

## High-Energy Neutron-Liquid He<sup>4</sup>-Scattering and the He<sup>4</sup> Condensate Density

R. D. Puff and J. S. Tenn

*Department of Physics, University of Washington, Seattle, Washington 98105*

(Received 11 August 1969)

A simple theory of high-energy neutron scattering from liquid He<sup>4</sup> is developed. The inelastic scattering cross section for this process is related, for sufficiently high momentum transfer, to two parameters characterizing the He<sup>4</sup> momentum distribution. These two parameters are the average kinetic energy per particle and the fraction of particles in the zero-momentum condensate. Comparison of the theory with recent experimental data indicates that the condensate fraction  $\rho_0/\rho$  is approximately 0.06 at  $T=1.27^\circ\text{K}$ .

### I. INTRODUCTION

It has long been supposed that a condensation of particles into the zero-momentum state occurs<sup>1</sup> in liquid He<sup>4</sup> below the  $\lambda$  transition temperature, in analogy with the condensation in the free Bose gas. An early estimate<sup>2</sup> of the relative condensate density  $\rho_0/\rho$  was 0.08, while more recent calculations<sup>3</sup> find values near 0.11, or even as large as 0.25.

In any event, our theoretical interpretation and understanding of liquid-helium phenomena depend on the existence of a condensate, although direct experimental measurement of  $\rho_0/\rho$  has not been made.

Hohenberg and Platzman<sup>4</sup> have suggested that the inelastic scattering of neutrons in the 1-eV energy range can be used to measure the momentum distribution of individual He<sup>4</sup> atoms and, thereby, the occupancy of the zero-momentum state. The energy and momentum transfer must be sufficiently high so that the neutron scatters from an individual He<sup>4</sup> atom; the resonant energy in the scattering process will then be  $\hbar\omega_0(k) = \hbar^2 k^2 / 2M_{\text{He}}$ . Hohenberg and Platzman analyze the conditions under which one might hope to resolve a "condensate peak" on top of a broad background distribution, and they conclude that such an observation may be possible with good energy resolution ( $\sim 1\%$ ) in the experiment.

In this paper, we will investigate the same neutron scattering process with a somewhat different theoretical analysis. We will be able to show that, although the ideal "peak on top of a broad background" will not occur, the nature of the rapidly sharpening cross section below  $T_\lambda$ , observed by Cowley and Woods<sup>5</sup> and more recently by Harling,<sup>6</sup> allows direct interpretation as a condensate contribution. We will use, for comparison of the theory with experiment, the higher energy data of Harling.<sup>6</sup> Our analysis of the condensate part of the cross section follows that of Hohenberg and Platzman<sup>4</sup>; and the reader should refer to their paper for this part of the calculation and for

a more complete discussion of the physical ideas involved.

### II. THEORY, COMPARISON WITH EXPERIMENT AND CONCLUSIONS

It is well known that the neutron-He<sup>4</sup> inelastic scattering cross section is given<sup>7</sup> in the Born approximation, for  $N$  helium atoms in thermal equilibrium in the target, by

$$\frac{d^2\sigma}{d\Omega d\epsilon_f} = \frac{M_n^2}{(2\pi)^3 \hbar^5} \frac{k_f}{k_i} \left| U(k) \right|^2 N \frac{S(k, \omega)}{1 - e^{-\beta \hbar \omega}}, \quad (1)$$

where  $M_n$  is the neutron mass,  $\hbar \vec{k} = \hbar(\vec{k}_i - \vec{k}_f)$  is the momentum transfer,  $\hbar \omega = \epsilon_i - \epsilon_f$  is the energy transfer, and  $U(k)$  is the Fourier transform of the neutron-helium atom interaction.  $U(k)$  can be replaced by a constant over the range of  $k$  appropriate here, and  $e^{-\beta \hbar \omega} \ll 1$  for energy transfers of interest. Equation (1) can then be written, as an inelastic cross section per scatterer, in the form

$$\frac{1}{N} \frac{d^2\sigma}{d\Omega d\epsilon_f} = \frac{\sigma_b}{8\pi^2} \left( 1 - \frac{\hbar \omega}{\epsilon_i} \right)^{1/2} \frac{S(k, \omega)}{\hbar}, \quad (2)$$

where  $\sigma_b = (1 + M_n/M_{\text{He}})^2 4\pi a^2$ ,

with  $a$  the scattering length for He atom-neutron scattering.  $\sigma_b$  is traditionally called the bound-helium-atom cross section, and in the analysis below we will take<sup>8</sup>  $\sigma_b = 1.13$  b. Since experimental determinations are usually expressed, for a given incident neutron energy, as a function of energy transfer and scattering angle  $\theta$ , the kinematic relation

$$k^2(\epsilon_i, \theta, \omega) = \frac{2M_n}{\hbar^2} \left\{ 2\epsilon_i \left[ 1 - \cos\theta \left( 1 - \frac{\hbar \omega}{\epsilon_i} \right)^{1/2} \right] - \hbar \omega \right\} \quad (3)$$

will be useful. The  $\omega$ -integrated quantity, or single differential cross section, can also be obtained experimentally, and is given by<sup>9</sup>

$$\begin{aligned} \sigma(\theta, \epsilon_i) &\equiv \int_0^{\epsilon_i} d(\hbar\omega) \frac{1}{N} \frac{d^2\sigma}{d\Omega d\epsilon_i} \\ &= \frac{\sigma_b}{8\pi^2} \int_0^{\epsilon_i/\hbar} d\omega \left(1 - \frac{\hbar\omega}{\epsilon_i}\right)^{1/2} S[k(\epsilon_i, \theta, \omega), \omega]. \end{aligned} \quad (4)$$

Now, the theoretical problem is the calculation of the function  $S(k, \omega)$  for liquid He<sup>4</sup>. This function is defined as the Fourier transform of the particle density commutator

$$\begin{aligned} S(k, \omega) &= \frac{1}{\rho} \int d^3r \int_{-\infty}^{\infty} dt e^{-i\mathbf{k}\cdot\mathbf{r} + i\omega t} \\ &\quad \times \langle [\rho(\mathbf{r}, t), \rho(0, 0)] \rangle. \end{aligned} \quad (5)$$

Here  $\rho(r,t)$  is the particle density operator  $\psi^\dagger(r,t) \times \psi(r,t)$  in the Heisenberg picture,  $\langle \rangle$  refers to the equilibrium thermal ensemble average, and  $\rho = \langle \rho(r,t) \rangle$ .

For noninteracting bosons,  $S(k, \omega)$  can be determined by familiar methods, and the result is

$$\begin{aligned} S^{\text{FP}}(k, \omega) &= 2\pi(\rho_0/\rho) \{ \delta[\omega - \omega_0(k)] - \delta[\omega + \omega_0(k)] \} \\ &\quad + \left( \frac{\pi\beta}{\omega_0(k)} \right)^{1/2} (\rho\lambda^3)^{-1} \\ &\quad \times \ln \left( \frac{1 - e^{-\beta[(1/4\omega_0)(\omega + \omega_0)^2 - \mu]}}{1 - e^{-\beta[(1/4\omega_0)(\omega - \omega_0)^2 - \mu]}} \right), \end{aligned} \quad (6)$$

where  $\omega_0(k) = k^2/2M$ ,  $\lambda$  is the thermal de Broglie wave length  $(2\pi\hbar^2/Mk_B T)^{1/2}$ , and  $\rho_0$  is the number density of particles in the zero-momentum mode. Recall that

$$\rho_0/\rho = \{1 - [T/T_c(\rho)]^{3/2}\},$$

$$\text{and } \mu = 0 \text{ for } T < T_c(\rho),$$

while  $\rho_0 = 0$  and  $\mu \neq 0$  for  $T > T_c(\rho) = (2\pi\hbar^2/Mk_B) [\rho/\xi(\frac{3}{2})]^{2/3}$ . The function  $S$  splits into two pieces. The zero-momentum condensation shows up as a  $\delta$  function, while a "background" contribution (the log term) emerges as a result of helium atoms not in the condensate.

Now, a realistic extension of Eq. (6) to real liquid He<sup>4</sup>, both above and below the  $\lambda$ -transition temperature, is required. We expect, for reasons discussed in Ref. 4, that there will be both a condensate contribution and a background contribution for He<sup>4</sup>, although the free-particle result in Eq. (6) is clearly not appropriate. Hohenberg and Platzman<sup>4</sup> analyzed the background contribution by

going back to the free-particle form

$$\begin{aligned} \frac{2\pi}{\rho} \int [d^3q/(2\pi)^3] n'(q) \{ \delta[\omega - \omega_0(\vec{q} + \vec{k}) + \omega_0(\vec{q})] \\ - \delta[\omega - \omega_0(\vec{q}) + \omega_0(\vec{q} + \vec{k})] \}, \end{aligned}$$

from which the above log term emerges for the free-particle momentum space distribution  $n'(q)$  for particles not in the condensate. Their analysis then includes some justification for employing the free-particle form together with the actual  $n'(q)$  for He<sup>4</sup>. Further analysis and numerical estimates then involve a knowledge of  $n'(q)$ , together with the possibility of broadening the  $\delta$  function in the integrand. We wish here to employ a somewhat different method, and our task is made simpler if we restrict our attention to the high- $k$  regime.

Consider first the free-particle solution (6) and observe that the background contribution becomes

$$\begin{aligned} [S^{\text{FP}}(k, \omega)]_{\text{background}} &\approx \left( \frac{\pi\beta}{\omega_0} \right)^{1/2} \frac{e^{\beta\mu}}{\rho\lambda^3} \\ &\quad \times (e^{-\beta(4\omega_0)^{-1}(\omega - \omega_0)^2} - e^{-\beta(4\omega_0)^{-1}(\omega + \omega_0)^2}), \end{aligned} \quad (7)$$

whenever  $\frac{1}{4}\beta\omega_0^{-1}(\omega \pm \omega_0)^2 - \beta\mu \gg 1$  or, since  $\mu \leq 0$  in general, whenever

$$\begin{aligned} \beta\omega_0(k) &\gg 1, \\ \left| \frac{\omega \pm \omega_0}{\omega_0} \right| &\gg \frac{2}{\beta\omega_0(k)}. \end{aligned} \quad (8)$$

In the classical high temperature limit,  $e^{\beta\mu} \rightarrow \rho\lambda^3 \rightarrow 0$ , there is of course no condensation, and (7) is the classical solution ( $e^{\beta\mu}/\rho\lambda^3 = 1$ ) for the full  $S(k, \omega)$ . However, the form (7) remains valid (for free particles) without the classical low-density or high-temperature limit condition, under the "high  $k$ , sufficiently off resonance" conditions (8).

Now, we might expect to find a similar simplification of the background contribution in the interacting system at sufficiently high  $k$ . The condition (8) is irrelevant, of course, but for some  $k$  values we might expect the background term to attain the classical Gaussian form, centered about the resonant position  $\pm \omega_0(k)$ . The relevant energy for comparison in (8) should not be  $\beta^{-1}$ , but something like the actual kinetic energy per particle in the He<sup>4</sup> system.

To make this supposition more precise, we may first supply an "experimental" justification, and then introduce some theoretical analysis to make quantitative predictions. First, an examination of experimental data<sup>6</sup> above  $T_\lambda$  ( $T = 4.2^\circ \text{K}$ ), where we need not consider a condensate contribution, shows that the cross section is quite close to a simple Gaussian shape in  $\omega$  for fixed  $k$ . The width

of the Gaussian is clearly not just  $k_B T$ , but the resonant position is  $\omega_0(k)$  for  $k$  in the experimental range ( $k \sim 12 - 16 \text{ \AA}^{-1}$ ).

In order to provide some theoretical component to these assertions, let us examine several exact relations<sup>10</sup> satisfied by the function  $S(k, \omega)$ .  $S(k, \omega)$  is an odd function of  $\omega$  which satisfies the following sum rules for all  $k$ :

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(k, \omega) \coth \frac{1}{2} \beta \omega = S(k), \quad (9)$$

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S(k, \omega) = \omega_0(k), \quad (10)$$

$$\begin{aligned} \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^3 S(k, \omega) \\ = \omega_0(k) [\omega_0^2(k) + 4 \langle \text{KE} \rangle / N] \omega_0(k) + C(k). \end{aligned} \quad (11)$$

Here,  $S(k)$  is the liquid-structure factor. This function rapidly approaches 1 for large  $k$  and can be approximated by 1 in the  $k$  region of interest ( $k \sim 12 - 16 \text{ \AA}^{-1}$ ). Furthermore,  $\coth \frac{1}{2} \beta \omega$  can be replaced by  $\omega/|\omega|$ , since  $|\frac{1}{2} \beta \omega| \gg 1$ , for all  $\omega$  contributing significantly to the integral at high  $k$ .  $C(k)$  is a complicated function of the two-body

helium potential and  $S(k)$ . The precise form of  $C(k)$  can be found in Ref. 10. However,  $C(k)$  is, for large  $k$ , much smaller than the other terms in Eq. (11). One finds<sup>11</sup>  $|C(k \approx 15 \text{ \AA}^{-1})| \lesssim 1400 (\text{°K})^2$ , while  $\omega_0(k \approx 15 \text{ \AA}^{-1}) \approx 1360 \text{ °K}$ .  $\langle \text{KE} \rangle / N$  is the actual kinetic energy per particle in the He<sup>4</sup>, and is approximately  $12 - 15 \text{ °K}$  at  $T = 0$ . Therefore, a set of approximate sum rules for high-experimental- $k$  values is

$$\int_0^{\infty} \frac{d\omega}{2\pi} S(k, \omega) \approx 1, \quad (12)$$

$$\frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega S(k, \omega) = \omega_0(k), \quad (13)$$

$$\begin{aligned} \frac{1}{2} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^3 S(k, \omega) \\ \approx \omega_0(k) \left[ \omega_0^2(k) + 4 \frac{\langle \text{KE} \rangle}{N} \omega_0(k) \right]. \end{aligned} \quad (14)$$

Now, we wish to employ Eqs. (12-14), together with a phenomenological Gaussian form for  $T > T_\lambda$ . If we take

$$S(k, \omega) \approx \left( \frac{\pi}{\frac{2}{3} \frac{\langle \text{KE} \rangle}{N} \omega_0(k)} \right)^{1/2} \left\{ \exp \left[ -\frac{1}{4} \left( \frac{2}{3} \frac{\langle \text{KE} \rangle}{N} \omega_0 \right)^{-1} (\omega - \omega_0)^2 \right] - \exp \left[ -\frac{1}{4} \left( \frac{2}{3} \frac{\langle \text{KE} \rangle}{N} \omega_0 \right)^{-1} (\omega + \omega_0)^2 \right] \right\} \quad (15)$$

for  $T > T_\lambda$ , then Eqs. (13) and (14) are satisfied identically, and Eq. (11) is satisfied to within exponentially small factors, since  $\frac{1}{4} \left[ \frac{2}{3} \frac{\langle \text{KE} \rangle}{N} \right]^{-1} \times \omega_0(k) \gg 1$ . The three sum rules for high  $k$  serve to fix the normalization, width, and resonant position once the odd Gaussian choice is made. The Gaussian form is, of course, not uniquely dictated by either the exact or the approximate high- $k$  sum rules. However, we have used here the physical argument that at large momentum transfer the helium-neutron collision takes place in a time short compared to helium-atom collision times. Consequently, the helium target consists, in some sense, of a thermal bath of "free" helium atoms characterized by their average kinetic energy. Use of the sum rules with a Gaussian form produces a quantitative statement from this physical picture, and Eq. (15) is of course trivially exact in the limit of zero interaction between He atoms. It will be observed that (15) is simply the classical free particle  $S(k, \omega)$ , with  $\frac{3}{2} k_B T$  replaced by the true  $\langle \text{KE} \rangle / N$  for He<sup>4</sup>. The contention is that the high- $k$  scattering experiment above  $T_\lambda$  measures essentially only a single moment of the momentum distribution; i.e., the kinetic energy.

The cross section has an essentially Gaussian form centered about  $\omega_0(k)$ , and the only parameter

at our disposal is  $\langle \text{KE} \rangle / N(T)$ . This is not to say that the cross section is Gaussian in  $\omega$  with  $\theta$  fixed (as seen directly in the experiment). Although  $k$  changes little over the range of observation,<sup>6</sup> the distinction between constant  $k$  and constant  $\theta$  is significant for numerical calculation. A comparison of widths for constant  $k$  and constant  $\theta$  plots makes this distinction obvious (the width at constant  $\theta$  in the experimental range is about half that at constant  $k$ , since the location of the resonance varies as  $k^2$ ). Although the theoretical analysis is simpler at constant  $k$ , the direct comparison with experiment is facilitated by calculation at constant  $\theta$ .

We now use Eq. (15) for  $T = 4.2 \text{ °K}$  to calculate the double differential cross section [Eq. (2)] as a function of  $\theta$  and  $\omega$  for an incident energy  $\epsilon_i = 0.1715 \text{ eV}$ . We then perform the integral indicated in Eq. (4) to obtain the single differential cross section  $\sigma(\theta, \epsilon_i)$ . A plot of  $\sigma(\theta, \epsilon_i = 0.1715 \text{ eV})$  is shown in Fig. 1 for a choice of  $\langle \text{KE} \rangle / N$  ( $T = 4.2 \text{ °K}$ ) equal to  $15 \text{ °K}$ . Experimental values, taken from the data of Harling<sup>6</sup> are also shown. The largest value of  $\theta (= 154.3 \text{ deg})$  represents, of course, the largest value of  $k$ . For small angles we expect the high- $k$  approximations to be invalid. Consequently, we concentrate on the large-angle scattering and plot the double differential cross sec-

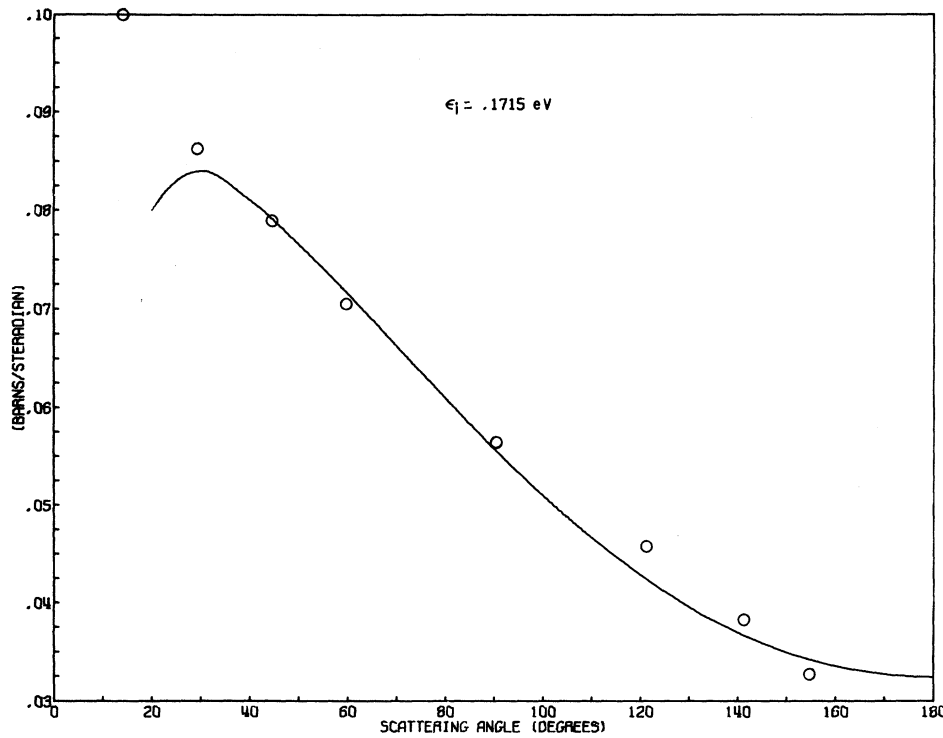


FIG. 1. Theoretical and experimental values for the single differential cross section, as a function of scattering angle, for incident neutron energy  $\epsilon_i = 0.1715$  eV and helium temperature  $T = 4.2$  K. The experimental results are taken from Ref. 6.

tion as a function of  $\omega$ , for incident energy  $\epsilon_i = 0.1715$  eV and  $\theta = 154.3$  deg. Again, we use  $\langle\langle KE \rangle\rangle/N$  ( $T = 4.2$  K) =  $15^\circ$  K to characterize  $S(k, \omega)$  according to Eq. (15). The results are shown in Fig. 2, together with experimental values for the same  $\epsilon_i$  and  $\theta$ . Values of  $\langle\langle KE \rangle\rangle/N$  from  $14.5$  to  $15.5$  K will serve almost as well, considering the resolution in the experiment; and we have not attempted to obtain more than a visual fit.

Agreement between theory and experiment seems reasonably good if we are willing to accept the value  $15^\circ$  K for  $\langle\langle KE \rangle\rangle/N$  at  $T = 4.2$  K. Present theoretical calculations of the kinetic energy per particle are confined to ground-state values; i.e., to  $\langle\langle KE \rangle\rangle/N(\rho, T = 0)$ . The cross section we are calculating here depends on  $\langle\langle KE \rangle\rangle/N(\rho, T)$ , with  $\rho = \rho(T)$  given by the density value along the vapor-pressure curve in order to compare with experiment. Experimentally,  $\rho(T)$  begins to decrease<sup>12</sup> rapidly above  $T_\lambda$  from the  $T = 0$  value  $m\rho(T = 0) = 0.145$  g/cm<sup>3</sup>. At  $4.2$  K, the density is somewhat less than 90% of this value. Various calculations of  $\langle\langle KE \rangle\rangle/N(\rho, T = 0)$  give values, at the  $T = 0$  equilibrium density, of 14.16,<sup>13</sup> 13.72,<sup>14</sup> and 14.06.<sup>15</sup> The same calculations produce numbers like 11.7,<sup>13</sup> 11.59,<sup>14</sup> and 11.60,<sup>15</sup> if the density is decreased by 10%. However, the apparent agreement between these results may be misleading because they are all variational calculations with the same type of (Jastrow) wave function. Furthermore, the calculations do not always predict the correct equilibrium density; the energy minimum in Ref. 13

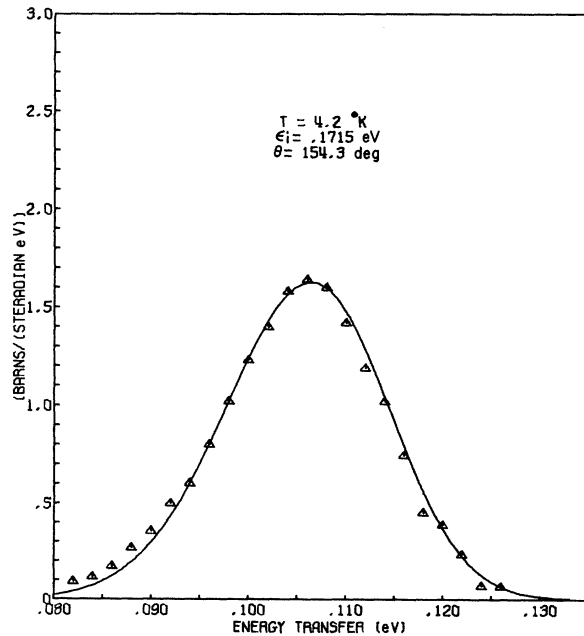


FIG. 2. Theoretical and experimental values for the double differential cross section, as a function of energy transfer for fixed scattering angle  $\theta = 154.3$  deg, for incident neutron energy  $\epsilon_i = 0.1715$  eV and helium temperature  $T = 4.2$  K. The experimental results are taken from Ref. 6.

and Ref. 14 occurs at 90% of the experimental density, where the kinetic energy has the lower value. A quite different type of calculation<sup>16</sup> (not a variational solution, with a different two-body potential) produces a still lower kinetic energy (10.2 °K) with a 5% error in density. All such calculations indicate that the  $T=0$  kinetic and potential energies are more rapidly varying functions of density than is their sum.

If we suppose for a moment that  $\langle\text{KE}\rangle/N(\rho, T=0)$  is known accurately, then since

$$\frac{\langle\text{KE}\rangle}{N}[\rho(T), T] = \frac{\langle\text{KE}\rangle}{N}[\rho(T), 0] + \int_0^T dT' \frac{\partial}{\partial T'} \frac{\langle\text{KE}\rangle}{N}[\rho(T), T'],$$

and since the derivative in the integrand is positive, we can be sure that  $\langle\text{KE}\rangle/N[\rho(T), T]$  lies above the ground-state value at the reduced density  $\rho(T)$ . A more complete statement can be made in the phonon region ( $T \lesssim 0.6$  °K), where  $\rho(T)$  has essentially its zero-temperature value and the second term in the above expression can be calculated. Since  $\langle\text{KE}\rangle = -m \partial F / \partial m |_{N, V, T}$ , where  $F$  is the Helmholtz free energy, we can relate  $F$  in the phonon region to the sound velocity, the mass derivative of which can then be related to the kinetic energy. Thus, one finds

$$\frac{\langle\text{KE}\rangle}{N}(\rho, T) = \frac{\langle\text{KE}\rangle}{N}(\rho, 0) - \frac{3}{2} \left\{ \frac{F}{N}(\rho, T) - \frac{F}{N}(\rho, 0) \right\} \times \left[ 1 + \frac{1}{mc^2} \frac{d}{d\rho} \rho^2 \frac{d}{d\rho} \frac{\langle\text{KE}\rangle}{N}(\rho, 0) \right],$$

where  $\{ \}$  =  $-(\pi^2/90\rho)(kT)^2/\hbar c)^3$ . The coefficient of the  $[ \ ]$  term in this expression is, therefore, only 0.03  $(T/T_\lambda)^4$  °K. Unless the factor  $[ \ ]$  is very large indeed,  $\langle\text{KE}\rangle/N[\rho(T), T] \approx \langle\text{KE}\rangle/N \times [\rho(0), 0]$  over the phonon region. Theoretical estimates indicate that  $[ \ ]$  is  $< 5$ .

The observations above lead us to believe that our choice of  $\langle\text{KE}\rangle/N = 15$  °K at  $T = 4.2$  °K, used to obtain a good visual fit of the theoretical cross section to experimental data, is not at all unreasonable. An increase in kinetic energy caused by an increase in temperature is offset by a corresponding decrease produced by a decrease in den-

sity.  $\langle\text{KE}\rangle/N[\rho(T), T]$  apparently does not change very much below 4 deg, if we accept the 15 °K estimate at 4.2 °K. For the  $T < T_\lambda$  analysis, we will see below that a lower bound on  $\langle\text{KE}\rangle/N[\rho(T), T]$  is required, and we might set this lower bound at 12 °K, in view of the uncertainties described above in theoretical calculations of  $\langle\text{KE}\rangle/N(\rho, T=0)$ .

Now it is clear that a smaller  $\langle\text{KE}\rangle/N$  will have the effect of sharpening the cross section. As the temperature is lowered, any *smaller* estimate for  $\langle\text{KE}\rangle/N[\rho(T), T]$  will make the cross section more peaked. We know that as  $T$  drops below  $T_\lambda$ , the presence of a condensate should also have the effect of sharpening the cross section, even if no small peak on top of the background contribution, as suggested by Hohenberg and Platzman, can be seen experimentally. We should find that the form (15) can be used for all  $T > T_\lambda$  with a reasonable estimate for  $\langle\text{KE}\rangle/N(T)$ . A slowly sharpening cross section, as the temperature is lowered, would indicate a slow decrease in kinetic energy. As we go below  $T_\lambda$ , however, the form (15) should fail badly. That is, we expect the cross section to become both highly peaked (too much so to be accounted for by a decrease in  $\langle\text{KE}\rangle/N$ ), and its *shape* should be distinct from that of the single Gaussian. The zero-momentum component introduces an additional term whose width is essentially temperature independent and whose relative weight is proportional to  $(\rho_0/\rho)(T)$ .

In order to analyze the condensate part, we will use the arguments of Hohenberg and Platzman<sup>4</sup> to estimate the condensate width, then apply the approximate high- $k$  sum rules to obtain a model for the full  $S(k, \omega)$ . We will assume that the condensate part has Gaussian shape, centered about  $\pm\omega_0(k)$ . Following Hohenberg and Platzman, we take the full width at half-maximum in the condensate peak to be

$$\Gamma = \rho\sigma k/M_{\text{He}}, \quad (16)$$

where  $\sigma$  is the He-He scattering cross section and  $\rho$  is the helium number density. In the range of  $k$  appropriate here,  $\sigma$  is not reduced appreciably from its  $k=0$  value<sup>4</sup> ( $\sigma \approx 2 \times 10^{-15}$  cm<sup>2</sup>). We may then construct a form for  $S(k, \omega)$  which includes both the properly weighted condensate and background terms:

$$S(k, \omega) = 2(\rho_0/\rho) \left\{ \pi / [\gamma_1(k)] \right\}^{1/2} \left( e^{-\gamma_1^{-1}(\omega - \omega_0)^2} - e^{-\gamma^{-1}(\omega + \omega_0)^2} \right) + 2(1 - \rho_0/\rho) \left\{ \pi / [\gamma_2(k)] \right\}^{1/2} \left( e^{-\gamma_2^{-1}(\omega - \omega_0)^2} - e^{-\gamma_2^{-1}(\omega + \omega_0)^2} \right), \quad (17)$$

where  $\gamma_i(k)$ , according to our assumption concerning the condensate width, is given by

$$\gamma_1(k) = \frac{1}{4\ln 2} \Gamma^2 = \Omega \omega_0(k), \quad \text{with } \Omega \equiv \frac{1}{2\ln 2} \frac{(\rho\sigma)^2}{M_{\text{He}}}. \quad (18)$$

The sum rules then further demand that

$$\gamma_2(k) = \left[ \left( \frac{8 \langle KE \rangle}{3N} - \frac{\rho_0}{\rho} \Omega \right) / \left( 1 - \frac{\rho_0}{\rho} \right) \right] \omega_0(k). \quad (19)$$

The numerical value of the constant  $\Omega$ , using the  $\sigma$  above and the  $T=0$  equilibrium helium density, is 1.40 °K. Therefore, since  $\rho_0/\rho < 1$  and  $\langle KE \rangle/N$  is about 14 °K, it is clear that the  $\Omega$  term in (19) represents a small correction. We furthermore expect, since  $\rho_0/\rho$  is probably  $\lesssim 0.10$ , that the denominator correction is small.

Above  $T_\lambda$ , when  $\rho_0/\rho = 0$ , Eqs. (17) and (19) reduce to the previous result (15). However, below  $T_\lambda$ , the quantity  $(\rho_0/\rho)[\rho(T), T]$  enters as an unknown parameter. Both parameters  $(\rho_0/\rho)$  and  $\langle KE \rangle/N$  are, in principle, determined by the momentum distribution for the He<sup>4</sup>,

$$n(q) = (2\pi)^3 \rho_0 \delta(\vec{q}) + n'(q), \quad \rho - \rho_0 = \int \frac{d^3q}{(2\pi)^3} n'(q), \quad (20)$$

$$\rho \langle KE \rangle / N = \int \frac{d^3q}{(2\pi)^3} \omega_0(q) m'(q),$$

and the independent calculation of  $n(q)$  remains a separate problem. The high- $k$  scattering results are described, from (17), in terms of the two quantities  $\rho_0/\rho$  and  $\langle KE \rangle/N$  above, once we have fixed the width of the condensate contribution.

We must now answer the following questions: First, for reasonable  $\rho_0/\rho$  and  $\langle KE \rangle/N$ , will the low-temperature cross section be seen as a distinct "bump on top of a background?" For  $\rho_0/\rho \lesssim 0.10$  and  $\langle KE \rangle/N \approx 14$  °K, it would seem that no small "bump" can be resolved by a visual check of the entire cross-section curve predicted by (17). Thus, even with infinite resolution in the experiment, the answer to this question, posed by Hohenberg and Platzman, seems to be *no*. This prediction seems to be verified experimentally, as we will see below.

However, a fairly rapid sharpening of the cross section below  $T_\lambda$  has been observed by Cowley and Woods<sup>5</sup> and by Harling.<sup>6</sup> Since our theoretical analysis is dependent on very high- $k$  approximations, we will use only the Harling data for numerical comparison. The basic question to be answered is now the following: Can the sharpening of the cross section below  $T_\lambda$  be ascribed entirely to a decrease in  $\langle KE \rangle/N$  with an assumed  $\rho_0/\rho = 0$  (no condensation)? That is, is it necessary to include a  $\rho_0/\rho$  somewhere between 0 and 0.1 in order to explain the behavior of the cross section at low temperatures?

The double differential cross section,<sup>6</sup> as a function of energy transfer for a scattering angle  $\theta = 154.3$  deg, for incident neutron energy  $\epsilon_i = 0.1715$  eV and helium temperature  $T = 1.27$  °K,

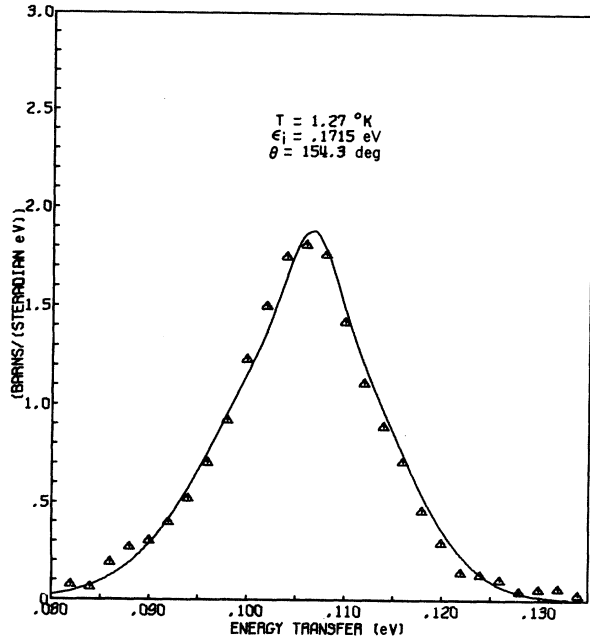


FIG. 3. Theoretical and experimental cross sections at 1.27 °K. The theoretical curve has been broadened by the resolution function appropriate to the data (Ref. 6). The kinetic energy per particle has been fixed initially at 14 °K, the most reasonable *a priori* value. The one remaining adjustable parameter,  $\rho_0/\rho$ , is found to be 0.07 by a least-square fit.

is shown in Fig. 3. The data shown here is an average of three experiments, each normalized to the same total cross section. The experimental results are broadened by an instrumental energy resolution<sup>6</sup> of  $\Gamma_R = 0.0042$ -eV full width at half-maximum. Since this resolution is comparable with our theoretical condensate width, the observed cross section should be compared with the convolution of the theoretical cross section and a resolution function

$$R(\omega - \omega') = (\pi \gamma_R)^{-1/2} \exp[-\gamma_R^{-1}(\omega - \omega')^2],$$

with  $\gamma_R = (4 \ln 2)^{-1} \Gamma_R^2$ . The "resolution broadened" theoretical cross section is also shown in Fig. 3.

In Fig. 3,  $\langle KE \rangle/N$  has been taken to be 14 °K. This represents our best *a priori* number for  $\langle KE \rangle/N$ ; that is, we have not adjusted it to improve the fit.  $\langle KE \rangle/N$  is rather restricted if we demand that it lie between the previous 4.2 ° result and a reasonable  $T=0$  value. It is probably closer to the  $T=0$  value, since  $\rho(T) \approx \rho(0)$  at this temperature.  $\rho_0/\rho$  has been chosen equal to 0.07 by a least-square fit of the "resolution broadened" theoretical curve to the experimental data between 0.090 and 0.120 eV. The mean-square deviation

$$z^2 \equiv \frac{1}{N} \sum_{i=1}^N [(\text{theory})_i - (\text{experimental})_i]^2$$

is equal to 0.0045 (b/sr eV)<sup>2</sup>.

The reasonable agreement between theory and experiment implies that the presence of a condensate can be used to interpret the sharpening of the cross section below  $T_\lambda$ . However, as discussed above, we really want to know how *necessary* the condensate is, in view of the uncertainties in  $\langle \text{KE} \rangle / N$ . Consequently, we next suppose that  $\rho_0/\rho = 0$  and adjust  $\langle \text{KE} \rangle / N$  to obtain a least-squares fit of the "resolution broadened" theory to the data. The result is shown in Fig. 4.  $\langle \text{KE} \rangle / N$  is 12.2 °K and the mean-square deviation is found to be  $z^2 = 0.0085$ .

The most we can say from this analysis is that the theory with adjustable condensate and a fixed theoretical estimate of kinetic energy per particle seems to be in better agreement with the data than the theory without a condensate and an adjustable kinetic energy. If the best  $\langle \text{KE} \rangle / N$  in the zero-condensate calculation were absurdly small, we would be in a better position to discard the possibility of the choice  $\rho_0/\rho = 0$ . However, 12.2 °K for  $\langle \text{KE} \rangle / N$  at  $T = 1.27$  °K is in our opinion *not* a sufficiently absurd number, and we can only note

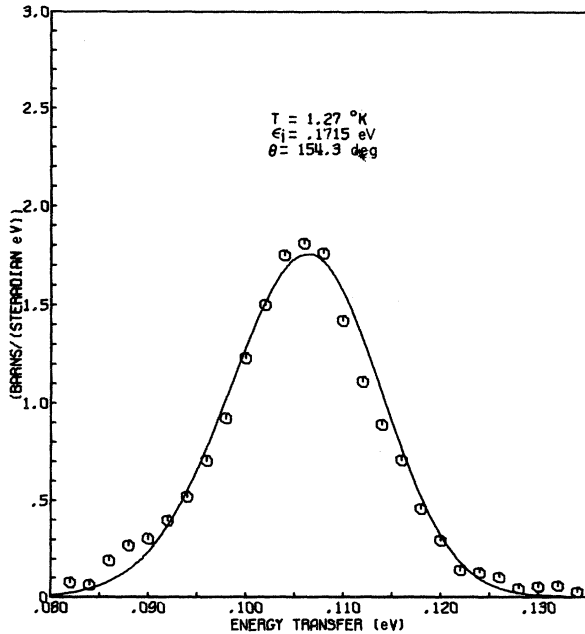


FIG. 4. Theoretical and experimental cross sections at 1.27 °K. The theoretical curve has been broadened by the resolution function appropriate to the data (Ref. 6). The condensate fraction  $\rho_0/\rho$  has been fixed initially at zero. The one remaining adjustable parameter  $\langle \text{KE} \rangle / N$  is then found to be 12.2 °K by a least-squares fit.

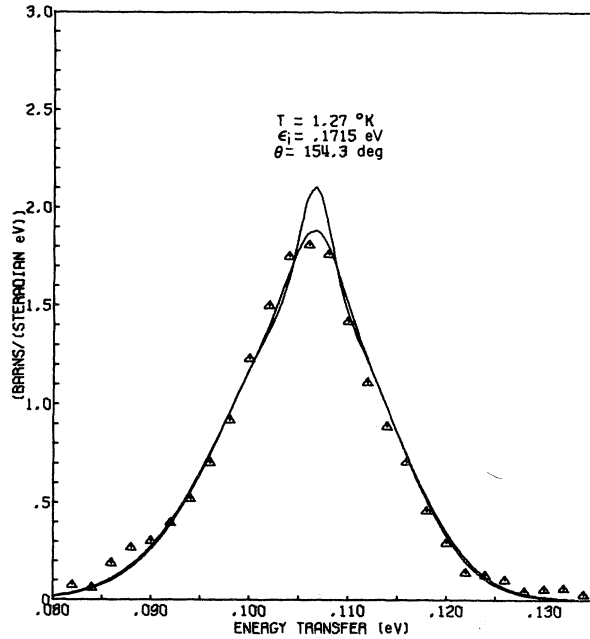


FIG. 5. Theoretical and experimental cross sections at 1.27 °K. The lower curve represents the best least-squares fit of the resolution-broadened theory to the data (Ref. 6).  $\rho_0/\rho$  is 0.062, and  $\langle \text{KE} \rangle / N$  is 13.5 °K. The upper curve shows the actual cross section predicted for these parameters without resolution broadening.

that the presence of a condensate improves the agreement with experiment.

If we admit the presence of a condensate on this basis and adjust both  $\rho_0/\rho$  and  $\langle \text{KE} \rangle / N$  to obtain the best mean-square fit of the "resolution broadened" theoretical curve to experiment, we achieve the results shown in Fig. 5. Here  $\langle \text{KE} \rangle / N = 13.5$  °K and  $\rho_0/\rho = 0.062$ , while the mean-square deviation is  $z^2 = 0.0043$ . This is our best determination of  $\langle \text{KE} \rangle / N$  and  $\rho_0/\rho$  at  $T = 1.27$  °K from the data shown. The upper curve shows the theoretical cross section for these parameters, while the lower curve shows the resolution-broadened result appropriate to the experimental conditions of Ref. 6.

In order to estimate the uncertainty in this  $\rho_0/\rho$  value, we should look again at the results above  $T_\lambda$ . Our theoretical picture makes sense only if  $\rho_0/\rho = 0$  at 4.2 °K. A least-squares fit of the  $\rho_0/\rho = 0$  resolution-broadened theory to the 4.2 °K data in Fig. 2 gives  $\langle \text{KE} \rangle / N = 14.8$  °K, with  $z^2 = 0.0020$ . Agreement seems remarkably good (i. e., like the curve in Fig. 2). On the other hand, if we allow the freedom of a nonzero condensate [i. e., use Eq. (17)] and adjust both parameters, the "best" least-squares fit produces  $\langle \text{KE} \rangle / N = 15.2$  °K and  $\rho_0/\rho = 0.022$ , with  $z^2 = 0.0014$ . This best fit, with a small condensate above  $T_\lambda$ , is meaningless. It reinforces the intuitive feeling that two free parameters may give a slightly better

fit to experimental data even though one of the parameters should be fixed *a priori*. The obvious conclusion to draw here is that differences in  $z^2$  of  $\sim 0.001$  are meaningless, and that we will not obtain  $\rho_0/\rho$  values to within better than  $\pm 0.03$  with the present data unless a better *a priori* number for  $\langle KE \rangle/N$  can be assigned to a given temperature. We therefore conclude that our theoretical interpretation of the data in Ref. 6 implies a condensate of  $\rho_0/\rho = 0.06 \pm 0.03$  at  $T = 1.27^\circ\text{K}$ .

It is now clear that reasonable agreement between the theoretical expression (17) and additional experimental data at high momentum transfer can be achieved. We should emphasize that a good "two-parameter fit" to any  $T < T_\lambda$  data, where the two parameters are Gaussian widths, is not at all convincing without a knowledge that the two parameters are related to  $\langle KE \rangle/N$  and  $\rho_0/\rho$  according to the demands of the sum-rule theory. The relatively narrow range of values possible for  $\langle KE \rangle/N$  and reasonable for  $\rho_0/\rho$  is the only thing that

makes any conclusion possible from a two-parameter fit. Further two-parameter fits to the data should be carried out in order to determine both  $\rho_0/\rho$  and  $\langle KE \rangle/N$  as functions of temperature within the limits dictated by experimental errors. Since statistical errors are less important than resolution-broadening effects here, it is perhaps better not to average-in data with the worst resolution (the  $\Gamma_R$  used above is an average resolution). Some of the Harling data,<sup>6</sup> with  $\Gamma_R = 0.0027$ , seems to show a more pronounced peak around the resonance, but careful analysis is necessary to determine if this is statistically significant.<sup>17</sup>

#### ACKNOWLEDGMENTS

We wish to thank Dr. O. K. Harling for making his experimental results available to us before publication, and Dr. W. D. McCormick for numerous discussions.

\*Work supported in part by the U.S. Atomic Energy Commission.

<sup>1</sup>F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II.

<sup>2</sup>O. Penrose and L. Onsager, *Phys. Rev.* **104**, 576 (1956).

<sup>3</sup>W. L. McMillan, *Phys. Rev.* **138**, A442 (1965); W. E. Parry and C. R. Rathbone, *Proc. Phys. Soc. (London)* **91**, 273 (1967). The latter authors report the higher value.

<sup>4</sup>P. C. Hohenberg and P. M. Platzman, *Phys. Rev.* **152**, 198 (1966).

<sup>5</sup>R. A. Cowley and A. D. B. Woods, *Phys. Rev. Letters* **21**, 787 (1968).

<sup>6</sup>O. Harling (to be published); and *Bull. Am. Phys. Soc.* **14**, 8 (1969).

<sup>7</sup>L. Van Hove, *Phys. Rev.* **95**, 249 (1954).

<sup>8</sup>Brookhaven National Laboratory Report No. BNL325, edited by M. D. Goldberg *et al.* (Associated Universities Inc., 1966), 2nd ed., Suppl. 2; and R. Genin *et al.*, *J. Phys. Radium* **24**, 21 (1963).

<sup>9</sup>After Eq. (4) we will use units  $\hbar = 1$  unless otherwise noted.

<sup>10</sup>R. D. Puff, *Phys. Rev.* **137**, A406 (1965).

<sup>11</sup>N. Mihara, Ph.D. thesis, University of Washington

(Seattle), 1968 (unpublished).  $C(k)$  oscillates around zero. The number given here is an approximate amplitude near  $k \sim 15 \text{ \AA}^{-1}$ . We will always neglect  $C(k)$ , but it is clear that a lower- $k$  analysis, by the same sum-rule method, can produce oscillations in the cross section width related to oscillations in both  $C(k)$  and  $[S(k) - 1]$ . Such oscillations have been observed in Ref. 5, where the momentum transfer is lower than that of Ref. 6. However, sufficiently accurate theoretical calculations of  $C(k)$  and  $[S(k) - 1]$  are not available. Furthermore, even with a good  $C(k)$  and  $[S(k) - 1]$ , it is not yet clear how far we may push a sum-rule theory based on Eqs. (9)–(11), and our analysis here is restricted to momentum transfers large enough so that we can use the simpler approximate sum rules, Eqs. (12)–(15), together with a simple Gaussian form for  $S(k, \omega)$ .

<sup>12</sup>J. Wilks, *Liquid and Solid Helium* (Clarendon Press, Oxford, England, 1967), see the Table in Appendix 1.

<sup>13</sup>W. L. McMillan, Ref. 3.

<sup>14</sup>D. Schiff and L. Verlet, *Phys. Rev.* **160**, 208 (1967).

<sup>15</sup>W. E. Massey and C. W. Woo, *Phys. Rev.* **164**, 256 (1967); and *Phys. Rev. Letters* **19**, 622 (1967).

<sup>16</sup>N. Mihara and R. D. Puff, *Phys. Rev.* **174**, 221 (1968).

<sup>17</sup>O. Harling (private communication).