

Self-consistent screening and approximate residual Landau interaction functions for the electron gas

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We formulate a new self-consistent approach which takes into account both exchange and collision processes consistent with the conserving approximation scheme in an electron gas. We extract the Landau Fermi-liquid parameters from this theory. We compute self-consistently the various system parameters such as the effective mass at the Fermi surface, the spin susceptibility, the compressibility, and the plasmon dispersion. We have calculated the Fermi-liquid parameters for various angles and for densities in the metallic range. All these are compared with our previous work on the subject which did not take account of the exchange and collision processes included here. We have thus considered in some detail, the effects of antiparallel spin correlations on various system properties.

I. INTRODUCTION

In an earlier paper¹ (to be referred to as I), we presented a self-consistent quasistatic screening approach for studying various properties of the homogeneous electron gas within the framework of the time-dependent Hartree-Fock theory. Essentially, in that scheme we first solved the integral equation for the irreducible vertex function representing the summation of all exchange-ladder diagrams, by taking the statically screened Coulomb interaction $V(\vec{q}) = 4\pi e^2 / (q^2 + \xi^2 k_F^2)$ as the exchange interaction function between the parallel spins. The solution was exact in the long-wavelength ($\vec{q} \rightarrow 0$) static ($\omega \rightarrow 0$) limit, and variational in other regions.² The screening parameter ξ^2 was then obtained self-consistently from the limiting value of the resulting longitudinal dielectric function $\epsilon(\vec{q}, \omega)$. This also leads to the self-consistent determination of the compressibility ratio κ_F/κ , the long-wavelength static paramagnetic susceptibility ratio χ/χ_F , and the plasma dispersion relation for the electron gas. That calculation indeed corresponds to a fully conserving approximation, satisfying the Ward identities identically,³ but its use of the time-dependent Hartree-Fock theory and the consequent neglect of the contribution to the irreducible vertex function Λ arising from spin-independent interaction beyond the average polarization field are not valid at metallic densities. In other words, the so-called collision diagrams for the vertex function must be included in our calculation, at least up to the lowest-order skeleton diagrams in V , i.e., of order V^2 with the full vertex function on one side, in order to describe the antiparallel spin-correlation correctly.⁴

In principle, this generalization will lead to a set of nonlinear integral equations as has recently been discussed by Rau and Rajagopal.⁵ They set up a variational method of obtaining χ/χ_F and κ/κ_F when such nonlinear equations govern these quantities. The final results are quite complicated. However, a less restricted set of diagrams consistent with conserving approximation schemes can be fruitfully incorporated in such a calculation, which will be discussed in the present paper. Apart from providing a more accurate method of obtaining the self-consistent screening parameter ξ^2 , such an extension of our earlier calculation would also lead to the correct result that χ/χ_F is no longer equal^{5,6} to κ/κ_F . For formulating the new self-consistent approach which takes care of both exchange and collisions, it is not necessary to solve the new integral equation for the vertex function. If we can extract the analytical forms of the frequency-independent residual Landau interaction function⁷

$$f(\vec{k}\sigma, \vec{k}'\sigma') \equiv f_{ex}(\vec{k}, \vec{k}')\delta_{\sigma\sigma'} + f_0(\vec{k}, \vec{k}') \quad (1.1)$$

between the quasiparticles of the charged system from such an analysis, we can use the well-known results of the Landau Fermi-liquid theory straight away to obtain κ_F/κ and the self-consistent screening parameter ξ^2 . It would also lead to the self-consistent determination of various other properties like m/m^* at the Fermi surface, χ/χ_F , and the plasma-dispersion in the long-wavelength limit. In Sec. II of this paper, we introduce the new vertex equation,⁸ in the so-called V_s approximation of Baym and Kadanoff. From the structure of this equation we extract the static interaction functions $f_{ex}(\vec{k}, \vec{k}')$ and $f_0(\vec{k}, \vec{k}')$. Of course $-f_{ex}(\vec{k}, \vec{k}')$

is nothing but our old $V(q = |\vec{k} - \vec{k}'|)$, defined earlier. For completeness in this section we also present the new form of $\epsilon(\vec{q}, \omega)$ obtained from variational solution of the resulting approximate vertex equation (with only static interactions f_{ex} and f_0). In Sec. III, we describe the application of the results of the Landau Fermi-liquid theory to our problem, for obtaining directly the self-consistent screening parameter ξ^2 and various other physical

$$\Lambda(K, Q) = 1 - i \sum_{K'} \bar{Y}_Q(K, K') G(K') G(K' + Q) \Lambda(K', Q), \tag{2.1}$$

$$\begin{aligned} \bar{Y}_Q(K, K') = \sum_{\sigma'} & \left(-V(K - K') \delta_{\sigma\sigma'} \right. \\ & \left. + i \sum_{K''} G(K + K'' + \frac{1}{2}Q) [G(K' + K'' + \frac{1}{2}Q) + G(K' - K'' + \frac{1}{2}Q)] V(\frac{1}{2}Q - K'') V(\frac{1}{2}Q + K'') \right), \end{aligned} \tag{2.2}$$

where $G(K)$ is the single-particle propagator with the Hartree-Fock self-energy¹ involving the function $V(Q)$, and where K, Q , etc., stand for four momenta (\vec{k}, ϵ) , $(\vec{q}, \hbar\omega)$, etc. In terms of the vertex function, the longitudinal dielectric function $\epsilon(Q)$ is given by

$$\epsilon(Q) = 1 + \frac{4\pi e^2}{q^2} 2i \sum_K G(K) G(K + Q) \Lambda(K, Q). \tag{2.3}$$

From an examination of Fig. 1 and Eq. (2.2), one finds that the dynamic interaction function $\bar{Y}_Q(K, K')$ contains two types of terms; the first one arises from the exchange interaction between the parallel spins, and the second one comes from the spin-independent collisions. After the trivial summation over spin σ' , \bar{Y}_Q is of course inde-

$$f_0(\vec{k}, \vec{k}') = - \sum_{\vec{k}''} |V(\vec{k}'')|^2 \left(\frac{\eta_{\vec{k}+\vec{k}''} - \eta_{\vec{k}'+\vec{k}''}}{(E_{\vec{k}}, -E_{\vec{k}'+\vec{k}''}) - (E_{\vec{k}} - E_{\vec{k}+\vec{k}''})} + \frac{\eta_{\vec{k}+\vec{k}''} + \eta_{\vec{k}-\vec{k}''} - 1}{(E_{\vec{k}}, -E_{\vec{k}',-\vec{k}''}) + (E_{\vec{k}} - E_{\vec{k}+\vec{k}''})} \right), \tag{2.5}$$

pendent of σ . Thus $f_{ex}(\vec{k}, \vec{k}') \delta_{\sigma\sigma'}$, and $f_0(\vec{k}, \vec{k}')$ must correspond to some limiting values of the first and second term, respectively, inside the large parentheses in Eq. (2.2). As far as the exchange part is concerned, we have already made the static approximation for $V(Q)$ in our earlier paper.¹ Thus, at least for $|\vec{k} - \vec{k}'| \ll K_F$, we have $f_{ex}(\vec{k}, \vec{k}') = -V(|\vec{k} - \vec{k}'|) = -4\pi e^2 / (|\vec{k} - \vec{k}'|^2 + \xi^2 k_F^2)$.

where $\eta_{\vec{k}}$'s are the zero-temperature Fermi functions. Note that our expression for $f_0(\vec{k}, \vec{k}')$ differs from another expression derived by Herring, Eq. (3.30) in Ref. 4, only in the fact that in our case we have the single-particle Hartree-Fock energies $E_{\vec{k}}$ in the denominators instead of the unperturbed energy $\hbar^2 k^2 / 2m$. However, since any additional contribution from the correction factor $(m \hbar_F / m)$ to f_0 is of higher order in the interaction, approximately we can still use something similar to Herring's final result which he obtained after an approximate integration of his expression for f_0 . We have found that for obtaining an exact agreement with the expression for the compressibility ratio in the high-density limit ($r_s \rightarrow 0$), up to all the terms of $O(r_s^2)$ (this may be obtained from the correla-

tion energy calculation of Gell-Mann and Brueckner,^{8,9,10} which will be discussed in Sec. IV, we have the identity q_D in Herring's expression for f_0 as $\xi k_F / \sqrt{2}$. However, to be consistent with the

II. THE VERTEX EQUATION APPROACH

If we sum all the exchange-ladder diagrams involving the interaction function $V(Q)$ and limit ourselves to the second-order skeleton collision diagrams (Fig. 1), the integral equation for the proper vertex function $\Lambda(K, Q)$ can be written⁸

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In the same spirit, we will reduce the second term inside the large parentheses in Eq. (2.2) to the form $f_0(\vec{k}, \vec{k}')$ by first taking the limit $Q = 0$, and then assuming that both K and K' are on the mass shell. Of course, $V(K'')$ is again taken to be the static interaction $V(\vec{k}'')$. This leads to

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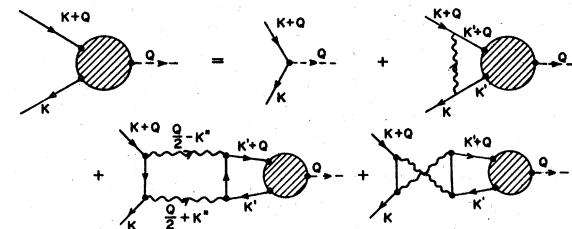


FIG. 1. Feynman diagrams for the vertex equation in the V_s approximation, including lowest-order collisions and exchange ladder graphs.

approximation (2.4) for $V(q)$, we will still take q_D to be ξk_F . Since ξ is determined self-consistently in the final analysis, this choice serves our purpose. We thus approximately write (as done by Herring⁴)

$$f_0(\vec{k}, \vec{k}') = - \frac{4\pi e^2 (m e^2 / 4\pi \hbar^2 k_F)}{\xi k_F (|\vec{k} + \vec{k}'|^2 + \xi^2 k_F^2)^{1/2}} \times \ln \left(\frac{(|\vec{k} + \vec{k}'|^2 + \xi^2 k_F^2)^{1/2} + \xi k_F}{(|\vec{k} + \vec{k}'|^2 + \xi^2 k_F^2)^{1/2} - \xi k_F} \right), \quad (2.6)$$

where in terms of the dimensionless density parameter r_s , $m e^2 / \pi \hbar^2 k_F = \alpha r_s / \pi$; $r_s^{-3} \equiv (\frac{4}{3}\pi n a_0^3)$, in terms of the Bohr radius a_0 , $\omega^3 \equiv 4/9\pi$.

We can now follow the variational method of Ref. 2 to solve the vertex Eq. (2.1) in which $\bar{Y}_Q(K, K')$ is replaced by the static interaction $f_{ex}(\vec{k}, \vec{k}') + 2f_0(\vec{k}, \vec{k}')$ as given by Eqs. (2.4) and (2.6). Such an approach leads to the new variational dielectric function in the form

$$\epsilon(\vec{q}, \omega) = 1 + \frac{8\pi e^2}{q^2} \frac{M^2(\vec{q}, \omega)}{M(\vec{q}, \omega) - J(\vec{q}, \omega) - K(\vec{q}, \omega)}, \quad (2.7)$$

where the new correction term $K(\vec{q}, \omega)$ arising from the spin-independent interaction f_0 is given by

$$K(\vec{q}, \omega) = -2 \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} f_0(\vec{k}, \vec{k}') M(\vec{k}', Q) M(\vec{k}, Q) \quad (2.8)$$

and where the functions $M(\vec{k}, Q)$, $M(\vec{q}, \omega)$, and $J(\vec{q}, \omega)$ are same as defined in I. The variational solution (2.7) is of course exact in the limit $\omega = 0$, $\vec{q} \rightarrow 0$, so that we can proceed as before to evaluate $\epsilon(\vec{q} \rightarrow 0, 0)$ to obtain the self-consistent ξ^2 . However, instead of doing that we will apply the more elegant and consistent Landau Fermi-liquid theory approach to our problem in Sec. III to achieve similar results.

III. APPLICATION OF THE LANDAU-THEORY APPROACH

In this section, we first summarize the results for various physical quantities in Landau's Fermi-liquid theory,¹¹ and explain the self-consistent screening idea in terms of these equations. As already introduced earlier, basic to Landau's theory is the interaction function, $f(\vec{k}\sigma, \vec{k}'\sigma')$, which represents the residual interaction energy between two charged quasiparticles on the Fermi surface, apart from the average polarization term. The specific-heat constant C , the spin susceptibility χ , and the compressibility κ can be obtained from the function f as follows. Define dimensionless interaction-functions $\tilde{f}_0(\vec{k}, \vec{k}')$ and $\tilde{f}_{ex}(\vec{k}, \vec{k}')$ by

$$\tilde{f}_0(\vec{k}, \vec{k}') = \frac{4E_F}{3n} f_0(\vec{k}, \vec{k}'); \quad \tilde{f}_{ex}(\vec{k}, \vec{k}') = \frac{4E_F}{3n} f_{ex}(\vec{k}, \vec{k}'), \quad (3.1)$$

where $3n/4E_F$ is the density states per unit volume at the Fermi surface. We get

$$C_F/C = m/m^* = 1 - \langle \mu(2\tilde{f}_0 + \tilde{f}_{ex}) \rangle, \quad (3.2)$$

$$\chi_F/\chi = 1 + \langle (1 - \mu)\tilde{f}_{ex} \rangle - 2\langle \mu\tilde{f}_0 \rangle, \quad (3.3)$$

$$\kappa_F/\kappa = 1 + \langle (1 - \mu)(2\tilde{f}_0 + \tilde{f}_{ex}) \rangle, \quad (3.4)$$

where the quantities with suffix F refer to the non-interacting free electrons. The angular brackets stand for the Fermi-surface average and $\mu = (\vec{k} \cdot \vec{k}')/k_F^2$. The dielectric constant in the static long-wavelength limit is related to the compressibility through the well-known equation¹²

$$\epsilon(q, 0) = 1 + \xi^2 k_F^2 / q^2 \quad (3.5)$$

with

$$\xi^2 = (4\alpha r_s / \pi)(\kappa / \kappa_F). \quad (3.6)$$

We also note that the plasma dispersion of the electron gas can be obtained from the Landau-Silin transport equation as¹³

$$\omega_p^2(q) \simeq \omega_p^2 + \frac{3}{5}(k_F^2/m^2)q^2 A, \quad (3.7)$$

where

$$A = 1 + \frac{1}{3} \langle (2\mu - 1)(\mu - 1)(2\tilde{f}_0 + \tilde{f}_{ex}) \rangle. \quad (3.8)$$

The value $A = 1$ corresponds to the RPA case (A was referred to in I as β/β_{RPA}). There is still some experimental interest in the measurement of this quantity,^{14,19,20} which is found to differ noticeably from unity.

We now turn to our main problem, namely, the elucidation of the phenomenological interaction function from a microscopic theory. As already discussed in Sec. II, the results of I turn out to correspond exactly to setting $f_0 = 0$. Thus the dimensionless interaction function \tilde{f}_{ex} at the Fermi surface is

$$\tilde{f}_{ex} = -\lambda / (1 + \frac{1}{2}\xi^2 - \mu), \quad (3.9)$$

where

$$\lambda = \alpha r_s / \pi. \quad (3.10)$$

The interaction function depends on ξ^2 , which in turn can be determined from f_{ex} through Eqs. (3.4) and (3.6) if f_0 is taken to be zero. These equations are combined to give an identity which defines the self-consistent screening problem of I. Expressed in this way, we can see that the main approximation scheme of I is identical to that of Watabe.¹⁵

As already discussed in the Introduction,¹⁶ the most serious shortcoming of the above approach

is in the omission of the antiparallel spin function f_0 which is expected to play an important role at metallic densities.¹⁶ In this work, we have corrected for this by choosing a nonzero f_0 . From Eq. (2.6), with \vec{k} and \vec{k}' on the Fermi surface, we get

$$\tilde{f}_0 = -\frac{\frac{1}{2}\lambda^2}{\xi[\xi^2 + 2(1 + \mu)]^{1/2}} \ln\left(\frac{(\xi^2 + 2 + 2\mu)^{1/2} + \xi}{(\xi^2 + 2 + 2\mu)^{1/2} - \xi}\right). \quad (3.11)$$

We are now in a position to repeat the self-consistent screening argument. Equations (3.9) and (3.11) specify the interaction function in terms of ξ^2 , and ξ^2 is obtained back from Eqs. (3.4) and (3.6). This leads to the new equation for ξ^2 :

$$\begin{aligned} \frac{4\lambda}{\xi^2} = 1 - \lambda \left[1 - \frac{\xi^2}{4} \ln\left(1 + \frac{4}{\xi^2}\right) \right] \\ + \frac{\lambda^2}{6} \left[2 + (6 + \xi^2) \ln \xi^2 \right. \\ \left. - \frac{(4 + \xi^2)^{3/2}}{\xi} \ln\left(\frac{(4 + \xi^2)^{1/2} + \xi}{(4 + \xi^2)^{1/2} - \xi}\right) \right]. \end{aligned} \quad (3.12)$$

This equation can be readily solved for ξ^2 as a function of $\lambda = \alpha r_s / \pi$, on a computer. The solution will be presented in Sec. IV. For completeness, we, however, list below the relevant averages which are necessary for our analysis. With $\beta^2 \equiv 1 + 4/\xi^2$, we get

$$\langle \tilde{f}_{\text{ex}} \rangle = -\frac{1}{2}\lambda \ln \beta^2, \quad (3.13)$$

$$\langle \mu \tilde{f}_{\text{ex}} \rangle = \frac{1}{2}\lambda \left[2 - (1 + \frac{1}{2}\xi^2) \ln \beta^2 \right], \quad (3.14)$$

$$\langle \tilde{f}_0 \rangle = \frac{1}{4}\lambda^2 \left\{ \ln \xi^2 - \beta \ln[(\beta + 1)/(\beta - 1)] \right\}, \quad (3.15)$$

$$\begin{aligned} \langle \mu \tilde{f}_0 \rangle = -\frac{1}{4}\lambda^2 \left\{ \frac{2}{3} + (1 + \frac{1}{3}\xi^2) \ln \xi^2 \right. \\ \left. - \frac{1}{3}\beta(1 + \xi^2) \ln[(\beta + 1)/(\beta - 1)] \right\}. \end{aligned} \quad (3.16)$$

IV. RESULTS AND DISCUSSIONS

We present the computed values of ξ^2 in Table I, and compare it with the previous result as well as the Thomas-Fermi result. It is clear that the new values of ξ^2 are much enhanced as a result of the

TABLE I. Screening parameter ξ^2 .

r_s	Present	Previous (I)	Thomas-Fermi
1	0.782	0.744	0.663
2	1.828	1.591	1.327
3	3.162	2.490	1.990
4	4.801	3.420	2.654
5	6.763	4.368	3.317
6	9.066	5.327	3.981

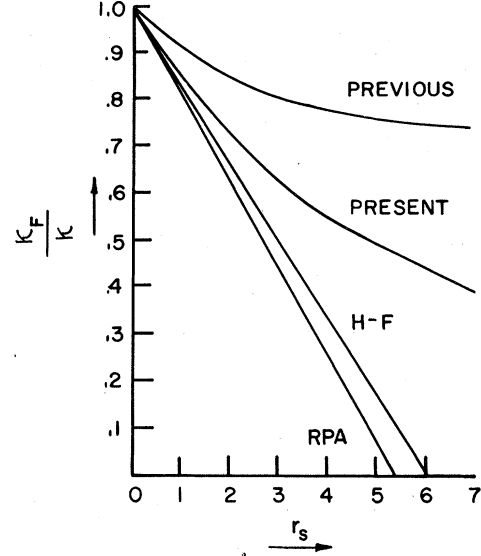


FIG. 2. Compressibility ratio κ_F/κ in various theories. The curve marked RPA is from Ref. 6.

antiparallel spin function f_0 . The compressibility ratio κ_F/κ is plotted as a function of r_s in Fig. 2, and, as expected, we find that it dips lower than the previous result. The blowing up of the compressibility, which signals an instability of the electron gas (presumably towards a Wigner solid) is absent in our theory (at least for $r_s < 70$). However, the compressibility does become very large and has interesting consequences for the magnetic susceptibility, which is discussed below.

Before discussing the results at metallic densities, let us analyze the high-density behavior of our solution. It is elementary to see that $\xi^2 \rightarrow 4\alpha r_s / \pi + O(r_s^2)$ as $r_s \rightarrow 0$, and hence we can di-

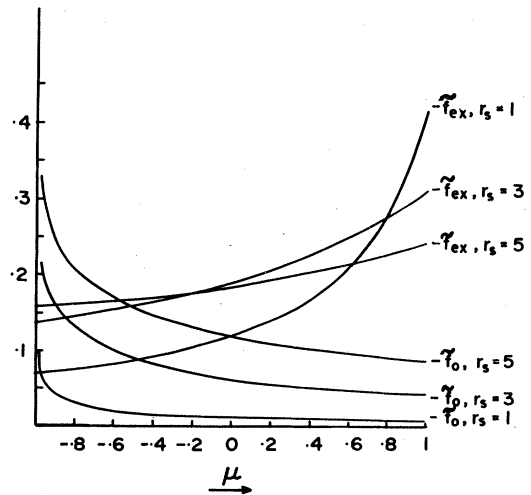


FIG. 3. Functions \tilde{f}_{ex} and \tilde{f}_0 vs $\mu (= \cos \theta_{KK'})$ for a few typical values of r_s .

TABLE II. Paramagnetic susceptibility χ/χ_F .

r_s	Present	Previous (I)	=TF	RPA ^a
1	1.136	1.122	1.144	1.155
2	1.224	1.199	1.271	1.311
3	1.273	1.251	1.392	1.477
4	1.295	1.289	1.512	1.658
5	1.300	1.317	1.635	1.859
6	1.296	1.338	1.761	2.086

^aB. S. Shastry, Ref. 6, 1976.

rectly get the high-density behavior of χ_F/χ and κ_F/κ from Eqs. (3.3), (3.4), and (3.13)–(3.16) as

$$\chi_F/\chi = 1 - \lambda + \frac{1}{2}\lambda^2 [C_1 - \ln\lambda], \quad (4.1a)$$

$$\kappa_F/\kappa = 1 - \lambda - C_2\lambda^2. \quad (4.2a)$$

These are to be contrasted with the results of I as $r_s \rightarrow 0$.

$$\chi_F/\chi = 1 - \lambda - \lambda^2 [\ln\lambda + C_3], \quad (4.1b)$$

$$\kappa_F/\kappa = \chi_F/\chi. \quad (4.2b)$$

The exact results in this limit are known to be^{6,10}

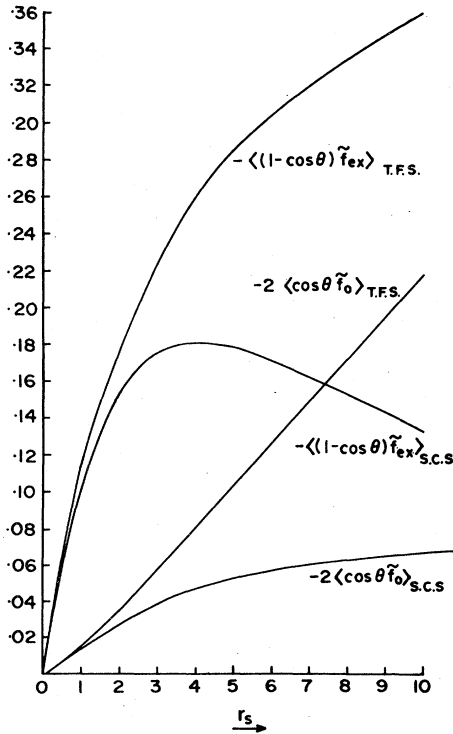


FIG. 4. Contributions from \tilde{f}_0 and \tilde{f}_{ex} to the spin susceptibility are plotted for various r_s . (TFS is Thomas-Fermi screening, SCS is self-consistent screening.)

TABLE III. Fermi-surface effective mass.

r_s	1	2	3	4	5	6
m^*/m	0.970	0.991	1.011	1.027	1.040	1.0489

$$\chi_F/\chi = 1 - \lambda + \frac{1}{2}\lambda^2 [0.306 - \ln\lambda], \quad (4.1c)$$

$$\kappa_F/\kappa = 1 - \lambda - (1 - \ln 2)\lambda^2. \quad (4.2c)$$

In deriving (4.1c) and (4.2c) the dynamically screened interaction is used as it should be. Thus the inclusion of the antiparallel spin function gives the correct logarithmic behavior in the high-density limit for both these quantities. The constants C_1 and C_2 are, however, not the same (we get $C_1 = \ln 4$, $C_2 = 1 - 2 \ln 2$). As discussed in Sec. II, this was already expected.

Turning to the metallic density ranges, we have plotted the functions \tilde{f}_0 and \tilde{f}_{ex} for various μ and r_s in Fig. 3, using the calculated ξ^2 . The function \tilde{f}_0 is seen to increase in magnitude with increasing r_s , and becomes more pronounced and peaked for $\mu = -1$. The function \tilde{f}_{ex} , on the other hand, becomes flatter at higher r_s . We present the computed values of the paramagnetic susceptibility in Table II. The new results are compared with our previous work I and the RPA results.⁶ We also present the results for the case when ξ^2 is taken to be the Thomas-Fermi value 4λ , and substituted in Eqs. (3.9), (3.11), and (3.4). These are quite close to those of I, but considerably smaller than the other two. To understand this situation further, we have plotted in Fig. 4, the two terms $-\langle(1-\mu)\tilde{f}_{ex}\rangle$ and $-2\langle\mu\tilde{f}_0\rangle$ for various densities in the new self-consistent ξ^2 case as well as in the Thomas-Fermi case. We first note that both terms are positive, i.e., both the exchange and the anti-

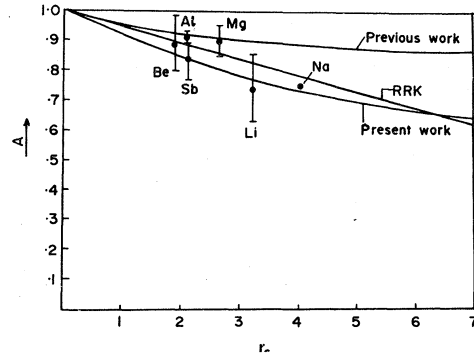


FIG. 5. Plasmon dispersion coefficient A for various values of r_s . The data on Mg and Na are from Refs. 19 and 20, and the rest from Ref. 14. The curve marked RRR is from Ref. 18.

parallel spin parts favor a large susceptibility enhancement. The antiparallel term contribution is seen to increase with increasing r_s in both cases, thus emphasizing its importance at metallic densities. The interesting point to note is that the large magnitude of ξ^2 in the self-consistent screening case depresses the contributions arising from both the exchange and antiparallel terms. This is a very significant result since it shows that a tendency towards a large compressibility (a singlet electron-hole property) is unfavorable towards a large susceptibility (a triplet electron-hole property). It should also be emphasized that the antiparallel spin interaction actually favors an enhancement of the spin susceptibility rather than otherwise, as is sometimes stated in literature. However, we must mention that our spin susceptibility is somewhat difficult to be reconciled with the recent experimental results of Kushida,

Murphy, and Hanabusa,¹⁷ who find that the RPA is extremely satisfactory, at least for $r_s < 4$.

The computed values of m^*/m are presented in Table III and seen to be very close to unity. We present the calculated curve for A in Fig. 5 and compare with our previous results as well as the unscreened HF result¹⁸ [obtained by setting $\tilde{f}_0 = 0$ and $\xi^2 = 0$ in Eq. (3.8)], $A = 1 - \frac{1}{3}\lambda$. The experimental data on magnesium and sodium are taken from the recent work of Chen¹⁹ and Gibbons *et al.*,²⁰ and the rest from Raether's review article.¹⁴ The overall agreement seems to be better with the present calculation.

In conclusion, we have proposed a self-consistent scheme for the electron gas which has the virtue of incorporating the exchange and the antiparallel spin correlations, and yet retains the ease with which most of the long-wavelength properties can be calculated.

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³Note that the order in which the limiting procedures for \vec{q} and ω has to be carried out on the vertex function has not been written correctly in Eq. (5) of Ref. 1. It should be $\lim_{\omega \rightarrow 0} \lim_{q \rightarrow 0} \Lambda(\vec{k}, q)$. This implies that the calculation in Ref. 1 satisfies the Ward identity exactly rather than, as stated there, only approximately.

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