Chapter 2

General properties of the dynamic structure function

In this chapter, the definition and general properties of the dynamic structure function of isotropic, infinite pure phase liquid and mixtures are reviewed. Most of the features described here are common to all kind of correlated systems, ranging from Helium liquids to nuclear matter and even finite nuclei. The discussion is focused on the density and the spin–density responses, as they provide the maximum information of the system that can be obtained from a standard neutron scattering experiment on condensed matter.

2.1 Definition of $S(q, \omega)$ and $S(q, t)$

The dynamic structure function or density response $S(q, \omega)$ of a fluid describes the way in which the system responds to a probe that transfers a fixed momentum $q$ and energy $\omega$ [Lov84][PN66][Gly94a] to the system. As the equilibrium local density at each point in space is given by the expectation value of the static operator

$$\rho(r) = \sum_{j=1}^{N} \delta(r - r_j) ,$$

(2.1)
its Fourier components of momentum $q \neq 0$ characterize the density fluctuations through the operators
\[ \rho_q = \sum_{j=1}^{N} e^{iqr_j} . \] 
while $\rho_{q=0} = \rho_0 \equiv \rho$ is the mean density that coincides with the actual particle density in unperturbed, homogeneous and infinite systems.

At zero temperature the system is in the ground state, but the presence of density fluctuations produces elementary excitations that make the wave function describing the system partially populate states of higher energy. A measure of the effects produced by the perturbation can be obtained by looking at the probability of coupling the resulting state to all the available states compatible with a net gain of energy and momentum $\omega$ and $q$. Written as a transition probability, and introducing explicitly the energy conservation constrain, the response per particle becomes
\[ S(q, \omega) = \frac{1}{N} \sum_{\{n\}} \left| \langle 0 | \rho_q^\dagger | n \rangle \right|^2 \delta(E_n - E_0 - \omega) , \] 
where $\{n\}$ is a complete set of eigenstates of the Hamiltonian $H$. Notice that this definition, although obtained in a different way, coincides with the one deduced from the analysis of the double differential cross section of the scattering process. Two important conclusion about the behavior of $S(q, \omega)$ can be drawn from it:

1) The strength of the response of a fluid in a single phase is non-negative.

2) The strength of the $T=0$ response of a fluid in a single phase is zero at negative energies.

The dynamic structure function $S(q, \omega)$ is also related to the density–density correlation factor $S(q, t)$ by Fourier transformation [Lov84]
\[ S(q, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \ e^{-i\omega t} S(q, t) , \]
a relation that can be inverted to yield
\[ S(q, t) = \frac{1}{N} \sum_{i,j}^{N} \langle e^{-iqr_i} e^{iqr_j(t)} \rangle \]
where $r_i$ and $r_j(t)$ are the position operators of particles $i$ and $j$ evaluated at times 0 and $t$, respectively. Here the brackets $\langle \ldots \rangle$ denote ground state expectation value, but this definition of $S(q, t)$ is readily generalized to finite temperatures replacing them...
2.1 Definition of $S(q,\omega)$ and $S(q, t)$

by a thermal average [Gri93]. Notice also that, in the $t \to 0$ limit, $S(q, t)$ in eq. (2.5) reduces to the static structure factor $S(q)$

$$\lim_{t \to 0} S(q, t) = S(q) \quad . \quad (2.6)$$

There are yet two additional asymptotic properties that are of major theoretical interest in the description of the high momentum transfer behavior of the dynamic structure function. The first one concerns the separation of the response in its coherent and incoherent parts and the way in which they contribute to the total $S(q, \omega)$, while the second one refers to the scaling relation satisfied by the incoherent response when $q \to \infty$.

The incoherent density–density correlation factor $S_{\text{inc}}(q, t)$ is defined as the response obtained when only the $i=j$ terms in the summation of eq. (2.5) are retained [SSC89]. The coherent density–density correlation factor is the difference between $S(q, t)$ and $S_{\text{inc}}(q, t)$, i.e., the sum of all the $i \neq j$ terms in the same expression [SSC89]

$$S_{\text{inc}}(q, t) = \frac{1}{N} \sum_{j} \left< e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{i\mathbf{q} \cdot \mathbf{r}_j(t)} \right> \quad (2.7)$$

$$S_{\text{coh}}(q, t) = \frac{1}{N} \sum_{i \neq j} \left< e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{i\mathbf{q} \cdot \mathbf{r}_j(t)} \right> \quad . \quad (2.8)$$

In this way, the incoherent and the coherent responses measure the effects induced by the correlations between the position of the same and of different atoms at different times, respectively.

It is easy to see that, in the $q \to \infty$ limit, the response of a system interacting through a potential bounded both from above and from below is entirely dominated by $S_{\text{inc}}(q, t)$. Indeed, denoting

$$O_j(q, t) = e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{i\mathbf{q} \cdot \mathbf{r}_j(t)} \quad , \quad (2.9)$$

the incoherent and the coherent responses read

$$S_{\text{inc}}(q, t) = \frac{1}{N} \left\langle \sum_{j=1}^{N} O_j(q, t) \right\rangle \quad (2.10)$$

$$S_{\text{coh}}(q, t) = \frac{1}{N} \sum_{i \neq j} \left< e^{i\mathbf{q} \cdot (\mathbf{r}_j - \mathbf{r}_i)} \sum_{j=1}^{N} O_j(q, t) \right> \quad (2.11)$$

and, if $q \gg \rho^{1/3}$ (where $\rho^{1/3}$ sets the characteristic length of the momentum scale), $S_{\text{coh}}(q, t)$ vanishes much more rapidly than $S_{\text{inc}}(q, t)$ due to the strong oscillations of
the exponential factor. Accordingly, the total contribution of the coherent response decreases with increasing $q$ and $S(q, t)$ reduces to $S_{\text{inc}}(q, t)$ when $q \to \infty$.

Consider now the incoherent term only. In the $q \to \infty$ limit the system gains both a high momentum and a high energy, and therefore the time interval associated to the scattering event is short compared to any characteristic time length of the fluid. The incoherent response can be written in the following form once the momentum translation operators act on the time evolution operator

$$S_{\text{inc}}(q, t) = \frac{1}{N} \sum_{j=1}^{N} \left< e^{-i \mathbf{q}_j \mathbf{r}_j} e^{i \mathbf{H}_j} e^{i \mathbf{q}_j \mathbf{r}_j} e^{-i \mathbf{H}_j} \right> = \frac{1}{N} \sum_{j=1}^{N} \left< e^{i \mathbf{u} \left( \mathbf{H} + \frac{1}{m} \mathbf{q} \mathbf{p}_j + \frac{q^2}{2m} \right)} e^{-i \mathbf{H}_j} \right>$$

$$= \frac{1}{N} \sum_{j=1}^{N} e^{i \mathbf{u} \frac{q^2}{2m}} \left< e^{i \mathbf{u} \left( \mathbf{H} + \frac{1}{m} \mathbf{q} \mathbf{p}_j \right)} e^{-i \mathbf{H}_j} \right> ,$$

and the leftmost exponential operator can be expanded using Zassenhaus formula [Wil67]

$$e^{\lambda(A+B)} = e^{\lambda A} e^{\lambda B} e^{-\frac{1}{2} \lambda^2 [A,B]} e^{\frac{1}{4} \lambda^3 [B,[A,B]] + \frac{1}{2} [A,[A,B]]} \ldots . \quad (2.12)$$

Identifying $\lambda$ with $it$, and keeping only the lowest $t$ power in the exponent, one arrives at

$$S_{\text{inc}}(q, t) = \frac{1}{N} e^{i \mathbf{u} \frac{q^2}{2m}} \sum_{j=1}^{N} \left< e^{i \frac{t}{m} \mathbf{q} \mathbf{p}_j} \right> . \quad (2.13)$$

The dynamic structure function can now be obtained by direct Fourier transformation

$$S_{\text{inc}}(q, \omega) = \frac{1}{2\pi N} \sum_{j=1}^{N} \int_{-\infty}^{\infty} dt \ e^{-i \omega \left( \frac{q^2}{2m} \right)} \left< e^{i \frac{t}{m} \mathbf{q} \mathbf{p}_j} \right>$$

$$= \frac{1}{2\pi v_q N} \sum_{j=1}^{N} \int_{-\infty}^{\infty} dx \ e^{-i \frac{v_q}{q} \left( \frac{\omega}{q} - \frac{q}{2} \right)} \left< e^{i x \mathbf{p}_j} \right> \quad (2.14)$$

where $x = v_q t$ and $v_q = q/m$, $\mathbf{v}_q$ being a vector of modulus $v_q$ parallel to $\mathbf{q}$. As $x$ is an integration variable, $v_q S_{\text{inc}}(q, \omega)$ does not depend separately on $q$ and $\omega$ but only through the single combination $Y = m\omega/q - q/2$, thus evidencing the most important scaling property of the dynamic structure function at high $q$’s (but not the only one [Bel92] [Sea84]). The variable $Y$ and the expression (2.14) are commonly known as the West scaling variable [Wes75] and the Impulse Approximation (IA) [HP66][SSC89][SS90], respectively. Alternatively, and as it is shown in the next chapter, the IA can be written in terms of the momentum distribution $n(k)$ as follows

$$S_{IA}(q, \omega) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{k} n(k) \delta \left( \frac{(k + q)^2}{2m} - \frac{k^2}{2m} - \omega \right) . \quad (2.15)$$
Notice that the scaling property is obtained on the basis that at high $q$ the trajectory described by the struck particle is a straight line, as the momentum and the energy absorbed from the probe are so large that collisions with the background particles do not appreciably modify its dynamic evolution. Corrections to this approximation are proportional to the strength of the correlations with the surrounding atoms, and so this picture can be completely distorted when the interatomic potential $V(r)$ becomes steeply repulsive or infinite and billiard ball collisions may occur. Nevertheless, it has been shown by Weinstein and Negele [WN82][NO88] that, even for the gas of hard spheres where $V(r)$ is infinite at distances smaller than one particle diameter, the scaling property holds although $S(q, \omega)$ is no longer given by eq. (2.15). This indicates that $Y$ scaling is of more general validity than the IA, and in fact it has been largely verified in systems like liquid Helium [SS90][SSSS89], nuclear matter in heavy nuclei [Day87] or the electron gas in metals [Pla89], where moderate and large momentum transfer can be experimentally achieved before internal degrees of freedom in the constituents are excited.

The previous definitions and properties are easily generalized to systems containing more than one component, as are the $^3$He–$^4$He mixtures. In these systems, the total dynamic structure function $S(q, \omega)$ is the sum of several terms, due to the different types of correlations present. In the case of Helium mixtures, the response resulting from a typical inelastic neutron scattering experiment [GS87][FGKSD90] has four terms, each one weighted with a suitable cross section and concentration factor

$$S(q, \omega) = \sigma_4 x_4 S^{(4,4)}(q, \omega) + \sigma_3 x_3 S^{(3,3)}(q, \omega)$$

$$+ 2 \sigma_3 \sigma_4 \sqrt{x_3 x_4} S^{(3,4)}(q, \omega) + \sigma_3 \sigma_3 x_3 x_3 S^{(3,3)}(q, \omega) . \quad (2.16)$$

The three terms corresponding to density excitations ($S^{(4,4)}(q, \omega)$, $S^{(3,3)}(q, \omega)$ and $S^{(3,4)}(q, \omega)$) are defined in terms of the $\alpha$–isotope density fluctuation operators

$$\rho^{(\alpha)}_q = 2 \sum_{j=1}^{N_a} e^{i \mathbf{q} \cdot \mathbf{r}_j} , \quad (2.17)$$

as

$$\sqrt{N_a N_\beta} S^{(\alpha, \beta)}(q, \omega) = \sum_n \left[ \langle 0 | \rho^{(\alpha)\dagger}_q | n \rangle \langle n | \rho^{(\beta)}_q | 0 \rangle ight.$$ 

$$+ \langle 0 | \rho^{(\beta)\dagger}_q | n \rangle \langle n | \rho^{(\alpha)}_q | 0 \rangle \right] \delta (E_n - E_0 - \omega) , \quad (2.18)$$

$\alpha$ being either 3 or 4.
General properties of the dynamic structure function

The spin of a $^3\text{He}$ atom is $1/2$ and so it can couple to the spin of the probe used in the scattering experiment, in case the latter is non-zero. This phenomenon produces magnetic scattering and is typically observed when the probe is a neutron. The contribution of the magnetic scattering to the total dynamic structure function is entirely contained in the spin-dependent dynamic structure function $S_f^{(3,3)}(q, \omega)$ [Sea76]

$$S_f^{(3,3)}(q, \omega) = \frac{1}{N_3 I(I + 1)} \sum_{\{n\}} | \langle n | I_q | 0 \rangle |^2 \delta (E_n - E_0 - \omega)$$  \hspace{1cm} (2.19)

that is written in terms of the spin density fluctuation operator

$$I_q = \sum_{j=1}^{N_3} I_j e^{i q r_j} ,$$  \hspace{1cm} (2.20)

$I_j$ being the spin operator of the $j$-th $^3\text{He}$ atom.

At this point, the only quantities that remain to be specified in eq. (2.16) are the cross sections $\sigma$. Their values have been reported by Sears [Sea86] for the $^3\text{He} - ^4\text{He}$ mixture and are $\sigma_4 = 1.34$, $\sigma_3 = 4.42$, $\sigma_{3,4} = 2.35$ and $\sigma_{3,I} = 1.19$ in units of barns. Notice that in practice the measurement of the $^3\text{He}$ response is difficult due to the high neutron absorption of the $^3\text{He}$ atoms, but this is somewhat compensated by the high $\sigma_3$ factor entering in (2.16).

2.2 Sum rules of $S(q, \omega)$

In general, the exact evaluation of $S(q, \omega)$ becomes a rather involved problem because it requires precise knowledge of the whole set of energy eigenstates of the Hamiltonian. Accordingly, different approximations must be considered in order to gather relevant information on the response. One of the most common techniques used to this end consist in evaluating the different energy-weighted sum rules satisfied by $S(q, \omega)$ and then infer from them its behavior. At zero temperature, the sum rules of the response of a pure phase are defined as

$$m_k(q) = \int_0^{\infty} d\omega \omega^k S(q, \omega) ,$$  \hspace{1cm} (2.21)

and for the $(\alpha, \beta)$ component of a mixture as

$$m_k^{(\alpha, \beta)}(q) = \int_0^{\infty} d\omega \omega^k S_{(\alpha, \beta)}^{(I)}(q, \omega) .$$  \hspace{1cm} (2.22)

Even though the information contained in a small set of energy moments is insufficient to completely characterize the response, this method has proved to be extremely...
2.2 Sum rules of $S(q, \omega)$

helpful in the analysis of the response of pure $^3$He [DS89], pure $^4$He [Str92] and $^3$He–$^4$He mixtures ([BDMP93]), and constitutes a capital ingredient in the recent phenomenological analysis of $S(q, \omega)$ proposed by Glyde [Gly94b]. Notice that the definitions given above are particular to $T = 0$, as in this limit the response contributes only at positive frequencies. In the general $T > 0$ case, $S(q, \omega)$ spreads over the whole energy axis and the definitions in (2.21) and (2.22) must be extended to integrate from $-\infty$ to $+\infty$.

Due to the energy integration, the $m(q)$ moments do not depend on the details of the excited states and reduce to ground state expectation values of commutators of the Hamiltonian and the density fluctuation operator

$$
m_k(q) = \int_0^\infty d\omega \omega^k S(q, \omega)$$

$$= \frac{1}{N} \sum_{\langle n \rangle} \int_0^\infty d\omega \omega^k |\langle n | \rho_q | 0 \rangle|^2 \delta(E_n - E_0 - \omega)$$

$$= \frac{1}{N} \sum_{\langle n \rangle} |\langle n | \rho_q | 0 \rangle|^2 (E_n - E_0)^k$$

$$\equiv \frac{1}{N} \sum_i \binom{k}{i} (-1)^{k-i} \left\langle \rho_q^i H^i \rho_q H^{k-i} \right\rangle . \quad (2.23)$$

Of course, the higher the order of the sum rule, the more involved its evaluation becomes. However, the lowest moments can be exactly expressed in terms of ground state quantities as the radial distribution function $g(r)$ or the two–particle density matrix $\rho_2$. In the following, the derivation of the first three moments of the response of a spinless system in a single phase (like pure $^4$He) is discussed. The generalization to the $^3$He–$^4$He mixtures is also presented.

2.2.1 The $m_0(q)$ moment

The zero order sum rule of $S(q, \omega)$ is immediately obtained setting $k = i = 0$ in eq. (2.23)

$$m_0(q) = \frac{1}{N} \left\langle \rho_q^i \rho_q \right\rangle \equiv S(q) , \quad (2.24)$$

and yields the definition of the static structure factor $S(q)$, as one would expect from the Fourier transform relation connecting $S(q, t)$ and $S(q, \omega)$, and the asymptotic condition reported in eq. (2.6).
2.2.2 The $m_1(q)$ moment ($f$–sum rule)

The expression of the first order energy–weighted sum rule of the dynamic structure function reads, from eq. (2.23)

$$m_1(q) = \frac{1}{N} \left\langle \rho_q^\dagger H \rho_q - \rho_q^\dagger \rho_q H \right\rangle = \frac{1}{N} \left\langle \rho_q^\dagger [H, \rho_q] \right\rangle,$$

(2.25)

but it can be brought to the following alternative form that simplifies its evaluation

$$m_1(q) = \frac{1}{2N} \left\langle \rho_q^\dagger H \rho_q - \rho_q^\dagger \rho_q H - H \rho_q \rho_q^\dagger + \rho_q^\dagger H \rho_q \right\rangle.$$

(2.26)

As the system under study is infinite and translationally invariant, the ground state has a well defined total momentum equal to zero, and the state generated from the action of $\rho_q$ on it originates a new state of net momentum $q$. As the system is also invariant under time reversal, the energy of the two states $\rho_q|0\rangle$ and $\rho_{-q}|0\rangle \equiv \rho_q^\dagger|0\rangle$ is the same, and hence

$$\left\langle \rho_q^\dagger H \rho_q \right\rangle \equiv \left\langle \rho_q H \rho_q^\dagger \right\rangle,$$

(2.27)

leading to the following double commutator expectation value

$$m_1(q) = \frac{1}{2N} \left\langle [\rho_q^\dagger, [H, \rho_q]] \right\rangle.$$

(2.28)

The inner commutators can be easily carried out and give

$$[H, \rho_q] = [T, \rho_q] = \frac{1}{2m} \sum_{j=1}^{N} \left[ e^{ijq r_j} (q \cdot p_j) + (q \cdot p_j) e^{ijq r_j} \right],$$

(2.29)

where $T$ is the kinetic energy operator. The first equality holds because both $\rho_q$ and the interatomic potential are function of the position operators only. Then, the outer commutator becomes

$$[\rho_q^\dagger, [H, \rho_q]] = \frac{1}{2m} \sum_{j=1}^{N} \left[ \rho_q^\dagger e^{ijq r_j} (q \cdot p_j) + (q \cdot p_j) e^{ijq r_j} \right] \equiv N \frac{q^2}{m},$$

(2.30)

showing that the first moment of the response, also known as the $f$–sum rule, takes the simple form

$$m_1(q) = \frac{q^2}{2m},$$

(2.31)

and depends on the details of the system only through the mass $m$ of its constituents. Notice that this result has been obtained on the basis that the system is in the ground state and that it is infinite, translationally invariant and invariant under time reversal transformations. These conditions are satisfied by a whole class of systems, and thus the range of validity of the $f$–sum rule is wide. Of course, the fact that $m_1(q)$ equals $q^2/2m$ is very interesting from the theoretical point of view because it imposes a severe model independent constrain on any realistic calculation of the response.
### 2.2.3 The $m_2(q)$ moment

In contrast to the simplicity of the previous two sum rules, $m_2(q)$ is more involved. From eq. (2.23) and rearranging terms, $m_2(q)$ can be written as

$$m_2(q) = \frac{1}{N} \left< [H, \rho_q] [\rho_q^4, H] \right>, \quad (2.32)$$

where the commutators inside the expectation value are the same as those appearing in eq. (2.29). The second order sum rule of $S(q, \omega)$ becomes then the sum of four different terms

$$m_2(q) = \frac{1}{N (2m)^2} \sum_{i,j=1}^{N} \left< e^{i q r_j (q \cdot p_j)} e^{-i q r_i (q \cdot p_i)} + e^{i q r_j (q \cdot p_j)} (q \cdot p_i) e^{-i q r_i} + (q \cdot p_j) e^{i q r_j} e^{-i q r_i} (q \cdot p_i) + (q \cdot p_j) e^{i q r_j} (q \cdot p_i) e^{-i q r_i} \right> \quad (2.33)$$

which can be separately evaluated. Using the relation

$$\left[ e^{-i q r_i}, (q \cdot p_j) \right] = q^2 \delta_{ij} e^{-i q r_j}, \quad (2.34)$$

the first term of eq. (2.33) becomes

$$I_1 = \left< e^{i q r_j (q \cdot p_j)} e^{-i q r_i (q \cdot p_i)} \right>$$
$$= -q^2 \delta_{ij} \left< e^{i q r_j} e^{-i q r_i} (q \cdot p_i) \right> + \left< e^{i q r_j} e^{-i q r_i} (q \cdot p_j) (q \cdot p_i) \right> \quad (2.35)$$

In the same way, the other terms read

$$I_2 = \left< e^{i q r_j (q \cdot p_j)} (q \cdot p_j) e^{-i q r_i} \right>$$
$$= q^4 \delta_{ij} \left< e^{i q r_j} e^{-i q r_i} \right> - q^2 \left< e^{i q r_j} e^{-i q r_i} (q \cdot p_j) \right> + I_1 \quad (2.36)$$

$$I_3 = \left< (q \cdot p_j) e^{i q r_j} e^{-i q r_i} (q \cdot p_i) \right>$$
$$= q^2 \left< e^{i q r_j} e^{-i q r_i} (q \cdot p_j) e^{-i q r_i} \right> + I_1 \quad (2.37)$$

and

$$I_4 = \left< (q \cdot p_j) e^{i q r_j} (q \cdot p_i) e^{-i q r_i} \right>$$
$$= -q^4 \left< e^{i q r_j} e^{-i q r_i} \right> + q^2 \left< e^{i q r_j} e^{-i q r_i} (q \cdot p_i) \right> + I_2. \quad (2.38)$$

Substituting now eqs. (2.35)–(2.38) in eq. (2.33), the $\omega^2$ sum rule of the dynamic structure function can be rearranged to yield

$$m_2(q) = \left( \frac{q^2}{2m} \right)^2 \left[ 2 - S(q) \right] + \frac{1}{N (2m)^2} \sum_{i,j=1}^{N} \left\{ 2q^2 \left< e^{i q r_j} e^{-i q r_i} (q \cdot (p_i - p_j)) \right> \right\}$$


\[ + 4 \left\langle e^{i\mathbf{q}_i \mathbf{r}_j} e^{-i\mathbf{q}_r \mathbf{r}_j} (\mathbf{q} \cdot \mathbf{p}_j)(\mathbf{q} \cdot \mathbf{p}_i) \right\rangle \]  \hspace{1cm} (2.39)

Taking into account the isotropy of the momentum distribution, the sum of the \( i = j \) terms in the curly brackets of eq. (2.39) becomes proportional to the kinetic energy per particle \( \langle t \rangle \)

\[
\frac{4}{N} \frac{1}{(2m)^2} \sum_{j=1}^{N} \left\langle (\mathbf{q} \cdot \mathbf{p}_j)^2 \right\rangle = \frac{1}{m^2} \frac{\nu}{(2\pi)^2 \rho} \int dk n(k) (\mathbf{k} \cdot \mathbf{k})^2 = \frac{2 \frac{q^2}{3}}{2m} \langle t \rangle  \hspace{1cm} (2.40)
\]

Terms with \( i \neq j \) are harder to evaluate due to the derivatives acting directly on the wave function. Nevertheless they can be computed replacing the second term inside the curly brackets of eq. (2.39) with

\[
2 \sum_{i \neq j} \left\langle e^{i\mathbf{q}_i \mathbf{r}_j} e^{-i\mathbf{q}_r \mathbf{r}_j} \left[ (\mathbf{q} \cdot \mathbf{p}_j)(\mathbf{q} \cdot \mathbf{p}_i) + (\mathbf{q} \cdot \mathbf{p}_i)(\mathbf{q} \cdot \mathbf{p}_j) \right] \right\rangle \hspace{1cm} (2.41)
\]

integrating the resulting expression by parts

\[
= 2N(N-1) \int dx^N e^{i\mathbf{q} \cdot \mathbf{x}} e^{-i\mathbf{q} \cdot \mathbf{x}} \left[ (\mathbf{q} \cdot \nabla_1 \Psi_0^*)(\mathbf{q} \cdot \nabla_2 \Psi_0) + (\mathbf{q} \cdot \nabla_2 \Psi_0^*)(\mathbf{q} \cdot \nabla_1 \Psi_0) \right]
+ 2iq^2 N(N-1) \int dx^N e^{i\mathbf{q} \cdot \mathbf{x}} e^{-i\mathbf{q} \cdot \mathbf{x}} \left[ \Psi_0^*(\mathbf{q} \cdot \nabla_1) - (\mathbf{q} \cdot \nabla_2) \right] \Psi_0 \hspace{1cm} (2.42)
\]

and noticing that the last term in eq. (2.42) cancels exactly with the first one inside the curly brackets of (2.39). Then, one is left with a single integral that can be written in the form

\[
4N(N-1) \int dx^N \cos(\mathbf{q} \cdot \mathbf{x}) \left[ (\mathbf{q} \cdot \nabla_1 \Psi_0^*)(\mathbf{q} \cdot \nabla_2 \Psi_0) \right] \equiv 4Nq^2 \tilde{D}(q) , \hspace{1cm} (2.43)
\]

\( \tilde{D}(q) \) being a function of the transferred momentum \( q \) that asymptotically goes to zero when \( q \rightarrow \infty \). Hence, the total \( m_2(q) \) sum rule reduces to

\[
m_2(q) = \left( \frac{q^2}{2m} \right)^2 \left[ 2 - S(q) \right] + \frac{q^2}{2m} \left[ \frac{2}{3} - \langle t \rangle \right] + \tilde{D}(q) \hspace{1cm} . \hspace{1cm} (2.44)
\]

Eventually, this can also be written in a more compact form if one realizes that, with \( \mathbf{P} = \sum_j \mathbf{p}_j \) being the total momentum operator, then

\[
\sum_{j=1}^{N} \left\langle (\mathbf{q} \cdot \mathbf{p}_j)(\mathbf{q} \cdot \mathbf{P}) \right\rangle = \sum_{j=1}^{N} \left\langle (\mathbf{q} \cdot \mathbf{p}_j)^2 \right\rangle + \sum_{i \neq j} \left\langle (\mathbf{q} \cdot \mathbf{p}_i)(\mathbf{q} \cdot \mathbf{p}_j) \right\rangle = 0 , \hspace{1cm} (2.45)
\]

and so the sum of the \( i = j \) terms inside the brackets of eq. (2.39) amounts

\[
- \frac{4}{N} \frac{1}{(2m)^2} \sum_{i \neq j} \left\langle (\mathbf{q} \cdot \mathbf{p}_i)(\mathbf{q} \cdot \mathbf{p}_j) \right\rangle = - \frac{1}{m^2} (N-1) \int dx^N \left[ (\mathbf{q} \cdot \nabla_1 \Psi_0^*)(\mathbf{q} \cdot \nabla_2 \Psi_0) \right] . \hspace{1cm} (2.46)
\]
2.2 Sum rules of \( S(q, \omega) \)

Equation (2.46) can be combined with the expression of the \( i \neq j \) terms in (2.43) to form a function of \( q \) known, after Feenberg [Fe69], as the kinetic structure factor \( D(q) \)

\[
\frac{q^2}{m^2} D(q) = \frac{N - 1}{m^2} \int dx^N \left[ \cos(q \cdot x_{12}) - 1 \right] (q \cdot \nabla_1 \Psi_0^*) (q \cdot \nabla_2 \Psi_0) \\
= \frac{N - 1}{m^2} \int dx_1 dx_2 \left[ \cos(q \cdot x_{12}) - 1 \right] (q \cdot \nabla_1) (q \cdot \nabla_2) \rho_2(x_1, x_2; x'_1, x'_2) \frac{\delta^4(x_1 - x'_1)}{x_1 - x'_1} 
\]

(2.47)

in terms of which the second energy weighted sum rule of the dynamic structure function reads

\[
m_2(q) = \left( \frac{q^2}{2m} \right)^2 \left[ 2 - S(q) \right] + \frac{q^2}{m^2} D(q) .
\]

(2.48)

Comparing the form of the kinetic structure factor to the form \( \tilde{D}(q) \) given in eq. (2.43), it is clear that the limiting value of \( D(q) \) is \( 2m \langle t \rangle / 3 \) when \( q \to \infty \) and 0 when \( q \to 0 \). The behavior of the kinetic structure factor between these limits strongly depends on the detailed structure of the ground state through the two-body density matrix, so it can not be easily described from general arguments.

The first estimation of \( D(q) \) for pure \(^4\)He was extracted by Dalfovo and Stringari [DS92] from a Path Integral Monte Carlo simulation by Pollock and Ceperley [PC87]. More recently, new upper an lower bounds for the spectrum of elementary excitations of pure \(^4\)He have been obtained using the first realistic calculation of \( D(q) \) [BCDMS95].

2.2.4 The \( m_3(q) \) moment

The third moment of the response can be written, from eq. (2.23) with \( k = 3 \), as the ground state expectation value

\[
m_3(q) = -\frac{1}{N} \langle 0 | [H, \rho_q^3] [H, [H, \rho_q]] | 0 \rangle 
\]

(2.49)

which, once again, can be brought to an alternative form that simplifies its evaluation

\[
m_3(q) = -\frac{1}{2N} \langle 0 | [H, \rho_q^2], [H, [H, \rho_q]] | 0 \rangle . 
\]

(2.50)

The commutator of \( H \) and \( \rho_q^3 \) has been reported in eq. (2.29) and the double commutator in the right becomes

\[
[H, H, \rho_q] = [T + V, [T, \rho_q]] = [T, [T, \rho_q]] + [V, [T, \rho_q]] ,
\]

(2.51)

thus leading to the following expression of the third moment of the response

\[
m_3(q) = -\frac{1}{2N} \langle 0 | [T, \rho_q], [T, [T, \rho_q]] | 0 \rangle - \frac{1}{2N} \langle 0 | [T, \rho_q], [V, [T, \rho_q]] | 0 \rangle .
\]

(2.52)
In eq. (2.52), \( m_3(q) \) is split two pieces that will be referred as kinetic and potential terms, respectively. From the result in eq. (2.29), the kinetic term can be easily calculated

\[
[T, [T, \rho_q]] = \frac{1}{(2m)^2} \sum_{i,j=1}^{N} \left[ p_i^2, e^{iqr_j}(q \cdot p_j) + (q \cdot p_j) e^{iqr_j} \right]
\]

\[
= \frac{1}{(2m)^2} \sum_{j=1}^{N} \left\{ 4e^{iqr_j}(q \cdot p_j)^2 + 4q^2 e^{iqr_j}(q \cdot p_j) + q^4 e^{iqr_j} \right\} ,
\]

and its contribution to the sum rule reads

\[
[[T, \rho_q], [T, \rho_q]] = \frac{1}{(2m)^3} \sum_{j=1}^{N} \left\{ 8q^2(q \cdot p_j)^2 - 4q^4(q \cdot p_j) - 2q^6 \right\} .
\]

The potential term in eq.(2.52) can be equally treated, but now the resulting expression includes derivatives of the interatomic potential

\[
[V, [T, \rho_q]] = \frac{1}{2m} \sum_{j=1}^{N} \left[ V(x_1, \ldots, x_N), e^{iqr_j}(q \cdot p_j) + (q \cdot p_j) e^{iqr_j} \right]
\]

\[
= \frac{i}{m} \sum_{j=1}^{N} e^{iqr_j} \left[ (q \cdot \nabla_j) V(x_1, \ldots, x_N) \right] ,
\]

where in the last line use has been made of the well known relations

\[
[x_j, F(p_1, \ldots, p_N)] = i \nabla_j F(p_1, \ldots, p_N)
\]

\[
[p_j, G(x_1, \ldots, x_N)] = -i \nabla_j G(x_1, \ldots, x_N) .
\]

Collecting everything, the total contribution of the potential term to \( m_3(q) \) becomes

\[
[[T, \rho_q], [V, [T, \rho_q]]] = -i \frac{q}{m^2} \sum_{j=1}^{N} (q \cdot \nabla_j) V - \frac{1}{m^2} \sum_{i,j=1}^{N} e^{iqr_j} e^{-iqr_i} (q \cdot \nabla_i) (q \cdot \nabla_j) V .
\]

The first term in right hand side of the last equation vanishes when the interatomic potential is pairwise and central

\[
V(r_1, r_2, \ldots, r_N) = \sum_{i<j=1}^{N} V(r_{ij}) ,
\]

while the ground–state expectation value of the second term can be expressed in configuration space as an integral of the potential weighted by the two–body radial distribution function \( g(r) \). Collecting the results in eqs. (2.54) and (2.57), and projecting on a complete basis of position eigenstates, one finally finds

\[
m_3(q) = \frac{\rho}{2m^2} \int d\mathbf{r} g(r) \left[ 1 - \cos(q \cdot \mathbf{r}) \right] \left[ (q \cdot \nabla)^2 V(r) \right] + \left( \frac{q^2}{2m} \right)^3 + \frac{q^4}{m} (t)
\]

which is the contribution of all the different terms to the third moment of the response.
2.3 Coherent and incoherent sum rules

The preceding set of sum rules is useful to study the behavior of the dynamic structure function at low and intermediate momentum transfers, where collective states dominate the spectrum of elementary excitations. However, the progressive reduction of $S_{\text{coh}}(q, \omega)$ at high $q$'s justifies a separated analysis of the coherent and incoherent responses, and of the specific sum rules satisfied by both functions.

Due to its definition in time space, eq. (2.7), the energy–weighted sum rules of the incoherent response must be deduced from a relation like (2.4) applied to $S_{\text{inc}}(q, \omega)$ and $S_{\text{inc}}(q, t)$. From the general properties of the Fourier transform

$$m_n^{\text{inc}}(q) = \int_{-\infty}^{\infty} \omega^n S_{\text{inc}}(q, \omega) \, d\omega$$

$$= \frac{1}{i^n} \frac{d^n}{dt^n} S_{\text{inc}}(q, t) \bigg|_{t=0}, \quad (2.60)$$

showing that each sum rule of $S_{\text{inc}}(q, \omega)$ is completely determined by a given coefficient of the Taylor series of $S_{\text{inc}}(q, t)$.

A formal expansion in powers of $t$ of the incoherent density–density correlation function can be easily derived from eq. (2.7)

$$S_{\text{inc}}(q, t) = \frac{1}{N} \sum_{j=1}^{N} \left< e^{-i\mathbf{q} \mathbf{r}_j} e^{i\mathbf{q} \mathbf{r}_j(t)} \right>$$

$$\equiv \left< e^{-i\mathbf{q} \mathbf{r}_1} e^{iHt} e^{i\mathbf{q} \mathbf{r}_1} e^{-iHt} \right> \quad (2.61)$$

with the aid of the Baker–Campbell–Hausdorff formula valid for arbitrary operators $A$ and $B$

$$e^{\lambda A} B e^{-\lambda A} \equiv B + \lambda [A, B] + \frac{1}{2} \lambda^2 [A, [A, B]] + \cdots. \quad (2.62)$$

Applying (2.62) to the rightmost operators in eq. (2.61), the desired expansion naturally emerges

$$S_{\text{inc}}(q, t) = 1 + it \left< e^{-i\mathbf{q} \mathbf{r}_1} \left[ H, e^{i\mathbf{q} \mathbf{r}_1} \right] \right>$$

$$+ \frac{1}{2!} (it)^2 \left< e^{-i\mathbf{q} \mathbf{r}_1} \left[ H, \left[ H, e^{i\mathbf{q} \mathbf{r}_1} \right] \right] \right>$$

$$+ \frac{1}{3!} (it)^3 \left< e^{-i\mathbf{q} \mathbf{r}_1} \left[ H, \left[ H, \left[ H, e^{i\mathbf{q} \mathbf{r}_1} \right] \right] \right] \right> + \cdots \quad (2.63)$$

where the matrix elements are time–independent. Accordingly, the formal Taylor expansion of $S_{\text{inc}}(q, \omega)$ gives rise to

$$m_0^{\text{inc}}(q) = 1 \quad (2.64)$$
General properties of the dynamic structure function

\[ m_1^{inc}(q) = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} [H, e^{i\mathbf{q}\cdot\mathbf{r}_1}] \rangle \]  
(2.65)

\[ m_2^{inc}(q) = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} [H, [H, e^{i\mathbf{q}\cdot\mathbf{r}_1}]] \rangle \]  
(2.66)

\[ m_3^{inc}(q) = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} [H, [H, [H, e^{i\mathbf{q}\cdot\mathbf{r}_1}]]] \rangle , \]  
(2.67)

while expressions for higher order terms may be equally deduced.

Equation (2.64) indicates that the zero order sum rule of the incoherent dynamic structure function is equal to 1 for all values of \( q \), reproducing the asymptotic value reached by \( S(q) \) when \( q \to \infty \) and hence stressing the tendency of the incoherent sum rules to reproduce those of the total \( S(q, \omega) \) at high \( q \)'s.

The expectation value entering in eq. (2.65) can be written in the form

\[ m_1^{inc}(q) = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} H e^{i\mathbf{q}\cdot\mathbf{r}_1} \rangle - \langle H \rangle , \]  
(2.68)

where

\[ e^{-i\mathbf{q}\cdot\mathbf{r}_1} H e^{i\mathbf{q}\cdot\mathbf{r}_1} = e^{-i\mathbf{q}\cdot\mathbf{r}_1} H (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N) e^{i\mathbf{q}\cdot\mathbf{r}_1} \]

\[ = H (\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{p}_1 + \mathbf{q}, \mathbf{p}_2, \ldots, \mathbf{p}_N) \]

\[ = H + \left[ \frac{(\mathbf{p}_1 + \mathbf{q})^2}{2m} - \frac{\mathbf{p}_1^2}{2m} \right] \]  
(2.69)

because \( \exp(i\mathbf{q}\cdot\mathbf{r}_1) \) is a momentum translation operator and the potential operator entering in the Hamiltonian is assumed to be velocity-independent. As a consequence, the first energy-weighted sum rule of \( S_{inc}(q, \omega) \) reduces to

\[ m_1^{inc}(q) = \left\langle H + \frac{\mathbf{q} \cdot \mathbf{p}_1}{m} + \frac{q^2}{2m} \right\rangle - \langle H \rangle \equiv \frac{q^2}{2m} \]  
(2.70)

because \( \langle \mathbf{q} \cdot \mathbf{p}_1 \rangle = \mathbf{q} \cdot \langle \mathbf{p}_1 \rangle = 0 \) due to space isotropy. Notice that this result coincides with that of the first moment of the total dynamic structure function, and so the \( f \)-sum rule is entirely exhausted by the incoherent response.

The calculation of \( m_2^{inc}(q) \) requires the evaluation of the following matrix element

\[ m_2^{inc}(q) = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} [H, [H, e^{i\mathbf{q}\cdot\mathbf{r}_1}]] \rangle \]

\[ = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} H^2 e^{i\mathbf{q}\cdot\mathbf{r}_1} - e^{-i\mathbf{q}\cdot\mathbf{r}_1} H e^{i\mathbf{q}\cdot\mathbf{r}_1} H - H e^{-i\mathbf{q}\cdot\mathbf{r}_1} H e^{i\mathbf{q}\cdot\mathbf{r}_1} + H^2 \rangle \]

\[ = \langle e^{-i\mathbf{q}\cdot\mathbf{r}_1} H^2 e^{i\mathbf{q}\cdot\mathbf{r}_1} \rangle - 2E_0 \left( E_0 + \frac{q^2}{2m} \right) + E_0^2 , \]  
(2.71)

where \( E_0 \) is the ground state energy that appears from the reiterated action of \( H \) on \( |0 \rangle \) and \( \langle 0 | \). The expectation value remaining in the right hand side of eq. (2.71) can
be evaluated introducing an identity in the form of two exponential operators between the two Hamiltonians

\[
\langle e^{-iq_r H^2} e^{iq_r} \rangle = \langle e^{-iq_r H} e^{iq_r} e^{-iq_r H} e^{iq_r} \rangle
\]

\[
= \left( \left[ H + \frac{q \cdot P_1}{m} + \frac{q^2}{2m} \right] + \left[ H + \frac{q \cdot P_1}{m} + \frac{q^2}{2m} \right] \right)
\]

\[
= E_0^2 + 2E_0 \frac{q^2}{2m} + \left( \frac{q^2}{2m} \right)^2 + \frac{1}{m^2} \langle (q \cdot P_1)^2 \rangle ,
\]

while the last expectation can be written in terms of the kinetic energy per particle \( \langle t \rangle \) as follows

\[
\frac{1}{m^2} \langle (q \cdot P_1)^2 \rangle = \frac{1}{m^2} \frac{q^2}{3} \langle \vec{p}_1^2 \rangle \equiv \frac{4}{3} \left( \frac{q^2}{2m} \right) \langle t \rangle .
\]

Collecting all the terms in (2.71), (2.72) and (2.73), the final expression of \( m_2^{inc}(q) \) reduces to

\[
m_2^{inc}(q) = \left( \frac{q^2}{2m} \right) + \frac{4}{3} \left( \frac{q^2}{2m} \right) \langle t \rangle
\]

which, recalling the high \( q \) behavior of \( D(q) \) and \( S(q) \), coincides with the asymptotic value reached by \( m_2(q) \) (see eq. (2.48)) when \( q \rightarrow \infty \).

The third energy weighted sum rule of the incoherent response can be worked out in the same way, as from eqs. (2.66) and (2.67) \( m_3^{inc}(q) \) and \( m_2^{inc}(q) \) are related through

\[
m_3^{inc}(q) = \langle e^{-iq_r [H, [H, e^{iq_r}]]} \rangle
\]

\[
= \langle e^{-iq_r} H [H, e^{iq_r}] \rangle - E_0 m_2^{inc}(q) .
\]

The first term in the last line of eq. (2.75) can be written explicitly as follows

\[
\langle e^{-iq_r} H [H, e^{iq_r}] \rangle
\]

\[
= \langle e^{-iq_r} H^3 e^{iq_r} - 2e^{-iq_r} H^2 e^{iq_r} H + e^{-iq_r} H e^{iq_r} H^2 \rangle
\]

\[
= \langle e^{-iq_r} H^3 e^{iq_r} \rangle - 2E_0 \langle e^{-iq_r} H^2 e^{iq_r} \rangle + E_0^2 \langle e^{-iq_r} H e^{iq_r} \rangle ,
\]

where the second and third terms in the last line have been already calculated in eqs. (2.72) and (2.69), respectively. The first term may be worked out as done before and becomes

\[
\langle e^{-iq_r} H^3 e^{iq_r} \rangle = \left( \left[ H + \frac{q \cdot P_1}{m} + \frac{q^2}{2m} \right] + \left[ H + \frac{q \cdot P_1}{m} + \frac{q^2}{2m} \right] \right)
\]

\[
= E_0^3 + E_0^3 \frac{q^2}{2m} + E_0 \left( 3 \left( \frac{q^2}{2m} \right)^2 + \frac{2}{m^2} \langle (q \cdot P_1)^2 \rangle \right)
\]

\[
+ \left( \frac{q^2}{2m} \right)^3 + \frac{1}{m^2} \langle (q \cdot P_1)^2 \rangle + \frac{1}{m^2} \langle (q \cdot P_1) H(q \cdot P_1) \rangle .
\]
The ground state expectation value of \((q \cdot p_1)\) has already been evaluated and is proportional to the kinetic energy per particle in the medium. The last term in (2.77) can also be evaluated writing

\[
\langle (q \cdot p_1)H(q \cdot p_1) \rangle = \langle (q \cdot p_1) [H, (q \cdot p_1)] \rangle - E_0 \langle (q \cdot p_1)^2 \rangle ,
\]

(2.78)

where

\[
\langle (q \cdot p_1) [H, (q \cdot p_1)] \rangle = \frac{1}{2} \langle \{[q \cdot p_1], [H, (q \cdot p_1)]\} \rangle = \frac{1}{2} \langle q \cdot \nabla_1 \rangle \sum_{j=2}^N V(r_{1j})
\]

(2.79)

from relations (2.56) and the specific form of the Hamiltonian. Therefore, the expectation value in eq. (2.78) reduces to an integral of the radial distribution function and the interatomic potential

\[
\langle (q \cdot p_1)H(q \cdot p_1) \rangle = \frac{1}{2} \left( \langle q \cdot \nabla_1 \rangle \right)^2 \sum_{j=2}^N V(r_{1j}) - E_0 \langle (q \cdot p_1)^2 \rangle
\]

\[= \frac{1}{2} \int dr \, g(r) (q \cdot \nabla)^2 V(r) - E_0 m^2 \rho \left( \frac{q^2}{2m} \right) \langle t \rangle .
\]

(2.80)

The final expression of the third moment of the incoherent response reads

\[m_3^{inc}(q) = \left( \frac{q^2}{2m} \right)^3 + 4 \left( \frac{q^2}{2m} \right)^2 \langle t \rangle + \frac{1}{2m \rho} \int dr g(r) (q \cdot \nabla)^2 V(r) .
\]

(2.81)

Compared to the expression of the third energy weighted sum rule of the total response reported in eq. (2.59), the result in the previous line shows that all the terms in \(m_3(q)\) except the one proportional to the integral of \(\cos(q \cdot r)\) are reproduced by \(m_3^{inc}(q)\). The excluded term, therefore, constitutes the contribution of the coherent response to the \(\omega^3\) sum rule of the total dynamic structure function.

### 2.4 Coherent and incoherent responses of the free systems

The separation of \(S(q, \omega)\) in its coherent and incoherent responses and the way in which they contribute to the total dynamic structure function are easily analyzed in the context of the free systems, where all the calculations are simple and can be analytically carried out [MBP96]. Great differences arise when the response of the free Bose gas is compared to the response of the free Fermi gas, so they should be separately studied. Of course, only statistical effects can be traced there, but these impose quite different constrains on the dynamics of the two systems which are reflected in an overall change of their responses.
2.4 Coherent and incoherent responses of the free systems

2.4.1 Free Bose gas

The zero temperature response of the free Bose gas is easily derived. The ground state wave function of this system is a constant that, normalized to unity in a large box of volume $\Omega$, reads

$$\Psi_0(r_1, r_2, \ldots, r_N) = \frac{1}{\Omega^{N/2}}. \tag{2.82}$$

The wave function of a generic excited state characterized by the occupation numbers $\{n_0, n_1, \ldots, n_{\infty}\}$ is

$$\Psi_{\{n_0, \ldots, n_{\infty}\}}(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N! n_0! n_1! \ldots n_{\infty}!}} \sum_{\pi} \phi_{\pi_1}(r_1)\phi_{\pi_2}(r_2) \cdots \phi_{\pi_N}(r_N) \tag{2.83}$$

where the summation runs over all the elements of the symmetric group $S_N$, labels $\pi_1, \pi_2, \ldots, \pi_N$ denote a given permutation of the (ordered) single–particle states occupied and the $\phi_m(r)$ orbitals are taken to be box–normalized plane waves.

The system is uncorrelated, and so the expectation value of the one–body operator $\rho_q$ is a sum of $N$ different single–particle terms. This means that the only excited states contributing to the matrix elements of $S(q, \omega)$ in eq. (2.3) are those where a single particle is promoted outside of the ground state. Momentum conservation forces the momentum of these states to be equal to the momentum of $\rho_q|0\rangle$, which is $q$. At the end, this severe constrain restricts the sum over $\{n\}$ to the single state

$$\Psi_q(r_1, r_2, \ldots, r_N) = \frac{1}{\sqrt{N!}} \sum_{j=1}^{N} e^{-iq\cdot r_j}. \tag{2.84}$$

Hence, the expression of the dynamic structure function reduces to a delta distribution

$$S(q, \omega) = \delta \left( \frac{q^2}{2m} - \omega \right), \tag{2.85}$$

thus showing that the response of the free Bose gas is a single peak of strength unity located at the quasielastic recoil energy $\omega = q^2/2m$.

The incoherent response $S_{\text{inc}}(q, \omega)$ can also be calculated. Due to the absence of an interatomic potential, eq. (2.13) becomes exact and $S_{\text{inc}}(q, \omega)$ is entirely given by the Impulse Approximation. In the free Bose gas all particles occupy the $k = 0$ state and the momentum distribution is a delta peak normalized to the total number of particles

$$n(k) = (2\pi)^3 \rho \delta(k) \tag{2.86}$$

that, once introduced in eq. (2.15), leads to the final form of the incoherent part of the response

$$S_{\text{inc}}(q, \omega) = \delta \left( \frac{q^2}{2m} - \omega \right). \tag{2.87}$$
This result indicates that $S_{\text{inc}}(q, \omega)$ is exactly equal to the total $S(q, \omega)$ reported above, showing that the $T = 0$ dynamic structure function of the system is completely incoherent, and that therefore $S_{\text{coh}}(q, \omega) = 0$ independently of the values of $q$ and $\omega$. This is not surprising because in the free Bose gas the movement of a particle does not affect the state of the others due to the absence of dynamical and statistical correlations.

### 2.4.2 Free Fermi gas

The $T = 0$ dynamic structure function of the free Fermi gas is given by the Lindhard function [Lin54], which substantially differs from the delta peak predicted in eq. (2.85) for bosons. The origin of the differences lies on the nature of the excitations produced by a density fluctuation of fixed energy and momentum, which are particle–hole pairs in Fermi systems. The Pauli principle strongly constrains these excitations, forbidding the promotion of particles to already occupied states and thus reducing the phase space available to each one.

As before, the incoherent dynamic structure function of the free Fermi gas is given by eq. (2.14)

$$S_{\text{inc}}(q, t) = \frac{1}{2\pi v_q N} \sum_{j=1}^{N} \int_{-\infty}^{\infty} dx \, e^{-ix\left(\frac{m\omega}{q} - \frac{q}{2}\right)} \left\langle e^{ixp_j} \right\rangle .$$

(2.88)

Under the same conditions, the coherent dynamic structure function can be written in the form

$$S_{\text{coh}}(q, \omega) = \frac{1}{2\pi v_q N(N - 1)} \sum_{i\neq j}^{N} \int_{-\infty}^{\infty} dx \, e^{-ix\left(\frac{m\omega}{q} - \frac{q}{2}\right)} \left\langle e^{-i\mathbf{q} \cdot \mathbf{r}_1} \right\rangle \left\langle e^{i\mathbf{q} \cdot (\mathbf{r}_2 - \mathbf{r}_1)} \right\rangle e^{ixp_i} .$$

(2.89)

Once projected on a complete basis of states in configuration space, the incoherent and the coherent responses become functions of the one- and the semi–diagonal two–body density matrices

$$S_{\text{inc}}(q, \omega) = \frac{1}{2\pi \rho v_q} \int_{-\infty}^{\infty} dx \, e^{-iyx} \rho_1(x)$$

(2.90)

$$S_{\text{coh}}(q, \omega) = \frac{1}{2\pi \rho v_q} \int_{-\infty}^{\infty} dx \, e^{-iyx} \int d\mathbf{r} \, e^{i\mathbf{q} \cdot \mathbf{r}} \rho_2(\mathbf{r}, 0; \mathbf{r} + \mathbf{x})$$

(2.91)

where $\rho$ is the particle number density, $Y$ is the West scaling variable, $v_q = q/m$ is the recoiling velocity of particle $j$, and $\rho_1$ and $\rho_2$ the one- and the semidiagonal two–body density matrices. The expression in eq. (2.90) is the Impulse Approximation, which exactly describes $S_{\text{inc}}(q, \omega)$ in free systems but that only reproduces the first term of
the $1/q$ series expansion of the response derived by Gersch and coworkers [GRS72] that is analyzed in the next chapter. Higher order terms in the series are in general related to integrals of the potential and vanish when describing the response of a free system.

Due to the close relation between the one–body density matrix $\rho_1(x)$ and the momentum distribution $n(k)$

$$n(k) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} \rho_1(r),$$

(2.92)

$S_{\text{inc}}(q, t)$ can be Fourier transformed to yield the standard representation of the IA

$$S_{\text{inc}}(q, \omega) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{k} n(k) \delta \left( \frac{(k + q)^2}{2m} - \frac{k^2}{2m} - \omega \right)$$

$$= \frac{\nu m}{4\pi^2 pq} \int_0^\infty k n(k) \, dk,$$

(2.93)

(2.94)

$\nu$ being the degeneracy of each single–particle state of definite momentum. The momentum distribution of the free Fermi gas is a Heaviside step function $n(k) = \theta(k_F - k)$ that allows for the occupation of states up to the Fermi surface only. Therefore, the integral in eq. (2.94) can be performed and the result, expressed in terms of a new set of dimensionless variables $\bar{q} = q/k_F$ and $\bar{\omega} = \omega/\epsilon_F$ with $\epsilon_F = k_F^2 / 2m$ the Fermi energy, is given by

$$S_{\text{inc}}(q, \omega) \equiv \frac{1}{\epsilon_F} S_{\text{inc}}(\bar{q}, \bar{\omega}) = \frac{3}{\epsilon_F 8\bar{q}} \left[ 1 - \frac{1}{4} \left( \frac{\bar{\omega}}{\bar{q}} - \frac{1}{\bar{q}} \right)^2 \right] \theta \left( 1 - \frac{1}{2} \left( \frac{\bar{\omega}}{\bar{q}} - 1 \right) \right),$$

(2.95)

which defines the dimensionless incoherent response $S_{\text{inc}}(\bar{q}, \bar{\omega})$.

In a similar way, the coherent response of the free Fermi gas can be brought to a form that closely resembles the IA

$$S_{\text{coh}}(q, \omega) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{k} n(k, -\mathbf{q}) \delta \left( \frac{(k + q)^2}{2m} - \frac{k^2}{2m} - \omega \right),$$

(2.96)

where $n(k, q)$ is the generalized momentum distribution introduced by Ristig and Clark [RC89][Ris79]

$$n(k, q) = \frac{1}{\nu N \rho} \int d\mathbf{r}_1 d\mathbf{r}_1' d\mathbf{r}_2 d\mathbf{r}_2' \rho_2(r_1, r_2; r_1', r_2') e^{i\mathbf{k} \cdot (r_1 - r_1')} e^{-i\mathbf{q} \cdot (r_1 - r_2)}$$

$$= \frac{1}{\nu} \int d\mathbf{r} d\mathbf{r}' \rho_2(r, 0; r', 0) e^{-i\mathbf{k} \cdot (r - r')} e^{-i\mathbf{q} \cdot r}.$$

(2.97)

(2.98)

Both the semidiagonal two–body density matrix and the generalized momentum distribution of the non–interacting system are easily derived

$$\rho_2(r_1, r_2; r_1', r_2) = \rho^2 \left[ \ell(k_F r_{11'}) - \frac{1}{\nu} \ell(k_F r_{12}) \ell(k_F r_{12'}) \right]$$

(2.99)

$$n(k, q) = \theta(k_F - k) \left[ (2\pi)^3 \rho \delta(q) - \theta(k_F - ||k - q||) \right].$$

(2.100)
where $\ell(z)$ is the statistical correlation function, characteristic in the variational analysis of homogeneous fermion systems

$$
\ell(z) = \frac{3}{z^3} \left[ \sin z - z \cos z \right].
$$

(2.101)

Inserting $n(k, q)$ (2.100) in eq.(2.96), the coherent response may be written as

$$
S_{\text{coh}}(q, \omega) = \frac{\nu}{(2\pi)^3 \rho} \int d\mathbf{k} \theta(k_F - k) \times \left[ (2\pi)^3 \rho \delta(q) - \theta(k_F - \|\mathbf{k} + \mathbf{q}\|) \right] \delta \left( \frac{(\mathbf{k} + \mathbf{q})^2}{2m} - \frac{k^2}{2m} - \omega \right)
$$

(2.102)

The $\delta(q)$ term in the integral contributes only at $q = 0$, while the other carries all the information at finite values of the momentum transfer and can be evaluated analytically

$$
S_{\text{coh}}(q, \omega) = \begin{cases} 
-\frac{1}{\epsilon_F} \frac{3}{8q} \left[ 1 - \frac{1}{4} \left( \frac{\omega}{q} - \bar{q} \right)^2 \right] & \text{if } 0 \geq \bar{\omega} \geq \bar{q}^2 - 2\bar{q} \\
-\frac{1}{\epsilon_F} \frac{3}{8q} \left[ 1 - \frac{1}{4} \left( \frac{\bar{\omega}}{q} + \bar{q} \right)^2 \right] & \text{if } 2\bar{q} - \bar{q}^2 \geq \bar{\omega} \geq 0 \\
0 & \text{for } \bar{q} \leq 2 \\
\end{cases}
$$

(2.103)

thus defining the dimensionless coherent response $S_{\text{coh}}(\bar{q}, \bar{\omega})$.

Several conclusions on the behavior of the coherent and the incoherent responses can be drawn from equations (2.95) and (2.103), some of them being also valid for realistic interacting systems.

The incoherent response $S_{\text{inc}}(\bar{q}, \bar{\omega})$ of the free Fermi gas is positive defined for all energies between $\bar{q}^2 - 2\bar{q}$ and $\bar{q}^2 + 2\bar{q}$, and vanishes out of this range. At fixed $\bar{q}$, $S_{\text{inc}}(\bar{q}, \bar{\omega})$ is a quadratic polynomial in $\bar{\omega}$ with its maximum located at $\bar{\omega} = \bar{q}^2$, thus being symmetric around this point. Hence, both $S_{\text{inc}}(\bar{q}, \bar{\omega})$ and its derivatives are continuous.

At momentum transfer $\bar{q} < 2$, $S_{\text{coh}}(\bar{q}, \bar{\omega})$ is non–zero and negative in the range $\bar{\omega} \in (\bar{q}^2 - 2\bar{q}, 2\bar{q} - \bar{q}^2)$. It is split in two different parts, one defined at negative energies and the other at positive ones. At fixed $\bar{q}$, both functions are quadratic polynomials in $\bar{\omega}$ that differ only in the sign of the linear coefficient. This peculiarity gives rise to a symmetric and continuous $S_{\text{coh}}(\bar{q}, \bar{\omega})$ that, at $\bar{\omega} = 0$, presents both a minimum and a discontinuity in the first derivative. At $\bar{q}$’s greater than twice the Fermi momentum, the coherent response vanishes.
2.4 Coherent and incoherent responses of the free systems

The total response \( S(\tilde{q}, \tilde{\omega}) \), which is the sum of \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) (2.95) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) (2.103), is the well-known Lindhard function [Lin54], [PN66] that becomes totally incoherent at \( \tilde{q} > 2 \). At \( \tilde{q} \)'s smaller than 2, both the coherent and the incoherent responses contribute and, even though they are of opposite sign in the free Fermi gas, the total response remains always positive. This is a general property of the dynamic structure function of all systems, as is apparent from eq. (2.3). For instance, if at a certain energy one of the two responses is negative, its absolute value has to be smaller than the value of the other one at that point, which should be positive, as this is the only way to produce a total \( S(q, \omega) \) that is either positive or zero.

This feature is particularly apparent at negative \( \omega \)'s, as the energy conserving delta appearing in the definition of \( S(q, \omega) \), eq. (2.3), forces the non-zero contributions to appear at positive energies only. The separation of the response in its coherent and incoherent terms breaks this constrain and both \( S_{\text{inc}}(q, \omega) \) and \( S_{\text{coh}}(q, \omega) \) can locate part of their strength at \( \omega < 0 \). However, as the total response is zero in this range, \( S_{\text{coh}}(q, \omega) \) has to be equal to \(-S_{\text{inc}}(q, \omega)\) at \( \omega < 0 \). This is once again a requirement for the response derived directly from its definition, and so does not depend on the kind of system under study. It is easy to check from equations (2.95) and (2.103) that this holds for the free Fermi gas.

Figures (2.1), (2.2) and (2.3) show the total response of the free Fermi gas and its incoherent and coherent parts at \( \tilde{q} = 0.01, \tilde{q} = 1 \) and \( \tilde{q} = 1.9 \). The upper plots show the Lindhard function (solid line), while \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) are drawn below (solid and dashed lines, respectively). There are three main regions at \( \tilde{q} \leq 2 \) where the Lindhard function changes its behavior due to the different \( \tilde{\omega} \) dependence of \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \). At negative \( \tilde{\omega} \)'s lying between \( \tilde{q}^2 - 2\tilde{q} \) and 0, \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) = -S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) and the total response vanishes. At positive energies smaller than \( 2\tilde{q} - \tilde{q}^2 \), the addition of the two responses cancel the terms quadratic in \( \tilde{\omega} \) (see equations (2.95) and (2.103)) and the total \( S(\tilde{q}, \tilde{\omega}) \) is linear. Finally, at \( \tilde{q}^2 + 2\tilde{q} \geq \tilde{\omega} \geq 2\tilde{q} - \tilde{q}^2 \) the coherent response vanishes and the dynamic structure function becomes entirely incoherent and quadratic in \( \tilde{\omega} \). Out of these limits all three functions are zero.

The different behavior of \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) is also reflected in figures (2.1) to (2.3). At very low values of the momentum transfer, both \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) are large, but strong cancellations produce the strength of the total \( S(\tilde{q}, \tilde{\omega}) \) to be drastically reduced. Notice that in this limit the region \( \tilde{\omega} \in (2\tilde{q} - \tilde{q}^2, \tilde{q}^2 + 2\tilde{q}) \) where \( S(\tilde{q}, \tilde{\omega}) \) has only incoherent contributions covers a range \( \Delta \tilde{\omega} = 2\tilde{q}^2 \ll 1 \), which is much smaller than the range where the two responses coexist. As a consequence, \( S(\tilde{q}, \tilde{\omega}) \) looks linear in \( \tilde{\omega} \) (see
General properties of the dynamic structure function

Figure 2.1: Comparison between the dimensionless Lindhard function (solid line) and the dimensionless incoherent and coherent dynamic structure functions (solid and dashed lines below, respectively) at \( \tilde{q} = 0.01 \).

When \( \tilde{q} \) increases, as seen in figure (2.2), both \( S_{\text{inc}}(\tilde{q}, \tilde{\omega}) \) and \( S_{\text{coh}}(\tilde{q}, \tilde{\omega}) \) are spread and quenched, but the former still shows a maximum well centered at \( \tilde{\omega} = \tilde{q}^2 \) and the latter a minimum at \( \tilde{\omega} = 0 \). The minimum of the coherent response coincides with the point where the two functions defined in eq. (2.103) join (\( \tilde{\omega} = 0 \)), and the different value between the left and right derivatives at that point produces a peak that sharpens with increasing \( \tilde{q} \). At \( \tilde{q} = 1 \) the range where the coherent response is non–zero becomes maximal, going from \( \tilde{\omega} = -1 \) to \( \tilde{\omega} = 1 \), but the incoherent response
2.4 Coherent and incoherent responses of the free systems

Figure 2.2: Same as in figure (2.1) but for $\tilde{q} = 1.0$.

has a wider range of existence, and the total $S(\tilde{q}, \tilde{\omega})$ presents two well differentiated regions, one linear and another quadratic in $\tilde{\omega}$. As $\tilde{q}$ rises above this value, $S_{coh}(\tilde{q}, \tilde{\omega})$ reduces both its magnitude and its range of definition and, in particular, at $\tilde{q} = 1.9$ becomes much smaller than $S_{inc}(\tilde{q}, \tilde{\omega})$ (see figure (2.3)), thus producing a total $S(\tilde{q}, \tilde{\omega})$ that is mostly incoherent.

Another useful tool in the study of the dynamic structure function are the energy weighted sum rules, which can be also derived for $S_{inc}(\tilde{q}, \tilde{\omega})$ and $S_{coh}(\tilde{q}, \tilde{\omega})$. As it has been mentioned, they are defined to be the moments of the different responses which,
Figure 2.3: Same as in figure (2.1) but for $\tilde{q} = 1.9$

in terms of the dimensionless variables $\tilde{q}$ and $\tilde{\omega}$, read

$$m^{(\alpha)}_{inc,(coh)}(\tilde{q}) = \int_{-\infty}^{\infty} d\tilde{\omega} \tilde{\omega}^\alpha S_{inc,(coh)}(\tilde{q},\tilde{\omega})$$

$$m^{(\alpha)}(\tilde{q}) = m^{(\alpha)}_{inc}(\tilde{q}) + m^{(\alpha)}_{coh}(\tilde{q}) = \int_{0}^{\infty} d\tilde{\omega} \tilde{\omega}^\alpha S(\tilde{q},\tilde{\omega}) .$$

Even though $m^{(\alpha)}_{inc}(\tilde{q})$ and $m^{(\alpha)}_{coh}(\tilde{q})$ integrate over all energies, $m^{(\alpha)}(\tilde{q})$, built from their sum, is an equivalent integral of the total $S(\tilde{q},\tilde{\omega})$ but obviously restricted to positive energies.
2.4 Coherent and incoherent responses of the free systems

The first moments read

\[
\begin{align*}
    m_{\text{inc}}^{(0)}(\bar{q}) &= 1 \\
    m_{\text{coh}}^{(0)}(\bar{q}) &= S(q) - 1 \\
    m_{\text{inc}}^{(1)}(\bar{q}) &= q^2 \\
    m_{\text{coh}}^{(1)}(\bar{q}) &= 0
\end{align*}
\]  

(2.106) (2.107) (2.108) (2.109)

and are the same in a correlated system replacing \( S(q) \) by the appropriate static structure factor. For the free Fermi gas, all odd moments of \( S_{\text{coh}}(\bar{q}, \bar{\omega}) \) cancel due to the symmetry of the coherent response around \( \bar{\omega} = 0 \), while even ones are related to derivatives of \( \rho_2 \). Furthermore, all odd order incoherent moments centered at \( \bar{\omega} = q^2 \) vanish. Particle correlations in realistic systems may cause the static structure factor to be greater or smaller than 1 as a function of \( q \). Even though this change in the sign of \( m_{\text{coh}}^{(0)}(q) \) can be obtained from a \( S_{\text{coh}}(q, \omega) \) symmetric around \( \omega = 0 \) that has no nodes, it seems more reasonable to think about a coherent response that has at least one point where the function changes sign, located in such a way that both \( m_{\text{coh}}^{(0)}(q) \) and \( m_{\text{coh}}^{(1)}(q) \) are fulfilled. Therefore, this difference in the behavior of the zero moment points towards a change in the structure of the coherent response entirely induced by particle correlations.

Concerning the contribution of \( S_{\text{inc}}(\bar{q}, \bar{\omega}) \) and \( S_{\text{coh}}(\bar{q}, \bar{\omega}) \) at \( \bar{\omega} < 0 \), moments (2.106) to (2.109) differ from those obtained integrating over positive energies only. In particular for the Fermi sea, the first moments of \( S_{\text{inc}}(\bar{q}, \bar{\omega}) \) integrated at \( \bar{\omega} > 0 \) are

\[
\begin{align*}
    \int_0^\infty d\bar{\omega} S_{\text{inc}}(\bar{q}, \bar{\omega}) &= 1 - \frac{3}{2} \int_{\bar{q}/2}^\infty \bar{k} \left( \bar{k} - \frac{\bar{q}}{2} \right) n(\bar{k}) d\bar{k} \\
    \int_0^\infty d\bar{\omega} \bar{\omega} S_{\text{inc}}(\bar{q}, \bar{\omega}) &= \bar{q}^2 + \frac{3\bar{q}}{4} \int_{\bar{q}/2}^\infty \bar{k} \left( \bar{k} - \frac{\bar{q}}{2} \right)^2 n(\bar{k}) d\bar{k}
\end{align*}
\]  

(2.110) (2.111)

and coincide with the previous ones at \( \bar{q} > 2 \) where \( S(\bar{q}, \bar{\omega}) = S_{\text{inc}}(\bar{q}, \bar{\omega}) \). The residual terms appearing in the right hand side of equations (2.110) and (2.111) are the manifestation of the negative energy contributions, and are the same in realistic systems when the incoherent response is described by the Impulse Approximation. Notice that in such systems the momentum distribution \( n(k) \) extends up to infinity, and therefore those terms contribute no matter how large \( \bar{q} \) is. Nevertheless, \( n(k) \) decreases rapidly with \( k \) and they become vanishingly small as \( \bar{q} \) increases.

In summary, a direct calculation of the coherent and incoherent density responses of the free Fermi gas reveals significant differences between them and with respect to
the total dynamic structure function. While the latter is known to be non-zero and positive at $\omega > 0$ only, none of those constrains apply to the coherent and the incoherent responses separately. In particular, and for the Fermi gas, $S_{\text{coh}}(q, \omega)$ is negative and symmetric around $\omega = 0$ and both $S_{\text{inc}}(q, \omega)$ and $S_{\text{coh}}(q, \omega)$ present non-negligible contributions at $\omega < 0$ that cancel exactly once added up. This cancellation also holds in any realistic system, a behavior that is also reflected in the energy weighted sum rules.

2.5 Sum Rules of $S(q, \omega)$ in the $^3\text{He}–^4\text{He}$ mixture

As it has been said, the dynamic structure factor of the $^3\text{He}–^4\text{He}$ mixture is the sum of four terms, each one corresponding the different type of density excitations that can be produced on the system. The definition of the energy weighted sum rules corresponding to each of the four terms of the response reported in eq. (2.16) has been given in eq. (2.22), and they can be analytically expressed in terms of ground state quantities using the same methods employed in the last section. Only the zero, first and third moments of $S(q, \omega)$ are analyzed here, as they involve simple ground state properties as are the kinetic energies per particle or the radial distribution functions, while they provide information enough to draw a qualitative sketch of the behavior of the response in the mixture.

2.5.1 The $m_0(q)$ moments

The zero order energy weighted sum rule of the density components of the response are given by

$$m_0^{(\alpha, \beta)}(q) = \frac{1}{\sqrt{N_\alpha N_\beta}} \langle 0 \mid \rho^{(\alpha)}_q \rho^{(\beta)}_q \mid 0 \rangle \equiv S^{(\alpha, \beta)}(q) ,$$

(2.112)

where $S^{(\alpha, \beta)}(q)$ are the $(\alpha, \beta)$-components of the static structure factor, related to the radial distribution function $g^{(\alpha, \beta)}(r)$ through

$$S^{(\alpha, \beta)}(q) = \delta_{\alpha \beta} + \sqrt{\rho_\alpha \rho_\beta} \int dr \left[ g^{(\alpha, \beta)}(r) - 1 \right] e^{iqr} .$$

(2.113)

The zero moment of the $^3\text{He}$ spin dependent component has the following form

$$m_0^{(3, f)}(q) = \frac{1}{N_3 I(I + 1)} \langle 0 \mid \mathbf{I}_q \cdot \mathbf{I}_q \mid 0 \rangle \equiv S^{(3, f)}(q)$$

(2.114)
which is the definition of the spin dependent static structure function \( S_I^{(3,3)}(q) \). The latter can be written in terms of the spin radial distribution function \( g_I^{(3,3)}(r) \) as

\[
S_I^{(3,3)}(q) = 1 + \rho_0 \int d\mathbf{r} \, g_I^{(3,3)}(r) e^{i\mathbf{q} \cdot \mathbf{r}},
\]

where

\[
g_I^{(3,3)}(r) = g_{I+}^{(3,3)}(r) - g_{I-}^{(3,3)}(r).
\]

In eq. (2.116), \( g_{I+}^{(3,3)}(r) \) and \( g_{I-}^{(3,3)}(r) \) are the radial distribution functions corresponding to the \(^3\)He atoms in a parallel or antiparallel spin configuration, respectively, and normalized such that \( g^{(3,3)}(r) = g_{I+}^{(3,3)}(r) + g_{I-}^{(3,3)}(r) \). In a system of spin \( I = 1/2 \) particles, the spin radial distribution functions read

\[
g_{I+}(r) = \sum_{\sigma = -1/2}^{1/2} g_{\sigma,\sigma}(r,0)
\]

\[
g_{I-}(r) = \sum_{\sigma = -1/2}^{1/2} g_{\sigma,-\sigma}(r,0)
\]

where the functions entering in the right hand side of this expression are defined as

\[
g_{\sigma_1,\sigma_2}(r,r') \equiv g_{\sigma_1,\sigma_2}(|r - r'|) = \frac{1}{p^2} \sum_{i,j} \langle 0 | P^{(i,j)}_{\sigma_1,\sigma_2} \delta(r - r_i) \delta(r' - r_j) | 0 \rangle
\]

in terms of the spin operators

\[
P^{(i,j)}_{\sigma_1,\sigma_2} = \left| \sigma_1^{(i)} \sigma_2^{(j)} \right\rangle \langle \sigma_1^{(i)} \sigma_2^{(j)} |
\]

which project the third component of the spin of particles \( i \) and \( j \) into the states \( \sigma_1 \) and \( \sigma_2 \), respectively.

All the ground state functions previously mentioned have been calculated in the HNC/FHNC framework at different \(^3\)He concentrations. The four different \( m_0(q) \) moments of \( S(q, \omega) \) in the \( x_3 = 0.01 \) and \( x_3 = 0.066 \) mixtures are shown in figure (2.4). Due to the low \(^3\)He concentration, the static structure factor of the \(^4\)He component is nearly the same as in the pure phase, while the \(^3\)He component behaves almost as a gas of free fermions. Due to the weakness of the spin correlations between \(^3\)He atoms in the mixture at low concentrations, \( S^{(3,3)}(q) \) and \( S_I^{(3,3)}(q) \) are close and similar to the corresponding response of a gas of free fermions at the same density where they are identical. In particular, for \( x_3 = 0.01 \) \( S^{(3,3)}(q) \) and \( S_I^{(3,3)}(q) \) are indistinguishable. Finally, \( S^{(3,4)}(q) \) is significantly different from zero for \( q \)’s below 3Å\(^{-1}\) approximately, and has not definite sign. This oscillating behavior reflects the fact that \( S^{(3,4)}(q, \omega) \) is not positively defined.
2.5.2 The \( m_1(q) \) moments

As in the case of pure phases, the first order sum rule of \( S(q, \omega) \) in the mixture takes a particularly simple form. The four different moments can be written, following the steps shown above, as the ground state expectation value of the following double commutators

\[
m_{1,(\alpha,\beta)}^{(\omega)}(q) = \frac{1}{2\sqrt{N_\alpha N_\beta}} \langle 0 | \left[ \rho_{q}^{(\alpha)}, \left[ H, \rho_{q}^{(\beta)} \right] \right] | 0 \rangle \quad (2.120)
\]

and

\[
m_{1,I}^{(3,3)}(q) = \frac{1}{2N_3 I (I + 1)} \langle 0 | \left[ I_q^+, \left[ H, I_q \right] \right] | 0 \rangle . \quad (2.121)
\]

The commutators can be explicitly carried out using the expression of the Hamiltonian and the excitation operators, and the result are the well known \( f \)-sum rules

\[
m_{1}^{(4,4)}(q) = \frac{q^2}{2m_4} \quad (2.122)
\]

\[
m_{1}^{(3,3)}(q) = m_{1,I}^{(3,3)}(q) = \frac{q^2}{2m_3} \quad (2.123)
\]
2.5 Sum Rules of $S(q, \omega)$ in the $^3\text{He}^{-4}\text{He}$ mixture

![Graph showing sum rules for $^3\text{He}^{-4}\text{He}$ mixture](image)

**Figure 2.5:** The $m_3^{(4,4)}(q)$ and $m_3^{(3,3)}(q)$ sum rules in the mixture at zero pressure and for $x_3 = 0.06$. The solid lines correspond to the total $m_3^{(4,4)}(q)$ and $m_3^{(3,3)}(q)$. The dashed lines show the potential contribution to the sum rules, i.e., the terms integrating the radial distribution functions in eqs. (2.125) and (2.126).

\[ m_1^{(3,4)}(q) = 0, \quad (2.124) \]

which do not depend on the special character of the particle correlations and thus supply rather strong model independent constrains to all the four terms entering in $S(q, \omega)$.

### 2.5.3 The $m_3(q)$ moments

The generalization of the calculation of $m_3(q)$ for pure phases to the mixture is straightforward. Again, one has to evaluate commutators between $\rho_q$, $I_q$ and the Hamiltonian $H$. At the end, one finds

\[
m_3^{(4,4)}(q) = \left( \frac{q^2}{2m_4^2} \right)^3 + 4 \left( \frac{q^2}{2m_4^2} \right)^2 \langle t_4 \rangle \\
+ \frac{\rho_4}{2m_4} \int d\mathbf{r} g^{(4,4)}(r) [1-\cos(\mathbf{q} \cdot \mathbf{r})] \left[ (\mathbf{q} \cdot \nabla)^2 V(r) \right] \quad (2.125)
\]
**General properties of the dynamic structure function**

**Figure 2.6:** $m^{(3,4)}_3(q)$ in a 0.06 $^3$He concentration mixture at $T = 0$ and zero pressure

\[
m^{(3,3)}_3(q) = \left( \frac{q^2}{2m_3} \right)^3 + 4 \left( \frac{q^2}{2m_3} \right)^2 \langle t_3 \rangle + \frac{\rho_3}{2m_3^2} \int \! d\mathbf{r} \; g^{(3,3)}(r) \left[ 1 - \cos(\mathbf{q} \cdot \mathbf{r}) \right] \left[ (\mathbf{q} \cdot \nabla)^2 V(R) \right] \tag{2.126}
\]

\[
m^{(3,3)}_{3,4}(q) = \left( \frac{q^2}{2m_3} \right)^3 + 4 \left( \frac{q^2}{2m_3} \right)^2 \langle t_3 \rangle + \frac{\rho_3}{2m_3^2} \int \! d\mathbf{r} \; \left[ g^{(3,3)}(r) - g^{(3,3)}_I(r) \cos(\mathbf{q} \cdot \mathbf{r}) \right] (\mathbf{q} \cdot \nabla)^2 V(r) \tag{2.127}
\]

\[
m^{(3,4)}_3(q) = -\left( \frac{\rho_3 \rho_4}{2m_3 m_4} \right)^{1/2} \int \! d\mathbf{r} \; g^{(3,4)}(r) \cos(\mathbf{q} \cdot \mathbf{r}) (\mathbf{q} \cdot \nabla)^2 V(r) \tag{2.128}
\]

where $\rho_\alpha$ and $\langle t_\alpha \rangle$ are the particle density and the kinetic energy per particle of the $\alpha$ isotope, respectively. Notice that the only ground state quantities required in the evaluation of these sum rules are the radial distribution functions (as in the case of $m_0(q)$) and the kinetic energy per particle of each isotope.

The four terms in eqs.(2.125)–(2.128) have been calculated using a variational description of the ground state. The $m_3(q)$ and $m_4(q)$ moments are shown in figure (2.5)
2.5 Sum Rules of $S(q, \omega)$ in the $^3\text{He} - ^4\text{He}$ mixture

![Graph showing the ratio between the density and spin-density $m_3(q)$ responses of $^3\text{He}$ in the mixture. The solid and dashed lines correspond to $x_3 = 0.06$ and $x_3 = 0.01$, respectively.](image)

**Figure 2.7:** Ratio between the density and spin-density $m_3(q)$ responses of $^3\text{He}$ in the mixture. The solid and dashed lines correspond to $x_3 = 0.06$ and $x_3 = 0.01$, respectively.

at zero pressure and for a 6% $^3\text{He}$ concentration mixture. The solid curves are the total moments $m_3^{(A)}(q)$ and $m_3^{(3)}(q)$, while the dashed lines correspond to the potential terms only, i.e., those integrating the different radial distribution functions. The spin dependent term of $^3\text{He}$ is indistinguishable from the density moment on the scale considered. The oscillating behavior of the potential parts reflects the general structure of the radial distribution functions and the shape of the potential. This is also apparent for the third moment of the cross term, which is plotted in figure (2.6).

### 2.5.4 Density and spin dependent $^3\text{He}$ dynamic structure factors

The previous sum rules can be used to study the role of the different kind of excitations in the response. In the $^3\text{He}$ case, both density and spin-density dependent excitations can be produced. Differences in the two responses $S^{(3,3)}(q, \omega)$ and $S^{(3,3)}_f(q, \omega)$ are known to be entirely due to the correlations present in the liquid, as in a free gas of fermions.
both responses are identical. Correlations between $^3$He atoms are weak in the mixture, as only low concentration mixtures are stable in the nature. Therefore, one could picture the $^3$He component as a gas of quasiparticles in a background of $^4$He atoms, where the density and spin dependent responses should be very close to each other. The extent to which this is true can be discussed by direct inspection of the sum rules previously calculated.

The ratio of the zero–order sum rules $m_0^{(3,3)}(q)/m_{0,I}^{(3,3)}(q)$ has been discussed above. The density and spin dependent static structure factors of $^3$He in the mixture are very close to each other, even at the maximum solubility value $x_3=0.066$ at $T=0$. The two functions are very similar, even at low $q$. As it is apparent from eqs. (2.123), the ratio $m_1^{(3,3)}(q)/m_{1,I}^{(3,3)}(q)$ is exactly equal to 1 at all $q$’s. Finally, the ratio $m_3^{(3,3)}(q)/m_{3,I}^{(3,3)}(q)$ at zero pressure and for two values of the concentration is plotted in figure (2.7). As can be seen, the two components are basically equal for $q$’s larger than $1\AA^{-1}$, approximately.

When all ratios $m_k^{(3,3)}(q)/m_{k,I}^{(3,3)}(q)$ are close to one, the effects of the spin correlations on the dynamic structure function are negligible and

$$S_I^{(3,3)}(q,\omega) \approx S^{(3,3)}(q,\omega) .$$

The previous analysis based on the zero, first and third moments of the response strongly support this statement. This is certainly true for wave vectors much larger than the Fermi momentum $k_F$, as in this limit the response is mostly dominated by its incoherent term. Actually, the incoherent density and spin–dependent responses are identical, as is easily verified

$$S_{I,\text{inc}}^{(3,3)}(q,t) = \left\langle \hat{I}_q^I(t) \cdot \hat{I}_q(0) \right\rangle_{\text{inc}}$$

$$\quad = \frac{1}{I(I+1)N_3} \sum_{j=1}^{N_3} \left\langle e^{iHt} I_q e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{-iHt} I_q e^{i\mathbf{q} \cdot \mathbf{r}_j} \right\rangle$$

$$\quad = \frac{1}{I(I+1)N_3} \sum_{j=1}^{N_3} \left\langle I_j e^{iHt} e^{-i\mathbf{q} \cdot \mathbf{r}_j} e^{-iHt} e^{i\mathbf{q} \cdot \mathbf{r}_j} \right\rangle$$

$$\quad = \frac{1}{N_3} \left\langle e^{-i\mathbf{q} \cdot \mathbf{r}_j(t)} e^{i\mathbf{q} \cdot \mathbf{r}_j} \right\rangle \equiv S_{\text{inc}}^{(3,3)}(q,t) .$$

The third line follows immediately from the second one because the interatomic potential considered here is spin–independent. Finally, spin operator dependencies disappear because $^3$He atoms are such that $I_q^J = \frac{1}{4} \sigma_q^J \equiv \frac{3}{4}, \sigma_j$ being the Pauli matrices. The result is nothing but the Fourier transform of the incoherent density response $S_{\text{inc}}^{(3,3)}(q,t)$. 
2.5 Sum Rules of $S(q, \omega)$ in the $^3$He–$^4$He mixture

![Diagram](image)

**Figure 2.8:** Relative contributions of the different ($\alpha, \beta$)-components to the $m_0(q)$ and $m_3(q)$ moments of the total dynamic structure function, as given in eqs. (2.131). Thick solid line: (4, 4); thin solid line: (3, 4); dashed line: (3, 3); dotted line: spin dependent (3, 3). All curves correspond to zero pressure and $^3$He concentration $x_3 = 0.06$.

For typical values of the momentum transfer in neutron scattering experiments, $q$ lies well above $k_F$ so that the difference between the density and the spin-dependent dynamic structure functions can be safely neglected. As an example, consider the values $q = 1\, \text{Å}^{-1}$ and $x = 0.045$ taken from ref. [FGKSD90]. With these numbers, $m_0/m_0,I = 0.966$ and $m_3/m_3,I = 1.044$. These numbers give a microscopic basis to approximation (2.129) used in the analysis of the experimental spectrum.

2.5.5 The cross term $S^{(3,4)}(q, \omega)$

The previous evaluation of the different moments of the response give useful information about the cross term $S^{(3,4)}(q, \omega)$. In fact, sum rules (2.112), (2.124) and (2.128) provide rigorous constraints to $S^{(3,4)}(q, \omega)$, and can be used to evaluate how much the cross term contributes to the total dynamic structure function.

To this end, one can compute the sum rules corresponding to each of the four terms
in the r.h.s. of eq. (2.21) and divide them by the same moments of the total \( S(q, \omega) \)

\[
m_k^{(4A)}(q) = \frac{1}{m_k(q)} \sigma_4 x_4 m_k^{(4A)}(q)
\]

\[
m_k^{(3,3)}(q) = \frac{1}{m_k(q)} \sigma_3 x_3 m_k^{(3,3)}(q)
\]

\[
m_k^{(3,3)}(q) = \frac{1}{m_k(q)} \sigma_3 x_3 m_k^{(3,3)}(q)
\]

\[
m_k^{(3,4)}(q) = \frac{1}{m_k(q)} \sigma_{34} \sqrt{x_3 x_4} m_k^{(3,4)}(q)
\]

(2.131)

where

\[
m_k(q) = \sigma_4 x_4 m_k^{(4A)}(q) + \sigma_3 x_3 m_k^{(3,3)}(q) + \sigma_3 x_3 m_k^{(3,3)}(q) + \sigma_{34} \sqrt{x_3 x_4} m_k^{(3,4)}(q)
\]

(2.132)

Cases with \( k = 0 \) and \( k = 3 \) are shown in figure (2.8) for zero pressure and temperature. It is apparent that \( S^{(3,4)}(q, \omega) \) gives a small contribution to the sum rules for \( q \) greater than 3Å\(^{-1}\) approximately, while its contribution at lower \( q \)'s is similar to the contribution of the \(^3\)He terms. In particular and for \( q \)'s between 1Å\(^{-1}\) and 2Å\(^{-1}\), \( m_0^{(3,4)} \) is negative while \( m_1^{(3,4)} \) is zero and \( m_3^{(3,4)} \) is positive. This is important as it indicates that \( S^{(3,4)}(q, \omega) \) has to be included in the analysis of the low \( q \) experimental data.

Measurements of the dynamic structure factor in the mixture have been analyzed neglecting this term, as it was considered that it must remain small at low \(^3\)He concentrations [FGKSD00]. As a consequence, unexpected results like a \( m^* = 2.95 m_3 \) \(^3\)He effective mass were obtained, in contrast to the \( m^* = 2.3 m_3 \) value resulting from both measurements of thermodynamic properties and theoretical calculations. Moreover, the reported area under the particle–hole peak is \( f = 0.37 \) while in a free quasiparticles model this should equal 1.

The experimental measurements were performed on a 4.5% \(^3\)He concentration mixture for \( q \)'s laying between 1Å\(^{-1}\) and 1.8Å\(^{-1}\). In this range the response shows two well separated peaks, corresponding to particle–hole excitations at low energies and phonon–roton excitations at higher energies. A background of multi–particle excitations, distributed on a much more broadened peak located at higher energies, is also observed. Whereas the qualitative behavior of the response is well understood, the fact that the total strength at the particle–hole peak is largely reduced from what it would be expected in a Fermi quasiparticle model posses a severe problem in the analysis of the data.
2.5 Sum Rules of $S(q, \omega)$ in the $^3\text{He}–^4\text{He}$ mixture

However, theory and experiment can be brought to agreement if one considers the following model of the total dynamic structure function [BDMP93]. Assume that $S(q, \omega)$ is the sum of

i) A peak centered around $\omega_{p-h} = q^2/2m^*_3$, where $m^*_3$ is the effective mass of a $^3\text{He}$ quasiparticle. The peak is the sum of $S^{(3,3)}(q, \omega)$ and $S^{(3,4)}(q, \omega)$. The latter is negative and follows approximately the shape of the $^3\text{He}$ peak.

ii) A narrow peak at the energy $\omega_0(q)$ of the phonon–roton branch, corresponding almost entirely to $S^{(4,4)}(q, \omega)$.

iii) A band of multiparticle excitations above $\omega_0(q)$, corresponding to a broad distribution of strength coming mainly from $S^{(4,4)}(q, \omega)$ and partly from $S^{(3,3)}(q, \omega)$ and $S^{(3,4)}(q, \omega)$; the latter being positive and having the same broad distribution as the other two. In particular, they have the same mean energy and broadness and in fact their values can be estimated from the corresponding values obtained from the pure $^4\text{He}$ response at the same density

$$\left| \frac{m_1}{m_{1\,mp}} \right| = 30K \quad \text{and} \quad \sqrt{\left| \frac{m_3}{m_{1\,mp}} \right|} = 65K.$$  \hspace{1cm} (2.133)

Therefore, in this model $S^{(3,4)}(q, \omega)$ is zero at the phonon–roton peak, negative at the particle–hole peak and positive in the band of multiparticle excitations.

A qualitative sketch of the model is shown in figure (2.9). With these assumptions and with approximation (2.129), it is possible to estimate how much strength contribute $S^{(3,3)}(q, \omega)$ and $S^{(3,4)}(q, \omega)$ to the particle–hole peak.

To this end one first writes a $^3\text{He}$ normalized response as follows

$$\hat{S}_{p-h}(q, \omega) = S^{(3,3)}_{p-h}(q, \omega) + \frac{2\sigma_{34}\sqrt{x_3(1-x_3)}}{(\sigma_3 + \sigma_{3f})x_3} S^{(3,4)}(q, \omega)$$  \hspace{1cm} (2.134)

that is equal to the considered contribution of $S(q, \omega)$ divided by $(\sigma_3 + \sigma_{3f})x$ at the particle–hole peak. Defining

$$b = \frac{\sigma_{34}\sqrt{x_3(1-x_3)}}{(\sigma_3 + \sigma_{3f})}$$  \hspace{1cm} (2.135)

then eq. (2.134) and its corresponding sum rules read

$$\hat{S}_{p-h}(q, \omega) = S^{(3,3)}(q, \omega) + b S^{(3,4)}(q, \omega)$$  \hspace{1cm} (2.136)

and

$$\hat{m}_{k|p-h} = m^{(3,3)}(q) + b m^{(3,4)}(q).$$  \hspace{1cm} (2.137)
Figure 2.9: Qualitative picture of the dynamic structure function in the mixture and for $q$’s between $1\text{Å}^{-1}$ and $1.5\text{Å}^{-1}$. The solid line is the total $S(q, \omega)$, the dotted line is the contribution of $S^{(3,3)}(q, \omega)$ at the particle–hole peak, and the dashed line is the contribution of $S^{(3,4)}(q, \omega)$ in the same region.

The experimental data of ref. [FGKSD90] was taken at $T=0.07K$, $q=1.3\text{Å}^{-1}$ and $x_3=0.045$ so $k_F=0.22\text{Å}^{-1}$ and $b=3.62$ in this case. The sum rules of the measured response at the particle–hole peak were obtained fitting a temperature-dependent Lindhard function with the effective mass $m_3^*$ and the total strength $f$ as free parameters. The resulting fits, in nice agreement with the measured response, lead to the following moments

\[
\hat{m}_0|_{p-h} = f = 0.37 \tag{2.138}
\]
\[
\hat{m}_1|_{p-h} = f \left( \frac{m_3}{m_3^*} \right) \frac{q^2}{2m_3} = 1.7K \tag{2.139}
\]
\[
\hat{m}_3|_{p-h} = f \left( \frac{m_3}{m_3^*} \right)^3 \left[ \frac{q^2}{2m_3} \right] \left[ 1 + \frac{12k_F^2}{5q^2} \right] = 40K . \tag{2.140}
\]

while the exact sum rules computed from the mixture calculations result in the values

\[
m_0^{(4,4)} = 0.393 \quad m_1^{(4,4)} = 10.22K \quad m_3^{(4,4)} = 36900K^3
\]
\[
m_0^{(3,3)} = 0.984 \quad m_1^{(3,3)} = 13.56K \quad m_3^{(3,3)} = 20600K^3
\]
2.5 Sum Rules of $S(q, \omega)$ in the $^3\text{He} - ^4\text{He}$ mixture

$$m_{0,1}^{(3,3)} = 0.999 \quad m_{1,1}^{(3,3)} = 13.56K \quad m_{3,1}^{(3,3)} = 19300K^3$$

$$m_{0}^{(3,4)} = -0.134 \quad m_{1}^{(3,4)} = 0 \quad m_{3}^{(3,4)} = 3400K^3.$$  (2.141)

Comparing the last column to eq. (2.140), it is apparent that the third moments of the response are almost entirely exhausted by multiparticle excitations. As a consequence $m_3^{(3,4)} \sim m_3^{(3,4)}|_{mp}$ and thus

$$\sqrt{\frac{m_3^{(3,4)}}{m_1^{(3,4)}}}|_{mp} = 65K \sim \sqrt{\frac{m_3^{(3,4)}}{m_1^{(3,4)}}}|_{mp}$$  (2.142)

from where $m_1^{(3,4)}|_{mp} = 0.8K$. With it and eq. (2.133), the zero moment of the cross term is found to be $m_0^{(3,4)}|_{mp} = 0.027$.

The contribution of the sum rules of $S^{(3,4)}(q, \omega)$ at the particle hole peak can now be extracted from the exact sum rules reported in (2.141)

$$m_{0}^{(3,4)}|_{p-h} = m_{0}^{(3,4)} - m_{0}^{(3,4)}|_{mp} = -0.16$$

$$m_{1}^{(3,4)}|_{p-h} = m_{1}^{(3,4)} - m_{1}^{(3,4)}|_{mp} = -0.8K,$$  (2.143)

and the sum rules of $S^{(3,3)}(q, \omega)$ read, inverting relations (2.137)

$$m_{0}^{(3,3)}|_{p-h} = m_{0}|_{p-h} - b \quad m_{0}^{(3,4)}|_{p-h} = 0.37 + 0.16b = 0.95$$  (2.144)

$$m_{1}^{(3,3)}|_{p-h} = m_{1}|_{p-h} - b \quad m_{1}^{(3,4)}|_{p-h} = 1.7 + 0.8b = 4.6K.$$  (2.145)

Therefore, the zero moment is almost 1 while the first moment is reduced by a factor $m_3^*/m_3 \sim 3$ with respect to the total $f$ sum rule. Both results are consistent with the Fermi quasiparticle model. The possible error in the last quantities due to the uncertainties in the ratios reported in (2.133) is found to be of the order of 10%. The final outcome of the model is that the strength missing in the measured particle–hole peak can be associated with a negative cross term $S^{(3,4)}(q, \omega)$. 
General properties of the dynamic structure function