

Statistical Mechanics of a Nonideal Boson Gas: Pair Hamiltonian Model*

MARSHALL LUBAN†‡§

*The Enrico Fermi Institute for Nuclear Studies, and Department of Physics,
University of Chicago, Chicago, Illinois*

(Received April 30, 1962)

This work is concerned with a microscopic model of a nonideal boson gas. The Hamiltonian is treated in a rigorous manner free of all approximations and, in particular, the Bogoliubov approximation of replacing the zero-momentum single-particle creation and destruction operators by a c number is entirely avoided. Utilizing a method due to Wentzel, the Hamiltonian is replaced by one involving products of two second quantized operators which, in general, can be diagonalized. This replacement is shown to be rigorously valid in the infinite volume limit for all temperatures despite the avoidance of the Bogoliubov approximation. It is found that the assumption of a positive-definite quasi-particle excitation spectrum $\epsilon(\mathbf{k})$ becomes untenable for temperatures T less than a critical value T_c , if the interparticle potential is described by a certain kernel which possesses positive eigenvalues only, corresponding to a sufficiently repulsive interparticle force. Assuming that $\epsilon(\mathbf{k})=0$ only for $\mathbf{k}=0$, it is found that for $T < T_c$ the system undergoes an Einstein condensation into the $\mathbf{k}=0$ single-particle state, and the integral equations characterizing the system are precisely the same as would be obtained if the Bogoliubov approximation were made, proving within the framework of this model the strict validity of this approximation procedure. The well-known criterion for an Einstein condensation

$v(0) > 0$, where $v(\mathbf{k})$ is the Fourier transform of the interparticle potential, is shown to be a weaker statement of our eigenvalue criterion. Further, in agreement with Girardeau and Arnowitt, it is found that an energy gap separates $\epsilon(0)$ and $\epsilon(\mathbf{k})$ for $k > 0$. An approximation method is developed for solving the integral equations which describe those systems which undergo an Einstein condensation, and it is shown that this method can be justified if $|T - T_c| \lesssim T_c/10$, and in cases of short-range repulsive interparticle forces and systems for which $\rho v(0)$ possesses a certain prescribed upper bound, ρ being the number of particles per unit volume. The transition temperature is found to be lower than the corresponding quantity for the ideal boson gas of the same density. A detailed discussion of the thermal properties of the system in the vicinity of T_c is also given. In an Appendix a general type of smeared Einstein condensation is assumed, and it is found that for systems in which this property occurs $\epsilon(\mathbf{k})$ is linear for small k . This ansatz is shown to be tenable only if $v(0) < 0$. Finally, by assuming an appropriate pseudopotential representation of a hard repulsive core and by including a weak, long-ranged attractive force between particles, $\epsilon(\mathbf{k})$ shows a non-monotonic behavior of the same qualitative type as observed in liquid He⁴.

I. INTRODUCTION

THIS work concerns itself with a microscopic model of a nonideal boson gas. One is motivated to make such a study for several reasons. Of the numerous phenomenological theories that have been developed in an attempt to explain the peculiar properties of liquid He⁴, that of Landau¹ has met with the greatest success. The main feature of Landau's work is a description of the energy-momentum spectrum of the elementary excitations in the liquid. Although the existence of such an excitation spectrum has been demonstrated experimentally,² one has at present only qualitative arguments and some semiquantitative calculations to support such a scheme theoretically.³ Furthermore, above approximately 1.6°K conclusions of the Landau theory fail to agree with experiment. In particular, the mechanism responsible for the lambda transition remains a complete mystery to it as well as to all other existing theories. A successful microscopic theory of liquid helium is therefore very much in demand.

One possible procedure for developing a first-principles theory for a system of $N > 2$ interacting particles is to replace the actual Hamiltonian by one which is readily diagonalized. Of course, for this procedure to be meaningful, one must provide convincing proof that the model system gives an accurate description of the actual system.

Representative of attempts along this line is the work of Bogoliubov.⁴ In this work Bogoliubov anticipates that at $T=0^\circ\text{K}$ a system of bosons which interact through a two-body potential that is predominantly positive possesses the property that the single-particle state of zero momentum is occupied by a finite fraction of the system (Einstein condensation). With this idea in mind he develops the following scheme for truncating the actual second-quantized Hamiltonian H : Ignore all terms of H but those involving two or more zero momentum creation and destruction operators a_0^\dagger, a_0 . This yields a Hamiltonian which we shall call H_1 . Now replace $a_0^{(\dagger)}$ by $N_0^{1/2}$, where N_0 is a c number of the same order of magnitude as N , the total number of particles. The resulting Hamiltonian, which we shall refer to as H_B , is easily diagonalized, and it describes a gas of non-interacting excitations or so called quasi-particles. In agreement with Landau's work the energy-momentum spectrum of these excitations is linear for small momenta.

Existing arguments for the relevance of H_B serving as a replacement for H run as follows⁵: If one attempts

* Supported in part by the U. S. Atomic Energy Commission.

† Presented as a thesis to the Department of Physics, University of Chicago, in partial fulfillment of the requirements for the Ph.D. degree.

‡ National Science Foundation Predoctoral Fellow.

§ Present address: Institute for Advanced Study, Princeton, New Jersey.

¹ L. D. Landau, *J. Phys. (U.S.S.R.)* **5**, 71 (1941); **11**, 91 (1947).

² D. G. Henshaw and A. D. B. Woods, *Phys. Rev.* **121**, 1266 (1961).

³ R. P. Feynman, *Progress in Low-Temperature Physics*, edited by J. C. Gorter (North-Holland Publishing Company, Amsterdam, 1955), Vol. I, Chap. II. M. Cohen and R. P. Feynman, *Phys. Rev.* **102**, 1189 (1956).

⁴ N. N. Bogoliubov, *J. Phys. (U.S.S.R.)* **11**, 23 (1947).

⁵ See, for example, K. A. Brueckner and K. Sawada, *Phys. Rev.* **106**, 1117 (1957).

to use perturbation theory to calculate the ground-state energy of H , with a gas of noninteracting particles serving as the unperturbed system, in the third and higher approximations one encounters integrals which diverge at low momenta. Furthermore, the severest divergence in each approximation order can be generated by H_1 alone. Taking the severity of a divergence as a measure of the disparity between the chosen unperturbed system and the actual system, we can anticipate that H_1 is a good replacement for H . Moreover, if ψ is the ground-state eigenfunction of H , the occupation of the $\mathbf{k}=0$ single-particle state by $N_0 \approx N$ particles implies that $\langle \psi | [a_0, a_0^\dagger] | \psi \rangle \langle \psi | a_0^\dagger a_0 | \psi \rangle^{-1} \approx 1/N$. It is, therefore, plausible to regard a_0, a_0^\dagger as identical operators to be replaced by $N_0^{1/2}$. The Hamiltonians H_1 and H_B are then anticipated to give similar, if not identical, results.

The present work deals with a model system described by a Hamiltonian \mathcal{H}_P which is essentially a somewhat generalized version of H_1 . One might, therefore, anticipate that \mathcal{H}_P will serve as a better replacement for H than does H_1 . In addition, the model possesses the highly attractive feature that it can be diagonalized as it stands. In particular, one can entirely avoid replacing $a_0^{(\dagger)}$ by a c number. Because this is a soluble model the following matters are open to study:

1. *Einstein condensation.* To our knowledge there exists no treatment which obtains as a derived result (in contrast to an assumption made at the outset) the existence of an Einstein condensation in a nonideal boson gas. Instead, one obtains an *a posteriori* inference that such is fact. Such a procedure is unsatisfactory in that it becomes difficult to obtain a quantitative criterion for the existence of the condensation. In particular, little is known of the effect upon the condensation of including a weakly attractive portion to the interparticle potential.

2. *Excitation spectrum.* Of further interest is the nature of the excitation spectrum in this model. Is the linear form at low momenta of the excitation spectrum derived by Bogoliubov a fortuitous result, or does one obtain this result even if further interactions are included? More generally, what are the effects of truncating a Hamiltonian?

3. *Phase transition.* Systems in which an Einstein condensation occurs are expected to undergo a phase transition at a finite temperature T_c . Consequently, the effect of the interparticle interactions on T_c and the thermodynamic properties of the system can serve within the context of this model as a test of London's hypothesis⁶ that the lambda transition in liquid He⁴ is to be interpreted as an Einstein condensation in a boson fluid.

4. *Validity of approximation procedures.* An outstanding feature of a soluble model is that it can serve as a

testing ground for various approximation procedures. In the present work one can test the validity of the Bogoliubov approximation⁷ not only for $T=0^\circ\text{K}$ but also for $T=T_c$ —where it is most suspect. The following remarks show the importance of such a test: (a) An immediate consequence of the Bogoliubov approximation is the decoupling of the $\mathbf{k}=0$ state from all other single-particle momentum states. But such a decoupling, in turn, implies a two-fluid description of the nonideal boson system. (b) Hugenholtz and Pines⁸ have stated the theorem that at $T=0^\circ\text{K}$ phonon modes will exist in any boson gas in which repulsive forces predominate. Their proof is contingent upon the validity for boson systems of the ground state linked cluster expansion,⁹ which in turn requires the validity of the Bogoliubov approximation.

In this work, we utilize a procedure developed by Wentzel¹⁰ to construct from \mathcal{H}_P a Hamiltonian \mathcal{H}^0 in which boson creation and destruction operators only appear quadratically. Employing statistical perturbation theory, one can prove fairly convincingly that for very large systems the volume-proportional part of the thermodynamic potential (Helmholtz free energy in the grand ensemble) determined by using \mathcal{H}^0 is the same as the corresponding quantity determined by using \mathcal{H}_P . For systems in which an Einstein condensation occurs, the proof of this result is closely related to the proof that the Bogoliubov approximation is strictly valid. The “thermodynamically equivalent” Hamiltonian \mathcal{H}^0 involves two functions to be found by solving a pair of coupled, nonlinear integral equations. The diagonalization of \mathcal{H}^0 can be affected but this requires great care. In fact, one finds an intimate connection between the properties of the interparticle potential, the presence of a zero in the excitation spectrum, and the existence of an Einstein condensation. These matters are discussed in Sec. II.

The discussion in Appendix E is closely related to that of Sec. II. In that Appendix we allow for a “smearing” of the Einstein condensation in momentum space, and we establish the relationship of such a smearing to the properties of the excitation spectrum as well as to the inclusion of a long-ranged, weakly attractive force between particles.

In Secs. III and IV, we display an approximation method for solving the integral equations which describe systems in which an Einstein condensation occurs. It is shown that this method can be justified if $T \approx T_c$, and if we restrict our attention to either weak, short-range repulsive interparticle forces, or to short-range repulsive forces and systems of low density. Section V is devoted to the evaluation of the thermodynamic po-

⁷ Henceforth, we shall call the approximation of replacing $a_0^{(\dagger)}$ by a c number, irrespective of its value, the Bogoliubov approximation.

⁸ N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

⁹ J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

¹⁰ G. Wentzel, Phys. Rev. **120**, 1572 (1960).

⁶ F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II.

tential and to the study of the phase transition. Finally, in Sec. VI we summarize the conclusions of our work.

In concluding this section we must mention that other studies of the present model have been made,¹⁰⁻¹³ but these use the Bogoliubov approximation and/or a variational theorem technique, and, in addition, do not attempt a complete analysis. Furthermore, there is a lack of unanimity in the conclusions of these authors.

II. DIAGONALIZATION

1. Thermodynamically Equivalent Hamiltonian

Imagine a large but finite cubic box of volume V containing N identical bosons each of mass m . We shall eventually allow N and V to approach infinity in such a way that the density $\rho = N/V$ is held constant.¹⁴ This will be achieved by constructing an infinite set of such systems, each with the same density ρ , with successive members of the set being characterized by increasingly larger values of V . The force between two particles will be assumed dependent only upon the distance separating them. The Hamiltonian of such a system expressed in the formalism of second quantization is¹⁵

$$H = \sum_{\mathbf{k}} (k^2/2m) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p}, \mathbf{q}} v(\mathbf{k}) a_{\mathbf{p}+\mathbf{k}}^\dagger a_{\mathbf{q}-\mathbf{k}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}}, \quad (1)$$

where $a_{\mathbf{k}}$ and $a_{\mathbf{k}}^\dagger$ are the usual boson destruction and creation operators, respectively, for single-particle plane wave states satisfying periodic boundary conditions with respect to V . The quantity $v(\mathbf{k})$ is the Fourier transform of the interparticle potential, and it is spherically symmetric: $v(\mathbf{k}) = v(k)$. It should be remarked that the existence of $v(k)$ forbids the use of potentials which for small distances r behave as r^{-n} , $n \geq 3$.

The Hamiltonian \mathcal{H}_P , called the "pair Hamiltonian," is obtained by ignoring all interaction terms of (1) with the exception of the following three types: (a) $\mathbf{k} = 0$; (b) $\mathbf{k} = \mathbf{q} - \mathbf{p}$, ($\mathbf{p} \neq \pm \mathbf{q}$); (c) $\mathbf{q} = -\mathbf{p}$, ($\mathbf{k} = 0$). That is,¹⁶

$$\begin{aligned} \mathcal{H}_P = & \sum_{\mathbf{k}} [(k^2/2m) - \mu] a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \\ & + (2V)^{-1} v(0) \left(\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right) \left[\left(\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \right) - 1 \right] \\ & + (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \pm \mathbf{k}} v(\mathbf{p} - \mathbf{k}) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \\ & + (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \mathbf{k}} v(\mathbf{p} - \mathbf{k}) a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_{-\mathbf{p}} a_{\mathbf{p}}. \quad (2) \end{aligned}$$

¹¹ D. N. Zubarev and Iu. A. Tserkovnikov, Doklady Akad. Nauk (S.S.S.R.) **120**, 991 (1958) [translation: Soviet Phys.—Doklady **3**, 603 (1958)].

¹² J. G. Valatin and D. Butler, Nuovo cimento **10**, 37 (1958).

¹³ M. Girardeau and R. Arnowitt, Phys. Rev. **113**, 755 (1959); M. Girardeau, J. Math. Phys. **3**, 131 (1962).

¹⁴ For brevity, we shall refer to this limit as the "volume limit."

¹⁵ We choose units so that $\hbar = 1$.

¹⁶ In Sec. I, we have made mention of the Hamiltonian H_1 which generates the severest divergence in each approximation order

We may refer to the last three terms of \mathcal{H}_P as representing forward, exchange, and pair scattering, respectively. In (2), the single-particle kinetic energy has been replaced by $(k^2/2m) - \mu$, where μ is a Lagrangian multiplier, the chemical potential, which will allow us to use the grand ensemble.¹⁷ Despite the presence of terms involving products of four operators, the thermal properties of \mathcal{H}_P in the volume limit can be determined in a rigorous manner utilizing Wentzel's "method of thermodynamically equivalent Hamiltonian."¹⁰

Following Wentzel, we define operators $B_{\mathbf{k}1}$, $B_{\mathbf{k}2}$ by

$$\begin{aligned} B_{\mathbf{k}1} &= a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - \xi_{\mathbf{k}}, \\ B_{\mathbf{k}2} &= a_{-\mathbf{k}} a_{\mathbf{k}} - \eta_{\mathbf{k}}, \end{aligned} \quad (3)$$

where the quantities $\xi_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ are real functions, of the nature of trial functions. In terms of these operators, we express \mathcal{H}_P as

$$\mathcal{H}_P = \mathcal{H}^0 + \mathcal{H}', \quad (4)$$

where

$$\begin{aligned} \mathcal{H}' = & (2V)^{-1} v(0) \sum_{\mathbf{k}, \mathbf{p}} B_{\mathbf{k}1}^\dagger B_{\mathbf{p}1} \\ & + (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \pm \mathbf{k}} v(\mathbf{p} - \mathbf{k}) B_{\mathbf{k}1}^\dagger B_{\mathbf{p}1} \\ & + (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \mathbf{k}} v(\mathbf{p} - \mathbf{k}) B_{\mathbf{k}2}^\dagger B_{\mathbf{p}2}, \end{aligned} \quad (5)$$

$$\mathcal{H}^0 = \mathcal{H}_P - \mathcal{H}' = \mathcal{U}$$

$$+ \sum_{\mathbf{k}} [f_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} h_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} a_{\mathbf{k}})]. \quad (6)$$

In (6), the c -number quantities \mathcal{U} , $f_{\mathbf{k}}$, and $h_{\mathbf{k}}$ are expressed in terms of the trial functions as

$$\begin{aligned} \mathcal{U} = & - (2V)^{-1} v(0) \sum_{\mathbf{k}, \mathbf{p}} \xi_{\mathbf{k}} \xi_{\mathbf{p}} - (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \pm \mathbf{k}} v(\mathbf{p} - \mathbf{k}) \xi_{\mathbf{k}} \xi_{\mathbf{p}} \\ & - (2V)^{-1} \sum_{\mathbf{k}, \mathbf{p} \neq \mathbf{k}} v(\mathbf{p} - \mathbf{k}) \eta_{\mathbf{k}} \eta_{\mathbf{p}}, \end{aligned} \quad (7)$$

$$\begin{aligned} f_{\mathbf{k}} = & (k^2/2m) - \mu + V^{-1} v(0) \left[\left(\sum_{\mathbf{p}} \xi_{\mathbf{p}} \right) - \frac{1}{2} \right] \\ & + V^{-1} \sum_{\mathbf{p} \neq \pm \mathbf{k}} v(\mathbf{p} - \mathbf{k}) \xi_{\mathbf{p}}, \end{aligned} \quad (8)$$

$$h_{\mathbf{k}} = V^{-1} \sum_{\mathbf{p} \neq \mathbf{k}} v(\mathbf{p} - \mathbf{k}) \eta_{\mathbf{p}}. \quad (9)$$

It is important to note that all of the above sums

when one attempts to calculate the ground state energy of (1) using perturbation theory. This Hamiltonian is given by the following truncated portion of \mathcal{H}_P :

$$H_1 = \sum_{\mathbf{k}} (k^2/2m) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2} N(N-1) V^{-1} v(0) + V^{-1} \sum_{\mathbf{k}} v(k) [a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_0^\dagger a_0 + \frac{1}{2} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_{-\mathbf{k}} a_{\mathbf{k}})]$$

(see reference 5). Further, H_B is given by

$$H_B = \sum_{\mathbf{k}} \{ [(k^2/2m) + (N_0/V) v(k)] a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + (N_0/2V) v(k) (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{-\mathbf{k}} a_{\mathbf{k}}) \} + N(N-1) v(0)/2V.$$

(A prime on a summation sign means that the $\mathbf{k} = 0$ term is to be omitted.)

¹⁷ We choose a script letter to denote the pair Hamiltonian so as to indicate explicitly that we are using the grand ensemble.

include \mathbf{k} and/or $\mathbf{p}=0$. The thermodynamic potentials associated with \mathcal{H}^0 and \mathcal{H}_P are

$$\Omega^0 = -\beta^{-1} \ln \text{Tr}[\exp(-\beta\mathcal{H}^0)], \quad (10a)$$

$$\Omega_P = -\beta^{-1} \ln \text{Tr}[\exp(-\beta\mathcal{H}_P)]. \quad (10b)$$

The quantity β^{-1} is the product of Boltzmann's constant κ and the absolute temperature T .

Thus far, the separation (4)–(6) has been purely formal. The point of Wentzel's method, however, is that for trial functions $\xi_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ which minimize Ω^0 , i.e.,

$$\partial\Omega^0/\partial\xi_{\mathbf{k}}=0, \quad \partial\Omega^0/\partial\eta_{\mathbf{k}}=0, \quad (11)$$

\mathcal{H}' fails to contribute to the volume-proportional part of Ω_P . That is to say, if \mathcal{H}^0 is constructed from $\xi_{\mathbf{k}}$ and $\eta_{\mathbf{k}}$ which satisfy (11), *in the volume limit the thermodynamic properties of the system given by the pair Hamiltonian (2) are determined by \mathcal{H}^0 alone.* The proof of this statement in the present work where we do not replace $a_0^{(\dagger)}$ by a c number is based on the fact that the fluctuations of $a_0^\dagger a_0$ and $a_0 a_0$ can be shown to be small. This question is discussed in Appendix A.

In the following, we shall employ the notation $\langle A \rangle$ for the ensemble average of a quantity A taken with respect to \mathcal{H}^0 :

$$\langle A \rangle = \text{Tr}\{\exp\beta(\Omega^0 - \mathcal{H}^0)A\}. \quad (12)$$

Using (6), (10a), and (12) one can show¹⁰ that (11) is satisfied if

$$\begin{aligned} \xi_{\mathbf{k}} &= \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle, \\ \eta_{\mathbf{k}} &= \langle a_{-\mathbf{k}} a_{\mathbf{k}} \rangle = \langle a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger \rangle. \end{aligned} \quad (13)$$

The ensemble average in (12) can be performed once \mathcal{H}^0 is diagonalized. For this purpose it is convenient to write \mathcal{H}^0 as

$$\mathcal{H}^0 = \mathcal{U} + \mathcal{H}^0_0 + \frac{1}{2} \sum_{\mathbf{k}}' \mathcal{H}^0_{\mathbf{k}}, \quad (14)$$

where

$$\mathcal{H}^0_0 = f_0 a_0^\dagger a_0 + \frac{1}{2} h_0 (a_0 a_0 + a_0^\dagger a_0^\dagger), \quad (15a)$$

$$\mathcal{H}^0_{\mathbf{k}} = f_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}}) + h_{\mathbf{k}} (a_{-\mathbf{k}} a_{\mathbf{k}} + a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger). \quad (15b)$$

Here and in the following, a prime on a summation sign means that the term with zero subscript is to be omitted. Following Bogoliubov,⁴ we introduce new destruction and creation operators $\alpha_{\mathbf{k}}$ and $\alpha_{\mathbf{k}}^\dagger$ defined by the linear transformation

$$a_{\mathbf{k}} = u_{\mathbf{k}} \alpha_{\mathbf{k}} + v_{\mathbf{k}} \alpha_{-\mathbf{k}}^\dagger \quad (\text{all } \mathbf{k}), \quad (16)$$

where $u_{-\mathbf{k}} = u_{\mathbf{k}}^*$, $v_{-\mathbf{k}} = v_{\mathbf{k}}^*$. To insure that these operators satisfy the Bose-Einstein commutation rules, one must impose the restriction

$$u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1. \quad (17)$$

Substitution of (16) into (15) yields an expression which is diagonal in the new representation if

$$f_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} + \frac{1}{2} h_{\mathbf{k}} (u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2) = 0. \quad (18)$$

The simultaneous Eqs. (17) and (18) possess a solution if $f_{\mathbf{k}} \neq \pm h_{\mathbf{k}}$:

$$u_{\mathbf{k}}^2 = \frac{1}{2} [(f_{\mathbf{k}}/\epsilon_{\mathbf{k}}) + 1], \quad v_{\mathbf{k}}^2 = \frac{1}{2} [(f_{\mathbf{k}}/\epsilon_{\mathbf{k}}) - 1], \quad (19)$$

where

$$\epsilon_{\mathbf{k}} = (f_{\mathbf{k}}^2 - h_{\mathbf{k}}^2)^{1/2}. \quad (20)$$

For this transformation to be physically meaningful it is necessary that $\epsilon_{\mathbf{k}}$ be real; i.e., $|h_{\mathbf{k}}|$ cannot exceed $|f_{\mathbf{k}}|$. Further, if $|f_{\mathbf{k}}| = |h_{\mathbf{k}}|$, i.e., $\epsilon_{\mathbf{k}} = 0$, Eq. (18) implies $u_{\mathbf{k}} = \pm v_{\mathbf{k}}$ which is incompatible with (17). That is to say, only for those values of \mathbf{k} for which the real functions $f_{\mathbf{k}}$ and $h_{\mathbf{k}}$ satisfy $|h_{\mathbf{k}}| < |f_{\mathbf{k}}|$ is (15) diagonalized by (16). We shall first restrict our discussion to the case for which $\epsilon_{\mathbf{k}} > 0$ for all \mathbf{k} .

2. Positive-Definite Excitation Spectrum

In this case \mathcal{H}^0 and Ω^0 are given by

$$\mathcal{H}^0 = \mathcal{U} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}}, \quad (21)$$

$$\Omega^0 = \mathcal{U} + \beta^{-1} \sum_{\mathbf{k}} \ln[1 - \exp(-\beta\epsilon_{\mathbf{k}})], \quad (22)$$

where

$$\mathcal{U} = \mathcal{U} + \frac{1}{2} \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - f_{\mathbf{k}}). \quad (23)$$

We may interpret (21) as follows: The Hamiltonian \mathcal{H}^0 describes an infinite set of independent harmonic oscillators whose excited states can be described in terms of noninteracting excitations or quasi-particles of momentum \mathbf{k} and energy $\epsilon_{\mathbf{k}}$. We rephrase an earlier statement: The entire thermodynamics of the pair Hamiltonian system is described by an ideal gas of quasi-particles.¹⁸ The remaining problem is to obtain $f_{\mathbf{k}}$, $h_{\mathbf{k}}$, and thus $\epsilon_{\mathbf{k}}$ in terms of the given quantities m , $\rho = N/V$, $v(k)$, and T .

We begin by noting that the number of quasi-particles populating the state \mathbf{k} at the temperature T is

$$\langle \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} \rangle = [\exp(\beta\epsilon_{\mathbf{k}}) - 1]^{-1}. \quad (24)$$

Further, using (12), (16), and (19) the following relations are easily proved

$$\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{2} [(f_{\mathbf{k}}/\epsilon_{\mathbf{k}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{k}}) - 1] = \xi_{\mathbf{k}}, \quad (25)$$

$$\langle a_{-\mathbf{k}} a_{\mathbf{k}} \rangle = -\frac{1}{2} (h_{\mathbf{k}}/\epsilon_{\mathbf{k}}) \coth \frac{1}{2}\beta\epsilon_{\mathbf{k}} = \eta_{\mathbf{k}}. \quad (26)$$

In the following we may imagine V to be so large that

¹⁸ We wish to stress that the thermodynamic equivalence of \mathcal{H}_P and \mathcal{H}^0 is not at all a trivial result. This remark is prompted by the fact that \mathcal{H}_P consists of products of four $a_{\mathbf{k}}^{(\dagger)}$ operators in contrast to \mathcal{H}^0 which is composed of products of two operators. Although it is quite popular in current many-body studies to linearize all equations of motion (random phase approximation), that is to say, to replace Eq. (1) by an alternate Hamiltonian composed of products of two rather than four operators, it is generally quite difficult to justify such a procedure. Such linearization schemes generally imply that the actual many-body system is equivalent to an infinite set of independent harmonic oscillators, whose excited states, therefore, are variously described in terms of noninteracting excitations or quasi-particles such as phonons, plasmons, etc. For the present model this description is valid because of the equivalence of \mathcal{H}_P and \mathcal{H}^0 .

$V^{-1} \sum_{\mathbf{k}} \dots$ can be replaced by $(2\pi)^{-3} \int d\mathbf{k} \dots$.¹⁹ Furthermore, we shall assume that $f_{\mathbf{k}}$ and $h_{\mathbf{k}}$ are spherically symmetric, i.e., $f_{\mathbf{k}} = f_k$, $h_{\mathbf{k}} = h_k$. Using (8), (9), (25), and (26), one finds the following coupled, nonlinear integral equations for $f(k)$ and $h(k)$:

$$f(k) = \frac{k^2}{2m} - \mu + \rho v(0) + \int_0^\infty dp p^2 J(k, p) \times \left[\frac{f(p)}{\epsilon(p)} \coth\left(\frac{1}{2}\beta\epsilon\right) - 1 \right], \quad (27)$$

$$h(k) = - \int_0^\infty dp p^2 J(k, p) \frac{h(p)}{\epsilon(p)} \coth\left(\frac{1}{2}\beta\epsilon(p)\right). \quad (28)$$

The quantity $J(k, p)$ is defined by

$$J(k, p) = (8\pi^2)^{-1} \int_{-1}^{+1} d\mu v[(k^2 + p^2 - 2kp\mu)^{1/2}]; \quad (29)$$

it is the angular average of $v(\mathbf{k} - \mathbf{p})$ for fixed magnitudes k and p . We remark that $J(k, p)$ is a real, symmetric kernel.

The chemical potential μ appearing in (27) is determined from the auxiliary condition

$$\rho = V^{-1} \sum_{\mathbf{k}} \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{4\pi^2} \int_0^\infty dk k^2 \left[\frac{f(k)}{\epsilon(k)} \coth\left(\frac{1}{2}\beta\epsilon\right) - 1 \right]. \quad (30)$$

Equations (20), (27), (28), and (30) are the basic equations for the model when $\epsilon(k)$ is positive-definite.

We note that (28) possesses the trivial solution $h(k) \equiv 0$ for all k . For this solution it follows from (20) that $\epsilon(k) = f(k)$,²⁰ which in turn means that the auxiliary condition (30) cannot be satisfied for temperatures below a critical value T_c [it obviously cannot be satisfied for $T = 0^\circ\text{K}$, since it is presupposed in this section that $\epsilon(k) > 0$ for all k]. Expressed precisely, T_c is the smallest value of T for which the equations

$$\epsilon(k) = \frac{k^2}{2m} - \mu + \rho v(0) + 2 \int_0^\infty dp p^2 J(k, p) \frac{1}{e^{\beta\epsilon} - 1}, \quad (31)$$

$$\rho = \frac{1}{2\pi^2} \int_0^\infty dk k^2 \frac{1}{e^{\beta\epsilon} - 1}, \quad (32)$$

are simultaneously satisfied. Continuing this argument, a positive-definite excitation spectrum for $T < T_c$ re-

¹⁹ Since $\epsilon_0 \neq 0$ it is clear from (25) that $\langle a_0^\dagger a_0 \rangle$ is a well behaved volume-independent quantity; i.e., there is no Einstein condensation in the system. The replacement of the sum by an integral is therefore valid. This matter is discussed in detail later in this section.

²⁰ Since $\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$ cannot be negative it follows from (25) that $f(k) > 0$ for all k .

quires the existence of a nontrivial solution to (28). The obvious question is: Under what conditions does (28) possess a nontrivial solution?

Multiply both sides of (28) by $\theta(k) = k^2(h/\epsilon) \coth\frac{1}{2}\beta\epsilon$ and integrate from $k=0$ to $k=\infty$:

$$- \int_0^\infty dk k^2 \frac{h^2(k)}{\epsilon(k)} \coth\left(\frac{1}{2}\beta\epsilon(k)\right) = \int_0^\infty dp \int_0^\infty dk \theta(k) J(k, p) \theta(p) \equiv (\theta, J\theta). \quad (33)$$

The left side of (33) is negative-semidefinite. If $J(k, p)$ is a kernel such that $(\theta, J\theta) \geq 0$ for all θ , it follows from (33) that for *all* temperatures the only solution to (28) is $h(k) \equiv 0$. Such a condition for real, symmetric kernels is well known in the theory of integral equations: All the eigenvalues of $J(k, p)$ are positive.²¹ For kernels of this type, if $T < T_c$ our ansatz of a positive-definite excitation spectrum becomes untenable; that is to say, for $T < T_c$ a zero must occur in the excitation spectrum.

It is a difficult task to phrase in a precise way this condition upon the eigenvalues of $J(k, p)$ in terms of the interparticle potential.²² Instead, we shall make several semiquantitative remarks.

It is easily shown²¹ that a necessary (but not sufficient) condition for $J(k, p)$ to be a J_+ kernel is that its diagonal elements be non-negative, i.e., $J(k, k) \geq 0$. By suitable change of variable, one can write this condition as

$$J(k, k) = \frac{1}{8\pi^2 k^2} \int_0^{2k} ds s v(s) \geq 0. \quad (34)$$

For small k , Eq. (34) becomes

$$J(k, k) \approx (4\pi^2)^{-1} v(0) \geq 0. \quad (35)$$

That is to say, that the space average of the interparticle potential be positive is a necessary condition for the presence of a zero in the excitation spectrum. This, of course, is the well-known criterion for phonon excitations.⁴ The following statements, which are proved in Appendix B, unfortunately show that (35) is a very ineffective expression of the necessary condition (34). (a) Equation (34) rules out the possibility of two-body bound states; (35) does not. (b) Even if $v(0) > 0$ and the interparticle potential does not allow for two-body bound states it is possible for (34) to be violated.

An interesting example where one can prove that a zero occurs in the excitation spectrum is provided by $v(k) = 4\pi a/m$, the hard sphere pseudopotential used by Lee, Huang, and Yang in their studies of the boson hard sphere gas.²³ In this case $(\theta, J\theta)$, proportional to (θ, θ) ,

²¹ See F. G. Tricomi, *Integral Equations* (Interscience Publishers, Inc., New York, 1957), Chap. 3.

²² For brevity, we shall call $J(k, p)$ a J_+ kernel if all its eigenvalues are positive.

²³ T. D. Lee, K. Huang, and C. N. Yang, Phys. Rev. **106**, 1135 (1957).

is positive-semidefinite. As a further example, if $J(k, p) = [4\pi^2 v(0)]^{-1} v(k)v(p)$ then $(\theta, J\theta) \geq 0$ as long as $v(0) > 0$.¹²

Thus far, we have exhibited an intimate connection between the properties of the eigenvalue spectrum of $J(k, p)$ and the existence of a zero in the quasi-particle excitation spectrum. This connection can be further extended to the question of the existence of an Einstein condensation in this model.

According to (25), the number of particles occupying the single-particle state \mathbf{k} is

$$\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle = \frac{1}{2} [(f_{\mathbf{k}}/\epsilon_{\mathbf{k}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{k}}) - 1].$$

For *all* temperatures and *all* values of \mathbf{k} the right side of this equation is finite and volume-independent. Crucial to obtaining this result was the assumption that \mathcal{H}^0 is diagonalized by (16)–(20), which in turn means that $\epsilon_{\mathbf{k}} \neq 0$. We, therefore, conclude that if $\epsilon_{\mathbf{k}}$ is positive-definite the system fails to undergo an Einstein condensation.²⁴

On the basis of these remarks, we can expect novel results if we study systems whose interparticle interactions are described by J_+ kernels. The remainder of this work concerns itself with such systems.

3. Zero in the Excitation Spectrum

In the previous discussion we have seen that if the eigenvalues of the kernel $J(k, p)$ defined by (29) are all positive, it follows that for temperatures less than T_c there exists at least one momentum value \mathbf{k} for which $h_{\mathbf{k}} = \pm f_{\mathbf{k}}$, i.e., $\epsilon_{\mathbf{k}} = 0$. We have also seen that in such an instance the transformation (16)–(20) fails to diagonalize $\mathcal{H}_{\mathbf{k}}^0$ given by Eq. (15). Consequently, the first equalities of (25) and (26) fail to hold for the momentum \mathbf{k} , thus making inapplicable all subsequent equations. We now modify our equations to allow for this possibility. It is essential to note that (13) continues to hold since the diagonalization of \mathcal{H}^0 was of no relevance to its derivation.

On the basis of the following remarks we shall assume throughout the rest of this work that $\epsilon_{\mathbf{k}} \neq 0$ for \mathbf{k} which do not vanish in the volume limit. If, on the contrary, $\epsilon_{\mathbf{k}} = 0$ for $\mathbf{k} = \mathbf{k}_0 \neq 0$, and if $\epsilon_{\mathbf{k}}$ is a continuous function of \mathbf{k} it follows that it is possible to impart a net momentum $\mathbf{k}_0 \neq 0$ to the system by expending a vanishingly small amount of energy, namely, by exciting a quasi-particle of momentum $\mathbf{k} \approx \mathbf{k}_0$. Such a situation, however, must be regarded as highly unphysical as long as \mathbf{k}_0 does not vanish in the volume limit. Since the continuity of $\epsilon_{\mathbf{k}}$ is merely a conjecture one should accept these re-

²⁴ One cannot speak of an Einstein condensation unless some momentum state(s) is(are) populated by a number of particles proportional to a positive power of the volume. From the point of view of the infinite set of systems which gives meaning to the operation $\lim_{V \rightarrow \infty, \rho = N/V = \text{constant}}$, there is no essential difference between two volume-independent functions, which is not the case for two functions one of which is volume-independent, the other proportional to V^x , $x > 0$.

marks not as a proof, but rather as giving plausibility to the assumed form of $\epsilon_{\mathbf{k}}$.

In the present section we shall assume that V is large but finite, and further that $\epsilon_0 = 0$, whereas $\epsilon_{\mathbf{k}} \neq 0$ for *all* nonzero values of \mathbf{k} . With this assumption the complete equations (25) and (26) apply only to nonzero \mathbf{k} . In the remainder of this section, unless written explicitly to the contrary, all momenta are nonzero. In this instance one finds the following equations²⁵ for $f_{\mathbf{k}}$ and $h_{\mathbf{k}}$:

$$f_{\mathbf{k}} = (k^2/2m) - \mu + \rho v(0) + V^{-1} \xi_0 v(k) + (2V)^{-1} \sum_{\mathbf{p}}' v(\mathbf{p} - \mathbf{k}) \times [(f_{\mathbf{p}}/\epsilon_{\mathbf{p}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{p}}) - 1], \quad (36a)$$

$$f_0 = -\mu + \rho v(0) + (2V)^{-1} \sum_{\mathbf{p}}' v(\mathbf{p}) \times [(f_{\mathbf{p}}/\epsilon_{\mathbf{p}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{p}}) - 1], \quad (36b)$$

$$h_{\mathbf{k}} = V^{-1} \eta_0 v(k) - (2V)^{-1} \sum_{\mathbf{p}}' v(\mathbf{p} - \mathbf{k}) \times (h_{\mathbf{p}}/\epsilon_{\mathbf{p}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{p}}), \quad (37a)$$

$$h_0 = -(2V)^{-1} \sum_{\mathbf{p}}' v(\mathbf{p}) (h_{\mathbf{p}}/\epsilon_{\mathbf{p}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{p}}). \quad (37b)$$

As mentioned previously, a prime on a summation sign means that the zero index term is to be omitted. Further, the auxiliary condition (30) is replaced by

$$\rho = (\xi_0/V) + (2V)^{-1} \sum_{\mathbf{k}} [(f_{\mathbf{k}}/\epsilon_{\mathbf{k}}) \coth(\frac{1}{2}\beta\epsilon_{\mathbf{k}}) - 1]. \quad (38)$$

The two seemingly independent quantities ξ_0 and η_0 will now be related.

Two choices are open for insuring that $\epsilon_0 = 0$. For argument's sake we take the factor $f_0 + h_0$ to be zero:

$$f_0 + h_0 = 0, \quad T < T_c. \quad (39)$$

By forming the following commutator

$$[a_0 a_0, \mathcal{H}^0] = 2f_0(a_0 a_0 - a_0^\dagger a_0 - 1/2), \quad (40)$$

one finds

$$\text{Tr}\{\exp\beta(\Omega^0 - \mathcal{H}^0)[a_0 a_0, \mathcal{H}^0]\} = 2f_0(\eta_0 - \xi_0 - 1/2) = 0. \quad (41)$$

The left side of (41) vanishes since the trace operation is invariant under a cyclic interchange of factors. Only in rare instances can we expect f_0 to vanish, so it follows that

$$\eta_0 = \xi_0 + 1/2. \quad (42)$$

The existence of an Einstein condensation in this system is easily seen. If η_0/V and ξ_0/V vanish in the volume limit, Eqs. (36)–(38) reduce to (27), (28), and (30). But these latter equations cannot be satisfied simultaneously since by assumption $J(k, p)$ is a J_+ kernel. There is no alternative but

$$\lim_{V \rightarrow \infty, \text{fixed } \rho} \xi_0/V = \lim_{V \rightarrow \infty, \text{fixed } \rho} \eta_0/V \neq 0, \quad T < T_c. \quad (43)$$

²⁵ For the present discussion it is safest to delay the limiting procedure of replacing sums by integrals.

That is to say, for $T < T_c$ the system undergoes an Einstein condensation.

Using (36b) and (37b), we find as a further consequence of (39) that

$$\mu = \rho v(0) + \frac{1}{4\pi^2} \int_0^\infty dk k^2 v(k) \left[\frac{f(k)}{\epsilon(k)} \coth(\tfrac{1}{2}\beta\epsilon) - 1 \right] - \frac{1}{4\pi^2} \int_0^\infty dk k^2 v(k) \frac{h(k)}{\epsilon(k)} \coth \tfrac{1}{2}\beta\epsilon(k). \quad (44)$$

We can now eliminate μ from (36)–(38) in favor of $s = \xi_0/V$, the density of particles occupying the $\mathbf{k}=0$ state:

$$f(k) = \frac{k^2}{2m} + sv(k) + \int_0^\infty dp p^2 [J(k, p) - J(0, p)] \times \left[\frac{f(p)}{\epsilon(p)} \coth(\tfrac{1}{2}\beta\epsilon) - 1 \right] + \int_0^\infty dp p^2 J(0, p) \frac{h(p)}{\epsilon(p)} \coth \tfrac{1}{2}\beta\epsilon(p), \quad (45)$$

$$h(k) = sv(k) - \int_0^\infty dp p^2 J(k, p) \frac{h(p)}{\epsilon(p)} \coth \tfrac{1}{2}\beta\epsilon(p), \quad (46)$$

$$\rho = s + \frac{1}{4\pi^2} \int_0^\infty dp p^2 \left[\frac{f(p)}{\epsilon(p)} \coth(\tfrac{1}{2}\beta\epsilon) - 1 \right], \quad (47)$$

$$f(0) = -h(0) = \int_0^\infty dk k^2 J(0, k) \frac{h(k)}{\epsilon(k)} \coth \tfrac{1}{2}\beta\epsilon(k). \quad (48)$$

Equations (45)–(48) which are applicable when $T < T_c$ complement (31) and (32) which describe the system above the transition temperature.

Two remarks are in order at this point: (a) In contrast to (28), the equation for $h(k)$ when $\epsilon(k)$ is positive-definite, Eq. (46) is not a homogeneous integral equation, and therefore it does not possess the trivial solution $h(k) \equiv 0$.

(b) Equations (45)–(47) have been obtained by Wentzel¹⁰ and by Zubarev and Tserkovnikov¹¹ in their respective studies of \mathcal{H}_P . In both studies use was made of the Bogoliubov approximation $a_0^{(\dagger)} = N_0^{1/2}$, but the methods for determining N_0 were somewhat different. One can, therefore, conclude that within the framework of the pair Hamiltonian the Bogoliubov approximation is rigorously valid for all temperatures $T < T_c$ for those systems characterized by J_+ kernels.

To conclude this section, we shall give a brief and incomplete analysis of (45)–(47) discussing first the structure of the excitation spectrum. For small k , Eqs.

(45), (46), and (48) give

$$f(k) = f(0) + sv(0) + O(k^2), \quad (49)$$

$$h(k) = -f(0) + sv(0) + O(k^2), \quad (50)$$

so that

$$\epsilon(k) \xrightarrow{k \rightarrow 0} [4sv(0)f(0) + O(k^2)]^{1/2}. \quad (51)$$

We therefore conclude, in agreement with Girardeau and Arnowitt,¹³ that a gap separates $\epsilon(0)$ ($=0$) and $\epsilon(k)$, $k \neq 0$. Equations (49) and (50) show clearly the role of the Einstein condensation in effecting (51). Furthermore, the discontinuous behavior of $f(k)$ and $h(k)$ is easily traced back to the definition of \mathcal{H}_P where in order to avoid repetition of terms it was necessary to impose index restrictions on the exchange and pair scattering terms.²⁶

We wish to emphasize that the result (51) does not satisfy a theorem due to Bogoliubov,^{27,28} that a system of bosons whose Hamiltonian satisfies a certain gauge condition possesses an excitation spectrum which is linear at low momenta. Specifically, Bogoliubov's theorem applies to a system whose Hamiltonian is invariant under the infinitesimal transformation $a_{\mathbf{k}} \rightarrow a_{\mathbf{k}}' = a_{\mathbf{k}} - i(a_{\mathbf{k}+\mathbf{q}} + a_{\mathbf{k}-\mathbf{q}})\delta\xi$, where \mathbf{q} is an arbitrary vector and $\delta\xi$ is an arbitrary infinitesimal c -number quantity. The complete Hamiltonian given by (1) is invariant under this transformation whereas \mathcal{H}_P and H_B (see footnote 16), truncated versions of (1) are not. As such the linear spectrum of H_B must be regarded as a fortuitous result.

Although we do not wish to discuss the solution of (45)–(47) in this section, it is nevertheless instructive to quote the results of an iterative procedure for solving these equations.

(a) Zeroth approximation [$v(k)=0$]:

$$\epsilon^0(k) = f^0(k) = k^2/2m, \quad h^0(k) = 0, \quad (52)$$

$$s^0/\rho = 1 - (T/T_c^0)^{3/2}, \quad \kappa T_c^0 = 2\pi[\zeta(\tfrac{3}{2})]^{-2/3}\rho^{2/3}/m. \quad (53)$$

Equations (52) and (53) describe the *ideal* boson gas.²⁹

(b) First approximation: The quantities f , h , ϵ , and s which appear on the right sides of (45)–(47) are replaced by their values obtained in the zeroth approximation. The left sides of these equations give the results of the

²⁶ This perhaps may explain why Valatin and Butler (see footnote 12) found $\epsilon(k) \propto k$ for small k .

²⁷ N. N. Bogoliubov, Dubna Report D-781, 1961 (unpublished).

²⁸ Hugenholtz and Pines (footnote 8) enunciated a similar theorem somewhat earlier, but, as mentioned in Sec. I, because they assumed for the complete Hamiltonian the validity of the replacement $a_0^{(\dagger)} = N_0^{1/2}$ their proof cannot be regarded as complete.

²⁹ We shall frequently encounter the quantity $\zeta(\sigma) = \sum_{n=1}^\infty n^{-\sigma}$, the Riemann zeta function. Values of this function are given in E. Jahnke and F. Emde, *Tables of Functions* (Dover Publications, Inc., New York, 1945), 4th ed., p. 273.

first approximation:

$$f^1(k) = \frac{k^2}{2m} + s^0 v(k) + 2 \int_0^\infty dp p^2 [J(k, p) - J(0, p)] \times \frac{1}{\exp(\beta p^2/2m) - 1}, \quad (54)$$

$$h^1(k) = s^0 v(k), \quad (55)$$

$$\epsilon^1(k) = [f^1(k)^2 - h^1(k)^2]^{1/2}, \quad (56)$$

$$\frac{s^1}{\rho} = 1 - \frac{1}{4\pi^2} \int_0^\infty dk k^2 \left[\frac{f^1(k)}{\epsilon^1(k)} \coth(\frac{1}{2}\beta\epsilon^1) - 1 \right]. \quad (57)$$

This iteration procedure can be continued in an obvious fashion. Equations (54)–(56) have been given by Zubarev and Tserkovnikov (ZT).¹¹ Since for small k the quantity $J(k, p) - J(0, p)$ is of order k^2 the excitation spectrum $\epsilon^1(k)$ is linear in this range. In fact at $T=0$ Eqs. (54)–(56) reduce to the values of f , h , and ϵ which describe H_B (see footnote 16). It should be mentioned that ZT refrained from continuing this iterative procedure since they felt that a treatment based on the Bogoliubov approximation $a_0^{(+)} = N_0^{1/2}$ should be valid only for weakly interacting bosons. However, since we have not made the Bogoliubov approximation we feel justified in continuing this iteration procedure. In particular, an energy gap, which already appears in the second approximation, is an inescapable characteristic of the pair Hamiltonian model.

It can be shown that the results of the first approximation can be obtained by considering a Hamiltonian which consists of the forward and exchange scattering terms of \mathcal{H}_P and only those pair scattering terms which were retained by Bogoliubov.^{4,16} This criticism of the work of ZT is of more general importance: If one wishes to obtain the correct consequences of the pair Hamiltonian model something approaching an exact solution of (31) and (32) and (45)–(47) is necessary. In particular, the above iteration procedure, whose zeroth approximation describes the ideal boson gas, appears ill-suited for this purpose except for systems of very weakly interacting bosons.

III. SOLUTION OF INTEGRAL EQUATIONS ($T \geq T_c$)

1. Preliminaries

In this and the following section we display an approximation method for solving the integral equations which describe the system when $J(k, p)$ is of the J_+ form (see Sec. II 2). This method can be justified if $|T - T_c| \lesssim T_c/10$, and if we restrict our attention to short range repulsive interactions and to systems for which $\rho v(0)$ possesses a certain prescribed upper bound. We shall first treat the case of $T \geq T_c$. The solution for $T < T_c$ forms the discussion of Sec. IV.

Above the transition temperature the excitation

spectrum of the system is found by solving the integral Eq. (31) subject to the auxiliary condition (32). For this purpose it is convenient to write (31) in the following equivalent form:

$$\epsilon(k) = \epsilon(0) + \frac{k^2}{2m} + 2 \int_0^\infty dp p^2 [J(k, p) - J(0, p)] \frac{1}{e^{\beta\epsilon} - 1}, \quad (58)$$

$$\epsilon(0) = -\mu + \rho v(0) + 2 \int_0^\infty dp p^2 J(0, p) \frac{1}{e^{\beta\epsilon} - 1}. \quad (59)$$

Note that $\epsilon(k)$ is a function of both k and T ; for brevity we have not written the latter dependence explicitly.

We shall briefly digress in order to study the form assumed by Eqs. (45)–(47) when the temperature is raised to T_c . At the transition temperature the density s of particles occupying the $k=0$ state is zero. Thus, the limiting form of (45)–(47) is

$$\epsilon(k) = \frac{k^2}{2m} + 2 \int_0^\infty dp p^2 [J(k, p) - J(0, p)] \frac{1}{e^{\beta\epsilon} - 1}, \quad (60)$$

$$\rho = \frac{1}{2\pi^2} \int_0^\infty dp p^2 \frac{1}{e^{\beta\epsilon} - 1}, \quad (61)$$

where $\beta_c = 1/\kappa T_c$. The resemblance between (32), (58), and (60), (61) is not accidental. Indeed, we expect that the equations which describe \mathcal{H}_P for $T < T_c$ become identical with those that apply for $T > T_c$ when $T \rightarrow T_c^-$. This is accomplished if $\epsilon(0, T_c) = 0$. The alternative, namely, that $\epsilon(k)$ is discontinuous for all k when $T = T_c$ is physically unacceptable, for such implies that the thermodynamic potential is discontinuous at that temperature.

We now return to the discussion of the solution of (58). It is convenient to measure the strength of the interparticle potential $V(r)$ in terms of an energy W rather than in terms of a coupling constant. The spatial variation of $V(r)$ is expressed in terms of the dimensionless quantity r/R , where R plays the role of a range parameter. Thus, we write

$$V(r) = W\phi(r/R). \quad (62)$$

The Fourier transform of $V(r)$ is given by

$$v(k) = 4\pi W R^3 \times \frac{1}{kR} \int_0^\infty dx x \phi(x) \sin kRx. \quad (63)$$

It is essential to note that $v(k)$ is a function of kR .

Throughout the remainder of this work we shall require ϕ to satisfy the following two conditions:

$$\phi(x) \geq 0 \quad (\text{all } x), \quad (64)$$

$$I_{2n}/I_4 \leq \frac{1}{6}(2n-1)! \quad (n \geq 3), \quad (65)$$

where

$$I_n = \int_0^\infty dx x^n \phi(x). \quad (66)$$

Using (29) and (63), one finds

$$J(k, k) = \frac{1}{\pi k^2} \int_0^\infty dr V(r) \sin^2 kr. \quad (67)$$

Because of (64) it follows that $J(k, k) \geq 0$ as is required of a J_+ kernel (see Sec. II 2).

Two examples will illustrate the nature of the requirement of Eq. (65). If $\phi(x) = e^{-x}/x$ and $x^{-2} \exp(-x^2)$, one finds

$$I_{2n}/I_4 = \frac{1}{6}(2n-1)!$$

and

$$\frac{1}{6}(2n-1)! 48[2^{2n}(n-1)!(2n-1)]^{-1},$$

respectively. Quite generally, Eq. (65) is satisfied if $\phi(x)$ rapidly decreases to zero when $x > 1$.

The purpose of (65) is twofold. First, it assures that $v(k)$ may be expanded as a Taylor series about $kR=0$ with a radius of convergence not smaller than $kR=1$. Specifically,

$$v(k) = v(0)[1 - (k^2/k_c^2)S(kR)], \quad kR < 1, \quad (68)$$

where

$$k_c^2 = 6(I_2/I_4)(1/R^2) > 0. \quad (69)$$

The precise form of $S(kR)$ is of little interest. The essential point is that because of (65), and this is the second purpose of that equation, $S(kR)$ satisfies the following inequality (consult Appendix C)

$$|S(kR) - 1| \leq \frac{(kR)^2}{1 - (kR)^2}, \quad kR < 1. \quad (70)$$

Define k_s as $k_s = (10R)^{-1}$. It follows from (70) that $S(kR)$ differs from unity by less than 1% as long as $k < k_s$. Note further that a small value of the range parameter R assures a large value of k_s . Similar considerations apply to $J(k, p)$, although in this case there is the added condition $k_c R \geq 1$. This latter condition is well satisfied if, as is the requirement for the validity of (65), $\phi(x)$ drops to zero rapidly when $x > 1$. In what we refer to as the "effective-mass approximation"³⁰

$$v(k) = v(0)(1 - k^2/k_c^2), \quad 0 \leq k \leq k_s, \quad (71a)$$

$$J(k, p) = J(0, p) - \frac{v(0)}{4\pi^2} \frac{k^2}{k_c^2}, \quad 0 \leq k, p \leq k_s. \quad (71b)$$

2. Method of Solution

We now proceed to display our approximation method for solving Eq. (58). Making use of (71b), we write

(58) as

$$\begin{aligned} \epsilon(k) = & [\epsilon(0) + k^2/2m] - \frac{v(0)}{2\pi^2} \frac{k^2}{k_c^2} \int_0^{k_s} dp p^2 \frac{1}{e^{\beta\epsilon} - 1} \\ & + 2 \int_{k_s}^\infty dp p^2 [J(k, p) - J(0, p)] \frac{1}{e^{\beta\epsilon} - 1}, \end{aligned} \quad (72)$$

$0 < k < k_s.$

We can anticipate that for a sufficiently small range parameter R the value of k_s is so large that $(e^{\beta\epsilon} - 1)^{-1}$ will serve as a strong convergence factor, so that one might be able to ignore the third term on the right side of (72). Indeed, using Eqs. (64) and (65) one can show (see Appendix C) that the *exact* solution of (58) has as a lower bound a rapidly increasing positive function of k : $\epsilon(k) \geq 0$, $\epsilon(k) \geq (k^2/2m) + [\epsilon(0) - 2\rho v(0)]$, whichever is larger. The consequence of this is that the ratio of the third term to the second term of (72) is less than

$$(k_s^2/2m\kappa T)^{1/2} \{ \exp\beta[(k_s^2/2m) - 2\rho v(0)] - 1 \}^{-1},$$

as long as $k_s^2/2m\kappa T_c \geq 9$ and $0 \leq T - T_c \leq T_c/10$. If, for example, $2\rho v(0) = \kappa T_c$ this ratio is less than 10^{-3} . For weak short-range forces, or for short-range forces and systems of low density, these conditions will be satisfied. For such cases, we feel justified to write (72) as

$$\epsilon(k) = \epsilon(0) + k^2/2m^*, \quad 0 \leq k \leq k_s, \quad (73)$$

where m^* , an effective mass, satisfies

$$\frac{1}{m^*} = \frac{1}{m} - \frac{1}{\pi^2} \frac{v(0)}{k_c^2} \int_0^{k_s} dk k^2 \frac{1}{\exp\beta[\epsilon(0) + k^2/2m^*] - 1}. \quad (74)$$

With the same accuracy and subject to the same conditions we can write (32) as

$$\rho = \frac{1}{2\pi^2} \int_0^{k_s} dk k^2 \frac{1}{\exp\beta[\epsilon(0) + k^2/2m^*] - 1}. \quad (75)$$

Comparison of (74) and (75) shows that

$$m^* = m[1 - 2m\rho v(0)/k_c^2]^{-1} > m. \quad (76)$$

Note that m^* is temperature independent. That the effective mass is larger than the true mass is a direct consequence of (64), the requirement that $V(r)$ be non-negative.

We now determine the transition temperature T_c . Because $\epsilon(0, T_c) = 0$, Eq. (75) becomes²⁹

$$\begin{aligned} \rho \simeq & \frac{1}{2\pi^2} \int_0^\infty dk k^2 \frac{1}{\exp(\beta_c k^2/2m^*) - 1} \\ & = \left(\frac{m^* \kappa T_c}{2\pi} \right)^{3/2} \zeta\left(\frac{3}{2}\right). \end{aligned} \quad (77)$$

³⁰ The reason for this terminology will become clear presently.

More important, for the same particle density the

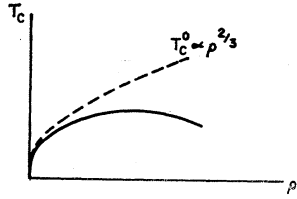


FIG. 1. Qualitative plot of the transition temperature T_c given by (79) as a function of density. The quantity T_c^0 is the corresponding quantity for the ideal boson gas.

product of m^* and T_c is equal to the corresponding quantity for the ideal boson gas; that is to say

$$m^* T_c = m T_c^0 \quad (\text{const } \rho), \quad (78)$$

where T_c^0 is the ideal gas transition temperature [see Eq. (53)]. Combining (76) and (78), it follows that

$$T_c = T_c^0 [1 - 2m\rho v(0)/k_c^2] < T_c^0. \quad (79)$$

A qualitative plot of T_c as a function of ρ is shown in Fig. 1.

As is well known, the lambda transition in liquid He⁴ occurs at $T_\lambda = 2.18^\circ\text{K}$, whereas the transition temperature in the ideal boson gas of the same density occurs at $T_c^0 = 3.13^\circ\text{K}$.³¹ The unanswerable question of course is whether the result (79), in particular $T_c < T_c^0$, is just fortuitous, being peculiar only to the present model, or possibly would result from more advanced models of systems of bosons interacting via repulsive forces.

It has been pointed out that $k_c R \geq 1$ must hold if (71b) is to be a good approximation to $J(k, p)$. It is then easy to see that (79) is valid only for very small differences $T_c^0 - T_c$. (With $k_s^2/2m = 9\kappa T_c$, $2\rho v(0) = \kappa T_c$, and $k_c = R^{-1}$ one finds $T_c^0 - T_c = 5.55 \times 10^{-4} T_c^0$.) We, therefore, cannot apply (79) to a discussion of the density dependence of the transition temperatures for which HeI and HeII are in equilibrium. Nevertheless, it is interesting that according to (79) the quantity $\partial T_c / \partial \rho$ is negative for sufficiently high densities (see Fig. 1). Indeed, the HeI-HeII equilibrium curve in the $T-1/\rho$ plane is so characterized.

It is unfortunate that we have been able to obtain an approximate solution of (32) and (58) only for the range of parameters previously mentioned. In view of the nontriviality of \mathcal{H}_P it would be interesting to determine the functional dependence of T_c on ρ for more general values of these parameters.

IV. SOLUTION OF INTEGRAL EQUATIONS ($T < T_c$)

In this section we present a method for obtaining an accurate approximate solution of Eqs. (45)–(47) in the temperature range $0 \leq T_c - T \leq T_c/10$. Because we are interested in the thermodynamic properties of the system in the immediate vicinity of the phase transition we shall not attempt to extend our treatment to lower temperatures.

Our method is based upon the following considerations. At $T = T_c$ the density s of particles occupying the

$\mathbf{k}=0$ state is zero, in which case the only solution of (46) is $h(k) \equiv 0$. Slightly below the transition temperature $h(k) = O(s)$; i.e., $h(k)$ is very nearly zero. This suggests the following: Consider a value of T only slightly smaller than T_c . Set $s=0$ in (45) and (46) and obtain the solution $\epsilon_0(k)$ of the resulting integral equation. Replace f , ϵ , and h on the right sides of (45) and (46) by $f_0(k) = \epsilon_0(k)$, and $h_0(k) \equiv 0$, respectively. The left sides of these equations are denoted by f_1 and h_1 . These results are used to repeat the process. This is shown explicitly in the following:

(a) Zeroth approximation ($s=0$):

$$h_0(k) = 0, \quad (80)$$

$$\epsilon_0(k) = f_0(k) = \frac{k^2}{2m} + 2 \int_0^\infty dp \, p^2 [J(k, p) - J(0, p)] \times \frac{1}{\exp[\beta \epsilon_0(p)] - 1}. \quad (81)$$

(b) First approximation:

$$h_1(k) = sv(k), \quad (82)$$

$$f_1(k) = sv(k) + \epsilon_0(k), \quad (83)$$

$$\epsilon_1(k) = \{\epsilon_0(k) [\epsilon_0(k) + 2sv(k)]\}^{1/2}. \quad (84)$$

(c) Second approximation:

$$h_2(k) = sv(k) - \int_0^\infty dp \, p^2 J(k, p) \frac{sv(p)}{\epsilon(p)} \coth \frac{1}{2} \beta \epsilon_1(p), \quad (85)$$

$$f_2(k) = \frac{k^2}{2m} + sv(k) + \int_0^\infty dp \, p^2 [J(k, p) - J(0, p)] \times \left[\frac{f_1(p)}{\epsilon_1(p)} \coth \left(\frac{1}{2} \beta \epsilon_1 \right) - 1 \right] + \int_0^\infty dp \, p^2 J(0, p) \frac{sv(p)}{\epsilon_1(p)} \coth \frac{1}{2} \beta \epsilon_1(p), \quad (86)$$

$$\epsilon_2(k) = +[f_2^2(k) - h_2^2(k)]^{1/2}. \quad (87)$$

It is instructive to give a physical interpretation of the equations of the zeroth approximation. Had we started with a Hamiltonian, say $\mathcal{H}_{f, s}$, consisting of only the forward and exchange scattering terms of \mathcal{H}_P , one can show that for $T \geq T_c$ the system would be described by Eqs. (31) and (32), the very equations which describe the *pair Hamiltonian* model in this temperature range. That is to say, the pair scattering terms of \mathcal{H}_P are of physical consequence only if the $\mathbf{k}=0$ single-particle state is populated by a finite fraction of the system, i.e., only if $T < T_c$. Now then, for T slightly smaller than T_c one expects that the pair scattering terms are playing a very minor role. Accordingly, for $T \approx T_c$ it is reason-

³¹ K. R. Atkins, *Liquid Helium* (Cambridge University Press, London, 1960).

able to totally ignore the pair scattering terms in the lowest approximation and simply use $\mathcal{H}_{f,e}$ to determine the excitation spectrum. Indeed, for $T < T_c$ the following equations describe $\mathcal{H}_{f,e}$:

$$\epsilon(k) = \frac{k^2}{2m} + sv(k) + 2 \int_0^\infty dp \, p^2 [J(k,p) - J(0,p)] \times \frac{1}{\exp[\beta\epsilon(p)] - 1}, \quad (88)$$

$$\rho = s + \frac{1}{2\pi^2} \int_0^\infty dp \, p^2 \frac{1}{\exp[\beta\epsilon(p)] - 1}. \quad (89)$$

For $T \approx T_c$ the quantity $sv(k)$ is effectively zero and (88) is then precisely (81). Our lowest approximation should be compared with that of Zubarev and Tserkovnikov [see (52)]. In their scheme for solving (45)–(47) the lowest approximation is the ideal boson gas. There is no doubt that in any approximation order our scheme gives results which have a closer resemblance to the exact solution of (45)–(47) than do those of Zubarev and Tserkovnikov.

For small k the quantity $J(k,p) - J(0,p)$ is of order k^2 . Thus, from Eqs. (80)–(87) one finds $\epsilon_0(k) = O(k^2)$, $\epsilon_1(k) = O(k)$, whereas

$$\epsilon_2(k) \xrightarrow[k \rightarrow 0]{} \Delta > 0.$$

Because $\epsilon_2(k)$ possesses an energy gap, evaluation of Ω^0 in Sec. V will be made using the results of the second approximation.

Applying to Eq. (81) the same procedure as was used to obtain an approximate solution of (58) we find $\epsilon_0(k) = k^2/2m^*$ ($0 \leq k \leq k_s$). In contrast to (76) the effective mass in the present case is (slightly) temperature dependent. As in Sec. III the validity of the approximation method for solving (81) implies that $(m^* - m)/m$ is very small, and that $T_c - T \lesssim T_c/10$. Since the kernel $J(k,p)$ decreases for large k , the exact solution of (81) approaches $k^2/2m$ in this limit. Further, since m^* is only slightly larger than m , in this temperature range we may for simplicity take $\epsilon_0(k) = k^2/2m$ for all k . Indeed, we have verified that this simplification does not affect the essentials of our results for the thermodynamic functions.³² Equations (80)–(84) are now written as

$$\epsilon_0(k) = k^2/2m, \quad (90)$$

$$h_1(k) = sv(k), \quad f_1(k) = sv(k) + k^2/2m,$$

$$\epsilon_1(k) = \left\{ \frac{k^2}{2m} \left[\frac{k^2}{2m} + 2sv(k) \right] \right\}^{1/2}. \quad (91)$$

³² It should be appreciated that our iteration scheme is of value for all $J(k,p)$. The unsatisfactory aspect of our work is that we can solve (81) only in limited cases.

Using Eq. (81), we can write $f_2(k)$ in the following useful form:

$$f_2(k) = \epsilon_0(k) + sv(k) - h_2(k) + \int_0^\infty dp \, p^2 \epsilon_0(p) [J(k,p) - J(0,p)] \times \left[\frac{1}{\epsilon_1(p)} \coth(\tfrac{1}{2}\beta\epsilon_1) - \frac{1}{\epsilon_0(p)} \coth(\tfrac{1}{2}\beta\epsilon_0) \right]. \quad (92)$$

Let us imagine that the right sides of Eqs. (85) and (92) have been expanded in powers of the small quantity s . It can be shown that to lowest order in s one can obtain f_2 and h_2 using the following simplified forms of Eqs. (85) and (92):

$$h_2(k) = -2 \int_0^\infty dp \, p^2 J(k,p) \frac{sv(p)}{\epsilon_1(p)} \frac{1}{\exp[\beta\epsilon_1(p)] - 1}, \quad (93)$$

$$f_2(k) = \epsilon_0(k) + sv(k) - h_2(k) + 2 \int_0^\infty dp \, p^2 \epsilon_0(p) [J(k,p) - J(0,p)] \times \left[\frac{1}{\epsilon_1(p)} \frac{1}{e^{\beta\epsilon_1} - 1} - \frac{1}{\epsilon_0(p)} \frac{1}{e^{\beta\epsilon_0} - 1} \right]. \quad (94)$$

Because of the strong convergence of the factor $(e^{\beta\epsilon_1} - 1)^{-1}$, we can replace $J(k,p)$ and $v(p)$ in Eq. (93) by $v(k)/4\pi^2$ and $v(0)$, respectively. One obtains

$$h_2(k) = -(2\pi)^{1/2} [v(k)/v_T] \omega^{1/2} \mathcal{G}(\omega), \quad \omega = sv(0)/\kappa T, \quad (95)$$

where

$$\mathcal{G}(\omega) = -\frac{\sqrt{2}}{\pi} \omega \int_0^\infty dt \left[\frac{(t^2 + 1)^{1/2} - 1}{t^2 + 1} \right]^{1/2} \frac{1}{e^{\omega t} - 1}, \quad (96)$$

and where

$$v_T = (2\pi/m\kappa T)^{3/2}. \quad (97)$$

In the remainder of this work we shall frequently encounter integrals similar to $\mathcal{G}(\omega)$. For illustrative purposes, we present a detailed evaluation of $\mathcal{G}(\omega)$ in Appendix D. For small values of ω

$$\mathcal{G}(\omega) = 1 - (2/\pi)^{1/2} (1.460) \omega^{1/2} + \dots \quad (98)$$

Thus, to lowest order in s

$$h_2(k) = -(2\pi\omega)^{1/2} [v(k)/v_T] + O(\omega). \quad (99)$$

Likewise, by replacing $J(k,p)$ in (94) by $J(k,0)$, and by using (91) one obtains

$$f_2(k) = \frac{k^2}{2m} + sv(k) + \frac{1}{v_T} [v(k) - v(0)] \times [\mathcal{F}(\omega) - \zeta(\tfrac{3}{2})] - h_2(k), \quad (100)$$

where

$$\mathcal{F}(\omega) = \frac{2}{\sqrt{\pi}} \omega^{3/2} \int_0^\infty dt \frac{[(t^2+1)^{1/2}-1]^{3/2}}{(t^2+1)^{1/2}} \frac{1}{e^{\omega t}-1}. \quad (101)$$

For small ω

$$\mathcal{F}(\omega) = 2.612 - 2(2\pi)^{1/2} \omega^{1/2} + 3(1.460)\omega + \dots \quad (102)$$

In the range $0 < k < k_s$ we use Eq. (71a), so that

$$f_2(k) = ck^2 + \nu, \quad 0 < k < k_s, \quad (103)$$

where

$$c = (1/2m) + 2(2\pi)^{1/2} (v(0)/v_T) (1/k_c^2) \omega^{1/2}, \quad (104)$$

and

$$\nu = sv(0) + (2\pi\omega)^{1/2} v(0)/v_T. \quad (105)$$

Also in this range the excitation spectrum is of the form

$$\epsilon_2(k) = [(ck^2 + D)(ck^2 + F)]^{1/2}, \quad (106)$$

where

$$\begin{aligned} D &= 2sv(0), \\ F &= (8\pi\omega)^{1/2} v(0)/v_T. \end{aligned} \quad (107)$$

Rather than D and F , we shall frequently use ν and λ where

$$\nu = \frac{1}{2}(D+F), \quad \lambda = (DF)^{1/2}. \quad (108)$$

Prior to evaluating the thermodynamic potential, we shall use Eq. (47) to determine the temperature dependence of the density s of particles occupying the single-particle state $\mathbf{k}=0$. We begin by writing (47) in the form

$$\begin{aligned} s = \rho - \frac{1}{4\pi^2} \int_0^\infty d\mathbf{p} \, p^2 \left[\frac{f_2(\mathbf{p})}{\epsilon_2(\mathbf{p})} - 1 \right] \\ - \frac{1}{2\pi^2} \int_0^\infty d\mathbf{p} \, p^2 \frac{f_2(\mathbf{p})}{\epsilon_2(\mathbf{p})} \frac{1}{e^{\beta\epsilon_2}-1}. \end{aligned} \quad (109)$$

Since the main contribution to the integrals of (109) comes from those values of \mathbf{p} less than k_s , we can use Eqs. (103) and (106) for $f_2(k)$ and $\epsilon_2(k)$, respectively. One obtains

$$\int_0^\infty d\mathbf{p} \, p^2 \left[\frac{f_2(\mathbf{p})}{\epsilon_2(\mathbf{p})} - 1 \right] = \frac{\sqrt{2}}{3c^{3/2}} \nu^{3/2} + O(s^{5/4}). \quad (110)$$

Similarly,

$$\begin{aligned} \int_0^\infty d\mathbf{p} \, p^2 \frac{f_2(\mathbf{p})}{\epsilon_2(\mathbf{p})} \frac{1}{\exp[\beta\epsilon_2(\mathbf{p})]-1} \\ = 2\pi^2 \left(\frac{\kappa T}{4\pi c} \right)^{3/2} \mathcal{G}(\beta\nu; \beta\lambda), \end{aligned} \quad (111)$$

where

$$\begin{aligned} \mathcal{G}(a; b) = \frac{2}{\sqrt{\pi}} a^{3/2} \int_0^\infty dt \, t \left[\frac{(t^2+1)^{1/2}-1}{t^2+b^2/a^2} \right]^{1/2} \\ \times \frac{1}{\exp[a(t^2+b^2/a^2)^{1/2}]-1}. \end{aligned} \quad (112)$$

For small values of a and b , one has

$$\mathcal{G}(a; b) = 2.612 - (2\pi)^{1/2} (a+b)^{1/2} + 1.460a - \frac{4}{3}(2\pi)^{-1/2} a^{3/2} + \dots \quad (113)$$

Retaining all terms of order s Eq. (109) becomes

$$\begin{aligned} s = \rho - \zeta\left(\frac{3}{2}\right) v_T^{-1} + (2\pi)^{1/2} v_T^{-1} [(\beta\nu + \beta\lambda)^{1/2} \\ - (2\pi)^{-1/2} (1.460)\beta\nu - \frac{1}{4}(2\pi)^{-3/2} (2.612)(\beta\nu)^2]. \end{aligned} \quad (114)$$

Note that if we set $v(0)=0$, i.e., no interaction between particles, Eq. (114) reduces to Eq. (53).

For the remainder of this discussion it will be useful to introduce the following parameters:

$$x = \frac{sv(0)}{2\pi\kappa T}, \quad y = \frac{v(0)}{v_T \kappa T}, \quad z = \frac{v(0)}{v_T} \frac{8\pi m}{k_c^2}. \quad (115)$$

When $s=0$, Eq. (114) reduces to $\rho = \zeta(\frac{3}{2}) v_T^{-1}$. Thus, $y \approx y_c = 0.383 \rho v(0)/\kappa T_c$ and $z \approx 4.814 \rho v(0)/(k_c^2/2m)^{-1}$. So as to satisfy the requirements of Sec. III, we must take $y_c \lesssim \frac{1}{2}$ and $z \lesssim 2 \times 10^{-3}$.

Making the change of variable $x^{1/4} = -qy^{1/2}$, so that $q \propto s^{1/4}$, Eq. (114) becomes a quartic (biquadratic) equation in the quantity q :

$$\Gamma(q) \equiv Aq^4 - Bq^3 - Cq^2 + q - \gamma = 0, \quad (116)$$

where

$$\begin{aligned} A &= 1 + 1.460y - 0.653y^2, \\ B &= \frac{3}{2}yz, \quad C = 1 - 1.460y, \end{aligned} \quad (117)$$

and

$$\gamma = \frac{2.612}{2\pi} \left(\frac{y_c T_c}{T} - y \right) \frac{1}{y^2} = \frac{1}{2\pi} \frac{\rho v_T^2}{v(0)} \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right]. \quad (118)$$

The quantity of interest is

$$s = 2\pi y q^4 / v_T. \quad (119)$$

So much for preliminaries. One can show that the positive real root of (116) is the only root which vanishes when $\gamma=0$ ($T=T_c$).³³

Formulas exist for the four roots of a quartic equation, but because they are so unwieldy they are ill suited for practical work. With the aid of a computer, one can obtain numerical values of the required root as a function of the coefficients A , B , C , and γ . The results are shown in Fig. 2. However, since s will appear as a parameter in the thermodynamic potential and its derivatives, we must also obtain a useful analytic expression for s . The following method which is valid for small values of γ , i.e., $T \approx T_c$, will give the required

³³ Because $\Gamma(\pm\infty) = +\infty$ and $\Gamma(0) < 0$, it follows that $\Gamma(q)$ possesses at least two real roots, one positive and the other negative. Further, one can show that for values of A , B , and C which are appropriate to our work the cubic equation $\Gamma'(q)=0$ has only one real root. Thus, $\Gamma(q)$ has no more than two real roots. Finally, using Descartes' rule one finds that if $\gamma=0$, then Eq. (116) is satisfied by $q=0$ and a negative real value of q .

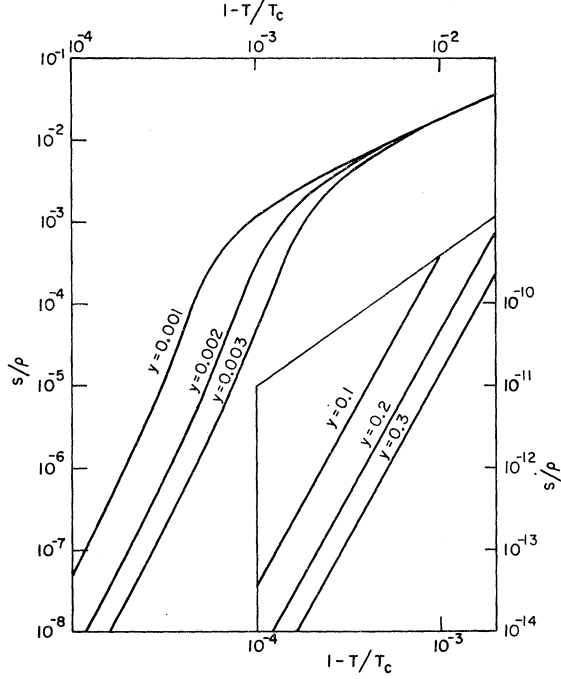


FIG. 2. Fractional population s/ρ of the $k=0$ single-particle state as a function of $1 - T/T_c$ for various values of $\gamma_c = 0.3828\rho v(0)/\kappa T_c$.

result.³⁴ This method can be used for algebraic equations of any degree. We write (116) as

$$q = \gamma + Cq^2 + Bq^3 - Aq^4.$$

On the right side of this expression, substitute for q the quantity $\gamma + Cq^2 + Bq^3 - Aq^4$. If this process is repeated, the terms involving q are of increasingly higher order in the small quantity γ . Through $O(\gamma^4)$ the desired root of (116) is

$$q = \gamma + C\gamma^2 + \gamma^3(B + 2C^2) + \gamma^4(5BC - A + 5C^3) + \dots, \quad \gamma \ll 1. \quad (120)$$

It is important to realize that for fixed positive values of $T_c - T$ we cannot allow $v(0)$ to approach zero in (120) and expect to obtain the ideal gas result (53). This is because $\gamma = O[k(T_c - T)/\rho v(0)]$ is no longer small when such a limit is taken.

Using Eqs. (117)–(120), we find that

$$s/\rho = O[(1 - T/T_c)^4] \quad \text{for } T \rightarrow T_c^-.$$

One can easily show that this behavior is due to a gap in the energy spectrum. Indeed, were we to use Eqs. (82)–(84), the first approximation results for f , h , and ϵ , because $\epsilon_1(k) \propto k$ for small k , we would find $s/\rho = O[(1 - T/T_c)^2]$.³⁵

³⁴ In general, this method gives a valid result only for $T_c - T$ considerably smaller than those for which (114) is an accurate approximation of Eq. (109). However, for the purpose of studying the phase transition it is the behavior of s for the limiting values $T \rightarrow T_c^-$ which is of greatest importance.

³⁵ One should be careful not to identify s with D_s , the superfluid mass density of the two-fluid model of liquid helium (see footnote 31). For $T \rightarrow T_\lambda^-$ the quantity D_s is of order $1 - T/T_\lambda$.

V. PHASE TRANSITION

1. Thermodynamic Functions ($T \geq T_c$)

The first part of this section is devoted to the study of the thermal properties of the system just above the transition temperature T_c . In this temperature range the low-momentum portion of the excitation spectrum is of the form $\epsilon(k) = \epsilon(0) + k^2/2m^*$ [see Eq. (73)]. Consequently, one might be tempted to describe the system as an ideal gas of particles of mass m^* . Alternately, because $\epsilon(0)$ does not coincide with $-\mu$ as it does for a gas of free particles, but instead they are related through (59), we can expect the thermal properties of the system to be somewhat different from those of the ideal boson gas.

In the present work it is of decided advantage to choose T , V , and ρ as independent “external” variables rather than T , V , and μ as is generally done. In terms of these variables one finds the pressure p , entropy S , mean number of particles N , and specific heat at constant volume C_V to be related to the thermodynamic potential Ω by

$$p = -(\partial\Omega/\partial V)_{T,\rho}, \quad (121)$$

$$S = -(\partial\Omega/\partial T)_{V,\rho} - N(\partial\mu/\partial T)_{V,\rho}, \quad (122)$$

$$N = -(\partial\Omega/\partial\mu)_{T,V}/(\partial\mu/\partial\rho)_{T,V}, \quad (123)$$

$$C_V = T(\partial S/\partial T)_{V,\rho}. \quad (124)$$

The thermodynamic potential Ω^0 can be written as [see (22) and (23)]³⁶

$$\begin{aligned} \Omega = -V \left[\frac{1}{2}\rho^2 v(0) + \frac{1}{2\pi^2} \int_0^\infty dk k^2 \frac{1}{e^{\beta\epsilon} - 1} \right. \\ \times \int_0^\infty dp p^2 J(k,p) \frac{1}{e^{\beta\epsilon} - 1} - \frac{1}{2\pi^2} \kappa T \\ \left. \times \int_0^\infty dk k^2 \ln(1 - e^{-\beta\epsilon}) \right]. \quad (125) \end{aligned}$$

Following the reasoning of Sec. III, because of the extreme rapidity with which the factor $(e^{\beta\epsilon} - 1)^{-1}$ drops to zero for large values of k , it is justifiable to approximate $J(k,p)$ by (71b), and $\epsilon(k)$ by (73) for all values of their respective arguments. In that event, Eq. (125) and the auxiliary condition (30) assume the form:

$$\Omega = -V(\kappa T/v_T^*) \times [1 - 3\rho v(0)m^*/k_c^2] g_{5/2}(z^*) - V\rho^2 v(0), \quad (126)$$

$$\rho = (1/v_T^*) g_{3/2}(z^*). \quad (127)$$

³⁶ Henceforth, we shall drop the superscript on Ω^0 since we shall restrict our attention to volumes so large that Ω^0 is equivalent to the true thermodynamic potential Ω_P .

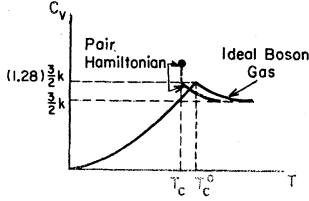


FIG. 3. Specific heat per particle as a function of temperature.

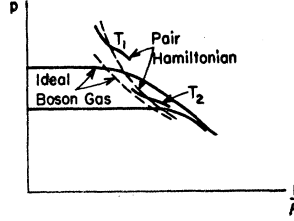


FIG. 4. Full lines and dashed lines denote isotherms and loci of points of condensation, respectively.

In (126) and (127)

$$g_\sigma(z^*) = \frac{1}{\Gamma(\sigma)} \int_0^\infty dx x^{\sigma-1} \frac{1}{(1/z^*)e^x - 1}, \quad (128)$$

$$z^* = \exp[-\beta\epsilon(0)], \quad (129)$$

and

$$v_T^* = (2\pi/m^* \kappa T)^{3/2}. \quad (130)$$

The chemical potential μ is related to $\epsilon(0)$ by (59). Using (71a) one finds

$$\mu = -\epsilon(0) + 2\rho v(0) - \frac{3}{2}v(0)(k_c^2/2m^*)^{-1}(\kappa T/v_T^*)g_{5/2}(z^*). \quad (131)$$

By combining (126) and (131), we find

$$\Omega + \rho V \mu = -V \kappa T [(1/v_T^*)g_{5/2}(z^*) - \rho \ln z^*] + V \rho^2 v(0), \quad (132)$$

$$\rho = (1/v_T^*)g_{3/2}(z^*). \quad (133)$$

Let us for the moment fix the density of our system at a value ρ . According to (76) this fixes the value of the effective mass $m^*/m = [1 - 2m\rho v(0)/k_c^2]^{-1}$. Now let us imagine a gas of noninteracting bosons of (real) mass $m^*(\rho)$, and of arbitrary density. The equations which describe this latter system, called i (ideal), are obtained from (132) and (133) by setting $v(0)=0$ wherever it appears explicitly, i.e., only in $V\rho^2 v(0)$:

$$\Omega_i + \rho_i V \mu_i = -V \kappa T [(1/v_T^*)g_{5/2}(z_i) - \rho_i \ln z_i], \quad (134)$$

$$\rho_i = (1/v_T^*)g_{3/2}(z_i), \quad (135)$$

and

$$z_i = \exp(\beta \mu_i). \quad (136)$$

It is important to realize that if the value of ρ_i is set equal to ρ , the quantities z_i and z^* are equal for all temperatures $T \geq T_c$. That is to say, $z^*(\rho, T) = z_i[\rho, T, m^*(\rho)]$. Now according to (122) and (124) the quantities S and C_V are obtained by differentiating $\Omega + \rho V \mu$ with respect to T , holding ρ and V constant. Since the term $V\rho^2 v(0)$ in (132) does not contribute to these derivatives we conclude that $S(\rho, T) = S_i[\rho, T, m^*(\rho)]$ and $C_V(\rho, T) = C_{V,i}[\rho, T, m^*(\rho)]$. That is to say, in this model, above the transition temperature the entropy and specific heat of a system of bosons of (real) mass m , and of density ρ are the same as those of a system of noninteracting bosons of real mass $m^*(\rho)$ and of density ρ . The temperature dependence of C_V is shown in Fig. 3. No such statement can be made about the pressure, for according

to (121) and (126) it follows that

$$p = (\kappa T/v_T^*) \times [1 - \frac{3}{2}\rho v(0)(k_c^2/2m^*)^{-1}]g_{5/2}(z^*) + \rho^2 v(0) \quad (137)$$

$$= p_i[\rho, T, m^*(\rho)] + \rho v(0)[\rho - \frac{3}{2}(\kappa T/v_T^*)(k_c^2/2m^*)^{-1}]. \quad (138)$$

We denote by ρ_c the value of the density associated with the transition point in the $p-1/\rho$ plane. So as to study the isotherms of the system we shall express p solely in terms of ρ and ρ_c . Specifically, we shall express z^* , m^* , v_T^* , and T in terms of these variables.

The quantity z^* is related to T and ρ through Eq. (133). Although it is impossible to express $g_{3/2}(z^*)$ in closed form in terms of familiar functions, one can express it as a rapidly converging power series when T is just above T_c . If σ is real, positive, and not an integer⁶

$$g_\sigma(x) = (-\ln x)^{\sigma-1} \Gamma(1-\sigma) + \sum_{n=0}^{\infty} \frac{1}{n!} \zeta(\sigma-n) (\ln x)^n, \quad (139)$$

where $\zeta(\sigma) = \sum_{n=1}^{\infty} n^{-\sigma}$ is the Riemann zeta function. With $\ln x = -\epsilon(0)/\kappa T$ the rapid convergence of the series in (139) is evident. Using (133) and retaining only the two terms of (139) which are of lowest order in $\ln x$, one finds

$$\epsilon(0) = -\kappa T \ln z^* = 0.543 \kappa T [1 - \rho v_T / \zeta(\frac{3}{2})]^2. \quad (140)$$

Referring to (76) and (130) one notes that v_T^* is density dependent for fixed T . Furthermore, it was shown in Sec. III 2 that for $T \geq T_c$ the excitation spectrum is correctly given by Eq. (73), only if $\rho v(0)(k_c^2/2m)^{-1}$ is very small compared to one. To lowest order in this small quantity one has

$$m^*(\rho) = m^*(\rho_c) [1 - (\rho_c - \rho)v(0)(k_c^2/2m)^{-1}], \quad (141)$$

$$v_T^*(\rho) = \zeta(\frac{3}{2}) \rho_c^{-1} [1 + \frac{3}{2}(\rho_c - \rho)v(0)(k_c^2/2m)^{-1}]. \quad (142)$$

Further, using Eqs. (76), (130), and (142) one finds

$$\kappa T_c = 3.313 \rho_c^{2/3} m^{-1} [1 - \rho_c v(0)(k_c^2/2m)^{-1}]. \quad (143)$$

Using Eqs. (140)–(143) and approximating $g_{5/2}(z^*)$ in the same way as $g_{3/2}(z^*)$, one obtains

$$p = 1.70 \rho_c^{5/3} m^{-1} \{ [1 - 1.06(1 - \rho/\rho_c)^2] - a_c [2.5 - 5.82(1 - \rho/\rho_c)^2] \} + \rho^2 v(0), \quad (144)$$

where

$$a_c = \rho_c v(0)(k_c^2/2m)^{-1}. \quad (145)$$

The locus of points of condensation is given by

$$p(\rho_c) = 1.70\rho_c^{5/3}m^{-1}(1 - 2.5a_c) + \rho_c^2v(0), \quad (146)$$

in contrast to

$$p^0(\rho_c) = 1.70\rho_c^{5/3}m^{-1} \quad (147)$$

for the ideal boson gas (particles of mass m). Schematic plots of these results are given in Fig. 4.

2. Thermodynamic Functions ($T < T_c$)

We now discuss the thermal properties of the system for temperatures just below T_c . In view of the complexity of the calculations, we shall limit our attention to $S(T_c-)$, $C_V(T_c-)$, $[\partial C_V(T_c-)/\partial T]_{\rho, V}$, and $p(\rho)$. For simplicity, we shall set $k_c = \infty$ in all calculations; i.e., we shall ignore terms of order $(k/k_c)^2$ in the low-momentum expansion of $v(k)$.³⁷

In the temperature range under consideration the density s of particles occupying the $\mathbf{k}=0$ state is of order $(1 - T/T_c)^4$. Because Ω and μ are functions of s , to obtain $\partial C_V(T_c-)/\partial T$ it will be necessary to retain all terms of order $s^{3/4}$. For this purpose it can be shown that instead of the complete expressions (7), (22), and (23) it suffices to consider the following reduced expression for Ω :

$$\begin{aligned} \Omega = & -\frac{1}{2\pi^2}V \left\{ \pi^2\rho^2v(0) \right. \\ & + \int_0^\infty dk k^2 \xi(k) \int_0^\infty dp p^2 J(k, p) \xi(p) \\ & + \int_0^\infty dk k^2 \frac{h(k)}{\epsilon(k)} \int_0^\infty dp p^2 \frac{h(p)}{\epsilon(p)} J(k, p) \frac{1}{e^{\beta\epsilon} - 1} \\ & + \int_0^\infty dk k^2 \frac{h(k)}{\epsilon(k)} \frac{1}{e^{\beta\epsilon} - 1} \int_0^\infty dp p^2 \frac{h(p)}{\epsilon(p)} J(k, p) \frac{1}{e^{\beta\epsilon} - 1} \\ & \left. - \frac{1}{2\pi^2}kT \int_0^\infty dk k^2 \ln(1 - e^{-\beta\epsilon}) \right\}, \quad (148) \end{aligned}$$

where $h(k)$ and $\epsilon(k)$ are given by (99) and (106), respectively. Once again the rapid decrease of $(f/\epsilon) - 1$ and $(e^{\beta\epsilon} - 1)^{-1}$ allows us to replace $J(k, p)$ by $J(0, 0) = v(0)/4\pi^2$, and $h(k)$ by $h(0)$ ³⁸ in the first and third integrals of (148). Using Eq. (47), one obtains

$$\int_0^\infty dk k^2 \xi(k) \int_0^\infty dp p^2 \xi(p) = \pi^2\rho^2v(0). \quad (149)$$

In order to determine the contribution of the third

³⁷ It should be remarked that if one performs the calculations of the present section avoiding the simplifying assumption $k_c = \infty$ the essentials of our results are unaffected.

³⁸ Here and in the following $h(0)$ actually means $h(k=0+)$. The discussion of Sec. II 3 shows that $h(k=0) \neq h(k=0+)$.

integral of (148), it is necessary to evaluate

$$\int_0^\infty dk \frac{k^2}{\epsilon(k) \exp[\beta\epsilon(k)] - 1} = \pi m^{3/2} k T v^{-1/2} \mathcal{E}(\beta v; \beta \lambda), \quad (150)$$

where

$$\begin{aligned} \mathcal{E}(a; b) = & -\frac{\sqrt{2}}{\pi} a \int_0^\infty dt t \left[\frac{(t^2 + 1)^{1/2} - 1}{(t^2 + 1)(t^2 + a^2/b^2)} \right]^{1/2} \\ & \times \frac{1}{\exp[a(t^2 + b^2/a^2)^{1/2}] - 1}. \quad (151) \end{aligned}$$

Using the technique discussed in Appendix D, for small values of a and b one obtains

$$\mathcal{E}(a; b) = a^{1/2}(a + b)^{-1/2} - (2/\pi)^{1/2}(1.460)a^{1/2} + \dots \quad (152)$$

The analysis of the second integral of (148) requires some care. For the integration over p we set $J(k, p) = J(k, 0)$ and $h(p) = h(0)$. On the other hand, all terms involving k are left intact. Further, using (99) and (106) we write

$$\begin{aligned} & \int_0^\infty dk k^2 v(k) \frac{h(k)}{\epsilon(k)} \\ & = \frac{h(0)}{v(0)} \int_0^\infty dk k^2 \frac{v^2(k)}{\epsilon(k)} \simeq h(0)v(0) \\ & \quad \times \int_0^{k_s} dk k^2 \frac{1}{[(D + k^2/2m)(F + k^2/2m)]^{1/2}} \\ & \quad + 2m \frac{h(0)}{v(0)} \int_{k_s}^\infty dk v^2(k). \quad (153) \end{aligned}$$

Through order $s^{3/4}$, one obtains

$$\begin{aligned} & \int_0^\infty dk k^2 v(k) h(k) / \epsilon(k) \\ & = -16\pi^3 k T y x^{1/2} [B(T_c) - 2y^{3/2} x^{1/4}], \quad (154) \end{aligned}$$

where

$$\begin{aligned} B(T) = & B(T_c) = \pi^{-1/2} y (k_s^2 / 2m k T)^{1/2} \\ & + [m / 4\pi^2 v(0)] \int_{k_s}^\infty dk v^2(k). \quad (155) \end{aligned}$$

The symbols x and y are defined by Eq. (115).

The last integral of (148) can be written as

$$\int_0^\infty dk k^2 \ln(1 - e^{-\beta\epsilon}) = -(2\pi^2 / v_T) \mathcal{K}(\beta v; \beta \lambda), \quad (156)$$

where

$$\begin{aligned} \mathcal{K}(a; b) = & -\frac{2}{\sqrt{\pi}} a^{3/2} \int_0^\infty dt t \left[\frac{(t^2 + 1)^{1/2} - 1}{t^2 + 1} \right]^{1/2} \\ & \times \ln[1 - \exp(a(t^2 + b^2/a^2)^{1/2})]. \quad (157) \end{aligned}$$

For small values of a and b , one has

$$\mathcal{K}(a; b) = 1.341 - 2.612a + \frac{4}{3}(2\pi)^{1/2}(a+b)^{1/2}(a-\frac{1}{2}b) - \frac{3}{2}(1.460)a^2 + \dots \quad (158)$$

Collecting these results, through $O(s^{3/4})$, one obtains

$$\Omega(T) = -V\{1.341(\kappa T/v_T) + \rho^2 v(0) + 2\pi^2 y(y-0.831)x^{1/2} + \frac{4}{3}\pi^2 y^{3/2}[1-8.760y+6B(T_c)]x^{3/4}\}. \quad (159)$$

Upon setting $k_c = \infty$ in Eq. (126) we see that Ω is continuous at the transition temperature as is to be expected. The first term of (159) is the value of Ω for the ideal boson gas for $T \leq T_c$.

It is to be emphasized that to obtain (159) we have expanded $(\beta\nu + \beta\lambda)^{-1/2}$, involving the quantity $(x^{1/4} + y^{1/2})^{-1}$, in increasing powers of $(x/y^2)^{1/4}$. Since $x/y^2 \propto (s/\rho)[\kappa T/\rho v(0)]$, it is clear that such an expansion is convergent for $T < T_c$ only if $v(0)$ is nonzero. That is to say

$$\lim_{v(0) \rightarrow 0} \Omega(T) \neq [\Omega(T)]_{v(0)=0}, \quad (160)$$

whereas

$$\lim_{v(0) \rightarrow 0} \lim_{T \rightarrow T_c^-} \Omega(T) = [\Omega(T_c)]_{v(0)=0}. \quad (161)$$

Note that (160) dictates that the double limiting process can only be performed in the order shown in (161). Furthermore, because of (160) we can expect that $S(T_c-)$, $C_V(T_c-)$, and $\partial C_V(T_c-)/\partial T$, which arise from derivatives of $\Omega(T)$, may not behave in the fashion of (161). Of course this curious situation is a consequence of the nature of the energy gap in the excitation spectrum.

The chemical potential μ is given by Eq. (44). Since we have just discussed the evaluation of all integrals appearing in this equation, we shall only quote the final result

$$\mu = \rho v(0)[1 + (T/T_c)^{3/2}] - 4\pi\kappa T y[1 + 0.730y - B(T_c)]x^{1/2} + 2\pi\kappa T y^{1/2} x^{3/4}. \quad (162)$$

We now proceed to write our expressions for Ω and μ in powers of $T_c - T$. Using Eqs. (115), (117)–(120), in a straightforward fashion, one obtains

$$x^{1/2} = 0.389y_c^{-1}[1 + (1.179 + 1.247y_c^{-1})(1 - T/T_c)] \times (1 - T/T_c)^2, \quad (163)$$

$$x^{3/4} = 0.2425y_c^{-3/2}(1 - T/T_c)^3,$$

where $y_c = y(T_c) = \rho v(0)/\zeta(\frac{3}{2})\kappa T_c$. Using (163), one finds that through order $(1 - T/T_c)^3$

$$\Omega(T) = -N\kappa\{0.5134(T/T_c)^{5/2} + (T_c - T)[a_1(1 - T/T_c) + a_2(1 - T/T_c)^2]\} - N\rho v(0), \quad (164)$$

and

$$\mu(T) = \rho v(0)[1 + (T/T_c)^{3/2}] - \kappa(T_c - T)[a_3(1 - T/T_c) + a_4(1 - T/T_c)^2], \quad (165)$$

where

$$\begin{aligned} a_1 &= -2.442 + 2.939y_c, \\ a_2 &= -3.048y_c^{-1} + 9.336 + (7.328b_c - 17.520)y_c, \\ a_3 &= 4.886 + (3.567 - 4.886b_c)y_c, \\ a_4 &= 4.570y_c^{-1} + (2.880 - 6.093b_c) - (2.929 - 1.568b_c)y_c. \end{aligned} \quad (166)$$

The quantity b_c , independent of $v(0)$, is given by

$$b_c = B(T_c)/y_c = \pi^{-1/2}(k_s^2/2m\kappa T_c)^{1/2} + 1.039\gamma(k_s^3/\rho)(k_s^2/2m\kappa T_c)^{-1}, \quad (167)$$

where γ is given by

$$\gamma = \int_{0.1}^{\infty} dx g^2(x), \quad (168)$$

and

$$v(k) = v(0)g(kR). \quad (169)$$

Using Eqs. (122) and (124), one obtains

$$S(T_c-) = N\kappa(1.2835 - 3.918y_c), \quad (170)$$

$$C_V(T_c-) = N\kappa[6.812 + (11.053 - 9.772b_c)y_c], \quad (171)$$

$$\begin{aligned} \left[\frac{\partial C_V}{\partial T}(T_c-) \right]_{\rho, v} &= \frac{N\kappa}{T_c} [(36.558b_c - 65.552) \\ &+ (134.726 - 63.148b_c)y_c - 9.132y_c^{-1}]. \end{aligned} \quad (172)$$

Several comments are in order at this point:

1. In Sec. V 1 we have seen that for $T > T_c$ the entropy per particle is the same as for an ideal boson gas. In particular, for a system of N particles $S(T_c+) = 1.2835N\kappa$. Comparison with (170) shows that

$$S(T_c-) = S(T_c+) - (3.918y_c)N\kappa. \quad (173)$$

That is to say, at the transition temperature there is associated a latent heat $(3.918y_c)\kappa T_c$ per particle. The latent heat is due to the fact that μ contains a term which is linear in $T_c - T$. We therefore conclude that the phase transition is of *first* order. Hypothetically, a perfect temperature resolution measurement of the specific heat would show a delta function behavior at T_c .

2. If we allow $v(0)$ to approach zero $S(T_c-)$ approaches the corresponding quantity for the ideal boson gas. In contrast,

$$\lim_{v(0) \rightarrow 0} C_V(T_c-) \neq C_V^0(T_c) = 1.925N\kappa,$$

$$\lim_{v(0) \rightarrow 0} \frac{\partial C_V}{\partial T}(T_c-) \neq \frac{\partial C_V^0}{\partial T}(T_c-) = 2.8875 \frac{N\kappa}{T_c}.$$

This situation has been anticipated earlier in this section.

3. Note the rather unexpected result that $C_V(T_c-) - C_V^0(T_c)$ decreases linearly for increasing values of y_c .

4. A graph of $\partial C_V(T_c-)/\partial T$ as a function of y_c for various values of b_c is given in Fig. 5. Since, as discussed in Sec. III 2, our results are valid only if $2\rho v(0) \leq \kappa T_c$, i.e., $y_c \leq 0.191$, the curves are not drawn for values of $y_c > 0.195$. One striking property of these curves is that for a large value of b_c the ordinate takes on a wide range of values. More interesting is the fact that for very small values of y_c the value of $\partial C_V(T_c-)/\partial T$ is proportional to $(-1/y_c)$. The situation is even more curious, for except in a narrow temperature region below T_c of width proportional to $\rho v(0)$ our expressions for s , Ω , and μ (and thus S , C_V , $\partial C_V/\partial T$) reduce to the corresponding values for the ideal boson gas. The existence of this narrow temperature range is most clearly seen from (116), the equation which we use to determine s . Note that for $v(0) \approx 0$ this equation is of the form

$$\Gamma(q) = q^4 - q^2 + q - \gamma = 0.$$

Now for large values of γ , i.e., $\rho v(0) \ll \kappa(T_c - T)$, the real positive root³³ of this equation is $q \approx \gamma^{1/4}$ so that $s \approx \rho[1 - (T/T_c)^{3/2}] = s^0$ [see Eq. (53)]. On the other hand, for values of T such that $\rho v(0) \lesssim \kappa(T_c - T)$ to obtain the desired root it is necessary to find the root of the full quartic equation, and it is evident that for such values of γ the quantity s no longer bears resemblance to s^0 . We can anticipate that the rapid change in the functional form of s in this narrow temperature region will cause an equivalent effect in C_V in the same temperature range. Indeed, to accommodate a situation where $C_V(T) \approx C_V^0(T)$ except for T such that $T_c - \rho v(0)/\kappa \leq T \leq T_c$, and $\partial C_V(T_c-)/\partial T \propto -\kappa T_c/\rho v(0)$ it seems necessary to assume that C_V shows a very high (positive) peak at approximately the middle of this temperature range.

It should be noticed that C_V must be such that the area under the curve bounded by $T = T_c - \rho v(0)/\kappa$ and $T = T_c -$ must vanish in the limit $v(0) \rightarrow 0$. This is a consequence of the fact that the entropy is continuous at T_c in this limit.

Without resorting to extensive numerical techniques, we do not see any method for studying the detailed shape of the specific heat curve just below T_c in the limit $v(0) \rightarrow 0$. To carry out such a study it would presumably be necessary to obtain expressions in closed form for s , Ω , and μ . Now our procedure for obtaining the desired root of the quartic (116) is valid only if $\gamma \ll 1$. Thus, it would be necessary to use the complete analytical expressions for the roots of a quartic. Of a more serious nature, it would be necessary to evaluate all integrals contributing to Ω and μ in closed form, and this is effectively impossible.

To conclude this section, we briefly discuss the iso-

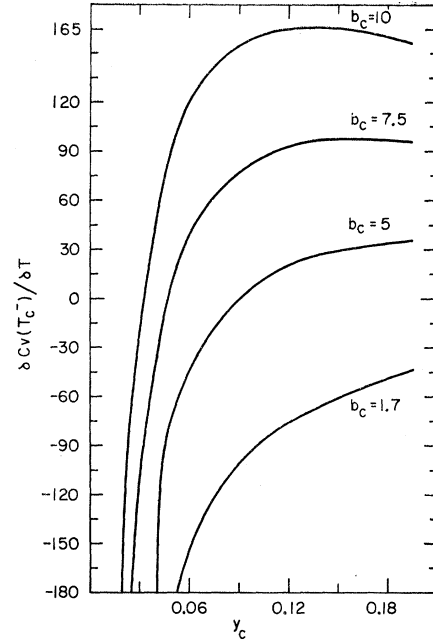


FIG. 5. Slope of the specific heat curve at $T = T_c -$ as a function of $y_c = 0.3828\rho v(0)/\kappa T_c$ for various values of the parameter b_c [see Eq. (167)].

therms. Using Eqs. (120), (121), and (159), one obtains

$$p = 1.70m^{-1}\rho_c^{5/3} + \rho^2 v(0) - F(\rho - \rho_c)^2 + G(\rho - \rho_c)^3, \quad (174)$$

where

$$\begin{aligned} F &= 1.306\kappa T_c(0.831 - y_c)\rho_c^{-1}, \\ G &= 1.086\kappa T_c[-0.831y_c^{-1} + 3.761 \\ &\quad + (2b_c - 5.840)y_c]\rho_c^{-2}. \end{aligned} \quad (175)$$

At the phase transition the pressure is continuous:

$$p(\rho_c+) = p(\rho_c-) = 1.70\rho_c^{5/3}m^{-1} + \rho_c^2 v(0).$$

Furthermore, $[\partial p(\rho_c)/\partial \rho^{-1}]_{T,V}$ is continuous having the value $-2\rho_c^3 v(0)$. These results are shown in Fig. 4.

VI. CONCLUSIONS

This work has concerned itself with a soluble model of a nonideal boson gas. Although the predicted behavior of the thermodynamic functions does not resemble that of liquid He^4 it has been possible to consider several questions which are of importance for an understanding of many-boson systems.

Without making any assumptions, it has been possible to formulate a quantitative criterion for the occurrence of an Einstein condensation. This criterion when satisfied also insures the presence of a zero in the quasi-particle excitation spectrum. Involved with this matter was the proof that the fluctuations of quantities like $a_0^\dagger a_0$ are small, and further, that within the context of the present model the Bogoliubov approximation of replacing the zero momentum creation and destruction

operators by a c number is justified. In addition, we have found that although the present model is a generalization of Bogoliubov's classic model, it predicts an excitation spectrum possessing an energy gap. The model also predicts a slight lowering of the transition temperature as compared to the ideal boson gas of the same density. So as to obtain this result, it was necessary to restrict our attention to weak short-range repulsive interparticle forces, or to short-range forces and to systems of low density. Because of these conditions, it was impossible to apply our results to liquid helium. Finally, it was found that the entropy and the specific heat have a finite discontinuity at the transition temperature.

One tends to conclude this study with a certain degree of disappointment, for it seems difficult to develop a soluble model which includes further terms of the total Hamiltonian (1). Involved with this is the following question of principle: Is there any hope of understanding the lambda transition as long as one restricts oneself to a description of the many-boson system in terms of noninteracting excitations? To answer this question it would surely be helpful to have available detailed experimental data for the dispersion curve of the excitations in the liquid in the vicinity of the λ point. The broadening of the spectrum of scattered neutrons with increasing temperature² of course indicates the decrease of the mean free path of the excitations. However, this does not preclude the possibility that using the experimental dispersion curve and treating the excitations as infinitely lived (so as to evaluate the partition function) one might properly describe the thermodynamical behavior of the system. In fact, it is possible³⁹ to cite examples where such a procedure is successful. Although from the point of view of the theory an answer in the negative would not be accepted jubilantly (the phrase "cooperative interactions between excitations" really means "proceed to diagonalize the nonlinear many-body Hamiltonian"), any answer would do much in helping to point the way to a successful soluble model.

ACKNOWLEDGMENTS

I wish particularly to express my deep gratitude to Professor Gregor Wentzel for his patient guidance and criticism with regard to the present work and, more generally, with regard to my studies of the past three years. Also I am indebted to Dr. Marvin Girardeau for several profitable conversations especially with respect to the subject matter of Appendix E. The kind assistance of Dr. Richard R. Chasman is also gratefully acknowledged. Finally, I wish to express my appreciation to the National Science Foundation for the award of a predoctoral fellowship during the years 1959–1962.

³⁹ T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958), Sec. 9.

APPENDIX A

In this Appendix we sketch the proof that \mathcal{H}' , defined by Eq. (5), fails to contribute to the volume-proportional part of the thermodynamical potential Ω_P . In particular, we shall limit our attention to systems in which an Einstein condensation occurs. Starting from Eqs. (10a) and (10b), in a straightforward manner one obtains

$$\exp\beta(\Omega^0 - \Omega_P) = \langle U(\beta) \rangle, \quad (\text{A1})$$

where

$$U(\beta) = \sum_{n=0}^{\infty} (-1)^n \times \int_{\beta > u_1 \cdots > u_n > 0} du_1 \cdots du_n \mathcal{H}'(u_1) \cdots \mathcal{H}'(u_n), \quad (\text{A2})$$

and

$$\mathcal{H}'(u) = [\exp(u\mathcal{H}^0)] \mathcal{H}' [\exp(-u\mathcal{H}^0)]. \quad (\text{A3})$$

The ensemble average in (A1) is defined by Eq. (12). Suppressing all integrals, the n th term of the sum in (A2) involves expressions of the form

$$V^{-n} \langle [B_0(\dagger)]^m \sum \cdots \sum^{(2n-m)} \alpha_{2n-m} \rangle, \quad 0 \leq m \leq 2n, \quad (\text{A4})$$

where α_{2n-m} involves the product of $2n-m$ operators B_k , $k \neq 0$. The $(2n-m)$ -fold sums include all *nonzero* momenta. For brevity, we have ignored the subscripts $\lambda = 1, 2$ of $B_{k\lambda}$.

Because of the independence of the contributions of different momentum states to \mathcal{H}^0 , Eq. (A4) can be written as

$$V^{-n} \langle [B_0(\dagger)]^m \rangle \sum \cdots \sum^{(2n-m)} \langle \alpha_{2n-m} \rangle. \quad (\text{A5})$$

As shown by Wentzel,¹⁰ for large volumes V

$$\begin{aligned} \sum \cdots \sum^{(2n-m)} \langle \alpha_{2n-m} \rangle &= O[V^{(n-m/2)}], & m \text{ even}, \\ &= O\{V^{[n-(m+1)/2]}\}, & m \text{ odd}. \end{aligned} \quad (\text{A6})$$

Thus, if⁴⁰

$$\begin{aligned} \langle [a_0^\dagger a_0 - \langle a_0^\dagger a_0 \rangle]^m \rangle &= O[V^{m/2}], & m \text{ even}, \\ &= O[V^{(m-1)/2}], & m \text{ odd}, \end{aligned} \quad (\text{A7})$$

each term (A4) gives a volume independent contribution to $\exp\beta(\Omega^0 - \Omega_P)$.

We now proceed to prove that (A7) is indeed satisfied. One can show,⁴¹ very generally, that if a quantity A possesses the property that $\langle (A - \langle A \rangle)^2 \rangle = O(V)$, then

$$\langle (A - \langle A \rangle)^{2n} \rangle = O(V^n), \quad (\text{A8})$$

and

$$\langle (A - \langle A \rangle)^{2n+1} \rangle = O(V^n). \quad (\text{A9})$$

⁴⁰ According to Eq. (42) $\langle a_0^\dagger a_0 \rangle = \langle a_0^\dagger a_0 \rangle$. Thus, (A7) is sufficiently general.

⁴¹ R. H. Fowler, *Statistical Mechanics* (Cambridge University Press, London, 1955), 2nd ed., p. 762.

It, therefore, suffices to prove that

$$\langle (a_0^\dagger a_0 - \langle a_0^\dagger a_0 \rangle)^2 \rangle = O(V).$$

For brevity, let $a_0^\dagger a_0 = n_0$, $\sum_{\mathbf{k}'} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} = \mathcal{N}'$, and $\sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} = \mathcal{N}$. Then⁴²,

$$\langle (n_0 - \langle n_0 \rangle)^2 \rangle = \langle (\mathcal{N}^2) - \langle \mathcal{N} \rangle^2 \rangle - \langle (\mathcal{N}'^2) - \langle \mathcal{N}' \rangle^2 \rangle. \quad (\text{A10})$$

Now it is well known that

$$\langle \mathcal{N}^2 \rangle - \langle \mathcal{N} \rangle^2 = -\beta z \left[\frac{\partial}{\partial z} \left(z \frac{\partial \Omega}{\partial z} \right) \right]_{T, V}, \quad (\text{A11})$$

where $z = \exp(\beta\mu)$. The fugacity z is volume independent, whereas $\Omega = O(V)$. Thus, the left side of (A11) is of order V . Further,

$$\begin{aligned} \langle \mathcal{N}'^2 \rangle - \langle \mathcal{N}' \rangle^2 = & \sum_{\mathbf{k}'} \left[\langle (a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'}) \rangle - \langle a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} \rangle^2 \right] \\ & - \langle (a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} a_{-\mathbf{k}'}^\dagger a_{-\mathbf{k}'}) \rangle - \langle a_{\mathbf{k}'}^\dagger a_{\mathbf{k}'} \rangle \langle a_{-\mathbf{k}'}^\dagger a_{-\mathbf{k}'} \rangle. \end{aligned} \quad (\text{A12})$$

Now each term of (A12) can be evaluated using (16)–(20); they are all volume independent. The sum is therefore of order V . Thus, the left side of (A10) is of order V .

We, therefore, conclude that if the sum of all terms (A4) which contribute to (A1) converges,⁴³ \mathcal{H}' fails to contribute to the volume proportional part of the thermodynamic potential Ω_P .

APPENDIX B

In the first part of this Appendix we shall prove that if the kernel $J(k, p)$, defined by (29), has only positive eigenvalues (J_+ kernel), two-body bound states are impossible.

If \mathbf{r} is the relative position vector of the two particles the Schrödinger equation is

$$-(1/2\mu)\nabla^2\psi(\mathbf{r}) + V(r)\psi(\mathbf{r}) = -W\psi(\mathbf{r}). \quad (\text{B1})$$

The reduced mass of the system is denoted by μ , and we assume that the interaction between the two particles is a function of their separation distance only. We further assume that the two particles form a bound state ($W > 0$).

For large values of \mathbf{r} the wave function drops rapidly to zero. It, therefore, follows that

$$\int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2\psi = -k^2\phi(\mathbf{k}), \quad (\text{B2})$$

where⁴⁴

$$\phi(\mathbf{k}) = \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \psi(\mathbf{r}). \quad (\text{B3})$$

⁴² Note carefully that it is the independence of the contributions of different momentum states to \mathcal{H}^0 which effects (A10).

⁴³ For a discussion on this point see G. Wentzel, *W. Heisenberg* (Vieweg, Braunschweig, 1961).

⁴⁴ If the two particles did not form a bound state

$$\int_{\tau} d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \nabla^2\psi + k^2 \int_{\tau} d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} \psi = \int_{\Sigma} d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} [\nabla\psi - i\mathbf{k}\psi] \neq 0,$$

where τ is the volume of integration and Σ is its surface.

Multiplying (B1) by $e^{i\mathbf{k}\cdot\mathbf{r}}$ and integrating over all space, one finds that $\phi(\mathbf{k})$ satisfies the following integral equation

$$-(W + k^2/2\mu)\phi(\mathbf{k}) = (2\pi)^{-3} \int d\mathbf{p} v(|\mathbf{k} - \mathbf{p}|) \phi(\mathbf{p}), \quad (\text{B4})$$

where

$$v(\mathbf{k}) = \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} V(r). \quad (\text{B5})$$

Let us confine our attention to s states, so that $\psi(\mathbf{r}) = \psi(r)$ and $\phi(\mathbf{k}) = \phi(k)$.

In this case (B4) can be written as

$$-(W + k^2/2\mu)\phi(k) = 2 \int_0^\infty dp p^2 J(k, p) \phi(p). \quad (\text{B6})$$

As in Sec. II 2, we multiply both sides of (B6) by $k^2\phi(k)$ and integrate from $k=0$ to $k=\infty$. The left side of the resulting equation is negative-semidefinite, whereas the right side is positive-semidefinite if $J(k, p)$ has only positive eigenvalues. That is to say, for J_+ kernels two-body bound states are impossible.

In the second part of this Appendix we shall give an example where the interparticle potential is predominantly positive, i.e., $v(0) > 0$, and unable to sustain two-body bound states, but yet $J(k, p)$ is not of the J_+ form.

Consider the potential $V(r) = -V_1$, ($0 < r < a$); V_2 , ($a < r < a+b$); 0, ($r > a+b$), where V_1 and V_2 are both positive. The space average of $V(r)$ is positive if $3V_2b > V_1a$. Further, $J(k, k)$ is proportional to

$$\begin{aligned} -V_1 \left(a - \frac{1}{2k} \sin 2ka \right) \\ + V_2 \left[b - \frac{1}{2k} \sin 2k(a+b) + \frac{1}{2k} \sin 2ka \right]. \end{aligned}$$

If $b \ll a$ and $k = a/\pi$, one has

$$J(k, k) \propto -V_1a + V_2bO(b^2/a^2).$$

In addition, we would like $V(r)$ to be such that the two-body system has no bound states. The Schrödinger equation is easily solved since we need only consider s states. One finds that bound states are absent if simultaneously $mV_2b^2 \ll 1$ and $4mV_1a^2/\pi^2 \lesssim 1$. It is easily seen that these last conditions are quite compatible with the earlier requirements $b \ll a$ and $3V_2b > V_1a$. Since $J(k, k) \geq 0$ is a necessary condition that $J(k, p)$ be of the J_+ form, the result claimed at the outset is proved.

As discussed in Sec. II 2, the two results of this Appendix show the inadequacy of the usual criterion $v(0) > 0$ for the existence of an Einstein condensation in boson systems.

APPENDIX C

The Fourier transform of the central interparticle potential $W\phi(r/R)$ is given by

$$v(k) = 4\pi WR^3(kR)^{-1} \int_0^\infty dx x \phi(x) \sin kRx. \quad (C1)$$

Expanding $\sin(kRx)$ in a Taylor series about $x=0$ and term-wise performing the integration, one obtains

$$v(k) = v(0)[1 - (k^2/k_c^2)S(kR)], \quad (C2)$$

where

$$S(kR) = \sum_{n=1}^{\infty} (-1)^{n-1} a_n (kR)^{2(n-1)}, \quad (C3)$$

and where

$$a_n = \frac{6}{(2n+1)!} \frac{I_{2n+2}}{I_4}. \quad (C4)$$

The quantities I_n and k_c^2 are defined by (66) and (69), respectively. Two examples will show the effect of the functional form of $\phi(x)$ upon the value of $k_c R$. If $\phi(x) = e^{-x}/x$ (screened Coulomb potential) and $\phi(x) = x^{-2} \exp(-x^2)$ one obtains $(k_c R)^2 = 1$ and $(k_c R)^2 = 12$, respectively. Quite generally, the more rapidly $\phi(x)$ decreases to zero for $x > 1$ the larger is the value of $k_c R$.

Because of Eqs. (64) and (65), it follows that $0 \leq a_n \leq 1$. For $kR < 1$, the power series $S(kR)$ converges absolutely since

$$|S(kR) - 1| \leq (kR)^2 \sum_{n=0}^{\infty} (kR)^{2n} = \frac{(kR)^2}{1 - (kR)^2}. \quad (C5)$$

The kernel $J(k, p)$, defined by Eq. (29), can be written as

$$J(k, p) = \frac{1}{8\pi^2 k p} \int_{|k-p|}^{k+p} dy y v(y), \quad (C6)$$

or as

$$J(k, p) = \frac{WR^3}{\pi} \int_0^\infty dx x^2 \phi(x) \frac{\sin kRx}{kRx} \frac{\sin pRx}{pRx}. \quad (C7)$$

For $(k+p)R < 1$, substitution of (C2) for $v(k)$ in (C6) yields

$$\left| J(k, p) - \frac{v(0)}{4\pi^2} \left(1 - \frac{k^2 + p^2}{k_c^2} \right) \right| \leq J(0, 0) (k_c R)^{-2} \times \left\{ \frac{1}{4k p R^2} \ln \frac{1 - R^2(k-p)^2}{1 - R^2(k+p)^2} - [1 + R^2(k^2 + p^2)] \right\}. \quad (C8)$$

For $k_c R \geq 1$ and $kR = pR = 1/10$ the right side of (C8) is less than 5×10^{-4} times the value of

$$J(0, 0) [1 - (k^2 + p^2)/k_c^2].$$

Because of Eq. (64), it follows that

$$\phi(x) \left(1 - \frac{\sin kRx}{kRx} \right) \frac{\sin pRx}{pRx} \leq \phi(x) \left(1 - \frac{\sin kRx}{kRx} \right)$$

for all values of x , k , and p . Using (C7), we conclude that for all p and k

$$0 < J(0, p) - J(k, p) < J(0, 0) - J(k, 0), \quad (C9)$$

$$|v(k)| < v(0).$$

According to (58)

$$|\epsilon(k) - \epsilon(0) - k^2/2m| \leq 2 \int_0^\infty dp p^2 |J(k, p) - J(0, p)| \frac{1}{e^{\beta\epsilon} - 1}. \quad (C10)$$

Using (C9) and (32), it follows that

$$|\epsilon(k) - \epsilon(0) - k^2/2m| \leq 2\rho v(0). \quad (C11)$$

This verifies the claim made in Sec. III 2.

Finally, we shall determine the ratio of the third term to the second term of Eq. (72). According to (C9) it suffices to obtain the ratio of $\int_0^{k_s} dp p^2 (e^{\beta\epsilon} - 1)^{-1}$ to $\int_{k_s}^\infty dp p^2 (e^{\beta\epsilon} - 1)^{-1}$. By writing $(e^{\beta\epsilon} - 1)^{-1}$ as a geometric series and by using Eq. (73), one obtains

$$\int_0^{k_s} dp p^2 \frac{1}{e^{\beta\epsilon} - 1} = \left(\frac{2\pi^2}{v_T^*} \right) \left(\frac{2}{\pi^{1/2}} \right) \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} \gamma(\frac{3}{2}, nk_s^2/2m^*kT) \times \exp[-n\beta\epsilon(0)], \quad (C12)$$

where⁴⁵

$$\gamma(\frac{3}{2}, y) = \int_0^y dx x^{1/2} e^{-x} = \frac{1}{2} \pi^{1/2} \operatorname{erf}(y^{1/2}) - y^{1/2} e^{-y}, \quad (C13)$$

and

$$\operatorname{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y dx e^{-x^2}. \quad (C14)$$

Finally, v_T^* is given by Eq. (130). If $k_s^2/2m^* = 9\kappa T_c$ it follows that the incomplete gamma function in (C12) can be replaced by $\gamma(\frac{3}{2}, \infty) = \frac{1}{2} \sqrt{\pi}$ with an error of less than 0.1% as long as $T - T_c \leq T_c/10$. Because of the narrowness of this temperature range, we shall set $T = T_c$ in the following. Using (C11), one finds in a similar manner

$$\int_{k_s}^\infty dp p^2 \frac{1}{e^{\beta\epsilon} - 1} \leq 2\pi^2 \rho \frac{1}{\Gamma(\frac{3}{2}) \zeta(\frac{3}{2})} \times \sum_{n=1}^{\infty} n^{-3/2} \Gamma(\frac{3}{2}, nk_s^2/2m\kappa T_c) \exp[2n\beta_c \rho v(0)], \quad (C15)$$

⁴⁵ In (C13) and (C16) we use the notation for the incomplete gamma function as given by Erdelyi *et al.*, *Higher Transcendental Functions* (McGraw-Hill Book Company, Inc., New York, 1953), Vol. II, Chap. IX.

where

$$\Gamma(\frac{3}{2}, y) = \Gamma(\frac{3}{2}) - \gamma(\frac{3}{2}, y). \quad (\text{C16})$$

Using the following asymptotic form⁴⁵

$$\Gamma(\frac{3}{2}, y) = e^{-y} y^{3/2} (y - \frac{1}{2})^{-1} \{1 - O[\frac{1}{2}/(y - \frac{1}{2})^2]\}, \quad (\text{C17})$$

the ratio of (C15) to (C12) is found to be less than

$$\frac{2}{\sqrt{\pi}} \frac{m}{m^*} \left(\frac{k_s^2}{2m^* k T_c} \right)^{1/2} \times \frac{1}{\exp\{\beta_c [(k_s^2/2m) - 2\rho v(0)]\} - 1}. \quad (\text{C18})$$

APPENDIX D

In this Appendix for illustrative purposes we evaluate the following integral

$$\mathcal{E}(\omega) = \frac{\sqrt{2}}{\pi} \omega \int_0^\infty dt \left[\frac{(t^2 + 1)^{1/2} - 1}{t^2 + 1} \right]^{1/2} \frac{1}{e^{\omega t} - 1}. \quad (\text{D1})$$

Employing the following identities⁴⁶:

$$\left[\frac{(t^2 + 1)^{1/2} - 1}{t^2 + 1} \right]^{1/2} = t^{1/2} \int_0^\infty du e^{-u} J_{1/2}(ut), \quad (\text{D2})$$

$$\int_0^\infty dt e^{-at} t^{1/2} J_{1/2}(ut) = \left(\frac{2}{\pi} \right)^{1/2} \frac{u^{1/2}}{u^2 + a^2}, \quad (\text{D3})$$

Eq. (D1) becomes

$$\mathcal{E}(\omega) = \frac{2}{\pi^{3/2}} \omega^{1/2} \int_0^\infty du e^{-\omega u} u^{1/2} \sum_{n=1}^\infty \frac{1}{u^2 + n^2}. \quad (\text{D4})$$

The quantity $J_{1/2}(ut)$ is a usual Bessel function. The infinite series in (D4) is easily evaluated using Poisson's sum formula⁴⁷

$$\sum_{n=1}^\infty \frac{1}{u^2 + n^2} = \frac{1}{2} \left(\frac{\pi}{u} + \frac{2\pi}{u} \frac{1}{e^{2\pi u} - 1} - \frac{1}{u^2} \right). \quad (\text{D5})$$

Thus,

$$\mathcal{E}(\omega) = \frac{\sqrt{2}}{\pi} \omega^{1/2} \int_0^\infty du u^{-1/2} \times \exp\left(-\frac{\omega u}{2\pi}\right) \left(\frac{1}{e^u - 1} - \frac{1}{u} + \frac{1}{2} \right). \quad (\text{D6})$$

Now by expanding e^{-au} and integrating term by term,

one finds

$$\int_x^\infty du u^{-1/2} e^{-au} \frac{1}{e^u - 1} \xrightarrow{x \rightarrow 0} \int_x^\infty du u^{-1/2} \frac{1}{e^u - 1} - a \Gamma(\frac{3}{2}) \zeta(\frac{3}{2}) + \frac{a^2}{2!} \Gamma(\frac{5}{2}) \zeta(\frac{5}{2}) + \dots, \quad (\text{D7})$$

where $\zeta(s)$ is the Riemann zeta function,²⁹ and $\Gamma(s)$ is the gamma function. Furthermore,

$$\int_x^\infty du u^{-3/2} e^{-au} \xrightarrow{x \rightarrow 0} \int_x^\infty du u^{-3/2} - 2\pi^{1/2} a^{1/2}, \quad (\text{D8})$$

and

$$\int_0^\infty du u^{-1/2} e^{-au} = \pi^{1/2} a^{-1/2}. \quad (\text{D9})$$

Finally,⁴⁸

$$\int_0^\infty du u^{-1/2} \left(\frac{1}{e^u - 1} - \frac{1}{u} \right) = \Gamma(\frac{1}{2}) \zeta(\frac{1}{2}). \quad (\text{D10})$$

By adding Eqs. (D7)–(D9) and making use of (D10), one obtains

$$\mathcal{E}(\omega) = 1 - (2/\pi)^{1/2} (1.460) \omega^{1/2} + (2/\pi) \omega - (2\pi)^{-3/2} (2.612) \omega^{3/2} + \dots \quad (\text{D11})$$

APPENDIX E⁴⁹

In Sec. II 2 we have seen that if the interparticle potential is characterized by a so called J_+ kernel, a zero must exist in the quasi-particle excitation spectrum for temperatures below a certain critical value T_c . In Sec. II 3, we made the assumption that $\epsilon_0 = 0$ and $\epsilon_k \neq 0$ for all $k \neq 0$. Among the consequences of this assumption were: (a) For $T < T_c$ the occupation number of the $k=0$ single-particle state is $O(V)$; (b) an energy gap separates ϵ_0 and $\epsilon_{k>0}$. We shall now assume that for $T < T_c$

$$\epsilon_k \neq 0, \quad (\text{all } k > k_0) \quad (\text{E1})$$

$$\langle a_k^\dagger a_k \rangle = O(V^{x(k)}), \quad (\text{all } k < k_0) \quad (\text{E2})$$

$$0 < x(k) = O(1) < 1, \quad (\text{E3})$$

$$\sum_{k < k_0} \langle a_k^\dagger a_k \rangle = O(V). \quad (\text{E4})$$

Note, in particular, that we have assumed that

$$V^{-1} \langle a_0^\dagger a_0 \rangle \xrightarrow{V \rightarrow \infty} 0.$$

⁴⁶ G. N. Watson, *Theory of Bessel Functions* (Cambridge University Press, London, 1944), 2nd ed., p. 386.

⁴⁷ P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), Part I, p. 467.

⁴⁸ E. C. Titchmarsh, *The Theory of the Riemann Zeta Function* (Oxford University Press, London, 1951), pp. 24–25.

⁴⁹ Several of the results of this Appendix have been obtained independently by Dr. M. Girardeau, *Phys. Fluids* (to be published).

The assumptions of (E1)–(E4) imply the following:

(i) $\langle a_k^\dagger a_k \rangle = O(1)$ for $k > k_0$, whereas $\epsilon_k = 0$ for $k < k_0$. (See end of Sec. II 2.)

(ii) $k_0 = O(V^{-y})$ where $y > 0$. [If k_0 were $O(1)$ the number of single-particle states for which $k < k_0$ would be $O(V)$. But then (E2) and (E4) would be contradictory.]

(iii) The number of states for which $k < k_0$ is $O(V^z)$, where $0 < z < 1$. (This follows from (E3).)

(iv) $\epsilon_k \neq 0$ for any nonzero value of k such that $k = O(1)$. [According to (ii), one need only consider a system whose volume is such that k_0 is less than the value of k under consideration.]

We now investigate the consequences of (E1)–(E4) upon the form of the quasi-particle excitation spectrum. For $k > k_0$ the complete Eqs. (25) and (26) are valid. Thus, for all values of \mathbf{k} we may write Eqs. (8) and (9) as

$$f_k = (k^2/2m) - \mu + \rho v(0) + V^{-1}v(k) \sum_{p < k_0} \xi_p + (2V)^{-1} \sum_{p > k_0} v(\mathbf{p} - \mathbf{k}) [(f_p/\epsilon_p) \coth(\frac{1}{2}\beta\epsilon_p) - 1], \quad (\text{E5})$$

$$h_k = V^{-1}v(k) \sum_{p < k_0} \eta_p - (2V)^{-1} \sum_{p > k_0} v(\mathbf{p} - \mathbf{k}) (h_p/\epsilon_p) \coth(\frac{1}{2}\beta\epsilon_p). \quad (\text{E6})$$

Since f_k and h_k are continuous functions of \mathbf{k} , if we choose $f_0 + h_0 = 0$ it follows that $f_k + h_k = 0$, and thus $\xi_k = \eta_k + O(1)$, for all $k < k_0$. Let

$$s = \lim_{V \rightarrow \infty, \text{ fixed } \rho} V^{-1} \sum_{k < k_0} \xi_k. \quad (\text{E7})$$

According to (E4) this quantity is nonzero for $T < T_c$. In the volume limit,

$$\mu = \rho v(0) + 2sv(0) + \int_0^\infty dp p^2 J(0, p) \left[\frac{f(p)}{\epsilon(p)} \coth(\frac{1}{2}\beta\epsilon) - 1 \right] - \int_0^\infty dp p^2 J(0, p) \frac{h(p)}{\epsilon(p)} \coth(\frac{1}{2}\beta\epsilon(p)), \quad (\text{E8})$$

$$f(k) = \frac{k^2}{2m} + s[v(k) - 2v(0)] + \int_0^\infty dp p^2 [J(k, p) - J(0, p)] \times \left[\frac{f(p)}{\epsilon(p)} \coth(\frac{1}{2}\beta\epsilon) - 1 \right] + \int_0^\infty dp p^2 J(0, p) \frac{h(p)}{\epsilon(p)} \coth(\frac{1}{2}\beta\epsilon(p)), \quad (\text{E9})$$

$$h(k) = sv(k) - \int_0^\infty dp p^2 J(k, p) \frac{h(p)}{\epsilon(p)} \coth(\frac{1}{2}\beta\epsilon(p)), \quad (\text{E10})$$

$$\rho = s + \frac{1}{4\pi^2} \int_0^\infty dk k^2 \left[\frac{f(k)}{\epsilon(k)} \coth(\frac{1}{2}\beta\epsilon) - 1 \right]. \quad (\text{E11})$$

It is important to note that according to Eqs. (E8)–(E11) the effects of the smeared Einstein condensation upon the thermal properties of the system are described solely in terms of one parameter, namely s . Conversely, s is the only property of the condensation which can be obtained from these equations. Although Ω^0 correctly gives the volume proportional part of Ω_P , it is only by including those corrections to Ω_P which are of lower order in V that one can determine the details of the smearing.⁵⁰

The properties of $\epsilon(k)$ for small k are easily determined from Eqs. (E9) and (E10): $f(k) + h(k) = O(k^2)$ whereas $f(k) - h(k) = 2f(0) + O(k^2)$. Thus

$$\epsilon(k) \xrightarrow{k \rightarrow 0} ck.$$

That is to say, the assumption of a “smeared” Einstein condensation of the form of (E2)–(E4) results in a linear low energy spectrum.

We now turn to the question, under what conditions are the assumptions of (E1)–(E4) tenable? For this purpose we shall make the simplifying assumption that $J(k, p)$ is a factorizable kernel. Although the assumption is true in only a very few cases we believe that the following conclusions are true more generally. Since $J(k, 0) = (4\pi^2)^{-1}v(k)$, in the factorized form

$$J(k, p) = [4\pi^2 v(0)]^{-1} v(k) v(p). \quad (\text{E12})$$

Equations (E9) and (E10) are now easily solved:

$$f(k) = -\frac{1}{2}(\gamma - \eta)v(0) + (k^2/2m) + \frac{1}{2}(\gamma + \eta)[v(k) - v(0)], \quad (\text{E13})$$

$$h(k) = \frac{1}{2}(\gamma - \eta)v(k) = -f(0)v(k)/v(0), \quad (\text{E14})$$

where

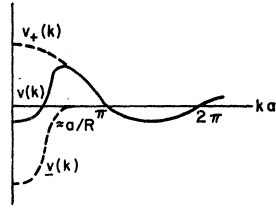
$$\gamma = 2s + \frac{1}{4\pi^2 v(0)} \int_0^\infty dk k^2 v(k) \times \left[\frac{f(k) - h(k)}{\epsilon(k)} \coth(\frac{1}{2}\beta\epsilon) - 1 \right], \quad (\text{E15})$$

$$\eta = \frac{1}{4\pi^2 v(0)} \int_0^\infty dk k^2 v(k) \left[\frac{f(k) + h(k)}{\epsilon(k)} \coth(\frac{1}{2}\beta\epsilon) - 1 \right]. \quad (\text{E16})$$

Equations (E11), (E15), and (E16) serve to determine the three unknown quantities γ , η , and s in terms of T , ρ , and $v(k)$.

⁵⁰ The author is indebted to Dr. M. Girardeau for the clarification of this point.

FIG. 6. Schematic plot of the Fourier transform $v(k)$ representing a two-body potential consisting of a repulsive hard core (pseudo-potential) and a weak, long ranged attractive portion.



According to Eq. (25), in order to insure that $\langle a_k^\dagger a_k \rangle \geq 0$ it is necessary that $f(k) \geq \epsilon(k) > 0$ for all $k > k_0$. Now because $f(k)$ is a continuous function of k , and, further, $k_0 = O(V^{-\nu})$, $\gamma > 0$, it follows that $f(0) > 0$. If we assume $v(0) > 0$, then according to (E13) it is necessary that $\gamma - \eta < 0$. But using (E14)–(E16), one finds

$$\frac{1}{2}(\gamma - \eta) = s + \frac{1}{4\pi^2 v^2(0)} f(0) \int_0^\infty dk k^2 \frac{v^2(k)}{\epsilon(k)} \coth[\frac{1}{2}\beta\epsilon(k)] > 0.$$

Only if $v(0) < 0$ is this contradiction avoided. The answer to our question is now clear: The smeared Einstein condensation of (E1)–(E4) can occur only if the interparticle potential is predominantly negative.

We now proceed to study the form of $\epsilon(k)$ in greater detail. For this purpose we choose a two-body potential composed of a hard core of diameter a , and an attractive potential of range $R \gg a$. For $v(k)$, we write

$$v(k) = v_+(0) \frac{\sin ka}{ka} + v_-(k), \quad (\text{E17})$$

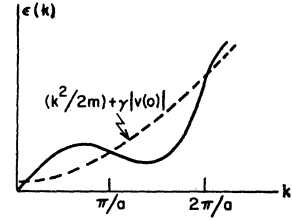
such that

$$v_+(0) > 0, \quad v_-(0) < 0, \quad v(0) < 0. \quad (\text{E18})$$

In (E17) the hard core is represented by the pseudo-potential $v_+(0) \times (\sin ka/ka)$.⁵¹ The assumption $R \gg a$ insures that $v(k) \approx v_+(k)$ for $k \gtrsim R^{-1}$. These properties of $v(k)$ are displayed in Fig. 6.

⁵¹ R. Abe, Progr. Theoret. Phys. (Kyoto) **19**, 699 (1958).

FIG. 7. Qualitative behavior of the quasi-particle excitation spectrum (E19) using a two-body potential whose Fourier transform is shown in Fig. 6.



According to (E13) and (E14), with $v(0) = -|v(0)|$

$$\epsilon(k) = \{[(k^2/2m) + \gamma|v(0)| + \gamma v(k)] \times [(k^2/2m) + \gamma|v(0)| + \eta v(k)]\}^{1/2}. \quad (\text{E19})$$

We note that $\epsilon(k) = (k^2/2m) + \gamma|v(0)|$ whenever $v(k) = 0$. That is to say, $\epsilon(k)$ intertwines itself with $(k^2/2m) + \gamma|v(0)|$. For the specific choice of (E17) and (E18) the nonmonotonic behavior of $\epsilon(k)$ is shown in Fig. 7.

We have not pursued the analysis of (E19) any further, for without the aid of a computer the evaluation of the integrals in (E11), (E15), and (E16), and thus the determination of γ , η , and s , is a prohibitively difficult task. Nevertheless, it is an exciting possibility that the peculiar properties of liquid He^4 are to be understood in terms of a *smeared* Einstein condensation of the type (E1)–(E4). The notorious results of those treatments⁵² which include an attractive portion to the interparticle potential within the framework of a usual Einstein condensation certainly provides incentive to attempt to verify the ideas of this Appendix.

In conclusion, we wish to add that $v_+(k)$ of (E17) is such that $J_+(k, p)$ is rigorously factorizable in the form (E12). Now because $R \gg a$, it seems likely that (E13) and (E14) are accurate solutions to (E9) and (E10) for $k \gtrsim R^{-1}$. In such an instance the nonmonotonic behavior of $\epsilon(k)$ would be assured.

⁵² See, for example, W. E. Parry and D. ter Haar, Ann. Phys. (New York) (to be published).