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# Oscillations and line shapes of $S(Q,\omega)$ in quantum fluids

B. Tanatar, E. F. Talbot, and H. R. Glyde
*Department of Physics, University of Delaware, Newark, Delaware 19716*
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The dynamic form factor $S(Q,\omega)$ of the quantum liquids $^3$He and $^4$He is evaluated in the range $3 \le Q \le 10$ Å$^{-1}$ within the random-phase approximation (RPA) beginning from the He-He pair potential. In $^4$He, the width $W(Q)$ of $S(Q,\omega)$ is found to oscillate with $Q$ as observed. These oscillations originate in the He-He interaction in the RPA. In $^3$He, $W(Q)$ agrees in magnitude with experiment but does not oscillate. This suggests $W(Q)$ is not simply related to the total He-He scattering cross section $\sigma(Q)$. The calculated $S(Q,\omega)$ has high-frequency tails which make the kinetic energy greater than expected from $W(Q)$ and a Gaussian $S(Q,\omega)$.

Studies of excitations in quantum fluids by inelastic neutron scattering at high momentum transfers have revealed many fascinating properties,[1-11] such as the condensate fraction[3-7] in liquid $^4$He, and some puzzles. We address two outstanding puzzles in the intermediate-momentum-transfer range. The observed scattering intensity is proportional to the dynamic form factor, $S(Q,\omega)$, where $\hbar Q$ ($\hbar\omega$) is the momentum (energy) of the excitation created by the neutron. First, Martel *et al.*[5] observed in liquid $^4$He that the full width at half maximum, $W(Q)$, of $S(Q,\omega)$ oscillated with $Q$ in the range $3 \le Q \le 10$ Å$^{-1}$. In a simple model, they related[2,5] the oscillations in $W(Q)$ to the oscillations in the $^4$He-$^4$He atom scattering cross section,[12] $\sigma(Q)$. This leads to $W(Q) \propto \sigma(Q)$. Since $\sigma(Q)$ for $^3$He-$^3$He scattering oscillates with $Q$ (see Fig. 1), oscillations in $W(Q)$ in $^3$He might also be expected. In liquid $^3$He, Mook[9] has recently observed that $W(Q)$ varied with $Q$ in the range $4 \le Q \le 7$ Å$^{-1}$, has a minimum at $Q \approx 5.5$ Å$^{-1}$, but does not apparently oscillate. We present a straightforward calculation of $S(Q,\omega)$ beginning from the pair interatomic potential[13] which reproduces the "oscillations" of $W(Q)$ in $^4$He but shows no oscillations in $^3$He. For $3 \le Q \le 10$ Å$^{-1}$ at least, $W(Q)$ may not be simply related to $\sigma(Q)$, as noted by Sears.[11]

Second, the ground-state energy and kinetic energy per atom, $\langle E_{\rm kin}\rangle$, of Fermi fluids are properties of fundamental interest.[14] The $\langle E_{\rm kin}\rangle$ is related to the second moment $M_2 = \int d\omega(\omega-\omega_R)^2 S_i(Q,\omega)$ of the incoherent $S_i(Q,\omega)$ by $\langle E_{\rm kin}\rangle = (3\hbar/4\omega_R)M_2$, where $\omega_R = \hbar Q^2/2m$ is the recoil frequency. If we assume at high $Q$ that $S \approx S_i$ and that $S(Q,\omega)$ is a Gaussian, the second moment $M_2$ may be obtained from the observed $W(Q)$ by the relation appropriate for Gaussian functions, $M_2 = W^2(Q)/8\ln 2$. In this way Sokol, Sköld, Price, and Kelb[8] and Mook,[9] respectively, obtained the first values of $\langle E_{\rm kin}\rangle = 8.1^{+1.7}_{-1.3}$ and 10.7 K, significantly below the most reliable theoretical values[14] of $\langle E_{\rm kin}\rangle \approx 13$ K. We find that $S(Q,\omega)$ is not a Gaussian. Rather it has tails[15] at large $\omega-\omega_R$ which make $M_2$ larger than expected for a Gaussian of equivalent $W$. Thus a $\langle E_{\rm kin}\rangle$ based on $W$ and a Gaussian assumption probably underestimates the true $\langle E_{\rm kin}\rangle$ in liquid $^3$He. We present calculations here mainly for $^3$He with some discussion of liquid $^4$He.

The $S(Q,\omega)$ in liquid $^3$He is the sum[16] of a coherent part, $S_c(Q,\omega)$, describing density excitations and a spin-dependent part, $S_I(Q,\omega)$, describing spin-density excitations,

$$S(Q,\omega) = S_c(Q,\omega) + \frac{\sigma_i}{\sigma_c} S_I(Q,\omega) . \tag{1}$$

Here $\sigma_i/\sigma_c$ is the ratio of the incoherent to coherent total neutron-$^3$He scattering cross section and is estimated[17] to be 0.25. For $^4$He, $\sigma_i = 0$. At $T=0$, each $S_a(Q,\omega)$

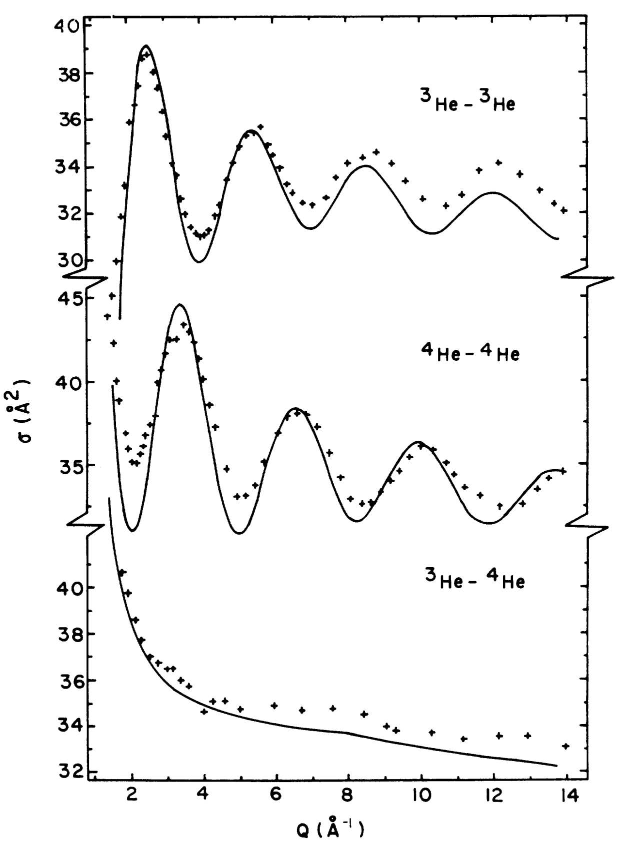


FIG. 1. Total He-He scattering cross sections. +, data (Ref. 12); ——, present calculations.

($\alpha=c,I$) is related to the imaginary part of the corresponding dynamic response function $\chi_\alpha(Q,\omega)$ by

$$S_\alpha(Q,\omega)=-\frac{1}{n\pi}\chi''_\alpha(Q,\omega) , \quad (2)$$

where $n$ is the number density.

To develop a model of $S(Q,\omega)$ for $Q\geq 4$ Å$^{-1}$, we assume that at high $Q$ short-range correlations between pairs of atoms are most important. These short-range correlations are well described by a $T$ matrix. A particle-hole ($p$-$h$) pair $(\mathbf{p}+\mathbf{Q},\mathbf{p}')$ excited by a neutron, interact and scatter to other $p$-$h$ pairs $(\mathbf{p}'+\mathbf{Q},\mathbf{p})$. The $T$ matrix, $\Gamma(k,k';P)$, describing this "dressed" particle interaction depends upon the relative momenta $2\mathbf{k}=(\mathbf{p}+\mathbf{Q})-\mathbf{p}'$, $2\mathbf{k}'=\mathbf{p}-(\mathbf{p}'+\mathbf{Q})$ and little on the center-of-mass momentum $\mathbf{P}=\mathbf{p}+\mathbf{p}'+\mathbf{Q}$. Here $|p|\sim|p'|\sim p_F=0.8$ Å$^{-1}$ in liquid $^3$He. At high $Q$, $Q\gg p$ or $p'$ and we assume that $\Gamma$ depends predominantly on $Q$ (and $\omega$). With this approximation, the exact integral equation for $\chi(Q,\omega)$ reduces to the random-phase-approximation (RPA) result,[18-20]

$$\chi_\alpha(Q,\omega)=\frac{\chi_0(Q,\omega)}{1-\Gamma^\alpha(Q,\omega)\chi_0(Q,\omega)} , \quad (3)$$

where

$$\chi_0(Q,\omega)=\frac{\hbar}{\Omega}\sum_{\mathbf{p}}\frac{n_{\mathbf{p}}-n_{\mathbf{p}+\mathbf{Q}}}{\hbar\omega-\varepsilon_{\mathbf{p}+\mathbf{Q}}+\varepsilon_{\mathbf{p}}+i\eta} \quad (4)$$

is the Lindhard function.[21] Here $\Gamma^\alpha$ is the spin-symmetric (spin-antisymmetric) interaction in the $\chi_c$ ($\chi_I$), $n_{\mathbf{p}}$ is the momentum distribution, and $\varepsilon_{\mathbf{p}}=\varepsilon^0_{\mathbf{p}}+\Sigma(\mathbf{p},\varepsilon_{\mathbf{p}})$ is the "dressed" single-particle energy calculated using the full $\Gamma(k,k';P)$. This RPA result in valid only for $Q\gg\langle p^2\rangle^{1/2}$ (and $Q\rightarrow 0$).

We consider two models. In the first (model 1), we approximate the full interaction $\Gamma(Q,\omega)$ in the fluid by the corresponding scattering amplitude or $t$ matrix for two atoms scattering in free space, $\Gamma_0(Q)$. In this simple case we ignore any Fermi- or Bose-liquid effects and use free-particle energies $\varepsilon^0_{\mathbf{p}}=p^2/2m$ in the equation[22] for $\Gamma_0(Q)$. Also $\Gamma_0(Q)$ depends only on $Q$ with $\hbar\omega$ set at the kinetic energy of the incoming pair. In model 1 we also use free-particle energies $\varepsilon^0_{\mathbf{p}}$ in $\chi_0$. The Fermi- or Bose-liquid effects enter only through the momentum distribution $n_{\mathbf{p}}$ in $\chi_0$.

In model 2 for $^3$He, we use the GFHF theory developed by Glyde and Hernadi.[23] In this case the $\Gamma(Q,\omega)$ in (3) is the Galitskii-Feynman (GF) $T$ matrix and the $\Sigma$ in $\varepsilon_{\mathbf{p}}$ is the Hartree-Fock (HF) self-energy, $\Sigma_{\rm HF}(\mathbf{p},\varepsilon_{\mathbf{p}})$. This includes Fermi-liquid effects, viz., the Fermi sea and renormalized $\varepsilon_{\mathbf{p}}=\varepsilon^0_{\mathbf{p}}+\Sigma_{\rm HF}$. The $\Sigma_{\rm HF}$ and $\Gamma$ were calculated iteratively until consistent with $v(r)$ as input. The GF $T$ matrix describes the interaction of a pair in the liquid via the potential $v(r)$ well, but the pair interaction induced via collective effects is ignored. At $Q\geq 6$ Å$^{-1}$ we found $\Gamma(Q,\omega)$ was well approximated by $\Gamma_0(Q,\omega)$, the free-atom $t$ matrix with energy dependence retained.

In Fig. 1 we show the total scattering cross section for two He atoms in free space calculated from our $\Gamma_0(Q)$. These are

$$\sigma_{3\text{-}3}=\tfrac{1}{4}(3A_o+A_e),\ \sigma_{4\text{-}4}=A_e,\ \sigma_{3\text{-}4}=\tfrac{1}{2}(A_o+A_e) , \quad (5)$$

where

$$A_{o,e}=\frac{1}{2\pi}\sum_{L\ \text{odd,even}}(2L+1)|\Gamma_{0L}(Q)|^2$$

are sums over the odd and even angular momentum components $\Gamma_{0L}$ (in length units) of $\Gamma_0$, respectively. The $\sigma_{3\text{-}3}$ and $\sigma_{4\text{-}4}$ differ only in the selection of the $L$ components dictated by statistics. They oscillate with $Q$ in agreement with the observed values of Feltgen *et al.*[12] Using the optical theorem, $\sigma_{3\text{-}3}=-(1/k)(\Gamma_0^{3\text{-}3})''$ and $\sigma_{4\text{-}4}=-(1/k)(\Gamma_0^{4\text{-}4})''$ where $\Gamma''_0$ is the imaginary part. This shows that the $\Gamma''_0(Q)$ clearly oscillate.

In the upper part of Fig. 2 we show $S(Q,\omega)$ in liquid $^3$He calculated using models 1 and 2. Also shown is $S^0_0$ calculated from $\chi_0$ using free particle energies in (4) as used in model 1, and $S_0^{\rm HF}$ calculated using GFHF energies $\varepsilon_{\mathbf{p}}$ in $\chi_0$. In each case we see that the interaction $\Gamma$ in the RPA contributes significantly to $S(Q,\omega)$. The $S(Q,\omega)$ also has high-frequency tails. In the bottom of Fig. 2 we compare model 2 for $Q=5.5$ Å$^{-1}$ with the scattering intensity observed by Mook[9] at constant scattering angle.

The width $W(Q)$ of $S(Q,\omega)$ in liquid $^3$He calculated from $S_0^{\rm HF}$ and models 1 and 2 is compared with the values observed by Sokol *et al.*[8] and by Mook[9] in Fig. 3. First, our calculated $W(Q)/Q$ is approximately constant for $Q\geq 5$ Å$^{-1}$ and in excellent agreement the values of Sokol *et al.* (observed for $12\leq Q\leq 15$ Å$^{-1}$). It also agrees reasonably well with the average value of 2.18 meV Å quoted by Mook[9] but does not show the increase with $Q$ between 5 and 7 Å$^{-1}$. For $S_0^{\rm HF}$ and models 1 and 2, $W(Q)/Q$ shows only very weak oscillations with $Q$. These oscillations are in phase with $\sigma_{3\text{-}3}$ shown in Fig. 1, especially in model 1. The oscillations originate from $\Gamma$ but are so weak in $S(Q,\omega)$ that effectively the oscillations in $\Gamma$ are not translated into $W(Q)$ for $^3$He. The $W(Q)/Q$ obtained from $S_0^{\rm HF}$also does not oscillate, although the imaginary part of the $\varepsilon_{\mathbf{p}}$ does oscillate with $p$ at high $p$. In general, models 1 and 2 reproduce the observed widths well and give similar results.

For liquid $^4$He, in Fig. 4 we compare our calculated $W(Q)$ using model 1 with the observed values of Martel *et al.*[5] We used the free-atom dispersion $\varepsilon^0_{\mathbf{p}}=p^2/2m$ and the free-particle Bose distribution $n_{\mathbf{p}}$ evaluated at $T=3.2$ K which is just above the Bose condensation temperature of a free Bose gas having the mass and number densities of liquid $^4$He. This leads to a narrow distribution $n_{\mathbf{p}}$. [The curves $B$ and $B'$ from Ref. 5 were obtained using $W(Q)\propto\sigma(Q)$ with magnitude set to agree with experiment by adjusting $\langle p^2\rangle$.] The oscillations in our calculated $W(Q)$ (magnitude aside) match the experimental values in phase and period as well as the curves $B$ and $B'$. The present model 1, using an energy-independent $\Gamma_0(Q)$ is not valid below $Q=4$ Å$^{-1}$. The present calculation involves only $\chi_0(Q,\omega)$ and an interaction $\Gamma_0(Q)$. As there are no oscillations in $\chi_0$, the oscillations in $W(Q)$ follow from those in the real and imaginary parts of $\Gamma_0(Q)$ entering the RPA in (3). Thus the observed oscillation of $W(Q)$ in $^4$He can be reproduced using (3) and (4) begin-

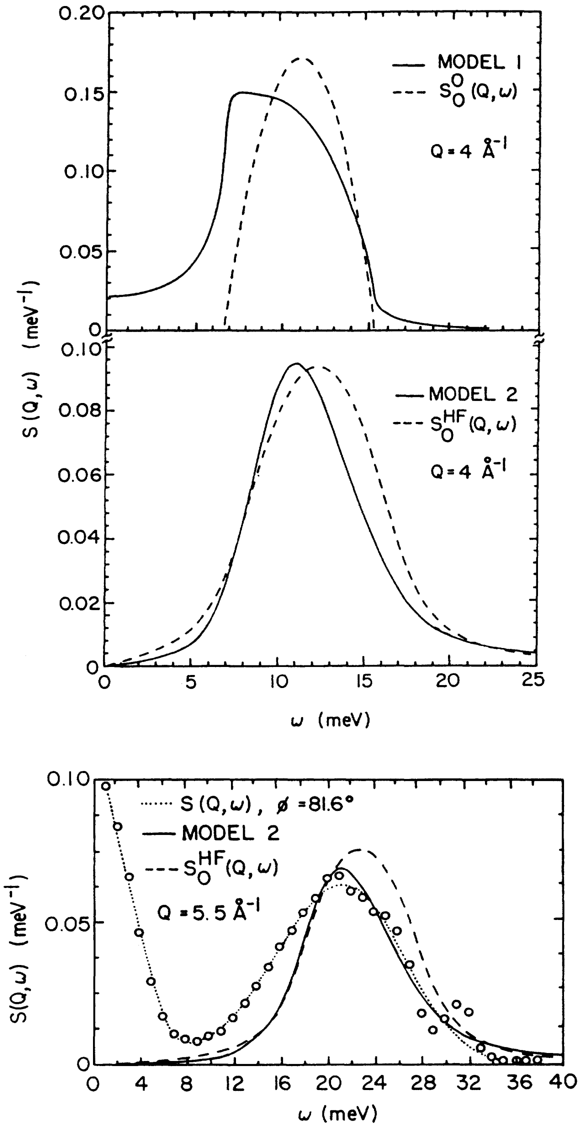


FIG. 2. Upper part is dynamic form factor in liquid $^3$He: ——, $S(Q,\omega)$ of Eq. (1) calculated using RPA models 1 and 2; ---, $S_0^0(Q,\omega)$ and $S_0^{HF}(Q,\omega)$ calculated from Eq. (4) using free-particle and GFHF energies $\varepsilon_p$, respectively. Lower part: scattered intensity observed ( · · · O · · · ) by Mook at constant angle $\phi$ in arbitrary units (Ref. 9); $S_0^{HF}(Q,\omega)$ (---) and $S(Q,\omega)$ (——) of model 2.

ning from $v(r)$. The same model does not give oscillations in $^3$He.

Returning to liquid $^3$He, we have calculated the second moments $M_2$ of $S(Q,\omega)$ shown in Fig. 2 and we find them to be large, due to the high- (and low-) frequency tails of $S(Q,\omega)$. Indeed, $M_2$ depends sensitively on the high-frequency behavior of $\Gamma(Q,\omega)$ and we have not been able to evaluate $M_2$ with confidence. However, $M_2$ is significantly larger than expected from our $W(Q)$ and the assumption of a Gaussian $S(Q,\omega)$, at least for $Q \leq 12$ Å$^{-1}$. Thus values of $\langle E_{\mathrm{kin}} \rangle$ inferred from $W(Q)$ and a

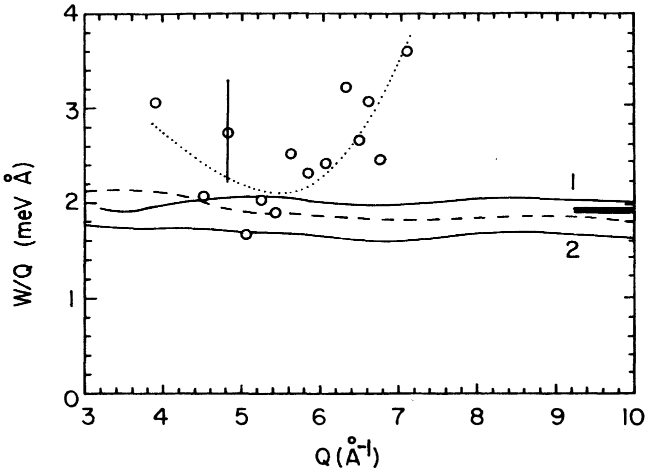


FIG. 3. Widths of $S(Q,\omega)$ in liquid $^3$He: Mook's data (O) and guide to eye (....); ——, present calculations using models 1 and 2, and using $S_0^{HF}$ alone (---); ▬▬, Sokol *et al.* observed $W(Q)/Q$ for $12 \leq Q \leq 15$ Å$^{-1}$.

Gaussian $S(Q,\omega)$ probably underestimate the $\langle E_{\mathrm{kin}} \rangle$ in liquid $^3$He.

In summary, the present results show that the oscillations in $W(Q)/Q$ with $Q$ in $S(Q,\omega)$ in $^4$He can be reproduced using a simple RPA model. In this model, the oscillations originate from the oscillations with $Q$ in the $T$-matrix interaction $\Gamma_0(Q)$ appearing in the RPA. There could be additional contributions in $^4$He to the oscillations in $W(Q)/Q$ from lifetime effects as proposed by Martel *et al.* We have not included these lifetime contributions to the oscillations in $^4$He. The same model (model 1) does not produce oscillations in $W(Q)/Q$ in $^3$He. Even when the lifetime effect is included (in $S_0^{HF}$) or both lifetime and interaction effects are included together in a full Fermi-fluid model (model 2), no oscillations are found in $^3$He. Thus we believe oscillations in $W(Q)/Q$ will not be

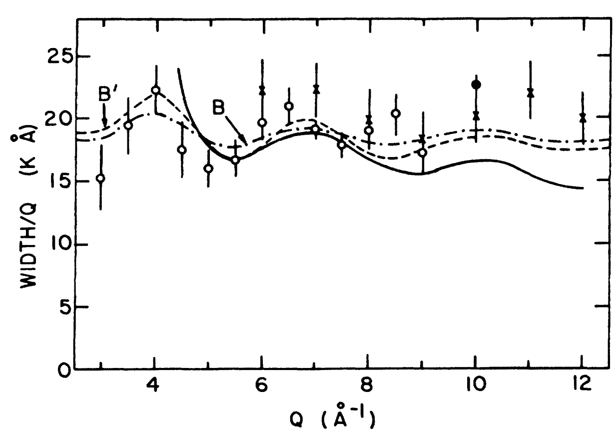


FIG. 4. Widths of $S(Q,\omega)$ in liquid $^4$He; O and × are data of Martel *et al.* (Ref. 5); $B$ and $B'$ model calculations from Ref. 5; ——, present width using model 1.

observed in $^3$He and therefore that $W(Q)$ may not be simply related to $\sigma(Q)$. As shown in Figs. 2 and 3, the magnitude of $W(Q)/Q$ and the shape of $S(Q,\omega)$ predicted by model 2 agrees quite well with the observed values in $^3$He. Given the controversial nature of the high-$\omega$ contribution to $S(Q,\omega)$, direct comparison of observed and calculated $S(Q,\omega)$ is therefore probably a better test of models of quantum liquids[10] than calculation of moments. Further work to refine the present results is necessary and in progress. Further experiments would be interesting.

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