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Excitation spectrum of a system of interacting bosons

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The Bogoliubov treatment of a weakly interacting Bose gas is extended by allowing macroscopic occupation of many single-particle quantum states. This generalization of having more than a single condensed mode gives rise to a nonuniform condensate and is being considered as a possible mechanism for the description of a dense strongly interacting Bose gas at low temperatures. The model with a repulsive δ-function interparticle potential gives an energy spectrum of elementary excitations or quasiparticles with both phonon and roton features. The values obtained for the roton minimum energy Δ and the speed of (first) sound agree reasonably well with inelastic-neutron-scattering data.

I. INTRODUCTION

The classic work of Bogoliubov[1] on a microscopic theory of superfluidity is successful in obtaining a phononlike low-momentum spectrum from a repulsive interaction. The crucial assumption for this weakly interacting Bose system is the macroscopic occupation of a single quantum state. In fact, this assumption is the fundamental feature of the existing microscopic theories of superfluidity and underlies, for instance, the perturbation theory for bosons.[2]

However, on the one hand, the results[3-5] for a dilute Bose gas are given in terms of an expansion parameter—the ratio of the scattering length to the correlation length—which is large when evaluated for ^{4}He. More importantly, however, the elementary excitation spectrum[4] does not give rise to the roton minimum observed with the neutron-scattering experiments.[6,7]

On the other hand, the variational calculation of Feynman,[8] although not a full microscopic theory, is particularly successful in obtaining the excitation curve for phonons and rotons—it relates the static form factor $S(\vec{k})$ to the energy $E_{\vec{k}}$ of an excitation. The agreement with the experimental excitation curve may be improved[9] by introducing a wave function which allows for back flow in order to conserve the current density for a roton. Nevertheless, in these variational calculations the experimental static form factor for scattering neutrons from the liquid is used as an input—instead of the pair potential between the atoms—in order to obtain the excitation spectrum.

In this work, we suggest a model for the description of a dense strongly interacting Bose gas which may describe the main features of real helium at low temperatures. The model supposes macroscopic occupation of many single-particle quantum states and is suggested by the integral representation[10]

$$n(\vec{p}) = \int \int \int f(T,\rho,\vec{u})\,\omega(\vec{p})\, dT\, d\rho\, d\vec{u} \; , \tag{1}$$

for the helium momentum distribution $n(\vec{p})$, where

$$\begin{aligned}\omega(\vec{p}) &= N\left[1-\left(\frac{T}{T_0}\right)^{3/2}\right]\delta(\vec{p}-m\vec{u}) \\ &\quad + \frac{V}{h^3}\,\frac{1}{e^{(\vec{p}-m\vec{u})^2/2mk_BT}-1}\,, \quad T<T_0, \\ &= \frac{V}{h^3}\,\frac{1}{Ae^{(\vec{p}-m\vec{u})^2/2mk_BT}-1}\,, \quad T>T_0,\end{aligned} \tag{2}$$

and the positive definite spectral function $f(T,\rho,\vec{u})$ is normalized to unity

$$\int\int\int f(T,\rho,\vec{u})\,dT\,d\rho\,d\vec{u} = 1\,. \tag{3}$$

Suppose that $F(T,\rho,\vec{u}) = f(T,\rho,u)$, then

$$\begin{aligned} n(p) &= \int_0^\infty d\rho \int_0^{T_0} dT \frac{N}{m}\left[1-\left(\frac{T}{T_0}\right)^{3/2}\right] f\left(T,\rho,\frac{p}{m}\right) \\ &+ \frac{2\pi V}{h^3 p}\int_0^\infty d\rho \int_0^{T_0} k_B T\, dT \int_0^\infty f(T,\rho,u)u\,du\,\ln\left(\frac{1-e^{-\frac{1}{2}(p+mu)^2/mk_BT}}{1-e^{-\frac{1}{2}(p-mu)^2/mk_BT}}\right) \\ &+ \frac{2\pi V}{h^3 p}\int_0^\infty d\rho \int_{T_0}^\infty k_B T\, dT \int_0^\infty f(T,\rho,u)u\,du\,\ln\left(\frac{A-e^{-\frac{1}{2}(p+mu)^2/mk_BT}}{A-e^{-\frac{1}{2}(p-mu)^2/mk_BT}}\right). \end{aligned} \tag{4}$$

If, for $T > T_0$, $f(T,\rho,u)$ is peaked around some value of T and $u = u_0$ such that $A \gg 1$, then the last term in (4) gives for $p \approx p_0 \equiv mu_0$, $pn(p) \sim e^{-\frac{1}{2}(p-p_0)^2/mk_BT}$. (Actually, we have a smeared-out Gaussian function.) This broad peak around some momentum p_0 is observed in neutron-scattering experiments and is identified with roton excitations.[11] Note that rotons appear here in the limit of Boltzmann statistics since we have to suppose that $A \gg 1$. Also, if, for $T < T_0$, $f(T,\rho,u)$ is peaked around some value of T and $u = u_c$, then the second term in (4) gives rise to a narrow peak in $pn(p)$ around $p = mu_c$—corresponding to a smeared-out logarithmic singularity. This peak is due clearly to the condensate since the spectral function which gives rise to it contributes to the condensate—the first integral in (4). [See also Eq. (22) of Ref. 10.] This peak appears in no calculation[11] of $pn(p)$.

Now it may be that the appearance of these peaks in $f(T,\rho,u)$ is not completely unrelated, that is, the structure of $pn(p)$ due to roton excitations and the condensate are related. In the succeeding sections a model with macroscopic occupation of many single-particle quantum states is introduced and we obtain the roton features of the experimentally observed excitation spectrum.

In the method of Bogoliubov, the dilute Bose gas at low temperatures is described by an asymptotically exact perturbation expansion in the density and in the potential. With respect to this perturbation theory, real helium is considered dense. Since macroscopic occupation of a single quantum state need not be true for sufficiently strong interaction, we see that macroscopic occupation of many single-particle quantum states may be a feature not only of a strongly interacting Bose gas, but also of a dense system as well.

II. MANY-CONDENSATE MODEL HAMILTONIAN

Consider the Hamiltonian[12]

$$\hat{H} = \sum_{\vec{k}} \epsilon_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{g}{2V} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3 \vec{k}_4} \delta_{\vec{k}_1+\vec{k}_2,\, \vec{k}_3+\vec{k}_4} \times a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} a_{\vec{k}_3} a_{\vec{k}_4} \tag{5}$$

for an interacting Bose gas with $\epsilon_{\vec{k}} = (\hbar^2 k^2/2m_{\mathrm{He}})$, where m_{He} is the mass of the helium atom. To first order, the constant matrix element g for the potential energy is related to the s-wave scattering length a in vacuum by $g = (4\pi\hbar^2 a/m_{\mathrm{He}})$.

Suppose we have macroscopic occupation of many discrete single-particle states, that is,

$$a_{\vec{k}} = \xi_{\vec{k}} \sqrt{N_0}, \quad \text{where } -1 \le \xi_{\vec{k}} \le 1 , \tag{6}$$

with the real c number $\xi^2_{\vec{k}}$ denoting the fraction of particles in the condensate with momentum $\vec{k}$ and

$$\xi_{\vec{k}} = \xi_{-\vec{k}} , \tag{7}$$

so that the average linear momentum of the condensate is zero—we choose the system with respect to which our condensate with N_0 particles is at rest.

If the leading terms in N_0 are kept after the replacement (6), the Hamiltonian (5) becomes[13]

$$\hat{H} = N_0 \sum_{\vec{k}} \xi^2_{\vec{k}} \epsilon_{\vec{k}} + \frac{gN_0^2}{2V} \sum_{\vec{q}} A^2_{\vec{q}} + \frac{gN_0^{3/2}}{V} \sum_{\vec{k}\vec{q}} (a^\dagger_{\vec{k}} + a_{\vec{k}}) A_{\vec{q}} \xi_{-\vec{k}+\vec{q}} + \sum_{\vec{k}} \epsilon_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}}$$
$$+ \frac{gN_0}{2V} \sum_{\vec{k}_1 \vec{k}_2} (A_{\vec{k}_1+\vec{k}_2} a^\dagger_{\vec{k}_1} a^\dagger_{\vec{k}_2} + 4A_{\vec{k}_1-\vec{k}_2} a^\dagger_{\vec{k}_2} a_{\vec{k}_1} + A_{\vec{k}_1+\vec{k}_2} a_{\vec{k}_1} a_{\vec{k}_2}), \tag{8}$$

where

$$A_{\vec{q}} \equiv \sum_{\vec{k}} \xi_{\vec{k}} \xi_{\vec{k}-\vec{q}} = A_{-\vec{q}} , \tag{9}$$

with the second equality in (9) following from (7). The quantity A_0 is identically equal to unity and

$$|\Psi(\vec{x})|^2 = \frac{N_0}{V} \sum_{\vec{q}} A_{\vec{q}} e^{i\vec{q}\cdot\vec{x}} , \tag{10}$$

with $\Psi(\vec{x})$ denoting the condensate wave function. Thus, macroscopic occupation of more than a single quantum state gives rise to a nonuniform condensate.

The Hamiltonian (8) reduces to Bogoliubov's case—condensation in the zero-momentum state only—for $\xi_{\vec{k}} = \delta_{\vec{k},0}$, that is, $A_{\vec{q}} = \delta_{\vec{q},0}$. In particular, the term linear in the creation and annihilation operators vanishes. The appearance of the linear term in (8) implies[14] further condensation in the states with momenta which are integral multiples of the momenta of the original states in the condensate, provided, of course, that the sum $\sum_{\vec{q}} \xi_{-\vec{k}+\vec{q}} A_{\vec{q}}$ does not vanish. Therefore, we may delete the linear term in (8) but with the consistency proviso that the condensate gets augmented by these added states: an infinite number.

Since

$$\hat{N} = N_0 + \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} , \tag{11}$$

then

$$\frac{N_0^2}{2V} + \frac{N_0}{V} \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} \approx \frac{N^2}{2V} . \tag{12}$$

Therefore, the final model Hamiltonian becomes

$$\begin{aligned}\hat{H} = &\frac{gN^2}{2V} \sum_{\vec{q}} A_{\vec{q}}^2 + N_0 \sum_{\vec{k}} \xi_{\vec{k}}^2 \epsilon_{\vec{k}} \\ &+ \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} \left(\epsilon_{\vec{k}} - \frac{gN_0}{V} \sum_{\vec{q}} A_{\vec{q}}^2 \right) \\ &+ \frac{gN_0}{2V} \sum_{\vec{k}_1 \vec{k}_2} (A_{\vec{k}_1 + \vec{k}_2} a_{\vec{k}_2}^\dagger a_{\vec{k}_1}^\dagger + 4A_{\vec{k}_1 - \vec{k}_2} a_{\vec{k}_2}^\dagger a_{\vec{k}_1} \\ &\qquad + A_{\vec{k}_1 + \vec{k}_2} a_{\vec{k}_2} a_{\vec{k}_1}) . \end{aligned} \tag{13}$$

The kinetic energy $N_0 \sum_{\vec{k}} \xi_{\vec{k}}^2 \epsilon_{\vec{k}}$ of the condensate can be made vanishingly small (see below) and, hence, the replacement (11) has not been applied to this term. The number of particles N_0 in the condensate is eliminated by considering $N = \langle \hat{N} \rangle$. Particle nonconservation may also be taken into account by introducing instead a chemical potential μ.

If one minimizes the quantity

$$N_0 \sum_{\vec{k}} \xi_{\vec{k}}^2 \epsilon_{\vec{k}} + \frac{gN_0^2}{2V} \sum_{\vec{k}} A_{\vec{q}}^2 - \mu N_0 , \tag{14}$$

with respect to $\xi_{\vec{k}}$ [or, equivalently, its Fourier transform $1/(N_0)^{1/2} \Psi(\vec{x})$], then one is lead to the Gross-Pitaevskii equation.[15] This, however, does not necessarily give the state of the system for given density and temperature. One should diagonalize (13) first and afterwards minimize the free energy with respect to the condensate wave function for fixed density and temperature. Therefore, in general, the condensate wave function does not satisfy the Gross-Pitaevskii equation.

The macroscopic occupation of a denumerably infinite number of single-particle quantum states does not give rise to any formal difficulty. Suppose we have macroscopic occupation of a finite number of single-particle quantum states with $\vec{k} = \vec{0}, \pm\vec{k}_0, \ldots, \pm M\vec{k}_0$, where M is a positive integer. Then the sum in (9), with $2M+1$ terms, gives that $A_{\vec{q}}$ is, in general, nonvanishing for $\vec{q} = \vec{0}, \pm\vec{k}_0, \ldots, \pm 2M\vec{k}_0$. Thus, from (8), we have terms of $(a_{\vec{k}}^\dagger + a_{\vec{k}})$ for $\vec{k} = \pm(M+1)\vec{k}_0, \ldots, \pm 2M\vec{k}_0$ and can consider both $a_{\vec{k}}$ and $a_{\vec{k}}^\dagger$ as macroscopic c numbers equal to $\xi_{\vec{k}}(N_0)^{1/2}$ with an asymptotic accuracy.[14] Therefore, we actually have macroscopic occupation of the states with $\vec{k} = \vec{0}, \pm\vec{k}_0, \ldots, \pm 2M\vec{k}_0$. Thus, we must begin our analysis again but now with macroscopic occupation of the states with $\vec{k} = \vec{0}, \pm\vec{k}_0, \ldots, \pm 2M\vec{k}_0$ and conclude, as before, that we must have macroscopic occupation of the states with $\vec{k} = \vec{0}, \pm\vec{k}_0, \ldots, \pm 4M\vec{k}_0$, and so on. Therefore, provided that the coefficient $\sum_{\vec{q}} \times A_{\vec{q}} \xi_{-\vec{k}+\vec{q}}$ of the term linear in the creation and annihilation operators in (8) converges, we obtain a sequence limiting to macroscopic occupation of a denumerably infinite number of single-particle quantum states. (Note that, in general, we can have finite sums over the variable $\vec{k}_0$.) Now we have by Cauchy's inequality that

$$-\left(\sum_{\vec{q}} A_{\vec{q}}^2 \right)^{1/2} \le \sum_{\vec{q}} A_{\vec{q}} \xi_{-\vec{k}+\vec{q}} \le \left(\sum_{\vec{q}} A_{\vec{q}}^2 \right)^{1/2} .$$

Therefore, in order to avoid any formal difficulty with the limiting sequence of condensates, we require that $\sum_{\vec{q}} A_{\vec{q}}^2$ be finite. [This quantity plays a fundamental role in our work (see below).]

III. DIAGONALIZATION PROBLEM

The diagonalization of the model Hamiltonian (13) is accomplished by the canonical transformation

$$a_{\vec{k}} = \sum_{\vec{k}'} \alpha_{\vec{k}\vec{k}'} b_{\vec{k}'} + \sum_{\vec{k}'} \beta_{\vec{k}\vec{k}'} b_{\vec{k}'}^\dagger \tag{15}$$

defining new creation and annihilation operators. The coefficients $\alpha_{\vec{k}\vec{k}'}$ and $\beta_{\vec{k}\vec{k}'}$ are assumed to be real and satisfy the relations

$$1 = \alpha\tilde{\alpha} - \beta\tilde{\beta} , \tag{16}$$

and

$$0 = \alpha\tilde{\beta} - \beta\tilde{\alpha} , \tag{17}$$

when expressed concisely in terms of matrices or tensors. ($\tilde{\alpha}$ denotes the transpose of α.) On substituting (15) into (13) we get

$$\begin{aligned}\hat{H} = &\frac{g}{2V} N^2 \sum_{\vec{k}} A_{\vec{q}}^2 + N_0 \sum_{\vec{k}} \xi_{\vec{k}}^2 \epsilon_{\vec{k}} \\ &+ \mathrm{Tr}\,(\tilde{\beta} h \beta + 2\tilde{\alpha} A \beta + 2\tilde{\beta} B \beta) + \sum_{\vec{k}} E_{\vec{k}} b_{\vec{k}}^\dagger b_{\vec{k}} , \end{aligned} \tag{18}$$

where the elements of the matrices h, A, and B are given, respectively, by

$$h_{\vec{k}\vec{k}'} = (\epsilon_{\vec{k}} - \frac{gN_0}{V} \sum_{\vec{q}} A_{\vec{q}}^2) \; \delta_{\vec{k}\vec{k}'} \equiv h_{\vec{k}} \delta_{\vec{k}\vec{k}'} , \tag{19}$$

$$A_{\vec{k}\vec{k}'} = \frac{gN_0}{2V} A_{\vec{k}+\vec{k}'} , \tag{20}$$

and

$$B_{\vec{k}\vec{k}'} = \frac{gN_0}{2V} A_{\vec{k}-\vec{k}'} . \tag{21}$$

The nondiagonal elements of $\hat{H}$ are made to vanish by the conditions

$$\tilde{\alpha}h\alpha+\tilde{\beta}h\beta+2\tilde{\alpha}A\beta+4\tilde{\alpha}B\alpha+4\tilde{\beta}B\beta+2\tilde{\beta}A\alpha=(E1)\,, \tag{22}$$

$$\tilde{\alpha}h\tilde{\beta}+\tilde{\alpha}A\alpha+4\tilde{\alpha}B\beta+\tilde{\beta}A\beta=0\,, \tag{23}$$

and

$$\tilde{\beta}h\alpha+\tilde{\beta}A\beta+4\tilde{\beta}B\alpha+\tilde{\alpha}A\alpha=0\,. \tag{24}$$

The notation (E1) indicates a diagonal matrix with elements $E_{\vec{k}}$.

On adding (22)–(24) we get

$$(\tilde{\alpha}+\tilde{\beta})(h+2A+4B)(\alpha+\beta)=(E1)\,. \tag{25}$$

On subtracting (23) and (24) from (22) we get

$$(\tilde{\alpha}-\tilde{\beta})(h-2A+4B)(\alpha-\beta)=(E1)\,. \tag{26}$$

Now (16) and (17) imply

$$(\alpha-\beta)(\tilde{\alpha}+\tilde{\beta})=1\,, \tag{27}$$

or its transpose

$$(\alpha+\beta)(\tilde{\alpha}-\tilde{\beta})=1\,. \tag{28}$$

Results (25)–(28) may be simplified by defining

$$\gamma\equiv\alpha+\beta,\quad\text{and }\delta\equiv\alpha-\beta\,, \tag{29}$$

which give

$$\tilde{\gamma}(h+2A+4B)\gamma=(E1)\,, \tag{30}$$

$$\tilde{\delta}(h-2A+4B)\delta=(E1)\,, \tag{31}$$

and

$$\gamma\tilde{\delta}=\delta\tilde{\gamma}=1\,. \tag{32}$$

Now, by (29)–(31), the term with the trace in (18) becomes

$$\mathrm{Tr}(\tilde{\beta}h\beta+2\tilde{\alpha}A\beta+4\tilde{\beta}B\beta)=\mathrm{Tr}\left[-\tfrac{1}{2}h-2B+\tfrac{1}{2}(E1)\right]. \tag{33}$$

Consequently, (18) becomes

$$\hat{H}=\frac{g}{2V}N^2\sum_{\vec{q}}A_{\vec{q}}^2+N_0\sum_{\vec{k}}\xi_{\vec{k}}^2\epsilon_{\vec{k}}+\frac{1}{2}\sum_{\vec{k}}\left(E_{\vec{k}}-\epsilon_{\vec{k}}+\frac{gN_0}{V}\sum_{\vec{q}}A_{\vec{q}}^2-\frac{2gN_0}{V}\right)+\sum_{\vec{k}}E_{\vec{k}}b_{\vec{k}}^\dagger b_{\vec{k}}\,. \tag{34}$$

Results (30)–(32) allow us to obtain a whole sequence of sum rules for even powers of the eigenvalue $E_{\vec{k}}$. We have

$$\sum_{\vec{k}}E_{\vec{k}}^{2n}=\mathrm{Tr}\left[(h+2A+4B)(h-2A+4B)\right]^n,\quad n=1,2,\cdots\,. \tag{35}$$

In particular for $n=1$ and $n=2$ we have

$$\sum_{\vec{k}}E_{\vec{k}}^2=\sum_{\vec{k}}\left[\epsilon_{\vec{k}}^2+\epsilon_{\vec{k}}\left(4g\frac{N_0}{V}-2g\frac{N_0C}{V}\right)+\frac{g^2N_0^2}{V^2}C(C-1)\right], \tag{36}$$

and

$$\begin{aligned}\sum_{\vec{k}}E_{\vec{k}}^4=\sum_{\vec{k}}\Bigg[&\epsilon_{\vec{k}}^4+\epsilon_{\vec{k}}^3\left(\frac{8gN_0}{V}-\frac{4gN_0C}{V}\right)+\epsilon_{\vec{k}}^2\left(\frac{6g^2N_0^2C^2}{V^2}-\frac{2g^2N_0^2C}{V^2}\right)\\&+\epsilon_{\vec{k}}\left(\frac{-4g^3N_0^3C^3}{V^3}-\frac{20g^3N_0^3C^2}{V^3}+\frac{10g^2N_0^2}{V^2}\sum_{\vec{k}'}\epsilon_{\vec{k}'}A_{\vec{k}'}^2+\frac{24g^3N_0^3}{V^3}\sum_{\vec{k}_1\vec{k}_2}A_{\vec{k}_1}A_{\vec{k}_2}A_{\vec{k}_1+\vec{k}_2}\right)\\&+\left(\frac{g^4N_0^4C^4}{V^4}+\frac{14g^4N_0^4C^3}{V^4}-\frac{10g^3N_0^3C}{V^3}\sum_{\vec{k}'}\epsilon_{\vec{k}'}A_{\vec{k}'}^2-\frac{24g^2N_0^4C}{V^4}\sum_{\vec{k}_1\vec{k}_2}A_{\vec{k}_1}A_{\vec{k}_2}A_{\vec{k}_1+\vec{k}_2}\right)\\&+\frac{9g^4N_0^4}{V^4}\sum_{\vec{k}_1\vec{k}_2\vec{k}_3}A_{\vec{k}_1}A_{\vec{k}_1+\vec{k}_2}A_{\vec{k}_2+\vec{k}_3}A_{\vec{k}_3}\Bigg)\Bigg]\,,\end{aligned} \tag{37}$$

where

$$C\equiv\sum_{\vec{q}}A_{\vec{q}}^2\geq1\,, \tag{38}$$

since $-1\leq A_{\vec{q}}\leq1$ for all $\vec{q}$ and $A_0=1$.

Note that in the simpler case of Bogoliubov $A_{\vec{k}}=\delta_{\vec{k},0}$, that is, $C=1$, and, hence, the $\vec{k}$th term of the sums in the sum rules may be identified formally and we obtain the classic result[1]

$$E_{B\vec{k}}^2=\epsilon_{\vec{k}}^2+2g(N_0/V)\epsilon_{\vec{k}}\,. \tag{39}$$

However, such a direct identification of $E_{\vec{k}}$ from the sum rules, for instance, from (36), is not valid in our more general case and would not satisfy (37).

The sum rules (35) suggest that

$$E_{\vec{k}}^2=\epsilon_{\vec{k}}^2+\epsilon_{\vec{k}}\left(\frac{4gN_0}{V}-\frac{2gN_0C}{V}\right)+\frac{g^2N_0^2}{V^2}C(C-1)+f_{\vec{k}}\,, \tag{40}$$

where the real function $f_{\vec{k}}$ is such that $\sum_{\vec{k}}\epsilon_{\vec{k}}^n f_{\vec{k}}=0$ for $n=0,1,2$ and leaves unchanged the sum rule (36). However, the added, probably oscillating, term $f_{\vec{k}}$ will make a contribution to (37) of the form

$$\sum_{\vec{k}} f_{\vec{k}}^2=\sum_{\vec{k}}\left(\frac{16g^2N_0^2}{V^2}(C-1)\epsilon_{\vec{k}}^2+\alpha_1\epsilon_{\vec{k}}+\alpha_0\right)\,, \tag{41}$$

where α_1 and α_0 are unknown constants, so that the sum rule (37) is satisfied. The coefficients α_1 and α_0 vanish for $C=1$, since $f_{\vec{k}}$ vanishes identically for $C=1$.

IV. EXCITATION SPECTRUM OF THE MODEL HAMILTONIAN

In Sec. III the simple form (34) was obtained for the model Hamiltonian (13). Also, the single-particle excitation energy $E_{\vec{k}}$ satisfies the infinite set of sum rules (35), two of which have been written out explicitly in (36) and (37).

From (30)–(32) we have the result

$$\tilde{\gamma}(h+2A+4B)(h-2A+4B)\tilde{\gamma}^{-1}=(E^2 1)\,, \tag{42}$$

where we have assumed $\delta=\tilde{\gamma}^{-1}$, that is, from (32) that $\tilde{\gamma}$ has an inverse matrix. Therefore, the square of the energies $E_{\vec{k}}^2$ of the elementary excitations or quasiparticles are the eigenvalues of the matrix $(h+2A+4B)(h-2A+4B)$. The corresponding eigenvalue equation is

$$h_{\vec{k}}^2\phi(\vec{k})+\frac{gN_0}{V}h_{\vec{k}}\sum_{\vec{k}'}A_{\vec{k}+\vec{k}'}\phi(\vec{k}')+\frac{3gN_0}{V}\sum_{\vec{k}'}h_{\vec{k}'}A_{\vec{k}+\vec{k}'}\phi(\vec{k}')+\frac{3g^2N_0^2}{V^2}\sum_{\vec{k}',\vec{k}''}A_{\vec{k}+\vec{k}''}A_{\vec{k}''+\vec{k}'}\phi(\vec{k}')=E^2\phi(\vec{k})\,, \tag{43}$$

where we assume that the eigenfunction satisfies $\phi(\vec{k})=\phi(-\vec{k})$, this assumption is by no means essential. In terms of Fourier transforms, (43) becomes

$$\left(\frac{\hbar^4}{4m_{\mathrm{He}}^2}\nabla^4+\frac{\hbar^2gN_0C}{m_{\mathrm{He}}V}\nabla^2+\frac{g^2N_0^2C^2}{V^2}\right)\phi(\vec{x})-\frac{\hbar^2g}{2m_{\mathrm{He}}}\nabla^2[\phi(\vec{x})|\Psi(\vec{x})|^2]-\frac{4g^2CN_0}{V}|\Psi(\vec{x})|^2\phi(\vec{x})+3g^2|\Psi(\vec{x})|^4\phi(\vec{x})-\frac{3g\hbar^2}{2m_{\mathrm{He}}}|\Psi(\vec{x})|^2\nabla^2\phi(\vec{x})=E^2\phi(\vec{x})\,, \tag{44}$$

where

$$\phi(\vec{x})\equiv\frac{1}{V}\sum_{\vec{k}}\phi(\vec{k})e^{i\vec{k}\cdot\vec{x}}\,. \tag{45}$$

Note that the condensate density $|\Psi(\vec{x})|^2$ is in principle determined by the minimization scheme mentioned at the end of Sec. II. Nevertheless, we may obtain important information on the excitation spectrum by considering the asymptotic behavior $(|\vec{x}|\to\infty)$ of (44). Now, from (10) and (38), we find by taking the mean value of the oscillations that

$$\lim_{|\vec{x}|\to\infty}|\Psi(\vec{x})|^2=N_0/V\,, \tag{46}$$

and

$$\lim_{|\vec{x}|\to\infty}|\Psi(\vec{x})|^4=\frac{N_0^2}{V^2}\sum_{\vec{q}}A_{\vec{q}}^2=\frac{N_0^2C}{V^2}\,. \tag{47}$$

These asymptotic values are valid for finite values of $|\vec{x}|$ if the macroscopic occupation occurs over a dense set of single-particle states. Thus, in the asymptotic region (44) becomes

$$\left(\frac{\hbar^4}{4m_{\mathrm{He}}^2}\nabla^4+\frac{\hbar^2gN_0C}{m_{\mathrm{He}}V}\nabla^2+\frac{g^2N_0^2C^2}{V^2}\right)\phi(\vec{x})-\frac{2\hbar^2gN_0}{m_{\mathrm{He}}V}\nabla^2\phi(\vec{x})-\frac{g^2CN_0^2}{V^2}\phi(\vec{x})=E^2\phi(\vec{x})\,. \tag{48}$$

Therefore, asymptotically $\phi(\vec{x})$ oscillates indefinitely and we have that $\phi(\vec{x})\sim e^{i\vec{k}\cdot\vec{x}}+e^{-i\vec{k}\cdot\vec{x}}$ is an eigenfunction of (48) with eigenvalue

$$E_{\vec{k}}^2=\epsilon_{\vec{k}}^2+\epsilon_{\vec{k}}\left(\frac{4gN_0}{V}-\frac{2gN_0C}{V}\right)+\frac{g^2N_0^2}{V^2}C(C-1)\,. \tag{49}$$

This result also follows directly from (43) for $|\vec{k}|\to\infty$. Note that expression (49) for $E_{\vec{k}}^2$ is positive definite since $C\geq 1$ and has a minimum for $C\geq 2$. It is clear that (49) cannot be valid for all values of $\vec{k}$ — since for $C>1$ it does not satisfy the sum rule (37) — however, it represents correctly the energy spectrum for large values of $|\vec{k}|$, that is, $f_{\vec{k}}$ in (40) is negligible. This can be inferred from the fact that (49) satisfies the sum rule (36) exactly but only gives the correct first two leading terms in (37). Also, the oscillating solution for $\phi(\vec{x})$ is only valid in the asymptotic region and, thus, for finite values of $\vec{k}$. As expected, (49) reduces to the correct result (39) of Bogoliubov when $C=1$.

The replacement of the constant g for the actual potential $V(\vec{k})$ in (5) gives rise to an artificial divergence of the form $\sum_{\vec{k}} 1/k^2$ in (34) when using (49). For $|\vec{k}| \to \infty$, (40) gives

$$E_{\vec{k}} = \epsilon_{\vec{k}} + \frac{2gN_0}{V} - \frac{gN_0C}{V} + \frac{g^2N_0^2}{2V^2}\frac{(3C-4)}{\epsilon_{\vec{k}}} - \frac{f_{\vec{k}}^2}{8\epsilon_{\vec{k}}^3} + \cdots . \tag{50}$$

Therefore, the diverging term in (34) becomes

$$\frac{1}{2}\sum_{\vec{k}}\left(\frac{g^2N_0^2}{2V^2\epsilon_{\vec{k}}}(3C-4) - \frac{f_{\vec{k}}^2}{8\epsilon_{\vec{k}}^3}\right) = -\tfrac{1}{4}C \cdot \frac{g^2N_0^2}{V^2}\sum_{\vec{k}}\frac{1}{\epsilon_{\vec{k}}}, \tag{51}$$

when using (41). With the aid of (51) the c-number term in (34) becomes

$$E = \frac{gN^2C}{2V} - \frac{gN_0^2C}{2V} + \frac{N_0^2C}{2V}\frac{4\pi a\hbar^2}{m_{\text{He}}} + N_0\sum_{\vec{k}}\xi_{\vec{k}}^2\epsilon_{\vec{k}} + \frac{1}{2}\sum_{\vec{k}}\left(E_{\vec{k}} - \epsilon_{\vec{k}} + \frac{gN_0C}{V} - \frac{2gN_0}{V} + \frac{g^2N_0^2C}{2V^2\epsilon_{\vec{k}}}\right), \tag{52}$$

where to second order in g, the s-wave scattering length a is given[2,16] by

$$\frac{4\pi a\hbar^2}{m_{\text{He}}} = g - \frac{g^2}{2V}\sum_{\vec{k}}\frac{1}{\epsilon_{\vec{k}}} . \tag{53}$$

If we now make the replacement (53) to first order in (52), we get

$$E = \frac{gN^2C}{2V} + N_0\sum_{\vec{k}}\xi_{\vec{k}}^2\epsilon_{\vec{k}} + \frac{1}{2}\sum_{\vec{k}}\left(E_{\vec{k}} - \epsilon_{\vec{k}} + \frac{gN_0C}{V} - \frac{2gN_0}{V} + \frac{g^2N_0^2}{2V^2}\frac{C}{\epsilon_{\vec{k}}}\right), \tag{54}$$

where the last sum converges.

In order to find the excitation spectrum in the low-momentum region we shall consider the solution of (44) in the neighborhood of the origin $|\vec{x}| = 0$. Now from (9) and (10) we find

$$|\Psi(\vec{x})|^2 = \frac{N_0}{V}\sum_{\vec{q}}A_{\vec{q}} - \frac{1}{6}\frac{N_0}{V}|\vec{x}|^2\sum_{\vec{q}}q^2A_{\vec{q}} + \cdots . \tag{55}$$

We shall suppose that $\sum_{\vec{q}} q^2|\xi_{\vec{q}}|$ is arbitrarily small, that is, the origin $q^2=0$ is an accumulation point of the set of condensate states and that $\sum_{\vec{q}}\xi_{\vec{q}}$ is finite, that is, $\Psi(\vec{x}=0)$ finite. Since

$$\sum_{\vec{q}}q^2A_{\vec{q}} = 2\left(\sum_{\vec{q}}\xi_{\vec{q}}\right)\left(\sum_{\vec{q}}q^2\xi_{\vec{q}}\right),$$

we have that $\sum_{\vec{q}} q^2A_{\vec{q}}$ is arbitrarily small and, hence, also the coefficients of the higher order terms in the series (55), of the form $\sum_{\vec{q}} q^{2m}A_{\vec{q}}$ with $m=2,3,\cdots$. Also, $\sum_{\vec{q}} q^2\xi_{\vec{q}}^2 \le \sum_{\vec{q}} q^2|\xi_{\vec{q}}|$ since $|\xi_{\vec{q}}| \le 1$; therefore, the condensate kinetic energy $N_0\sum_{\vec{q}}\xi_{\vec{k}}^2\epsilon_{\vec{k}}$ is arbitrarily small.

On substituting (55) in (44), we get

$$\left[\frac{\hbar^4}{4m_{\text{He}}^2}\nabla^4 + \frac{\hbar^2gN_0C}{m_{\text{He}}V}\nabla^2 - \frac{2g\hbar^2N_0}{m_{\text{He}}V}\left(\sum_{\vec{q}}A_{\vec{q}}\right)\nabla^2 + \frac{g^2N_0^2C^2}{V^2} + \frac{\hbar^2gN_0}{2m_{\text{He}}V}\sum_{\vec{q}}q^2A_{\vec{q}} - \frac{4g^2N_0^2C}{V^2}\sum_{\vec{q}}A_{\vec{q}} + \frac{3g^2N_0^2}{V^2}\left(\sum_{\vec{q}}A_{\vec{q}}\right)^2\right]\phi(\vec{x}) = E^2\phi(\vec{x}). \tag{56}$$

A solution of the linear differential Eq. (56) is $\phi(\vec{x}) \sim (e^{i\vec{k}\cdot\vec{x}} + e^{-i\vec{k}\cdot\vec{x}})$ and, hence, the eigenvalue becomes

$$E_{\vec{k}}^2 = \epsilon_{\vec{k}}^2 - \frac{2gN_0C}{V}\epsilon_{\vec{k}} + \frac{4gN_0}{V}\epsilon_{\vec{k}}\sum_{\vec{q}}A_{\vec{q}} + \frac{\hbar^2gN_0}{2m_{\text{He}}V}\sum_{\vec{q}}q^2A_{\vec{q}} + \frac{g^2N_0^2C^2}{V^2} - \frac{4g^2N_0^2C}{V^2}\ \frac{4gN_0^2C}{V^2}\sum_{\vec{q}}A_{\vec{q}} + \frac{3g^2N_0^2}{V^2}\left(\sum_{\vec{q}}A_{\vec{q}}\right)^2 . \tag{57}$$

This result for the excitation spectrum also follows directly from (43) for $|\vec{k}| \to 0$. If we require a phononlike behavior for our excitation spectrum (57), then we must have that

$$\frac{g^2N_0^2C^2}{V^2} - \frac{4g^2N_0^2C}{V^2}\sum_{\vec{q}}A_{\vec{q}} + \frac{3g^2N_0^2}{V^2}\left(\sum_{\vec{q}}A_{\vec{q}}\right)^2 = 0 , \tag{58}$$

that is, $C \equiv \sum_{\vec{q}} A_{\vec{q}}^2 = \sum_{\vec{q}} A_{\vec{q}}$. [The solution $\sum_{\vec{q}} A_{\vec{q}}^2 = 3\sum_{\vec{q}} A_{\vec{q}}$ of (58) is not acceptable since $E_{\vec{k}}^2$ must be positive definite.] Consequently, (57) becomes

$$E_{\vec{k}}^2 = \epsilon_{\vec{k}}^2 + \frac{2gN_0C}{V}\epsilon_{\vec{k}} + \frac{gN_0}{V}\sum_{\vec{q}}\epsilon_{\vec{q}}A_{\vec{q}} . \tag{59}$$

Therefore, the phononlike behavior is achieved since $\sum_{\vec{q}}\epsilon_{\vec{q}}A_{\vec{q}}$ has been made arbitrarily small so that

$$E_{\vec{k}} \approx \left(\frac{2gN_0C}{V}\epsilon_{\vec{k}}\right)^{1/2} \text{ for } \frac{2gN_0}{V} \gg \epsilon_{\vec{k}} \gtrsim \sum_{\vec{q}}\epsilon_{\vec{q}}A_{\vec{q}} \to 0 . \tag{60}$$

It should be remarked that our requirement of a phonon branch for the excitation spectrum must be based purely on an attempt to agree with experimental findings. The known theorems,[5] albeit based on a term by term examination of the perturbation series, stating that the quasiparticle spectrum cannot exhibit a gap assume macroscopic occupation of only one single-particle quantum state, the zero-momentum state, and, hence, are not applicable here.

As remarked at the end of Sec. II, the thermodynamic state of the system is determined by minimizing the Helmholtz free energy with respect to the condensate wave function $\Psi(\vec{x})$ for given fixed density and temperature. Therefore, $\Psi(\vec{x})$, as well as

$$C \equiv \sum_{\vec{q}} A_{\vec{q}}^2 = \frac{V\int|\Psi(\vec{x})|^4 d\vec{x}}{[\int|\Psi(\vec{x})|^2 d\vec{x}]^2}$$

$$= 1 + \frac{V^2}{N_0^2}\frac{1}{V}\int\left(|\Psi(\vec{x})|^2 - \frac{N_0}{V}\right)^2 d\vec{x},$$

depends implicitly on density and temperature. Consequently, our Hamiltonian (13) or (34) depends not only on density but also on temperature through its explicit dependence on C. Therefore, the c-number term in (34), given also by E in (54), represents the ground-state energy only when evaluated at $T=0$.

Since the Bogoliubov result is contained in our general model given by the Hamiltonian (13), we believe that our work is an extension of Bogoliubov's method for a dense strongly interacting Bose gas at low temperatures. Thus, we expect to recover the asymptotically exact perturbative result of Bogoliubov in the limit of a dilute gas with very weak potential. That is, $C \to 1$ for $N/V \to 0$ and $g \to 0$ at low temperatures. However, this has not been shown rigorously since we do not have an expression for $E_{\vec{k}}$ for all values of $\vec{k}$.

Note that Bogoliubov's result, $C=1$, follows for two quite distinct cases: The usual one of a uniform condensate, with $|\Psi(\vec{x})|^2 = (N_0/V)$, and that of a nonuniform condensate such that $1/V\int[|\Psi(\vec{x})|^2 - (N_0/V)]^2 d\vec{x}$ vanishes in the thermodynamic limit. Therefore, in the cases with $C>1$, the dispersion of the condensate density with respect to the distribution $1/V$ remains finite in the thermodynamic limit.

A very interesting possibility for a condensate density with $C \equiv \sum_{\vec{q}} A_{\vec{q}}^2 = \sum_{\vec{q}} A_{\vec{q}} > 1$ occurs when $|\Psi(\vec{x})|^2$ has the same nonzero value, which must be $(N_0/V)C$, in (infinitely many) distinct regions of space with total volume V_1 and is otherwise zero. Then $C = V/V_1$ and from (44) one obtains the exact excitation spectra $E_{\vec{k}}^2 = \epsilon_{\vec{k}}^2 + 2g(N_0/V)C\epsilon_{\vec{k}}$ in the regions of nonzero condensate density and $E_{\vec{k}}^2 = [\epsilon_{\vec{k}} - g(N_0/V)C]^2$ in the regions of space where the condensate density vanishes identically. Now, the accumulation of condensate states about the zero-momentum single-particle state implies that the above condensate droplets must coalesce, thus forming a single large drop. It is evident that the vanishing nature of the condensate density in regions far away from this drop must be modified, so that (46) be satisfied. Therefore, the latter condition, together with the incoherence effect of (47), modifies the condensate and, consequently, modifies both spectra to the ones found previously, given by (60) and (49).

V. SUMMARY AND DISCUSSION

In Sec. IV, it is shown that the model Hamiltonian (13), containing macroscopic occupation of many single-particle quantum states, gives rise to the structure and elementary excitations of liquid helium, especially below the λ transition. In the classic work of Bogoliubov on the dilute weakly interacting Bose gas, the assumption of macroscopic occupation of the zero-momentum state produced the correct long-wavelength phonon behavior in the excitation spectrum. We now have shown that macroscopic occupation of a dense set of single-particle states — in an infinitesimal neighborhood of the zero-momentum state — gives the roton feature missing in Bogoliubov's original result, while preserving the phonon nature of the long-wavelength excitations.

The excitation spectrum given by (49) and (60) may be compared with the experimental results for the Landau parameters for rotons and the speed of ordinary (first) sound. We shall suppose that (49) is valid down to the region of the roton minimum, that is, $f_{\vec{k}}$ in (40) is negligible. Now (49) may be written

$$E_{\vec{k}}^2 = [\epsilon_{\vec{k}} - (gN_0/V)(C-2)]^2 + (g^2N_0^2/V^2)(3C-4). \tag{61}$$

Thus, for $C \geq 2$, $E_{\vec{k}}$ has a minimum at $\epsilon_{\vec{k}} = (gN_0/V)(C-2)$. Considering (61) near its minimum, we can identify the roton parameters, an energy gap Δ, an effective mass μ_r, and a momentum p_0, and find

$$\Delta = (gN_0/V)(3C-4)^{1/2}, \tag{62}$$

$$\mu_r = m_{\mathrm{He}}\frac{(3C-4)^{1/2}}{2(C-2)}, \tag{63}$$

and

$$p_0^2 = 2m_{\mathrm{He}}(gN_0/V)(C-2). \tag{64}$$

Note that (61) is a parabola in the variable p^2, not in the momentum p, and is qualitatively consistent with the asymmetry found[17] about p_0. (However, in Ref. 18 they see no indications of this asymmetry.)

From (62)–(64) we obtain the relation

$$\mu_r = m_{\mathrm{He}}^2\Delta/p_0^2, \tag{65}$$

between the roton parameters. For temperature and density variations of the Landau parameters for rotons, relation (65) gives

$$\delta\mu_r/\mu_r = \delta\Delta/\Delta - 2(\delta p_0/p_0)\,. \qquad (66)$$

At the saturated vapor pressure[18] and 1.3 °K, (66) gives for the density derivatives of the Landau parameters −1.1 for the left-hand side and −1.68 for the right-hand side.

The position of the roton minimum p_0 at all pressures and temperatures is related to the density ρ by the simple expression[18] $[p_0(\rho)/\hbar] = A\rho^{1/3}$ with $A = 3.64\ \mathrm{cm\,g^{-1/3}\,\AA^{-1}}$. Therefore, (66) gives

$$\delta\mu_r/\mu_r = \delta\Delta/\Delta \qquad (67)$$

for the temperature dependence of μ_r and Δ at constant density. Thus, μ_r is temperature dependent.[18] Relationship (67) was used[19] to find values of $\mu_r(\rho, T=0)$ from the data at finite temperatures. However, it would be more appropriate to use (66) since the density variation of the second term in (66) is appreciable.

Result (60) gives for the phonon velocity

$$c = (gN_0C/m_{\mathrm{He}}V)^{1/2}\,, \qquad (68)$$

which reduces, with the help of (63) and (64), to

$$c = \frac{p_0}{m_{\mathrm{He}}\sqrt{2}}\,\frac{[1+4(\mu_r^2/m_{\mathrm{He}}^2)]^{1/2}}{[\frac{1}{4}+\frac{3}{4}(1+\frac{32}{9}\mu_r^2/m_{\mathrm{He}}^2)^{1/2}]^{1/2}} \approx \frac{p_0}{m_{\mathrm{He}}\sqrt{2}}\left(1+\frac{4}{3}\frac{\mu_r^2}{m_{\mathrm{He}}^2}\right) \qquad (69)$$

with neglect of higher powers of μ_r/m_{He}. Note that the phonon velocity is proportional to N_0/V, as in early microscopic theories, but we now have the factor C which drastically modifies it. We shall identify the phonon velocity with the macroscopic sound velocity.

Since the roton momentum p_0 depends only on the density, we see that the speed of ordinary (first) sound is almost independent of the temperature in agreement with experimental results[20] and depends on density as $\rho^{1/3}$. The slight temperature dependence in (69) has the effect of reducing the velocity with increasing temperature also in agreement with the data, since μ_r decreases with increasing temperature at constant pressure.[18]

Our identification of the phonon velocity with the macroscopic sound velocity c may be partially justified by the following consideration. If at zero temperature c is related to the density ρ by $c = \alpha\rho^\beta$ with α and β constants, then the ground-state energy is related to c by $E = [m_{\mathrm{He}}Nc^2/2\beta(2\beta+1)]$. In our case, by considering the leading term in (54) and (68), we obtain $(N_0/N) = \beta(2\beta+1)$ so that $0<\beta\le\frac{1}{2}$. We have seen above that $\beta=\frac{1}{3}$ and, hence, $(N_0/N)=\frac{5}{9}$ which compares favorably with $(N_0/N)=\frac{1}{10}$ (see below). Note that in Bogoliubov's case $\beta=\frac{1}{2}$ so that $(N_0/N)=1$.

If we use the experimental values for two of the roton parameters, say the momentum p_0 and the effective mass μ_r, then by (65) and (69) we may deduce the energy gap Δ and the speed of ordinary (first) sound c. Using the experimental results $\mu_r = 0.16\ m_{\mathrm{He}}$ and $p_0/\hbar = 1.91\ \mathrm{\AA}^{-1}$ for liquid helium at 1.12 °K under its normal vapor pressure,[6] we get from (65) and (69) that $\Delta/k_B = 7$ °K and $c = 218$ m/sec, which are in reasonable agreement with the experimental value[6] of $(\Delta/k_B) = 8.6$ °K and the zero-temperature velocity of $c = 238$ m/sec.

For the parameters C and (gN_0/V) we obtain from (63) and (64) that $C = 32$ and $(gN_0/V) = 1\times10^{-16}$ erg. Therefore, the phonon branch (60) is valid for $0 \le k \ll 2.76\ \mathrm{\AA}^{-1} \approx \sqrt{2}(p_0/\hbar)$. To first order, from (53), $gN/V = (4\pi a\hbar^2N/m_{\mathrm{He}}V) = 1\times10^{-15}$ erg, where we have used[5] $a = 2.2$ Å and $m_{\mathrm{He}}N/V = 0.145$ g/cm³. Hence, $N_0/N = \frac{1}{10}$ and agrees with the depletion of the condensate which is believed to be about 90%. Note, however, that our approximation (12) may preclude taking this result for the fractional depletion of the condensate seriously.

The exact results[21] in the long-wavelength limit for the density-density Green's function and the single-particle Green's function at zero temperature, which establish that both functions have only a single pole, corresponding to the macroscopic sound velocity, as q and ω become small, are not obviously valid here since we have macroscopic occupation of many single-particle states. This has the disadvantage that one has no rigorous means of determining the macroscopic sound velocity from the single-particle Green' s function. Nonetheless, we have identified the characteristic velocity of the long-wavelength excitations with the speed of macroscopic sound velocity. In the Appendix, however, we have proved that our model for He II does lead to the basic equivalence of the field and density fluctuations.

In closing it should be remarked that the findings in this work should have a strong bearing on the microscopic theory of superfluidity as well as on theories where macroscopic occupation of single-particle states plays a fundamental role, for instance, the structure of superconducting ground states. Of course, some of the results of this new model for He II can be regarded as obtainable from a more conventional approach, a theory based on a single-state condensate, but with an appropriate self-energy approximation.[22] However, any microscopic theory of liquid helium must eventually wrestle with the fundamental question of the nature of the condensate.[23]

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APPENDIX

The quasiparticle Hamiltonian (34), with the excitation spectrum $E_{\vec{k}}$ given by (49) and (60), allows us to calculate the thermodynamic quantities of He II at temperatures near absolute zero. Now, inelastic neutron scattering from the density fluctuations in He II also gives rise to an excitation spectrum. Experimentally, these spectra are found to be the same[7]; however, within the context of a microscopic theory, it is not at all obvious how they are related. A further question is the equivalence of the field and density fluctuations.[24]

Here we give the results for the single-particle temperature Green's function and the density correlation function. Throughout this Appendix, we use the notation of the finite-temperature formalism of Ref. 2.

The Fourier transform of the single-particle temperature Green's function, for the helium atom field operators, is given by

$$\mathcal{G}(\vec{q},\vec{q};\omega_n) = -\beta\hbar N_0 V\xi_{\vec{q}}^2\delta_{\omega_n,0} + V\sum_{\vec{k}}\frac{(\alpha_{\vec{q}\vec{k}})^2}{i\omega_n - \hbar^{-1}E_{\vec{k}}} - V\sum_{\vec{k}}\frac{(\beta_{\vec{q}\vec{k}})^2}{i\omega_n + \hbar^{-1}E_{\vec{k}}}, \tag{A1}$$

and the anomalous Green's function by

$$\mathcal{G}_{12}(\vec{q},\vec{q};\omega_n) = -\beta\hbar N_0 V\xi_{\vec{q}}^2\delta_{\omega_n,0} + V\sum_{\vec{k}}\frac{\alpha_{\vec{q}\vec{k}}\beta_{-\vec{q}\vec{k}}}{i\omega_n - \hbar^{-1}E_{\vec{k}}} - V\sum_{\vec{k}}\frac{\alpha_{-\vec{q}\vec{k}}\beta_{\vec{q}\vec{k}}}{i\omega_n + \hbar^{-1}E_{\vec{k}}}, \tag{A2}$$

with $\omega_n = 2n\pi/\beta\hbar$ and $\beta = 1/k_BT$. The excitation spectrum $E_{\vec{k}}$ is that given in the text but with $\epsilon_{\vec{k}}$ replaced by $\epsilon_{\vec{k}} - \mu$ where μ is the chemical potential of the helium atoms. The coefficients $\xi_{\vec{q}}$, $\alpha_{\vec{q}\vec{k}}$, and $\beta_{\vec{q}\vec{k}}$ are those of (6) and (15).

The Fourier transform of the density correlation function is given by

$$\begin{aligned}\mathfrak{D}(\vec{q},\vec{q};\omega_n) = {} & \beta\hbar R(\vec{q})\delta_{\omega_n,0} + \sum_{\vec{k}}\frac{[\chi_{\vec{k}}(\vec{q}) + \omega_{\vec{k}}(-\vec{q})]^2}{i\omega_n - \hbar^{-1}E_{\vec{k}}} - \sum_{\vec{k}}\frac{[\chi_{\vec{k}}(-\vec{q}) + \omega_{\vec{k}}(\vec{q})]^2}{i\omega_n + \hbar^{-1}E_{\vec{k}}} + \sum_{\vec{k}_1\vec{k}_2}\frac{[M_{\vec{k}_1\vec{k}_2}(\vec{q}) + N_{\vec{k}_1\vec{k}_2}(-\vec{q})]^2(n_{\vec{k}_1} - n_{\vec{k}_2})}{i\omega_n + \hbar^{-1}(E_{\vec{k}_1} - E_{\vec{k}_2})} \\ & + \sum_{\vec{k}_1\vec{k}_2}\frac{P_{\vec{k}_1\vec{k}_2}(\vec{q})[P_{\vec{k}_1\vec{k}_2}(\vec{q}) + P_{\vec{k}_2\vec{k}_1}(\vec{q})](1 + n_{\vec{k}_1} + n_{\vec{k}_2})}{i\omega_n - \hbar^{-1}(E_{\vec{k}_1} + E_{\vec{k}_2})} - \sum_{\vec{k}_1\vec{k}_2}\frac{P_{\vec{k}_1\vec{k}_2}(-\vec{q})[P_{\vec{k}_1\vec{k}_2}(-\vec{q}) + P_{\vec{k}_2\vec{k}_1}(-\vec{q})](1 + n_{\vec{k}_1} + n_{\vec{k}_2})}{i\omega_n + \hbar^{-1}(E_{\vec{k}_1} + E_{\vec{k}_2})} \\ & + 2\sum_{\vec{k}}\frac{P_{\vec{k}\vec{k}}^2(\vec{q})(1 + 2n_{\vec{k}})}{i\omega_n - 2\hbar^{-1}E_{\vec{k}}} - 2\sum_{\vec{k}}\frac{P_{\vec{k}\vec{k}}^2(-\vec{q})(1 + 2n_{\vec{k}})}{i\omega_n + 2\hbar^{-1}E_{\vec{k}}},\end{aligned} \tag{A3}$$

where

$$\chi_{\vec{k}}(\vec{q}) = (N_0)^{1/2}\sum_{\vec{k}_1}\alpha_{\vec{k}_1\vec{k}}\,\xi_{\vec{k}_1-\vec{q}}, \tag{A4}$$

$$\omega_{\vec{k}}(\vec{q}) = (N_0)^{1/2}\sum_{\vec{k}_1}\beta_{\vec{k}_1\vec{k}}\,\xi_{\vec{k}_1-\vec{q}}, \tag{A5}$$

$$M_{\vec{k}_1\vec{k}_2}(\vec{q}) = \sum_{\vec{k}_1'}\alpha_{\vec{k}_1'\vec{k}_1}\alpha_{\vec{k}_1'+\vec{q}\,\vec{k}_2}, \tag{A6}$$

$$N_{\vec{k}_1\vec{k}_2}(\vec{q}) = \sum_{\vec{k}_1'}\beta_{\vec{k}_1'\vec{k}_1}\beta_{\vec{k}_1'+\vec{q}\,\vec{k}_2}, \tag{A7}$$

$$P_{\vec{k}_1\vec{k}_2}(\vec{q}) = \sum_{\vec{k}_1'}\alpha_{\vec{k}_1'\vec{k}_1}\beta_{\vec{k}_1'-\vec{q}\,\vec{k}_2}, \tag{A8}$$

and

$$R(\vec{q}) = -4\sum_{\vec{k}}M_{\vec{k}\vec{k}}(\vec{q})N_{\vec{k}\vec{k}}(\vec{q})n_{\vec{k}}(n_{\vec{k}}+1) - \sum_{\vec{k}}M_{\vec{k}\vec{k}}^2(\vec{q})n_{\vec{k}}(2n_{\vec{k}}+1) - \sum_{\vec{k}}N_{\vec{k}\vec{k}}^2(\vec{q})(2n_{\vec{k}}^2 + 3n_{\vec{k}} + 1), \tag{A9}$$

with

$$n_{\vec{k}} = (e^{\beta E_{\vec{k}}} - 1)^{-1}. \tag{A10}$$

In the simpler case of Bogoliubov,

$$\alpha_{\vec{k}\vec{k}_1}^{(B)} = u_k\delta_{\vec{k},\vec{k}_1}, \quad\text{and}\quad \beta_{\vec{k}\vec{k}_1}^{(B)} = -v_k\delta_{\vec{k},-\vec{k}_1}. \tag{A11}$$

Therefore,

$$\chi_{\vec{k}}^{(B)}(\vec{q}) = (N_0)^{1/2}u_k\,\delta_{\vec{k},\vec{q}}, \tag{A12}$$

$$\omega_{\vec{k}}^{(B)}(\vec{q}) = -(N_0)^{1/2}v_k\,\delta_{\vec{k},-\vec{q}}, \tag{A13}$$

$$M_{\vec{k}_1\vec{k}_2}^{(B)}(\vec{q}) = u_{k_1}u_{k_2}\delta_{\vec{k}_1+\vec{q},\vec{k}_2}, \tag{A14}$$

$$N_{\vec{k}_1\vec{k}_2}^{(B)}(\vec{q}) = v_{k_1}v_{k_2}\delta_{\vec{k}_1-\vec{q},\vec{k}_2}, \tag{A15}$$

and

$$P_{\vec{k}_1\vec{k}_2}^{(B)}(\vec{q}) = -u_{k_1}v_{k_2}\delta_{\vec{q}-\vec{k}_2,\vec{k}_1}. \tag{A16}$$

These values give the usual expressions for the Green's functions in the Bogoliubov approximation provided, of course, that we neglect all but the first three terms in (A3). [Recall that for homogeneous systems, $\mathcal{G}(\vec{q},\vec{q}';\ \omega_n) = V\delta_{\vec{q},\vec{q}'}\mathcal{G}(\vec{q},\omega_n)$ and $\mathcal{D}(\vec{q},\vec{q}';\omega_n) = V\delta_{\vec{q},\vec{q}'}\mathcal{D}(\vec{q},\omega_n)$.] In particular, in the Bogoliubov approximation, with the help of (A1)–(A3) and (A11)–(A13), one finds

$$\mathcal{D}^{(B)}(\vec{q},\omega_n) = \frac{N_0}{V}\sum_{\alpha,\beta}\mathcal{G}^{(B)}_{\alpha\beta}(\vec{q},\omega_n). \tag{A17}$$

The condensate considered in the text is composed of a large number of different states with the single state $(\vec{k}=0)$ as a point of accumulation. Therefore, (A4) and (A5) become

$$\chi_{\vec{k}}(\vec{q}) = \sqrt{V}\,\Psi(\vec{x}=0)\,\alpha_{\vec{q}\vec{k}}\ , \tag{A18}$$

and

$$\omega_{\vec{k}}(\vec{q}) = \sqrt{V}\,\Psi(\vec{x}=0)\beta_{\vec{q}\vec{k}}\,. \tag{A19}$$

If we retain only the second and third terms of (A3), we get, with the help of (A1), (A2), (A18), and (A19), that

$$\mathcal{D}(\vec{q},\vec{q};\omega_n) = |\Psi(\vec{x}=0)|^2\sum_{\alpha,\beta}\mathcal{G}_{\alpha\beta}(\vec{q},\vec{q};\omega_n). \tag{A20}$$

Therefore, in our model for He II, the elementary excitations [poles of $\mathcal{G}(\vec{q},\vec{q};\omega_n)$] are the same as the density fluctuations [poles of $\mathcal{D}(\vec{q},\vec{q};\omega_n)$], the dynamic structure factor

$$S(\vec{q},\omega) = -(\pi\hbar)^{-1}\,\mathrm{Im}\,\mathcal{D}(\vec{q},\vec{q};\omega_n\,|_{i\omega_n\to\omega+i0^+}\,.$$

It was shown in the text that the smeared condensate gives rise to a phonon branch in the excitation spectrum. Now it has been shown that it also leads to the basic equivalence of the field and density fluctuations. Therefore, it seems that the fundamental requirement for the occurrence of the equivalence is the existence of a phonon spectrum as $k\to 0$.

Another consequence of the condensate accumulation around the state with $\vec{k}=0$ is that for fixed $\vec{q}$ one would expect the coefficient $\alpha_{\vec{q}\vec{k}}$ to have a peak around the value $\vec{k}=\vec{q}$ ($\beta_{\vec{q}\vec{k}}$ to have a peak around the value $\vec{k}=-\vec{q}$), the limit of the smeared condensate to the Bogoliubov case. Therefore, the smeared condensate gives rise to a smearing of the pole in $\mathcal{G}(\vec{q},\vec{q};\omega_n)$ and, consequently, in $\mathcal{D}(\vec{q},\vec{q};\omega_n)$.

The additional terms in (A3), which are usually neglected in the Bogoliubov approximation,[22,25] are due to the two-quasiparticle continuum. Unfortunately, our lack of knowledge of the values of the discontinuities along the cuts does not permit us to analyze these terms. It is possible, however, that these terms may be connected with the multiphonon component seen in inelastic neutron scattering.[7]

Since the temperature and density dependence of the condensate fraction is of experimental interest [see, for instance, A. D. B. Woods and V. F. Sears, Phys. Rev. Lett. 39, 415 (1977)], we include here the explicit result for N_0/N which follows from (63) and (64)

$$\frac{N_0}{N} = \frac{3}{8}\,\frac{p_0^2}{m_{\mathrm{He}}}\frac{V}{gN}\left[\left(1+\frac{32}{9}\,\frac{\mu_r^2}{m_{\mathrm{He}}^2}\right)^{1/2} - 1\right].$$

Now[18] $p_0(\rho)/\hbar = A\rho^{1/3}$ with $A = 3.64\ \mathrm{cm}\,g^{-1/3}\,\mathrm{\AA}^{-1}$ and by (53) $g = 4\pi a\hbar^2/m_{\mathrm{He}}$ so that

$$\frac{N_0}{N} = \frac{3}{32\pi}\,\frac{m_{\mathrm{He}}A^2}{a}\,\frac{1}{\rho^{1/3}}\left[\left(1+\frac{32}{9}\,\frac{\mu_r^2}{m_{\mathrm{He}}^2}\right)^{1/2} - 1\right]$$

$$\approx 2.14\,\frac{1}{\rho^{1/3}}\,\frac{\mu_r^2}{m_{\mathrm{He}}^2}$$

with ρ is g/cm^3.

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