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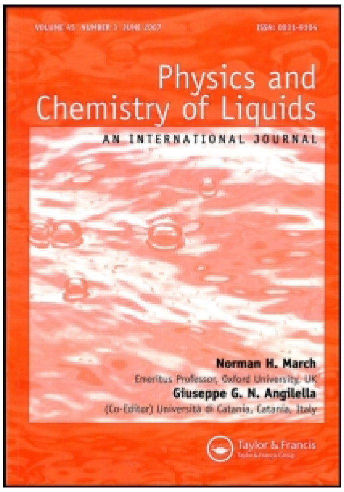

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Letter

FIRST-ORDER DENSITY MATRIX, PAIR-DISTRIBUTION FUNCTION AND STRUCTURE FACTOR OF A FERMI LIQUID

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Where overlap exists, results of the free Fermi gas in D dimensions agree between the studies of Lee and Long [*Phys. Rev., E*, **52**, 189 (1995)] and our own previous works. We add some results of the effect of intractions in the three-dimensional electron liquid phase relating to the first-order density matrix, the electron-pair function, and the structure factor.

Keywords: Fermi liquid; density matrix; structure factor; pair distribution.

Lee and Long [1] have discussed the free Fermi gas in D dimensions, an area we have also worked on [2, 3]. In regions of overlap, the findings are in accord for (i) the first-order density matrix, (ii) the structure factor and hence (iii) the electron-pair function – the Fourier transform of (ii).

Here we want to add some comments on the interacting uniform electron liquid, where the $D = 3$ case has been studied by us [4–8] as well as by other workers [9, 10]. Denoting the free Fermi gas results of (i)–(iii) above by $\gamma_0(|\mathbf{r} - \mathbf{r}'|)$, $S_0(q)$ and $g_0(r)$, the interacting cases will be denoted by omitting the subscript zero. The $D = 3$ form of γ_0 referred to in [5, 3] and [1], with $\mathbf{R} = \mathbf{r} - \mathbf{r}'$:

$$\gamma_0(R) = \rho \frac{3[\sin(k_F R) - (k_F R)\cos(k_F R)]}{(k_F R)^3} \tag{1}$$

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is replaced [5] in the interacting case by

$$\gamma(\mathbf{r};\mathbf{r}') \equiv \gamma(R) = \frac{2}{\Omega}\sum_{\mathbf{k}} n(k)\, e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')}$$

$$= \frac{1}{\pi^2 R}\int_0^{\infty} dk\, n(k) k \, \sin(kR), \tag{2}$$

where Ω is the volume of the normalization box for N electrons, ρ is the electron density $\rho = N/\Omega = (\frac{4}{3}\pi a_B^3 r_s^3)^{-1}$, the Fermi momentum k_F in terms of density is $k_F = (3\pi^2\rho)^{1/3}$, and a_B denotes the Bohr radius $a_B = \hbar^2/(me^2)$. The function $n(k)$ is the natural orbital occupation number, $0 \leqslant n(k) \leqslant 1$. Such a compact form (2) of the exact density matrix follows from the fact that plane waves are natural orbitals not only for the noninteracting uniform electron system, but also for the interacting case in the electron liquid paramagnetic phase.

In order to find the physical interpretation of $n(k)$ let us recall the relation between the one-particle density matrix in position space, $\gamma(\mathbf{r};\mathbf{r}')$, and that in momentum space, $\Gamma(\mathbf{p};\mathbf{p}')$, namely [11] (a version for the case of a finite normalization volume):

$$\Gamma(\mathbf{p};\mathbf{p}') = \frac{1}{\Omega}\int_{\Omega} d^3r \int_{\Omega} d^3r'\, e^{-i(\mathbf{r}\mathbf{p}-\mathbf{r}'\mathbf{p}')}\gamma(\mathbf{r};\mathbf{r}'). \tag{3}$$

After inserting the first form of $\gamma(\mathbf{r};\mathbf{r}')$ in Eqn. (2) we obtain from Eqn. (3)

$$\Gamma(\mathbf{p};\mathbf{p}') = 2n(p)\delta_{\mathbf{p},\mathbf{p}'} \tag{4}$$

(factor 2 reflects equal occupancy of spin-up and spin-down subsystems). From Eqn. (4) taken on the diagonal it turns out that $n(p)$ is equivalent to the momentum distribution function of the interacting electron liquid.

It should be mentioned that $\gamma(R)$ in Eqn. (2) can be written in terms of the function $A_I(r)$, inverstigated and discussed in [8], in connection with a similar problem of the reference response function (see also [7]). This relation reads

$$\gamma(R) = \frac{1}{\pi^2 R} A_I(R/2). \tag{5}$$

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While the noninteracting density matrix (1) can be expanded around the diagonal as a Taylor series in powers of R^2:

$$\gamma_0(R) = \rho\left[1 - \frac{(\hbar k_F)^2}{10m} R^2 + \frac{(\hbar k_F)^4}{280m^2} R^4 + O(R^6)\right], \tag{6}$$

the expansion of the interaction counterpart [5] is of asymptotic character:

$$\gamma(R) = \rho[1 + t_2(r_s)R^2 + t_4(r_s)R^4 + t_5(r_s)R^5 + \ldots]. \tag{7}$$

The small-R properties of $\gamma(R)$ are determined by the behavior of $n(k)$ at large k, which is known from the work of Kimball [12] to be

$$n(k) = \frac{8\rho^2 g(0, r_s)}{a_B^2} \frac{1}{k^8} + \text{higher order terms}, \tag{8}$$

where $g(r, r_s)$ is the pair-correlation function at interelectronic separation r.

The coefficients t_i shown in Eqn. (7) can be calculated directly by means of differentiation of $R\gamma(R)$ (or $A_l(R/2)$, [8]) to obtain

$$t_2 = -\frac{1}{3}\frac{m}{\hbar^2}\langle T\rangle, \tag{9}$$

$$t_4 = \frac{1}{30}\left(\frac{m}{\hbar^2}\right)^2 \langle T^2\rangle, \tag{10}$$

$$t_5 = -\frac{1}{180\pi}\frac{\rho}{a_B^2} g(0, r_s). \tag{11}$$

The value of t_5 obtained by the methods of [8] confirmed the earlier result [5]. Existence (or not) of higher order non-analytic terms in the asymptotic expansion (7) depends on analytic properties of $n(k)$ beyond the terms shown explicity in Eqn. (8). The averaged 1-st and 2-nd power of the kinetic energy T per particle, occurring in Eqns. (9) and (10) is given [8] by

$$\langle T^l\rangle = \frac{\int d^3p\, n(p)\left(\frac{(\hbar p)^2}{2m}\right)^l}{\int d^3p\, n(p)}. \tag{12}$$

In connection with t_5 in Eqn. (11) proportional to $g(0, r_s)$ it is relevant to comment that Lee and Long [1] write "for the non-ideal Fermi gas, $g(r=0)$ and $g'(r=0)$ are believed to be a strong function of r_s". Two points are to be made in the above context. The first is that the electron-electron cusp condition, the analogue in jellium of Kato's theorem for the electron-nuclear cusp in atoms reads, according to Kimball [12];

$$\left(\frac{\partial g(r, r_s)}{\partial r}\right)\bigg|_{r=0} = \frac{g(0, r_s)}{a_B}, \tag{13}$$

Furthermore, very recently, Overhauser [13] has given a valuable approximate analytic form he has fitted for $g(0, r_s)$, namely

$$g(0, r_s) = \frac{32}{(8 + 3r_s)^2} \tag{14}$$

for $D = 3$ jellium, which evidently tends to the free Fermi gas value of $\frac{1}{2}$ as r_s tends to zero.

As shown earlier[5] and as Eqn. (9) demonstrates, $t_2(r_s)$ is proportional to the averaged kinetic energy per particle $\langle T \rangle$. Using the virial theorem [4, 9] the result of Gell-Mann and Brueckner [14] for the correlation energy allows the small-r_s form of $\langle T \rangle$ to be established, a $\ln r_s$ term entering its expansion [4, 5].

The asymptotic large-r expansion of $A_l(r)$, obtained also in [8], leads immediately to such an expansion of $\gamma(R)$ in Eqn. (5). While details can be readily found in [8], we summarize them by indicating that the leading term of $\gamma(R)$ is $\propto \cos(k_F R)/R^2$, similar to that in (1), but with the coefficient reduced by the electron-electron interaction, since it is given by the discontinuity Z_F in $n(k)$ at k_F, which satisfies $Z_F < 1$ for $r_s > 0$. Besides oscillatory terms, the large-R expansion may contain non-oscillatory components, the lowest being $\propto R^{-4}$, with a coefficient determined by the linear term in k of $n(k)$ expanded around $k = 0$.

Finally we shall comment on the effect of interactions on the long-wave behavior of the electron liquid structure factor $S(q)$ and also on the (partially) related problem of the long-distance behavior of the pair function $g(r)$. As discussed for $D = 3$ in [10, 2] and [1], $S_0(q) \propto q$ at small q and this linear term is removed by the electron-electron interactions, a term $\propto q^2$ being introduced thereby with a coefficient involving the zero-point energy of the plasmons $\frac{1}{2}\hbar\omega_p$. However, Pines and Nozières [10], see also Holas and March [6], propose that, in addition, the interaction removes from

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$S_0(q)$ also the term $\propto q^3$, the first 'nonanalyticity' at the origin of the wavenumber q space appearing in $S(q)$ at $O(q^5)$. In turn, by Fourier transform, such a contribution leads [6] to a (non-oscillatory-see below) decay term in $\{g(r)-1\}$ proportional to r^{-8} at large r. But the point $q=2k_F$, i.e. the diameter of the Fermi sphere, remains non-analytic in the presence of electron-electron interactions, with a long-range contribution to $\{g(r)-1\}$ of the form $\propto \cos(2k_Fr)/r^4$. This is then the dominant non-analyticity in $S(q)$ as regards the long-range behavior of $\{g(r)-1\}$, whereas in $S_0(q)$ both non-analytic points at $q=0$ and at $2k_F$ contribute terms of the range r^{-4}, the latter times, of course, an oscillatory factor $\cos(2k_Fr)$. In this latter term, only the coefficient is affected by switching on the electron-electron interactions, its amplitude being thereby reduced from the free Fermi gas form.

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