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Three-particle correlations in the ground state of a Bose fluid*

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The two- and three-particle distribution functions of the weakly interacting Bose gas in its ground state are studied via the calculation of their Fourier transforms. The form obtained for the three-particle distribution function shows that the familiar convolution approximation is not correct even in the lowest nontrivial order of perturbation theory. For the special case of the charged Bose gas at high density, the two-particle distribution function is obtained to second order in the expansion parameter $r_s^{3/4}$, a result which disagrees with a recent calculation. The discrepancy is traced to a use of the convolution approximation for the three-particle distribution function. Finally, Landau's theory of quantum hydrodynamics is employed to relate the long-range part of the three-particle distribution function to the Grüneisen constant. These results emphasize the need to treat properly the dynamic three-particle correlations in any quantitative theory of liquid helium.

For liquid He^4 in its ground state and low-lying excited states, three-particle correlations are physically significant because the density is large and the interactions of the particles are strong. Nevertheless, most quantitative estimates of the ground-state wave function are based on the Jastrow form

$$\Phi(\vec{r}_1,\ldots,\vec{r}_N)=\prod_{i<j}\exp[\tfrac{1}{2}u(\vec{r}_i-\vec{r}_j)],$$

an explicit product of two-particle functions. Variational calculations based on this choice of wave function are in semi-quantitative agreement with experiment.[1] Substantial improvement of this wave function requires the introduction of a factor containing three-particle functions of the form

$$\prod_{i<j<k}\exp[\tfrac{1}{2}w(\vec{r}_i,\vec{r}_j,\vec{r}_k)],$$

as suggested by Feenberg[2] and Woo.[3] A preliminary estimate of the modifications of the ground-state energy and structure factor introduced by this generalization of the Jastrow function has been made by Campbell,[4] but the corresponding variational calculation has not yet been attempted.

From an alternative point of view, adopted here, three-particle correlations can be characterized by the three-particle distribution function $p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ of the ground state. This function is defined as the joint probability density of finding one (distinct) particle at each of the locations $\vec{r}_1$, $\vec{r}_2$, and $\vec{r}_3$. Feenberg[2,5] has summarized what little is known about $p^{(3)}$. Approximate forms for the three-particle distribution function have been used in theoretical calculations of the excitation spectrum,[6,7] ground-state energy,[8] and cross section for light scattering.[9] The most common approximations are the convolution approximation and the Kirkwood superposition approximation, as discussed in Ref. 5. The convolution approximation is known to be superior to the Kirkwood approximation, but little is known about the magnitude of the errors caused by the convolution approximation.

The purpose of this paper is to supply some new, albeit limited, information regarding the three-particle distribution function in the ground state of a Bose fluid. In Sec. I it is expressed in terms of the two- and three-particle structure functions $S(k)$ and $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$, and a convenient method for the calculation of S and T is derived. Perturbation calculations for the weakly interacting Bose gas are presented in Sec. II; one finds that the convolution approximation for $p^{(3)}$ fails to correctly describe three-particle correlations even in the lowest, nontrivial order of perturbation theory. As a subsidiary calculation the structure function $S(k)$ is given to two orders in perturbation theory. In Sec. III the special case of the charged Bose gas at high density is considered, and the leading correction to the structure factor is evaluated numerically. It is shown that the discrepancy with Bhattacharyya and Woo's calculation[10] of this correction is due to their use of the convolution approximation for the three-particle distribution function. Section IV contains a simple calculation of the long-range part of the three-particle distribution function as given by quantum hydrodynamics for liquid helium, together with a discussion of the validity of the result.

I. TWO- AND THREE-PARTICLE DISTRIBUTION FUNCTIONS AND A METHOD FOR THEIR COMPUTATION

The functions $p^{(2)}(\vec{r}_1,\vec{r}_2)$ and $p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ are defined by

$$p^{(2)}(\vec{r}_1,\vec{r}_2)\equiv\langle\psi^\dagger(\vec{r}_1)\psi^\dagger(\vec{r}_2)\psi(\vec{r}_2)\psi(\vec{r}_1)\rangle \tag{1a}$$

and

$$p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3) \equiv \langle \psi^\dagger(\vec{r}_1)\psi^\dagger(\vec{r}_2)\psi^\dagger(\vec{r}_3)\psi(\vec{r}_3)\psi(\vec{r}_2)\psi(\vec{r}_1)\rangle, \tag{1b}$$

where $\psi(\vec{r})$ and $\psi^\dagger(\vec{r})$ are the usual destruction and creation operators for the boson field, and the angular brackets indicate the expectation value in the ground state. In terms of the density operator

$$\rho(\vec{r}) \equiv \psi^\dagger(\vec{r})\psi(\vec{r}), \tag{2}$$

these functions may be rewritten in the form

$$p^{(2)}(\vec{r}_1,\vec{r}_2) = \langle \rho(\vec{r}_1)\rho(\vec{r}_2)\rangle - n\delta(\vec{r}_1-\vec{r}_2), \tag{3a}$$

and

$$\begin{aligned} p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3) = {} & \langle \rho(\vec{r}_1)\rho(\vec{r}_2)\rho(\vec{r}_3)\rangle \\ & - \delta(\vec{r}_1-\vec{r}_2)\langle\rho(\vec{r}_1)\rho(\vec{r}_3)\rangle \\ & - \delta(\vec{r}_2-\vec{r}_3)\langle\rho(\vec{r}_2)\rho(\vec{r}_1)\rangle \\ & - \delta(\vec{r}_3-\vec{r}_1)\langle\rho(\vec{r}_3)\rho(\vec{r}_2)\rangle \\ & + 2n\delta(\vec{r}_1-\vec{r}_2)\delta(\vec{r}_2-\vec{r}_3), \end{aligned} \tag{3b}$$

with $n \equiv \langle \rho(r)\rangle$ a constant, under the assumption of translational invariance. The presence of translational invariance makes it desirable, in addition, to deal with the Fourier components of the density operator,

$$\rho_{\vec{k}} \equiv \int d^3\vec{r}\, e^{i\vec{k}\cdot\vec{r}}\rho(\vec{r}), \tag{4}$$

rather than the density operator itself. Thus one is led to introduce the two- and three-particle structure functions S and T:

$$S(k) \equiv N^{-1}\langle \rho_{\vec{k}}\rho_{-\vec{k}}\rangle, \quad k \neq 0, \tag{5a}$$

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) \equiv N^{-1}\langle \rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}\rangle, \quad \vec{k}_1,\vec{k}_2,\vec{k}_3 \neq 0, \tag{5b}$$

where N is the total number of particles, and the function $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ vanishes unless $\vec{k}_1+\vec{k}_2+\vec{k}_3=0$. In terms of S and T one has

$$\langle\rho(\vec{r}_1)\rho(\vec{r}_2)\rangle = n^2 + n^2N^{-1}\sum_{\vec{k}}{}' e^{i\vec{k}\cdot(\vec{r}_2-\vec{r}_1)}S(k), \tag{6a}$$

and

$$\begin{aligned}\langle\rho(\vec{r}_1)\rho(\vec{r}_2)\rho(\vec{r}_3)\rangle = {} & n^3 + n^3N^{-2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}{}' e^{-i(\vec{k}_1\cdot\vec{r}_1+\vec{k}_2\cdot\vec{r}_2+\vec{k}_3\cdot\vec{r}_3)}T(\vec{k}_1,\vec{k}_2,\vec{k}_3) \\ & + n^3N^{-1}\sum_{k}{}'(e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} + e^{i\vec{k}\cdot(\vec{r}_2-\vec{r}_3)} + e^{i\vec{k}\cdot(\vec{r}_3-\vec{r}_1)})S(k), \end{aligned} \tag{6b}$$

where the primes mean that terms with any wave vector equal to zero are excluded. The substitution of Eqs. (6a) and (6b) into Eqs. (3a) and (3b) gives $p^{(2)}(\vec{r}_1,\vec{r}_2)$ in terms of $S(k)$ and gives $p^{(3)}(\vec{r}_1,\vec{r}_2,\vec{r}_3)$ in terms of $S(k)$ and $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$. Thus further considerations may be restricted to the structure functions S and T, which are regarded as containing the two- and three-particle correlations, respectively.

A convenient method for the computation of these structure functions involves the functional differentiation of energy eigenvalues. For a Hamiltonian H, consider the related Hamiltonian

$$H^* = H + N^{-2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}{}' A_{\vec{k}_1,\vec{k}_2,\vec{k}_3}\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}, \tag{7}$$

where the discrete values of the vectors $\vec{k}_i$, $i=1,2,3$, in the sum are determined by the usual periodic boundary conditions. It is convenient (but not necessary) to assume that the function $A_{\vec{k}_1,\vec{k}_2,\vec{k}_3}$ is symmetric in its arguments and vanishes unless $\vec{k}_1+\vec{k}_2+\vec{k}_3=0$. An eigenstate $|\phi^*\rangle$ of H^* with eigenvalue E^* has the property that

$$\frac{\partial E^*}{\partial A_{\vec{k}_1,\vec{k}_2,\vec{k}_3}} = 3!N^{-2}\langle\phi^*|\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}|\phi^*\rangle,$$

with the consequence that, for the ground state of H,

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) = \frac{N}{3!}\left(\frac{\partial E^*}{\partial A_{\vec{k}_1,\vec{k}_2,\vec{k}_3}}\right)_{A=0}, \tag{8}$$

where the definition (5b) of $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ has been employed and the subscript $A=0$ means that one must set $A_{\vec{k}_1,\vec{k}_2,\vec{k}_3}=0$ after performing the differentiation. Thus the three-particle structure factor may be calculated by means of a simple differentiation once the ground-state energy of the Hamiltonian H^* is known. This technique is often particularly useful because a given approximation for the ground-state energy E^* immediately yields a corresponding approximation for $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$.

The calculation of the two-particle structure function $S(k)$ may be performed in the same way. The potential energy operator has the form

$$U = \tfrac{1}{2}\Omega^{-1}\sum_{\vec{k}} v(\vec{k})[\rho_{\vec{k}}\rho_{-\vec{k}} - N],$$

where Ω is the volume and $v(\vec{k})$ is the Fourier transform of the interparticle potential. If the dependence of the ground state energy E upon $v(\vec{k})$ is known for $v(\vec{k})$ close to its "physical" value, then one has

$$S(k)=1+(2/n)\,\partial E/\partial v(\vec{k}), \tag{9}$$

for $k\neq 0$.

II. WEAKLY INTERACTING BOSE GAS: GROUND-STATE ENERGY AND STRUCTURE FUNCTIONS

The calculation of the ground-state energy, including in the Hamiltonian the three-phonon term in Eq. (7), is most easily accomplished using a theory in which the density operator $\rho_{\vec{k}}$ enters the analysis in a direct way. Thus it is inconvenient to employ the standard theory of Bogoliubov,[11] for which the operators $a_{\vec{k}}$ and $a_{\vec{k}}^{\dagger}$ (destruction and creation operators for particles in plane-wave states) serve as variables. More convenient would be the method of correlated basis functions in the uniform limit,[5,12] using a Jastrow function as the zero-order approximation to the ground state. A method using density and phase operators as variables[13] could also be used. Finally, the method of "auxiliary variables" of Bogoliubov and Zubarev[14] is suitable for the present calculation, and will be used here.

Bogoliubov and Zubarev wrote the Hamiltonian in the form

$$H=H_0+H', \tag{10a}$$

where

$$H_0=E_0+\sum_{\vec{k}}{}' \eta(k)\, b_{\vec{k}}^{\dagger} b_{\vec{k}}, \tag{10b}$$

with

$$\eta(k)\equiv \hbar^2k^2/2m\lambda_k^2, \tag{10c}$$

and

$$\lambda_k^4\equiv\frac{\hbar^2k^2/2m}{\hbar^2k^2/2m+2nv(k)}\,. \tag{10d}$$

The zero-order energy E_0 is given by

$$E_0=\tfrac{1}{2}n^2\Omega v(0)+\tfrac{1}{2}\sum_{\vec{k}}\left[\eta(k)-\hbar^2k^2/2m-nv(k)\right]. \tag{10e}$$

The operators $b_{\vec{k}}$ are defined for $k\neq 0$ by

$$b_{\vec{k}}=\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial q_{\vec{k}}}+q_{-\vec{k}}\right), \qquad q_{\vec{k}}=(2N)^{-1/2}\lambda_k^{-1}\rho_{\vec{k}}. \tag{10f}$$

The perturbation term H' in Eq. (10a) will not be written out explicitly; it may be found in Ref. 14 or 15. The term H' is a trilinear form in the operators $b_{\vec{k}}$ and $b_{\vec{k}}^{\dagger}$.[16] Bogoliubov and Zubarev have calculated the ground-state energy to second order in H'.

The problem at hand is the calculation of the ground-state energy to the same order and using the same techniques as Bogoliubov and Zubarev, but the Hamiltonian to be used is the modified Hamiltonian H^* of Eq. (7). With Eq. (10f), Eq. (7) may be written as

$$H^*=H+N^{-1/2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}{}' \lambda_{k_1}\lambda_{k_2}\lambda_{k_3}A_{\vec{k}_1,\vec{k}_2,\vec{k}_3} \times(b_{\vec{k}_1}+b_{-\vec{k}_1}^{\dagger})(b_{\vec{k}_2}+b_{-\vec{k}_2}^{\dagger})(b_{\vec{k}_3}+b_{-\vec{k}_3}^{\dagger}).$$

Because the correction to H in this equation is a trilinear form in the operators $b_{\vec{k}}$ and $b_{\vec{k}}^{\dagger}$, it may be treated as a perturbation on an equal footing with the physical perturbation H' appearing in Eq. (10a). Repeating the procedure of Bogoliubov and Zubarev, one finds the ground-state energy E^* of the Hamiltonian H^* to be

$$E^*=E_0^*+E_1^*+E_2^*+\cdots, \tag{11a}$$

where

$$E_0^*=E_0, \tag{11b}$$

$$E_1^*=0, \tag{11c}$$

and

$$E_2^*=-\frac{2}{3N}\sum_{\vec{k}_1,\vec{k}_2}(\eta_1+\eta_2+\eta_3)^{-1}\left(\frac{\hbar^2}{8m}\vec{k}_1\cdot\vec{k}_2\frac{\lambda_3}{\lambda_1\lambda_2}(1-\lambda_1^2)(1-\lambda_2^2)+\text{c.p.}+3\lambda_1\lambda_2\lambda_3A_{123}\right) \times\left(\frac{\hbar^2}{8m}\vec{k}_1\cdot\vec{k}_2\frac{\lambda_3}{\lambda_1\lambda_2}(1+\lambda_1^2)(1+\lambda_2^2)+\text{c.p.}+3\lambda_1\lambda_2\lambda_3A_{123}\right). \tag{11d}$$

In Eq. (11d), $\vec{k}_3$ is defined equal to $-\vec{k}_1-\vec{k}_2$; the arguments $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ of various functions have been suppressed in favor of the indices 1, 2, and 3; and the notation $f_{123}+\text{c.p.}$ means $f_{123}+f_{231}+f_{312}$.

Given Eqs. (11a)–(11d) for the ground-state energy, the calculation of the structure functions $S(k)$ and $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ to this order in perturbation theory is an exercise in differentiation. With Eq. (8), one obtains for the three-particle structure function the expression

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3)=-\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0}\left(\frac{k_1^2}{\lambda_1^2}+\frac{k_2^2}{\lambda_2^2}+\frac{k_3^2}{\lambda_3^2}\right)^{-1} \times\left[\vec{k}_1\cdot\vec{k}_2\,\lambda_3^2(1+\lambda_1^2\lambda_2^2)+\text{c.p.}\right]. \tag{12}$$

This equation has been obtained previously by Sunakawa, Yamasaki, and Kebukawa,[17] but they did not note its significance. In the present context, Eq. (12) is interesting because it contradicts the convolution approximation. The convolution approximation for $T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ is[2]

$$T_c(\vec{k}_1, \vec{k}_2, \vec{k}_3) = \delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0} S(k_1) S(k_2) S(k_3). \tag{13}$$

As will be shown shortly, the structure factor, in lowest order of perturbation theory, is given by

$$S_0(k) = \lambda_k^2 , \tag{14}$$

so that, for the weakly interacting Bose gas, the convolution approximation assumes the form

$$T_c(\vec{k}_1, \vec{k}_2, \vec{k}_3) \cong \delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0} \lambda_1^2\lambda_2^2\lambda_3^2, \tag{15}$$

at variance with Eq. (12). Both Eqs. (12) and (15) attain the proper limiting value for the ideal Bose gas (i.e., in the limit $\lambda_i^2 \to 1$, $i = 1, 2, 3$), but there is otherwise little similarity. While the convolution approximation has proved empirically useful for the ground state of liquid helium, the present result shows that it gives an incorrect description of the three-particle correlations of the ground state of a weakly interacting Bose gas, even to lowest nontrivial order in perturbation theory.

For the computation of $S(k)$ it is necessary to differentiate the ground-state energy with respect to $v(\vec{k})$, according to Eq. (9). The differentiation of $E_0^* = E_0$ of Eq. (10e) yields

$$S_0(k) = \lambda_k^2 , \tag{16a}$$

in agreement with Eq. (14). Since $E_1^* = 0$, one sees further that

$$S_1(k) = 0. \tag{16b}$$

Prior to the differentiation of E_2^* of Eq. (11d), it is convenient to rewrite it (for $A_{123} = 0$) in the form[18]

$$\begin{aligned} E_2 = {} & \frac{\hbar^2}{16Nm} \sum_{\vec{k}_1,\vec{k}_2} k_3^2(1-\lambda_1^2)(1-\lambda_2^2)(1-\lambda_3^2) \\ & - \frac{\hbar^2}{48Nm} \sum_{\vec{k}_1,\vec{k}_2} \left(\frac{k_1^2}{\lambda_1^2} + \frac{k_2^2}{\lambda_2^2} + \frac{k_3^2}{\lambda_3^2}\right)^{-1} (\lambda_1\lambda_2\lambda_3)^{-2} \\ & \times [\vec{k}_1 \cdot \vec{k}_2 \, \lambda_3^2(1-\lambda_1^2)(1-\lambda_2^2) + \text{c.p.}]^2 . \end{aligned} \tag{17}$$

Differentiating this expression with respect to $v(\vec{k})$, one finds the second-order correction to $S(k)$:

$$\begin{aligned} S_2(k_1) = \frac{1}{16N} \sum_{\vec{k}_2} \Bigg[& 4\lambda_1^6\left(1 + \frac{k_2^2}{k_1^2} + \frac{k_3^2}{k_1^2}\right)(1-\lambda_2^2)(1-\lambda_3^2) + (\Delta E_{123}\lambda_2^2\lambda_3^2)^{-1}\left(\Delta E_{123}{}^{-1} - \frac{2m\lambda_1^2}{\hbar^2 k_1^2}\right) \\ & \times\left(\frac{\hbar^2}{m}\vec{k}_1 \cdot \vec{k}_2\lambda_3^2(1-\lambda_1^2)(1-\lambda_2^2) + \text{c.p.}\right)^2 - (\Delta E_{123}\lambda_2^2\lambda_3^2)^{-1}\left(\frac{4m\lambda_1^4}{\hbar^2 k_1^2}\right)\left(\frac{\hbar^2}{m}\vec{k}_1 \cdot \vec{k}_2\lambda_3^2(1-\lambda_1^2)(1-\lambda_2^2) + \text{c.p.}\right) \\ & \times\left(\frac{\hbar^2}{m}\vec{k}_1 \cdot \vec{k}_2\lambda_3^2(1-\lambda_2^2) + \frac{\hbar^2}{m}\vec{k}_1 \cdot \vec{k}_3\lambda_2^2(1-\lambda_3^2) - \frac{\hbar^2}{m}\vec{k}_2 \cdot \vec{k}_3(1-\lambda_2^2)(1-\lambda_3^2)\right)\Bigg], \end{aligned} \tag{18}$$

where

$$\vec{k}_3 \equiv -\vec{k}_1 - \vec{k}_2,$$

and

$$\Delta E_{123} = \frac{\hbar^2}{2m}\left(\frac{k_1^2}{\lambda_1^2} + \frac{k_2^2}{\lambda_2^2} + \frac{k_3^2}{\lambda_3^2}\right).$$

This result has been obtained previously,[13] but is rederived here for application to the charged Bose gas at high density, where it represents the exact leading correction to the structure factor.

III. CHARGED BOSE GAS AT HIGH DENSITY

The analysis to this point has employed the method of "auxiliary variables" of Bogoliubov and Zubarev,[14] together with a convenient form of perturbation theory. It must be recognized that the ordering of the perturbation series has been accomplished in a formal way; to give a unique classification to the terms appearing in perturbation theory it is necessary to introduce an expansion parameter. For this purpose the high-density charged Bose gas with neutralizing background has been chosen.

The Fourier transform $v(k)$ of the interparticle potential assumes the form

$$\begin{aligned} & v(k) = 4\pi e^2/k^2, \quad k \neq 0, \\ & v(0) = 0. \end{aligned} \tag{19}$$

Properties such as the ground-state energy are then functions of a single dimensionless parameter, the average interparticle spacing in units of the Bohr radius,

$$r_s \equiv \left(\frac{3}{4\pi n}\right)^{1/3} \frac{me^2}{\hbar^2} \ll 1. \tag{20}$$

For example, the ground-state energy per particle, measured in units of $me^4/2\hbar^2$ is

$$E/N = -0.8031 r_s{}^{-3/4} + 0.0275 + \cdots . \tag{21}$$

The first term arises from Eq. (10e) for E_0, once the specific form (19) is used for $v(k)$ and the sum is converted to an integral. It was first obtained by Foldy.[19] The second term, proportional to $r_s{}^0$, arises from Eq. (17) for E_2 or, equivalently, from Eq. (11d) for E_2^* with $A_{123} = 0$. It was first obtained by Brueckner.[20]

An expansion in powers of $r_s^{3/4}$ for the structure factor, analogous to Eq. (21) for the ground-state energy, has the form

$$S(k) = f_0(t) + f_1(t)\, r_s^{3/4} + \cdots , \tag{22}$$

where t is a dimensionless wave vector, defined by

$$t = k(\hbar^2/16mne^2)^{1/4}.$$

The function $f_0(t)$ may be extracted from Eqs. (10d), (16a), and (19):

$$f_0(t) = t^2(1+t^4)^{-1/2}. \tag{23}$$

The function $f_1(t)$ is similarly extracted from Eq. (18), after converting the sum to an integral.[21] The integration was performed numerically and the result is displayed in Fig. 1. The asymptotic behaviors of $f_1(t)$ are

$$f_1(t) \sim 0.065t^4 \quad \text{as } t \to 0 \tag{24a}$$

and

$$f_1(t) \sim 0.423t^{-4} \quad \text{as } t \to \infty. \tag{24b}$$

Also shown in Fig. 1 is the result of an independent calculation by Bhattacharyya and Woo of the same function.[10] The disagreement is evident. Their unpublished data points[23] show the largest percentage discrepancy at small t, where they find

$$f_1^{\mathrm{BW}}(t) \sim 0.043t^4, \quad t \to 0,$$

about 30% less than the values given by Eq. (24a). The difference between $f_1(t)$ and $f_1^{\mathrm{BW}}(t)$ is due to Bhattacharyya and Woo's use of the convolution approximation for the three-particle structure function, as will be clear shortly.

Bhattacharyya and Woo employed the powerful method of correlated basis functions to study the excitation spectrum of the charged Bose gas in the high-density limit. Starting with the optimum Jastrow function as the correlation function (ground-state wave function), they computed the excitation spectrum $\hat{\epsilon}(k)$ to two orders in $r_s^{3/4}$. This result agrees with previous work by Ma and Woo.[22] Next, the calculation was repeated using the exact ground state as the correlation function, to obtain the (same) excitation spectrum $\epsilon(k)$ to two orders in $r_s^{3/4}$. The function $\epsilon(k)$ depends explicitly on the exact structure functions $S(k)$ and $T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$. Making the convolution approximation (13) for $T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$, they obtained $\epsilon(k)$ as a function of $S(k)$ alone, and used the equality between $\epsilon(k)$ and $\hat{\epsilon}(k)$ to extract $S(k)$ itself to two orders in $r_s^{3/4}$.

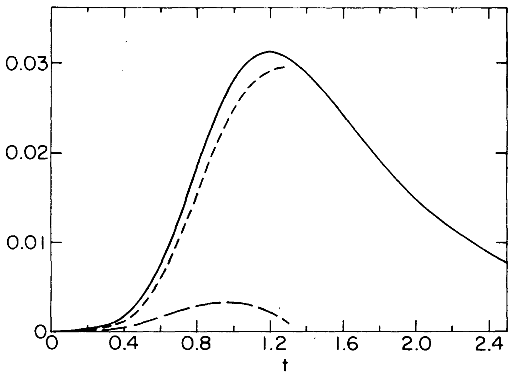

FIG. 1. Solid line: leading correction $f_1(t)$ to the structure factor for the charged Bose gas at high density, as a function of the dimensionless wave vector t. Short dashes: the result $f_1^{\mathrm{BW}}(t)$ reported in Ref. 10. Long dashes: the function $\Delta f_1(t)$ computed as a correction to $f_1^{\mathrm{BW}}(t)$.

Using the theory of correlated basis functions we present a corrected calculation of $\epsilon(k)$, the energy of an excitation, using the exact ground state as the correlation function. Following Bhattacharyya and Woo, one finds

$$\epsilon(k) = \epsilon_0(k) + \epsilon_2(k) + \cdots , \tag{25a}$$

where

$$\epsilon_0(k) = \hbar^2 k^2/2mS(k), \tag{25b}$$

$$\epsilon_2(k_1) = \tfrac{1}{2}\sum_{\vec{k}_2} \frac{|\langle -\vec{k}_1|H|\vec{k}_2, \vec{k}_3\rangle|^2}{\epsilon_0(k_1) - \epsilon_0(k_2) - \epsilon_0(k_3)} , \tag{25c}$$

with

$$\begin{aligned} \langle -\vec{k}_1|H|\vec{k}_2, \vec{k}_3\rangle = -(\hbar^2/2m)[NS(k_1)S(k_2)S(k_3)]^{-1/2} \\ \times [\vec{k}_1 \cdot \vec{k}_2 S(k_3) + \vec{k}_1 \cdot \vec{k}_3 S(k_2) \\ + k_1^2 S^{-1}(k_1)\, T(\vec{k}_1, \vec{k}_2, \vec{k}_3)] . \end{aligned} \tag{25d}$$

Momentum conservation in the matrix element makes the notation $\vec{k}_3 \equiv -\vec{k}_1 - \vec{k}_2$ convenient. The one- and two-phonon (or plasmon) states appearing in Eqs. (25c) and (25d) are formed by multiplying one or two factors of $\rho_{\vec{k}}$, respectively, by the exact ground state. These states are then normalized and made orthogonal to one another and the ground state by means of the Gram-Schmidt orthogonalization procedure. It should be emphasized that Eq. (25d) is exact for an arbitrary interacting Bose system of infinite extent, subject only to the restrictions that $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ are not zero and that no pair of these vectors are identical.

Since $\epsilon_2(k)$ in Eq. (25c) is a small correction to the excitation spectrum, the functions $S(k)$ and $T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ which are necessary for its evaluation may be replaced by their values in the lowest, nontrivial order of perturbation theory, given by Eqs. (16a) and (12), respectively. Bhattacharyya and Woo incorrectly used Eq. (13) for $T(\vec{k}_1, \vec{k}_2, \vec{k}_3)$ in Eq. (25d) to obtain the value for the correction to the excitation spectrum, which we designate as

$\epsilon_2^{\mathrm{BW}}(k)$. Since their method for the calculation of the leading correction to the structure factor involves the comparison of two distinct perturbation expansions for $\epsilon(k)$, the difference between $\epsilon_2^{\mathrm{BW}}(k)$ and $\epsilon_2(k)$ contributes a correction to their value for $S_2(k)$, i.e.,

$$\Delta S_2(k) = (2mS_0^2(k)/\hbar^2k^2)[\epsilon_2(k) - \epsilon_2^{\mathrm{BW}}(k)]\,. \tag{26}$$

For the charged Bose gas at high density the function $\Delta S_2(k)$ was obtained by evaluating the necessary integrals numerically. The function

$$\Delta f_1(t) \equiv r_s^{-3/4}\Delta S_2(t(16\pi mne^2/\hbar^2)^{1/4})$$

is displayed in Fig. 1. With this correction, the results of Bhattacharyya and Woo[10] agree with our result (obtained by direct calculation), to within the 1% accuracy of the numerical integrations. Therefore, the function $\Delta f_1(t)$ is a direct quantitative measure of the error caused by the convolution approximation for the three-particle structure function.

The analysis in Chap. 2 of Feenberg's monograph[5] can be employed to prove that the convolution approximation is exact in leading order *if* the actual ground-state wave function is a Jastrow function. (Bhattacharyya and Woo evidently assumed that a Jastrow function could adequately represent the ground state.) The failure of this approximation thus shows that a Jastrow function is not sufficiently flexible to represent the ground state. Errors, similar to those found here, must be expected in the theory of the ground state of liquid ^{4}He if the convolution approximation is employed or if the wave function is assumed to have the Jastrow form.

IV. QUANTUM HYDRODYNAMICS AND THE THREE-PARTICLE STRUCTURE FUNCTION OF LIQUID HELIUM

In order to obtain some quantitative information about the structure function $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ of the liquid-helium ground state we turn to Landau's theory of quantum hydrodynamics.[24,25] The Hamiltonian has the form

$$H = \int d^3r\,[\tfrac{1}{2}m\rho(\vec{r})\vec{v}^2(\vec{r}) + \mathcal{E}(\rho(\vec{r}))]\,, \tag{27}$$

where $\vec{v}(r)$ is an operator representing the hydrodynamic flow velocity and $\mathcal{E}(\rho)$ is the energy per unit volume of the stationary liquid at the density ρ. The function $\mathcal{E}(\rho)$ may be expanded about the equilibrium point $\rho = n$ as

$$\mathcal{E}(\rho) = \mathcal{E}(n) + \tfrac{1}{2}(mc^2/n)\rho'^2 + \tfrac{1}{6}(mc^2/n^2)(2u-1)\rho'^3 + \cdots\,, \tag{28}$$

where $\rho'(\vec{r})$ is the density-fluctuation operator $\rho(\vec{r}) - n$, c is the speed of sound, and u is the Grüneisen constant

$$u \equiv (n/c)\,\partial c/\partial n. \tag{29}$$

For the present purposes the velocity operator $\vec{v}(\vec{r})$ may be regarded as irrotational; it may be written in terms of a phase operator $\sigma(\vec{r})$:

$$\vec{v}(\vec{r}) = (\hbar/m)\nabla\sigma(\vec{r}). \tag{30}$$

Landau's commutation relations[24] for $\rho(\vec{r})$ and $\vec{v}(\vec{r})$ then reduce to simple canonical forms in terms of $\rho'(\vec{r})$ and $\sigma(\vec{r})$:

$$[\sigma(\vec{r}),\rho'(\vec{r}\,')] = -i\delta(\vec{r}-\vec{r}\,'), \tag{31a}$$

$$[\sigma(\vec{r}),\sigma(\vec{r}\,')] = [\rho'(\vec{r}),\rho'(\vec{r}\,')] = 0. \tag{31b}$$

The quadratic part of the Hamiltonian (27) may be immediately diagonalized:

$$H_0 \equiv \int d^3r\,[\tfrac{1}{2}mn\vec{v}^2(\vec{r}) + \mathcal{E}(n) + \tfrac{1}{2}(mc^2/n)\rho'^2(\vec{r})] \tag{32a}$$

$$= \Omega\mathcal{E}(n) + \sum_{\vec{k}}\hbar ck(\pi_{\vec{k}}^\dagger\pi_{\vec{k}} + \tfrac{1}{2}), \tag{32b}$$

where the phonon creation and destruction operators are defined for $\vec{k} \neq 0$ by

$$\rho_{\vec{k}} = -i(N\hbar k/2mc)^{1/2}(\pi_{\vec{k}}^\dagger - \pi_{-\vec{k}}), \tag{33a}$$

$$\sigma_{\vec{k}} = \tfrac{1}{2}(2mc/N\hbar k)^{1/2}(\pi_{\vec{k}} + \pi_{-\vec{k}}^\dagger), \tag{33b}$$

where

$$\sigma_{\vec{k}} \equiv \Omega^{-1}\int d^3r\, e^{-i\vec{k}\cdot\vec{r}}\sigma(\vec{r}), \tag{34}$$

and $\rho_{\vec{k}}$ is defined in Eq. (4). Inspection of Eq. (32b) shows that the ground-state energy is ill-defined unless an ultraviolet cutoff is introduced. Such behavior must be expected in any hydrodynamic theory, of course, and indicates that any results must be restricted to long wavelengths.

The ground state $|\phi_0\rangle$ of H_0, i.e., the vacuum of the operators $\pi_{\vec{k}}$ and $\pi_{\vec{k}}^\dagger$, does not represent the ground state of the full Hamiltonian (27) accurately enough to give nontrivial information concerning the three-particle structure function. The zero-order result for $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ is

$$N^{-1}\langle\phi_0|\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}|\phi_0\rangle = 0, \tag{35}$$

because $\rho_{\vec{k}}$ is a linear function of $\pi_{\vec{k}}$ and $\pi_{-\vec{k}}^\dagger$. For this reason it is necessary to consider the effect of the trilinear terms in Eq. (27):

$$H_1 \equiv \int d^3r\,\{\tfrac{1}{2}m\rho'(\vec{r})\vec{v}^2(\vec{r}) + \tfrac{1}{6}(mc^2/n^2)(2u-1)[\rho'(\vec{r})]^3\}. \tag{36}$$

Taken to lowest order, H_1 introduces a three-phonon correction $|\phi_1\rangle$ to the unperturbed ground state $|\phi_0\rangle$,[26]

$$|\phi_1\rangle = -\frac{1}{3!}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3}{}' \frac{\langle\phi_0|\pi_{\vec{k}_1}\pi_{\vec{k}_2}\pi_{\vec{k}_3}H_1|\phi_0\rangle}{\hbar c(k_1+k_2+k_3)} \times \pi^\dagger_{\vec{k}_1}\pi^\dagger_{\vec{k}_2}\pi^\dagger_{\vec{k}_3}|\phi_0\rangle. \tag{37}$$

Thus the three-particle structure factor is given to lowest order by

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) = N^{-1}(\langle\phi_0|\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}|\phi_1\rangle + \langle\phi_1|\rho_{\vec{k}_1}\rho_{\vec{k}_2}\rho_{\vec{k}_3}|\phi_0\rangle). \tag{38}$$

With Eqs. (4), (33), (34), (36), and (37), together with the properties of the operators $\pi_{\vec{k}}$ and $\pi^\dagger_{\vec{k}}$, the necessary matrix elements can be evaluated to obtain the explicit result

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) = -\tfrac{1}{4}\delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0}\frac{\hbar^2}{m^2c^2}\left(\frac{k_1k_2k_3}{k_1+k_2+k_3}\right) \times\left((2u-1)+\frac{\vec{k}_1\cdot\vec{k}_2}{k_1k_2}+\frac{\vec{k}_2\cdot\vec{k}_3}{k_2k_3}+\frac{\vec{k}_3\cdot\vec{k}_1}{k_3k_1}\right), \tag{39}$$

valid for $k_i \ll n^{1/3}$, $i=1,2,3$. Higher-order contributions to $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ contain sums over wave vectors which diverge or depend upon an arbitrary ultraviolet cutoff. Thus, if quantum hydrodynamics is to yield a sensible result for the structure function $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$, that result is given by Eq. (39).

One interesting feature of the hydrodynamic form (39) for T is that it is negative, since $u \cong 2.84$ for liquid helium at zero pressure.[27] On the other hand, for k_1, k_2, and k_3 large compared to $n^{1/3}$, interactions in the liquid should be unimportant[28] and the positive ideal-gas value for T will be attained,

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) = \delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0}, \quad k_1,k_2,k_3 \gg n^{1/3}. \tag{40}$$

Consider a triangle with sides $\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ with variable size but fixed shape. Then T has the form

$$T(\vec{k}_1,\vec{k}_2,\vec{k}_3) = Ag(k_1),$$

where A is a positive constant depending on u and the angles of the triangle, and $g(k_1)$ is a function of k_1 alone. Then $g(k_1)$ is negative and proportional to k_1^2 for small k_1, and attains a positive value at large k_1. Thus the function $g(k_1)$ must have at least one minimum and must cross through zero in the intermediate region $k_1 \sim n^{1/3}$.

Since the hydrodynamical result (39) for the three-particle structure function is apparently new, and since the use of quantum hydrodynamics for this case may be subject to some question, it is highly desirable to make any possible checks of the formula. One such check is the special case of the weakly interacting Bose gas with short-range interactions, a special case of the formulas developed in Sec. II. For this case, the speed of sound is

$$c = [nv(0)/m]^{1/2},$$

and, with Eq. (29), the Grüneisen constant is

$$u = \tfrac{1}{2}.$$

Substituting these values into Eq. (39), one finds complete agreement with the long-wavelength limit of Eq. (12), verifying the result of quantum hydrodynamics for this case.

A much more significant check can be made by employing the theory of correlated basis functions[2,5] to calculate the strength of the three-phonon vertex for liquid helium. Equation (25d) gives the strength of this vertex, if $S(k)$ and $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ are known. The long-wavelength behavior of $S(k)$ is[29]

$$S(k) = \hbar k/2mc, \quad k \to 0,$$

and that of $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ is given by Eq. (39). For phonons "on the mass shell," i.e., assuming energy conservation, Eq. (25d) reduces to

$$\langle -\vec{k}_1|H|\vec{k}_2,\vec{k}_3\rangle = \delta_{\vec{k}_1+\vec{k}_2+\vec{k}_3,0}(\hbar^3c/2mN)^{1/2}(u+1)[(k_2+k_3)k_2k_3]^{1/2}, \tag{41}$$

where the vectors $-\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ are very nearly parallel since the phonon spectrum is approximately linear at long wavelengths. The corresponding matrix element given by quantum hydrodynamics has the same numerical value,[30]

$$\langle 0|\pi_{-\vec{k}_1}H_1\pi^\dagger_{\vec{k}_2}\pi^\dagger_{\vec{k}_3}|0\rangle = \langle -\vec{k}_1|H|\vec{k}_2,\vec{k}_3\rangle, \tag{42}$$

provided $-\vec{k}_1$, $\vec{k}_2$, and $\vec{k}_3$ are nearly parallel, even though these matrix elements are different when taken off the mass shell. The damping of sound waves in superfluid helium at low temperatures proceeds via this three-phonon vertex. Detailed theoretical calculations[31-33] depend upon the precise shape of the excitation spectrum at long wavelengths, but are in fair agreement with extensive experiments.[34-36] Thus one is led to the belief that the matrix element (41) is reliable. The only serious assumption necessary for the derivation of Eq. (41) is that the long-wavelength limit of $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ is given by Eq. (39). Thus the relation (39) for the small-k behavior of $T(\vec{k}_1,\vec{k}_2,\vec{k}_3)$ is indirectly supported by experimental measurements.

V. CONCLUDING REMARKS

The three-particle structure function in the ground state of a Bose fluid has been discussed at some length. The model of the charged Bose gas at high density shows that the convolution approximation fails to describe even the leading correction to the ideal gas. More generally, it is clear that a quantitative theory of the ground state and low-lying states of liquid helium requires an accurate dynamical treatment of the three-particle correlations. Empirical approximations for the three-particle structure function[6-8] or restriction of the ground-state wave function to the Jastrow form[1,37,38] immediately obliterate the three-particle correlations and preclude a quantitative theory. A study of the three-particle structure function has yielded some dynamical information, but a systematic theory—perhaps a generalization of the Jastrow theory—is clearly required for the future.

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