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LETTER TO THE EDITOR

The relation between the static structure factor and the ‘density–density’ response function in the long-wave limit

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Abstract. A relationship between the static structure factor and the ‘density–density’ response function in the long-wave limit is established for the case of arbitrary parameters of a system. The structure factor of the degenerate ideal Fermi gas is also examined.

Studying the static structure factors of disordered systems is of great importance in describing the properties of the latter for the following two reasons. First, the structure factors enter into most of the relations for thermodynamic functions and for kinetic coefficients of disordered systems. Second, they are directly measurable by scattering from a disordered system of neutrons, x-rays, and electrons (Pines 1963, Temperley *et al* 1968).

Besides, the development of a theory for the systems of strongly interacting particles involves poorly controllable approximations (because of the absence of any small parameters). In this case, the general relations (i.e. independent of interaction intensity) for the correlation functions of a system that, when satisfied, corroborate the self-consistency of the theory, become particularly important.

The present work establishes a relationship between the static structure factor and the ‘density–density’ response function in the long-wave limit for the case of an arbitrary system. The structure factor of the degenerate ideal Fermi gas is also examined.

The static structure factor $S(q)$

$$hS(q) = V^{-1} \langle \delta \hat{n}_q(0) \delta \hat{n}_{-q}(0) \rangle \quad (1)$$

is known (Lifshitz and Pitaevsky 1978) to be related to the retarded ‘density–density’ Green function

$$L^R(q, \omega) = -\frac{i}{\hbar V} \int_0^\infty dt \exp(i\omega t) \langle [\delta \hat{n}_q(t), \delta \hat{n}_{-q}(0)] \rangle \quad (2)$$

as

$$nS(q) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(q, \omega) \quad (3)$$

$$S(q, \omega) = -2\hbar(1 - \exp(-\hbar\omega/T))^{-1} \text{Im } L^R(q, \omega). \quad (4)$$

Here, $\langle \dots \rangle$ is the averaging with the equilibrium statistical Gibbs operator for an examined system, V is the volume of the system, T is the temperature of the system,

$$\delta \hat{n}_q = \int dr \delta \hat{n}(r) \exp(-iqr)$$

$\delta \hat{n}(r)$ is the fluctuation operator of the particle number density in a system characterised by the mean density n [\hat{a}, \hat{b}] = $\hat{a}\hat{b} - \hat{b}\hat{a}$, and

$$\hat{a}(t) = \exp(i\hat{H}t/\hbar)\hat{a}\exp(-i\hat{H}t/\hbar) \quad (5)$$

where \hat{H} is the Hamiltonian of the system. The relations (1) and (2) should hold in the thermodynamic limit, namely, $N \rightarrow \infty$, $V \rightarrow \infty$, and $n = N/V$, where N is the total mean number of particles in a system.

The importance of (3) and (4) ensues from the fact that the function $L^R(q, \omega)$ is directly related to the temperature Green function $L^T(q, i\Omega_n)$:

$$L^T(q, i\Omega_n) = \frac{1}{2} \int_{-1/T}^{1/T} d\tau \exp(i\Omega_n \tau) L^T(q, \tau) \quad (6)$$

$$L^T(q, \tau) = \begin{cases} -V^{-1} \langle \delta \hat{n}_q(\tau) \delta \hat{n}_{-q}(0) \rangle & \tau > 0 \\ -V^{-1} \langle \delta \hat{n}_{-q}(0) \delta \hat{n}_q(\tau) \rangle & \tau < 0 \end{cases} \quad (7)$$

which is to be calculated by the purposely designed diagram technique (Abrikosov *et al* 1962). In (6) and (7), $\Omega_n = 2\pi nT$, $n = 0, \pm 1, \dots$;

$$\hat{a}(\tau) = \exp[(\hat{H} - \mu\hat{N})\tau] \hat{a} \exp[-(\hat{H} - \mu\hat{N})\tau] \quad (8)$$

where \hat{N} is the operator of the total particle number and μ is the chemical potential. Using the spectral representation of the functions $L^R(q, \omega)$ and $L^T(q, i\Omega_n)$ (Abrikosov *et al* 1962), it can readily be verified that

$$L^R(q, 0) = L^T(q, 0). \quad (9)$$

(6) and (7) can be used to demonstrate (Abrikosov *et al* 1962) that

$$T \sum_{\Omega_n} L^T(q, i\Omega_n) = \hbar \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \cotanh\left(\frac{\hbar\omega}{2T}\right) \text{Im} L^R(q, \omega). \quad (10)$$

Considering that the dynamic structure factor $S(q, \omega)$ satisfies the relation (Lifshitz and Pitaevsky 1978)

$$S(q, -\omega) = \exp(-\hbar\omega/T) S(q, \omega) \quad (11)$$

we obtain from (4) and (10):

$$T \sum_{\Omega_n} L^T(q, i\Omega_n) = -nS(q). \quad (12)$$

As shown by Bobrov and Trigger (1988)

$$L^T(q, i\Omega_n) \sim q^2 \quad (13)$$

at $\Omega_n \neq 0$ and as $q \rightarrow 0$, whereas $L^T(q, i\Omega_n) \sim q^2/\Omega_n^2$ at $\Omega_n \rightarrow \infty$, so that the series

$$\sum_{\Omega_n \neq 0} L^T(q, i\Omega_n)$$

is convergent. Therefore,

$$nS(q \rightarrow 0) = -TL^T(q \rightarrow 0, 0) \quad (14)$$

or, if (9) is allowed for,

$$nS(q \rightarrow 0) = -TL^R(q \rightarrow 0, 0) \quad (15)$$

In the case of classical systems ($\hbar \rightarrow 0$), the stricter proposition

$$nS(q) = -TL^R(q, 0) \tag{16}$$

is valid. This follows from (3) and (4) and from the Kramers–Kronig relations (Zubarev 1971) for $L^R(q, \omega)$. It is expedient to note here that the obtained relation (15) is quite a general result.

From (15) it follows that the structure factor of temperature-degenerate systems has to be calculated carefully. Consider the example of the degenerate ideal Fermi gas of particles with spin $S = \frac{1}{2}$. If we assume that $T = 0$ when calculating $S(q)$ and $L^R(q, 0)$, then, as is well known (Pines and Noziers 1966)

$$S(q) = \begin{cases} 3q/4q_F - q^3/16q_F^3 & 0 \leq q \leq 2q_F \\ 1 & q > 2q_F \end{cases} \tag{17}$$

$$L^R(q \rightarrow 0, 0) = -3n/2\varepsilon_F \tag{18}$$

where $q_F = (3\pi^2n)^{1/3}$ is the Fermi wave factor, $\varepsilon_F = \hbar^2q_F^2/2m$ is the Fermi energy, and m is the particle mass. At $T = 0$, from (17) and (18) it follows that (16) is valid, but the question arises whether (17) for $S(q)$ is valid at $T \ll \varepsilon_F$, where $T \neq 0$.

In the case of non-interacting particles with spin $S = \frac{1}{2}$, we find from (1):

$$nS(q) = 2 \int \frac{d^3p}{(2\pi)^3} f_p(1 - f_{p+q}) \tag{19}$$

$$f_p = [1 + \exp((\varepsilon_p - \mu)/T)]^{-1} \tag{20}$$

where $\varepsilon_p = \hbar^2p^2/2m$. If we put $T = 0$ in (19) and (20), then

$$nS(q) = \int_{\substack{p < q_F \\ |p+q| > q_F}} \frac{d^3p}{(2\pi)^3} \tag{21}$$

whence the relation (17) ensues. Examine the behaviour of $S(q)$ (19) for small wave vectors q at $T \neq 0$

$$\begin{aligned} nS(q) &= 2 \int \frac{d^3p}{(2\pi)^3} \left(f_p(1 - f_p) - \frac{1}{2}f_p \frac{\partial^2 f_p}{\partial p_\alpha \partial p_\beta} q_\alpha q_\beta \right) + \overline{O}(q^2) \\ &= T \left(\frac{\partial n}{\partial \mu} \right)_T - \varepsilon_q \frac{\partial}{\partial \mu} \int \frac{d^3p}{(2\pi)^3} \left(\frac{\varepsilon_p}{T} \left(\frac{2}{3}f_p^2 - \frac{8}{15}f_p^3 \right) - f_p^2 \right)_T + \overline{O}(q^2). \end{aligned} \tag{22}$$

At $T \ll \varepsilon_F$, $\mu = \varepsilon_F$ and $f_p^m = f_p$ where $m = 1, 2, \dots$, so

$$\left(\partial n / \partial \mu \right)_T = 3n/2\varepsilon_F \tag{23}$$

$$S(q) = 3T/2\varepsilon_F + \varepsilon_q/6T + 3\varepsilon_q/4\varepsilon_F + \overline{O}(q^2). \tag{24}$$

Thus, the relation (16) for the ideal Fermi gas is satisfied rigorously at $0 < T \ll \varepsilon_F$, whereas the relation (17) for $S(q)$ appears to be invalid. The fact is that as well as the conventional dimensionless parameters T/ε_F and $\varepsilon_q/\varepsilon_F$ the parameter T/ε_q also appears in the calculation of $S(q)$.

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