Sum Rules and Spin Multipair Excitations in Liquid ^{3}He

F. Dalfovo and S. Stringari

Dipartimento di Fisica, Università di Trento, 38050 Povo, Italy
and Istituto Nazionale di Fisica Nucleare, Gruppo Collegato di Trento, 38050 Povo, Italy

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Multipair excitations in liquid ^{3}He at low temperature are investigated using a sum-rule approach. The $m_3 = \int S(\mathbf{q},\omega)\omega^3 d\omega$ sum rule is calculated microscopically by properly accounting for short-range correlations. The average spin multipair (mp) energy $\omega^i_{31}[m^i_3(\text{mp})/m^i_1(\text{mp})]^{1/2}$ is found to be $\sim$50 K in the low-q limit. A rigorous lower bound for the multipair contribution to the static form factor in the low-q limit is derived. The relative importance of coherent and spin-dependent multipair excitations is also discussed.

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After the first measurements with inelastic neutron scattering on liquid ^{3}He at the Institut Laue-Langevin[1] and at Argonne National Laboratory[2] several experimental and theoretical works have been devoted to the study of elementary excitations in normal liquid ^{3}He (see Ref. 3 for a recent review). Recently it has been shown[4] that multiple particle-hole excitations play an important role in characterizing the dynamic form factor of ^{3}He for wave vectors in the range 0.3 $\text{Å}^{-1} \le q \le 2.0$ Å^{-1} giving rise to a significant coupling with the zero sound mode. The resulting spectrum of elementary excitations has been found to be in good agreement with the theoretical calculations of Hess and Pines[5] based on the polarization potential theory by Aldrich and Pines.[6]

The purpose of this Letter is to investigate some properties of multipair excitations at low temperature using a microscopic approach based on sum rules. In particular we calculate the average energy of the spin-dependent multipair excitations in the low-q limit through the ratio of two sum rules and discuss the relative importance of coherent and spin-dependent excitations as a function of the wave vector q. In the long-wavelength limit the spin multipair excitations are expected to contribute more to sum rules than do the coherent counterparts since current conservation requires the latter contribution be of higher order in q.[7] As an ingredient of our analysis we use the HFDHE2 interatomic potential by Aziz *et al.*[8] recently employed in microscopic calculations[9-11] on the ground state of liquid ^{3}He. The sum-rule approach has been already employed in liquid ^{4}He[12-14] for a systematic analysis of the phonon-roton spectrum as well as of the multiphonon contribution to the dynamic form factor.

The k moments of the coherent and spin-dependent parts of the dynamic form factor

$$S(\mathbf{q},\omega) = S_c(\mathbf{q},\omega) + \frac{\sigma_i}{\sigma_c} S_i(\mathbf{q},\omega) \qquad (1)$$

entering the inelastic cross section are defined by the following relation:

$$m_k^{c(i)} = \int \omega^k S_{c(i)}(\mathbf{q},\omega)\,d\omega\,. \qquad (2)$$

In Eq. (1) σ^c and σ^i are the coherent and incoherent scattering cross sections, respectively [$\sigma^i/\sigma^c \simeq 0.25$ (Ref. 15)]. At zero temperature one can straightforwardly derive the following sum rules for the moments m_1 and m_3:

$$m_1 = \tfrac{1}{2}\langle 0|[F_q^\dagger,[H,F_q]]|0\rangle\,, \qquad (3)$$

$$m_3 = \tfrac{1}{2}\langle 0|[[F_q^\dagger,H],[H,[H,F_q]]]|0\rangle\,; \qquad (4)$$

these involve commutators between the Hamiltonian of the system and the excitation operator F_q, where

$$F_q = \sum_j e^{i\mathbf{q}\cdot\mathbf{r}_j}, \quad F_q = \sum_j \sigma_j^z e^{i\mathbf{q}\cdot\mathbf{r}_j}$$

in the coherent and spin-dependent case, respectively (σ^z is the third component of the Pauli spin matrix). In Eqs. (3) and (4) $|0\rangle$ is the ground state relative to the Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V(|\mathbf{r}_i - \mathbf{r}_j|)\,, \qquad (5)$$

where $V(|\mathbf{r}_i - \mathbf{r}_j|)$ is the central helium-helium potential. (In the case of ^{3}He one should add a magnetic dipole-dipole interaction among the nuclear spin; this term is negligible and will be ignored in the present work.)

For small values of the wave vector it is possible to distinguish in the moments m_k a contribution arising from the single pair excitations (1p-1h), occurring at energies of the order of qv_f, and a contribution coming from multipair excitations, occurring at higher energies. The former excitations are well accounted for by the Landau theory of Fermi liquids,[7] yielding the following results for the sum rules m_1 and m_3 in the low-q limit[16] ($\hbar=1$):

$$m_1^c(\text{1p-1h})=N\frac{q^2}{2m}, \qquad (6)$$

$$m_3^c(\text{1p-1h})=N\frac{q^4}{m^2}\frac{3}{5}\epsilon_F(1+\tfrac{5}{9}F_0^s+\tfrac{4}{45}F_2^s), \qquad (7)$$

$$m_1^i(\text{1p-1h})=N\frac{q^2}{2m}\frac{(1+\frac{1}{3}F_1^a)}{(1+\frac{1}{3}F_1^s)}, \qquad (8)$$

$$m_3^i(\text{1p-1h})=N\frac{q^4}{m^2}\frac{3}{5}\epsilon_F\frac{(1+\frac{1}{3}F_1^a)^2}{(1+\frac{1}{3}F_1^s)^2}\times(1+\tfrac{5}{9}F_0^a+\tfrac{4}{45}F_2^a), \qquad (9)$$

where F_l^s and F_l^a are the usual Landau parameters, $\epsilon_F=p_F^2/2m^*$ is the Fermi energy, with $m^*=m(1+F_1^s/3)$, and N is the total number of particles. As discussed in Ref. 16 the quantity

$$\omega_{31}^c(\text{1p-1h})=\left[\frac{m_3^c(\text{1p-1h})}{m_1^c(\text{1p-1h})}\right]^{1/2}=q\left[\frac{6\epsilon_F}{5m}(1+\tfrac{5}{9}F_0^s+\tfrac{4}{45}F_2^s)\right]^{1/2}$$

provides an excellent estimate of the zero sound frequency and, in particular, accounts for the distortions of the Fermi surface which characterize such a mode. The present knowledge of the Landau parameters[17] [$F_0^s=9.15$, $F_0^a=-0.70$, $F_1^s=5.27$, $F_1^a=-0.55$, and $F_2^s\simeq F_2^a\simeq 0$ at saturated vapor pressure (SVP)] permits a rather safe determination of such sum rules. Results (6)-(9) can be derived starting from Eqs. (3) and (4) using suitable spin-dependent effective interactions and an uncorrelated ground state. This corresponds to evaluating the moments (2) within the random-phase approximation (RPA).

In the following we will discuss the results for the sum rules (3) and (4) employing the bare spin-independent Hamiltonian (5). By explicitly carrying out the commutators of Eqs. (3) and (4) one finds the following results (see Refs. 12, 18, and 19):

$$m_1^c=m_1^i=N\frac{q^2}{2m}, \qquad (10)$$

$$m_3^c=N\left[\frac{q^6}{8m^3}+\frac{q^4}{m^2}\langle E_K\rangle+\frac{n_0q^2}{2m^2}\int g(r)(1-\cos qz)\nabla_z^2V(r)d\mathbf{r}\right], \qquad (11)$$

$$m_3^i=N\left[\frac{q^6}{8m^3}+\frac{q^4}{m^2}\langle E_k\rangle+\frac{n_0q^2}{2m^2}\int[g(r)-g^\sigma(r)\cos qz]\nabla_z^2V(r)d\mathbf{r}\right], \qquad (12)$$

having chosen $\mathbf{q}$ along the z axis. Note that results (10)-(12) are rigorous results for m_1 and m_3 holding at any value of q. In Eqs. (11) and (12) $\langle E_k\rangle$ and n_0 are the kinetic energy per particle and the particle density, respectively. The quantities

$$g(r)=n_0^{-2}\sum_{\sigma_1\sigma_2}G(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2),$$

$$g^\sigma(r)=n_0^{-2}\sum_{\sigma_1\sigma_2}\sigma_1\sigma_2G(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)$$

(with $\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2$) are the radial and spin radial distribution functions and $G(\mathbf{r}_1\sigma_1\mathbf{r}_2\sigma_2)$ is the usual correlation function. It is worth noting that, differently from m_1^i(1p-1h), the sum rule m_1^i is not affected by the interaction as a consequence of the local (velocity independent) and spin-independent nature of the bare interaction (5). This result indicates that 1p-1h excitations, characterizing the dynamic form factor in the low-q and low-ω region and properly accounted for by the Landau theory, do not exhaust the energy-weighted sum rule in the spin channel, an important contribution coming from the multipair excitations located at higher energies. The relevant results from the sum rule m_1 in the spin channel including the distinction between the 1p-1h and the multipair contributions are discussed in Ref. 20. Results (6)-(9), accounting for 1p-1h excitations in the low-q limit, can be generalized to higher values of q using the framework of the RPA with suitable spin-dependent effective interactions. In general such calculations will not exhaust the m_1 sum rule (10) in the spin channel unless multipair effects are explicitly included in the formalism as done, for example, in Ref. 5. Equations (11) and (12) provide a useful way to explore interesting properties of the dynamic form factor in liquid ^{3}He using microscopic ingredients. In fact, microscopic calculations of the ground state of liquid ^{3}He starting from the interatomic potential and accounting for short-range correlations are now available.[9-11]

In the low-q limit the m_3 sum rules get the following simplified form:

$$\lim_{q\to 0}m_3^c=N\frac{q^4}{m^2}\left[\langle E_k\rangle+\frac{n_0}{4}\int g(r)z^2\nabla_z^2V(r)d\mathbf{r}\right], \qquad (13)$$

$$\lim_{q\to 0}m_3^i=N\frac{n_0q^2}{m^2}\int g_{\uparrow\downarrow}(r)\nabla_z^2V(r)d\mathbf{r}, \qquad (14)$$

with the spin-up–spin-down radial distribution function defined by $g_{\uparrow\downarrow}=\frac{1}{2}(g-g^\sigma)$. Equations (13) and (14) reveal that the coherent and spin-dependent sum rules m_3 exhibit a different q dependence, consistent with the general arguments of Ref. 7. The origin of such a difference between m_3^c and m_3^i is easily understood by looking at the low-q behavior of the commutators $[H,F_q]$ entering Eq. (4). In the coherent case one has

$$\left[H,\sum_j e^{i\mathbf{q}\cdot\mathbf{r}_j}\right]_{\mathbf{q}\to 0}\to\frac{\mathbf{q}}{m}\cdot\sum_j\mathbf{p}_j,$$

and hence m_3^c vanishes at the order q^2 as a consequence of current conservation. In the spin-dependent case, vice versa, one has

$$\left[H,\sum_j \sigma_j^z e^{i\mathbf{q}\cdot\mathbf{r}_j}\right]_{\mathbf{q}\to 0} \rightarrow \frac{\mathbf{q}}{m}\cdot\sum_j \sigma_j^z \mathbf{p}_j .$$

Since the spin current is not conserved, one finds a q^2 effect in m_3^i.

It is worth noting that the nonvanishing of the integral of Eq. (14) is a pure effect of dynamic correlations in the ground state. Mean-field calculations, based on the random-phase approximation or on Landau theory, account only for Pauli correlations in the ground state (Slater determinant) and consequently give rise to a constant value for $g_{\uparrow\downarrow}$ ($=\frac{1}{2}$). The q^2 term in m_3^i then vanishes, consistent with the result of Eq. (9). (An exception is provided by inhomogeneous Fermi systems, e.g., atomic nuclei, for which the term in q^2 in the m_3 sum rule for spin and/or isospin excitations is different from zero in the mean-field scheme.)

The above results prove that in the low-q limit the m_3^i sum rule is entirely dominated by multipair effects. On the other hand the multipair contribution to m_1^i is easily calculated in the same limit using Eqs. (8) and (10). One finds[20]

$$m_1^i(\mathrm{mp}) = m_1^i(\text{1p-1h}) \underset{\mathbf{q}\to 0}{\rightarrow} N\frac{q^2}{2m}\frac{1}{3}\frac{F_1^s-F_1^a}{1+\frac{1}{3}F_1^s} . \qquad (15)$$

Combining results (14) and (15) one can evaluate the ω_{31}^i multipair excitation energy in the spin channel, defined by

$$\omega_{31}^i(\mathrm{mp}) = \left[\frac{m_3^i(\mathrm{mp})}{m_1^i(\mathrm{mp})}\right]^{1/2} \underset{\mathbf{q}\to 0}{\rightarrow} \left[\frac{1+\frac{1}{3}F_1^s}{F_1^s-F_1^a}\frac{6n_0}{m}\int g_{\uparrow\downarrow}(r)\nabla_z^2 V(r)\,d\mathbf{r}\right]^{1/2} . \qquad (16)$$

Using the radial distribution function by Viviani *et al.*,[11] which includes central, triplet, and spin correlations in the ground state, and the above reported values for F_1^s and F_1^a, we obtain $\omega_{31}^i(\mathrm{mp}) \simeq 50$ K at SVP. We emphasize that $\omega_{31}(\mathrm{mp})$ cannot in general be identified with the peak energy of multipair excitations. In fact, similarly to what happens in ^{4}He, one expects the mp component of the dynamic form factor to be significantly fragmented and the m_3 sum rule rather sensitive to the high-energy components. This can explain why the above value for ω_{31}^i is higher than the value of the peak energy of the spin mp excitations ($\sim$20 K) recently employed by Hess and Pines in their phenomenological analysis of $S(\mathbf{q},\omega)$.

Results (14) and (15) permit us to find a rigorous lower bound for the multipair contribution to the static form factor

$$S_q = m_0(q)/N = N^{-1}\int S(\mathbf{q},\omega)\,d\omega$$

in the low-q limit. In fact, from the inequality $(m_3/m_1)^{1/2} \geq m_1/m_0$ and using Eqs. (14) and (15), one finds

$$S_q^i(\mathrm{mp}) \geq q^2 \left[\frac{(F_1^s-F_1^a)^3}{(1+\frac{1}{3}F_1^s)^3}\frac{1}{216 n_0 m}\left(\int g_{\uparrow\downarrow}(r)\nabla_z^2 V(r)\right)^{-1}\right]^{1/2} \simeq 0.1 q^2 , \qquad (17)$$

where q is given in Å^{-1}. The coefficient of Eq. (17) is a factor of 2 smaller than the one determined in the phenomenological analysis of Ref. 20. Comparing result (17) with the single-pair contribution to S_q,[20,21] one notes that for wave vectors $q > 0.5$ Å^{-1} the multipair contribution (17) to the static form factor is not negligible.

Concerning the role of the coherent multipair excitations, the numerical comparison between the results of Eq. (7) and Eq. (13) reveals that they practically exhaust ($\sim$90%) the sum rule m_3^c. This suggests that the study of the ratio m_3^c/m_3^i [see Eqs. (11) and (12)] can provide a quantitative estimate (a part from the factor σ^i/σ^c) of the relative importance of the multipair excitations in the coherent and spin channels as a function of q. Figure 1 shows that for $q > 0.5$ Å^{-1} the mp excitations are more important in the spin channel than in the coherent one.

Finally, we note that the explicit evaluation of the integrals entering Eqs. (3) and (4) requires a rather accurate knowledge of the short-range effects in the distribu-

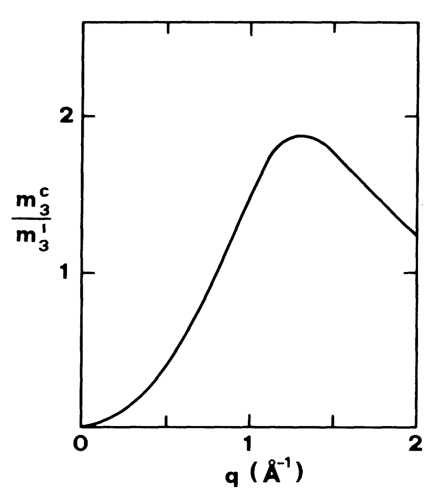

FIG. 1. Ratio m_3^c/m_3^i vs q, from Eqs. (11) and (12).

tion functions. In this context it is interesting to remark that the microscopic results of Refs. 10 and 11, obtained employing very different approaches, provide quite similar results for $g^{\uparrow\downarrow}$ in the spatial range relevant to the integral (14), and hence they give quite similar results for ω_{31}^{i}. Conversely, the differences are more pronounced in $g(r)$, the resulting value for m_3^s in the low-q limit being higher by 30% with the calculations of Ref. 10.

The present formalism can be naturally extended to discuss the effects of multiparticle excitations in other systems, such as ^{4}He, ^{3}He-^{4}He mixtures, and polarized ^{3}He. A detailed analysis will be presented in a future work.

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