# Structure Factor of the Electron Liquid from the Moment Sum Rules*

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The structure factor of the electron liquid at metallic densities is calculated from a nonlinear integral equation, derived earlier by Kuglar, using the low-order frequency-moment sum rules of the spectral function of the density response function. The results for the structure factor and the pair-correlation function are compared with those of Vashishta and Singwi.

Using some rigorous inequalities and sum rules obeyed by the spectral function of the density response function, Mihara and Puff[1] obtained a nonlinear integral equation for the static structure factor of interacting bosons. They applied this equation with considerable success to the calculation of some ground-state properties of liquid $He^4$. Based on that work, Kugler[2] derived (but did not solve) the following integral equation for the static structure factor $S(k)$ of the electron liquid in the ground state:

$$\left(\frac{\omega_0(k)}{S(k)}\right)^2 = \left(\frac{\omega_0(k)}{S_0(k)}\right)^2 + \omega_p^2 + G_3(k) \,, \tag{1}$$

where

$$S_0(k) = \begin{cases} \frac{3}{4}k/k_F - \frac{1}{16}k^3/k_F^3 \,, & 0 \le k \le 2k_F \\ 1 \,, & 2k_F \le k \,, \end{cases} \tag{2}$$

is the static structure factor of the noninteracting fermions in the ground state; $\omega_0(k) = \hbar k^2/2m$ is the free-particle excitation spectrum; $\omega_p = (4\pi n e^2/m)^{1/2}$ is the plasma frequency; $n$ is the uniform electron density; and

$$G_3(k) = \frac{e^2}{m\pi}\int_0^\infty dq\, q^2[S(q)-1] \times\left[\frac{5}{6} - \frac{q^2}{2k^2} + \frac{k}{4q}\left(\frac{q^2}{k^2}-1\right)^2 \ln\left|\frac{q+k}{q-k}\right|\right] , \tag{3}$$

is the potential contribution to the third frequency moment[2,3] of the spectral function of the density response function. In this note we present the self-consistent solution of the integral equation for the static structure factor and thus obtain the pair correlation function of an electron liquid at metallic densities and compare it with the best available results of Vashishta and Singwi[4] (VS).

The important features of this integral equation

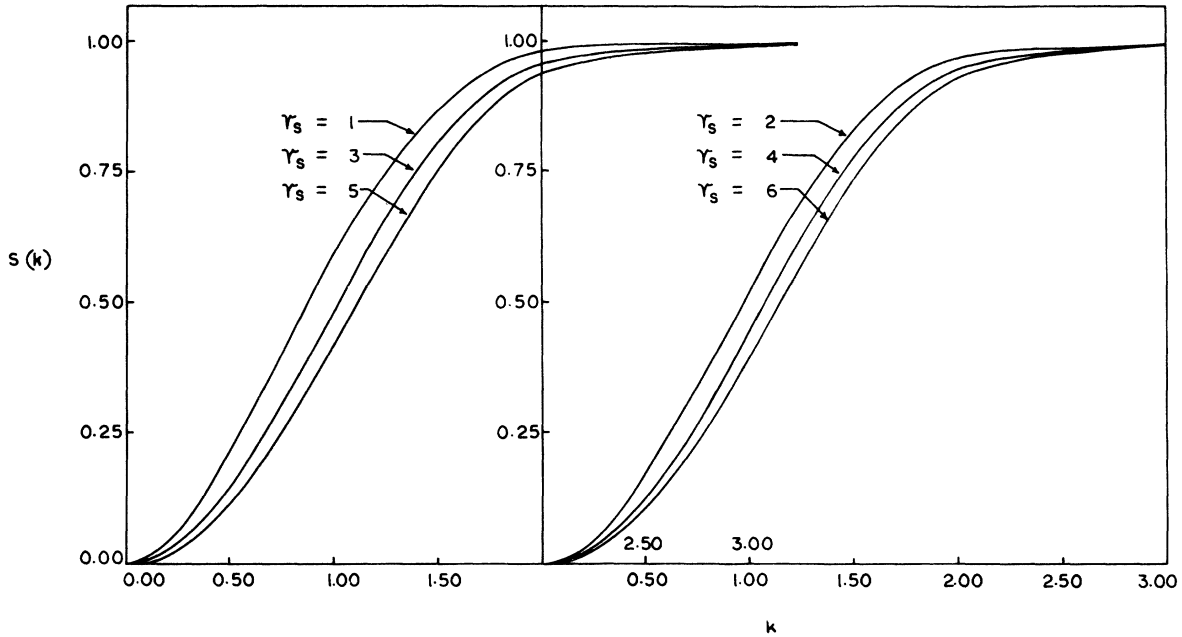


FIG. 1. Self-consistent values of the ground-state static structure factors $S(k)$ of the electron liquid vs $k$ for $r_s = 1-6$. Here $k$ is measured in units of $k_F$.

are that it is consistent with the moment sum rules and leads to the exact result for $S(k)$ in the long-wavelength limit (i.e., $k \to 0$). On the other hand, in the limit of large $k$ it is easy to see that

$$G_3(k) = \tfrac{2}{3}\omega_p^2[g(0) - 1] , \tag{4}$$

where $g(0)$ is the pair correlation function evaluated at the origin. We thus obtain from Eq. (1), in the limit of very large $k$, the result

$$S(k) - 1 = a/k^4 , \tag{5}$$

where $k$ is measured in the units of $k_F$ and

$$a = -0.1474 r_s[1 + 2g(0)] , \tag{6}$$

where $r_s$ is the electron-density parameter. This asymptotic form of $S(k)$ seems to be an interesting result obtained from the integral equation.

In order to solve Eq. (1) numerically, it is convenient to write it in the dimensionless form:

$$S^2(k) = \frac{Ck^4}{1 + Ck^4/S_0^2(k) + G_3(k)} , \tag{7}$$

where

$$C = \frac{3\pi}{16}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s} \tag{8}$$

and

$$G_3(k) = \frac{3}{4}\int_0^\infty dq\, q^2[S(q) - 1] \times\left[\frac{5}{6} - \frac{q^2}{2k^2} + \frac{k}{4q}\left(\frac{q^2}{k^2} - 1\right)^2 \ln\left|\frac{q+k}{q-k}\right|\right] . \tag{9}$$

It is evident from Eq. (7) that $S(k)$ is a function of $G_3(k)$, but according to Eq. (9), $G_3(k)$ itself is a functional of the structure factor. Thus $S(k)$ and $G_3(k)$ can be determined self-consistently from these equations. We have solved them self-consistently for the entire metallic-density range. After five iterations, our $G_3(k)$ was consistent within 0.1% for small $r_s$ and within 0.5% for large $r_s$ values. This results in higher consistency in $S(k)$.

The self-consistent values of the structure factor obtained above are plotted in Fig. 1, for $r_s = 1$–6. Our $S(k)$ are almost the same as those of VS upto at least two significant figures, for $r_s = 1$ and

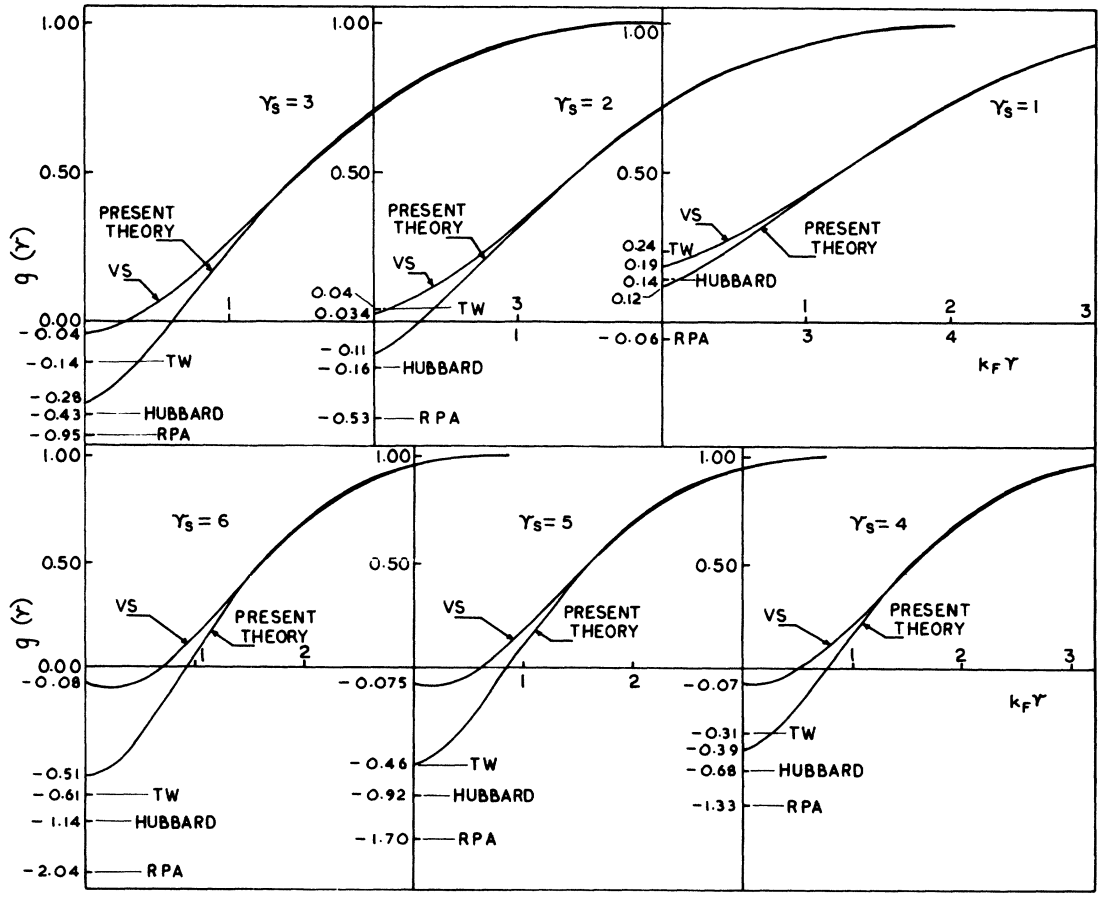


FIG. 2. Pair correlation function $g(r)$ versus $k_F r$ for $r_s = 1$–6. Values of $g(0)$ in some other theories are also marked. Note that the values of $g(0)$ marked from the theory of Hubbard and the RPA are not according to the scale.

2. For $3 \leq r_s \leq 6$, our $S(k)$ values are lower by about 1–3% from those of VS in the range $1 < k < 3$ and, in the rest of the region, both the values agree up to at least two significant figures. Thus the differences are so small that the two curves cannot be distinguished within the accuracy of the graph paper used. However, as seen below, the small differences in the structure factors, especially for large $k$, affects the pair correlation function at small $r$, which is found to be more negative as compared to that of VS.

Using the calculated values of the structure factor, we have estimated the pair correlation function $g(r)$ which is defined as

$$g(r) = 1 + \frac{3}{2r} \int_0^\infty dq\, q[\sin(qr)][S(q) - 1] , \qquad (10)$$

where $q$ and $r$ are expressed in the units of $k_F$ and $k_F^{-1}$, respectively. The results are shown in Fig. 2 for various values of $r_s$ and are compared with the corresponding results from the theory of VS. For the sake of comparison, values of $g(r)$ in the theory of Toigo and Woodruff[5] (TW), Hubbard, and in the random-phase approximation (RPA) are also mentioned. The values of $g(r)$ for small interparticle distance become negative for $r_s \geq 2$. Thus for low densities our $g(r)$ is poorer as compared to that of VS. For small $r_s$, our $g(r)$ is slightly inferior to that of TW, but for larger $r_s$ our $g(r)$ is better than that of TW.

To summarize, we have calculated the structure factor of the electron liquid self-consistently, from an integral equation obtained from low-order-moments relations. The values obtained for the structure factor agree very closely with those of VS. Also the integral equation yields an exact relation for the structure factor in the limit of very-small wave vectors and in the asymptotic limit it leads to $S(k) - 1 = O(1/k^4)$. Further, it is also consistent with the low-order frequency-moment relations. Although it leads to a finite pair correlation function at the origin, the quality of the pair correlation function at the origin is not good as compared to that of VS.

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