# High-Momentum Response of Liquid $^3$He

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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 $^3$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 semidiagonal 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 good agreement with available deep-inelastic neutron scattering data.

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Inelastic neutron scattering is the most efficient tool to explore the structure and dynamics of quantum liquids $^4$He and $^3$He since the dynamic structure function $S(q, \omega)$ is readily obtained from the double differential scattering cross section [1]. 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 allow 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 $q \rightarrow \infty$ 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 $k_F$ [2]. 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 [3–5]. 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, cannot 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 [6–10] 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 Azuah *et al.* [11], and more recently by Senesi *et al.* [12], 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.* [8] using the bosonic formalism of Carraro and Koonin [6]. Their results [8] 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 [1,13] has revealed significant differences between the *experimental* and theoretical $^3$He momentum distributions at equilibrium density [11].

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 semidiagonal two-body density matrix

$\rho_2(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1, \boldsymbol{r}_2)$. 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 $^4$He is concerned, most theories introduce FSE as a convolution in energies, which turn into an algebraic product in time representation. Hence, FSE are included by means of a new function $R(q, t)$ which multiplies $S_{\text{IA}}(q, t)$ to obtain the total response, $S(q, t) = S_{\text{IA}}(q, t)R(q, t)$. This convolutive approach is clearly ambiguous when applied to fermions because, contrary to the Bose case, $S_{\text{IA}}(q, t)$ has an infinite number of nodes, a fact that leads to a singular definition of $R(q, t)$. In order to overcome this serious drawback that emerges from a direct translation of the FSE theories for bosons to fermions, we have used an alternative formulation that can be considered a natural extension of Gersch-Rodriguez theory [14] to fermionic systems. In previous works [15,16], we have applied this theory to evaluate FSE in $^4$He-$^3$He mixtures, but there the fermionic corrections are much smaller due to the low $^3$He concentrations.

At high $q$, the density-density correlation factor $S(q, t)$ can be well approximated by

$$S(q, t) = \frac{1}{N!} e^{i\omega_q s/v_q} \int d\boldsymbol{r}_1 \ldots d\boldsymbol{r}_N \rho_N(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N; \boldsymbol{r}_1 + \boldsymbol{s})$$
$$\times \exp\left[\frac{i}{v_q} \sum_{j=2}^{N} \int_0^s \Delta V(\boldsymbol{r}_{1j}, \boldsymbol{s})\right], \tag{1}$$

with $\omega_q = q^2/2m$, $\boldsymbol{v}_q = \boldsymbol{q}/m$, $\boldsymbol{s} = \boldsymbol{v}_q t$, and $\Delta V(\boldsymbol{r}, \boldsymbol{u}) = V(\boldsymbol{r} - \boldsymbol{u}) - V(\boldsymbol{r})$. Equation (1) is derived assuming that the atom struck by the neutron recoils in a medium of nonmoving $^3$He atoms. $S(q, t)$ is still hard to evaluate using Eq. (1) since it implies an integration over the complete semidiagonal $N$-body density matrix of the system, which is essentially the square of the ground-state wave function. In $^4$He, a truncated cumulant expansion of Eq. (1) leads to the Gersch-Rodriguez expression for the FSE [14]. Recently, this formalism has proven its efficiency by reproducing $^4$He DINS data with high accuracy [7]. On the contrary, the nodal structure of $\rho_N$ in a Fermi system prevents a straightforward application of these methods.

In order to extend the FSE theory to $^3$He, one introduces an auxiliary $N$-body density matrix $\rho_N^{\text{B}}$ corresponding to a system of spinless bosons with the mass, density, and interatomic potential of $^3$He. $\rho_N^{\text{B}}$ is positive and then it can be used as the starting point of a cumulant expansion of the response function. In terms of $\rho_N^{\text{B}}$, a convenient decomposition of $\rho_N$ turns out to be

$$\rho_N(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N; \boldsymbol{r}'_1) = \rho_1(r_{11'})\left[\frac{1}{\rho_1^{\text{B}}(r_{11'})}\rho_N^{\text{B}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N; \boldsymbol{r}'_1)\right]$$
$$+ \Delta\rho_N(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N; \boldsymbol{r}'_1), \tag{2}$$

$\rho_1^{\text{B}}(r_{11'})$ being the one-body density matrix extracted from $\rho_N^{\text{B}}$. In the thermodynamic limit, $\rho_1^{\text{B}}(r_{11'})$ factorizes from $\rho_N^{\text{B}}$, and thus the first term in Eq. (2) corresponds to an artificial $N$-body density matrix containing fermionic correlations between points 1 and $1'$ only.

Inserting $\rho_N$ (2) in $S(q, t)$ (1), the $^3$He response becomes

$$S(q, t) = S_{\text{IA}}(q, t)R(q, t) + \Delta S(q, t), \tag{3}$$

with $S_{\text{IA}}(q, t)$ the exact $^3$He IA, and $R(q, t)$ the Gersch-Rodriguez FSE function calculated with the bosonic semidiagonal two-body density matrix $\rho_2^{\text{B}}(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1)$,

$$R(q, t) = \exp\left\{-\frac{1}{\rho_1^{\text{B}}(r_{11'})} \int d\boldsymbol{r}\rho_2^{\text{B}}(\boldsymbol{r}, 0; \boldsymbol{r} + \boldsymbol{s})\right.$$
$$\left.\times \left[1 - \exp\left(\frac{i}{v_q} \int_0^s ds' \Delta V(\boldsymbol{r}, \boldsymbol{s}')\right)\right]\right\}. \tag{4}$$

The new additive term $\Delta S(q, t)$ in Eq. (3) is a consequence of $\Delta\rho_N$ introduced in Eq. (2). The leading contribution to the FSE at high $q$ depends on the semidiagonal 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:

$$\frac{1}{\rho}\Delta\rho_2(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1) = \rho_1(r_{11'})G(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1)$$
$$+ \rho_{1\text{D}}(r_{11'})F(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1). \tag{5}$$

The form factors $G(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1)$ and $F(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}'_1)$ can be expressed in terms of auxiliary functions defined in the FHNC theory, and $\rho_{1\text{D}}(r_{11'})$ is positive everywhere and similar to a bosonic one-body density matrix [17,18]. Therefore, $\rho_{1\text{D}}(r_{11'})$ can be used as the basis of a cumulant expansion by simply adding and subtracting it to $\Delta\rho_N$. The resulting additive correction $\Delta S(q, t)$ is, to the lowest order,

$$\Delta S(q, t) = e^{i\omega_q s/v_q} \frac{1}{\rho}\rho_{1\text{D}}(r_{11'})\left\{\exp\left[-\frac{1}{\rho_{1\text{D}}(s)} \int d\boldsymbol{r}\Delta\rho_2(\boldsymbol{r}, 0; \boldsymbol{r} + \boldsymbol{s})\left[1 - \exp\left(\frac{i}{v_q} \int_0^s ds' \Delta V(\boldsymbol{r}, \boldsymbol{s}')\right)\right]\right] - 1\right\}. \tag{6}$$

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 [19] $Y = m\omega/q - q/2$, suggests as usual to write the response $(q/m)S(q, \omega)$ as a Compton profile,

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

$J(Y) = 1/(2\pi^2\rho) \int_{|Y|}^{\infty} dk k n(k)$ being the IA.

The microscopic functions entering the high-momentum response $J(q, Y)$ (7) are the one-diagonal and semidiagonal 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 [20,21]. At the equilibrium density $\rho_0 = 0.273\sigma^{-3}$ ($\sigma = 2.556$ Å), $n(k)$ is well parametrized by

$$n(x) = \begin{cases} a_0 - a_3 x^3 & x \le 1, \\ (b_0 + b_1 x + b_2 x^2) e^{-b_t x} & x > 1, \end{cases} \qquad (8)$$

with $x = k/k_F$, $k_F$ being the Fermi momentum. The set of parameters that best fit $n(k)$ (8) 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 quasiparticle 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 semidiagonal 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 [7]. 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

TABLE I. Parameters of $n(k)$ (8) at $\rho_0$.

| | |
|---|---|
| $a_0$ | 0.481 319 |
| $a_3$ | 0.084 295 6 |
| $b_0$ | 1.390 56 |
| $b_1$ | 0.157 930 |
| $b_2$ | 0.082 983 2 |
| $b_t$ | 2.313 98 |

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 [7]. 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$^{-1}$) producing a simultaneous decrease of the FSE corrections and a widening of the IRE. The IRE function estimated by Azuah *et al.* [11] is shown in Fig. 2 scaled by a factor of 0.1. The theoretical response $J(q, Y)$, shown in the figure, has been folded with the experimental IRE function $I(q, Y)$ to make a direct comparison possible. The kinks of $J(q, Y)$ at $Y = \pm k_F$ present in the IA, are completely washed out by the
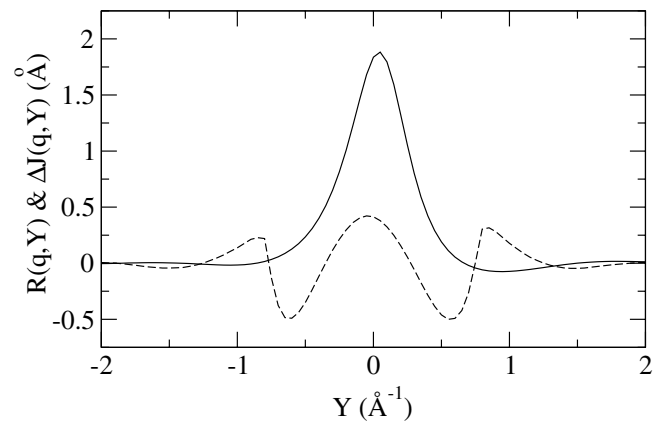


FIG. 1. FSE broadening function $R(q, Y)$ (solid line) and additive correction $\Delta J(q, Y)$ (dashed line) at $q = 19.4$ Å$^{-1}$ and $\rho_0$. $\Delta J(q, Y)$ is multiplied by a factor of 20 to fit into the scale.
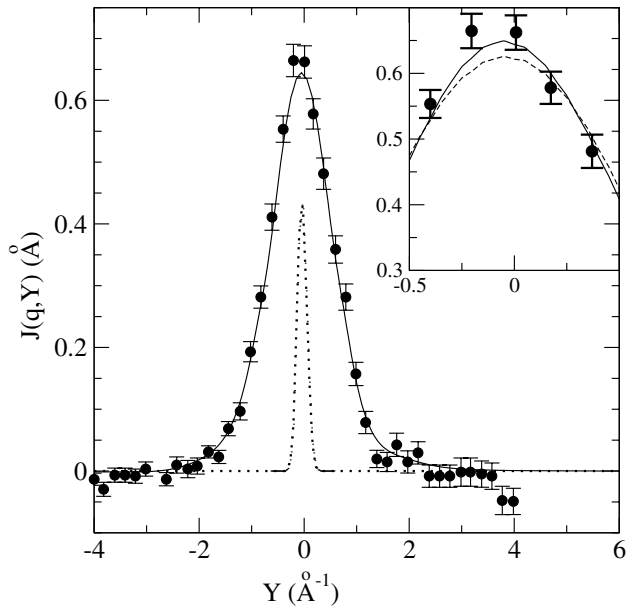
FIG. 2. $^3$He response at $q = 19.4$ Å$^{-1}$ and $\rho_0$ (solid line), folded to the IRE function (dotted line). The points with error bars are the experimental data from Ref. [11]. The instrumental resolution function [11] has been divided by a factor of 10 to fit into the scale. The inset shows $J(q, Y)$ near the peak with (solid line) and without (dashed line) the additive correction $\Delta J(q, Y)$.

successive folding with $R(q, Y)$ and $I(q, Y)$, although $\Delta J(q, Y)$ introduces additional structure around those points. The most remarkable feature is the enhancement of the strength of the response around the peak due to the new additive term introduced in the present approach (see the inset in Fig. 2). This small but significant increase of strength allows for the first time to reproduce the available $^3$He DINS experimental data.

To summarize, we have presented a FSE formalism suitable to study the dynamic structure function of a Fermi liquid like liquid $^3$He at large momentum transfer. The method is a natural extension of the Gersch-Rodriguez theory for bosons. According to the present formulation, $J(q, Y)$ results from the convolution of the IA with a purely bosonic FSE broadening function, which incorporates the short-range correlations induced by the interatomic potential, plus an additive correction term that takes into account Fermi statistics effects in the FSE. The results obtained are in good agreement with DINS data, comparable for the first time to the accuracy previously achieved in the study of the high-$q$ response of liquid $^4$He. The two key features behind the present

results are, on one hand, the use of a realistic momentum distribution provided by the DMC method, and on the other, the explicit introduction of Fermi corrections in the FSE. The latter effect is estimated at the lowest order, but its inclusion allows for a significant improvement and a better knowledge of specific mechanisms influencing the FSE in liquid $^3$He.

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