Analysis of line shapes observed in the scattering of thermal neutrons from superfluid ^{4}He

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The line shapes, energies, and linewidths of elementary excitations in superfluid ^{4}He have been studied as a function of scattering vector (q) and temperature by neutron scattering. Near the roton minimum, a harmonic-oscillator line shape provides a significantly better representation of the observed spectra than the more often employed Lorentzian form. The parameter characterizing the energy of the excitation is found to depend strongly on the analytic form of the dynamical structure factor $S(q,\omega)$ used to analyze the data. Linewidths, on the other hand, appear to be nearly independent of both q and the analytic form used to represent $S(q,\omega)$ between 0.75 and 2.0 Å^{-1}.

I. INTRODUCTION

In spite of the fact that superfluid ^{4}He has been extensively studied, its properties are still not well understood, particularly on a microscopic scale. Most of the available microscopic information comes from x-ray and neutron scattering studies, x rays being used primarily to investigate the static structure of the liquid and neutrons both its static and dynamical properties. Of the dynamical studies, the most complete to date is probably that of Cowley and Woods,[1] who looked at the energies and intensities of the excitations and at the temperature dependence of the linewidths at small and large values of the scattering vector q. Linewidth studies at scattering vectors near the roton minimum have also been made by Dietrich *et al.*[2] and light scattering studies of roton linewidths at lower temperatures have been reported by Greytak and Yan.[3] Little attention has, however, been paid to linewidths at intermediate values of q and even less to the actual shape of the spectrum.

Recently, Halley and Hastings[4] derived a specific form for the dynamical structure factor $S(q,\omega)$ for liquid ^{4}He at finite temperatures which Halley[5] has compared with an earlier Lorentzian form put forward by Cohen.[6] Halley and Hastings proposed for the dynamical structure factor in the roton region an expression of the form

$$S_H(q,\omega)=\frac{A\,\omega}{1-e^{\hbar\omega\beta}}\left(\frac{4\Gamma}{(\omega^2-E^2/\hbar^2)^2+4\Gamma^2\omega^2}\right), \quad (1)$$

(which we will call the harmonic-oscillator line shape[7]), while Cohen suggested a Lorentzian form

$$S_L(q,\omega)=\frac{A\,\omega}{1-e^{\hbar\omega\beta}}\left(\frac{\Gamma}{(\omega+E/\hbar)^2+\Gamma^2}+\frac{\Gamma}{(\omega-E/\hbar)^2+\Gamma^2}\right). \quad (2)$$

In both expressions β represents $1/k_BT$, and Γ, E, and A are considered to be functions of q and T.

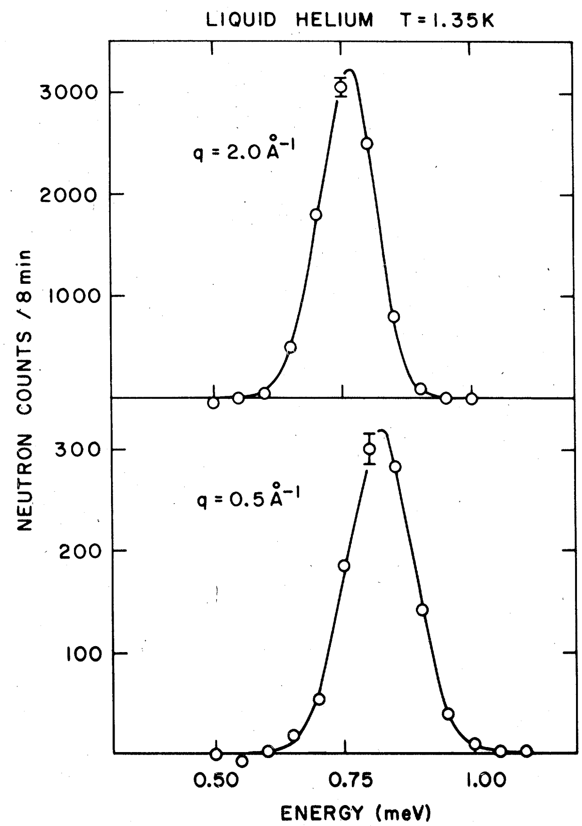

FIG. 1. Neutron scattering spectra at $T=1.35$ K. The solid lines represent the computed best fits to the data using either Eq. (1) or (2) (which are effectively interchangeable in the limit of small damping, i.e., low temperature).

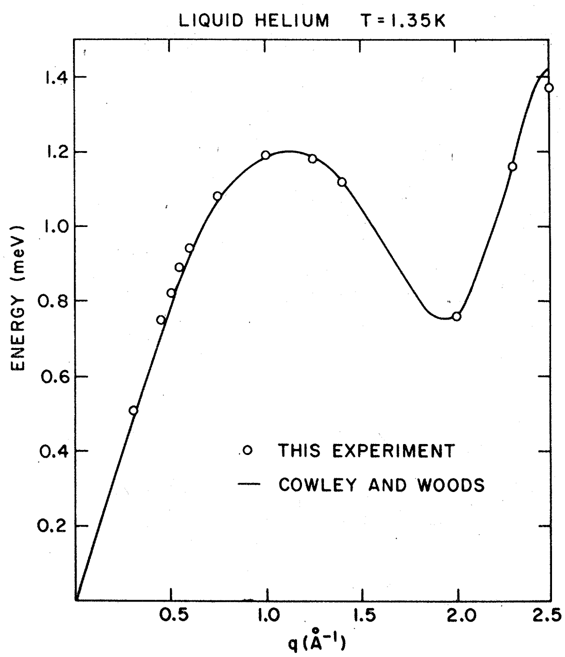

FIG. 2. Comparison of excitation energies observed at $T = 1.35$ K (open circles) with data of Ref. 1 (solid line).

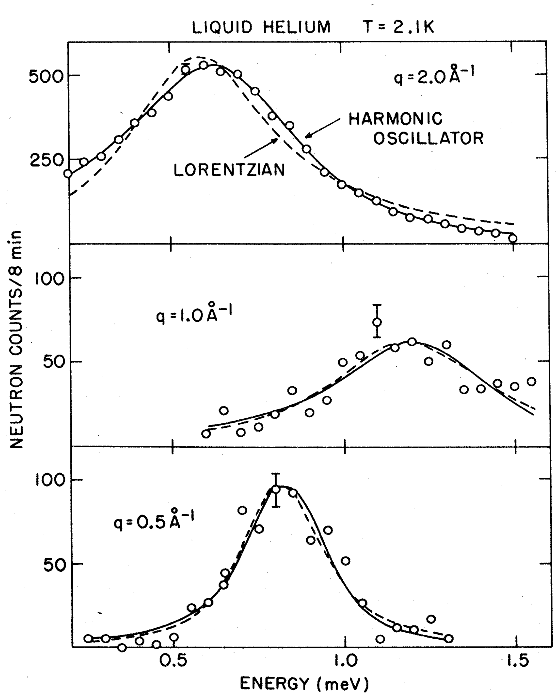

FIG. 3. Constant q scans at 2.1 K. Solid lines, best fits of S_H; dashed lines, best fits of S_L to the data. At $q = 2.0$ Å^{-1} the harmonic oscillator form S_H provides a better representation of the data than the Lorentzian form S_L. Elsewhere, the two are virtually indistinguishable.

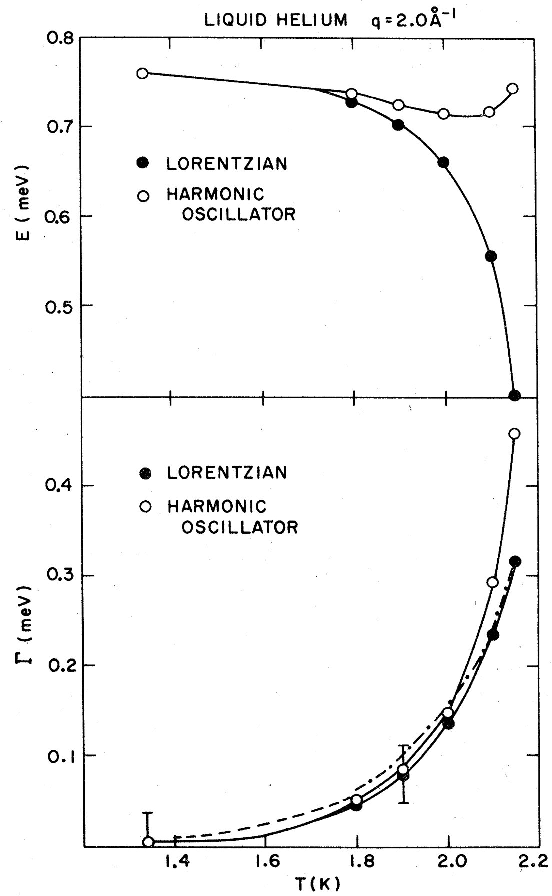

FIG. 4. Temperature variation of the fitting parameters E and Γ for S_H and S_L at $q = 2.0$ Å^{-1}. Also plotted are values of Γ from Ref. 2 (dashed line) and Ref. 3 (dot-dashed line). It is evident that E and Γ are model dependent (particularly the former) and have meaning *only* in the context of whatever form of dynamical structure factor is used to analyze the data. The solid lines are guides to the eye and have no theoretical significance.

II. EXPERIMENTAL DETAILS AND DATA ANALYSIS

The line-shape measurements to be compared with the above expressions were made on a triple-axis neutron spectrometer at the Brookhaven High Flux Beam Reactor with the incident neutron energy fixed at 5 meV. Curved pyrolytic graphite crystals were used for both monochromator and analyzer; a *Be* filter was mounted in front of the monochromator to remove neutrons with energies greater than 5 meV from the beam. Horizontal collimation before and after the monochromator and analyzer was 40 min full width at half-maximum (FWHM). The nominal energy resolution of the spectrometer was 0.15-meV FWHM using the 002 Bragg reflection from both monochromator and analyzer. In all cases spectra

TABLE I. Energy parameter E (meV) for fits of the experimental spectra to the harmonic-oscillator and Lorentzian forms of the dynamical structure factor.

	T (K)						
q (Å^{-1})	1.34	1.46	1.80	1.90	2.00	2.10	2.15
			Harmonic oscillator				
0.30	0.51						
0.45	0.75	0.75	0.74				
0.50	0.82	0.82	0.81	0.81	0.83	0.84	
0.55	0.88	0.89	0.88				
0.60	0.94	0.94	0.93	0.93		0.93	
0.75	1.08	1.09	1.08	1.07	1.07	1.18	
1.00	1.19	1.19	1.18	1.13	1.17	1.25	
1.25	1.18	1.18	1.16	1.16	1.18	1.25	
1.40	1.12	1.11	1.10	1.09	1.11	1.11	
2.00	0.76		0.74	0.72	0.72	0.72	0.74
2.30	1.16						
2.50	1.37						
			Lorentzian				
0.30	0.51						
0.45	0.75	0.74	0.73				
0.50	0.82	0.82	0.80	0.80	0.80	0.81	
0.55	0.88	0.88	0.87				
0.60	0.94	0.94	0.92	0.92		0.90	
0.75	1.08	1.08	1.07	1.06	1.04	1.09	
1.00	1.19	1.19	1.18	1.12	1.14	1.18	
1.25	1.18	1.18	1.15	1.15	1.14	1.15	
1.40	1.12	1.11	1.10	1.08	1.07	1.04	
2.00	0.76		0.73	0.70	0.66	0.55	0.40
2.30	1.16						
2.50	1.37						

were taken by scanning the outgoing neutron energy with fixed momentum transfer.

The sample consisted of 50 cm^3 of liquid ^{4}He in a thin walled cylindrical aluminum container mounted inside a pumped ^{4}He cryostat. Temperatures were measured by means of a calibrated Ge resistor; temperature uncertainties were of the order of 0.05 K. Since the spectra are observed experimentally with an instrument of finite q and ω resolution, the suggested forms of $S(q, \omega)$ had first to be folded with an analytic representation of the spectrometer resolution function before comparisons could be made with the data. Using the resolution function of Cooper and Nathans[8] together with the normalization of Chesser and Axe,[9] we performed an appropriate convolution for each experimental scan adjusting the parameters Γ, E, and A to minimize the weighted variance (χ^2).

III. RESULTS AND DISCUSSION

Scans were made at saturated vapor pressure over a wide range of momenta for $1.35 \leq T \leq 2.15$ K. Two of the lowest temperature scans are shown in Fig. 1 together with the best fitting computed line shapes. In Fig. 2 the excitation energies obtained from the 1.35 K data are compared with those observed by Cowley and Woods[1] at 1.1 K. Agreement is generally satisfactory; there are minor discrepancies at small q but they are within experimental error.

Best fitting values of the parameters for each analytic form of $S(q, \omega)$ are given in Tables I and II. It should be noted that all scans made at 1.35 and 1.46 K are resolution limited. In these cases we can only say that the intrinsic linewidth parameter Γ is less than 0.03 meV for all q below 1.46 K.

TABLE II. Linewidth parameter Γ (meV) for fits of the experimental spectra to the harmonic-oscillator and Lorentzian forms of the dynamical structure factor.

	T (K)				
q (Å^{-1})	1.80	1.90	2.00	2.10	2.15
		Harmonic oscillator			
0.45	0.036				
0.50	0.048	0.072	0.10	0.11	
0.55	0.044				
0.60	0.044	0.071		0.15	
0.75	0.052	0.071	0.14	0.26	
1.00	0.054	0.084	0.15	0.25	
1.25	0.058	0.092	0.17	0.28	
1.40	0.048	0.089	0.16	0.21	
2.00	0.050	0.084	0.15	0.29	0.46
		Lorentzian			
0.45	0.036				
0.50	0.049	0.074	0.10	0.11	
0.55	0.042				
0.60	0.044	0.072		0.18	
0.75	0.053	0.073	0.15	0.28	
1.00	0.056	0.084	0.15	0.27	
1.25	0.058	0.092	0.17	0.29	
1.40	0.049	0.090	0.16	0.23	
2.00	0.047	0.078	0.13	0.23	0.32

In the small damping limit (which applies at low temperatures) the two forms of $S(q,\omega)$ are indistinguishable and the parameters of best fit become identical. With increasing temperature, however, the damping increases and differences between the two forms become apparent. Figure 3 shows the best fits of the two analytic forms to scans at $q = 0.5$, 1.0, and 2.0 Å^{-1} with a sample temperature of 2.1 K. At 2.0 Å^{-1}, one can see a distinct difference in the quality of fit. Clearly, the harmonic oscillator line shape is superior; the mean value of χ^2 for scans at and above 1.8 K is 2.6 for S_H while for S_L it is 12.6! (We suspect that χ^2 is greater than unity even for the damped oscillator form because we have failed to take proper account of the background and have not corrected for small distortions introduced by multiphonon contributions to the scattering.)

At other values of q, S_L, and S_H fit the data almost equally well. In Fig. 3, S_L seems to be slightly the better choice for $q < 2.0$ Å^{-1}. Indeed, the values of χ^2 for S_L at and above 1.8 K are (on average) smaller, but the differences are probably not statistically significant.

Where S_H and S_L are different enough to be distinguishable, they yield values for the excitation parameters, particularly the nominal excitation energy E, which differ considerably. This is evident in Fig. 4 which is a plot of the temperature dependence of E and Γ as obtained from each form of $S(q,\omega)$. When the Lorentzian form is used, E and Γ are not strongly correlated and accurately reflect the peak position and half-width at half-maximum of the observed spectrum. The harmonic oscillator form on the other hand yields strongly correlated values of E and Γ which do not relate as well to the peak position and half width. S_L may, in fact, be the more useful form experimentally because its parameters are uncorrelated and have unambiguous meanings. Nevertheless, in the roton region, S_H is a significantly better representation of the data. In any event, it seems clear from our results that any definition of roton energies at higher temperatures has meaning only within the context of the analytic form in which the dynamic structure factor is represented.

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