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Local-field corrections of three-dimensional electron liquids

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Abstract. The static local-field corrections satisfying the compressibility, f-, and third moment sum rules exactly have been obtained for three-dimensional electron liquids. Our results also satisfy the non-negativity condition of the pair correlation function at origin, because they reproduce the static structure factors or the pair correlations obtained by the Fermi hypernetted chain method. An appropriate dynamic local-field correction has been introduced to satisfy the third moment sum rule exactly. We check the moment sum rules numerically for $q = 1.5q_F$, for example.

1. Introduction

The local-field correction $G(q)$ is the most important quantity in studying the static properties of electron liquids; it has been studied by many authors [1, 2]. However, a $G(q)$ which satisfies all the physical requirements including sum rules has not been found yet. The compressibility sum rule may be satisfied more easily than the frequency moment sum rules, except for the f-sum rule. One understands that the higher order frequency moment sum rules are satisfied when an appropriate dynamic local-field correction is given. The dynamic local-field correction may be defined in two different forms. One of them is derived as follows: the induced density fluctuation is written as [3]

$$\tilde{\rho}_q(\omega) = \tilde{\chi}^0(q,\omega)\{\Phi^{\text{ext}}(q,\omega) + v(q)[1 - \tilde{G}(q,\omega)]\tilde{\rho}_q(\omega)\} \tag{1}$$

where $\tilde{\rho}_q(\omega)$ is the Fourier component of the induced density fluctuation and $v(q)$ the Fourier transform of the Coulomb interaction. Niklasson [3] has shown that $\tilde{\chi}^0(q,\omega)$ is the modified Lindhard function, in which the Fermi distribution function is the exact one for the interacting system. Since the response function is defined by

$$\tilde{\rho}_q(\omega) = \chi(q,\omega)\Phi^{\text{ext}}(q,\omega) \tag{2}$$

the dynamic local-field correction $\tilde{G}(q,\omega)$ can be defined in terms of the response function by combining equations (1) and (2). It is

$$\chi(q,\omega) = \frac{\tilde{\chi}^0(q,\omega)}{1 - v(q)[1 - \tilde{G}(q,\omega)]\tilde{\chi}^0(q,\omega)}. \tag{3}$$

Equation (3) may be regarded as a definition of the dynamic local-field correction.

One may write the other definition, which is often used, as

$$\chi(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v(q)[1 - G(q,\omega)]\chi^0(q,\omega)} \tag{4}$$

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where $\chi^0(q,\omega)$ is the true non-interacting density response function (the Lindhard function). The superscript 0 means non-interacting in what follows. The definition (4) is usually taken for practical calculations because the Fermi distribution of the non-interacting system at $T = 0$ is simple and the latter fact makes calculations easy.

It is meaningful to discriminate $G(q,\omega)$ from $\tilde{G}(q,\omega)$ and obtain the former instead of the latter to use the definition (4) in studying the dynamic properties of many-electron systems. Since our purpose in this work is to obtain the static local-field correction $G(q)$ of equation (4), we only consider the static part of the dynamic local-field correction. A generally known behaviour of the static local-field correction $\tilde{G}(q)$ is that it increases quadratically at small q and approaches a constant as q approaches infinity. There may be a hump around $q = 2q_F$, q_F being the Fermi wave vector. The quadratically increasing behaviour at small q is guaranteed by the compressibility sum rule. On the other hand, the large-q limit, $\tilde{G}(\infty) = \frac{2}{3}[1 - g(0)]$, $g(0)$ being the pair correlation function at origin, has been given by Niklasson [3] and Vignale [4].

The explicit difference between the two local-field corrections can be obtained by equating equations (3) and (4). One may write the difference as

$$G(q) - \tilde{G}(q) = \frac{1}{v(q)}\left(\frac{1}{\chi^0(q)} - \frac{1}{\tilde{\chi}^0(q)}\right). \tag{5}$$

The right-hand side of equation (5) is proportional to q^4 for small q. Thus $\tilde{G}(q)$ and $G(q)$ have the same quadratic behaviour at small q, which may be constrained by the compressibility sum rule. However, a remarkable difference between $\tilde{G}(q)$ and $G(q)$ appears in the large-q regime. The large-q behaviour of $G(q)$ has been studied by Holas [5], and also by Lee and Hong [6]. They showed that $G(q)$ increases quadratically as q approaches infinity. The large-q expansion of equation (5) is

$$G(q) = \tfrac{2}{3}[1 - g(0)] + \frac{3\pi}{16\alpha r_s}(\tfrac{4}{3}\delta\langle K\rangle q^2 + \tfrac{16}{5}\delta\langle K^2\rangle - \tfrac{16}{9}\delta\langle K\rangle^2) + O(q^{-2}) \tag{6}$$

where $\alpha = (4/9\pi)^{1/3}$, $\delta\langle K\rangle = \langle\varepsilon_k\rangle - \langle\varepsilon_k\rangle^0$, $\delta\langle K^2\rangle = \langle\varepsilon_k^2\rangle - \langle\varepsilon_k^2\rangle^0$ and $\delta\langle K\rangle^2 = \langle\varepsilon_k\rangle^2 - (\langle\varepsilon_k\rangle^0)^2$, r_s is the average distance between electrons measured in units of Bohr radius. Here the angle brackets mean the average and ε_k is the kinetic energy per particle. Holas [5] has produced the same expansion as equation (6). As far as we know, there is no report on the study of the difference between $\tilde{G}(q)$ and $G(q)$. The purpose of this paper is to obtain the static part $G(q)$ of equation (4) instead of $\tilde{G}(q)$ of equation (3).

Since finding an exact $G(q,\omega)$ is a very difficult problem, there have been many attempts via the static approximation for $G(q,\omega)$, such as

$$\chi(q,\omega) = \frac{\chi^0(q,\omega)}{1 - v(q)[1 - G(q)]\chi^0(q,\omega)} \tag{7}$$

in studying the dynamic and the static properties of the electron liquids. Many forms of $G(q)$ have been presented in terms of equation (7) [1, 2, 7]. But it should be emphasized that only the first frequency moment sum rule (f-sum rule) is satisfied when equation (7) is used as a density response function.

There are two important points which must be checked for the $G(q)$ obtained by a particular theory. One is to check the sum rules and the other is the non-negativity condition for the pair-correlation function $g(r)$ at origin. No existing $G(q)$s satisfy these

requirements simultaneously to our knowledge. Iwamoto, Krotscheck and Pines (IKP) [7] and Neilson, Świerkowski, Sjölander and Szymański (NSSS) [8] have obtained $G(q)$ in terms of equation (7) for three and two dimensions, respectively. Their results satisfy the f-sum rule, the compressibility sum rule and the condition $g(0) \geqslant 0$ for any density simultaneously, but do not satisfy the third moment sum rule. The condition $g(0) \geqslant 0$ has been guaranteed by using the numerical data of the structure factor in their method. The compressibility sum rule can be satisfied by using a constraint [1, 9] which is expressed by the correlation energy whose precise values may be given by the Monte Carlo calculation [10]. However, to satisfy the third moment sum rule one needs an appropriate dynamic local-field correction. Of course, there are higher order frequency moments in principle. But the exact fifth and higher moments have not been obtained for the quantum system. Therefore, the third moment is the highest available moment one can use to check the frequency moment sum rule for the time being.

This paper is comprised as follows. We briefly introduce formal theory to obtain the dynamic local-field correction satisfying the third moment sum rule, and explain the method of this work in §2. In §3, we show our results for the static local-field corrections and make a comparison with others. We also give some discussions in this section.

2. Methods

Our object, in this work, is to find $G(q)$ satisfying the condition $g(0) \geqslant 0$, and satisfying the compressibility, f-, and third moment sum rules simultaneously. As we mentioned earlier, the first two may be satisfied through the method of IKP or NSSS by using the numerical data for the structure factor. But to satisfy the third moment sum rule, one needs an appropriate form of $G(q, \omega)$. Some years ago, Hong and Lee [11] presented a systematic approximation method to obtain the density response function satisfying the higher order moment sum rules exactly as the order of the approximation increases. The formalism has been reviewed recently by Hong and Kim [12] and has also appeared in other papers [6, 13]. Therefore, we do not need to repeat it here.

However, we show briefly how a $G(q, \omega)$ satisfying the third moment sum rule exactly is constructed. A numerical test is also given later in this work. The density response function (4), may be related to the relaxation function $\Xi(z)$ by [14]

$$\chi(q, z)/\chi(q) = 1 - z\Xi(z)|_{z=-i\omega+0^+} \tag{8}$$

where $\Xi(z)$ is represented by a continued fraction [15]:

$$\Xi(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{\ddots}}}. \tag{9}$$

In equation (9), $\Delta_1 = (\dot{\rho}_q, \dot{\rho}_q)/(\rho_q, \rho_q)$ and $\Delta_2 = (\ddot{\rho}_q, \ddot{\rho}_q)/(\dot{\rho}_q, \dot{\rho}_q) - \Delta_1$. The continued fraction can be expanded [16] as

$$\Xi(z) = \frac{1}{z} - \frac{\Delta_1}{z^3} + \frac{\Delta_1(\Delta_1 + \Delta_2)}{z^5} - \frac{\Delta_1[(\Delta_1 + \Delta_2)^2 + \Delta_2\Delta_3]}{z^7} + \cdots \tag{10}$$

where the inner product written above is the Kubo scalar product [17], and $(\rho_q, \rho_q) = -\chi(q)$. One can identify each frequency moment as

$$\langle\omega^1\rangle = -\Delta_1\chi(q) = (\dot{\rho}_q, \dot{\rho}_q) \tag{11}$$

$$\langle\omega^3\rangle = -\Delta_1(\Delta_1 + \Delta_2)\chi(q) = (\ddot{\rho}_q, \ddot{\rho}_q) \tag{12}$$

and so on by substituting equation (10) into equation (8).

Let us replace Δ_ν by Δ_ν^0 for $\nu \geqslant 2$ in equation (9) or (10); then the response function (8) satisfies the f-sum rule exactly and the higher moment sum rules approximately. We call this the first-order approximation in this paper. In a similar way, if we replace Δ_ν by Δ_ν^0 for $\nu \geqslant 3$, the response function satisfies the f- and the third moment sum rules exactly and the rest approximately. This is called the second-order approximation. According to this method, the dynamic local-field corrections corresponding to each approximation are as follows:

$$G^{(1)}(q,\omega) = G(q) \tag{13}$$

$$G^{(2)}(q,\omega) = G(q) + \eta_2 Q(q,\omega)/v(q)\chi^0(q) \tag{14}$$

$$\vdots$$

where $\eta_2 = \Delta_2/\Delta_2^0 - 1$ and $Q(q,\omega) = \chi^0(q)/\chi^0(q,\omega) + \omega^2/\Delta_1^0 - 1$. On the other hand, it is well known that for electron liquids the first and the third moments [18] are given by

$$\langle\omega^1\rangle = \frac{nq^2}{m} \tag{15}$$

$$\langle\omega^3\rangle = \frac{nq^2}{m}\left(\frac{q^4}{4m^2} + \frac{2q^2}{m}\langle\epsilon_k\rangle + \omega_p^2[1 - I(q)]\right) \tag{16}$$

where $\omega_p^2 = 4\pi ne^2/m$ and

$$I(q) = N^{-1}\sum_{k\neq 0,q}\left(\frac{(\boldsymbol{q}\cdot\boldsymbol{k})^2}{q^2k^2}\right)[S(\boldsymbol{k}) - S(\boldsymbol{k}-\boldsymbol{q})] \tag{17}$$

where N is the number of particles. We set $\hbar = 1$ in this work. This expression can be transformed to an integral form [12]. By using equations (11), (12), (15), (16), and the definition of η_2, we obtain the following relation for $\eta_2(q)$:

$$\eta_2(q) = \frac{\omega_p^2}{\Delta_2^0}\left(G(q) - I(q) + \frac{2q^2}{m\omega_p^2}(\langle\epsilon_k\rangle - \langle\epsilon_k\rangle^0)\right). \tag{18}$$

It is important to note that, since $\eta_2 \neq 0$, equation (18) is just a corrected version of equation (3.10) in IKP [7]. We will present the form of $\eta_2(q)$ later in this paper.

Now we are in a situation to perform our object of finding the static part $G(q)$ given in equation (14). To do this, we separate the structure factor into two parts, i.e. one given by the continuum excitations which range from $\omega = 0$ to $\omega = (2q + q^2)/2m$ and the other given by the plasmon excitation at $\omega = \omega_p(q)$. The formula is well known [19] and is

$$S(q) = -\frac{3q^2}{8\alpha r_s}\int_0^{q^2+2q}\mathrm{Im}\varepsilon^{-1}(q,\omega)\,\mathrm{d}\omega + \frac{3\pi q^2}{8\alpha r_s}\left(\frac{\partial \mathrm{Re}\varepsilon(q,\omega)}{\partial\omega}\right)^{-1}_{\omega=\omega_p(q)} \tag{19}$$

where the dielectric function

$$\varepsilon(q,\omega)^{-1} = 1 + (4\pi e^2/q^2)\chi(q,\omega) \tag{20}$$

and $\omega_p(q)$ is the plasmon energy at wave vector q. In equation (19), we express ω and q in units of Fermi energy and Fermi momentum, respectively. $G(q)$ is included in $\varepsilon(q,\omega)$ through equations (14) and (20).

In equation (19), all quantities are known except $S(q)$, $\langle\epsilon_k\rangle$ in η_2 and $G(q)$. Therefore, once the first two are given, $G(q)$ may be obtained. We use numerical data for $S(q)$ provided by Krotscheck [20] and for $\langle\epsilon_k\rangle$ by Monte Carlo calculation [10] to find $G(q)$ via equation (19). The structure factors given by Krotscheck are shown in figure 1 for several densities. The function $I(q)$, equation (17), has also been drawn in figure 2 by using the structures of figure 1. Very accurate numerical calculations have been performed in differentiation, integration and finding zeros of $\varepsilon(q,\omega)$. Our $G(q)$ gives rise to the $S(q)$ of the left-hand side of equation (19), as given by Krotscheck. Therefore, our $G(q)$ yields non-negative $g(r)$.

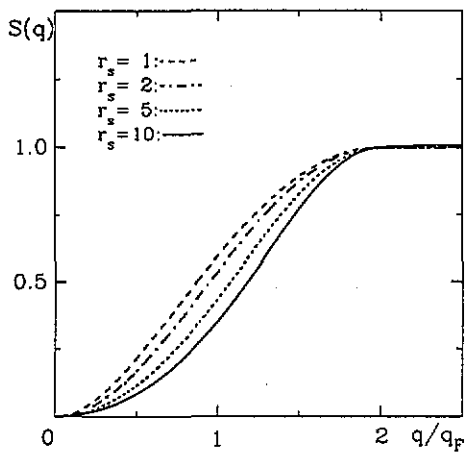

Figure 1. The structure factors obtained by Krotscheck [20] using the Fermi hypernetted chain method.

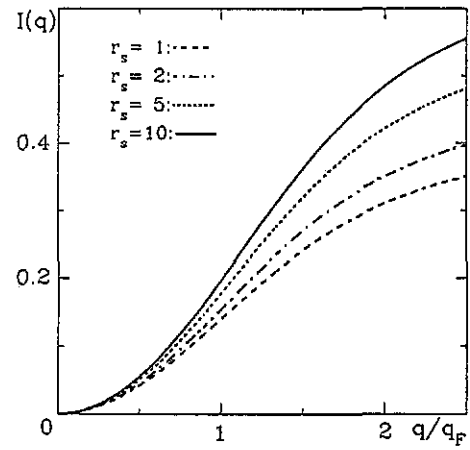

Figure 2. The forms of $I(q)$ obtained by using the data of figure 1.

We meet some difficulties for small q ($q < 0.5q_F$) because the numerical data for $S(q)$ do not satisfy the compressibility sum rule. This difficulty is remedied by using the constraint [1, 9] imposed by the compressibility sum rule which gives the correct quadratic line of $G(q)$ for small q. The smooth connection between the quadratically increasing line starting from $q = 0$ and the line obtained by equation (19) is achieved by using $\eta_2(q)$. The method used by NSSS for two dimensions is the same as ours when $\eta_2 = 0$.

3. Results and discussion

We obtain $\eta_2(q)$ in the course of finding $G(q)$ from equation (19). This function is crucial in both the smooth connection of $G(q)$ and to satisfy the third moment. We plot $\eta_2(q)$ in figure 3 for $r_s = 2$, 5 and 10. Here we discuss η_2 a little more. An exact analytic study of η_2 has been given by Hong *et al* [13] for a classical one-component plasma in two dimensions at $\Gamma = 2$, $\Gamma = e^2/(k_B T)$. The latter is the only case where the structure factor is known analytically [21]. In addition, for the classical one-component plasma $G(q)$ is simply related to the structure factor and $\langle\varepsilon_k\rangle = \langle\varepsilon_k\rangle^0$. The form of the exact η_2 is quite

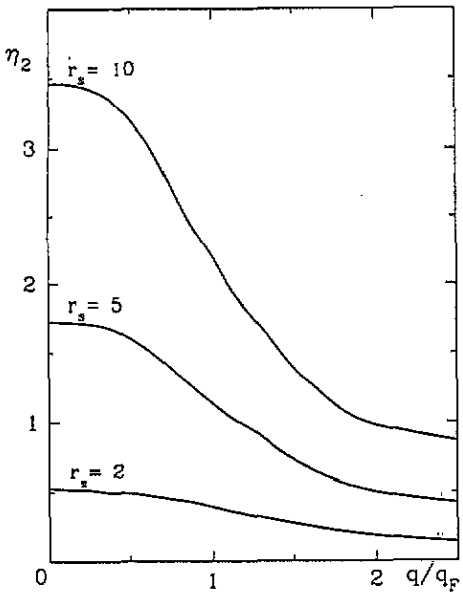

Figure 3. $\eta_2(q)$ for $r_s = 2$, 5 and 10.

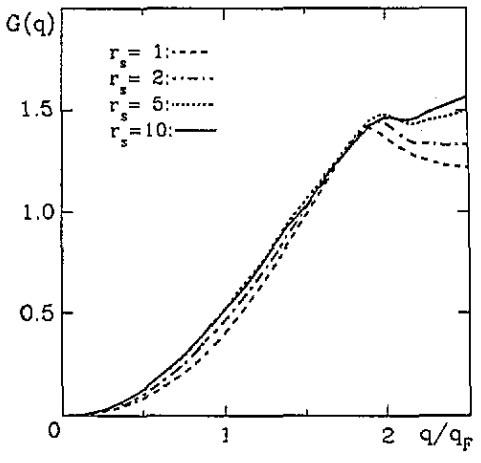

Figure 4. $G(q)$ of equation (14) for $r_s = 1$, 2, 5 and 10.

similar to those plotted in figure 3. In figure 4, we plot our second-order (equation (14)) results for the same densities as in figure 1.

A remarkable change with density is seen for $q \geqslant 2$, where $G(q)$ increases rapidly as density decreases. In figure 5, we finally plot our first- and second-order results and also those given by Utsumi and Ichimaru (UI) [22] for comparison. Our first-order result is practically the same as that of IKP [7], because our method is similar to theirs even though their results are obtained by using a self-consistent iteration. It is also interesting to note that the $G(q)$ of UI is very close to our first-order result. This fact suggests that UI's results are quite good as a static approximation.

We check the third moment sum rule for the densities of figure 1 by comparing equation (16) with

$$\langle\omega^3\rangle = -\frac{1}{\pi}\int_{-\infty}^{\infty}\omega^3 \mathrm{Im}\chi(q,\omega)\,\mathrm{d}\omega. \tag{21}$$

In table 1, we show the results of checking the third moment sum rule at $q = 1.5q_F$, for instance. One can see that only the second-order result satisfies the third moment sum rule exactly. As density decreases, the response function using the static approximation for $G(q,\omega)$ satisfies the third moment sum rule worse and worse. This is expected, since the region of validity of the static approximation (13) is a high-density regime, as for the random phase approximation. We have also checked the f-sum rule. It is satisfied exactly for all cases.

We now make some final remarks on our results. Since the numerical data [20] for $S(q)$ are restricted up to $q = 2.5$, one cannot see the quadratically increasing behaviour at large q mentioned above. However, it may be seen from this analysis if Kimball's large-q behaviour for $S(q)$ is used for very large q [23]. An interesting fact for our result is that the values of $G(q)$ in figure 4 are usually larger than other results [1, 2, 7]. The values around

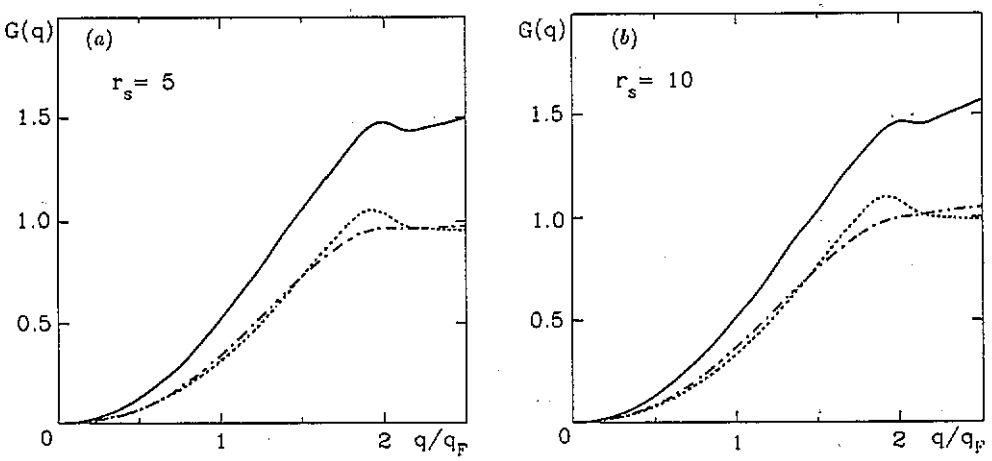

Figure 5. The local-field corrections of Eqs. (13) (chain curve) and (14) (full curve) for $r_s = 5$ and 10. The dotted curves are the cases of UI [22].

Table 1. Values of the third moment: $\langle\omega^3\rangle$ obtained from equation (16) and the first-order, UI and second-order results from equation (21) at $q = 1.5q_F$, respectively.

r_s	$\langle\omega^3\rangle$	First order	%	UI	%	Second order	%
1	25.4889	24.1451	94.73	24.2004	94.95	25.4887	100.00
2	27.5537	24.7058	89.66	24.7718	89.90	27.5534	100.00
5	33.8617	26.2345	77.48	26.2315	77.47	33.8606	100.00
10	43.7609	28.4945	65.11	28.2079	64.46	43.7598	100.00

peak are larger than unity even for high density ($r_s = 1$), and the peak becomes more of a shoulder as density is lowered. This reflects the fact that $G(q)$ must be distinguished from $\tilde{G}(q)$. It may also be interesting to compare our results with results obtained by Holas *et al* [24] and Brosens *et al* [25], whose $G(q)$ are the static parts of their $G(q, \omega)$, as ours are. As far as we know, the latter results do not satisfy the requirements mentioned above simultaneously.

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References

[1] Ichimaru S 1982 *Rev. Mod. Phys.* **54** 1017
[2] Singwi K S, Tosi M P, Land R H and Sjölander A 1968 *Phys. Rev.* **176** 589

Vashishta P and Singwi K S 1972 *Phys. Rev.* B **6** 875
Hubbard J 1957 *Proc. R. Soc.* A **243** 336
Toigo F and Woodruff T O 1970 *Phys. Rev.* B **2** 3958
[3] Niklasson G 1974 *Phys. Rev.* B **10** 3052
[4] Vignale G 1988 *Phys. Rev.* B **38** 6445
[5] Holas A 1987 *Strongly Coupled Plasma Physics* ed F J Rogers and H E Dewitt (New York: Plenum)
[6] Lee M H and Hong J 1989 *J. Phys.: Condens. Matter* **1** 3876
[7] Iwamoto N, Krotscheck E and Pines D 1984 *Phys. Rev.* B **29** 3936
[8] Neilson D, Świerkowski L, Sjölander A and Szymański J 1991 *Phys. Rev.* B **44** 6291
[9] Iwamoto N 1984 *Phys. Rev.* A **30** 3289
[10] Ceperley D M and Alder B J 1980 *Phys. Rev. Lett.* **45** 566
Vosko S H, Wilk L and Nusair M 1980 *Can. J. Phys.* **58** 1200
[11] Hong J and Lee M H 1985 *Phys. Rev. Lett.* **55** 2375
[12] Hong J and Kim C 1991 *Phys. Rev.* A **43** 1965
[13] Hong J, Park J and Lee M H 1989 *Phys. Rev.* B **40** 1528
[14] Jindal V K, Singh H B and Pathak K N 1977 *Phys. Rev.* B **15** 252 and also see [11]
[15] Lee M H 1983 *J. Math. Phys.* **24** 2512
Mori H 1965 *Prog. Theor. Phys.* **34** 399
[16] Dupuis M 1967 *Prog. Theor. Phys.* **37** 502
[17] Kubo R 1957 *J. Phys. Soc. Jpn.* **12** 570 and also see Lee M H 1983 *J. Math. Phys.* **24** 2512
[18] Puff R D 1965 *Phys. Rev.* **137** A406
Pathak K N and Vashishta P 1973 *Phys. Rev.* B **7** 3649
[19] Pines D and Nozières P 1966 *Theory of Quantum Liquids* (New York: Benjamin) p 212
[20] Krotscheck E Fermi hypernetted chain data for $S(q)$ via private communication
[21] Jancovici B 1981 *Phys. Rev. Lett.* **46** 389
[22] Utsumi K and Ichimaru S 1980 *Phys. Rev.* B **22** 4912
[23] Kimball J C 1973 *Phys. Rev.* A **7** 1648
[24] Holas A, Aravind P K and Singwi K S 1979 *Phys. Rev.* B **20** 4912
[25] Brosens F, Devreese J T and Lemens L F 1980 Phys. Rev. B **21** 1363