

## Scattering of Electromagnetic Radiation from Liquid He<sup>3</sup>†

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The Landau theory of Fermi liquids is used to calculate the frequency power spectrum of density fluctuations in liquid He<sup>3</sup>. Light-scattering intensities from "zero" sound, first sound, and quasiparticle-hole pairs are computed in detail. Finite-temperature x-ray structure factors are compared with experimental values and agreement is obtained within the considerable scatter of the experimental points. Light-scattering experiments are feasible and would provide detailed confirmation of Landau theory.

Although the Landau theory of Fermi liquids is an old and respected theory,<sup>1</sup> some of its very specific predictions for light- and x-ray-scattering experiments have not been computed in detail. In a previous letter<sup>2</sup> the Landau prediction for the ground-state x-ray structure factor was computed. These calculations are here extended to the finite-temperature regime. More important, the recent advances in light-scattering technology<sup>3,4</sup> make it feasible to provide much-needed confirmation of the Landau theory of liquid He<sup>3</sup>. The purpose of this paper is to provide detailed numerical predictions of the frequency power spectrum of scattered light.

The cross section for an unpolarized photon to scatter off a single helium atom is well known<sup>5</sup>:

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \alpha^2 (1 + \cos^2\theta) \chi^{-4} \quad (\text{light}), \quad (1a)$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \left( \frac{e^2}{mc^2} \right)^2 (1 + \cos^2\theta) |F(Q)|^2 \quad (\text{x ray}). \quad (1b)$$

In Eqs. (1),  $\alpha$  is the atomic polarizability,  $\chi$  is the wavelength of the photon divided by  $2\pi$ ,  $F(Q)$  is the electronic form factor, i. e., the Fourier transform of the electron number density, and

$$Q = (2/\lambda) \sin \frac{1}{2}\theta, \quad (2)$$

is the momentum transferred to the photon. For liquid He<sup>3</sup> the effects of scattered-amplitude interference from different atoms can be taken into account via the fluctuation-dissipation theorem, yielding<sup>5</sup>

$$\frac{d^2\hbar}{d\Omega d\omega} = \frac{d\sigma}{d\Omega} \frac{\hbar\omega}{\pi} (1 - e^{-\hbar\omega/k_B T})^{-1} \frac{\text{Im}\chi(Q, \omega)}{\omega}, \quad (3)$$

where  $\omega = \omega_i - \omega_f$  is the frequency shift in the scattered photon. We have expressed the scattered-photon distribution so that  $h_{\text{tot}}$  (the extinction coefficient) represents the inverse-mean-free-path length of the photon in the liquid. The crucial function to be calculated is  $\chi(Q, \omega)$ , i. e., the linear re-

sponse in the density  $\delta\rho$  to an external periodic potential  $\delta U_{\text{ext}}$  proportional to  $e^{i(\vec{Q}\cdot\vec{r}-\omega t)}$ . Present resolution allows x-ray experiments to measure only

$$\frac{d\hbar}{d\Omega} = \int d\omega \frac{d^2\hbar}{d\Omega d\omega} = \rho \frac{d\sigma}{d\Omega} S(Q). \quad (4)$$

We have calculated  $\chi(Q, \omega)$  by putting the external potential  $\delta U_{\text{ext}}$  into the Landau-Boltzmann equation and finding the resulting response  $\delta\rho$  in the density of quasiparticles.<sup>2</sup> Two approximations were made: (i) The collision integral was replaced by a single collision time in a manner consistent with the conservation laws. (ii) Only two nonzero Landau parameters<sup>6</sup>  $F_0$  and  $F_1$  were assumed in the spin symmetric part of the quasiparticle interaction function. The resulting  $\chi(Q, \omega)$  can be expressed in terms of a "dimensionless" frequency

$$\nu = \omega/QV_F \quad (5)$$

and "dimensionless" collision time

$$\sigma = \tau_c QV_F, \quad (6)$$

where  $V_F$  is the Fermi velocity  $p_F/m^*$ . We take<sup>7</sup>

$$\tau_c = (1.46 \times 10^{-12} \text{ sec} \text{ } ^\circ\text{K}^2)/T^2 \quad (7)$$

to assure that the first-sound mode is damped by the measured viscosity. The final result is in basic agreement with Abrikosov and Khalatnikov<sup>8</sup>; the Landau prediction is

$$\chi(Q, \omega) = \chi_L(\nu, \sigma), \quad (8a)$$

$$(3\pi^2\hbar^3/m^*p_F)\chi_L(\nu, \sigma) = (1 + \frac{1}{3}F_1)[\nu_0^2 - \varphi(\nu, \sigma) - \nu^2]^{-1}, \quad (8b)$$

where

$$\nu_0^2 = \frac{1}{3}(1 + F_0)(1 + \frac{1}{3}F_1), \quad (9a)$$

$$\varphi = (1 + \frac{1}{3}F_1)\nu[(1/3s)(1 + 1/W) - s], \quad (9b)$$

$$s = \nu + i/\sigma, \quad (9c)$$

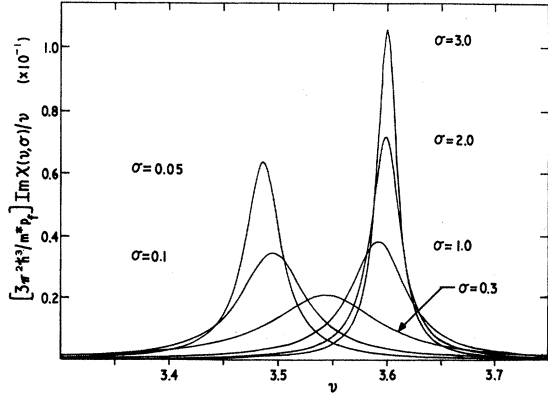


FIG. 1. Light-scattering intensity plotted against "dimensionless" frequency  $\nu$ , for several "dimensionless" relaxation times  $\sigma$ . The choice of  $\sigma$  covers scattering in the first-sound ( $\sigma=0.05, 0.1$ ) transition ( $\sigma=0.3$ ) and zero-sound ( $\sigma=1.0, 2.0$ , and  $3.0$ ) regimes.

$$W = \frac{1}{2}s \ln[(s+1)/(s-1)] - 1. \quad (9d)$$

All of the predictions of the Landau theory for the finite-temperature frequency power spectrum of density oscillations are contained in Eqs. (8) and (9) in a very implicit form. For this reason we have made detailed numerical calculations of

$$\frac{\text{Im}\chi_L(\nu, \sigma)}{\nu} = Q v_F \frac{\text{Im}\chi(Q, \omega)}{\omega}. \quad (10)$$

Using the values shown in Figs. 1 and 2, together with Eqs. (3) and (10), allows one to compute the frequency power spectrum of scattered light in considerable detail for a range of temperatures and wavelengths.

In Fig. 1 we have plotted the "zero-" and first-sound peaks. The peak corresponds to an incident photon creating one phonon of sound. As the tem-

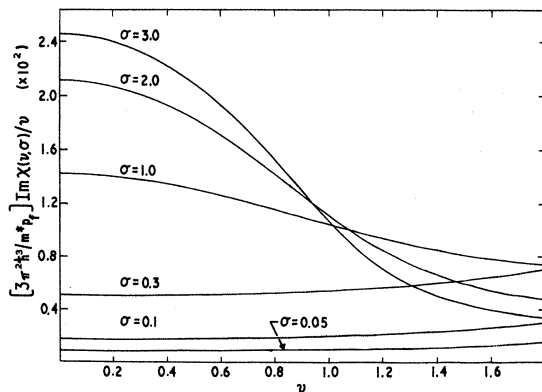


FIG. 2. Continuation of the plots in Fig. 1, for small values of  $\nu$ , where for  $\sigma \geq 1$  quasiparticle-hole pairs dominate the scattering.

perature is lowered, the peak first broadens and starts to shift from the first- to zero-sound regime. Further lowering of the temperature narrows the zero-sound peak. The shift takes place at temperatures of the order of 50 mK and is accessible to experiment.

In Fig. 2 we have plotted the intensity due to a photon creating a single quasiparticle-hole pair. The intensity shows up as a broad central peak which *increases*<sup>9</sup> as the temperature is lowered. This is in contrast to a typical heat-diffusion peak, which would decrease with lowered temperature but which is entirely negligible in liquid He<sup>3</sup> at low temperatures. The central quasiparticle-hole-pair intensity is small in comparison with the sound-wave peak (about 0.1%), but it is clearly distinguishable from background effects and would be most valuable to observe, since it is a prediction unique to a Landau quasiparticle theory.

Using the sum rule

$$S(Q) = (\hbar/\pi\rho) \int_{-\infty}^{+\infty} (1 - e^{-\hbar\omega/k_B T})^{-1} \text{Im}\chi(Q, \omega) d\omega, \quad (11)$$

one can predict finite-temperature x-ray structure factors from the Landau function  $\chi_L(\nu, \sigma)$ . By far the dominant contributor to the integral in Eq. (11) is the sound-wave peak.

In Fig. 3 we have plotted  $S(Q)$  for a range of temperatures and find that finite-temperature effects are negligible even for the smallest  $Q$  values measured experimentally. Agreement between theory and experiment is qualitatively good considering the scatter in the experimental points presently available.<sup>10,11</sup> What is needed is more precise experimental points to reduce the scatter.

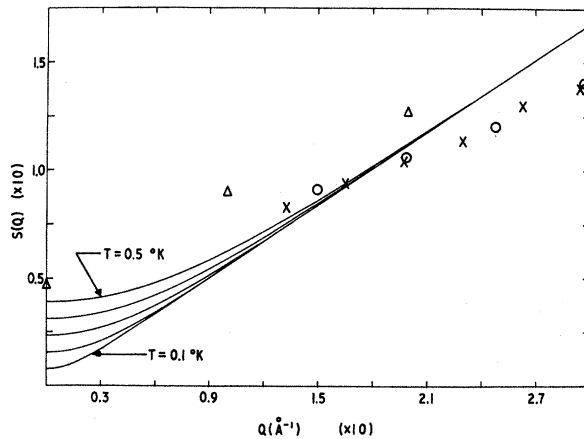


FIG. 3. Plot of  $S_T(Q)$  for temperatures from 0.1 to 0.5 K, at intervals of 0.1 superimposed over existing data at  $T=0.56$  (Ref. 11), 0.41, and 0.36 K (Ref. 10) represented by triangles, circles, and crosses, respectively.

In conclusion we wish to make two points: (i) Light-scattering measurements of the zero- to first-sound transition in liquid He<sup>3</sup> would be valuable and are possible. (ii) More difficult but even more

valuable would be the detection of quasiparticle-hole pairs by light scattering, since this would constitute an experimental confirmation of a particular prediction of the Landau theory.

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<sup>1</sup>L. D. Landau, *Zh. Eksperim. i Teor. Fiz.* **30**, 1054 (1956) [*Sov. Phys. JETP* **3**, 920 (1956)]; **32**, 59 (1957) [**5**, 101 (1957)]; **34**, 262 (1958) [**7**, 182 (1958)]. See also A. A. Abrikosov and I. M. Khalatnikov, *Rept. Progr. Phys.* **XXII**, 329 (1959).

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<sup>3</sup>R. A. Smith, *Contemp. Phys.* **12**, 523 (1971).

<sup>4</sup>C. J. Pailin, W. F. Vinen, E. R. Pike, and J. M. Vaughn, *J. Phys. C* **4**, 225 (1971).

<sup>5</sup>See, for example, L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media* (Pergamon, London, 1960), Chaps. XIV and XV.

<sup>6</sup>Our definition is the same as that used by D. Pines and P. Nozieres, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I. We use the values

$F_0 = 6.25$  and  $F_1 = 10.8$ .

<sup>7</sup>See, for recent viscosity value, M. P. Bertinat, D. S. Betts, D. F. Brewer, and G. J. Butterworth, *Phys. Rev. Letters* **28**, 472 (1972). We find  $\eta$  via the relationship  $\eta = \frac{1}{5} \pi \tau_\eta v_F^2 (1 + \frac{1}{3} F_1)$ .

<sup>8</sup>A. A. Abrikosov and I. M. Khalatnikov, *Zh. Eksperim. i Teor. Fiz.* **34**, 198 (1958) [*Sov. Phys. JETP* **7**, 135 (1958)]; **41**, 544 (1961) [**14**, 389 (1961)]. The original paper treated the collision integral incorrectly; however, we are in agreement with the latter result (second paper).

<sup>9</sup>As the temperature is lowered from first- to "zero-" sound regime the central peak first increases and then decreases (below about 20 °mK) since an over-all  $T$  factor has begun to dominate.

<sup>10</sup>R. B. Hallock, *Phys. Rev. Letters* **26**, 618 (1971).

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## Optimized Jastrow Factor and Consistent Phonons in Quantum Crystals

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Optimization of the short-range correlation function in the Jastrow-Nosonow-Koehler form of trial ground-state wave function for quantum crystals, by functional minimization of the ground-state energy, is proved to result automatically in phonon frequencies which are fully consistent: frequencies defined from the one-phonon excitation energy and from the Gaussian portion of the ground-state wave function are identical.

Considerable progress has been achieved<sup>1,2</sup> in recent years in constructing wave functions and phonon dynamical matrices for quantum crystals, where the possibility of hard-core collisions must be dealt with explicitly. Nevertheless, certain disturbing difficulties have resisted treatment. The major problem<sup>2</sup> is that of ambiguity in the definition of the phonon frequencies; those appearing in the phonon zero-point portion of the ground state wave function do not agree with those appearing in the excitation energy of the one-phonon state. Another problem is the conceptual difficulty of specifying the separation of the ground-state wave function into short- and long-range correlation parts. Although the former is to be represented by a Jastrow function, and the latter by a phonon Gaussian function, in fact both are of the same functional form and cannot be distinguished analytically. Finally, the problem of how best to choose the short-range correlation function has given rise

to a substantial literature.<sup>1</sup>

In this paper we demonstrate that all three problems are in fact closely related and can be resolved simultaneously. We show that when the short-range correlation function is determined by the variational requirement of functionally minimizing the ground-state energy, subject to a constraint which uniquely separates the pair distribution function into a short-range and a phonon part, then the previous ambiguity in the phonon dynamical matrix also disappears.

As a starting point we use the Koehler adaptation<sup>2</sup> of the method of correlated basis functions. First a trial ground-state wave function is exhibited for the solid,

$$|0\rangle = \left( \prod_{i<j} f_{ij}(\vec{r}_{ij}) \right) \exp \left( - \sum_{i<j} \frac{1}{4} \vec{u}_{ij} \cdot \vec{\Gamma}_{ij} \cdot \vec{u}_{ij} \right), \quad (1)$$

where the Jastrow-Nosonow factors  $f_{ij}$  are specifically intended to account for short-range hard-core