Density and spin-density excitations in normal-liquid ^{3}He

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In bulk Fermi liquids such as liquid ^{3}He and nuclear matter the quasiparticle effective mass is enhanced at the Fermi surface and reduces to the bare mass far from the Fermi surface. We incorporate this central physical feature into the density and spin-density dynamics of normal-liquid ^{3}He and obtain good agreement with recent high-resolution neutron-scattering experiments. Existing theories up to this time using quadratic quasiparticle dispersion do not reproduce experiment. [S0163-1829(97)05010-8]

Recent high-resolution inelastic-neutron-scattering measurements of excitations in normal-liquid ^{3}He (Refs. 1 and 2) show that existing theories and models cannot describe the dynamic response of this fundamental Fermi liquid. A clear understanding of simple Fermi liquids is a prerequisite for addressing more complex highly correlated systems.

Both density and nuclear spin-density fluctuations in liquid ^{3}He are observed in neutron-scattering measurements.[3] At long wavelengths and up to wave vectors $Q \sim 1$ Å^{-1}, the density response is dominated by a single collective zero-sound mode. The mode energy is well described using the random-phase approximation (RPA) and a quasiparticle interaction which is an extension to finite Q of the Landau interaction.[4–6] These models use a quasiparticle effective mass $m^*=2.8$ times the bare ^{3}He mass at saturated vapor pressure (SVP), a value taken from Landau-Fermi-liquid theory[7] used for describing thermodynamic and transport properties. The spin-density response displays a ''paramagnon'' resonance at low energies. The improved resolution of the measurements in Ref. 1 provided detailed information on the line shape of the paramagnon resonance. It has been shown[2] that the line shape cannot be described by RPA models using $m^*=2.8$, nor by the paramagnon model[8] which uses the bare mass $m^*=1$. Moreover, the paramagnon model cannot be extended to describe the density fluctuations. A good description of the paramagnon line shape can be obtained with a simple RPA model by arbitrarily setting $m^*=1.9$ combined with a fitted interaction parameter. However, this value of m^* is inconsistent with Landau theory, with the observed zero-sound dispersion and the fact that the zero-sound mode exists up to a wave vector of the order of 1.4 Å^{-1}.

Very generally, the single quasiparticle energy $\epsilon(k)$ in Fermi liquids shows a flattening at the Fermi surface, $k=k_F$. This flattening can be represented as an enhancement of the effective mass at the Fermi surface.[9] The effective mass $m^*(k)$ is a function of wave vector k and takes its maximum value at $k=k_F$ ($k_F=0.785$ Å^{-1} at SVP in liquid ^{3}He). Sufficiently far above (or below) k_F, $m^*(k)$ reduces to the bare mass, $m^*=1$. The behavior of the quasiparticle energy may also be described as an energy-dependent effective mass, $m^*(\omega)$, which takes its maximum value at $\omega=\epsilon_F$ (ϵ_F is the Fermi energy). For ''on-shell'' energies, the two descriptions are equivalent. Microscopic calculations in nuclear matter,[10] liquid ^{3}He,[11] and other Fermi liquids predict this enhancement. It originates from the renormalization of the quasiparticle mass by density and spin-density fluctuations. Thermodynamic properties at low temperatures, such as the specific heat, reflect the mass enhancement near k_F since only excitations close to the Fermi surface are sampled. On the other hand, neutron-scattering measurements at larger Q values excite quasiparticles having wave vectors k far from k_F, and $m^*(k)$ is sampled for a range of k values. Thus we expect to observe a somewhat different average $\langle m^*(k)\rangle$ in the two measurements.

In this report, we present a simple model of both the density and spin-density response of normal-liquid ^{3}He that incorporates an $\epsilon(k)$ that flattens at $k=k_F$ represented by an $m^*(k)$ enhanced at k_F. We also use the Landau parameters to represent the quasiparticle-quasiparticle interaction and include the Q dependence of the static interaction to the extent known from microscopic calculations. Within a simple RPA, we obtain a good description of both the ''paramagnon'' line shape and of the zero-sound energy for $Q \simeq 1$ Å^{-1}. The model may be extended readily to higher Q values by including multiquasiparticle excitations that requires going beyond the RPA.

Neutron scattering measures directly the sum of the density $S_c(Q,\omega)$ and the spin-density $S_I(Q,\omega)$ components of the dynamic structure factor, $S(Q,\omega)=S_c(Q,\omega)+(\sigma_i/\sigma_c)S_I(Q,\omega)$, where σ_c and σ_i are the coherent and incoherent scattering cross sections, respectively, $S_{c,I}(Q,\omega)$ is proportional to the imaginary part of the dynamic susceptibility $\chi_{c,I}(Q,\omega)$. The exact equation for $\chi(Q,\omega)$ reduces to the RPA expression

$$\chi_{c,I}(Q,\omega)=\frac{\chi_0(Q,\omega)}{1-I_{s,a}(Q,\omega)\chi_0(Q,\omega)}, \tag{1}$$

if the quasiparticle-quasiparticle interaction $I_{s,a}(k_1\omega_1,k_2\omega_2,Q\omega)$, where $k_1(\omega_1)$ and $k_2(\omega_2)$ are the wave vectors (energies) of two interacting quasiparticles and

$Q(\omega)$ is the wave vector (energy) transfer in the scattering process,[3] is approximated by an interaction $I_{s,a}(Q,\omega)$ that depends only on Q and ω. Here $\chi_0(Q,\omega)$ is the susceptibility of the independent (noninteracting) quasiparticles *and* I_s and I_a are the spin symmetric and spin antisymmetric interactions, respectively. This approximation is valid at $Q\to 0$, where both k_1 and k_2 are close to k_F. We expect it to become increasingly poor as Q increases. Multiparticle-hole excitations are also neglected in Eq. (1).

Secondly, we assume that the quasiparticle energy $\epsilon(k,\omega)$ is real and consider only "on-shell" energies, i.e., $\epsilon(k,\omega)=\epsilon(k,\epsilon_k)=\epsilon_k$, so that ϵ_k depends only on k. In this limit, $\chi_0(Q,\omega)$ reduces to the Lindhard function

$$\chi_0(Q,\omega)=\frac{2}{V}\sum_k \frac{n_k-n_{k+Q}}{\omega+i\eta-(\epsilon_{k+Q}-\epsilon_k)}, \tag{2}$$

where n_k is the Fermi function and V is the volume. The effective mass $m^*(k)$ is defined in terms of the quasiparticle energy ϵ_k as[7]

$$m^*(k)=\frac{\hbar^2 k}{m_3}\left(\frac{d\epsilon_{k'}}{dk'}\right)^{-1}_{k'=k}. \tag{3}$$

We introduce a model for $m^*(k)$ by representing it by a simple cosine function that peaks at the Landau value $m^*=2.8$ at $k=k_F$ and falls to a lower value on each side of k_F. How rapidly $m^*(k)$ falls to $m^*=1$ is not accurately predicted by microscopic calculations.[10,11] However, comparison of a calculated $S(Q,\omega)$ with observed data at $Q\sim 2$ Å^{-1} suggests that an aggregate m^* of 1.5–2 still appears in $S(Q,\omega)$ at this large Q value.[12] We therefore allow $m^*(k)$ to fall to a constant value $m_0\geqslant 1$ outside a range $|k-k_F|<fk_F$ where f sets this range. For $|k-k_F|<fk_F$ we chose the form $m^*(k)=m_0+(m^*-m_0)[1+\cos\{(k-k_F)\pi/fk_F\}]/2$. The model has two parameters, m_0 and f. We find, using the data from Refs. 1 and 2, that the spin-density response requires $m_0<2$, while the density response requires $m_0>1$. The results are largely insensitive to the analytic form chosen for $m^*(k)$ (Gaussian, cosine, inverse cosine) and to the value of m_0 ($1.0\leqslant m_0\leqslant 2.0$). The $m^*(k)$ should fall from $m^*=2.8$ to $m^*=m_0$ within $k_F/2$ from the Fermi surface. A good compromise is $m_0=1.7$ and $f=0.35$. The dynamic response of liquid ^{3}He up to $Q=1$ Å^{-1} depends chiefly on $m^*(k)$ in the region $|k-k_F|<fk_F\approx k_F/3$, i.e., on $m^*(k)$ near k_F, as set out below.

The inset of Fig. 1 shows the model $m^*(k)$ for different values of m_0. The quasiparticle energy ϵ_k was obtained by integrating Eq. (3) numerically. Figure 1 shows ϵ_k for $m_0=1.7$ and $f=0.35$: a clear flattening of ϵ_k is seen at k_F, where $m^*(k)=m^*=2.8$. The Fermi energy of the model ϵ_F lies somewhat above the Landau-Fermi energy.

The Lindhard function for the nonparabolic ϵ_k is obtained by numerical integration of Eq. (2). As expected, the resulting $\chi_0(Q,\omega)$, shown in Fig. 2, has a strong low-energy enhancement reflecting $m^*(k_F)=2.8$ but a longer tail than for a constant $m^*=2.8$.

We use the Landau interaction ($dn/d\epsilon$ is the density of states at the Fermi surface)

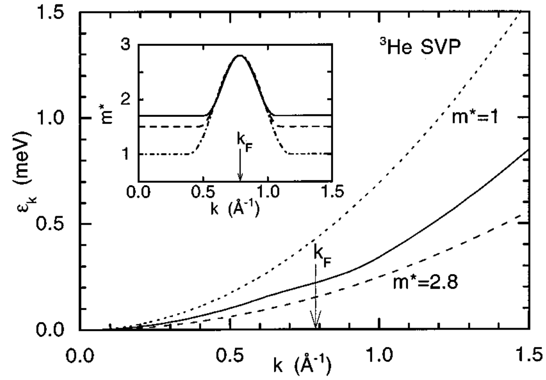

FIG. 1. The quasiparticle energy ϵ_k obtained from Eq. (3) and the model $m^*(k)$ for the parameters $m_0=1.7$, $f=0.35$ (solid line), compared with the free-particle ϵ_k for $m^*=2.8$ (dashed line) and $m^*=1$ (dotted line). The inset shows the model $m^*(k)$ for $m_0=1.7$, $f=0.35$ (solid line), $m_0=1.5$, $f=0.4$ (dashed line), and $m_0=1$, $f=0.5$ (dash-dotted line).

$$\left(\frac{dn}{d\epsilon}\right)I_{s,a}(Q,\omega)=F_0^{s,a}(Q)+\frac{F_1^{s,a}(Q)}{1+F_1^{s,a}(Q)/3}\left(\frac{\omega}{v_F Q}\right)^2, \tag{4}$$

in Eq. (1) with Q-dependent Landau parameters $F_{0,1}^{s,a}(Q)$ that reduce to the usual "Landau" values at $Q=0$, i.e., $F_{0,1}^{s,a}(0)=F_{0,1}^{s,a}$. The Q dependence of $F_{0,1}^{s,a}(Q)$ is guided by microscopic calculations. Figure 3 shows as the dotted line $F_0^s(Q)$ calculated by Clements *et al.*[13] This $F_0^s(Q)$ contains the effect of density and spin-density fluctuations to second order which increases $F_0^s(Q)$ at low Q. However, the calculated $F_0^s(Q)$ still lies below the observed Landau value. For consistency with Landau theory, we have further increased $F_0^s(Q)$ so that $F_0^s(0)=9.3$, the Landau value at SVP. The

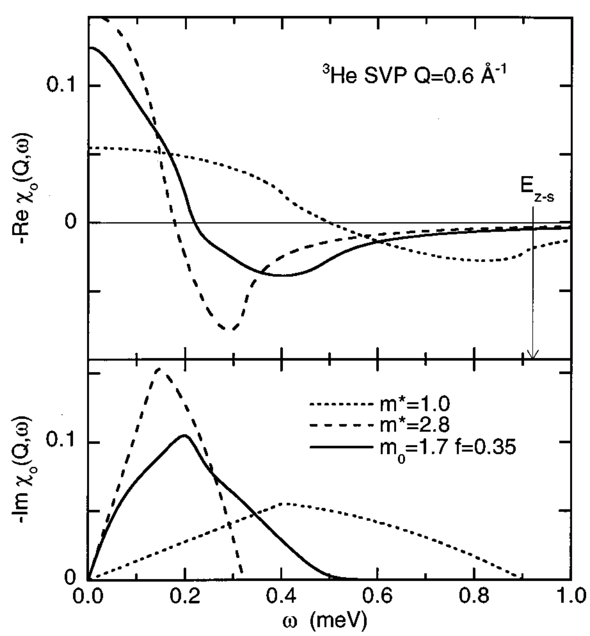

FIG. 2. $\chi_0(Q,\omega)$ at $Q=0.6$ Å^{-1} given by Eq. (2) and the model $m^*(k)$ for the parameters $m_0=1.7$, $f=0.35$ (solid line) and for the free particle ϵ_k using $m^*=2.8$ (dashed line) and $m^*=1$ (dotted line).

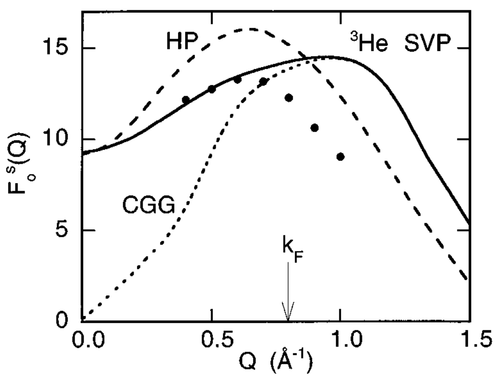

FIG. 3. Q dependence of $F_0^s(Q)$. The solid line shows the $F_0^s(Q)$ used, which is based on the microscopic calculation Clements, Greeff, and Glyde (CGG) (Ref. 13) (dotted line) and modified to reproduce the Landau parameter in the limit $Q \to 0$. For comparison, the polarization-potential result Hess and Pines (HP) (Ref. 5) is also shown. The dots show the values of $\alpha_Q F_0^s(Q)$ obtained from a fit to the observed zero-sound dispersion.

resulting $F_0^s(Q)$, given by the solid line in Fig. 3, is similar to the static interaction obtained by Hess and Pines[5] from a fit to the zero-sound energy. Clements *et al.* found that $F_0^a(Q)$ is nearly independent of Q, and for simplicity we use a constant $F_0^a(Q) = F_0^a = -0.695$, the Landau value independent of Q. $F_1^s(Q)$ was obtained by requiring that the coherent $S_c(Q,\omega)$ fulfill the f-sum rule at each Q value, neglecting multipair contributions. Little is known about $F_1^a(Q)$ and we used the Landau value $F_1^a = -0.55$.

This defines the model, which treats the density and spin-density excitations on an equal footing and reduces to Landau theory in the limit $Q \to 0$. The aim is to determine whether a simple enhancement of the effective mass near k_F can provide agreement with experiment for $Q \leqslant 1$ Å^{-1}.

Calculations of the spin-dependent dynamic structure factor $S_I(Q,\omega)$ are compared with experiment in Fig. 4. To set the stage, Fig. 4(a) shows the paramagnon[8] result, which uses $m^* = 1$ and a single interaction parameter, and the Landau result,[5,6] which uses $m^* = 2.8$ and the Landau interaction Eq. (4) with constant parameters $F_{0,1}^a$. Clearly, these two models do not reproduce the observed $S_I(Q,\omega)$. Figure 4(b) shows $S_I(Q,\omega)$ calculated using the present $\epsilon(k)$ obtained for $m_0 = 1.7$ and $f = 0.35$ as well as for $m_0 = 1$ and $f = 0.5$, using the Landau interaction. Both curves agree well with the observed $S_I(Q,\omega)$. This shows that an $m^*(k)$ enhanced at k_F reproduces $S_I(Q,\omega)$ well and that $S_I(Q,\omega)$ for $Q \leqslant 1$ Å^{-1} is most sensitive to $m^*(k)$ for k near k_F, $|k - k_F| < k_f/3$. We have compared theory and experiment for $Q = 0.6$ Å^{-1}, since this Q value ($< k_F$) is low enough for the theory to be valid and the intrinsic width of $S_I(Q,\omega)$ is considerably broader than the instrumental resolution width. The calculated $S_I(Q,\omega)$ was convolved with the Gaussian instrumental resolution function of width 0.08 meV. The low-energy tail of the zero-sound excitation has also been included in the calculations since the two excitations overlap and this contribution appears in the data. Comparisons at other wave vectors ($0.4 < Q < 1.0$ Å^{-1}) lead to similar conclusions.

Figure 5 shows the zero-sound mode energy calculated

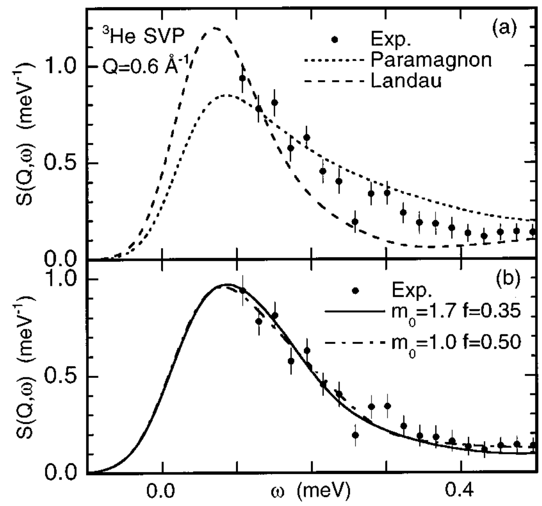

FIG. 4. Low-energy part of $S(Q,\omega)$ for liquid ^{3}He at $Q = 0.6$ Å^{-1} and SVP. (a) The paramagnon model ($m^* = 1$) is too extended in energy, while the Landau model ($m^* = 2.8$) is too sharp and has too little intensity at higher energies. (b) Excellent agreement is obtained with the model $m^*(k)$ for different parameters m_0 and f as shown. Experimental data are from Ref. 2.

from the denominator of $\chi_c(Q,\omega)$ in Eq. (1) with the present model of $m^*(k)$ and the interaction (4) compared with experiment. The mode energy is essentially an extension of the zero-sound velocity with some upward or anomalous dispersion arising from the initial increase of $F_0^s(Q)$ with Q, as pointed out already in Ref. 4. Calculations of the zero-sound energy with the model $m^*(k)$ using $m_0 = 1.7$ and $f = 0.35$ differ little from the "Landau calculation"[4–6] using a constant $m^* = 2.8$ (Fig. 5). The calculated mode energy and its weight Z_Q agree with experiment without including multiquasiparticle-hole (MPH) contributions up to $Q \simeq 0.7$ Å^{-1}. MPH excitations begin to appear in the observed $S_c(Q,\omega)$ at 0.8 Å^{-1}. When these are important, the particle-hole part of $\chi_0(Q,\omega)$ in Eq. (1) must be correspondingly reduced, by a factor $\alpha_Q < 1$. This reduces the product

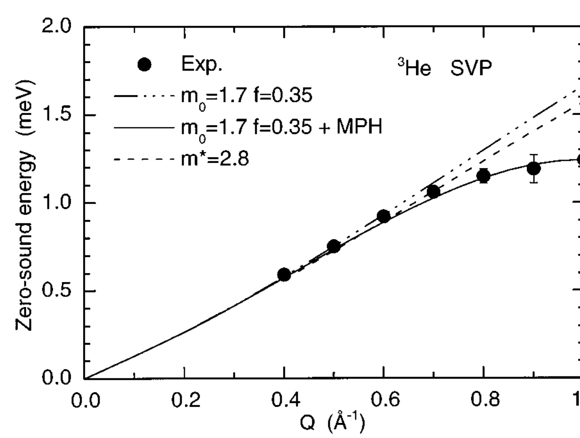

FIG. 5. Zero-sound dispersion for liquid ^{3}He obtained from Eq. (1) for a constant $m^* = 2.8$ (dashed line) and for the model $m^*(k)$ for $m_0 = 1.7$ and $f = 0.35$ (dash-dotted line) without including multiquasiparticle-hole (MPH) contributions. The solid line includes the effect of MPH. Experimental data are from Ref. 2.

$I_c(Q,\omega)\chi_0(Q,\omega)$ in Eq. (1) to $\alpha_Q I_c(Q,\omega)\chi_0(Q,\omega)$ which lowers the mode energy.[4–6]. In Fig. 3, we show how much $F_0^s(Q)$ must be decreased by α_Q to obtain agreement with experiment up to $Q=1$ Å^{-1} within the present model. In a following publication we will incorporate MPH contributions to $S_c(Q,\omega)$ fully, which will allow us to extend the model to higher Q values. Our goal here is to show that the model $m^*(k)$ depicted in Fig. 1 can provide a consistent explanation of both the density and spin-density excitations up to $Q\approx 1$ Å^{-1}.

In summary, we have presented a simple model of the density and spin-density response of normal-liquid ^{3}He which incorporates the enhancement of the effective mass to the Landau theory value $m^*=2.8$ at the Fermi surface and a smooth reduction of $m^*(k)$ to a lower value $m_0=1.7$ away from the Fermi surface. The results are insensitive to the value of m_0 within the range $1.0\leqslant m_0\leqslant 2.0$. The f value should lie within $0.3\leqslant f\leqslant 0.5$, i.e., $m^*(k)$ falls to m_0 within a relatively short distance from the Fermi surface. The model reproduces the spin-density response $S_I(Q,\omega)$ within observed precision and the zero-sound mode energy up to $Q=1$ Å^{-1}. Since m^* falls below 2.8, some Landau damping of the zero-sound mode is obtained in this model at low Q values ($0.5\leqslant Q\leqslant 1$ Å^{-1}) which partially explains the large observed width in this Q range. The model treats density and spin-density excitations consistently and reduces to the Landau-Fermi-liquid theory at low Q and low T.

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[1] R. Scherm, K. Guckelsberger, B. Fåk, K. Sköld, A.J. Dianoux, H. Godfrin, and W.G. Stirling, Phys. Rev. Lett. **59**, 217 (1987).
[2] B. Fåk, K. Guckelsberger, R. Scherm, and A. Stunault, J. Low Temp. Phys. **97**, 445 (1994).
[3] H.R. Glyde, *Excitations in Liquid and Solid Helium* (Oxford University Press, Oxford, 1994).
[4] C.H. Aldrich III, C.J. Pethick, and D. Pines, Phys. Rev. Lett. **37**, 845 (1976); C.H. Aldrich III and D. Pines, J. Low Temp. Phys. **32**, 689 (1978).
[5] D.W. Hess and D. Pines, J. Low Temp. Phys. **72**, 247 (1988).
[6] H.R. Glyde and F.C. Khanna, Phys. Rev. Lett. **37**, 1692 (1976); Can. J. Phys. **55**, 1906 (1977); **58**, 343 (1980).
[7] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. 1.
[8] M.T. Béal-Monod, J. Low Temp. Phys. **37**, 123 (1979); **39**, 231 (1980).
[9] G.E. Brown, *Many-Body Problems* (North-Holland, Amsterdam, 1972).
[10] C. Mahaux, P.F. Bortignon, R.A. Broglia, and C.H. Dasso, Phys. Rep. **120**, 1 (1985).
[11] B.L. Friman and E. Krotscheck, Phys. Rev. Lett. **49**, 1705 (1982); E. Krotscheck and R.A. Smith, Phys. Rev. B **27**, 4222 (1983); H.R. Glyde and S.I. Hernadi, *ibid.* **28**, 141 (1983).
[12] H.R. Glyde and S.I. Hernadi, Phys. Rev. B **29**, 4926 (1984).
[13] B.E. Clements, C.W. Greeff, and H.R. Glyde, Phys. Rev. B **44**, 5216 (1991).