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Electron correlation functions at metallic densities*†

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A nonlinear integral equation is obtained for the static structure factor of an electron liquid. The equation is exact both in the small- and large-wave-vector limits. It has been solved self-consistently and values of the structure factor thus obtained are used to calculate the pair-correlation function of the system. The results are found to be almost positive over the entire metallic density range. An integral equation for the magnetic structure factor is also obtained which is exact for large wave vectors. The spin pair-correlation functions of the electron liquid are calculated using the self-consistent values of the magnetic structure factor obtained by solving the integral equation. The quality of various spin pair-correlation functions is quite good as compared to those obtained from earlier calculations.

I. INTRODUCTION

A few years ago, Mihara and Puff[1] (MP) derived a nonlinear integral equation for the ground-state static structure factor of interacting bosons and applied it with reasonable success to study some ground-state properties of liquid ^{4}He. Following similar arguments Kuglar[2] obtained an integral equation for the static structure factor $S(k)$ of an interacting electron gas. This equation has recently been solved self-consistently by us.[3] The results for the pair-correlation function $g(r)$ were comparable with many of the earlier calculations[4-8] but remained negative for small interparticle separations. This is because the integral equation of Kuglar is rigorously valid only for small k. It is not expected to yield a positive pair correlation function for small r because $g(0)$, to a greater extent, is determined by the asymptotic behavior of $S(k)$. We have looked into Kuglar's derivation of the integral equation and it is found that there is some arbitrariness in the derivation. This arbitrariness has now been removed by constraining the integral equation to satisfy the exact asymptotic result[9,10] for the static structure factor. In this way, we obtain an integral equation for $S(k)$ which is exact for large k. This equation and the integral equation of Kuglar are solved self-consistently. For intermediate wave vectors, we obtain the structure factor by smoothly joining the small- and large-k values of $S(k)$. From this, we suggest another prescription for obtaining the structure factor which is equally good for intermediate k. In this way, we obtain an integral equation which is exact both in small- and large-k limits. This equation is solved self-consistently. We find that the electron pair-correlation function that is subsequently calculated, remains almost positive over the entire metallic-density range.

Recently, we derived[11] a nonlinear integral equation for the magnetic structure factor $\tilde{S}(k)$ which is expected to be good for small k. This equation was solved self-consistently. It was found that the quality of various spin pair-correlation functions was comparable with some of the earlier calculations[12,13] but the results were not quite satisfactory for small interparticle separations. We now derive an integral equation for the magnetic structure factor which is exact for large k. A prescription similar to that of $S(k)$ for intermediate wave vectors is used to obtain an integral equation which is assumed to be valid for all k. The values of $\tilde{S}(k)$ obtained by self-consistently solving this integral equation are used to calculate various spin pair-correlation functions. The present results for the spin correlation function with antiparallel spins [i.e., $g_{\uparrow\downarrow}(r)$] are positive over the entire metallic-density range. The values of the spin pair-correlation function with parallel spins [i.e., $g_{\uparrow\uparrow}(r)$] are negative for small r as in all the earlier theories but the magnitude is very small. These results are compared with those based on earlier theories.[8,12,13]

The general formalism of the paper is described in Sec. II. The integral equations for $S(k)$ and $\tilde{S}(k)$ are derived there. From these, a coupled nonlinear integral equation for $S(k)$ and $\tilde{S}(k)$ has also been obtained. The integral equations for $S(k)$ and $\tilde{S}(k)$ are solved in Sec. III and the results obtained for various pair correlation functions are discussed. Section IV contains our concluding remarks.

II. GENERAL FORMALISM

A. Integral equation for $S(k)$

We start with the following integral equation[2] for the static structure factor:

$$\left(\frac{\omega(k)}{S(k)}\right)^2 = \left(\omega^2(k) + \frac{4\omega(k)\langle T_{\mathrm{KE}}\rangle}{\hbar} + \omega_p^2 + G_3(k)\right) - t_d(k), \tag{1}$$

where $t_d(k) \geqslant 0$ for all k and $\langle T_{\mathrm{KE}} \rangle$ is the exact kinetic energy per electron. In Eq. (1),

$$G_3(k) = \frac{e^2}{m\pi} \int_0^\infty dq\, q^2 [S(q)-1]\, T(k,q), \tag{2}$$

where

$$T(k,q) = \frac{5}{6} - \frac{q^2}{2k^2} + \frac{k}{4q}\left(\frac{q^2}{k^2}-1\right)^2 \ln\left|\frac{k+q}{k-q}\right|. \tag{3}$$

Further

$$\omega(k) = \hbar k^2/2m$$

and

$$\omega_p = (4\pi n e^2/m)^{1/2}$$

is the plasma frequency. The function $t_d(k)$ in Eq. (1) can be determined by following the arguments in Ref. 11 and Eq. (1) becomes

$$\left(\frac{\omega(k)}{S(k)}\right)^2 = \left(\frac{\omega(k)}{S_0(k)}\right)^2 + \omega_p^2 + G_3(k) + \frac{4\omega(k)\Delta(T_{\mathrm{KE}})}{\hbar} - h_d(k), \tag{4}$$

where

$$S_0(k) = \begin{cases} \dfrac{3}{4}\dfrac{k}{k_F} - \dfrac{1}{16}\dfrac{k^3}{k_F^3}, & 0 \leqslant k \leqslant 2k_F \\ 1, & 2k_F \leqslant k \end{cases},$$

is the structure factor of a noninteracting electron gas. Further in Eq. (4), $\Delta(T_{\mathrm{KE}}) = \langle T_{\mathrm{KE}} \rangle - \langle T_{\mathrm{KE}} \rangle_f$, where $\langle T_{\mathrm{KE}} \rangle_f$ is the kinetic energy per electron for a free electron gas and

$$h_d(k) = t_d(k) - t_{df}(k), \tag{5}$$

where $t_{df}(k)$ is the value of $t_d(k)$ for the noninteracting electron gas. It can be seen from Eq. (1) that to have a nondivergent pair correlation function at the origin, the dominant contribution to function $h_d(k)$ must have the value $4\omega(k)\, \Delta(T_{\mathrm{KE}})/\hbar$, for large k. In view of this one chooses

$$h_d(k) = 4\omega(k)\, \Delta(T_{\mathrm{KE}})/\hbar \tag{6}$$

for all k. Then from Eqs. (4) and (6), one obtains

$$\left(\frac{\omega(k)}{S(k)}\right)^2 = \left(\frac{\omega(k)}{S_0(k)}\right)^2 + \omega_p^2 + G_3(k). \tag{7}$$

This integral equation, which is exact only for small k, was derived by Kuglar[2] and self-consistently solved by us.[3]

However, the choice of function $h_d(k)$ as given by Eq. (6) is arbitrary because one can always add some constant on the right-hand side of Eq. (6) and still get a finite $g(0)$. To avoid this arbitrariness, we make use of an exact asymptotic result for $S(k)$ to determine the function $h_d(k)$. It has recently been found[9,10] that

$$\lim_{k \to \infty} k^4 [S(k) - 1] = -(8k_f^3/3\pi a_0) g(0), \tag{8}$$

where k_F is the Fermi wave vector and a_0 is the first Bohr radius. Using this expression in Eq. (4), we obtain

$$h_d(k) = 4\,\omega(k)\Delta\,(T_{\mathrm{KE}})/\hbar + \tfrac{1}{3}\omega_p^2\, [g(0) - 1] \tag{9}$$

This leads to an integral equation

$$\left(\frac{\omega(k)}{S(k)}\right)^2 = \left(\frac{\omega(k)}{S_0(k)}\right)^2 + \omega_p^2 + G_3(k) + \tfrac{1}{3}\,\omega_p^2\, [g(0) - 1] \tag{10}$$

which being exact in large-k limit, automatically ensures a well-behaved $g(0)$.

It may be noted that in the large-k limit, the functional behavior of $k^4\, [S(k) - 1]$ as given by integral equation (7) is similar[3] to that given by the exact result (8) but the coefficient of $g(0)$ is somewhat different. Similarly in the small-k limit, $S(k)$ as given by integral equation (10) goes to zero as k^2 but its coefficient is not exact. Thus the integral equations (7) and (10) are exact only in small- and large-k limits, respectively. We rewrite these equations into a single integral equation as

$$\left(\frac{\omega(k)}{S(k)}\right)^2 = \left(\frac{\omega(k)}{S_0(k)}\right)^2 + \omega_p^2 + G_3(k) + \tfrac{1}{3}\,\eta(k)\omega_p^2 [g(0) - 1], \tag{11}$$

where

$$\eta(k) = \begin{cases} 1 & \text{for large } k, \\ 0 & \text{for small } k. \end{cases} \tag{12}$$

The important features of this integral equation are that it is consistent with the frequency moment sum rules and gives the free-fermion structure factor in the appropriate limit. Further, it yields exact results for $S(k)$ both in the small- and large-k limits. It also gives a finite pair-correlation function at the origin. Moreover, this integral equation being exact for large k, is expected to yield a positive $g(0)$ over the entire metallic density range. However, at present we do not know the function $\eta(k)$.

B. Integral equation for $\tilde{S}(k)$

In Ref. 11, while deriving an integral equation for the magnetic structure factor, we had

$$\left(\frac{\omega(k)}{\tilde{S}(k)}\right)^2 = \left(\frac{\omega(k)}{S_0(k)}\right)^2 + I_3(k) + \frac{4\omega(k)\Delta(T_{\mathrm{KE}})}{\hbar} - h_S(k), \tag{13}$$

where

$$I_3(k)=\frac{e^2}{m\pi}\int_0^\infty dq\,q^2\,\{[\tilde S(q)-1][\tfrac{2}{3}+T(k,q)]-\tfrac{2}{3}[S(q)-1]\},\tag{14}$$

and as in earlier section

$$h_S(k)=t_S(k)-t_{Sf}(k),$$

where suffix s refers to spin density. In order to have a finite $\tilde g(0)$, the spin pair-correlation function at the origin, we chose $h_S(k)=4\times\omega(k)\Delta(T_{\mathrm{KE}})/\hbar$, in the Ref. 11, and arrived at an integral equation

$$\left(\frac{\omega(k)}{\tilde S(k)}\right)^2=\left(\frac{\omega(k)}{S_0(k)}\right)^2+I_3(k).\tag{15}$$

In the long-wavelength limit, this equation leads to[11]

$$\lim_{k\to 0}\tilde S(k)=\left(\frac{3}{1-g_{\uparrow\downarrow}(0)}\right)^{1/2}\frac{\hbar k^2}{2m\omega_p},\tag{16}$$

where $g_{\uparrow\downarrow}(0)$ is the antiparallel spin pair-correlation function at the origin. The parallel and antiparallel spin pair-correlation functions are obtained from $g(r)$ and $\tilde g(r)$ using the relations

$$g_{\uparrow\uparrow}(r)=g(r)+\tilde g(r)$$

and

$$g_{\uparrow\downarrow}(r)=g(r)-\tilde g(r).$$

It may be noted that the expression (16) for the magnetic structure factor is similar to the corresponding exact result for $S(k)$.

However, there is an arbitrariness in the choice of function $h_S(k)$ as was the case with the first choice of $h_d(k)$ in Sec. II A. Here also we use another exact result[9] for $\tilde S(k)$ which reads as

$$\lim_{k\to\infty}k^4[\tilde S(k)-1]=-(8k_F^3/3\pi a_0)\tilde g(0).\tag{17}$$

This relation when used in Eq. (13) leads to

$$h_S(k)=4\,\omega(k)\Delta(T_{\mathrm{KE}})/\hbar+\omega_p^2[g(0)-1]/3\,.\tag{18}$$

It is interesting to note that this expression is exactly the same as that of $h_d(k)$ obtained earlier [Eq. (9)]. From Eqs. (13) and (17), we obtain an integral equation

$$\left(\frac{\omega(k)}{\tilde S(k)}\right)^2=\left(\frac{\omega(k)}{S_0(k)}\right)^2+I_3(k)+\tfrac{1}{3}\,\omega_p^2[g(0)-1],\tag{19}$$

for the magnetic structure factor. This equation is exact in the large k limit and also gives a finite value for $\tilde g(0)$. Combining Eqs. (15) and (19), we get an integral equation

$$\left(\frac{\omega(k)}{\tilde S(k)}\right)^2=\left(\frac{\omega(k)}{S_0(k)}\right)^2+I_3(k)+\tfrac{1}{3}\eta(k)\omega_p^2[g(0)-1].\tag{20}$$

Here we assume the function $\eta(k)$ to be the same as defined earlier, because $S(k)$ and $\tilde S(k)$ behave in the same way for small as well as large k. Integral equation (20), being exact in the large-k limit, is expected to yield the spin pair-correlation function of good quality.

Corresponding to three integral equations (7), (10), and (11) for $S(k)$ we have analogous integral equations (15), (19), and (20) for $\tilde S(k)$. Out of these, the first set consisting of Eqs. (7) and (15) is good for small k alone and the second set comprising of Eqs. (10) and (19) is exact only for large k. While the third set consisting of Eqs. (11) and (20) is expected to be good for all wave vectors. Eliminating the common term in the first set of equations, we obtain the following coupled integral equation for $S(k)$ and $\tilde S(k)$:

$$\left(\frac{\omega(k)}{S(k)}\right)^2=\left(\frac{\omega(k)}{\tilde S(k)}\right)^2+\omega_p^2+\Delta(k),\tag{21}$$

where

$$\Delta(k)=I_3(k)-G_3(k)=\frac{e^2}{m\pi}\int_0^\infty dq\,q^2\,[\tilde S(q)-S(q)][\tfrac{2}{3}+T(k,q)].\tag{22}$$

The second set [i.e., Eqs. (10) and (19)] also yield the same coupled equation (21). This only means (and this has already been seen) that the contribution which was left over in Eqs. (7) and (15) and which is now taken into account in Eqs. (10) and (19), is the same in all these four equations. It follows from the foregoing that Eq. (21) should be valid for all k. It may also be noted that the Eqs. (11) and (20) also lead to the same coupled integral equation (21).

III. SELF-CONSISTENT SOLUTION AND THE RESULTS

A. Solution for $S(k)$ and the results

We shall now solve the integral equation (9) numerically. The dimensionless form of this equation is

$$S^2(k)=Ck^4/\{1+Ck^4/S_0^2(k)+G_3(k)+\tfrac{1}{3}\eta(k)\omega_p^2[g(0)-1]\},\tag{23}$$

where now

$$G_3(k)=3/4\int_0^\infty dq\,q^2[S(q)-1]T(k,q)\tag{24}$$

and[14]

$$C = 3\pi/16\alpha r_s\,, \quad \alpha = (4/9\pi)^{1/3}. \tag{25}$$

Clearly, $S(k)$ and $G_3(k)$ can be determined self-consistently from Eqs. (23) and (24) provided $\eta(k)$ is known. To know this, we follow a method similar to that followed by Nozières and Pines[15] in the calculation of the correlation energy of an interacting electron gas. We first solve Eq. (23) with $\eta(k) = 1$ and obtain a set of self-consistent values of $S(k)$ which are thus good for large k. Then we set $\eta(k) = 0$ in Eq. (23). The resulting integral equation has already been solved by us[3] and the set of self-consistent values of $S(k)$ obtained from this equation are good only for small k. These two sets of values of $S(k)$ (one of which is valid for small k and the other for large k) are plotted in Fig. 1(a) for $r_s = 4$. The structure factor is expected to be a smoothly varying function of k for intermediate wave vectors. Therefore, to get the values of $S(k)$ for intermediate k, we smoothly join the above two curves to obtain the resultant dotted curve. The two curves can be seen to join smoothly about the plasmon cutoff wave vector $k_C = 0.47\, r_s^{\frac{1}{2}} \simeq 1$. It is expected also because for small k the structure factor is dominated by plasmons and the maximum value of k (in units of k_F) upto which the plasmons are the well-defined modes[15] of the system is

$$k_C = \left(\frac{4\alpha r_s}{3\pi}\right)^{1/2} \simeq 0.47\, r_s^{1/2}. \tag{26}$$

Taking this value of k_C as the critical wave vector, we solve Eq. (23) with three different choices of $\eta(k)$. These are, respectively, a step function, a Gaussian and a Lorentzian function:

$$\eta(k) = \Theta\,(k - k_C); \tag{27}$$

$$\eta(k) = \exp\,(-k_C{}^2/k^2); \tag{28}$$

$$\eta(k) = k^2/(k^2 + k_C^2). \tag{29}$$

The results given by these $\eta(k)$'s differ only slightly and thus we choose simplest of them—the step function (27). Now we solve the integral equation (23) self-consistently for the entire metallic-density range. The self-consistent values of the structure factor for $r_s = 2$, 4, and 6 are plotted in Fig. 1(b). It is noted with satisfaction that these values of $S(k)$ for $r_s = 4$, are almost the same, as obtained from the dotted curve in Fig. 1(a).

The self-consistent values of $S(k)$ are used to calculate the pair-correlation function which is defined as

$$g(r) = 1 + \frac{3}{2r}\int_0^\infty dq\, q[S(q) - 1]\sin qr. \tag{30}$$

The results obtained for $g(r)$ are plotted in Fig. 2, only for $r_s = 2$, 4, and 6 and are compared with the corresponding results of Vashishta and Singwi[4] (VS). It is important to note that the present $g(r)$ is positive for all values of r up to $r_s = 4$. For $r_s > 4$, it is negative only for very small values of r; however, its magnitude is so small that for all practical purposes, it may be taken to be zero. Thus, it indicates that the integral equation (23) is valid over the entire metallic-density range and that our choice of k_C as the plasmon cutoff wave vector is also good.

To give an idea of the quality of the pair-correlation function for all r_s values of interest, we have plotted $g(0)$ vs r_s in Fig. 3. The values of

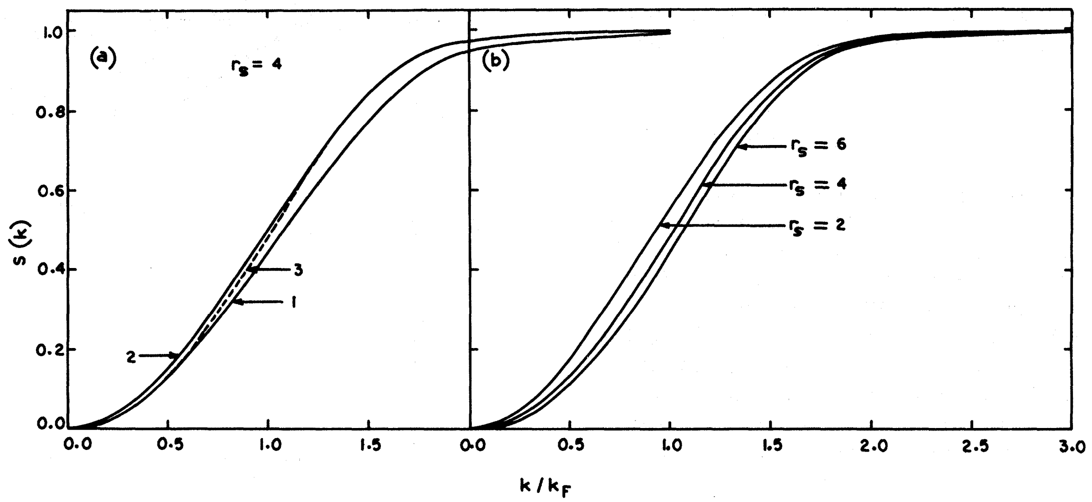

FIG. 1. (a) Self-consistent values of structure factor, $S(k)$ vs k for $r_s = 4$. Curves 1 and 2 are obtained from the integral equations (7) and (10), respectively. Curve 3 is obtained by smoothly joining the curves 1 and 2 for intermediate wave vectors. (b) Self-consistent values of structure factor, $S(k)$ vs k for $r_s = 2$, 4, and 6.

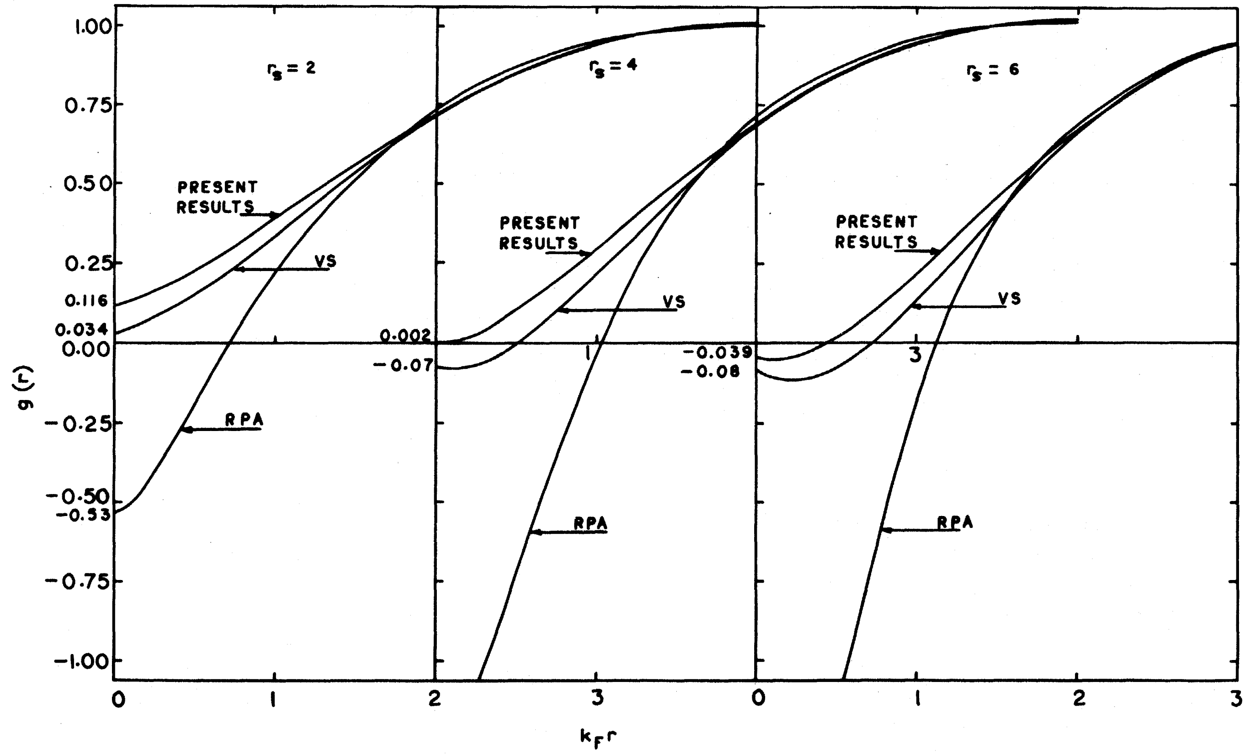

FIG. 2. Pair-correlation function, $g(r)$ vs $k_F r$ for $r_s = 2$, 4, and 6.

$g(0)$ from the theory of Singwi *et al.*[5] lies almost on the present curve and are thus not shown separately. The present results are compared with other results from earlier theories which includes random-phase approximation (RPA); Hubbard's approximation; moment-conserving approximations to Toigo and Woodruff[6] (TW) and that of Pathak and Vashishta[7] (PV); generalized RPA of VS,[4] and that of Hasegawa and Shimizu[8] (HS).

B. Solution for $\tilde{S}(k)$ and the results

The integral equation (20) for the magnetic structure factor can be solved self-consistently along with Eq. (14), provided the values for $S(k)$ are known. For that, we have used the values of $S(k)$ obtained in Sec. III A and have thus calculated the self-consistent values of $\tilde{S}(k)$ for the electron-density range encountered in metals.

The self-consistent values of the magnetic structure factor are used to calculate the spin pair-correlation function which is defined as

$$\tilde{g}(r) = \frac{3}{2r} \int_0^\infty dq\, q\,[\tilde{S}(q) - 1] \sin qr. \qquad (31)$$

The values of $\tilde{g}(r)$ are computed for $r_s = 1$ to 6.

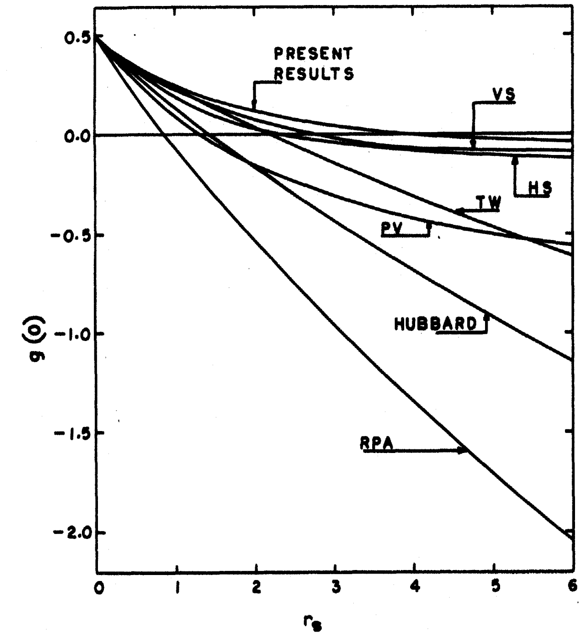

FIG. 3. Values of the pair-correlation function at the origin, $g(0)$ vs r_s.

The results for $g(r)$ for the corresponding r_s values have already been computed in Sec. III A. These values of $g(r)$ and $\bar{g}(r)$ are used to calculate the spin pair-correlation functions with antiparallel spins and parallel spins separately. We have evaluated these correlation functions over the entire metallic-density range. The results for $g_{\uparrow\downarrow}(r)$ and $g_{\uparrow\uparrow}(r)$ are presented in Figs. 4(a) and 4(b), respectively, for $r_s = 4$ only. The curves for other r_s values follow the expected pattern. To discuss the quality of these correlation functions over the range of metallic densities, we have plotted $g_{\uparrow\downarrow}(0)$ and $g_{\uparrow\uparrow}(0)$ as functions of r_s in Figs. 4(c) and 4(d), respectively. The results are compared with earlier calculated values in RPA, generalized RPA of Lobo *et al.*[12], and HS.[8] It is clear from Fig. 4(c) that the present $g_{\uparrow\downarrow}(0)$ satisfies the requirement

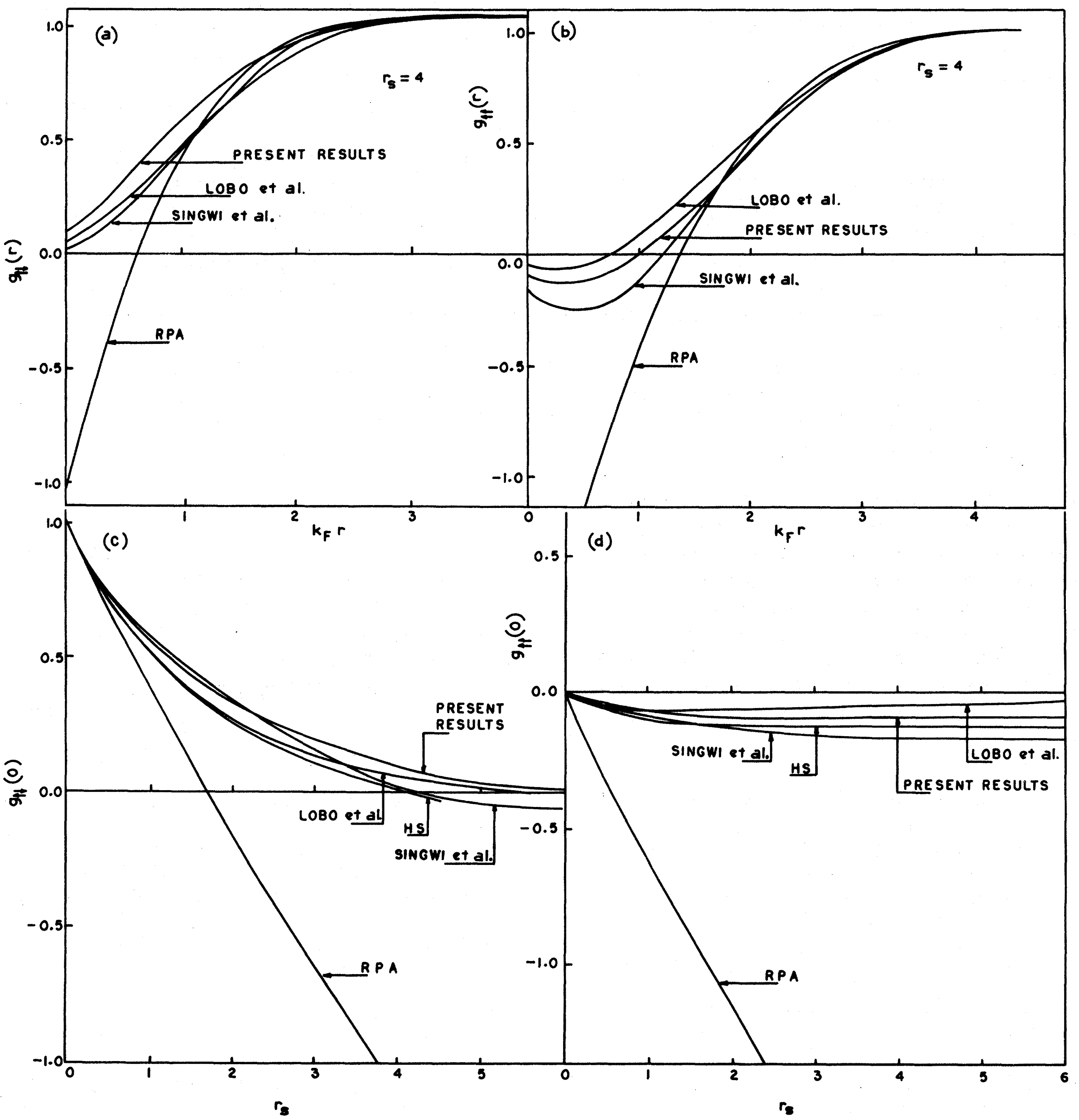

FIG. 4. (a) Spin pair-correlation function, $g_{\uparrow\downarrow}(r)$ vs $k_F r$ for $r_s = 4$. (b) Spin pair-correlation function, $g_{\uparrow\uparrow}(r)$ vs $k_F r$ for $r_s = 4$. (c) Values of the spin pair-correlation function at the origin, $g_{\uparrow\downarrow}(0)$ vs r_s. (d) Values of the spin pair-correlation function at the origin, $g_{\uparrow\uparrow}(0)$ vs r_s.

of positive definiteness over the entire metallic-density range as is the case in the theory of Lobo *et al.* [It may be noted that $g_{\uparrow\downarrow}(0)$ in the theory of Lobo *et al.* is slightly negative at $r_s \simeq 6$, while the present $g_{\uparrow\downarrow}(0)$ is positive even well beyond $r_s = 6$.] The results of HS (Ref. 8) seem to become negative for $r_s > 4$. As regards $g_{\uparrow\uparrow}(0)$, the present results are negative as in all the earlier theories. However, the magnitude is quite small. It can be seen from Fig. 4(d) that the present curve lies in between the curves of HS and Lobo *et al.* Thus, one can say that the overall quality of the present spin pair-correlation functions is almost as good as in the theory of Lobo *et al.* and is better than that obtained from other theories.

IV. CONCLUDING REMARKS

The main results in the present paper are the three expressions (11), (20), and (21). Of these, (11) is the integral equation for static structure $S(k)$. This integral equation is exact both in the small- and long-wavelength limit. Further, it is consistent with the frequency moment sum rules and also yields the free-fermion structure factor in the appropriate limit. The derivation of this integral equation is soundly based on the low-order moment sum rules and known exact results for the structure factor. However, there is some arbitrariness in the choice of function $\eta(k)$. The basic requirement on function $\eta(k)$ is that its value should be 0 and 1 in the small- and large-k limits, respectively. This could be accomplished through many choices of $\eta(k)$. However, we have found numerically that our results are not quite sensitive to the particular choice of $\eta(k)$ and thus we have chosen its simplest form which is given by step function about the plasmon cut-off wave vector. The quality of the pair-correlation function, obtained by using the self-consistent values of $S(k)$ as given by Eq. (11), is good over the entire metallic-density range. It gives *a posteriori* justification for the above procedure.

Expression (20) is the integral equation for the magnetic structure factor, $\tilde{S}(k)$ and its special features are similar to those of integral equation (11). The derivation of this equation is also based on exact results. But again there is an arbitrariness in the choice of function $\eta(k)$ which we have assumed to be same as choosen for solving the integral equation (11). The good quality of various spin-correlation functions over the entire metallic-density range, obtained by self-consistently solving Eq. (20), ensures the reasonableness of this assumption.

The another important expression (21) is the coupled integral equation between $S(k)$ and $\tilde{S}(k)$. If either $S(k)$ or $\tilde{S}(k)$ is known, the other can be calculated from Eq. (21) self-consistently. In the long-wavelength limit, using result (16) for $\tilde{S}(k)$ in Eq. (21), one obtains the corresponding exact result for $S(k)$ and vice versa. Similarly using the exact result (8) for $S(k)$ in Eq. (21) in the large-k limit, we get the corresponding exact result (17) for $\tilde{S}(k)$ and vice versa. Thus it may be hoped that the integral equation (21) may turn out to be an exact relation.

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