High momentum response of liquid $^3$He

F. Mazzanti,1 A. Polls,2 J. Boronat,3 and J. Casulleras3

1 Departament d’Electrònica, Enginyeria i Arquitectura La Salle, Pg. Bonanova 8, Universitat Ramon Llull, E-08022 Barcelona, Spain

2 Departament d’Estructura i Constituents de la Matèria, Diagonal 645, Universitat de Barcelona, E-08028 Barcelona, Spain

3 Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Campus Nord B4-B5, E-08034 Barcelona, Spain

(Dated: March 22, 2022)

A final-state-effects formalism suitable to analyze the high-momentum response of Fermi liquids is presented and used to study the dynamic structure function of liquid $^4$He. The theory, developed as a natural extension of the Gersch-Rodriguez formalism, incorporates the Fermi statistics explicitly through a new additive term which depends on the semi-diagonal two-body density matrix. The use of a realistic momentum distribution, calculated using the diffusion Monte Carlo method, and the inclusion of this additive correction allows for a good agreement with available deep-inelastic neutron scattering data.

PACS numbers: 67.55.-s, 61.12.Bt

Inelastic neutron scattering is the most efficient tool to explore the structure and dynamics of quantum liquids $^3$He and $^4$He since the dynamic structure function $S(q,\omega)$ is readily obtained from the double differential scattering cross-section. The range of momenta $q$ transferred to the system determines the kind of microscopic information that can be extracted. The most interesting regimes correspond to low and high $q$’s. At low $q$, the scattering data allows for the determination of the low-energy excitation spectrum. In the opposite limit, known as deep-inelastic neutron scattering (DINS), $q$ is so high that single-particle properties of the system become accessible.

It is well known that in the $q \to \infty$ limit, $S(q,\omega)$ approaches the impulse approximation (IA). The only ingredient to calculate the response in IA is the momentum distribution $n(k)$, a fundamental function in the study of $^4$He, $^3$He, and the $^4$He-$^3$He mixture. The boson and fermion quantum statistics of $^4$He and $^3$He, respectively, introduce significant differences in their corresponding momentum distributions. Liquid $^4$He presents a macroscopic occupation of the zero-momentum state, characterized by its condensate fraction $n_0$; $n(k)$ of liquid $^3$He, considered as a normal Fermi liquid, shows a discontinuity at the Fermi momentum $k_F$. Nowadays, different theoretical calculations of $n(k)$ ranging from variational theory, based on the (Fermi-)hypernetted-chain equations (F)HNC, to the more exact diffusion Monte Carlo (DMC) method are in an overall quantitative agreement. However, a direct comparison with experimental data is not possible due to instrumental resolution effects (IRE) and, more fundamentally, to final state effects (FSE). From the theoretical side, the problem is that the IA does not account completely for the scattering in most of the DINS experiments since the transferred momenta are not high enough. Therefore, FSE which take into account the interactions of the struck atom with the medium can not be disregarded.

The search for an unambiguous experimental signature of $n_0$ in liquid $^4$He using DINS has originated a great deal of theoretical and experimental work for the last two decades. At present, theoretical predictions for both the FSE and the IA provide a satisfactory description of the experimental measurements, with an overall agreement on the value of the condensate fraction, $n_0 \sim 9\%$ at the equilibrium density. It is worth noticing that FSE in superfluid $^4$He are enhanced due to $n_0$ and therefore, even at the highest momenta achieved in the laboratory, FSE play a fundamental role. Comparatively, few works have been devoted to the analysis of the high-$q$ response of liquid $^3$He. The main reasons underlying this situation are, from the experimental side, the large neutron absorption of $^3$He, and from the theoretical one, the difficulties the Fermi statistics of $^3$He introduces in the quantum many-body calculations. The most accurate data have been reported by Azuaah et al. and more recently by Senesi et al., but only the first one was carried out at the equilibrium density. FSE in $^3$He have been taken into account by Moroni et al. using the bosonic formalism of Carraro and Koonin. Their results show less strength at the peak than the experimental $S(q,\omega)$, pointing to possible limitations of the formalism when applied to a Fermi liquid. On the other hand, an analysis of the experimental data based on cumulant expansions has revealed significant differences between the experimental and theoretical $^3$He momentum distributions at equilibrium density.

We present in this letter results for the high-$q$ response of $^3$He using a theoretical formalism that incorporates explicitly and consistently the Fermi statistics to
the FSE. The inputs required are the momentum distribution \( n(k) \) and the semi-diagonal two-body density matrix \( \rho_2(r_1, r_2; r_1', r_2') \). Both are obtained from microscopic theory: \( n(k) \) from a DMC calculation, and \( \rho_2 \) from variational FHNC. The results obtained for \( S(q, \omega) \) reproduce the experimental data better than previous estimations, pointing to non-negligible Fermi contributions to the FSE.

As long as the Fermi system prevents from a straightforward application of the FSE, corrections are much smaller due to the low \(^3\text{He} \) density.

The form factors \( \rho_2^B(r_1, r_2; r_1', r_2') \) being the one-body density matrix extracted from \( \rho_2^B \). In the thermodynamic limit, \( \rho_2^B(r_11') \) factorizes from \( \rho_{1N}^B \), and thus the first term in Eq. (2) corresponds to an artificial -body density matrix containing fermionic correlations between points 1 and 1 only.

Inserting \( \rho_{1N}^B \) in \( S(q, t) \), the \(^3\text{He} \) response becomes

\[
S(q, t) = S_{1A}(q, t) R(q, t) + \Delta S(q, t),
\]

with \( S_{1A}(q, t) \) the exact \(^3\text{He} \) IA, and \( R(q, t) \) the Gersch-Rodriguez FSE function calculated with the bosonic semi-diagonal two-body density matrix \( \rho_2^B(r_1, r_2; r_1', r_2') \),

\[
R(q, t) = \exp \left[ -\frac{1}{\rho_{11'}(q, t)} \int dr \rho_2^B(r, 0; r + s) \times \left[ 1 - \exp \left( i \int_0^s ds' \Delta V(r, s') \right) \right] \right].
\]

The new additive term \( \Delta S(q, t) \) in Eq. (3) is a consequence of \( \Delta \rho_{1N}^B \) introduced in Eq. (2). The leading contribution to the FSE at high \( q \) depends on the semi-diagonal two-body density matrix, and then \( \Delta \rho_2 \) is required for the calculation of \( \Delta S(q, t) \). A cluster expansion in the framework of the FHNC formalism allows for an estimation of \( \Delta \rho_2 \) according to the following structure,

\[
\frac{1}{\rho} \Delta \rho_2(r_1, r_2; r_1') = \rho_1(r_{11'})G(r_1, r_2; r_1') + \rho_{1B}(r_{11'})F(r_1, r_2; r_1') .
\]

The form factors \( G(r_1, r_2; r_1') \) and \( F(r_1, r_2; r_1') \) can be expressed in terms of auxiliary functions defined in the FHNC theory, and \( \rho_{1B}(r_{11'}) \) is positive everywhere and similar to a bosonic one-body density matrix. Therefore, \( \rho_{1B}(r_{11'}) \) can be used as the basis of a cumulant expansion by simply adding and subtracting it to \( \Delta \rho_{1N} \). The resulting additive correction \( \Delta S(q, t) \) is, to the lowest order,

\[
\Delta S(q, t) = e^{i \omega q / v_q} \rho_{1D}(r_{11'}) \left\{ \exp \left[ -\frac{1}{\rho_{1D}(s)} \int dr \Delta \rho_2(r, 0; r + s) \left[ 1 - \exp \left( i \int_0^s ds' \Delta V(r, s') \right) \right] \right] - 1 \right\} .
\]
Finally, a Fourier transform of $S(q, t)$ provides the dynamic structure function $S(q, \omega)$. Furthermore, the scaling properties of the IA, in terms of the West variable $Y = m\omega/q - q/2$, suggests as usual to write the response $(q/m)S(q, \omega)$ as a Compton profile,

$$J(q, Y) = \int dY' J(Y') R(q, Y - Y') + \Delta J(q, Y) , \quad (7)$$

$$J(Y) = 1/(2\pi^2 \rho) \int Y dk n(k)$$

being the IA.

The microscopic functions entering the high-momentum response $J(q, Y)$ are the one- and the semi-diagonal two-body density matrices of the actual system and its bosonic counterparts. The most relevant quantity is the one-body density matrix, or equivalently the momentum distribution, which is used to evaluate $J(Y)$. We have estimated the $^3$He momentum distribution using the DMC methodology that has recently proved to be very accurate in the calculation of the $^3$He equation of state at zero temperature \[10, 20, 21\]. At the equilibrium density $\rho_0 = 0.273 \, \sigma^{-3}$ ($\sigma = 2.556$ Å), $n(k)$ is well parameterized by

$$n(x) = \begin{cases} a_0 - a_3x^3 & x \leq 1 \\ (b_0 + b_1x + b_2x^2)e^{-b_3x} & x > 1 \end{cases} \quad (8)$$

with $x = k/k_F$, $k_F$ being the Fermi momentum. The set of parameters that best fit $n(k)$ is reported in Table I. The kinetic energy per particle, related to the second moment of $n(k)$, is 12.3 K and the discontinuity of $n(k)$ at the Fermi surface is $Z = 0.236$. The value of $Z$, which defines the strength of the quasi-particle pole, is rather small, indicating that the system is strongly correlated. On the other hand, the tail of the momentum distribution extends up to high momenta generating significant high-energy wings in $J(q, Y)$. The present $n(k)$ is in overall agreement with the DMC one from Ref. \[3]\.

The semi-diagonal two-body density matrix $\rho_2$, and the auxiliary bosonic functions $\rho_1^B$ and $\rho_2^B$, have been obtained in the framework of the FHNC and HNC theories using a Jastrow-Slater variational wave function. It is well known that this trial wave function is not accurate enough if the main objective is to get a good upper-bound to the energy. This is not however the aim of the present letter. In fact, we have shown in previous work that a Jastrow wave function can efficiently account for the FSE in $^4$He \[5\]. Certainly, short-range correlations, which dominate the FSE, are already contained in the Jastrow-Slater approximation. Accordingly, the diagrammatic analysis for $^3$He has been performed at the two-body level, thus making the analysis easier.

The FSE broadening function $R(q, Y)$ at $\rho_0$ and a momentum transfer $q = 19.4$ Å$^{-1}$ is shown in Fig. 1. This value of $q$ has been used throughout this work since it corresponds to the momentum reported in the experimental data by Azuah et al. \[11\]. $R(q, Y)$ has been calculated in the bosonic approximation and then its structure is similar to the FSE function of $^4$He \[3\]. When $q$ increases $R(q, Y)$ narrows and sharpens, becoming a delta function in the $q \to \infty$ limit.

The $^3$He additive correction $\Delta J(q, Y) = (q/m)\Delta S(q, Y)$ at the same density and momentum transfer is also shown in Fig. 1. This function, which introduces fermionic correlations to the FSE, presents a shape that is entirely different from that of $R(q, Y)$. The strong oscillations that appear in the region $Y \approx \pm k_F$ modify the shape of the IA response around these points. Furthermore, a central peak centered at $Y = 0$ enhances the strength of the total response at the origin. Out of this region ($|Y| \gtrsim k_F$), $\Delta J(q, Y)$ is much smaller and its correction to the response becomes negligible. Further analysis indicates that $\Delta J(q, Y)$ decays to zero in the high momentum transfer limit. This fact, together with the limiting condition $R(q \to \infty, Y) \to \delta(Y)$, indicates that the total response asymptotically approaches $J(Y)$ when $q \to \infty$.

The final result of the $^3$He response at $q = 19.4$ Å$^{-1}$ is shown in Fig. 2. We compare our results with the DINS data of Azuah et al. \[11\] because their data correspond to densities around the equilibrium density $\rho_0$, and also because their experimental setup produces a rather narrow instrumental resolution function. More recent data \[12\] are focused at higher liquid densities and to the solid phase. In this experiment, the momentum transfer is much larger ($q \sim 90$ to 120 Å$^{-1}$) produc-

| $a_0$ | 0.481319 |
| $a_3$ | 0.0842956 |
| $b_0$ | 1.39056 |
| $b_1$ | 0.157930 |
| $b_2$ | 0.0829832 |
| $b_3$ | 2.31398 |

**TABLE I**: Parameters of $n(k)$ at $\rho_0$. 

![Image](image-url)
formulation, Rodriguez theory for bosons. According to the present for-mer. The method is a natural extension of the Gersch- 

data, comparable for the first time to the accuracy pre-

The results obtained are in good agreement with DINS 

that takes into account Fermi statistics effects in the FSE. The latter effect is estimated at the lowest or-

ner but its inclusion allows for a significant improvement 

and a better knowledge of specific mechanisms influenc-

the FSE in liquid \( ^3 \)He.

This work has been partially supported by Grants No. 

BFM2002-01868 and BFM2002-00466 from DGI (Spain) 

and Grants No. 2001SGR-00064 and 2001SGR-00222 

from the Generalitat de Catalunya.

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