Momentum Distribution in Liquid ^{4}He at $T = 1.1$ and 4.2 K

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A new analysis of neutron-scattering results for liquid ^{4}He, which reduces the effects of interference and final-state interactions, yields model-independent results for the momentum distribution function, $n(\vec{p})$. At $T=4.2$ K, $n(\vec{p})$ is found to be Gaussian but at $T=1.1$ K it has an exponential tail at large p and is enhanced near $p=0$. An analysis of the temperature change in $n(\vec{p})$ gives a value of $(6.9\pm 0.8)\%$ for the condensate fraction at $T=1.1$ K.

It is generally believed that the unique properties of superfluid ^{4}He arise from the macroscopic occupation of the zero-momentum state. Theoretical calculations[1-6] suggest that at $T=0$ the fraction of atoms in the zero-momentum state, n_0, is approximately 10%. In recent years there has been considerable interest in attempting to obtain n_0 experimentally from neutron-scattering results at large momentum transfer, $\hbar Q$. This method[7] is based on the fact that in the large-Q limit, where the impulse approximation is asymptotically exact, the dynamic structure factor, $S(Q,\omega)$, is the Doppler spectrum characteristic of the momentum distribution,[8] $n(\vec{p})$, of the atoms in the initial state. These quantities are related by the expression

$$p n(\vec{p}) = \lim_{Q\to\infty} -\frac{1}{2\pi}\left(\frac{\hbar Q}{m}\right)^2 \frac{\partial}{\partial\omega} S(Q,\omega), \quad (1)$$

in which m is the atomic mass, $p=(m/\hbar Q)(\omega-\omega_r)$, and $\hbar\omega_r \equiv (\hbar Q)^2/2m$ is the recoil energy.

For any finite value of Q, $S(Q,\omega)$ and the corresponding $n(\vec{p})$ are to some extent distorted by final-state interactions and interference effects which are neglected in the impulse approximation and which vanish only asymptotically in the limit $Q\to\infty$. In addition, the experimentally determined $S(Q,\omega)$ is broadened by effects of finite instrumental resolution.

The effect of final-state interactions can be reduced considerably[9] by symmetrizing $S(Q,\omega)$ about ω_r before computing $n(\vec{p})$. This procedure is based on the fact that final-state-interaction effects are of order Q^{-1} in $S(Q,\omega)$ but are only of order Q^{-2} in the symmetrized $S(Q,\omega)$. In the present work, the magnitude of the residual final-state interactions in the symmetrized $S(Q,\omega)$ is estimated as in Ref. 9 to be about 4%. The distortion of the experimentally determined $n(\vec{p})$ by interference effects in $S(Q,\omega)$ can be minimized by averaging the $n(\vec{p})$ results over a suitable range of Q values as discussed below.

The resolution-broadened dynamic structure factor is given approximately by

$$S_R(Q,\omega) = \int_{-\infty}^{\infty} R(\omega-\omega')S(Q,\omega')\,d\omega', \quad (2)$$

where $R(\omega)$ denotes the normalized instrumental resolution function. Hence, if $n(\vec{p})$ is of the form

$$n(\vec{p}) = n_0\delta(\vec{p}) + n'(\vec{p}), \quad (3)$$

where n_0 is the condensate fraction and $n'(\vec{p})$ the contribution from the uncondensed atoms, the corresponding resolution-broadened quantity is

$$n_R(\vec{p}) = n_0\Delta(\vec{p}) + n_R'(\vec{p}), \quad (4)$$

where

$$\Delta(\vec{p}) = -(2\pi p)^{-1}\,dR(p)/dp, \quad (5)$$

and

$$n_R'(\vec{p}) = \int_{-\infty}^{\infty} (p'/p) R(p-p') n'(\vec{p}')\,dp', \quad (6)$$

in which $R(p)dp \equiv R(\omega)d\omega$. It can be shown that $\int \Delta(\vec{p})d^3p = 1$.

In this Letter we present the results of a new analysis of previously reported measurements[10] of the neutron scattering from liquid ^{4}He at $T=1.1$ and 4.2 K. The measurements were performed with a triple-axis crystal spectrometer operated in the constant-Q mode with a fixed scattered-neutron energy. The data used were taken at two different sets of resolution conditions[11] with $40 \leqslant Q \leqslant 80$ nm^{-1}. The neutron data were analyzed with the help of the moment theorems, as described previously,[12] to obtain normalized, resolution-broadened $S(Q,\omega)$ distributions. Each of these was then smoothed, symmetrized about ω_r, and differentiated numerically to obtain the corresponding resolution-broadened $n(\vec{p})$ distribution from Eq. (1). These $n(\vec{p})$ distributions[13] were then averaged so as to minimize the distortion

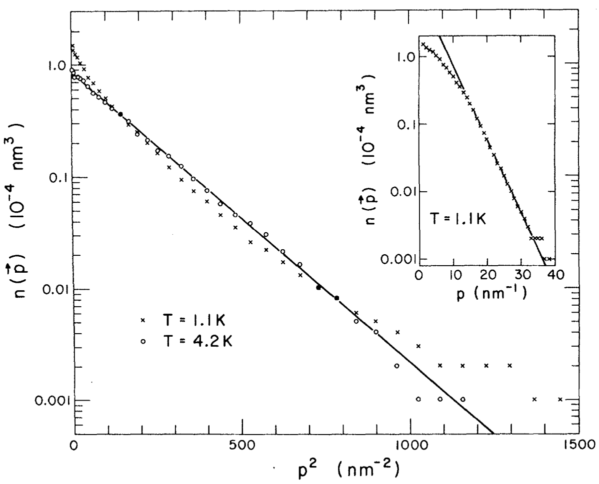

FIG. 1. The momentum distribution in liquid ^{4}He at $T=1.1$ and 4.2 K as a function of p^2 and (inset) at $T=1.1$ K as a function of p. These results were obtained as described in the text from nine scattered-neutron distributions (Ref. 10) in the range $60 \leq Q \leq 80$ nm^{-1}.

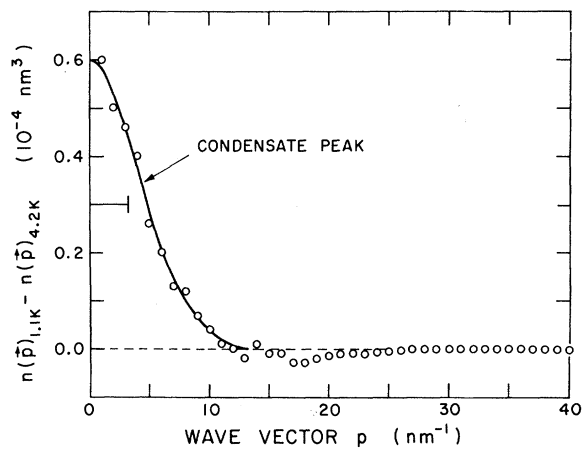

FIG. 2. Temperature change in the momentum distribution in liquid ^{4}He between 4.2 and 1.1 K. The horizontal line indicates the resolution width.

due to interference effects and to improve the statistical accuracy of the final results.

Figure 1 shows the results for $n(\vec{p})$ at $T=1.1$ and 4.2 K obtained from an average of nine distributions in the range $60 \leq Q \leq 80$ nm^{-1}. The validity of the averaging procedure is confirmed by the fact that the results are changed by less than 5% if we average, instead, over 16 distributions in the range $40 \leq Q \leq 80$ nm^{-1}. We employ the 60 to 80 nm^{-1} averages because they are less sensitive to interference effects and have slightly better resolution. It is seen that at $T=4.2$ K $n(\vec{p})$ is Gaussian so that p_x, p_y, and p_z are statistically independent.[14] When the temperature is reduced to 1.1 K, $n(\vec{p})$ becomes enhanced at both small and large p and depressed at intermediate p. It is evident from the inset part of Fig. 1 that when $p \gtrsim 15$ nm^{-1}, $n(\vec{p})$ is exponential rather than Gaussian.

The enhancement in $n(\vec{p})$ at small p is shown more explicitly in Fig. 2 where it is seen to consist of a peak centered at $p=0$ with a width which is slightly greater than the instrumental width. We interpret this as the condensate peak whose relatively small intrinsic width reflects the effect of residual final-state interactions. Assuming that $n_0=0$ at 4.2 K, we find from the integrated intensity of the condensate peak that $n_0=(6.9\pm0.8)\%$ at $T=1.1$ K. The value of n_0 at $T=0$ is probably somewhat larger. For example, if we were to assume that n_0 scales with temperature in the same way as in an ideal Bose-Einstein gas,[15] we would find that $n_0=(10.8\pm1.3)\%$ at $T=0$ which is in good agreement with theoretical values,[1-6] based on variational ground-state wave functions, which range from 8% to 13%.

The procedure we have used to obtain n_0 is based on the tacit assumption that $n'(\vec{p})$ is regular at $p=0$. In fact, in an ideal Bose-Einstein gas below the λ point[15] $n'(\vec{p})$ has a p^{-2} singularity at $p=0$ and an approximate calculation[16] indicates that this is also true in liquid ^{4}He. Although such a singularity will tend to be softened when effects of finite instrumental resolution are taken into account, it may still lead to a small enhancement[17] of the apparent value of n_0.

It is worth remarking that the basic effect on which our estimate of n_0 is based is already evident in the raw neutron data.[10] In particular, the slope of $S(Q,\omega)$ near the peak is larger at $T=1.1$ K than at $T=4.2$ K so that, near $p=0$, $n(\vec{p})$ is likewise larger at $T=1.1$ K.

The average kinetic energy per atom is found from the $n(\vec{p})$ distributions to have the value 13.2 K at $T=1.1$ K and the value 13.6 K at $T=4.2$ K. These values have been corrected for effects of finite instrumental resolution and are in agreement with results obtained from a recent analysis[18] of the frequency moments of $S(Q,\omega)$.

Figure 3 shows a comparison of our results at $T=1.1$ K (circles) with previously determined results for[9] $Q=100$ nm^{-1} and[19] $Q=150$ nm^{-1}. We believe the discrepancies are primarily due to interference effects which distort the apparent

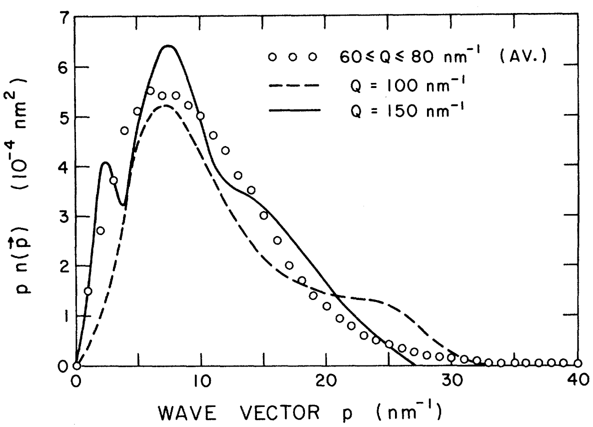

FIG. 3. Comparison of the present Q-averaged results (circles) at $T=1.1$ K with those of Ref. 9 (dashed curve) and Ref. 19 (solid curve).

$n(\vec{p})$ distributions when determined from experiments at a single value of Q and which are minimized when the appropriate Q averaging is performed. Such distortions may also account for the non-Gaussian $n(\vec{p})$ results which were obtained at $T=4.2$ K in earlier work.[7,19,20] The feature at $p\simeq 2$ nm^{-1} in the $Q=150$ nm^{-1} distribution in Fig. 3 was interpreted in Ref. 19 as the resolution-broadened condensate peak and a value $n_0=(1.8\pm 1.0)\%$ was obtained. This feature is not present in our Q-averaged distribution. Further experiments may help resolve this discrepancy.

In conclusion, we have shown that smooth, precise, and, we believe, accurate $n(\vec{p})$ distributions can be obtained from neutron-scattering experiments at moderately large Q values provided the results are suitably corrected for final-state interactions and interference effects. Figure 2 suggests that the absence of a clearly resolved condensate peak in $n(\vec{p})$ itself below the λ point may be due more to inadequate instrumental resolution than to residual final-state interactions. We hope to clarify this point in future experiments aimed at studying the temperature dependence of n_0.

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[1]O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

[2]W. L. McMillan, Phys. Rev. 138, A442 (1965).

[3]D. Schiff and L. Verlet, Phys. Rev. 160, 208 (1967).

[4]W. P. Francis, G. V. Chester, and L. Reatto, Phys. Rev. A 1, 86 (1970).

[5]M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A 9, 2178 (1974).

[6]M. L. Ristig, P. M. Lam, and J. W. Clark, Phys. Lett. 55A, 101 (1975); P. M. Lam and C. C. Chang, Phys. Lett. 59A, 356 (1976); P. M. Lam, J. W. Clark, and M. L. Ristig, Phys. Rev. B 16, 222 (1977).

[7]This method has been reviewed by H. W. Jackson, Phys. Rev. A 10, 278 (1974).

[8]More precisely, $\vec{p}$ denotes the wave vector of a ^{4}He atom so that the momentum is actually $\hbar\vec{p}$. The distribution function $n(\vec{p})$ is normalized such that $\int n(\vec{p})\,d^3p=1$.

[9]P. Martel, E. C. Svensson, A. D. B. Woods, V. F. Sears, and R. A. Cowley, J. Low Temp. Phys. 23, 285 (1976).

[10]R. A. Cowley and A. D. B. Woods, Can. J. Phys. 49, 177 (1971).

[11]The data used are designated in Table II of Ref. 10 as having analyzer angles of 40° and 36°.

[12]E. C. Svensson, P. Martel, V. F. Sears, and A. D. B. Woods, Can. J. Phys. 54, 2178 (1976).

[13]In what follows we shall, for simplicity, omit the subscript R since it is clear from the context whether or not we are referring to resolution-broadened momentum distributions. The full width at half-maximum of the resolution function $R(p)$ is 6.3 ± 0.3 nm^{-1}.

[14]It was shown by Maxwell in 1859 that the converse is also true; i.e., for an isotropic system in which p_x, p_y, and p_z are statistically independent, $n(\vec{p})$ is necessarily Gaussian. See *The Scientific Papers of James Clerk Maxwell*, edited by W. D. Niven (Dover, New York, 1965), Vol. I, p. 380.

[15]F. London, *Superfluids* (Wiley, New York, 1954), Vol. II, p. 40.

[16]L. Reatto and G. V. Chester, Phys. Rev. 155, 88 (1967).

[17]If we were to ignore instrumental resolution effects, the enhancement would be about 27% so that the actual enhancement is expected to be much less than this.

[18]A. D. B. Woods and V. F. Sears, to be published.

[19]H. A. Mook, Phys. Rev. Lett. 32, 1167 (1974).

[20]L. J. Rodriguez, H. A. Gersch, and H. A. Mook, Phys. Rev. A 9, 2085 (1974).