Extraction of the condensate fraction from the momentum distribution in superfluid ^{4}He

A. Griffin
Department of Physics and Scarborough College, University of Toronto, Toronto, Ontario, Canada M5S 1A7
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High-momentum neutron scattering data can be used to find the momentum distribution $n(\mathbf{p})$ of atoms in superfluid ^{4}He. The analysis of these data is complicated because the momentum distribution of the noncondensate atoms has an anomalous contribution which depends on the presence of the Bose condensate. We discuss a new way of estimating this contribution and show that the resulting values of the condensate fraction $n_0(T)$ are quite different from those given in the recent literature.

By using high-momentum neutron scattering where the impulse approximation is adequate, one can find the momentum distribution $n(\mathbf{p})$ of the atoms in liquid ^{4}He. Following Sears, Svensson, Martel, and Woods,[1] this can be written in the form

$$n(\mathbf{p})=n_0\delta(\mathbf{p})+(1-n_0)n^*(\mathbf{p},\,T) \;, \tag{1}$$

where $n^*(\mathbf{p})$ is the momentum distribution of the noncondensate atoms (normalized to unity). Of course, the experimental values of $n(\mathbf{p})$ are broadened by instrumental resolution and final-state effects. Experimentally, it is found that $n^*(\mathbf{p},T)$ is not very temperature dependent for $T>T_\lambda$. Theoretically, however, it is known that in the superfluid phase $n^*(\mathbf{p},T)$ has an anomalous contribution which is condensate induced. In particular, one has[2,3]

$$n^*(\mathbf{p},T=0\text{ K})\sim\frac{n_0mc}{2(2\pi)^3\hbar\rho}\frac{1}{p}\text{ as }p\to 0 \;, \tag{2}$$

where c is the sound velocity and ρ is the density. Taking these facts into account, Sears *et al.* introduced the useful decomposition

$$\tilde{n}(T)n^*(\mathbf{p},\,T)=\tilde{n}(T)n^*(\mathbf{p},T_\lambda)+\delta n^*(\mathbf{p},T) \;, \tag{3}$$

where $\delta n^*(\mathbf{p},T)$ is the condensate-dependent part of $n^*(\mathbf{p},T)$ and $\tilde{n}(T)\equiv 1-n_0(T)$ is the fraction of noncondensate atoms at temperature T. Using this ansatz and assuming that the broadened condensate peak extends to p_c, Sears *et al.* found that

$$n_0=\frac{\epsilon}{1-\beta+\gamma} \;, \tag{4}$$

with

$$\epsilon=\int_0^{p_c}dp\,4\pi p^2[n(\mathbf{p},T)-n^*(\mathbf{p},T_\lambda)] \;, \tag{5}$$

$$\beta=\int_0^{p_c}dp\,4\pi p^2\,n^*(\mathbf{p},T_\lambda) \;, \tag{6}$$

$$n_0(T)\gamma=\int_0^{p_c}dp4\pi p^2\delta n^*(\mathbf{p},T) \;. \tag{7}$$

Here it is assumed that $\delta n^*(\mathbf{p},T)$ is proportional to the condensate fraction $n_0(T)$ [this assumption is consistent with (2) and will be discussed at length later in this paper]. While ϵ and β can be obtained directly from experiment, γ requires some theoretical expression for $\delta n^*(\mathbf{p},T)$. All these quantities depend on the cutoff momentum p_c, which was ~ 1.2 Å^{-1} in Ref. 1.

Sears *et al.*[1] first emphasized the importance of including the effect of $\delta n^*(\mathbf{p},T)$ [i.e., the γ term in (4)] if one was to extract a reliable estimate of the condensate fraction. They obtained a simple expression for γ based on

$$\delta n^*(\mathbf{p},T)=\frac{n_0mk_BT}{(2\pi)^3\hbar^2\rho n_s}\frac{1}{p^2}+\frac{n_0mc}{2(2\pi)^3\hbar\rho}\frac{1}{p}, \tag{8}$$

where $n_s(T)$ is the superfluid fraction. The cutoff in (7) was defined as the value p_0, where the two terms in (8) are of equal magnitude. This cutoff is found to be $2k_BT/\hbar cn_s(T)$. It is very small (~ 0.2 Å^{-1}) at $T=1$ K, but increases rapidly with temperature. At $T=2.1$ K, one has $p_0\sim 1$ Å^{-1} and hence $\gamma\sim 3$. However, as discussed elsewhere,[2] the expression in (8) is incorrect. In particular, the first term is only valid for $cp\leqslant k_BT/\hbar$, while the second term is only valid for $cp\geqslant k_BT/\hbar$.

In the present note, we attempt to put the approach used in Ref. 1 to calculate γ on a firmer footing. With our new procedure, however, we find a value of γ which is quite substantial, even at low temperatures. This leads to revised values of $n_0(T)$ which are quite different from those of Ref. 1. The main conclusion of this paper is not in our specific numerical results for $n_0(T)$. Rather, it is that until one has a good estimate of γ, one *cannot* extract meaningful estimates of $n_0(T)$ from the momentum distribution. In future work, it is the determination of $\delta n^*(\mathbf{p},T)$ which should be emphasized. In this regard, we believe the unusual exponential tail[4,5] which $n(\mathbf{p},T=1\text{ K})$ exhibits in the high-momentum region $p\geqslant 1.5$ Å^{-1} is of special interest, since it is probably associated with the existence of the condensate. It would be worthwhile to study the temperature dependence of the exponential tail—it may be a more direct way of measuring $n_0(T)$.

To begin, we note that a decomposition such as in (3) seems quite reasonable in terms of our current ideas about the nature of the elementary excitations in superfluid ^{4}He in conjunction with the role of the condensate broken symmetry. We recall that (see, for example, Ref. 2)

$$(1-n_0)n^*(\mathbf{p},T)=\int_0^\infty\frac{d\omega}{2\pi}A(\mathbf{p},\omega)[2N^0(\omega)+1] \;, \tag{9}$$

where $A(\mathbf{p},\omega)$ is the single-particle spectral density and $N^0(\omega)$ is the Bose distribution. In a liquid such as ^{4}He, one expects to find a well-defined collisionless density oscillation (essentially a zero-sound–type mode in the noncondensate atoms).[6,7] Since the condensate fraction is always less than

$\sim 10\%$, the frequency ω_p of this mode will not be much different below the superfluid transition from what it is above (this is consistent with experimental data). However, a crucial difference below T_λ is that this zero-sound mode has finite weight in $A(\mathbf{p},\omega)$ due to the effect of the broken symmetry.[7] Thus, we expect $A(\mathbf{p},\omega)$ to be given by

$$A(\mathbf{p},\omega)=2\pi z(\mathbf{p},n_0)\delta(\omega-\omega_p)+A_{inc}(\mathbf{p},\omega;\tilde{n}) \ . \tag{10}$$

Here $z(\mathbf{p},n_0)$ is some weight function which vanishes with n_0, while $A_{inc}(\mathbf{p},\omega)$ is a broad (nonresonant) spectrum which describes the damped single-particle excitations which arise in any liquid. Since the condensate fraction is so small, we do not expect $A_{inc}(\mathbf{p},\omega)$ to be very much different above and below T_λ, although it will clearly depend on the relative number of noncondensate atoms $\tilde{n}$.

Using (10) in (9), we have

$$\tilde{n}(T)n^*(\mathbf{p},T)=z(\mathbf{p},n_0(T))[2N^0(\omega_p)+1] + \int_0^\infty \frac{d\omega}{2\pi}A_{inc}(\mathbf{p},\omega;\tilde{n})[2N^0(\omega)+1] \ . \tag{11}$$

Above T_λ, only the second term is present. Since experimentally $n^*(\mathbf{p},T>T_\lambda)$ is only weakly temperature dependent[1] up to 4 K, we conclude that $A_{inc}(\mathbf{p},\omega)$ is dominated by frequencies $\hbar\omega >> 4$ K and we can limit ourselves to the zero-point contribution in the second term. We are thus led to the following microscopic identification of the terms in (3):

$$n^*(\mathbf{p},T_\lambda)=\frac{1}{\tilde{n}}\int_0^\infty \frac{d\omega}{2\pi}A_{inc}(\mathbf{p},\omega;\tilde{n}) \ , \tag{12}$$

$$\delta n^*(\mathbf{p},T)=z(\mathbf{p},n_0(T))[2N^0(\omega_p)+1] \ . \tag{13}$$

At $T=0$ K, Gavoret and Nozières[3] have made a direct calculation of $A(\mathbf{p},\omega)$ for small $\mathbf{p}$ and ω, obtaining the result (10) with $\omega_p=cp$ and

$$z(\mathbf{p},n_0(0))=\frac{n_0 mc}{2(2\pi)^3\hbar\rho}\frac{1}{p} \ . \tag{14}$$

We shall make the key *assumption* that this expression is equally valid at *finite* temperatures in the collisionless region defined by $cp \geqslant k_BT/\hbar$, except that now the condensate fraction depends on the temperature of interest. It is, of course, *not* correct in the hydrodynamic region[2,8] $cp \leqslant k_BT/\hbar$. However, we are ultimately interested in calculating γ in (7), and the dominant contribution to the momentum integral will come from the region $p \geqslant k_BT/\hbar c$ (we recall that at $T \sim 2$ K, $k_BT/\hbar c \sim 0.1$ Å^{-1}). Thus, it is sufficient to limit ourselves to the zero-point contribution and hence we use the approximation

$$n_0\gamma=\int_0^{p_c} dp\, 4\pi p^2 z(\mathbf{p},n_0(T)) \ . \tag{15}$$

This gives

$$\gamma=\frac{mc}{8\pi^2\hbar\rho}p_0^2=0.85[p_0(\text{Å}^{-1})]^2 \ , \tag{16}$$

as the contribution for wave vectors up to p_0. Assuming that (14) is probably valid in the phonon region where $\omega_p=cp$, we estimate $p_0 \sim 0.7$ Å^{-1}, which gives $\gamma \simeq 0.42$. Unfortunately, this estimate leaves out the contributions from higher momentum (between 0.7 and 1.2 Å^{-1}), where we have no justification in using (14). However, we emphasize that even at $T=0$ K, this estimate says that $\gamma \geqslant 0.4$. The reason that the value of γ obtained in Ref. 1 was so small at $T=1$ K was that the cutoff used in (7) was based on the incorrect expression (8), which led to a value $p_0 \sim 0.2$ Å^{-1}.

A very physical way of understanding (14) is based on relating phase fluctuations of the order parameter and density fluctuations.[9] Assuming that the latter have a frequency ω_p, one is led to a more general version of (14), namely,

$$\delta n^*(\mathbf{p},T)=\frac{n_0(T)m\omega_p}{2(2\pi)^3\hbar\rho}\frac{1}{p^2}=n_0(T)B(\mathbf{p}) \ . \tag{17}$$

This gives a simple way of including the contribution to γ from the region where the excitations are no longer given by $\omega_p=cp$. Using the experimental values of the phonon-maxon-roton dispersion relation, we have calculated

$$\gamma=\int_0^{p_c} dp\, 4\pi p^2 B(\mathbf{p}) \ . \tag{18}$$

Our results are shown in Fig. 1. Of course, it should be emphasized that the dominant contribution to γ is coming from the larger values of p, where the validity of (14) and (17) has *not* been proven. On the other hand, our calculation is based on a reasonable extrapolation of what we know about Bose-condensed liquids and is probably about the best we can do at the present time. Thus, it would seem that γ is substantial (in the general range 0.5–1.0). As shown in Table I, our result for $n_0(T)$ is considerably smaller at low temperatures and considerably larger at high temperatures, relative to those obtained in Ref. 1. With regard to our small result for n_0 at 1 K, we recall that the best Monte Carlo calculations[5,10] give $n_0=0.09$ at $T=0$ K.

Mook[11] has also carried out measurements of the momentum distribution which he analyzed using (4). Due to better resolution, Mook's values for p_c were considerably smaller than in Ref. 1. In Table I, we reanalyze his data using the appropriate $\gamma(p_c)$ in Fig. 1. The values of $n_0(T)$ we obtain are in good agreement with those based on the data in Ref. 1.

We briefly mention a completely different approach to the calculation of $\delta n^*(\mathbf{p},T)$, which we have found gives results

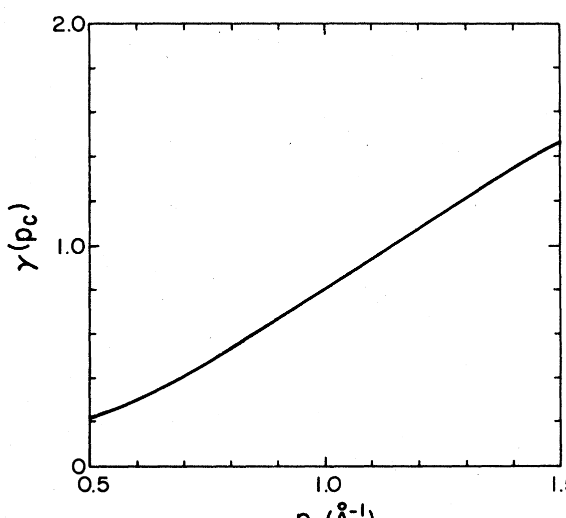

FIG. 1. Plot of $\gamma(p_c)$ in (7) as a function of the cutoff momentum p_c. These results are based on the generalized Gavoret-Nozières expression in (17).

TABLE I. The condensate fraction $n_0(T)$ as given by (4) using the results in Fig. 1 and the data in Refs. 1 and 11.

Ref.	T (K)	p_c (Å^{-1})	ϵ	β	γ	n_0 (T)
1	1.0	1.3	0.079	0.49	1.21	0.046
1	2.12	1.1	0.029	0.36	0.96	0.018
11	0.47	0.90	0.077	0.28	0.66	0.056
11	1.50	0.89	0.076	0.27	0.66	0.055
11	2.12	0.62	0.020	0.13	0.33	0.017

roughly similar to those based on the generalized Gavoret-Nozières expression (17). We assume that

$$\delta n^*(\mathbf{p},T) = z(\mathbf{p},n_0(T)) = n_0(T)B(\mathbf{p}) \ , \quad (19)$$

where the function $B(\mathbf{p})$ is taken to be temperature independent. This is a reasonable generalization of (14), but at the present time must be viewed as an assumption. Making use of (19) in (3), we have, at $T=0$ K,

$$\tilde{n}(0)n^*(\mathbf{p},\ T=0\ \text{K}) = \tilde{n}(0)n^*(\mathbf{p},T_\lambda) + n_0(0)B(\mathbf{p}) \ ,$$

or

$$B(p) = \frac{\tilde{n}(0)}{n_0(0)}[n^*(\mathbf{p},\ T=0\ \text{K}) - n^*(\mathbf{p},T_\lambda)] \ . \quad (20)$$

This is a useful expression since $n^*(\mathbf{p},\ T=0\ \text{K})$ is known from computer calculations.[5,10,12,13] For $n^*(\mathbf{p},T_\lambda)$, we argue that this momentum distribution is expected to be a Gaussian[4,14,15] with a width which can be related to the average kinetic energy K_0,

$$n(\mathbf{p},T_\lambda) = \left(\frac{3}{2\pi}\right)^{3/2} \frac{1}{\bar{p}^3} e^{-3p^2/2\bar{p}^2} \ , \quad (21)$$

where $K_0 = \hbar^2\bar{p}^2/2m$. Taking into account that the average kinetic energy is only slightly temperature dependent in liquid ^{4}He,[16] one can use the value $K_0 = 14.5$ K obtained from computer calculations at $T=0$ K.[5,10] With this procedure, we have found that the results for $4\pi p^2 B(p)$ predicted by (17) and (20) are in rough agreement up to $p \sim 1.3$ Å^{-1}. This gives a separate piece of evidence that our estimate of $\gamma(p_c)$ in Fig. 1 is reasonable.

Other experimental methods have given much larger values of $n_0(T)$ at low temperatures,[17] but the microscopic basis of these methods is weak. In assessing our results, we emphasize that (14) has only been proven[2,3] to be correct for small p and *may* be absent at larger momentum. If anything, the generalized form (17) underestimates the falloff of $\delta n^*(\mathbf{p},T)$ at larger values of p. Thus, our estimate of $\gamma(p_c)$ in Fig. 1 is probably too large and the correct values of n_0 should be somewhat larger than those given in Table I. Broadening of $\delta n^*(\mathbf{p},T)$ due to resolution and final-state effects does not alter γ very much. Furthermore, neutron scattering experiments with better resolution and at larger momentum transfers are of high priority, since then one could carry out the analysis based on (4) with a much smaller value of p_c. On the theoretical side, what is really needed are direct computer calculations of $n^*(\mathbf{p},T)$ and $n_0(T)$ as a function of the temperature.[18]

Recently, neutron scattering has been used to obtain $n(\mathbf{p},T)$ in liquid ^{4}He under a variety of pressures.[15] However, it would seem difficult to incorporate the effect of $\delta n^*(\mathbf{p},T)$ in the simple method of data analysis used by Sokol, Simmons, Price, and Hilleke based on Gaussians.

In conclusion, we call attention to the interesting exponential tail[4,5] which $n(\mathbf{p})$ exhibits for $p \gtrsim 1.5$ Å^{-1}, at least at low temperatures. We suggest that the difference between the Gaussian and exponential tail should be identified with $\delta n^*(\mathbf{p},T)$ in the large-momentum region and hence should be proportional to $n_0(T)$ if our ansatz (19) is still correct in this region. In this large-p region, $n(\mathbf{p})$ is extremely small, so that this region makes a negligible contribution to the momentum integrals in (5)–(7). However, a careful study of the temperature dependence of this high-p exponential tail might be a separate way of confirming the ansatz (19) as well as measuring $n_0(T)$ without all the complications which occur at small p. Further experimental work on this topic seems highly desirable.

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