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approximate expression for $n(\vec{k})$ is found if one starts with the exact relation $\rho_{\vec{k}} = \sum_{\vec{k}'} a_{\vec{k}+\vec{k}}^\dagger a_{\vec{k}'}$ and replaces it by the dominant terms, so that $\rho_{\vec{k}} \rightarrow a_{\vec{k}}^\dagger a_{\vec{k}} + a_{\vec{k}}^\dagger a_0$, and then eliminates the Bogoliubov transformation parameter from the two equations $n(\vec{k}) = \langle a_{\vec{k}}^\dagger a_{\vec{k}} \rangle_0$ and $NS(k) = \langle \rho_{-\vec{k}} \rho_{\vec{k}} \rangle_0$. The expectation value here is taken with respect to the ground state that is present after diagonalization of the zeroth-order Hamiltonian. One must also use $N_0 \approx N$ to find the stated equation for $n(\vec{k})$.

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²¹We are indebted to Dr. W. E. Massey for first suggesting to us that this representation for $\rho_{\vec{k}}$ is valid even for a realistic model of He⁴. In a private communication from Dr. E. Feenberg, we have also learned that this same relation has been derived independently by C. E. Campbell.

High-Energy Neutron Scattering from Liquid He⁴

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The scattering of high-energy neutrons from liquid He⁴ is discussed in terms of the Gram-Charlier series expansion of the incoherent scattering function. It is shown that the series falls naturally into two parts. The first part, which corresponds to keeping only the leading term in each coefficient in the limit of large momentum transfer κ can be summed exactly and gives the impulse approximation (IA). The second part, which vanishes in the limit $\kappa \rightarrow \infty$, describes the effect of final-state interactions which are neglected in the IA. The first two coefficients in the latter series are evaluated and indicate that final-state interactions are not negligible in the recent experiments of Cowley and Woods, a fact which probably explains why these authors failed to see a sharp peak, due to the condensate, which had been predicted by Hohenberg and Platzman on the basis of the IA. It is also shown that final-state interactions produce a shift in the position of the maximum of the energy distribution of scattered neutrons, and the calculated value is in rough agreement with the value observed by Cowley and Woods.

1. INTRODUCTION

In recent years slow-neutron inelastic scattering experiments¹⁻³ have provided much information about the energies and lifetimes of the quasi-particles which characterize the low-lying excited states of liquid He⁴. Hohenberg and Platzman⁴ have pointed out that experiments at large energy and momentum transfers are also of considerable interest since such experiments are, in principle, capable of yielding the single-particle momentum distribution in liquid helium. This pos-

sibility arises from the fact that for sufficiently large momentum transfers the scattering can be described in terms of the impulse approximation^{5,6} (hereafter abbreviated IA). In the IA, the scattering atom recoils as if it were free so that the energy distribution of scattered neutrons is the Doppler profile characteristic of the momentum distribution in the initial state. In particular, the existence⁷ of a zero-momentum condensate below the λ point will produce a sharp peak in the spectrum of the scattered neutrons and the relative intensity of this peak equals the fraction of

atoms in the condensate.

Cowley and Woods⁸ have recently measured the scattering cross section of liquid HeII for neutrons with momentum transfers in the range 2–9 Å⁻¹ and find no evidence of a sharp peak in the spectrum. This is presumably due to the effect of final-state interactions which are neglected in the IA and which, among other things, will produce a broadening of the peak.

Hohenberg and Platzman's derivation of the IA relies on an intuitive argument and does not provide a basis for a rigorous discussion of the effect of final-state interactions. In the present paper, an alternative derivation of the IA will be presented which is based on the Gram-Charlier series expansion of the incoherent scattering function. The series falls naturally into two parts. The first part, which corresponds to keeping only the leading term in each coefficient in the limit of large momentum transfer κ , can be summed exactly and gives the IA. The second part vanishes in the limit $\kappa \rightarrow \infty$ and represents the effect of final-state interactions. The first two coefficients in the latter series are evaluated and indicate that final-state interactions are not at all negligible in the experiments of Cowley and Woods.

In Sec. 2, a general expression for the incoherent scattering function is derived. This expression leads immediately to the IA although the derivation, like that of Hohenberg and Platzman, depends on physical intuition and does not allow for a discussion of final-state interactions. A formally exact derivation of the IA based on the Gram-Charlier expansion is presented in Sec. 3. Finally, in Sec. 4, the effect of final-state interactions is discussed.

2. INCOHERENT SCATTERING FUNCTION

Consider a system of N He⁴ atoms of mass m enclosed in a volume of space Ω and in thermal equilibrium with a heat bath at temperature T . Since He⁴ is a totally coherent scatterer, the cross section for the scattering of neutrons from states with wave vector \vec{k}_0 to states with wave vector \vec{k} is given by⁹

$$d^2\sigma/d\Omega d\omega = Na^2(k/k_0)S(\kappa, \omega), \quad (1)$$

where a is the bound scattering length of a nucleus, $\vec{\kappa} = \vec{k}_0 - \vec{k}$ is the momentum, and $\omega = (\hbar/2m') \times (k_0^2 - k^2)$ the energy, in units of \hbar , transferred to the helium in the scattering process, m' being the neutron mass. The scattering function is given by

$$S(\kappa, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} F(\kappa, t) dt, \quad (2)$$

where

$$F(\kappa, t) = \frac{1}{N} \sum_{i,j=1}^N \langle e^{-i\vec{\kappa} \cdot \vec{r}_i(0)} e^{i\vec{\kappa} \cdot \vec{r}_j(t)} \rangle. \quad (3)$$

Here $\vec{r}_j(t)$ is the position operator for the j th atom in the Heisenberg picture and the brackets $\langle \dots \rangle$ denote a thermal average.

The structure factor $F(\kappa, 0)$ observed in x-ray¹⁰ and neutron¹¹ diffraction experiments is essentially equal to unity when $\kappa > 4$ Å⁻¹ indicating that for such large momentum transfers only the incoherent terms in (3), i. e., those with $i=j$, are important. In what follows, the interference terms $i \neq j$ will, accordingly, be neglected.

Since the interatomic forces in liquid helium can be assumed to be velocity-independent, the incoherent intermediate scattering function can be expressed in the form^{12,13}

$$F(\kappa, t) = e^{i\omega_\gamma t} \langle g(\vec{\kappa}, t) \rangle, \quad (4)$$

where $\omega_\gamma = \hbar\kappa^2/2m$ is the recoil energy and

$$g(\vec{\kappa}, t) = e^{i(H/\hbar + \vec{\kappa} \cdot \vec{v})t} e^{-iHt/\hbar} \quad (5)$$

Here H is the Hamiltonian and \vec{v} the velocity of one particular He atom, hereafter referred to as the scattering atom. The quantity (5) obeys the equation

$$d[g(\vec{\kappa}, t)]/dt = i\kappa g(\vec{\kappa}, t) v_\kappa(t), \quad (6)$$

where v_κ is the component of \vec{v} in the direction of $\vec{\kappa}$. The iterated solution of this equation,

$$g(\vec{\kappa}, t) = 1 + \sum_{n=1}^{\infty} (i\kappa)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \times \int_0^{t_{n-1}} dt_n v_{\kappa}(t_n) \dots v_{\kappa}(t_2) v_{\kappa}(t_1), \quad (7)$$

can be summed explicitly by introducing a time-ordering operator \mathcal{T} , defined such that

$$\begin{aligned} \mathcal{T}[v_{\kappa}(t_2)v_{\kappa}(t_1)] &= v_{\kappa}(t_2)v_{\kappa}(t_1), \quad t_2 < t_1; \\ &= v_{\kappa}(t_1)v_{\kappa}(t_2), \quad t_2 > t_1. \end{aligned} \quad (8)$$

The result, substituted into (4), gives

$$F(\kappa, t) = e^{i\omega_\gamma t} \langle \mathcal{T} \exp[i\vec{\kappa} \cdot \int_0^t \vec{v}(t') dt'] \rangle. \quad (9)$$

The IA can be obtained intuitively from (9) by noting¹⁴ that as $\kappa \rightarrow \infty$ the right-hand side is appreciably different from zero only if $t \rightarrow 0$, in which case $\vec{v}(t')$ can be replaced by $\vec{v}(0)$. Thus, as $\kappa \rightarrow \infty$,

$$F(\kappa, t) \rightarrow e^{i\omega_\gamma t} \langle e^{i\vec{\kappa} \cdot \vec{v}t} \rangle \equiv F_{\text{IA}}(\kappa, t). \quad (10)$$

For an ideal gas the IA is, in fact, exact for all κ because \vec{v} is then a constant of the motion. In general, therefore, the physical assumption involved in the IA is that the scattering atom recoils as if it were free. It will be noted that in the IA interatomic interactions are neglected only in the final state and not in the initial state because the thermal average in (10) refers to the interacting system and not to a system of independent particles.

The scattering function for the IA is

$$S_{\text{IA}}(\kappa, \omega) = \langle \delta(\omega - \omega_{\vec{r}} - \vec{\kappa} \cdot \vec{v}) \rangle, \quad (11)$$

in which the δ function expresses conservation of energy and momentum. In second quantization this becomes

$$\begin{aligned} S_{\text{IA}}(\kappa, \omega) &= \left\langle \frac{1}{N} \sum_{\vec{q}, \vec{q}'} \delta(\omega - \omega_{\vec{r}} - \hbar \vec{\kappa} \cdot \vec{q}/m) \delta_{\vec{q}, \vec{q}'} a_{\vec{q}}^{\dagger} a_{\vec{q}'} \right\rangle \\ &= \sum_{\vec{q}} f_{\vec{q}} \delta(\omega - \omega_{\vec{r}} - \hbar \vec{\kappa} \cdot \vec{q}/m), \end{aligned} \quad (12)$$

where $a_{\vec{q}}^{\dagger}$ and $a_{\vec{q}}$ are the boson creation and annihilation operators for particles with momentum $\hbar \vec{q}$ and $f_{\vec{q}} \equiv N^{-1} \langle a_{\vec{q}}^{\dagger} a_{\vec{q}} \rangle$ is the fraction of particles in the state \vec{q} when the system is in thermal equilibrium at temperature T . Equation (12) is the form of the IA obtained by Hohenberg and Platzman⁴ by a different method. Since $f_{\vec{q}}$ depends only on the magnitude of \vec{q} for an isotropic system such as liquid helium, (12) can be expressed in the thermodynamic limit ($N \rightarrow \infty$, $\Omega \rightarrow \infty$, with $N/\Omega = \text{const}$)

$$\begin{aligned} S_{\text{IA}}(\kappa, \omega) &= f_0 \delta(\omega - \omega_{\vec{r}}) \\ &+ \frac{m\Omega}{4\pi^2 \hbar \kappa} \int_{(m/\hbar \kappa)(\omega - \omega_{\vec{r}})}^{\infty} f_{\vec{q}} q dq. \end{aligned} \quad (13)$$

While the derivation of the IA given above is intuitively appealing, it is not rigorous. Neither does it provide a useful basis for discussing the effect of final-state interactions. An alternative derivation which attempts to overcome these difficulties will be given in Sec. 3.

3. GRAM-CHARLIER SERIES

Consider the Hermite polynomials $H_n(x)$ which are defined¹⁵ by the generating function

$$e^{2xy - y^2} = \sum_{n=0}^{\infty} \frac{2^n}{n!} y^n H_n(x), \quad (14)$$

and are given explicitly by

$$H_n(x) = [(-)^n / 2^n] e^{x^2} d^n e^{-x^2} / dx^n. \quad (15)$$

With $x = (\omega - \omega_{\vec{r}}) / 2\alpha$ and $y = i\alpha t$, where α will be defined later, it follows from (14) that

$$e^{i\omega t} = e^{i\omega_{\vec{r}} t - (\alpha t)^2} \sum_{n=0}^{\infty} \frac{(2i\alpha t)^n}{n!} H_n\left(\frac{\omega - \omega_{\vec{r}}}{2\alpha}\right). \quad (16)$$

On substituting this identity into the inverse of (2), one finds

$$F(\kappa, t) = e^{i\omega_{\vec{r}} t - (\alpha t)^2} \sum_{n=0}^{\infty} \epsilon_n(\kappa) (i\alpha t)^n, \quad (17)$$

where

$$\epsilon_n(\kappa) = (2^n / n!) \int_{-\infty}^{\infty} H_n((\omega - \omega_{\vec{r}}) / 2\alpha) S(\kappa, \omega) d\omega. \quad (18)$$

Hence, from the orthonormality relation

$$\int_{-\infty}^{\infty} H_n(x) H_m(x) e^{-x^2} dx = (\pi^{1/2} n! / 2^n) \delta_{nm}, \quad (19)$$

one obtains the following Gram-Charlier expansion¹⁶ of the incoherent scattering function

$$\begin{aligned} S(\kappa, \omega) &= \frac{1}{2\pi^{1/2}\alpha} \exp\left\{-\left(\frac{\omega - \omega_{\vec{r}}}{2\alpha}\right)^2\right\} \\ &\times \sum_{n=0}^{\infty} \epsilon_n(\kappa) H_n\left(\frac{\omega - \omega_{\vec{r}}}{2\alpha}\right). \end{aligned} \quad (20)$$

The first few terms in this series have previously been considered by Nelkin and Parks^{17,18} and, classically, by Nijboer and Rahman.¹⁹

In general, $H_n(x)$ is an n th-order polynomial of the form

$$H_n(x) = \sum_{m=0}^n a_{nm} x^m, \quad (21)$$

where $a_{nm} = 0$ unless $n + m$ is even. The coefficients in (20) are therefore given by

$$\epsilon_n(\kappa) = \frac{2^n}{n!} \sum_{m=0}^n \frac{a_{nm} s_m(\kappa)}{(2\alpha)^m}, \quad (22)$$

in which $s_m(\kappa)$ is the m th central moment of the scattering function

$$\begin{aligned} s_m(\kappa) &= \int_{-\infty}^{\infty} (\omega - \omega_{\vec{r}})^m S(\kappa, \omega) d\omega \\ &= (-i)^m \langle d^m [g(\vec{\kappa}, 0)] / dt^m \rangle. \end{aligned} \quad (23)$$

The parameter α will be chosen in the usual way by requiring that $\epsilon_2(\kappa) = 0$. Thus,

$$\alpha = \left\{ \frac{1}{2} s_2(\kappa) \right\}^{1/2} = \kappa \left\{ \frac{1}{2} \langle v_\kappa^2 \rangle \right\}^{1/2}, \quad (24)$$

and $\epsilon_0(\kappa) = 1$, $\epsilon_1(\kappa) = \epsilon_2(\kappa) = 0$,

$$\epsilon_3(\kappa) = \frac{1}{3} \sqrt{2} [s_3(\kappa)/s_2(\kappa)^{3/2}], \quad (25)$$

$$\epsilon_4(\kappa) = \frac{1}{6} [s_4(\kappa)/s_2(\kappa)^2] - \frac{1}{2}, \text{ etc.}$$

The first six moments are given in Appendix A from which it is evident that in general

$$s_m(\kappa) = \kappa^m \langle v_\kappa^m \rangle + \begin{cases} 0, & m=0, 1, 2 \\ O(\kappa^{m-1}), & m=3, 5, \dots \\ O(\kappa^{m-2}), & m=4, 6, \dots \end{cases} \quad (26)$$

Hence, from (22),

$$\epsilon_n(\kappa) = \zeta_n + \xi_n(\kappa), \quad (27)$$

$$\text{where } \zeta_n = \frac{2^n}{n!} \sum_{m=0}^n a_{nm} \frac{\langle v_\kappa^m \rangle}{\{2 \langle v_\kappa^2 \rangle\}^{m/2}}, \quad (28)$$

$$\text{and } \xi_n(\kappa) = \begin{cases} 0, & n=0, 1, 2 \\ \kappa_3/\kappa, & n=3 \\ (\kappa_4/\kappa)^2, & n=4 \\ \kappa_n/\kappa + O(\kappa^{-3}), & n=5, 7, \dots \\ (\kappa_n/\kappa)^2 + O(\kappa^{-4}), & n=6, 8, \dots \end{cases} \quad (29)$$

It can be shown with the help of (A2) that

$$\kappa_3 = \frac{2^{1/2} \hbar \langle \Delta V \rangle}{18m^2 \langle v_\kappa^2 \rangle^{3/2}}, \quad \kappa_4^2 = \frac{\langle \vec{F}^2 \rangle}{18m^2 \langle v_\kappa^2 \rangle^2}, \quad (30)$$

where V is the total potential energy of the system and $\vec{F} = -\nabla V$ is the total force on the scattering atom.

Substituting (27) into (20), one finds

$$S(\kappa, \omega) = S_{\text{IA}}(\kappa, \omega) + S_{\text{FS}}(\kappa, \omega), \quad (31)$$

where $S_{\text{IA}}(\kappa, \omega)$

$$= \frac{1}{2\pi^{1/2}\alpha} \exp \left\{ - \left(\frac{\omega - \omega_r}{2\alpha} \right)^2 \right\} \sum_{n=0}^{\infty} \xi_n H_n \left(\frac{\omega - \omega_r}{2\alpha} \right), \quad (32)$$

$$\text{and } S_{\text{FS}}(\kappa, \omega) = \frac{1}{2\pi^{1/2}\alpha} \exp \left\{ - \left(\frac{\omega - \omega_r}{2\alpha} \right)^2 \right\} \times \sum_{n=3}^{\infty} \xi_n(\kappa) H_n \left(\frac{\omega - \omega_r}{2\alpha} \right). \quad (33)$$

It is shown in Appendix B that (32) is identical to the expression (11) for the impulse approximation. Thus, $S_{\text{FS}}(\kappa, \omega)$ represents the effect of final-state interactions on the scattering function. According to (29) $\xi_n(\kappa)$ vanishes in the limit $\kappa \rightarrow \infty$. Provided, therefore, that the Gram-Charlier expansion is uniformly convergent so that the limit $\kappa \rightarrow \infty$ commutes with the sum over n , $S_{\text{FS}}(\kappa, \omega)$ also vanishes in this limit and

$$S(\kappa, \omega) \rightarrow S_{\text{IA}}(\kappa, \omega), \quad \text{as } \kappa \rightarrow \infty. \quad (34)$$

This completes the derivation of the impulse approximation.

4. FINAL-STATE INTERACTIONS

Consider first the classical limit in which the velocity distribution of the atoms is Maxwellian. In this case one can easily show that $\xi_n = \delta_{n0}$ and $S_{\text{IA}}(\kappa, \omega)$ is a simple Gaussian. Also, $\xi_n(\kappa)$ is different from zero only if n is even and $\xi_4(\kappa) \sim \kappa^{-2}$ while the higher-order terms are all²⁰ of order κ^{-4} . Thus, the asymptotic behavior of $S_{\text{FS}}(\kappa, \omega)$ for large κ is given classically by the $n=4$ term in (33).

This is no longer true when quantum effects are important, as is the case in liquid He, and one would have to sum the series (33) in order to be able to discuss in detail the effect of final-state interactions on the scattering function. To calculate $\xi_n(\kappa)$ for arbitrary n seems to be prohibitively difficult.

One can, however, obtain $\xi_3(\kappa)$ and $\xi_4(\kappa)$ with the help of (30) and the values of these quantities provide an approximate lower bound on the value of κ for which the IA is valid. In particular, κ must be much larger than κ_3 and κ_4 . It is shown in Appendix C that for liquid He at $T=0$, $\kappa_3 = 4.2 \text{ \AA}^{-1}$, and $\kappa_4 \approx 1.6 \text{ \AA}^{-1}$. Final-state interactions are, therefore, clearly not negligible in the experiments of Cowley and Woods⁸ in which $2 < \kappa < 9 \text{ \AA}^{-1}$. This evidently explains why these authors failed to see the zero-momentum peak in (13).

It was assumed in the derivation of (34) that the interference terms in (3) can be neglected when κ is large. The complete coherent scattering function, including the interference terms, can, of course, also be expanded in the form (20). For example, one finds¹⁹ that in the classical limit, with $\alpha = \kappa(kT/2m)^{1/2}$,

$$\epsilon_0(\kappa) = S(\kappa), \quad \epsilon_2(\kappa) = 1 - S(\kappa),$$

$$\epsilon_4(\kappa) = (N/6\Omega\kappa^2 kT) \int (1 - \cos \kappa x)$$

$$\times \frac{\partial^2 \phi(r)}{\partial x^2} g(r) d\vec{r} + \frac{1}{2} [S(\kappa) - 1],$$

where $S(\kappa) \equiv F(\kappa, 0)$ is the structure factor, $\phi(r)$ is the pair potential, and $g(r)$ is the pair correlation function. It is evident that the values of the above coherent ϵ_n 's oscillate about the values of the corresponding incoherent ϵ_n 's. These oscillations, which arise from the hard core of the interatomic potential, are large in the neighborhood of the first diffraction maximum ($\kappa = 2 \text{ \AA}^{-1}$ in liquid He) but die out faster than κ^{-2} as $\kappa \rightarrow \infty$. In general, therefore, one would not expect the interference terms to destroy the validity of (34). Neither would one expect them to have any effect on the region of κ values in which the impulse approximation predominates since this region lies well above the region of the first diffraction maximum.

Hohenberg and Platzman⁴ argue that the broadening of the zero-momentum peak due to final-state interactions is a simple lifetime effect and estimate the width of the peak assuming that the recoiling atom collides independently with the other atoms in the system. Under these assumptions they find a width proportional to κ . Since the width of the spectrum of the uncondensed atoms [i. e., the second term in (13)] also increases linearly with κ , the zero-momentum peak does not, according to Ref. 4, approach a δ function in the high- κ limit (unless, of course, the recoil energy is so high as to invalidate the assumption that the atoms interact via a hard-core velocity-independent potential).

On the other hand, Eq. (34) implies that the width of the zero-momentum peak increases, if at all, more slowly than κ so that the peak becomes in effect a δ function for large κ . This result is consistent with the recent model calculation by Egelstaff and Mountain¹⁴ who find a width proportional to κ^s , where $s \leq \frac{1}{3}$. Equation (34) depends for its validity on the assumption that the Gram-Charlier series is uniformly convergent. If this is true, the broadening of the zero-momentum peak is not a simple lifetime effect of the type considered in Ref. 4.

The value of ω at which $S(\kappa, \omega)$ is a maximum, can be obtained by differentiating (20) and one finds

$$\omega_{\max} = \omega_{\gamma} - \Delta + O(\kappa^{-2}), \quad (35)$$

where

$$\Delta = (2 \langle v_{\kappa}^2 \rangle)^{1/2} \left(\frac{\frac{3}{4} K_2 - \frac{15}{8} K_3 + \dots}{1 + \frac{15}{4} \zeta_4 - \frac{105}{8} \zeta_6 + \dots} \right). \quad (36)$$

The data of Cowley and Woods²¹ at $T = 1.1^\circ \text{K}$ are consistent with (35) with $\Delta = 12 \pm 4^\circ \text{K}$. It is found with the help of the velocity distribution calculated by McMillan²² that for v_{κ} in units of 10^4 cm s^{-1} ,

$$\langle v_{\kappa}^2 \rangle = 1.96, \quad \langle v_{\kappa}^4 \rangle = 13.2, \quad \langle v_{\kappa}^6 \rangle = 142. \quad (37)$$

$$\text{Hence, } \zeta_4 = \frac{1}{6} \frac{\langle v_{\kappa}^4 \rangle}{\langle v_{\kappa}^2 \rangle^2} - \frac{1}{2} = 0.092,$$

$$\zeta_6 = \frac{1}{30} \frac{\langle v_{\kappa}^6 \rangle}{\langle v_{\kappa}^2 \rangle^3} - \frac{1}{6} \frac{\langle v_{\kappa}^4 \rangle}{\langle v_{\kappa}^2 \rangle^2} + \frac{1}{3} = -0.039. \quad (38)$$

With $\kappa_3 = 4.2 \text{ \AA}^{-1}$ (Appendix C), and ignoring the remaining terms in (36), one finds a value $\Delta = 26^\circ \text{K}$. The discrepancy between this and the observed value is probably not due entirely to the higher-order terms in (36) which have been neglected because the values of ζ_4 and ζ_6 are very sensitive to the values of the quantities (37). For example, a change in the values of $\langle v_{\kappa}^n \rangle$ by 10% can change the denominator of (36) by a factor of 3.

To summarize, the scattering of high-energy neutrons from liquid He⁴ has been discussed in terms of the Gram-Charlier series expansion of the incoherent scattering function. It was shown that the impulse approximation is obtained if one retains only the leading term in each coefficient in the limit of large momentum transfer κ . A formal expression for the effect of final-state interactions, which are neglected in the IA, is given by (33). The coefficients $\xi_n(\kappa)$ have not been evaluated for arbitrary n so that one cannot at present give a detailed discussion of the effect of final-state interactions on the shape of the scattering function. However, the calculated values of $\xi_3(\kappa)$ and $\xi_4(\kappa)$ do provide a lower limit on the values κ for which the IA is valid and it was found that final-state interactions were not negligible in the recent experiments of Cowley and Woods.⁸ It was also shown, in agreement with the data of Cowley and Woods,²¹ that final-state interactions produce a shift in the position of the maximum in the energy distribution of the scattered neutrons.

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APPENDIX A: MOMENTS OF $S(\kappa, \omega)$

Rahman, Singwi, and Sjölander¹³ have calculated the first four moments of the incoherent scattering function by substituting (7) into (23). Their results, extended to sixth order, are

$$s_0(\kappa) = 1, \quad s_1(\kappa) = 0, \quad s_2(\kappa) = \kappa^2 \langle v_{\kappa}^2 \rangle,$$

$$s_3(\kappa) = -i\kappa^2 \langle v_{\kappa} v_{\kappa}' \rangle, \quad s_4(\kappa) = -\kappa^2 \langle v_{\kappa} v_{\kappa}'' \rangle + \kappa^4 \langle v_{\kappa}^4 \rangle,$$

$$s_5(\kappa) = i\kappa^2 \langle v_{\kappa} v_{\kappa}''' \rangle - i\kappa^4 [\langle v_{\kappa} (v_{\kappa}^3)' \rangle]$$

$$+\langle v_{\kappa}^2(v_{\kappa}^2)'\rangle + \langle v_{\kappa}^3 v_{\kappa}'\rangle, \quad (\text{A1})$$

$$s_6(\kappa) = \kappa^2 \langle v_{\kappa} v_{\kappa}^m \rangle - \kappa^4 [\langle v_{\kappa} (v_{\kappa}^3)^m \rangle \\ + \langle v_{\kappa}^2 (v_{\kappa}^2)^m \rangle + \langle v_{\kappa}^3 v_{\kappa}^m \rangle + \langle v_{\kappa} (v_{\kappa} (v_{\kappa}^2)')' \rangle \\ + \langle v_{\kappa} (v_{\kappa}^2 v_{\kappa}')' \rangle + \langle v_{\kappa}^2 (v_{\kappa} v_{\kappa}')' \rangle] + \kappa^6 \langle v_{\kappa}^6 \rangle,$$

in which the primes denote differentiation with respect to t . With the help of the general rule $\langle AB' \rangle = -\langle A'B \rangle$, the third and fourth moments can be expressed in the more familiar forms^{12,23}

$$s_3(\kappa) = \hbar \kappa^2 \langle \Delta V \rangle / 6m^2, \\ s_4(\kappa) = \kappa^2 \langle \vec{F}^2 \rangle / 3m^2 + \kappa^4 \langle v_{\kappa}^4 \rangle, \quad (\text{A2})$$

in which V is the total potential energy of the system and $\vec{F} = -\vec{\nabla}V$ is the total force on the scattering atom.

APPENDIX B: PROOF OF EQUIVALENCE OF EQUATIONS (11) AND (32)

From Eq. (28),

$$\xi_n = \frac{2^n}{n!} \left\langle \sum_{m=0}^n a_{nm} \left(\frac{v_{\kappa}}{(2\langle v_{\kappa}^2 \rangle)^{1/2}} \right)^m \right\rangle \\ = (2^n/n!) \langle H_n [v_{\kappa} / (2\langle v_{\kappa}^2 \rangle)^{1/2}] \rangle \\ = (2^n/n!) \langle H_n (\vec{\kappa} \cdot \vec{v} / 2\alpha) \rangle. \quad (\text{B1})$$

Hence, (32) becomes

$$S_{\text{IA}}(\kappa, \omega) = \frac{1}{2\pi^{1/2}\alpha} \exp \left\{ - \left(\frac{\omega - \omega_r}{2\alpha} \right)^2 \right\} \\ \times \sum_{n=0}^{\infty} \frac{2^n}{n!} \left\langle H_n \left(\frac{\vec{\kappa} \cdot \vec{v}}{2\alpha} \right) \right\rangle H_n \left(\frac{\omega - \omega_r}{2\alpha} \right) \\ = \frac{1}{2\alpha} \left\langle \exp \left\{ - \left(\frac{\omega - \omega_r}{2\alpha} \right)^2 \right\} \right. \\ \left. \times \sum_{n=0}^{\infty} \frac{2^n}{\pi^{1/2} n!} H_n \left(\frac{\omega - \omega_r}{2\alpha} \right) H_n \left(\frac{\vec{\kappa} \cdot \vec{v}}{2\alpha} \right) \right\rangle \\ = \langle \delta(\omega - \omega_r - \vec{\kappa} \cdot \vec{v}) \rangle, \quad (\text{B2})$$

which is identical to (11). The last line of (B2) follows from the completeness relation for the Hermite polynomials

$$e^{-x^2} \sum_{n=0}^{\infty} \frac{2^n}{\pi^{1/2} n!} H_n(x) H_n(x') = \delta(x - x'). \quad (\text{B3})$$

APPENDIX C: VALUE OF κ_3 AND κ_4

The interatomic forces in liquid helium will be assumed to be additive so that

$$V = \sum_{i>j=1}^N \phi(|\vec{r}_j - \vec{r}_i|), \quad (\text{C1})$$

where $\phi(r)$ is the pair potential. Hence,

$$\langle \Delta V \rangle = \frac{N}{\Omega} \int_0^{\infty} \left\{ \frac{d^2 \phi(r)}{dr^2} + \frac{2}{r} \frac{d\phi(r)}{dr} \right\} g(r) 4\pi r^2 dr, \quad (\text{C2})$$

in which $g(r)$ is the pair correlation function. McMillan²² has calculated $g(r)$ for liquid He⁴ at $T=0$ assuming a trial ground-state wave function of the Jastrow type and a Lennard-Jones potential,

$$\phi(r) = 4\epsilon [(\sigma/r)^{12} - (\sigma/r)^6], \quad (\text{C3})$$

in which $\epsilon = 10.22^\circ\text{K}$ and $\sigma = 2.556 \text{ \AA}$. With McMillan's $g(r)$ it is found that $\langle \Delta V \rangle = 613 \text{ erg cm}^{-2}$ and, hence, from (30) and (37) that $\kappa_3 = 4.2 \text{ \AA}^{-1}$.

$$\text{In general, } \vec{F} = -\vec{\nabla}V = \sum_{j=1}^{N'} \vec{F}_j, \quad (\text{C4})$$

where \vec{F}_j is the force which the j th atom exerts on the scattering atom and the prime on the summation indicates that the value of j corresponding to the scattering atom itself is to be excluded. Thus,

$$\langle \vec{F}^2 \rangle = \sum_{j=1}^{N'} \langle \vec{F}_j^2 \rangle + \sum_{i \neq j=1}^{N'} \langle \vec{F}_i \cdot \vec{F}_j \rangle. \quad (\text{C5})$$

The second term in this expression is an interference term arising from three-body correlations which tends to cancel the first term.

In the classical limit one need not know the three-body correlation function in order to calculate $\langle \vec{F}^2 \rangle$ because it can be shown by integration by parts that²⁴

$$\langle \vec{F}^2 \rangle = \langle (\vec{\nabla}V)^2 \rangle = kT \langle \Delta V \rangle, \quad (\text{C6})$$

and, according to (C2), the last part of the right-hand side of (C6) is determined by the pair correlation function alone. At $T=0$, $\langle \vec{F}^2 \rangle = 0$ and the cancellation effect in (C5) is complete. This is, of course, just a reflection of the fact that at $T=0$ all the atoms are at rest at their equilibrium positions.

In a quantum system such as liquid He the atoms are not at rest at $T=0$ but execute zero-point motion which is associated with a nonvanishing value of $\langle \bar{F}^2 \rangle$. Let us write

$$\langle \bar{F}^2 \rangle = k T_{\text{eff}} \langle \Delta V \rangle, \quad (\text{C7})$$

where T_{eff} is an effective temperature which approaches the real temperature as $T \rightarrow \infty$ and quantum effects disappear. One can easily verify that for a simple harmonic oscillator

$$k T_{\text{eff}} = m \langle v_{\kappa}^2 \rangle, \quad \text{for all } T. \quad (\text{C8})$$

This equation is also true classically. To the extent, therefore, that the zero-point motion in liquid helium is either simple harmonic, or simulates classical motion at a finite temperature, Eqs. (C7) and (C8) can be used to estimate $\langle \bar{F}^2 \rangle$ and one finds a value $0.80 \times 10^{-12} \text{ dyn}^2$. This estimate is not likely to be very accurate but can be expected to be of the right order of magnitude. Hence, from (30), it is found that $\kappa_4 \approx 1.6 \text{ \AA}^{-1}$.

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