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Microscopic calculation of the excitation spectrum of superfluid helium-4*†

Gerald W. Goble and Donald H. Kobe
Department of Physics, North Texas State University, Denton, Texas 76203

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The Hartree-Fock-Bogoliubov equations for a homogeneous boson system at finite temperature are derived using linearized operator equations of motion. By a partial decoupling of two of the equations, a temperature-dependent form of the Lippmann-Schwinger equation for a local t matrix emerges naturally with a fully dressed energy denominator. In order to use a realistic potential the theory is phenomenologically modified by (i) redefining the chemical potential to remove an unphysical energy gap, and (ii) removing (possibly divergent) Hartree-Fock-like terms from the single-particle energy. The resulting set of coupled nonlinear integral equations is solved self-consistently for the Morse-dipole-dipole and the Frost-Musulin potentials. The excitation spectra obtained are in qualitative agreement with the observed phonon-roton spectrum, but the temperature dependence is given incorrectly. The calculations were made at a realistic density and the condensate fraction is about 60% at absolute zero.

I. INTRODUCTION

The energy spectrum of He II has been the subject of great interest for over three decades. Landau[1] originally postulated a two-branch spectrum to fit thermodynamic data on He II. Six years later[2] he found that a single-branch spectrum with a phonon part at low momentum which smoothly connected to a roton part at higher momentum gave better agreement with the data. A decade later Cohen and Feynman[3] predicted that the excitation spectrum should be observable by inelastic neutron scattering. During the next few years, intense effort by several groups[4] resulted in the experimental confirmation of Landau's single-branch phonon-roton spectrum.

There have been two main theoretical approaches to the calculation of the phonon-roton spectrum. Bogoliubov[5] showed that the energy spectrum of a weakly interacting boson system should be phononlike at small momentum by partially diagonalizing the Hamiltonian. His spectrum involved the Fourier transform of the potential, which is infinite for most realistic potentials. Feynman,[6] using a trial wave function and the energy variational principle, later showed that both the phonon and roton parts of the spectrum could be obtained if the experimental liquid-structure factor were used. Although the phonon part of the spectrum was well described, the roton minimum obtained by Feynman was high by a factor of about 2. Using a more sophisticated trial wave function which took into account backflow, Feynman and Cohen[7] calculated the roton minimum to within about 20% of the experimental value.

In an attempt to refine the calculation of Feynman and Cohen,[7] Burke, Major, and Chester[8] used a more general variation function and improved the roton energy only slightly. Unfortunately, they did not obtain good agreement with the phonon spectrum. In fact, the low-momentum part of the spectrum calculated from the variational principle was even less than the observed phonon spectrum for some values.

Ironically, attempts to improve the Bogoliubov spectrum also met with difficulties. When the correlations between particles of equal but opposite momentum were treated more carefully, a gap was discovered[9] in the excitation spectrum at zero momentum. This gap is unphysical,[10] but by calculating high-order diagrams several authors[11] have shown that this gap vanishes. To apply the theory to a system with a hard-core potential between the particles, Brueckner and Sawada[12] replaced the bare potential in the Hamiltonian by a t matrix calculated from a Lippmann-Schwinger (LS) equation before making the Bogoliubov transformation.[5] This procedure gave an expression for the excitation spectrum similar to the one obtained by Bogoliubov,[5] except that the Fourier transform of the potential was replaced by the t matrix. Since the t matrix for realistic potentials is finite, the excitation spectrum is now also finite. Brueckner and Sawada[12] assumed that essentially all the particles were in the zero-momentum state, and obtained a phonon-roton spectrum in qualitative agreement with Landau's.[2] Unfortunately, when Parry and ter Haar[13] took the depletion of the zero-momentum state into account self-consistently, they showed that in the Brueckner-Sawada[12] calculation there were 2.7 times as many particles excited out of the zero-momentum state as were in the system. When they performed a self-consistent calculation using a fixed condensate fraction of 0.50, the roton dip vanished.

Since these first calculations, several others using realistic potentials have been attempted to obtain the phonon-roton spectrum from first principles. Many other calculations have been made using model potentials with some adjustable parameters. In a later section some of these theories are compared with the calculations given here.

The need for yet another microscopic calculation of the excitation spectrum of He II perhaps requires some justification. In the present theory, it is shown that a *t* matrix emerges naturally from the Bogoliubov canonical transformation when correlations between particles of equal and opposite momentum are taken into account.[14] Thus the potential does not have to be replaced in an *ad hoc* way by the *t* matrix at the beginning. In addition the theory given here, which is a modified Hartree-Fock-Bogoliubov (HFB) theory[15] of homogeneous boson systems, can be extended to finite temperatures in a way similar to that used in superconductivity.[16] The temperature dependence of the boson spectrum has not previously been calculated from a microscopic theory, presumably because even the zero-temperature theory becomes extremely complicated. In addition, several new realistic interatomic potentials have recently become available for He^4 by fitting data on the gaseous phase and on phase shifts obtained from helium beam experiments.[17] Thus, for these reasons it was felt that another calculation of the energy spectrum of He II was in order.

The results obtained for the energy spectrum at zero temperature are only in qualitative agreement with the observed phonon-roton spectrum, but there are no arbitrary parameters to adjust in the theory. The phonon and roton features of the spectrum are clearly visible, however. Unfortunately, the temperature dependence of the spectrum is given incorrectly. The calculated speed of sound decreases as the temperature is increased, whereas the observed speed is essentially constant.[18] The calculated roton minimum increases with temperature, in contrast to the decrease observed experimentally.[19]

One interesting aspect of the calculation here is that the *t* matrix is local, and so in configuration space it can be compared with the bare potential. The *t* matrix is an effective interaction which takes into account the short-range correlation induced into the wave function by the strongly repulsive potential. As might be expected, the effective potential is very much like the bare potential at large interatomic distances, but at short range it is much less repulsive.

In Sec. II, the linearized equation of motion for the annihilation operator of an interacting boson system is obtained at finite temperatures. In Sec. III the linearized equation is solved to obtain the HFB theory for a homogeneous system at finite temperature. Two of the resulting equations are partially decoupled in Sec. IV without any approximation to give a local, temperature-dependent *t* matrix with a fully dressed energy denominator. Since some unphysical features, like an energy gap, occur in the HFB theory, it is phenomenologically modified in Sec. V to give a set of equations that can be solved for a realistic potential. The solution of the set of coupled nonlinear integral equations is briefly discussed in Sec. VI. The results are given in Sec. VII and physically interpreted. In Sec. VIII the calculated results are compared with other calculations. Section IX gives an evaluation of the theory.

II. LINEARIZED EQUATION OF MOTION

The first use of linearized operator equations of motion in the context of boson systems was made by Bogoliubov.[5] He approximated the Hamiltonian by replacing the operator a_0 by the c number $N_0^{1/2}$, and retained only the quadratic part. The linearized operator equations of motion were solved by a canonical transformation. The method was again used in boson systems by Valatin and Butler,[20] but they do not make the Bogoliubov approximation of replacing a_0 by a c number. Instead, they treated the system, including the condensate, as being composed of pairs, in analogy with the theory of superconductivity.[15] Their method was extended to finite temperatures ($T \neq 0$) by Evans and Imry.[21]

For inhomogeneous boson systems the linearized operator equations of motion were first used by Gross[22] in a semiclassical theory of boson wave fields. A completely quantum-mechanical version at zero temperature which took into account both the single-particle condensate and the pairing correlations was developed by Kobe.[23] The finite-temperature generalization was only recently given by Fetter,[24] but his treatment of the condensate is slightly different. The plane-wave solutions for the inhomogeneous system give the equations for the homogeneous system at finite temperature. However, since the method has not previously been applied directly to homogeneous boson systems at finite temperature taking into account both the single-particle condensate and pairing correlations, it is given here to review and to establish the notation.

The solution of the linearized equation of motion gives the Hartree-Fock-Bogoliubov (HFB) theory for a homogeneous boson system at finite temperature. The HFB theory can also be obtained from Green's functions,[25,26] the Gibbs-Bogoliubov free-energy variational principle,[25,27] Bogoliubov's principle of compensation of dangerous diagrams to lowest order,[25,28] and the method of thermodynamically equivalent Hamiltonians.[29,30]

The Hamiltonian for an interacting many boson system is[31]

$$H=\sum_{1}(e_1-\mu)a_1^\dagger a_1+\tfrac{1}{2}\sum_{1234}\langle 12|V|34\rangle a_1^\dagger a_2^\dagger a_3 a_4\,, \tag{2.1}$$

where 1 stands for $\vec{k}_1$, 2 for $\vec{k}_2$, etc. The kinetic energy of the particles with mass m is $e_k=k^2/2m$, and μ is the chemical potential. The matrix elements of the two-body potential $\langle 12|V|34\rangle$ are symmetrized. The creation operators $a_k^\dagger$ and the annihilation operators a_k satisfy the usual boson commutation relations.

For the operator a_k in the Heisenberg picture, the equation of motion is

$$i\dot{a}_k=[a_k,H]\,. \tag{2.2}$$

If the Hamiltonian in Eq. (2.1) is substituted into Eq. (2.2), the nonlinear operator equation

$$i\dot{a}_k=(e_k-\mu)a_k+\sum_{jpq}\langle kj|V|pq\rangle a_j^\dagger a_p a_q \tag{2.3}$$

is obtained.

For a boson system there can be macroscopic occupation of the zero-momentum state, which must carefully be taken into account. A shift canonical transformation[32]

$$a_k=b_k+\phi_0\delta_{k0}\,, \tag{2.4}$$

can be made to new "quasiparticle" operators b_k, which are the same as the particle operators for $k\neq 0$, but describe excitations about the condensate amplitude ϕ_0 for $k=0$.[33] The condensate amplitude ϕ_0 is a c number, and will be considered as time independent for the homogeneous system.

When Eq. (2.4) is substituted into Eq. (2.3), the nonlinear equation for the operator b_k is

$$\begin{aligned} i\dot{b}_k=&(e_k-\mu)b_k-\mu\phi_0\delta_{k0}+\langle k0|V|00\rangle\phi_0^3\\ &+\sum_{jpq}\langle kj|V|pq\rangle[b_j^\dagger b_p b_q+\phi_0\delta_{j0}b_p b_q+2\phi_0\delta_{p0}b_j^\dagger b_q\\ &+\phi_0^2\delta_{p0}\delta_{q0}b_j^\dagger+2\phi_0^2\delta_{j0}\delta_{p0}b_q]\,. \end{aligned} \tag{2.5}$$

This equation can be linearized by the standard method[34] of replacing all possible pairs of operators by their average values in the appropriate grand canonical ensemble. When the linearization of Eq. (2.5) is performed, the result is

$$i\dot{b}_k=(-\mu+\langle 00|V|00\rangle\phi_0^2+f_0+g_0)\phi_0\delta_{k0}+U_k b_k+\Delta_k b_{-k}^\dagger\,. \tag{2.6}$$

The dressed single-particle energy U_k is defined as

$$U_k=e_k-\mu+2\langle k0|V|0k\rangle\phi_0^2+f_k\,, \tag{2.7}$$

where the Hartree-Fock term

$$f_k=2\sum_{p}\langle kp|V|pk\rangle\langle b_p^\dagger b_p\rangle \tag{2.8}$$

describes the direct plus exchange scattering of a particle in the state $\vec{k}$ with one in the state $\vec{p}$ back to the same states. The term $2\langle k0|V|0k\rangle\phi_0^2$ describes the direct plus exchange scattering of a particle in the state $\vec{k}$ with one in the condensate, back to the same states. The pair potential Δ_k is defined as

$$\Delta_k=\langle k,-k|V|00\rangle\phi_0^2+g_k\,, \tag{2.9}$$

where the first term describes the excitation of a pair of particles from the condensate to the states $\vec{k}$ and $-\vec{k}$. The second term is defined as

$$g_k=\sum_{p}\langle k-k|V|-pp\rangle\langle b_{-p}b_p\rangle\,, \tag{2.10}$$

and describes the scattering of a pair of particles with momentum $\vec{p}$ and $-\vec{p}$ and amplitude $\langle b_p b_{-p}\rangle$ to the states $\vec{k}$ and $-\vec{k}$.

III. HARTREE-FOCK-BOGOLIUBOV THEORY

The linearized equation of motion of Sec. II is solved in this section to obtain the HFB theory.[25-30] Different authors, however, have different results regarding the energy gap, the chemical potential, and the density. The results obtained here are identical to the ones obtained by applying the Gibbs-Bogoliubov free-energy principle and the compensation of the lowest-order dangerous diagrams.[28]

The coefficient of the unit operator in Eq. (2.6) can be equated to zero, which gives the equation

$$[-\mu+\langle 00|V|00\rangle\phi_0^2+f_0+g_0]\phi_0=0\,. \tag{3.1}$$

If the condensate amplitude $\phi_0\neq 0$, this equation determines the chemical potential.

A canonical transformation[5] on the operator b_k to Bogoliubov quasiparticles (BQP's) can now be made, which gives

$$b_k=u_k\gamma_k+v_k\gamma_{-k}^\dagger\,. \tag{3.2}$$

In order for the BQP's to be bosons, the BQP creation and annihilation operators, $\gamma_k^\dagger$ and γ_k, respectively, must satisfy boson commutation relations. The coefficients in Eq. (3.2) must then satisfy

$$u_k^2-v_k^2=1\,, \tag{3.3}$$

in addition to being even functions of $\vec{k}$. The BQP operator $\gamma_k(\tau)$ in the Heisenberg picture is assumed to oscillate with the BQP energy E_k,

$$\gamma_k(\tau)=\gamma_k e^{-iE_k\tau}, \tag{3.4}$$

where τ is the time.

When Eq. (3.2) is substituted into Eq. (2.6), Eq. (3.4) is used, and the coefficients of the creation and annihilation operators separately equated to zero, the two equations

$$E_k u_k = U_k u_k + \Delta_k v_k \tag{3.5}$$

and

$$-E_k v_k = U_k v_k + \Delta_k u_k, \tag{3.6}$$

are obtained. In order for these homogeneous equations to have a nontrivial solution, the determinant of the coefficients must vanish. The BQP energy,

$$E_k=(U_k^2-\Delta_k^2)^{1/2}, \tag{3.7}$$

is thus obtained. Equations (3.5) and (3.6) can now be solved to give

$$u_k^2+v_k^2=U_k/E_k, \tag{3.8}$$

and

$$2u_k v_k=-\Delta_k/E_k, \tag{3.9}$$

when Eq. (3.3) is used.

The average particle occupation number, calculated in terms of the grand canonical ensemble for free BQP's, is

$$\langle b_p^\dagger b_p\rangle = v_p^2+(u_p^2+v_p^2)\bar{n}_p, \tag{3.10}$$

when Eq. (3.2) is used. The average BQP occupation number is given by

$$\bar{n}_p=[\exp(\beta E_p)-1]^{-1}, \tag{3.11}$$

where $\beta=(k_B T)^{-1}$, k_B is Boltzmann's constant, and T is the absolute temperature. The pair amplitude is

$$\langle b_p b_{-p}\rangle = u_p v_p(1+2\bar{n}_p), \tag{3.12}$$

when Eq. (3.2) is substituted into the average defined in terms of the grand canonical ensemble for free BQP's.

The chemical potential μ can be determined from Eq. (3.1) if the condensate amplitude is nonzero, which gives

$$\mu=\langle 00|V|00\rangle\phi_0^2+f_0+g_0. \tag{3.13}$$

When this equation is used in Eq. (2.7), along with Eq. (2.9), the single-particle energy is

$$\begin{aligned}U_k={}&e_k+(f_k-f_0)-(g_k+g_0)+\Delta_k\\&+[2\langle k0|V|0k\rangle-\langle k-k|V|00\rangle-\langle 00|V|00\rangle]\phi_0^2.\end{aligned} \tag{3.14}$$

This expression is used in Eq. (3.7) to obtain the BQP energy. When the resulting BQP energy is evaluated at $k=0$, a gap

$$E_0=2\phi_0[-g_0\langle 00|V|00\rangle]^{1/2}, \tag{3.15}$$

occurs in the excitation spectrum.[9]

In order to obtain the energy spectrum in the HFB theory, it is necessary to obtain Δ_k and U_k self-consistently, subject to the constraint in Eq. (3.7). When Eqs. (2.10), (3.12), and (3.9) are substituted into Eq. (2.9), an integral equation,

$$\begin{aligned}\Delta_k={}&\langle k-k|V|00\rangle\phi_0^2\\&-\sum_p\langle k-k|V|-pp\rangle(\Delta_p/2E_p)\coth(\tfrac{1}{2}\beta E_p),\end{aligned} \tag{3.16}$$

is obtained. When Eqs. (2.8), (3.10), (3.3), and (3.8) are substituted into Eq. (2.7), the equation

$$\begin{aligned}U_k={}&e_k-\mu+2\langle k0|V|0k\rangle\phi_0^2\\&+\sum_p\langle kp|V|pk\rangle[(U_p/E_p)\coth(\tfrac{1}{2}\beta E_p)-1]\end{aligned} \tag{3.17}$$

is obtained. These two equations are coupled through Eq. (3.7) in a highly nonlinear way. Before they can be solved self-consistently, the number of particles in the zero-momentum state ϕ_0^2 must be determined.

The average of the number operator in the free BQP grand canonical ensemble is

$$\langle\hat{N}\rangle=\phi_0^2+\sum_p\langle b_p^\dagger b_p\rangle. \tag{3.18}$$

When Eqs. (3.10), (3.3), (3.11), and (3.8) are substituted into Eq. (3.18) the result is

$$N=\phi_0^2+\tfrac{1}{2}\sum_p[(U_p/E_p)\coth(\tfrac{1}{2}\beta E_p)-1], \tag{3.19}$$

when $\langle\hat{N}\rangle$ is equated to the actual number of particles N. Dividing Eq. (3.19) by the volume of the system Ω, we obtain an equation for the density $\rho=N/\Omega$ in terms of the condensate density or the density in the zero-momentum state $\rho_0=\phi_0^2/\Omega$.

For a local potential between the particles, the matrix element of the potential is

$$\langle\vec{k}\vec{l}\,|V|\vec{p}\vec{q}\rangle=(2\Omega)^{-1}[V_{k-q}+V_{k-p}]\delta(\vec{k}+\vec{l},\vec{p}+\vec{q}), \tag{3.20}$$

where Ω is the volume. The Kronecker delta $\delta(\vec{k}+\vec{l},\vec{p}+\vec{q})$ is unity if momentum is conserved, and is zero otherwise. The Fourier transform of the local two-body potential $V(r)$ is

$$V_q=\int d^3r\, e^{i\vec{q}\cdot\vec{r}}\,V(r), \tag{3.21}$$

which depends only on the magnitude of $\vec{q}$. All the equations of this section are simplified by using the local potential and taking the infinite-volume limit.

IV. THE REACTION OPERATOR

A reaction operator or t matrix naturally emerges in this theory, as a result of a partial decoupling of Eq. (3.16) for Δ_k and Eq. (3.19) for ϕ_0^2. This t matrix in momentum space t_k is shown to be a local function $t(r)$ in configuration space.[35] The function $t(r)$ plays the role of an effective interaction. In many theories a t matrix is inserted in an *ad hoc* manner at the start.[12]

An operator t is defined such that it has matrix elements given by

$$\langle k - k \,|\, t \,|\, 00 \rangle \equiv \Delta_k / \phi_0^2 . \tag{4.1}$$

Then Eq. (3.16) divided by ϕ_0^2 becomes

$$\langle k - k \,|\, t \,|\, 00 \rangle = \langle k - k \,|\, V \,|\, 00 \rangle + \sum_p \frac{\langle k - k \,|\, V \,|\, -p p \rangle \langle p - p \,|\, t \,|\, 00 \rangle}{-2E_p} \coth(\tfrac{1}{2}\beta E_p) . \tag{4.2}$$

Equation (4.2) is a Lippmann-Schwinger (LS) equation for the t matrix or reaction operator. The t matrix in Eq. (4.2) describes the excitation of a pair of particles from the condensate to the states $\vec{k}$ and $-\vec{k}$. The energy denominator is fully dressed, since it is the BQP energy E_p in Eq. (3.7) which appears, rather than e_p or U_p. A novel feature of Eq. (4.2) is that the t matrix is temperature dependent through the factor $\coth(\frac{1}{2}\beta E_p)$, which goes to unity as the temperature $T = (k_B \beta)^{-1}$ goes to zero.

If it is assumed that the potential and the reaction operator are both local, the form of Eq. (3.20) may be used for both. Equation (4.2) reduces to

$$t_k = V_k - (2\pi)^{-3} \int d^3p \; V_{k-p} (t_p / 2E_p) \coth(\tfrac{1}{2}\beta E_p) , \tag{4.3}$$

in the infinite-volume limit.

Since a realistic potential $V(r)$ has a strongly repulsive core, it is easier to solve Eq. (4.3) by transforming to configuration space. Since the integral in Eq. (4.3) is of the convolution form, we obtain

$$t(r) = V(r) - V(r) \int_0^\infty dr' \, K(r, r') t(r') , \tag{4.4}$$

where the kernel is

$$K(r, r') = (r'/\pi r) \int_0^\infty dp \, E_p^{-1} \sin(pr) \times \sin(pr') \coth(\tfrac{1}{2}\beta E_p) . \tag{4.5}$$

The Fourier transform of $t(r)$,

$$t_k = 4\pi \int_0^\infty dr \, r^2 [\sin(kr)/kr] t(r) , \tag{4.6}$$

is needed to obtain the energy spectrum from Eqs. (3.20), (4.1), and (3.7). However, the energy spectrum in Eq. (3.7) is not valid for a realistic potential with a strongly repulsive core. The gap in Eq. (3.15) would be infinite for some potentials, while the terms $(f_k - f_0) - (g_k + g_0)$ in Eq. (3.14) could be overwhelmingly large compared to the bare kinetic energy e_k and the pair potential Δ_k. Thus to obtain a theory applicable to a realistic potential it is necessary to make some modifications.

V. MODIFICATION OF THE THEORY FOR A REALISTIC POTENTIAL

Some phenomenological modifications are made in this section to make the theory applicable to a system of He^4 atoms. These modifications should occur naturally if higher-order corrections are calculated,[11] but this is very difficult to show.

There is no gap in the observed excitation spectrum of He II at zero momentum.[36] The gap in Eq. (3.15) can be removed phenomenologically by subtracting $2g_0$ from the chemical potential in Eq. (3.13). Then the energy U_k in Eq. (3.14) can be written as

$$U_k = T_k + \Delta_k , \tag{5.1}$$

where the single-particle energy T_k is

$$T_k = e_k + (f_k - f_0) - (g_k - g_0) . \tag{5.2}$$

The BQP energy in Eq. (3.7) then becomes

$$E_k = [T_k (T_k + 2\rho_0 t_k)]^{1/2} , \tag{5.3}$$

when Eqs. (5.1), (4.1), and (3.20) are used. The condensate density is $\rho_0 = \phi_0^2 / \Omega$.

For a realistic potential the terms $(f_k - f_0) - (g_k - g_0)$ that modify the single-particle energy in Eq. (5.2) can be overwhelmingly large. For the sake of simplicity they are dropped here, but a more careful treatment of the problem would result in their being dressed by higher-order diagrams.[37] One possibility is that the potential in these terms is replaced by a t matrix.[38] The BQP energy spectrum in Eq. (5.3) then becomes

$$E_k = [e_k (e_k + 2\rho_0 t_k)]^{1/2} , \tag{5.4}$$

so it is necessary to calculate ρ_0 and t_k self-consistently. Equation (5.4) is the same form as obtained by Bogoliubov[5] except that ρV_k has been replaced by $\rho_0 t_k$. Brueckner and Sawada[39] obtained a similar form, but with ρ instead of ρ_0.

The condensate density can be calculated from Eq. (3.19). From Eq. (5.1) the function U_k in the approximation we are using here is

$$U_k = e_k + \rho_0 t_k \,, \tag{5.5}$$

when Eqs. (4.1) and (3.20) are used. If Eq. (3.19) is divided by the volume Ω, the condensate density

$$\rho_0 = \rho - (2\pi)^{-2} \int_0^\infty dp\, p^2 \{[(e_p + \rho_0 t_p)/E_p] \times \coth(\tfrac{1}{2}\beta E_p) - 1\} \tag{5.6}$$

is obtained in the infinite-volume limit. This equation and Eq. (4.3) were solved self-consistently for ρ_0 and t_k for two different realistic potentials to obtain the energy spectrum E_k in Eq. (5.4). The method of solution of these coupled equations is discussed in Sec. VI.

VI. CALCULATIONS

The system of equations comprising Eqs. (4.4)–(4.6), (5.4), and (5.6) were solved self-consistently at various temperatures on an IBM 360/50 computer for two different potentials. The interatomic helium potentials used are the Morse–dipole–dipole-2 (MDD2) potential and the Frost-Musulin (FM) potential given by Bruch and McGee.[17]

A detailed discussion of the numerical methods and the program used is beyond the scope of this paper.[40] However, the general method used is outlined below. For a given temperature, an energy was assumed in Eq. (4.5), and the kernel calculated by means of a 32-point Gauss quadrature from 0 to 6 Å^{-1} and also from 6 to 50 Å^{-1}.

Equation (4.4) for the reaction operator $t(r)$ was solved by the Fredholm method. The integral equation was converted into a set of 50 algebraic equations, which were solved by the Gauss-Jordan elimination method.[41] The integral in Eq. (4.4) was truncated at 10 Å, and equations were obtained at every 0.2-Å interval of r.

The Fourier transform of the reaction operator $t(r)$, the t matrix t_k, was calculated from Eq. (4.6) in two steps. The integration was performed using 32-point Gauss quadratures from 0 to 6 Å, and also from 6 to 50 Å.

The next step in the procedure was to calculate the condensate density ρ_0 using Eq. (5.6) into which Eq. (5.4) for E_p was substituted. The resulting equation then becomes

$$\rho_0 = \rho - (2\pi)^{-2} \int_0^\infty dp\, p^2 \{(e_p + \rho_0 t_p)(e_p^2 + 2e_p \rho_0 t_p)^{-1/2} \coth[(\tfrac{1}{2}\beta)(e_p^2 + 2e_p\rho_0 t_p)^{1/2}] - 1\} \,. \tag{6.1}$$

Since ρ_0 appears on the right-hand side under the integral, it was necessary to solve Eq. (6.1) by an iterative method. For a given system density ρ, an initial ρ_0 was assumed and the equation iterated. Convergence to a solution to within less than one part in 10^5 was obtained after fewer than ten iterations. The integral was performed using 32-point Gauss quadratures from 0 to 40 Å^{-1}, since the contribution beyond 40 Å^{-1} was negligible. Increasing the number of steps in the interval did not affect the value of the integral to the accuracy of the calculation. The system density ρ chosen was 0.0219 atoms Å^{-3}, corresponding to the experimental value extrapolated to zero pressure and temperature.

With the value of the condensate density ρ_0 determined, the energy spectrum E_k in Eq. (5.4) was calculated. This energy spectrum was used as the input in Eq. (4.5) to calculate the kernel values, and the whole process was repeated until self-consistency was attained. Up to ten iterations were required to give convergence to all values of the energy E_k to less than one part in 10^4.

VII. RESULTS

The results of the solution of the set of coupled nonlinear integral equations discussed in Sec. VI are given in this section and discussed.

The local reaction operator $t(r)$, which is an effective interaction, calculated from the MDD2 potential at the temperatures 0.00, 2.00, and 3.14 K is shown in Fig. 1. The corresponding curves for the FM potential are shown in Fig. 2. The dotted curve shows the original potential, so the effect of the short-range correlations, induced in the wave function by the strong short-range repulsion, is to weaken significantly the repulsion. The form of $t(r)$ for large r is a curve of the general shape of $V(r)$, since the integral in Eq. (4.4) decreases as r^{-1}. The structure in the curve for $r < 2$ Å is essentially due to the phonon-roton behavior of the energy spectrum E_p in Eq. (5.4) which occurs in Eq. (4.5). In particular the small hump at about 1.5 Å is correlated with the roton dip in E_p. As the temperature is increased, the term $\coth(\tfrac{1}{2}\beta E_p)$ in Eq. (4.5) becomes larger,

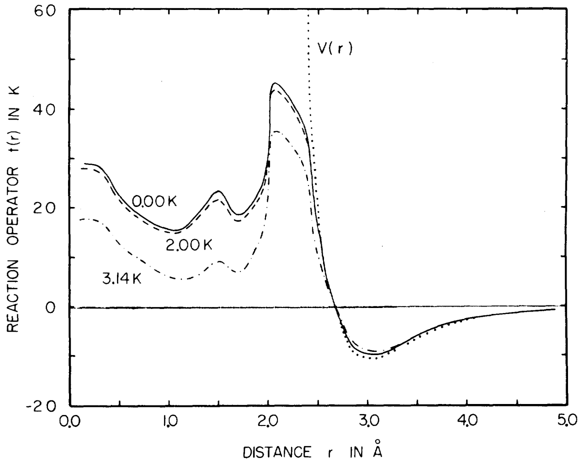

FIG. 1. Reaction operator $t(r)$ as a function of the interatomic distance calculated from the Morse-dipole-dipole-2 (MDD2) potential (dotted curve) of Ref. 17 at temperatures of 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve).

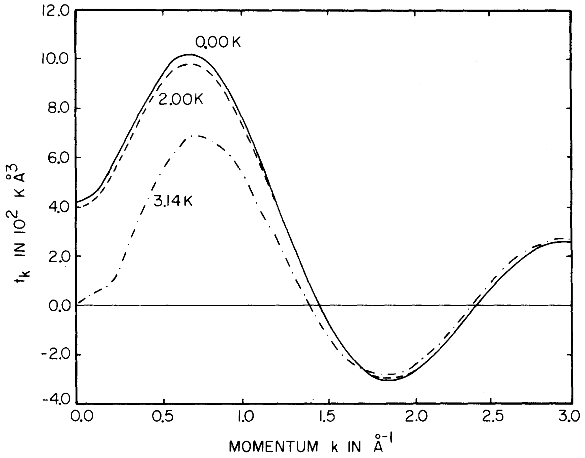

FIG. 3. t matrix t_k as a function of momentum k calculated from the MDD2 potential for the temperatures 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve).

which makes $t(r)$ in Eq. (4.4) smaller. For higher temperatures the volume integral of $t(r)$ decreases. The values of $t(r)$ for $r < 2$ Å are generally larger for the FM potential than for the MDD2 potential, since the former is more repulsive than the latter. The MDD2 potential is finite at the origin, whereas the FM potential is infinite.

That the effective interaction, the reaction operator $t(r)$, is less repulsive than the potential is to be expected. The product of the effective potential $t(r)$ and the wave function for a noninteracting pair of particles is equal to the bare potential multiplied by the correlated pair wave function. The correlated pair wave function goes to zero as the bare potential becomes infinite, and therefore the product is finite. Since the unperturbed pair wave function is finite, the effective interaction, or reaction operator, is also finite even at small interatomic distances.[42]

The t matrix t_k, which is the Fourier transform of $t(r)$, is shown in Fig. 3 for the MDD2 potential for the temperatures 0.00, 2.00, and 3.14 K. The corresponding curves for the FM potential are shown in Fig. 4. As the temperature increases the volume integral of $t(r)$ decreases. However, the volume integral of $t(r)$ is the t matrix at zero

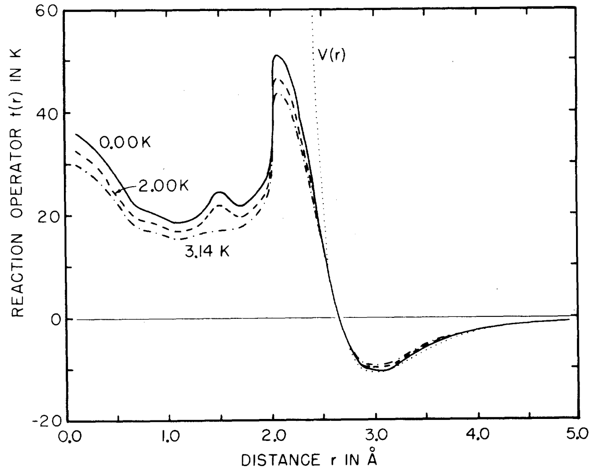

FIG. 2. Reaction operator $t(r)$ as a function of the interatomic distance calculated from the Frost-Musulin (FM) potential (dotted curve) of Ref. 17 at temperatures of 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve).

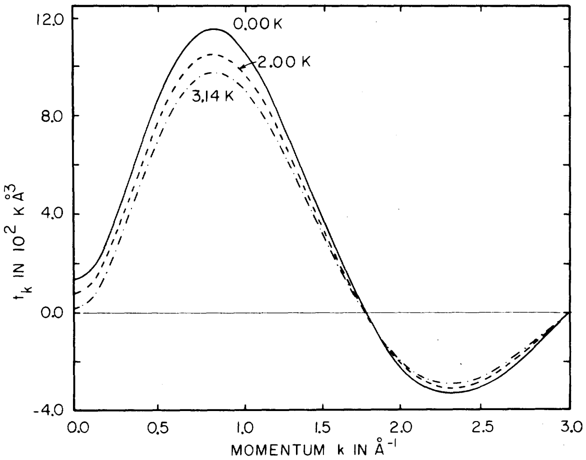

FIG. 4. t matrix t_k as a function of the momentum k calculated from the FM potential for the temperatures 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve).

momentum t_0. This value must be greater than zero in order for the excitation spectrum in Eq. (5.4) to be real. At sufficiently high temperatures t_0 becomes negative and the energy spectrum in Eq. (5.4) becomes imaginary. From both Figs. 3 and 4 the value of t_0 at 3.14 K is nearly zero, and for a temperature of 3.15 K the value of t_0 would become negative, which indicates a breakdown in the theory.

The ratio of the condensate density to the system density ρ_0/ρ calculated as a function of the temperature is shown in Fig. 5. For the temperature $T_c = 3.14$ K, Eq. (5.6) has two solutions. One solution corresponds to the ideal Bose-gas transition temperature with condensate density $\rho_0 = 0$, and energy spectrum $E_k = e_k = k^2/2m$, at a system density of $\rho = 0.0219$ atom Å^{-3}. Another solution exists, however, for $\rho_0 \neq 0$ and $E_k \neq e_k$, so there is a finite discontinuity in the ρ_0/ρ curve at T_c. For temperatures above 3.14 K there is no solution for $\rho_0 \neq 0$. Thus this theory of interacting bosons reduces to the ideal Bose gas at temperatures above 3.14 K. In other words, the bare BQP become bare particles for $\rho_0 = 0$ at the temperature 3.14 K and above.[43] When $\rho_0 = 0$ our derivation of the LS equation in Eq. (4.2) is invalid, because we cannot divide by zero in Eq. (4.1).

The fraction of the particles in the zero-momentum state at zero temperature calculated here is 59.5% for the MDD2 potential and 56.8% for the FM potential. The zero-momentum density slowly decreases with increase in temperature. Consequently as the temperature increases, the energy spectrum in Eq. (5.4) has a decreasing speed of sound and a less-pronounced roton minimum.

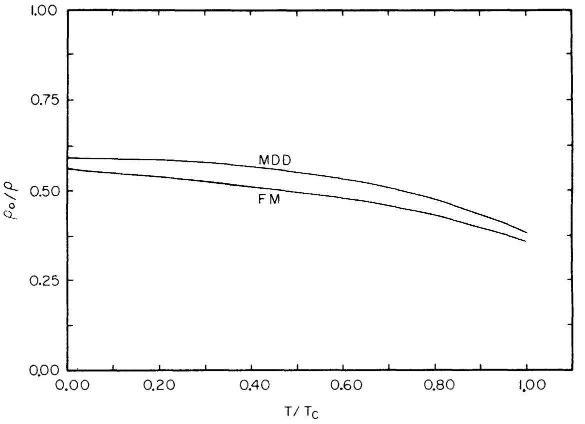

FIG. 5. Condensate fraction ρ_0/ρ as a function of the temperature ratio T/T_c calculated from the MDD2 and FM potential. The transition temperature of the ideal Bose gas is $T_c = 3.14$ K at the density $\rho = 0.0219$ atoms Å^{-3}. The experimental condensate ratio is 0.024 ± 0.01 at 1.2 K (Ref. 45).

However, at 3.14 K there is a discontinuity in ρ_0, which means that the energy spectrum abruptly changes from one with a phonon part for $\rho_0 \neq 0$ to the energy spectrum for a free particle for $\rho_0 = 0$.

Using the theory of Gersch, Rodriguez, and Smith[44] on the high-energy scattering of neutrons by He II, Mook, Scherm, and Wilkinson[45] found the condensate fraction to be 2.4 ± 1% at 1.2 K. This value is smaller than the 8.8 ± 1.3% found by Harling[46] at 1.27 K, or the value of 6% at 1.27 K found by Puff and Tenn.[47] Our calculated value thus is much larger than the experimental, but on the other hand it is positive, in contrast to some previous calculations.[12,13]

The energy spectra E_k calculated from Eq. (5.4) for the temperatures 0.00, 2.00, and 3.14 K are shown in Fig. 6 for the MDD2 potential. The corresponding spectra for the FM potential are shown in Fig. 7. The open circles are the experimental data of Cowley and Woods[48] at 1.12 K and the dotted curve is the free-particle energy $e_k = k^2/2m$. The fit to the experimental points is only qualitative, but it must be emphasized that there are no adjustable parameters in this theory which is completely self-consistent for a realistic potential and density. The spectrum calculated from the MDD2 potential at zero temperature is a somewhat better fit to the data than the spectrum calculated from the FM potential at zero temperature.

The slope of the phonon part of the spectrum gives the speed of sound in the liquid. Both potentials give a speed of sound that is too small.

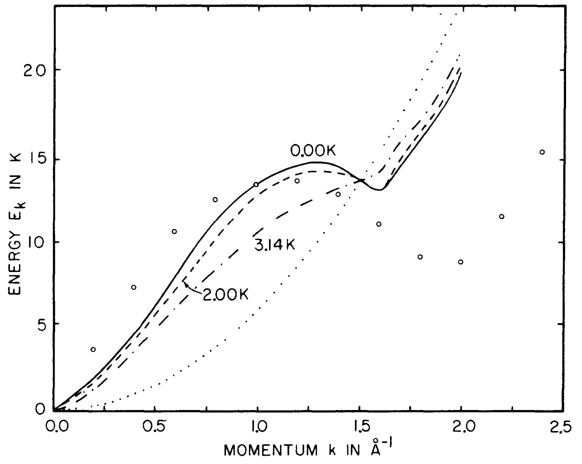

FIG. 6. Excitation spectra E_k as a function of momentum k calculated from the MDD2 potential for the temperatures 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve). The free-particle spectrum is given by the dotted curve. The open circles are the experimental data of Cowley and Woods (Ref. 48) at 1.12 K.

Worse yet, the experimental speed of sound is approximately constant from zero temperature to temperatures above the λ transition.[18] In our calculation the speed of sound decreases with an increase in temperature, contrary to experiment.

In both Figs. 6 and 7 the roton minima are higher, shallower, and occur at smaller momentum than the experimental roton minimum. The experimental roton minimum decreases with an increase in temperature,[19] while the calculated roton minimum in Fig. 6 increases and becomes shallower with an increase in temperature. However, in Fig. 7 there is a small decrease in the roton energy, but the dip becomes shallower at higher temperatures. The conclusion is that, while at low temperatures the modified HFB theory used here may be qualitatively correct, it gives generally the wrong temperature dependence for the speed of sound and the roton minimum. However, the modified HFB theory cannot be expected to be valid at higher temperatures, since the BQP's become more like free particles.

Since the excitation spectrum E_k is only in qualitative agreement with the experimental spectrum, a calculation of the heat capacity would give very poor results indeed. Especially at temperatures somewhat less that T_c the heat capacity would be poor. At lower temperatures where the phonons would dominate, the characteristic T^3 behavior is obtained.[1,2]

VIII. COMPARISON WITH OTHER WORK

While the results of Sec. VII are only in qualitative agreement with experiment, they compare very favorably with previous self-consistent microscopic calculations using realistic potentials. The emphasis in this section is on a comparison with theories that use realistic potentials. Many other calculations using model potentials have been made. However, since they have adjustable parameters, their agreement with the excitation spectrum may be fortuitous. In any case, they would not be expected to fit the data on gaseous helium.

Brown and Coopersmith[49] using a Slater-Kirkwood potential and an Yntema-Schneider potential obtain excitation spectra that, while having phonon-roton form, are too large by an order of magnitude. For the Slater-Kirkwood potential their depletion is 10%, while for the Yntema-Schneider potential their depletion is 7%. Our value of about 40% is closer to the experimental value[45] of 97.6% than theirs. Their approach is to use the HFB theory as obtained by Wentzel[29] and Luban,[30] and to replace the bare potential everywhere by a K matrix, which is a t matrix involving bare energy denominators. Since they also do this in Eq. (3.16) from which we obtained the LS equation in Eq. (4.2) for the t matrix, their procedure involves "teeing the tee." Presumably this procedure involves over-counting of diagrams and may explain their large energy. Their calculation is done only at zero temperature, although it could have been done at finite temperature as well.

In another recent calculation of the excitation spectrum, Østgaard[42] uses an extension of the Brueckner and Sawada theory.[12] His calculation also involves replacing the potential by the t matrix calculated from a LS equation using the reference-spectrum method,[50] which removes the energy denominator in the LS equation from the chain of self-consistency. The Hamiltonian is then partially diagonalized by using the Bogoliubov transformation. His spectrum is too high by about a factor of 2, while his depletion is 39–44%. The calculation is also done only at zero temperature.

Østgaard[51] was the first to plot the reaction operator in configuration space. Since his t matrix is nonlocal, it is a function of the relative coordinates between the atoms as well as the momentum. Even though he used a different method than ours, he obtained curves similar to our Figs. 1 and 2 for the reaction operator.[51] In his calculation of the reaction operator, he had to divide the potential acting on the perturbed pair wave function by the unperturbed wave function. Since the unperturbed wave function has nodes, the reaction operator is infinite at some points, but these were

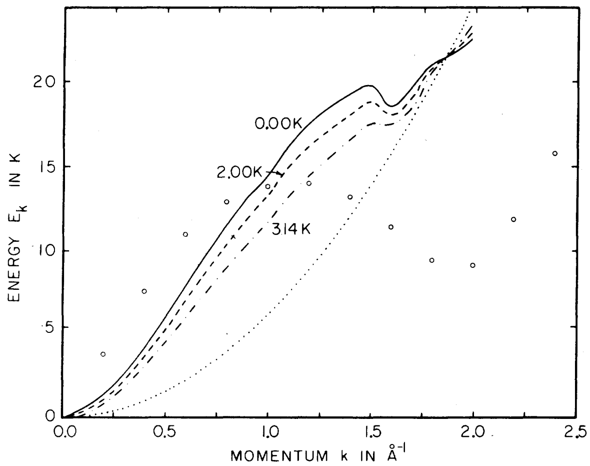

FIG. 7. Excitation spectra E_k as a function of the momentum k calculated from the FM potential for the temperatures 0.00 K (solid curve), 2.00 K (dashed curve), and 3.14 K (dot-dashed curve). The free-particle spectrum is given by the dotted curve. The open circles are the experimental data of Cowley and Woods (Ref. 48) at 1.12 K.

numerically smoothed. His reaction operator lacks structure for $r < 2$ Å, since he used a reference spectrum[50] in the energy denominator of the LS equation.

An earlier calculation by Byckling[52] attempted to extend the Brueckner and Sawada[12] theory by using an anomalous self-energy introduced by Beliaev.[53] However, his calculation for the zero-momentum density for hard spheres and the Lennard-Jones potential is not done self-consistently. The input depletion value for the Lennard-Jones potential was 24% and the output depletion was 132%, which is not a physically meaningful result. Therefore the qualitative agreement he obtained for the excitation spectrum is probably fortuitous.

Some model calculations have been made for the condensate density. Luban and Grobman,[54] using the temperature-dependent Bogoliubov theory with a constant interaction, obtain a transition temperature T_{c2} which is higher than the ideal Bose gas and gives a heat capacity divergent at the transition temperature with a critical exponent of $\frac{1}{2}$. Their condensate density has an infinite slope at a finite value, so there is a finite discontinuity in ρ_0.

On the other hand, Reatto and Straley,[55] using a spherically symmetric δ-function shell potential, obtained a curve for ρ_0 similar to Luban and Grobman.[54] In addition they found that ρ_0 decreased smoothly from T_{c2} with decreasing temperature below T_{c2} until it became zero at the transition temperature T_c for an ideal gas. Thus their condensate density ρ_0 is double valued above T_c. Which value of ρ_0 should have been chosen could have been determined by calculating the free energy. Grobman and Luban[56] imply that the higher value is the physical value. We have a temperature dependent t matrix t_k in Figs. 3 and 4, for which the spectrum becomes imaginary at the same temperature at which $\rho_0 = 0$ is a solution. Therefore, we are not faced with double-valued functions, but have a discontinuous change in ρ_0 and E_k at the ideal-Bose-gas transition temperature T_c.

A number of authors have used model potentials for systems of interacting bosons. Goble and Trainor[57] have made an extensive study of the Brueckner and Sawada[12] hard-core model as modified by Parry and ter Haar.[13] They find a qualitative agreement with experiment as well as a meaningful depletion. On the other hand, their study of the hard-core pseudopotential theory of Liu and Wong[58] gave somewhat different results, but were qualitatively the same. Since both theories purport to describe the hard-sphere boson system, the discrepancy needs to be clarified.

Another calculation based on the Brueckner and Sawada[12] theory has been made by Khanna and Phukan.[59] By using an effective mass and an attractive well, in addition to the hard core, they obtain a spectrum which is generally lower than the experimental one, but is in qualitative agreement with it. Their density is realistic, but contrary to Parry and ter Haar,[13] they obtain a negligible depletion. Their depletion is not obtained self-consistently, but estimated from a formula derived in a previous paper.[60] Thus it appears that even their qualitative agreement is fortuitous.

Another approach that has become popular is the density and velocity operator theory of Sunakawa, Yamasaki, and Kebukawa.[61] The energy spectrum they obtain is the same as the Bogoliubov spectrum with ρV_k instead of $\rho_0 V_k$. By using a soft core followed by an attractive square well, they were able to fit the observed phonon-roton spectrum quite well. The question of condensate fraction does not enter this theory. In a later paper[62] the authors used a Morse potential truncated at about 36 K to obtain even better agreement with the experimental spectrum. Their truncation value is roughly the average of the repulsive part for our self-consistent reaction operator in Figs. 1 and 2. In this theory based on density and velocity operators, there is a question of the existence of some of the operators[63] and of the convergence of the expansion of the inverse density operator.

IX. CONCLUSION

An original feature of this work is that a t matrix emerges in a natural way from the Bogoliubov canonical transformation when pairing correlations are taken into account. The t matrix obtained here is of a generalized form since a completely dressed energy denominator occurs, and the t matrix is explicitly temperature dependent. The calculations given here are the first to obtain the temperature dependence self-consistently from a microscopic theory using a realistic potential.[64]

The primary conclusion of this work is that, while qualitative agreement with the experimental spectrum is obtained by using the modified HFB theory with a realistic potential and density, the temperature dependence of the spectrum predicted by the modified HFB theory is incorrect. This behavior is in marked contrast with superconductivity,[15] where a free-electron model is valid above the transition temperature. There is always the possibility that without the phenomenological modifications, the summation of BQP self-energy diagrams in higher order,[37] along with the finite-temperature extension of Bogoliubov's principle of dangerous diagrams,[28] the theory could be brought into agreement with experiment. The dressing would be considerable, however, since the unperturbed Hamiltonian is not quantitatively correct. The question of the validity of the perturbation expansion is open, since there is no small expansion parameter.

On the other hand, compared with other microscopic calculations of the excitation spectrum of He II discussed in Sec. VIII, the agreement with experiment is not bad. Those theories involve the *ad hoc* insertion of the t matrix, or a use of a model potential. The temperature dependence of the excitation spectrum is not calculated, and even at zero temperature their agreement with experiment is at best only qualitative.

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