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Corrections to the Impulse Approximation for High-Energy Neutron Scattering from Liquid Helium*

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Corrections to the impulse approximation for scattering from a many-body system are derived in the form of a series in inverse powers of the momentum transfer k. The coefficients in this series are written in terms of the two-body interaction potential and the particle-density matrices. Application is made to the case of high-energy neutron scattering from liquid helium. Evaluation of correction terms corresponding to a single helium-helium collision during the neutron-helium interaction time indicates (a) a shift in the peak of the incoherent-scattering cross section toward lower energy by a constant amount, and (b) an asymmetry of the cross section with respect to neutron energy loss about its peak value. Numerical estimates are given for these two effects for $k = 14.3$ Å^{-1}. Evaluation of condensate broadening due to multiple He-He collisions shows that the condensate-scattering contribution has a width proportional to $k^{1/2}$, and is thus distinguishable from the main noncondensate peak whose width is proportional to k. Estimates are given for requirements on experimental-resolution functions necessary to preserve this evidence of a distinct condensate contribution.

I. INTRODUCTION

The inelastic cross section for neutrons on He^4 liquid is given in the Born approximation[1] by

$$\frac{d^2\sigma}{d\Omega\, d\epsilon_f} = \frac{\sigma_b k_f}{4\pi\hbar k_i} S(k,\ \omega)\ , \qquad (1)$$

where $\hbar\vec{k} = \hbar\vec{k}_i - \hbar\vec{k}_f$ is the momentum transferred to the helium, $\hbar\omega = \epsilon_i - \epsilon_f$ is the energy transfer, and $\sigma_b = 1.13$ b.[2] The dynamic structure factor $S(k,\ \omega)$ is the Fourier transform of the density-density correlation function $S(k,\ t)$:

$$2\pi S(k,\ \omega) = \int_{-\infty}^{\infty} dt\, e^{-i\omega t} S(k,\ t)\ , \qquad (2)$$

where

$$NS(k,\ t) = \sum_{j,l} \langle e^{-i\vec{k}\cdot\vec{r}_l(0)} e^{i\vec{k}\cdot\vec{r}_j(t)} \rangle\ . \qquad (3)$$

The average value of the time-dependent density-density correlation function in Eq. (3) is in general taken over a canonical ensemble in equilibrium at temperature T. In the present work, we will restrict ourselves to $T = 0$. Equation (3) contains the Heisenberg operator $\vec{r}_j(t)$ defined for all j and t by

$$\vec{r}_j(t) = e^{iHt/\hbar}\, \vec{r}_j e^{-iHt/\hbar} \tag{4}$$

The complexity of the liquid ground state makes it necessary to employ severe approximations to calculate $S(k, \omega)$. The most widely accepted approximations are limited to either small momentum transfers or to asymptotically large values of k. Little progress has been made in the evaluation of $S(k, \omega)$ for intermediate values of k.

The interest in inelastic neutron scattering for large momentum transfers is largely based on the fact that the approximation asymptotically valid in this region, the impulse approximation, provides a fairly direct connection between liquid helium's single-particle momentum distribution and $S(k, t)$ [see Eq. (24) below]. This connection has been employed to compare a theoretical prediction of the He^4-momentum distribution with experimental determinations of $S(k, \omega)$.[3] A problem with this approach is that experiments have been limited to only moderately large values of k, for example, 14.3 $Å^{-1}$,[4] and a strict criterion for evaluating the accuracy of the impulse approximation has been lacking.

This paper presents a derivation and evaluation of correction terms to the impulse approximation. In Sec. II, we express the exact $S(k, t)$ as a series in inverse powers of k, the momentum transfer. In Sec. III, the coefficients of these powers of k^{-1} are expressed in terms of the two-body interaction potential and the two-particle density matrix. In Sec. IV, these general results are specialized to the case of helium.

We find that these corrections shift the peak of the incoherent scattering toward lower energy by a constant amount, which depends on the hard-core radius in the two-body interaction potential. Choosing the hard-core radius to agree with the average of the observed peak shift in the momentum transfer region from about 3 to 9 $Å^{-1}$,[5] we predict a 1% shift in peak value for $k = 14.3$ $Å^{-1}$. A concomitant slight asymmetry of the cross section with respect to neutron energy loss accompanies this peak shift. The condensate scattering contribution, which is given by a δ function in energy in the impulse approximation is broadened by interactions into a curve with a width proportional to $k^{1/2}$. Since the main noncondensate peak has a width proportional to k, the condensate contribution remains visible as a distinct spike in the dynamic structure factor for large k. Such structure is broadened by experimental energy resolution, and we find that with energy resolution of about 3.4 meV, corresponding to experiments performed at $k = 14.3$ $Å^{-1}$, the shape of the scattering cross section versus energy transfer has only a single broad peak. A reduction in this energy resolution by about a factor of 2 is found to preserve the distinct condensate contribution in the inelastic scattering cross section.

II. DERIVATION OF SERIES EXPANSION

Substitute Eq. (4), with its right-hand side multiplied by unity in the form $e^{i\vec{k}\cdot\vec{r}_j} e^{-i\vec{k}\cdot\vec{r}_j}$, into Eq. (3). The result, putting $\hbar = 1$, is

$$NS(k, t) = \sum_{j,l} \langle e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{-i\vec{k}\cdot\vec{r}_j} e^{iHt} e^{i\vec{k}\cdot\vec{r}_j} e^{-iHt} \rangle . \tag{5}$$

Now make use of the identity

$$e^{-i\vec{k}\cdot\vec{r}_j} e^{iHt} e^{i\vec{k}\cdot\vec{r}_j} = e^{iH't} ,$$

where

$$H' \equiv H(\vec{r}_1, \ldots, \vec{r}_N ; \vec{p}_1, \ldots, \vec{p}_j + \vec{k}, \ldots, \vec{p}_N)$$
$$= H + \omega_k + L_j ,$$

with

$$\omega_k = k^2/2m , \quad L_j = \vec{k}\cdot\vec{p}_j/m .$$

The density-density correlation function now has the form

$$NS(k, t) = e^{i\omega_k t} \sum_{j,l} \langle e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{i(H + L_j)t} e^{-iHt} \rangle . \tag{6}$$

The proposed expansion results from utilizing the following relation, valid for arbitrary operators A and B:

$$e^{A+B} = e^A T_\lambda \exp\left(\int_0^1 e^{-\lambda A} B e^{\lambda A} d\lambda\right) . \tag{7}$$

Here T_λ is an operator, similar to the time-ordering symbol, which arranges operators containing the parameter λ so that in the series expansion of the exponential, the operator associated with the smallest value of λ appears farthest to the right. In Eq. (7) we make the identifications

$$A = iL_j t = it\,\vec{v}_k\cdot\vec{p}_j , \quad B = iHt ,$$

where $\vec{v}_k = \vec{k}/m$. With these substitutions, the integrand in Eq. (7) becomes

$$(it) e^{-i\lambda(\vec{v}_k t)\cdot\vec{p}_j} H e^{i\lambda(\vec{v}_k t)\cdot\vec{p}_j} = it H'' ,$$

where

$$H'' = H(\vec{r}_1, \ldots, \vec{r}_j - \lambda\vec{v}_k t, \ldots, \vec{r}_N ; \vec{p}_1, \ldots, \vec{p}_N)$$
$$\equiv H(\vec{r}_j - \lambda\vec{v}_k t) .$$

The substitution of Eq. (7) into Eq. (6) therefore yields

$$NS(k, t) = e^{i\omega_k t} \sum_{j,l} \langle e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{i(\vec{v}_k t)\cdot\vec{p}_j} \times T_\lambda \exp\left[it \int_0^1 H(\vec{r}_j - \lambda\vec{v}_k t) d\lambda\right] e^{-itH} \rangle . \tag{8}$$

Using pictorial arguments, a physical interpretation may be made of the above equation. Considering the jth term in Eq. (8) as representing the interaction of a neutron with the jth helium atom, $\omega_k + L_j$ may be taken as the kinetic energy transferred to the atom. Similarly, the shifted Hamiltonian, $H(\vec{r}_j - \vec{v}_k t\lambda)$, arises from the motion of the jth atom through the media of its neighbors. The combination of the two Hamiltonian operators in Eq. (8) measures this change in interaction energy of the helium atoms during the neutron-helium collision time t. Neglecting operator noncommutativity, Eq. (8) represents the addition of these changes in kinetic and potential energy of the struck helium atom.

We next introduce new variables $\vec{x} = \vec{v}_k t$, $\vec{y} = \lambda\vec{x}$. With these replacements, the Fourier transform indicated in Eq. (2) becomes

$$2\pi N v_k S(k, \omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \sum_{j,l} \langle e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{i\vec{x}\cdot\vec{p}_j} \times T_y \exp[(i/v_k)\int_0^x H(\vec{r}_j - \vec{y})\,dy]\, e^{-ixH/v_k}\rangle \,, \quad (9)$$

where

$$\Omega = (\omega - \omega_k)/v_k \,. \quad (10)$$

A simplification in the remaining calculations results from the fact that the average $\langle\cdots\rangle$ is to be taken over a single state, the ground state $|\psi_0\rangle$. Let $E_0 = H|\psi_0\rangle$ represent the energy of this state. Equation (9) can then be written as

$$2\pi N v_k S(k, \omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \sum_{j,l} \langle\psi_0| e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{i\vec{x}\cdot\vec{p}_j} \times T_y \exp\{(i/v_k)\int_0^x [H(\vec{r}_j - \vec{y}) - E_0]\,dy\}|\psi_0\rangle \,. \quad (11)$$

The y-ordered exponential is thus seen to generate a series in decreasing powers of v_k:

$$T_y \exp\{(i/v_k)\int_0^x [H(\vec{r}_j - \vec{y}) - E_0]\,dv\}\,|\psi_0\rangle = \sum_{n=0}^{\infty} (1/v_k)^n |\psi_n\rangle \,. \quad (12)$$

Using the abbreviation

$$U_j(\vec{y}) = \sum_{m\neq j} [V(\vec{r}_j - \vec{y}, \vec{r}_m) - V(\vec{r}_j, \vec{r}_m)] \quad (13)$$

and noting the relations

$$H(\vec{r}_j - \vec{y}) = H + U_j(\vec{y}) \,,$$

$$(H - E_0)U_j(\vec{y})|\psi_0\rangle = [H, U_j(\vec{y})]|\psi_0\rangle \,,$$

the "states" $|\psi_n\rangle$ appearing in the expansion, Eq. (12), can be simply expressed in terms of the ground state $|\psi_0\rangle$:

$$|\psi_1\rangle = i\int_0^x [H(\vec{r}_j - \vec{y}) - E_0]\,dy\,|\psi_0\rangle = i\int_0^x U_j(\vec{y})\,dy\,|\psi_0\rangle \,, \quad (14)$$

$$|\psi_2\rangle = i^2 \int_0^x dy [H(\vec{r}_j - \vec{y}) - E_0] \times \int_0^y dy'\,[H(\vec{r}_j - \vec{y}\,') - E_0]|\psi_0\rangle = i^2 \int_0^x dy \int_0^y dy' \{U_j(\vec{y})U_j(\vec{y}\,') + [H, U_j(\vec{y}\,')]\}|\psi_0\rangle \quad (15)$$

and so on. In the discussion which follows, explicit expressions for other $|\psi_n\rangle$ are not needed.

At this point we recall that in the separation of $S(k, \omega)$ into an incoherent (i) and a coherent (c) part,

$$S(k, \omega) = S^i(k, \omega) + S^c(k, \omega) \,. \quad (16)$$

The incoherent part $S^i(k, \omega)$ is obtained by summing, in Eq. (3), only those terms having $j = l$; the coherent part $S^c(k, \omega)$ is the sum of the remaining $j \neq l$ terms. The substitution of Eq. (12) into Eq. (11) thus yields a series for coherent and incoherent parts of $S(k, \omega)$:

$$2\pi v_k S^i(k, \omega) = \sum_{n=0}^{\infty} (1/v_k)^n F_n{}^i(\Omega) \,, \quad (17)$$

$$2\pi v_k S^c(k, \omega) = \sum_{n=0}^{\infty} (1/v_k)^n F_n{}^c(k, \Omega) \,, \quad (18)$$

where

$$N F_n{}^i(\Omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \textstyle\sum_j \langle\psi_0| e^{i\vec{x}\cdot\vec{p}_j}|\psi_n\rangle \,, \quad (19)$$

$$N F_n{}^c(k, \Omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \times \sum_{j\neq l} \langle\psi_0| e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)} e^{i\vec{x}\cdot\vec{p}_j}|\psi_n\rangle \,. \quad (20)$$

The energy transfer ω appears in both incoherent and coherent series expansions only through the variable $\Omega = (\omega - \omega_k)/v_k$. A simple physical interpretation of this quantity is provided in the discussion of the impulse approximation, given after Eq. (25) below.

The momentum transfer k appears in $S^i(k, \omega)$ as a power series in k^{-1}, the expansion coefficients depending only on the variable Ω. The coefficients of k^{-1} in $S^c(k, \omega)$ depend not only on Ω, but also on k through the phase factor $e^{i\vec{k}\cdot(\vec{r}_j - \vec{r}_l)}$. For large momentum transfer k, we expect rapid oscillations in this phase factor which will result in very small coherent contributions. Thus at large momentum transfer, the dynamic structure factor $S(k, \omega)$ can be well approximated by retaining only the first few terms of Eq. (17).

We now proceed to evaluate the first few expansion functions F_n. It will be seen that $F_0{}^i$ is intimately related to the single-particle momentum distribution, and thus to the one-particle density matrix. Next, two-particle correlations will be shown to be represented by $F_0{}^c$ and $F_1{}^i$, for which description the two-particle density matrix is required. Progressing in this fashion, one sees that successively higher-order terms in the preceding series describe the participation of increasing number of particles in the system response characterized by $S(k, \omega)$.

III. EVALUATION OF TERMS

We first evaluate $F_0{}^i$. In Eq. (19) replace the sum of N terms by a single term multiplied by N. We then have

$$F_0{}^i(\Omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \langle \psi_0 | e^{i\vec{x}\cdot\vec{p}_1} | \psi_0 \rangle \ .$$

Letting φ_0 be the real-valued ground-state wave function, this becomes

$$F_0{}^i(\Omega) = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \int \cdots \int d^3r_1 d^3r_2 \cdots d^3r_N \times \varphi_0(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)\varphi_0(\vec{r}_1+\vec{x}, \vec{r}_2, \ldots, \vec{r}_N)$$
$$= N^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \int d^3r_1 \rho_1(\vec{r}_1, \vec{r}_1+\vec{x}) \ , \quad (21)$$

where $\rho_1(\vec{r}_1, \vec{r}_1+\vec{x}) = \langle \psi^+(\vec{r}_1)\psi(\vec{r}_1+\vec{x})\rangle$ is the one-particle density matrix. Since, by translational invariance of the ground state this is independent of $\vec{r}_1$, the term $F_0{}^i$ can be written as

$$F_0{}^i(\Omega) = \rho^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \rho_1(0, x) \ . \quad (22)$$

In order to obtain a relation between $F_0{}^i$ and the ground-state momentum distribution n_p, we evaluat the expectation value in Eq. (22) in momentum representation:

$$\rho_1(0, x) = V^{-1} \sum_p N_p e^{i\vec{p}\cdot\vec{x}} \ ,$$

where V is the volume of the system and N_p is the number of atoms with momentum p. Then

$$F_0{}^i = 2\pi n_0 \delta(\Omega) + (2\pi\rho)^{-1} \int_{|\Omega|}^{\infty} p n_p dp \ , \quad (23)$$

where n_0 is the condensate fraction, and $n_p = N_p/N$. Comparing this result with Eqs. (6)–(8) of Ref. 3, combined here as

$$S^{IA}(k, \omega) = (n_0/v_k)\delta(\Omega) + (4\pi^2\rho v_k)^{-1}\int_{|\Omega|}^{\infty} p n_p dp \ , \quad (24)$$

we see that

$$S^{IA}(k, \omega) = (2\pi v_k)^{-1} F_0{}^i(\Omega) \ .$$

Thus the impulse approximation is given by the first term of the series expansion (17) of the incoherent part of $S(k, \omega)$. Reference 3 gave a pictorial description of the events described in $S^{IA}(k,\omega)$ which identified the variable $|\Omega|$ in Eq. (24) (called $p_{\min}$ in Ref. 3) as the magnitude of the smallest helium momentum parallel to $\vec{k}$ which will give the neutron the energy loss ω.

We next consider $F_0{}^c$. The double sum in Eq. (20) is replaced by a single term multiplied by the number $N(N-1)$ of such terms. Then

$$F_0{}^c(k, \Omega) = (N-1)\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \langle \psi_0 | e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} e^{i\vec{x}\cdot\vec{p}_1} | \psi_0 \rangle . \quad (25)$$

The expectation value in Eq. (25) is

$$\langle \psi_0 | e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} e^{i\vec{x}\cdot\vec{p}_1} | \psi_0 \rangle = \int \cdots \int d^3r_1 \cdots d^3r_N \times e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} \varphi_0(\vec{r}_1, \ldots, \vec{r}_N)\varphi_0(\vec{r}_1+\vec{x}, \ldots, \vec{r}_N)$$
$$= [N(N-1)]^{-1}\int d^3r_1 d^3r_2 e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} \times \rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2) \ , \quad (26)$$

where $\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2)$ stands for the two-particle density matrix:

$$\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2) = \langle \psi^\dagger(\vec{r}_1)\psi^\dagger(\vec{r}_2)\psi(\vec{r}_1+\vec{x})\psi(\vec{r}_2)\rangle \ . \quad (27)$$

So, then we have

$$F_0{}^c(k, \Omega) = N^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \int d^3r_1 d^3r_2 e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)} \times \rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2)$$
$$= \rho^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \int d^3r\, e^{i\vec{k}\cdot\vec{r}} \times \rho_2(\vec{r}, 0; \vec{r}+\vec{x}, 0) \ . \quad (28)$$

The Fourier transform of the sum of the two quantities calculated thus far is of fundamental significance. Equation (8) shows that at $t=0$, the only nonzero contributions to $S(k, t=0) = \int_{-\infty}^{\infty} S(k,\omega)d\omega$ are those from $F_0{}^i$ and $F_0{}^c$. Taking the Fourier transforms of these quantities, we therefore have

$$S(k) = S(k, t=0)$$
$$= 1 + \rho^{-1}\int d^3r\, e^{i\vec{k}\cdot\vec{r}} \rho_2(\vec{r}, 0; \vec{r}, 0)$$
$$= 1 + \rho\int d^3r\, e^{i\vec{k}\cdot\vec{r}}[g(r)-1] + N\delta_{k,0} \ , \quad (29)$$

where $S(k)$ is the static structure factor, and

$$g(r) = \rho_2(\vec{r}, 0; \vec{r}, 0)/\rho^2$$

is the pair-correlation function. Now for large k, $S(k) \approx 1$,[6] so the above result supports the previous suggestion that at large momentum transfer the coherent contribution will be quite small in comparison with the incoherent one.

We now proceed to the evaluation of the next function, $F_1{}^i$. From Eqs. (14) and (19),

$$NF_1{}^i(\Omega) = i\int_{-\infty}^{\infty} dx\, e^{-i\Omega x} \sum_j \langle \psi_0 | e^{i\vec{x}\cdot\vec{p}_j} \times \int_0^x \sum_{m\neq j} [V(\vec{r}_j - \vec{y}, \vec{r}_m) - V(\vec{r}_j, \vec{r}_m)] dy | \psi_0 \rangle \ . \quad (30)$$

Again we replace the sums over j and m by a single term multiplied by $N(N-1)$. The expectation value appearing in that term is

$$\langle \psi_0 | e^{i\vec{x}\cdot\vec{p}_1} \int_0^x [V(\vec{r}_1 - \vec{y}, \vec{r}_2) - V(\vec{r}_1, \vec{r}_2)] dy | \psi_0 \rangle$$
$$= \int \cdots \int d^3r_1 \cdots d^3r_N \varphi_0(\vec{r}_1, \ldots, \vec{r}_N) \int_0^x dy [V(\vec{r}_1+\vec{x}-\vec{y}, \vec{r}_2) - V(\vec{r}_1+\vec{x}, \vec{r}_2)] \varphi_0(\vec{r}_1+\vec{x}, \vec{r}_2, \ldots, \vec{r}_N)$$
$$= [N(N-1)]^{-1}\int d^3r_1 d^3r_2 \rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2) \int_0^x dy [V(\vec{r}_1+\vec{y}, \vec{r}_2) - V(\vec{r}_1+\vec{x}, \vec{r}_2)] \ .$$

Substituting this into Eq. (30) we obtain

$$F_1{}^i(\Omega) = i\rho^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\int d^3r\, \rho_2(\vec{r},\ 0,\ \vec{r}+\vec{x},\ 0) \times \int_0^x dy[V(\vec{r}+\vec{y}) - V(\vec{r}+\vec{x})]\ . \quad (31)$$

The coherent part of F_1, $F_1{}^c$, is obtained from Eqs. (14) and (20). It is clear from these equations that $F_1{}^c$ now contains in general three distinct particle coordinates: two coordinates $\vec{r}_j$, $\vec{r}_l$ coming from the factor $e^{i\vec{k}\cdot(\vec{r}_j-\vec{r}_l)}$ in Eq. (20) and a third coordinate $\vec{r}_m$ from the potential energy of interaction. Such terms will involve the three-particle density matrix, and we neglect these, by choosing $\vec{r}_m = \vec{r}_l$. Then, repeating the steps leading to Eq. (31) for $F_1{}^i$, we get the same expression for $F_1{}^c$, except that a factor $e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}$ must be inserted in the integral. The total contribution of coherent and incoherent terms in F_1 is therefore

$$NF_1 \cong i\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\int d^3r_1 d^3r_2\, \rho_2(\vec{r}_1,\ \vec{r}_2;\ \vec{r}_1+\vec{x},\ \vec{r}_2) \times (1+e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}) \times \int_0^x dy[V(\vec{r}_1+\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)]\ . \quad (32)$$

Finally, we consider the term F_2 given by Eqs. (15), (19), and (20). That part of $|\psi_2\rangle$ in Eq. (15) quadratic in the interactions $V(\vec{r}_i,\ \vec{r}_j)$ yields a contribution to F_2 which we call $F_2{}^q$. Utilizing the same procedure as in obtaining F_1, it can be written in the form

$$NF_2{}^q = i^2\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\int d^3r_1 d^3r_2 (1+e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)})\,\rho_2(\vec{r}_1,\ \vec{r}_2,\ \vec{r}_1+\vec{x},\ \vec{r}_2) \times \int_0^x dy[V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)]\int_0^y dy'[V(\vec{r}_1+\vec{x}-\vec{y}\,',\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)]\ . \quad (33)$$

In obtaining Eq. (33) we have again neglected terms involving three-particle correlations and also terms involving four-particle correlations.

The second-term on the right-hand side of Eq. (15) involves the commutator $[H,\ U_j(y)]$ which can be expressed as

$$[H,\ U_j(\vec{y})] = (2m)^{-1}[p_j{}^2,\ U_j(\vec{y})] = -(2m)^{-1}[\nabla_j{}^2 U_j(\vec{y}) + 2\vec{\nabla}_j U_j(\vec{y})\cdot\vec{\nabla}_j].$$

This term contributes a factor $F_2{}^l$ to F_2:

$$NF_2{}^l = -i^2(2m)^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\int d^3r_1 d^3r_2 (1+e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)})\int_0^x dy\,(x-y) \times\{\rho_2(\vec{r}_1,\ \vec{r}_2;\ \vec{r}_1+\vec{x},\ \vec{r}_2)\,\nabla_1{}^2[V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)] + 2(\vec{\nabla}_1[V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)])\cdot[\vec{\nabla}_1'\rho_2(\vec{r}_1,\ \vec{r}_2,\ \vec{r}_1'+\vec{x},\ \vec{r}_2)]|_{\vec{r}_1'=\vec{r}_1}\}\ . \quad (34)$$

The results of this section are summarized with the formulas

$$2\pi v_k S(k,\ \omega) = F_0 + (i/v_k)F_1 + (i/v_k)^2 F_2 + \cdots\ , \quad (35)$$

$$NF_0 = \int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\ \int d^3r_1\,\rho_1(\vec{r}_1,\ \vec{r}_1+\vec{x}) + \int d^3r_1 d^3r_2\, e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)}\,\rho_2(\vec{r}_1,\ \vec{r}_2,\ \vec{r}_1+\vec{x},\ \vec{r}_2)]\ , \quad (36)$$

$$NF_1 \cong i\int_{-\infty}^{\infty} dx e^{-i\Omega x}\int d^3r_1 d^3r_2\ (1+e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)})\,\rho_2(\vec{r}_1,\ \vec{r}_2;\ \vec{r}_1+\vec{x},\ \vec{r}_2)\int_0^x dy\,[\,V(\vec{r}_1+\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2],\quad (37)$$

$$NF_2 \cong i^2\int_{-\infty}^{\infty} dx e^{-i\Omega x}\int d^3r_1 d^3r_2\,(1+e^{i\vec{k}\cdot(\vec{r}_1-\vec{r}_2)})\,\{(\rho_2(\vec{r}_1,\ \vec{r}_2;\vec{r}_1+\vec{x}_1,\vec{r}_2) \times \int_0^x dy\,[\,V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+x,\ \vec{r}_2)]\int_0^y dy'\,[\,V(\vec{r}_1+\vec{x}-\vec{y}\,',\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)\,] - (2m)^{-1}\int_0^x dy\,(x-y)\ \nabla_1{}^2[\,V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)\,]) - m^{-1}\int_0^x dy\,(x-y)\,(\vec{\nabla}_1[\,V(\vec{r}_1+\vec{x}-\vec{y},\ \vec{r}_2) - V(\vec{r}_1+\vec{x},\ \vec{r}_2)\,])\cdot\vec{\nabla}_1'\rho_2(\vec{r}_1,\ \vec{r}_2,\ \vec{r}_1'+\vec{x},\ \vec{r}_2)|_{\vec{r}_1'=\vec{r}_1}\}. \quad (38)$$

For a free-particle system, only F_0 given by Eq. (36) is nonzero. The second term in this equation in momentum representation modifies the factor n_p appearing in Eq. (24) to $n_p(1 \pm n_{|\vec{p}+\vec{k}|})$, the plus sign for bosons and the minus sign for fermions. This, of course, is the proper factor for excitation of a free particle from momentum $\vec{p}$ to one of momentum $\vec{p}+\vec{k}$.

This formulation of corrections to the impulse approximation appears to be applicable to any system for which the particle motions are nonrelativistic.[8] The correction terms given above are not quite exact, in that we have neglected contributions from three- and four-particle correlations.

This neglect appears to be equivalent to the ladder approximation in a graphical representation of the effect of interactions on $S(k, \omega)$. Evaluation of these correction terms requires knowledge of both the interparticle interactions and also the off-diagonal elements of the ground-state two-particle density matrix.

IV. NUMERICAL RESULTS

In this section we determine the effects of the above correction terms on the cross section for the inelastic scattering of neutrons from superfluid helium at momentum transfer $k = 14.3$ Å^{-1}. Three effects are produced: (a) a shift in the peak of $S(k, \omega)$ from the location $\omega_k = k^2/2m$ of the impulse approximation, (b) the introduction of a very slight shape asymmetry about the new peak location, and (c) the broadening, from the δ function given in the impulse approximation, of the condensate contribution to $S(k, \omega)$.

Effects (a) and (b) above are produced by the incoherent part of F_1, given in Eq. (31). Consider a pictorial description of the events which this term describes. One of the two interacting helium particles (1 in our notation) is struck by a neutron, acquires a velocity $\vec{v}_k$ which we take to be along the z axis, and travels a distance $x = v_k t$ in time t. The term F_1 describes a single scattering of this helium particle 1 with its neighbor 2 during this excursion through the distance x, the scattering occurring at any distance from zero to x. This intermediate distance is represented by the coordinate y in Eq. (37), and the integral over y measures the change in the potential energy of a pair of helium atoms because of their relative motion. This potential-energy change, brought about by a displacement x of a helium atom, clearly depends on the angle between $\vec{x}$ (taken to be along z) and the relative coordinate $\vec{r}_1 - \vec{r}_2$, the change being most drastic for a given value of $\vec{x}$ when this angle is zero.
(head-on collision of two helium atoms). The helium-helium potential energy $V(\vec{r}_1, \vec{r}_2)$, which we represent by the Lennard-Jones potential, has essentially a hard core, becoming highly repulsive for interhelium separations less than a distance $r_0 \approx 2.0$ Å. Final configurations having interparticle separations less than r_0 are removed from the integral in F_1 by the density matrix $\rho_2(\vec{r}_1, \vec{r}_2, \vec{r}_1 + \vec{x}, \vec{r}_2)$, which prevents displacements x which bring the two helium atoms within this hard-core region. However, it is still possible to have intermediate y coordinates in F_1 for which $V(\vec{r} + \vec{y})$ is unphysically large. For example, with $\vec{r}_1 - \vec{r}_2$ in the negative z direction, we can choose an $\vec{x}$ (along z) larger than $2r_0$ so that although $\vec{r}_1 + \vec{x} - \vec{r}_2$ is outside the hard-core region, hence allowed by ρ_2, the smaller distance $\vec{r}_1 + \vec{y} - \vec{r}_2$ may be inside the hard-core region, with nothing in F_1 to remove such unphysical configurations. Their removal would apparently require considering the entire sequence of terms F_n for all n, and summing their contributions to build up the necessary two-particle correlations which prevent core penetration at intermediate distances y. We will assume that if one could carry out this difficult program, the result would be simply to limit all intermediate distances y to values such that $\vec{r}_1 + \vec{y} - \vec{r}_2$ also remains outside the hard-core region, and hence we will add this restriction to the integral over y in F_1. Since in our final form, values for x which contribute measurably to F_1 are considerably less than the distance $2r_0$ at which the above trouble arises, little effect on our final results should come from this imposed restriction on y. We proceed to approximate the density matrix $\rho_2(\vec{r}_1, \vec{r}_2, \vec{r}_1 + \vec{x}, \vec{r}_2)$ first for small interparticle separations, then for large-particle separations, and finally, we choose a form which includes both regions.

Viewing ρ_2 as a scalar product in $(N-2)$-particle Fock space,

$$\rho_2 = (\langle \varphi_0 | \psi^\dagger(\vec{r}_1) \psi^\dagger(\vec{r}_2)) \, (\psi(\vec{r}_1 + \vec{x}) \psi(\vec{r}_2) | \varphi_0 \rangle),$$

the Schwartz inequality yields

$$|\rho_2| \le \langle \varphi_0 | \psi^\dagger(\vec{r}_1) \psi^\dagger(\vec{r}_2) \psi(\vec{r}_2) \psi(\vec{r}_1) | \varphi_0 \rangle^{1/2} \times \langle \varphi_0 | \psi^\dagger(\vec{r}_2) \psi^\dagger(\vec{r}_1 + \vec{x}) \psi(\vec{r}_1 + \vec{x}) \psi(\vec{r}_2) | \varphi_0 \rangle^{1/2} .$$

Assuming that the ground state of liquid helium can be represented by an everywhere positive wave function, one can remove the absolute value symbol, yielding

$$\rho_2(\vec{r}_1, \vec{r}_2, \vec{r}_1 + \vec{x}, \vec{r}_2) \le \rho^2 g^{1/2}(\vec{r}_1, \vec{r}_2) g^{1/2}(\vec{r}_2, \vec{r}_1 + \vec{x}) . \quad (39)$$

When $x = 0$, the inequality in Eq. (39) becomes an equality. The equality would also hold for any two-particle system with an everywhere positive wave function, for which case the right-hand side is just the product of the two-particle ground-state wave functions $\varphi_0(\vec{r}_1, \vec{r}_2) \varphi_0(\vec{r}_1 + \vec{x}, \vec{r}_2)$, which is equal to ρ_2 by definition. For these reasons we expect the right-hand side of Eq. (39) to be a good approximation to ρ_2 for small values of x and all values of $\vec{r}_1 - \vec{r}_2$.

For large values of $|\vec{r}_1 - \vec{r}_2|$ and $|\vec{r}_1 + \vec{x} - \vec{r}_2|$, we expect ρ_2 to be given by the Hartree-Fock approximation

$$\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1 + \vec{x}, \vec{r}_2) \cong \rho \rho_1(\vec{r}_1, \vec{r}_1 + \vec{x}) + \rho_1(\vec{r}_1, \vec{r}_2) \rho_1(\vec{r}_2, \vec{r}_1 + \vec{x}). \quad (40)$$

The one-particle density matrices appearing in Eq. (40) can be evaluated utilizing a Gaussian fit to the ground-state momentum distribution, $n_p = 0.45 \, e^{-ap^2}$, with $a = 0.642$ Å^2.[3] Then

$$\rho(\vec{r}_1, \vec{r}_1 + \vec{x}) = V^{-1} \textstyle\sum_p N_p e^{i \vec{p} \cdot \vec{x}} = \rho_0 + \rho \, e^{-x^2/4a} , \quad (41)$$

where we neglect the difference between $\rho' = \rho - \rho_0$ ($\rho_0 = N_0/V$) and ρ in the second term on the right-hand side of Eq. (41). The exchange term in the Hartree-Fock approximation is

$$\rho_1(\vec{r}_1, \vec{r}_2)\,\rho_1(\vec{r}_2, \vec{r}_1+\vec{x}) = \rho_0^2 + \rho_0\,\rho\,(e^{-(\vec{r}_1-\vec{r}_2)^2/4a} + e^{-(\vec{r}_1-\vec{r}_2+\vec{x})^2/4a}) + \rho^2 e^{-(\vec{r}_1-\vec{r}_2)^2/4a}\, e^{-(\vec{r}_1-\vec{r}_2+\vec{x})^2/4a} . \quad (42)$$

This is small compared to the first term on the right-hand side of Eq. (40) and we neglect it, so that the large distance behavior of ρ_2 is taken to be

$$\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2) \cong \rho\,\rho_0 + \rho^2 e^{-x^2/4a} . \quad (43)$$

Noting that the correlation functions in the small-distance approximation of Eq. (39) both approach unity as their arguments increase, we see that we can join the noncondensate large distance part of ρ_2 given by Eq. (43) smoothly on the small-distance approximation of Eq. (39) with the single approximation for all distances,

$$\rho_2(\vec{r}_1, \vec{r}_2; \vec{r}_1+\vec{x}, \vec{r}_2) = \rho^2 g^{1/2}(\vec{r}_1, \vec{r}_2)\, g^{1/2}(\vec{r}_1+\vec{x}, \vec{r}_2)\, e^{-x^2/4a} . \quad (44)$$

To this we must add the condensate part, $\rho_2{}^c \cong \rho\,\rho_0$ valid only for large distances, $|\vec{r}_1 - \vec{r}_2| \rangle R$. Contributions to the scattering coming from this condensate part will be considered at the end of this section. Estimates[7] indicate that $g^{1/2}(r)$ is zero for $r \leq 2$ Å, then rises sharply to approach unity at $r \approx 3$ Å, and exhibits small rapidly damped oscillations about unity for $r \gtrsim 3$ Å. We will replace the above described behavior of $g^{1/2}(r)$ by a step function with a core radius of r_0,

$$g^{1/2}(r) = \theta(r - r_0) , \quad (45)$$

where $\theta(x) = 1$ for $x > 0$, zero otherwise. Thus we allow with equal probability amplitude any displacement of the interparticle separation of a pair of helium atoms outside of the hard core r_0, and prohibit any displacements which would penetrate the core. We subsequently treat the core radius r_0 as a fitting parameter.

Then $F_1{}^i$ is given by

$$F_1^i = 4\pi\rho \int_0^\infty dx\, \sin\Omega x e^{-x^2/4a} \int dr\, r^2 V(r) \int_0^x dy \int_{-1}^{+1} d\eta [\theta(r^2 + y^2 - 2ry\eta - r_0^2) \times \theta(r^2 + (x-y)^2 + 2r(x-y)\eta - r_0^2) - \theta(r^2 + x^2 - 2rx\eta - r_0^2)] , \quad (46)$$

where $\eta = \cos\varphi$, φ the angle between $\vec{r}$ and the z axis, which is the chosen direction of the momentum transfer $\vec{k}$. The integration over η and y is straightforward, but tedious. The following result is obtained:

$$F_1{}^i = 4\pi\rho \int_0^\infty dx e^{-x^2/4a} \sin\Omega x \int_{r_0}^{r_0+x} r^2 V(r) dr \times \left[\frac{r^2 - r_0^2}{r} \ln\frac{x}{r - r_0} + r - r_0 - x\right] . \quad (47)$$

Into this equation we substitute for $V(r)$ the Lennard-Jones potential[7]

$$V(r) = 4\epsilon\,[(\sigma/r)^{12} - (\sigma/r)^6] \quad (48)$$

($\epsilon = 10.22$ °K, $\sigma = 2.556$ Å). The subsequent integration over r is simplified by a cubic fit

$$(r - r_0)\ln\frac{r_0}{r - r_0} \cong C_0 + C_1 r + C_2 r^2 + C_3 r^3 \quad (49)$$

to the logarithmic term. The final integration over x is performed numerically using 20 terms of the power series expansion of $\sin\Omega x$, enabling $F_1{}^i$ to be expressed for a given value of r_0 as a polynomial in Ω.

The results of these calculations are presented graphically in Fig. 1, in which the leading correction $(2\pi\hbar v_k)^{-1} F_1{}^i(\Omega)$ to the quantity $v_k S^{IA}(k, \omega)$ is depicted as a function of Ω for values of r_0 between 2.0 and 2.4 Å. Since F_1 is an odd function of Ω, the correction term is represented for only positive values of Ω. Now $v_k S^{IA}(k, \omega)$ is an even function of Ω, so the dominant effect of the addition of this odd in Ω correction term is a shift in peak location:

$$v_k S(k, \omega) = v_k S^{IA}(k, \omega) + (2\pi\hbar v_k)^{-1} F_1{}^i(\Omega) \quad (50)$$

is a function which attains its maximum value, not at the free-particle energy ω_k of the impulse approximation, but instead at a lower energy ω_k' given by $(\omega_k' - \omega_k) = -|\Omega_k|\, v_k$, where Ω_k is that value of Ω at which $v_k S^{IA}(k, \omega)$ and $(2\pi\hbar v_k)^{-1} F_1{}^i(\Omega)$ have opposite slopes, i.e., from Eq. (24) Ω_k is the solution of

$$-(4\pi^2\rho)^{-1}\, p n_p \Big|_{p=|\Omega_k|} = (2\pi\hbar v_k)^{-1}\, dF_1(\Omega)/d\Omega \Big|_{\Omega=\Omega_k} . \quad (51)$$

Graphical analysis indicates that the solution Ω_k of this equation will be small, $\Omega_k \cong 0.1$ Å^{-1}. For these small values of Ω_k, both n_p for $p = \Omega_k$ and $dF_1/d\Omega$ can be replaced by their values at $\Omega_k = 0$. Then referring to the equation for n_p given immediately above Eq. (41), we have

$$\Omega_k = -\left[\frac{2\pi\rho m}{0.45\hbar^2}\left(\frac{dF_1}{d\Omega}\right)_0\right] \frac{1}{k} .$$

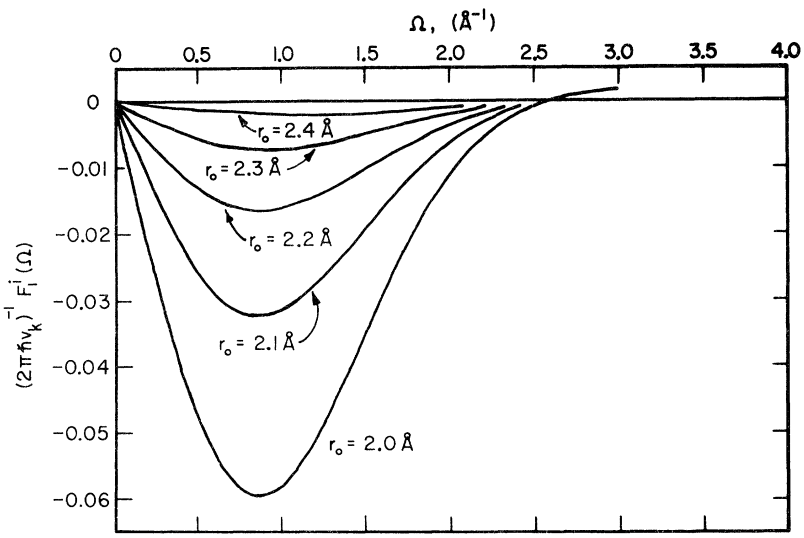

FIG. 1. The quantity $(2\pi\hbar v_k)^{-1} F_1{}^i(\Omega)$ given by Eq. (47) vs Ω for selected values of the hard-core radius r_0, and for $k=14.3$ Å^{-1}.

The absolute peak shift

$$\omega_k{}' - \omega_k = \Omega_k v_k \tag{52}$$

is thus independent of k, whereas the fractional peak shift

$$(\omega_k{}' - \omega_k)/\omega_k = 2\Omega_k/k \tag{53}$$

is proportional to k^{-2}.

In the above discussion, the quantities ω_k' and Ω_k depend upon the still undetermined core radius r_0. The value of this adjustable parameter is chosen to be $r_0 = 2.1$ Å by requiring that Eq. (52) reproduce the mean peak shift $\omega_k' - \omega_k \approx -12$ °K observed for $4 \lesssim k \lesssim 9$ Å^{-1} by Cowley and Woods.[5] Then at the higher momentum transfer $k = 14.3$ Å^{-1}, Eq. (53) predicts a fractional peak shift $|\omega_k' - \omega_k|/\omega_k \approx 1\%$, which is in agreement with the 0.6% shift reported by Harling.[4]

Having fixed r_0 at 2.1 Å, we can assess the asymmetry in $S(k,\omega)$ produced by the F_1 term. In Fig. 2 we show, as a line of long dashes, the noncondensate contribution to $v_k S^{IA}(k,\omega)$ vs Ω obtained in Ref. (3) using McMillan's n_p values.[7] The short-dashed line in the figure is the quantity $(2\pi\hbar v_k)^{-1} F_1{}^i(\Omega)$ for $r_0 = 2.1$ Å and $k = 14.3$ Å^{-1}, and the sum of these two quantities is the total $v_k S(k,\omega)$ represented by the solid line in Fig. 2. The asymmetry in $S(k,\omega)$ about its shifted peak position is very slight, and probably within experimental resolution.

Finally, we estimate the condensate broadening. We have up until now ignored the effects of final-state interactions on the condensate contribution coming from the first term on the right-hand side of Eq. (43) for ρ_2, $\rho\rho_0$, which should hold for interparticle separations larger than some value R. One procedure for accounting for these would be to work out the contributions coming from F_1 and F_2 in Eqs. (37) and (38) using a series expansion of the potential difference term $V(\vec{r}+\vec{x}-\vec{y}) - V(\vec{r}+\vec{x})$ in powers of x and y. Integration over the volume yields a power series in x multiplied by the factor $e^{-i\Omega x}$, which then has to be integrated over x through-

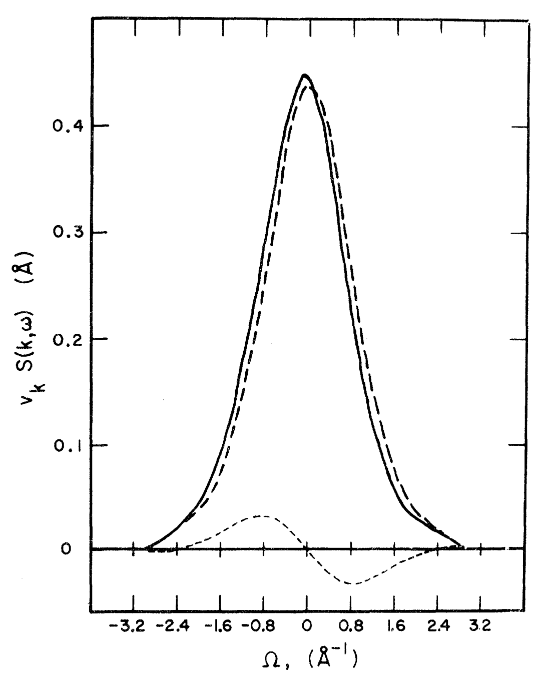

FIG. 2. Graph of $v_k S(k,\omega)$ vs $\Omega = (\omega - \omega_k)/v_k$. Long-dashed line is the impulse approximation, $v_k S^{IA}(k,\omega)$, omitting the condensate contribution, and utilizing the computer results of Ref. 7 for n_p. Short-dashed line is $(2\pi\hbar v_k)^{-1} F_1{}^i(\Omega)$, the correction to the impulse approximation for $r_0 = 2.1$ Å, and $k = 14.3$ Å^{-1}. The solid line is the sum of these two.

out the x region in which the series expansion is valid. The effects on the condensate given in the impulse approximation by a δ function are both a shift in the position of the peak (induced by terms odd in x) and an alteration of its shape (by terms even in x).

A simpler procedure is obtained by summing all contributions not involving derivatives of the potentials or density matrices [for example, neglect the last two terms in Eq. (38)].[9] This sum is simply an exponential, and yields a total correction term $\tilde{S}_0(k,\Omega)$ for the condensate part $S_0(k,\omega)$ given by

$$2\pi\tilde{S}_0(k,\Omega)=\rho_0 v_k^{-1}\int_{-\infty}^{\infty} dx e^{-i\Omega x}\int_{r>R} d^3r \times\left(\exp\{(i/v_k)\int_0^x [V(\vec{r}+\vec{x}-\vec{y})-V(\vec{r}+\vec{x})]\,dy\}-1\right). \tag{54}$$

We now assume that at large r, where $V(r)$ varies relatively slowly, a sufficiently good approximation to the exponential term is obtained by the first term in a series expansion of the difference in potential in powers of x and y:

$$\int_0^x dy\,[V(\vec{r}+\vec{x}-\vec{y})-V(\vec{r}+\vec{x})]\cong -\frac{x^2}{2}\frac{dV}{dr}\eta, \tag{55}$$

where η is the cosine of the angle between $\vec{r}$ and the z axis. Integrating over this angle yields the result

$$2\pi\tilde{S}_0(k,\Omega)=\rho_0 v_k^{-1}\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\int_R 4\pi r^2\,dr \times\left[\frac{\sin(\alpha x^2 dV/dr)}{(\alpha x^2 dV/dr)}-1\right], \tag{56}$$

where $\alpha=(2v_k)^{-1}$. Since all except large values of r are excluded from the above integration, we neglect effects of short-range repulsive forces and use for $V(r)$ only the attractive tail of the Lennard-Jones: $V(r)\cong -4\epsilon(\sigma/r)^6$. The r integration in Eq. (56) is performed by expanding the above quantity in square brackets in a power series and integrating term by term:

$$\int_R^{\infty} r^2 dr\left[\frac{\sin(\alpha x^2 dV/dr)}{\alpha x^2 dV/dr}-1\right] = R^3\sum_{n=1}^{\infty}\frac{(-1)^n}{(14n-3)(2n+1)!}(\alpha x^2 dV/dR)^{2n} \cong CR^3\left[\frac{\sin(\alpha x^2 dV/dR)}{\alpha x^2 dV/dR}-1\right]. \tag{57}$$

The approximation in Eq. (57) is suggested by the observation that, except for the factor $(14n-3)^{-1}$ in the nth term, the sum appearing in the first line of this equation is precisely the power-series expansion of the quantity in square brackets in the second line. In making this approximation, we have assumed that the quantity $\alpha x^2 dV/dR$ is small in comparison with unity, but this assumption appears to be no worse than that made in obtaining Eq. (55). Some attempt is made to adjust for the extraneous factors $(14n-3)^{-1}$ by introducing an over-all multiplicative constant C; inspection of the leading term indicates $C\approx 1/11$.

Combining Eqs. (56) and (57) we obtain the correction $2\pi v_k\tilde{S}_0(k,\Omega)$

$$= n_0\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}\,4\pi\rho CR^3\left[\frac{\sin(\alpha x^2 dV/dR)}{\alpha x^2 dV/dR}-1\right] \tag{58}$$

which is seen to be zero for a noninteracting system. This final-state condensate contribution is to be added to the corresponding impulse-approximation quantity

$$2\pi v_k S_0^{IA}(k,\Omega)=n_0\int_{-\infty}^{\infty} dx e^{-i\Omega x}. \tag{59}$$

The δ function of the impulse approximation will therefore be removed by the (-1) term in square brackets of Eq. (58) provided that the parameters C and R satisfy

$$4\pi\rho CR^3=1. \tag{60}$$

The following discussion bases the choice of R upon certain physical considerations. This value of R, when substituted into Eq. (60), yields a value of C which agrees well with our previous estimate of this adjustment parameter.

The total condensate contribution to $S(k,\omega)$ is thus given by

$$2\pi v_k S_0(k,\Omega)=n_0\int_{-\infty}^{\infty} dx\, e^{-i\Omega x}(\sin ax^2)/ax^2, \tag{61}$$

where $a=(2v_k)^{-1}(dV/dR)$. The approximations introduced in Eqs. (55) and (57) appear to enhance the oscillatory character of the integrand in Eq. (61). Qualitatively, one expects the integral in Eq. (57) to be a maximum at $x^2=0$, and to fall off to very small values for an x^2 value which makes the sine function go to zero, i.e., $x^2=2\pi v_k/(dV/dR)$. Our result has this behavior but in addition predicts small oscillations in x, and consequently, in Ω. The integral in Eq. (61) can be evaluated in closed form, and the result is[10]

$$2\pi v_k S_0(k,\Omega)=n_0\left\{\frac{|\Omega|}{a}\pi\left[S\left(\frac{|\Omega|}{2\sqrt{a}}\right)-C\left(\frac{|\Omega|}{2\sqrt{a}}\right)\right]+\frac{2}{a}(a\pi)^{1/2}\sin\left(\frac{\Omega^2}{4a}+\frac{\pi}{4}\right)\right\}, \tag{62}$$

where S and C are Fresnel integrals,

$$S(x)=\frac{2}{(2\pi)^{1/2}}\int_0^x \sin t^2\,dt, \qquad C(x)=\frac{2}{(2\pi)^{1/2}}\int_0^x \cos t^2\,dt. \tag{63}$$

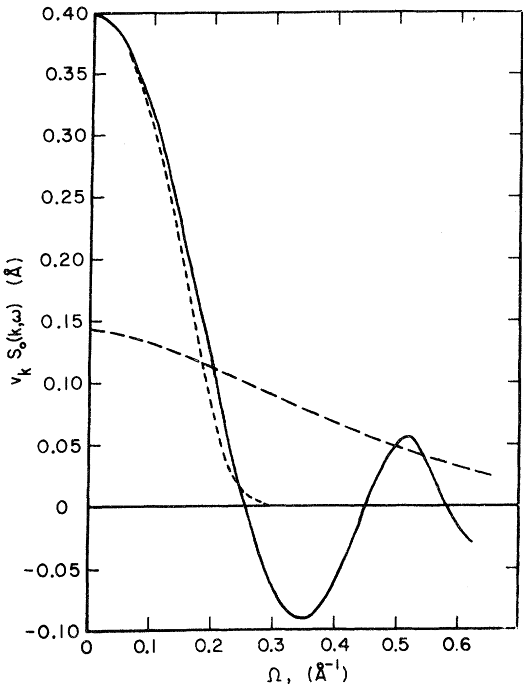

FIG. 3. Condensate contribution $v_k S_0(k, \omega)$ for $k = 14.3$ Å^{-1}. The long-dashed line is the phenomenological lifetime broadened δ function [Eq. (18) of Ref. 3]. Solid curve is Eq. (62). Short-dashed line is obtained from solid curve as described in the text.

Numerical evaluation of $S_0(k, \Omega)$ requires a choice of the distance R at which ρ_2 is well approximated by its asymptotic form. We select R by asking for a distance at which the pair correlation $g(r)$ given by computer calculations is within, for example, 10% of its asymptotic value [we may invoke the same criterion for the normalized one-particle density matrix $\rho_1(0, r)/\rho$ with approximately the same result].[7] This criterion sets $R \gtrsim 4$ Å, and we take $R = 4$ Å, which yields the largest dV/dR, and hence overestimates the condensate broadening. The condensate fraction ρ_0/ρ is chosen to be 0.11, consistent with computer results of Ref. (7).

A plot of $v_k S_0(k, \omega)$ vs Ω, shown in Fig. 3 as a solid line, exhibits the expected damped oscillations for increasing values of Ω. For comparison purposes, we show as a long-dashed line the phenomenologically lifetime-broadened $v_k S_0(k, \omega)$ previously utilized in Ref. 3. We arbitrarily remove the oscillations by replacing the solid line curve by the short-dashed line. This latter curve is drawn using the fact that the total area under the curve is fixed by the condensate fraction.

Finally, we combine the condensate contribution to $v_k S_0(k, \omega)$ (short-dashed line of Fig. 3) with the noncondensate contribution (solid line of Fig. 2) to get the total $v_k S(k, \omega)$ shown in Fig. 4. We have assumed that the peak of the condensate contribution is shifted equally with that of the noncondensate contribution.

In Ref. 3, a detailed comparison was made between the experimental inelastic cross section for neutron scattering from helium at 1.265 °K and theoretical predictions of the impulse approximation (see Fig. 7 of Ref. 3). That comparison indicated that the experimental data were consistent with a very small value for the condensate fraction, and we placed an upper limit of 3% on this quantity.

The only discernible change in that comparison which is introduced by the present treatment is the sharpening of the condensate contribution over the previous lifetime-broadened estimate. Figure 5 shows the experimental data of Harling[4] and the theoretical prediction, including experimental resolution broadening. The instrumental resolution function has a full width at half-maximum $\Delta E = 3.4$ meV. As Fig. 5 indicates, the distinct condensate contribution evident in the dynamic structure factor of Fig. 4 is so broadened by instrumental resolution that in the scattering cross section it cannot be distinguished from the noncondensate contribution. However, it is evident that the theoretical condensate fraction $n_0 = 0.11$ is too large. The discrepancy between theory and experiment can be removed by arbitrarily reducing the condensate

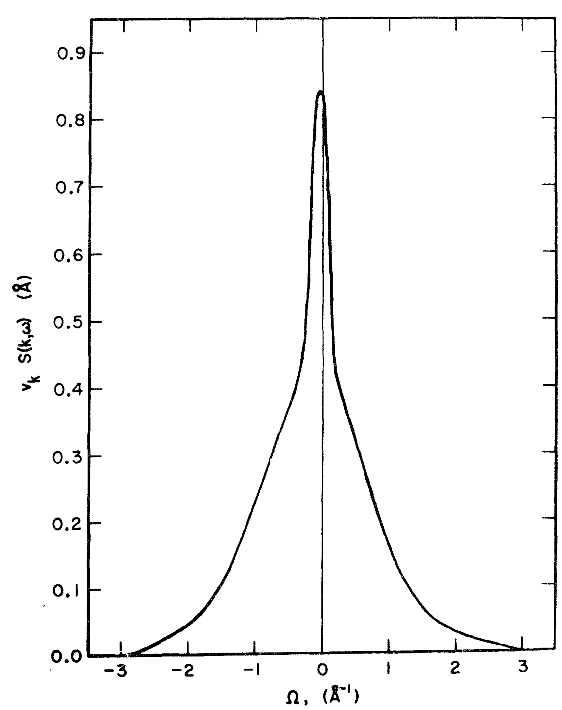

FIG. 4. Total $v_k S(k, \omega)$ for $k = 14.3$ Å^{-1}, including final state corrections and a condensate fraction $n_0 = 0.11$.

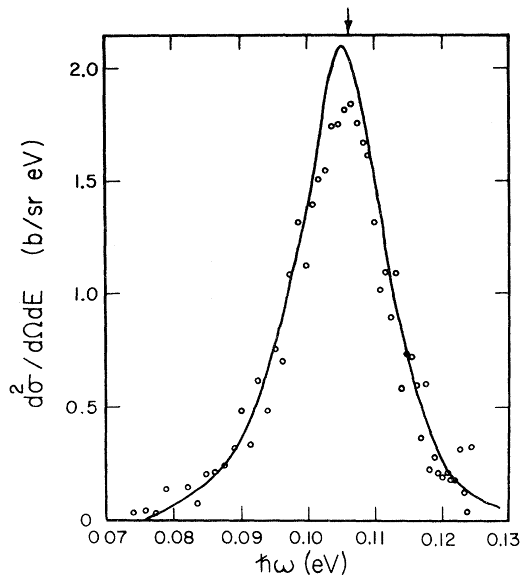

FIG. 5. Inelastic cross section for neutrons on He^4 liquid at 1.265 °K vs energy transfer $\hbar\omega$. Circles are the experimental data from Ref. 4. Solid line is present calculation which includes a condensate fraction $n_0 = 0.11$. The arrow on the top locates ω_k, the free-particle peak.

fraction to a much smaller value, which we estimate to be somewhat less than the value $n_0 = 0.03$ we previously found in Ref. 3.

It would clearly be desirable to preserve, in the predicted resolution-broadened inelastic cross section, the distinct condensate contribution pressent in $S(k, \omega)$, shown in Fig. 4. To this end, we have varied the energy resolution ΔE to see its effect on scattering cross section, and conclude that experimental resolutions $\Delta E \lesssim 2$ meV would preserve in the cross section the characteristic structure induced by the condensate in $S(k, \omega)$.

V. DISCUSSION

We have found that final-state corrections to the impulse approximation make only small changes in the noncondensate part of the incoherent dynamic structure factor $S^i(k, \omega)$, for momentum transfers $k = 14$ Å^{-1}. In particular, shape changes of $S(k, \omega)$ as a function of ω, the energy transfer [which would destroy the unique connection between $S(k, \omega)$ and ground-state momentum distribution n_p] are found to be insignificant. The broadening of the condensate contribution to $S(k, \omega)$ by these final-state effects is found to vary as $k^{1/2}$, [this can be seen by expanding the Fresnel integrals in Eq. (63) in powers of Ω for small values of Ω] and is less than that predicted by a phenomenological lifetime broadening, which increases linearly with k. Since the width of the noncondensate contribution to the scattering also increases linearly with k, it is clear that the condensate should appear as a discernible spike in the dynamic structure factor for large k. In particular, numerical estimates show that this large-k behavior is achieved for $k = 14$ Å^{-1}, which corresponds to experimental conditions using reactor neutrons. Presently attainable experimental energy resolutions of the order of 3.4 meV obscure this condensate contribution, producing an inelastic cross section whose energy dependence is given by a curve with a single broad peak. Comparison with Harling's experiment does not materially change our previous estimate of an upper limit of 0.03 for the condensate fraction.

Improvement of experimental energy resolutions by about a factor of 2 over those previously achieved should preserve the structure in the inelastic cross section induced by the distinct condensate contribution.

Our numerical estimates leading to these results have involved two essential parameters of the two-particle density matrix: the hard-core radius r_0 and the interhelium separation distance R at which the density matrix is judged to have achieved its asymptotic value. Lacking precise estimates of the off-diagonal behavior of ρ_2, we resorted to phenomenological arguments to determine R, and to experimental results to determine r_0.

We have made rough numerical estimates of coherent contributions to $S(k, \omega)$ (not reported here) which indicate them to be completely negligible for $k = 14$ Å^{-1}. We have unsuccessfully tried to accurately estimate coherent contributions to $S(k, \omega)$ for lower values of k, in the range from about 4 to 9 Å^{-1}, where experimental results show oscillations in k for both peak location and half-width of the inelastic cross section.[5] Unfortunately the integrations over the variables η and y in Eq. (46) for these coherent parts have so far proven intractable.

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[6]Experimental values for $S(k)$ are apparently limited to values of $k \lesssim 6\,\text{Å}^{-1}$ [see D. G. Henshaw, Phys. Rev. 119, 9 (1960)]. These results give oscillations in $S(k)$ about the value unity with a minimum and second broad maximum in the region of $k = 3.0$ and $4.7\,\text{Å}^{-1}$, respectively, which are 12 and 3% below and above the mean value of unity. There is a suggestion of a third shallow minumum at $k \approx 5.8\,\text{Å}^{-1}$, which is about 1% below unity.

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[8]An interesting pedagogical example is afforded by a one-dimensional harmonic oscillator, with classical frequency of oscillation ω_c, for which the exact solution of $S(k,t)$ can easily be written down in closed form. The series expansion of this exact $S(k,t)$ in powers of the assumed small parameter $\omega_c/(k^2/2m)$ is seen to generate the same sequence of terms as those provided by F_1^i, F_2^i, etc., for this simple model.

[9]We have verified that these two terms in Eq. (38) make negligible contributions to any condensate contribution to F_2.

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Streaming Instabilities in Relativistic Magnetoplasmas

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Stability of superluminous and subluminous waves propagating transverse to the direction of the external uniform magnetic field is investigated in streaming relativistic homogeneous plasmas. In the relativistic regime for $\Omega < ck$ (Ω being the electron cyclotron frequency and k the characteristic wave number), the superluminous waves remain stable as in the absence of external magnetic field; however, for the subluminous waves, the magnetic field has a tendency towards destabilization. For $\Omega \gg ck$, the superluminous waves are dynamically unstable for all streaming velocities U, which are smaller than U_c, or for magnetic fields Ω, which are greater than Ω_c, but for the waves with frequencies $\omega \ll \Omega$ ($\Omega \gg ck$), there exists a minimum streaming velocity above which the system is unstable. In the nonrelativistic regime the system is unstable if streaming is much larger than the thermal velocity but otherwise stable. The unstable region is bounded by $\Omega_{\min}$ and $\Omega_{\max}$; $\Omega_{\min}$ being kv_t (v_t being the electron thermal velocity) and $\Omega_{\max}$ being kU.

I. INTRODUCTION

The superluminous waves (waves with phase velocities exceeding the velocity of light), which are excited in a plasma by thermal fluctuations, do not exhibit any resonance effects, i.e., there is no Landau damping or growth[1,2] associated with these waves. Recently it was shown by the author that in streaming relativistic plasmas, the superluminous waves[3] propagating transverse to the direction of relative streaming U in the absence of any external magnetic field are absolutely stable, but the subluminous waves[4] in such systems are dynamically unstable for $U \geq 0.09c$. Such relativistic plasmas one encounters in nature as well as in laboratory (thermonuclear plasmas) with the difference that there is magnetic field associated with them. It would be interesting to investigate the effect of magnetic field on these waves. In nonrelativistic counterstreaming magnetoplasmas, it was shown by Lee,[5] by Tzoar and Yang,[6] and by Buti and Lakhina[7] that the magnetic field decreases the growth rate of instability of the transverse waves.

Following Buti,[3,4] here we have considered the propagation of superluminous ($\omega > ck$) as well as subluminous ($\omega < ck$) waves, in counterstreaming (relativistic or nonrelativistic streaming) relativistic plasmas in the presence of uniform magnetic field which is taken along the direction of relative streaming but transverse to the direction of wave propagation. For strong fields, namely, $\Omega \gg ck$ in the relativistic regime, i.e., $kT \ll mc^2$, the superluminous waves are found to be stable for all streaming velocities $U > U_c$, whereas the waves with frequencies $\omega \ll \Omega$ are unstable only if the streaming velocity is greater than a certain minimum velocity. For weak magnetic fields ($\Omega < ck$), however, the superluminous waves are absolutely stable but subluminous waves are dynamically unstable and the region of instability increases with the magnetic field.

In the nonrelativistic regime, i.e., $kT \gg mc^2$, these transverse waves are unstable in a region $kv_t < \Omega < kU$ provided $U \gg v_t$. In Sec. II, the general dispersion relation is derived and Secs. IV and V deal with the discussion of dispersion relation in the relativistic and nonrelativistic limit, respectively.