Relationships between the pair-correlation function, the superfluid fraction, and the condensate fraction in liquid ^{4}He

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It is shown that the Woods-Svensson decomposition of the dynamic structure factor $S(Q, \omega)$ into superfluid and normal-fluid components implies relationships between $S(Q)$ and the superfluid fraction $n_s = \rho_s/\rho$ and between $g(r)$ and n_s, which are very well borne out by experiment. Combining our new relationship between $g(r)$ and n_s with that between $g(r)$ and the condensate fraction n_0 proposed by Hyland, Rowlands, and Cummings then gives an explicit relationship between n_0 and n_s for all temperatures in the superfluid phase.

About two years ago, Woods and Svensson[1] found that new neutron inelastic scattering results[1,2] for the temperature dependence of the dynamic structure factor $S(Q, \omega)$ of liquid ^{4}He were very well described by the relationship[3]

$$S(Q, \omega) = n_s S_s(Q, \omega) + n_n S_n(Q, \omega) , \qquad (1)$$

where $n_s = \rho_s/\rho$ and $n_n = 1 - n_s$ are the superfluid and normal-fluid fractions. This remarkable decomposition of $S(Q, \omega)$ into components with weights proportional to the hydrodynamic quantities n_s and n_n at values of Q far beyond the hydrodynamic regime was, at the time, presented simply as an empirical relationship which gave a very good description of the data.

In this paper, we first outline the theoretical justification for the decomposition (1), summarizing the recent work of Griffin,[4] and Griffin and Talbot.[5] We then point out that (1) implies analogous decompositions for the static structure factor $S(Q)$ and the pair-correlation function $g(r)$. These relationships between $S(Q)$ and n_s and between $g(r)$ and n_s are shown to be very well borne out by the results of a recent high-accuracy neutron-diffraction determination[6] of $S(Q)$ and $g(r)$ for a wide range of temperatures.

Our relationship between $g(r)$ and n_s opens a new route for obtaining insight into the relationship between superfluidity and Bose-Einstein condensation. In 1938, London[7] first advanced the hypothesis that the λ transition in liquid ^{4}He is closely related to the phenomenon of Bose-Einstein condensation. More than four decades have since passed and, although it is generally believed that superfluidity in liquid ^{4}He is indeed a direct consequence of the mac-

roscopic occupation of the zero-momentum state, an explicit relationship between the superfluid fraction n_s and the condensate fraction n_0 has never been established. By combining our relationship between $g(r)$ and n_s with that between $g(r)$ and n_0 proposed by Hyland *et al.*,[8] we obtain an explicit relationship between n_s and n_0 covering the entire superfluid range $0 \leq T \leq T_\lambda$.

Subsequent to the proposal of the decomposition (1) by Woods and Svensson,[1] one of us[4] pointed out that in the well-known microscopic theory of a condensed Bose liquid, $S(Q, \omega)$ is composed of a condensate part (which vanishes if $n_0 = 0$) and a regular part. Moreover, a rigorous argument was given which showed that, at least in the phonon region, the quasiparticle resonance in the condensate part had a weight proportional to the superfluid fraction n_s, in agreement with the Woods-Svensson ansatz (1). In a recent extension[5] of this work, the regular part $[S_R(Q, \omega)]$ of $S(Q, \omega)$ has been evaluated using the simple "bubble approximation" with Bogoliubov propagators, and it is found that there are two contributions to $S_R(Q, \omega)$. One is due to excitation of two quasiparticles and vanishes (because of coherence factors) if $n_0 = 0$. This contribution is associated with what Woods and Svensson[1] call the multiphonon part of the superfluid component. The other contribution $[S_R^{th}(Q, \omega)]$ to $S_R(Q, \omega)$ is due to neutron scattering from a Bose gas of thermally excited quasiparticles and is clearly what Woods and Svensson[1] call the normal-fluid contribution (it vanishes at $T = 0$, but is finite for $T > T_\lambda$). In the evaluation of $S_R^{th}(Q, \omega)$, we note that, in the temperature region $1-2.17$ K, rotons make the dominant contribution to all properties and, in particular, one has[9] $n_n(T) \sim T^{-1/2} e^{-\Delta/T}$, where Δ is the roton energy. In this temperature re-

gion, we need only consider the rotons in evaluating $S_R^{th}(Q, \omega)$ and further, since one can use a Boltzmann distribution for rotons, it immediately follows that $S_R^{th}(Q, \omega)$ will be proportional to $e^{-\Delta/T}$ and hence to $n_n(T)$ to a very good approximation (for further details, see Ref. 5).

We thus see that both terms in (1) follow quite naturally from the microscopic theory of an interacting Bose-condensed system, at least for $T \gtrsim 1$ K. At lower temperatures, and especially in the phonon-dominated region ($T \lesssim 0.6$ K), the Woods-Svensson ansatz may not be strictly correct since, in this region, one would not expect[5] the normal-fluid part to be simply related to $S(Q, \omega)$ for $T \gtrsim T_\lambda$. In this region, however, the normal-fluid part is negligibly small.

In view of the strong support, both experimental[1] and theoretical,[4,5] for the decomposition (1) of $S(Q, \omega)$, one is clearly justified in using it to obtain the analogous relationships for the static structure factor $S(Q) = \int S(Q, \omega) \, d\omega$ and the pair-correlation function,

$$g(r) = 1 + (2\pi^2 \rho r)^{-1} \int Q[S(Q) - 1] \sin Qr \, dQ \quad ,$$

namely,

$$S(Q) = n_s S_s(Q) + n_n S_n(Q) \tag{2}$$

and

$$g(r) = n_s g_s(r) + n_n g_n(r) \quad . \tag{3}$$

The temperature dependence of the quantities $S_s(Q, \omega)$ and $S_n(Q, \omega)$ in (1) (see Ref. 1 for details) essentially disappears when one integrates over ω to obtain (2). The quantities $S_s(Q)$ and $g_s(r)$ may thus be simply interpreted as the values of $S(Q)$ and $g(r)$ at very low temperatures, where $n_s = 1$ and $n_n = 0$. (In practice, $T = 1$ K, where $n_s = 0.993$, is sufficiently low.) Similarly, $S_n(Q)$ and $g_n(r)$ are the values of $S(Q)$ and $g(r)$ at a temperature T^* just above T_λ, where $n_s = 0$ and $n_n = 1$. (As in Ref. 1, we will use $T^* = 2.27$ K.)

Recent high-accuracy neutron-diffraction results[6] for $S(Q)$ and $g(r)$ allow a detailed test of the temperature variations predicted by (2) and (3), and this is shown in Fig. 1 for a selected set of Q and r values. We see that the agreement between the solid curves given by (2) and (3) and the experimental values[6] is generally very good.[10] This good agreement is further strong evidence that (1) is essentially correct. In calculating the solid curves we have used the n_s values of Maynard[11] supplemented at temperatures less than 1.2 K by the values of Brooks and Donnelly.[12] The relationship (2) does not work very well in the hydrodynamic limit ($Q \rightarrow 0$), and this is expected from the work of Griffin,[4] but it is seen
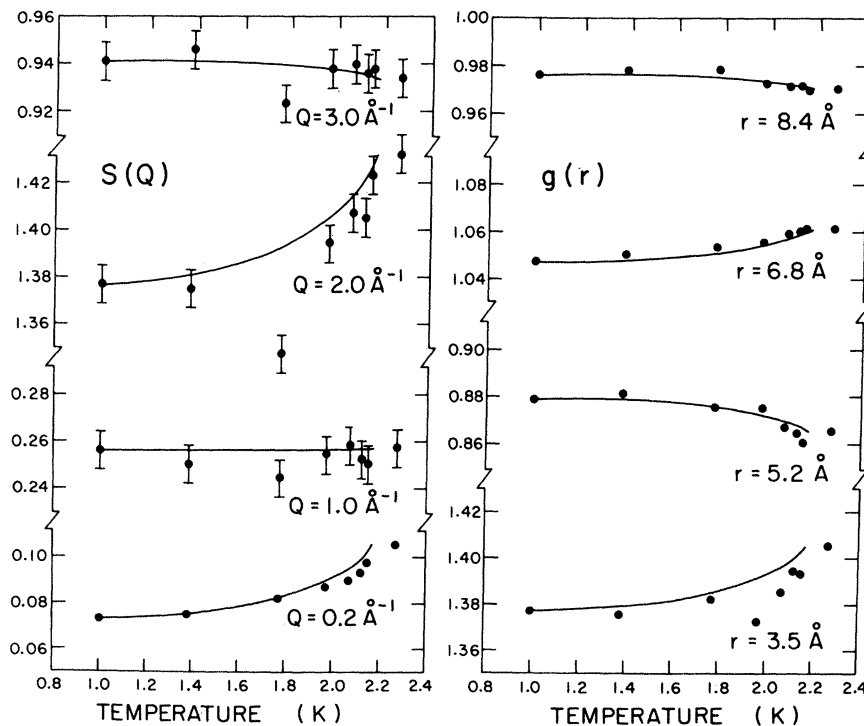

FIG. 1. Comparison between the experimental values (Ref. 6) of $S(Q)$ and $g(r)$ for liquid ^{4}He and the values (solid curves) calculated from Eqs. (2) and (3) using the n_s values of Refs. 11 and 12.

(Fig. 1) to give a good description for Q as small as 0.2 Å^{-1}. Note that (2) and (3) are both correct in the large-argument limits where $S(Q) = 1$ and $g(r) = 1$, and that (3) is also correct at small r since $g(r) = 0$ for $r \lesssim 2$ Å.

One now has the possibility of combining any known relationship between $g(r)$ and the condensate fraction n_0 with (3) to obtain an explicit relationship between n_s and n_0. About ten years ago, Hyland et al.[8] in fact proposed that

$$g(r) - 1 = (1 - n_0)^2 [g_n(r) - 1] \ . \tag{4}$$

This relationship has recently been used[13,14] together with the results of Ref. 6 to obtain values of n_0 for seven temperatures in the range $1.00 \le T \le 2.15$ K. These studies[13,14] give an extrapolated value of n_0 at $T = 0$ in good agreement with the best theoretical estimates, and, further, show that the behavior of $g(r)$ as a function T which is implied by (4) is, at least for $r \gtrsim 6$ Å, very well borne out by experiment. (See Refs. 13 and 14 for details.) By applying (4) to new x-ray-diffraction results for $g(r)$, Robkoff et al.[15] have also obtained a value of n_0 for liquid helium at 1.67 K and saturated vapor pressure which is in excellent agreement with the values in Refs. 13 and 14.

The above is strong experimental support for (4), but it is not proof of its validity. Strictly speaking, what is found[14] is that the experimental results[6] for $g(r)$ are very well described by the relationship

$$g(r) - 1 = f(T)[g_n(r) - 1] \ , \tag{5}$$

where, for $r \gtrsim 6$ Å, $f(T)$ is, to within the experimental uncertainty, independent of r and decreases monotonically with decreasing T from the value 1.002 ± 0.038 at 2.15 K to the value 0.762 ± 0.035 at 1.00 K. The quantity $g(r) - 1$, which is a measure of the spatial correlations of the atoms, is thus observed to decrease monotonically with decreasing temperature in the superfluid phase whereas it increases monotonically[6,14] with decreasing temperature in the normal phase. This continuous weakening of the spatial correlations as the temperature is lowered in the superfluid phase is believed[8] to be a direct consequence of the condensation into the zero-momentum state. Such an interpretation seems plausible since the "condensate atoms," being completely delocalized because of the Heisenberg uncertainty principle, might be expected not to contribute to the spatial correlations at large r. If this is indeed true, and if we regard $g_n(r)$ as the pair-correlation function for the "uncondensed atoms," then $f(T)$ should simply be the probability that a pair of atoms are not in the condensate, i.e.,

$$f(T) = [1 - n_0(T)]^2 \ . \tag{6}$$

Guided by the experimental observations, one is thus led to (4). We offer this simple physical in-

terpretation because the theoretical justification of (4) given in Ref. 8 is not very convincing and has recently been criticized.[16] In particular, in their derivation, Hyland et al.[8] completely ignore the role of anomalous correlation functions which are known to be of crucial importance in condensed Bose systems. In spite of this criticism, (4) may still be correct for reasons other than those given in Ref. 8.

A very recent study[17] has in fact given support for (4). In this study, values of n_0 for 1.00, 1.10, and 2.12 K have been obtained directly from the momentum distributions for the ^4He atoms deduced from neutron inelastic scattering measurements of the dynamic structure factor $S(Q, \omega)$ at large values of Q. This is a completely different method from that of Hyland et al.,[8] and it has a much more rigorous theoretical foundation.[18] The fact that the new values of n_0 are in very good agreement with those obtained[13,14] by application of (4) is independent evidence that (4) is a good approximation.

The empirical relationship (5) can be combined with (3) to give

$$n_s(T) = \frac{1 - f(T)}{1 - f(0)} \ . \tag{7}$$

To the extent that (6) is valid, we then find that

$$n_s(T) = \frac{n_0(T)[2 - n_0(T)]}{n_0(0)[2 - n_0(0)]} \ . \tag{8}$$

We thus have obtained an explicit relationship between n_s and n_0 for all temperatures in the superfluid phase.

An important implication of (8) is that n_s and n_0 have the same critical exponent as $T \to T_\lambda$. Josephson[19] has shown that, in the critical region near T_λ, $n_0 \propto (T_\lambda - T)^{2\beta}$ and $n_s \propto (T_\lambda - T)^{2\beta - \eta \nu'}$. Hence, if (8) is correct in this limit, $\eta \nu' = 0$. The exponent ν' is known[20] to be approximately 0.67, but η is indeed believed[20,21] to be very small, perhaps 0.03 to 0.04. Equation (8) also predicts that n_s and n_0 will have the same temperature dependence in the limit $T \to 0$ which is not correct since it is known that, as $T \to 0$, n_0 varies[22] as $1 - AT^2$ whereas n_s varies[23] as $1 - BT^4$. This shortcoming is not surprising since, as we have noted above, the relation (1) [on which (3), and hence (8), is based] may well not be correct in the phonon-dominated region ($T \lesssim 0.6$ K). In this region, however, the variations of n_s and n_0 are negligibly small and hence this limitation is of little importance.

A very important advantage of knowing the relationship between n_s and n_0 is that it would open a new possibility for an accurate determination of the temperature dependence of n_0. Experimental determinations[13-15,17] of n_0 are very difficult and time consuming and it may never be possible to determine n_0 directly with high precision at a great many tempera-

tures, particularly at temperatures near T_λ where n_0 is very small. On the other hand, n_s can be determined very precisely[11,24] over the entire temperature range, and the recent studies[13-15,17] give considerable hope that reasonably accurate values of n_0 can be determined at at least a few relatively low temperatures. These values could then be combined with the precise $n_s(T)$ values to give, via (8) or an improved relationship, accurate values of n_0 for all temperatures.

In this paper we have shown that the decompositions, (2) and (3), of $S(Q)$ and $g(r)$ into superfluid and normal-fluid components with weights n_s and n_n are very well borne out by experiment. This is additional strong evidence that the original decomposition of $S(Q,\omega)$ into such components proposed by Woods and Svensson[1] is indeed a good approximation. This decomposition has also been supported by the recent calculations of Griffin[4] and Griffin and Talbot[5] who have argued that forms such as (1), and hence (2) and (3), arise naturally as a direct consequence of the existence of a Bose condensate in an interacting system.

It is also worth noting that (2) and (3) can be rewritten

$$S(Q) - S_s(Q) = n_n[S_n(Q) - S_s(Q)]$$

and

$$g(r) - g_s(r) = n_n[g_n(r) - g_s(r)] \ .$$

These forms emphasize the fact that the changes in $S(Q)$ and $g(r)$ as we increase the temperature are proportional to the normal-fluid fraction, which in turn is proportional to the number of thermally excited rotons for $T \geq 1$ K. In fact, Reatto and co-workers[25,26] have proposed that the anomalous temperature dependences of $S(Q)$ and $g(r)$ for superfluid ^{4}He are a direct consequence of the thermal excitation of rotons. Their calculations, which are based on a finite-temperature generalization of the well-known zero-temperature Feynman variational calculation of $S(Q)$, give reasonably good agreement with the observed[6] variations of $S(Q)$ (see Ref. 26 and also Fig. 17 of Ref. 6). The precise connection between this approach and the microscopic theory of a Bose-condensed system used by Griffin[4] and by Griffin and Talbot[5] is not clear at present.

The existence of (3) gives rise to a new possibility of obtaining an explicit relationship between the condensate fraction and the superfluid fraction, and we have proposed a tentative relationship, (8), based on (4). While (4) does not at present have a rigorous theoretical foundation, it is found[13,14] to be consistent with the existing experimental data, and it has a simple physical interpretation. It is also supported by the fact that the values of n_0 obtained[17] in a very recent study based on a different method agree very well with those obtained[13,14] by application of (4).

To the extent that we take (3) as being correct, our relationship (8) is equivalent to the ansatz (4) of Hyland et al.[8] Our new relationship (3) has thus enabled us to replace the postulated[8] relationship (4) between n_0 and $g(r)$ by a relationship (8) between n_0 and n_s. It is hoped that future theoretical work will be able to give directly the explicit relationship between n_0 and n_s.

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