of a Bose System of Hard Spheres and its Low-Temperature Properties. Physical Review 106, 1135 (1957).

5. Girardeau, M. and Arnowitt, R. Theory of Many Boson Systems: Pair Theory. Physical Review 113, 755 (1959).

6. Wentzel, G. Thermodynamically Equivalent Hamiltonian for Some Many-Body Problems. Physical Review 128, 965 (1960).

7. Valatin, J. G. and Butler, D. On the Collective Properties of a Boson System. Nuovo Cimento 10, 37 (1958).

8. Feynman, R. P. Atomic Theory of the Two-Fluid Model in Liquid Helium. Physical Review 94, 262 (1954).

9. Feynman, R. P. and Cohen, M. Energy Spectrum of the Excitations in Liquid Helium. Physical Review 102, 1189 (1956).

10. Suhl, H. and Werthamer, N. R. Higher Random-Phase Approximations in the Many-Body Problem. Physical Review 122, 359 (1961).

11. Werthamer, N. R. and Suhl, H. Renormalization of Many-Fermion Momentum-Space Distributions in Higher Random Phase Approximations. Physical Review 125, 1402 (1962).

12. Landau, L. D. and Lifshitz, E. M. Statistical Physics. Reading, Mass., Addison-Wesley Publishing Company, Inc., 1958.

13. Pines, D. The Many Body Problem. New York, W. A. Benjamin, Inc., 1961.

14. Miller, A., Pines, D., and Nozieres, P. Elementary Excitations in Liquid Helium. Physical Review 127, 1452 (1962).

15. Huang, K. and Klein, A. Phonons in Liquid Helium. Annals of Physics 30, 203 (1964).

16. Anderson, P. W. and Schrieffer, J. R. The Many Body Problem. New York, W. A. Benjamin, Inc., 1961.

17. Foldy, L. L. Charged Boson Gas. Physical Review 124, 649 (1961).

18. Bassichis, W. and Foldy, L. L. Analysis of the Bogoliubov Method Applied to a Simple Boson Model. Physical Review 133, A 935 (1964).

VIII. ACKNOWLEDGEMENTS

The author wishes to pay tribute to his major professors, past and present, each of whom are responsible for his intellectual development. They are:

1. Dr. J. J. Brady; who taught me to look for simplicity in physics, perhaps out of necessity.
2. Dr. D. C. Lu; a nice guy who deserved more.
3. Dr. D. J. Zaffarano; whose "white elephant" proportional counter drove me into theoretical physics.
4. Dr. N. Bernardes; he left me in a big hole, but I got out! Besides, South America is great!
5. Dr. M. Schutzer; who had some interesting ideas.
6. Dr. R. Good; a stand off, only he won.
7. Dr. J. M. Keller; his penetrating questions and relentless demands changed my heuristic arguments into concrete axioms, which is a contribution of real value. Besides that, he saw me through, a task which required monumental patience and understanding.

Whatever are my attainments in physics, I <u>owe</u> a great measure of it to Dr. Keller and his predecessors.

IX. APPENDIX A

This appendix demonstrates that the fluctuation terms previously neglected in evaluating the equation of motion are indeed small. The fluctuation terms arise because certain operators are replaced by their average values. Following Suhl and Werthamer (10), in their treatment of the electron gas, the contribution to the equation of motion from the fluctuation of the number operator is included by adding to b_p^+ a term proportional to $\sum_k V(k)[N_{p-k} - a_{p-k}^+ a_{p-k}]a_p^+$, just as the triple operator product is added to a_p^+ in forming Eq. 30. A solution of Eq. 21 for this operator is, to second order in the extended RPA, equivalent to finding a simultaneous solution for Eqs. 33, 34, and

$$[H,(N_{p-k} - a_{p-k}^+ a_{p-k})a_p^+]|0\rangle = \omega(p)(N_{p-k} - a_{p-k}^+ a_{p-k})a_p^+|0\rangle \qquad (147)$$

With Eq. 147, the fluctuation term contained in Eq. 23 may be evaluated, from which its relative contribution to the equation of motion is determined.

By expanding the commutator, Eq. 147 becomes

$$[\omega(p) - T_p][N_{p-k} - a_{p-k}^+ a_{p-k}]a_p^+ = \sum_{y,\lambda} V(\lambda)[a_{p-k}^+ a_{y-\lambda}^+ a_y a_{p-k-\lambda}$$

$$- a_{y-\lambda}^+ a_{p-k+\lambda}^+ a_y a_{p-k}]a_p^+ + \sum_\lambda [V(\lambda)a_{p-k+\lambda}^+ a_{p-\lambda}^+ a_{p-k}$$

$$- V(\lambda)a_{p-k}^+ a_{p-\lambda}^+ a_{p-k-\lambda} - V(k)a_{\lambda+k}^+ a_{p-k}^+ a_\lambda] \qquad *(148)$$

Following Suhl and Werthamer (10), Eq. 148 is approximated by replacing number operators with their ground state expectation values in only the interaction part of the equation. Such a replacement essentially reduces the demonstration of this appendix to a self-consistency argument. After making all replacements in Eq. 148, the result is

$$[\omega(p) - T_p][N_{p-k} - a^+_{p-k}a_{p-k}]a^+_p = \sum_\lambda N_p[V(\lambda)a^+_{p-k}a^+_{p-\lambda}a_{p-k-\lambda}$$

$$+ V(k)a^+_{p-k}a^+_{\lambda+k}a_\lambda - V(\lambda)a^+_{p-\lambda}a^+_{p-k+\lambda}a_{p-k}]. \qquad *(149)$$

By operating from the left with $\sum_{k'} V(k)$, Eq. 149 can be put into the form of the fluctuation term which appears in Eq. 23. That is

$$\sum_k V(k)[N_{p-k} - a^+_{p-k}a_{p-k}]a^+_p$$

$$= \sum_{q,k}{}' N_p V(k)\left[\frac{V(p-k-q) + V(k) - V(p-q)}{\omega(p) - T_p}\right]a^+_{p-k}a^+_{q+k}a_q. \qquad *(150)$$

The substitution of this result into Eq. 23 gives

$$[H,a^+_p] = [T_p + K(p)]a^+_p$$

$$+ \sum_{q,k}{}' V(k)\left\{1 - \left[\frac{V(p-k-q) + V(k) - V(p-q)}{\omega(p) - T_p}\right]N_p\right\}a^+_{p-k}a^+_{q+k}a_q. \qquad *(151)$$

By comparing Eq. 151 with Eq. 103, which is the equation of motion considered in deducing the results of Part 3 in Chapter III, it appears that if

$$N_p\left[\frac{V(p-k-q) + V(k) - V(p-q)}{\omega(p) - T_p}\right] \ll 1$$

over the interval specified by Ineqs. 104, then the fluctuation term is of negligible importance. Over this interval, the above inequality is approximated by

$$\left(\frac{N_p}{N}\right)\frac{NV(p)}{\omega(p) - T_p} \ll 1 \qquad (152)$$

Since $NV(p)$ is on the order of the potential energy per particle, the quantity $NV(p)[\omega(p) - T_p]^{-1}$ is on the order of unity except for momenta very near the origin, and since N_p/N is certainly infinitesmal for all momenta on the order of or greater than δ and probably for all momenta other than zero, Ineq. 152 is satisfied everywhere except possibly very near the origin. In fact, by substituting Eq. 86 for N_p into Ineq. 152, the inequality is shown to be satisfied to order N^{-1} for all $p \neq 0$. Thus, the neglect of the fluctuation term appears to be justified for the many-boson problem studied in this paper. A similar argument may be constructed for the fluctuation of the operator products $a_p^+ a_{-p}^+$.

X. APPENDIX B

The extended RPA is an infinite sequence of approximations designed to yield the best linearized equation of motion for the operator that generates the elementary excitations of the system. The usual procedure is to terminate this sequence after a desired number of operations and then to neglect the remaining non-linear terms. The non-linear terms that remain after the second order of approximation in the many-boson problem are designated by Q in Eq. 107. In this appendix it will be shown that these terms actually give no contribution to the equation of motion within the bounds of the approximations that have been used and, therefore, their neglect is completely justified.

To calculate the contribution to the equation of motion from the triple term in Eq. 103, Eq. 34 was evaluated in an approximate way. This result yielded singles, triples, and the uncontractable quintuples Q.

$$Q = \overline{\sum_{m,n}} V(n)[a^+_{m-n} a^+_{p+n-k} a^+_{q+k} a_m a_q$$

$$+ a^+_{m-n} a^+_{q+k+n} a^+_{p-k} a_m a_q - a^+_{m-n} a^+_{p-k} a^+_{q+k} a_{q-n} a_m] \tag{153}$$

where the bar over the sum indicates that no subscript of any a^+ coincides with the subscript of any a in each term. That is, all possible number operators have been extracted from Q. These Q terms can be included in the equation of motion by evaluating Eq. 35 in conjunction with Eqs. 33 and 34. The quintuple commutator in Eq. 35 yields, upon contraction, triple, quintuple, and uncontractable septuple terms. It is the triples extracted from the quintuple commutator that couple the Q terms to the triples in Eq. 103. It has already been argued that the triple product in

Eq. 103 contributes to the equation of motion only in the momentum interval bounded by Ineqs. 104 and, as a result, all other triple terms have been discarded. Therefore, in evaluating the contribution from Q, to the same order of approximation, only triple terms that contribute in this interval need be retained. No such terms exist. Since the Q commutator couples the quintuple terms to the triple terms and since all higher order commutators must couple with Eqs. 33 and 34 through Q, all higher order terms may also be neglected. Thus, Eqs. 33 and 34 represent a complete set of coupled equations for determining the excitation spectrum. Mathematically, the Q terms may be carried through the formalism, in which case Eq. 110 becomes

$$\sum_{q,k}{}' V(k)a^+_{p-k}a^+_{q+k}a_q = -\sum_k \frac{K(k)V(k)N_{p-k}a^+_p}{\omega(p)+T_p+K(p)} + \sum_{q,k}{}' \frac{V(k)Q}{\omega(p)+T_p+K(p)}$$

$$= -\sum_k \frac{K(k)V(k)N_{p-k}a^+_p}{\omega(p)+T_p+K(p)} + \frac{1}{\omega(p)} \sum_{q,k}{}' \frac{V(k)[H,Q]}{\omega(p)+T_p+K(p)} \qquad *(154)$$

The second sum on the right hand side of Eq. 154 contains no triple terms in the momentum region specified by Ineqs. 104. Therefore, it has no effect on the linearization of Eq. 103 and may be discarded.

XI. APPENDIX C

In this appendix a test of some of the approximations made earlier in the text is performed on He II. This is accomplished by taking advantage of the experimentally known excitation spectrum for liquid helium. To evaluate K(k), the Fourier transform of the potential is approximated by an equivalent hard sphere potential of radius a. This approximation while not completely satisfactory, is expected to be an adequate representation for V(p) at small momenta.

$$K(k) = \sum_p V(p-k)N_p \approx \sum_p \frac{4\pi a}{m\,\Omega} N_p \approx \frac{4\pi a N}{m\,\Omega} \qquad (155)$$

where Ω is the volume of the system

$$a \approx 2.5 \times 10^{-13} \text{ cm}$$

$$\rho = \frac{mN}{\Omega} \approx .15 \text{ gm/cm}^3$$

$$m \approx 6.7 \times 10^{-24} \text{ gms}$$

These values yield

$$K(k) \approx 75^\circ K$$

$$T_k = 6\, k^2 \,{}^\circ K$$

where k is given in inverse angstroms A^{-1}. From Eqs. 86 and 87, N_p is

$$N_p = \frac{1}{2}\left[\frac{T_p + K(p)}{\omega(p)} - 1\right]$$

The result for N_p is given on Fig. 3, from which the effective width of the momentum distribution is estimated to be less than .1 A^{-1}. That is

$$\delta < .1\, A^{-1} \qquad (156)$$

Earlier in the text it was shown that a necessary and sufficient condition for $|\frac{\alpha(k)}{\beta(k)}| \approx 1$, for $|\underset{\sim}{k}| \leq \delta$ was that

$$\frac{\omega(k)}{\mu(k)} \ll 1 \qquad \text{for} \qquad |\underset{\sim}{k}| \leq \delta .$$

Using the above calculated values for He II

$$\frac{\omega(k)}{\mu(k)} \leq .026$$

for all $|\underset{\sim}{k}| \leq .1\ A^{-1}$. We therefore conclude that even for coupling as strong as in He II, the approximate result derived for $\eta(p)$ in Part 2 of Chapter III is valid.

In Appendix A it was shown that the neglect of fluctuation terms is permissible if

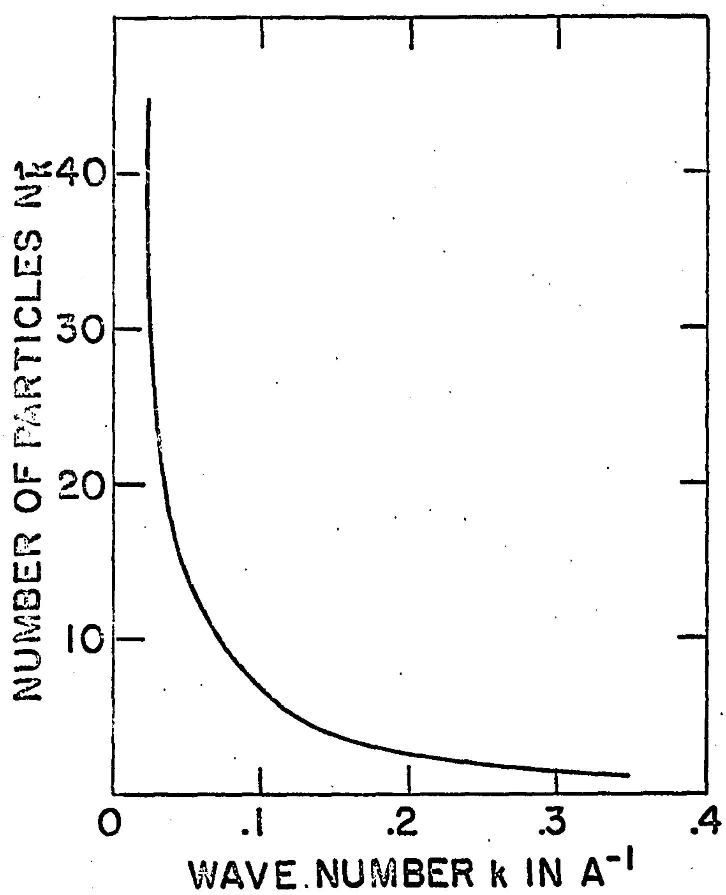
$$(\frac{N_p}{N}) \frac{NV(p)}{\omega(p) - T_p} \ll 1.$$

By substituting Eq. 86 for N_p into this inequality, it becomes

$$\frac{1}{N} [\frac{NV(p)}{2}(\frac{1}{T_p} - \frac{1}{\omega(p)})] \ll 1.$$

From the substitution of values appropriate to He II, into this expression, it is evident that the inequality holds for all momenta different from zero. The conclusion is that, even for He II, the momentum distribution function is sufficiently local so that all approximations which depend on this locality are valid.

Fig. 3. The momentum distribution function for He II


NUMBER OF PARTICLES N_k
10
20
30
40
0
.1
.2
.3
.4
WAVE NUMBER k IN A^{-1}