Spin correlations in the low-density electron system

F. Green
Commonwealth Scientific and Industrial Research Organization, Division of Radiophysics, Epping 2121, Sydney, Australia

D. Neilson and L. Świerkowski
School of Physics, University of New South Wales, Kensington 2033, Sydney, Australia

J. Szymański
Telecom Australia Research Laboratories, 770 Blackburn Road, Clayton 3168, Australia

D. J. W. Geldart
Physics Department, Dalhousie University, Halifax, Nova Scotia, Canada B3H 3J5

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We have calculated the spin susceptibility $\chi_\sigma(\mathbf{q},\omega)$ within a microscopic model over the full range of densities of the electron liquid in the paramagnetic state. Electron-electron interactions are described by static random-phase-approximation screening modified by a local-field correction which takes into account the exchange-correlation hole in the low-density regime. We focus attention on the dynamic properties of the system, calculating the spin-spin susceptibility $\chi_\sigma(\mathbf{q},\omega)$. Our results can be represented in terms of a complex Stoner-like enhancement function $I(\mathbf{q},\omega)$ with an explicit dependence on the wave number $\mathbf{q}$ and frequency ω. We find except for very large $\mathbf{q}$ and ω that $I(\mathbf{q},\omega)$ has only a weak functional dependence on $\mathbf{q}$ and ω and is nearly real, justifying the original Stoner approximation for a wide range of $\mathbf{q}$ and ω. We find when $I(\mathbf{q},\omega)$ does develop a $\mathbf{q}$ dependence, that this corresponds to a buildup of short-range spin correlations in the system that goes beyond the scope of the original Stoner model. Our results provide a first-principles determination of the density dependence of the Stoner enhancement factor. Finally, we find that paramagnons persist well away from the ferromagnetic transition.

I. INTRODUCTION

The ground state of the electron gas at high density has uniform density and is paramagnetic. As the density is lowered interaction-induced correlations between electrons become strong enough to cause a spontaneous transition to a spin-polarized ferromagnetic state. The formation of this new phase is accompanied by a change in symmetry of the ground state. The ferromagnetic ground state has a net magnetization and exhibits long-range order. At still lower densities, the spin-polarized electron gas undergoes a second phase transition by crystallizing to form a Wigner solid. Estimates of the critical densities for these phase transitions are available from Monte Carlo data.[1] In terms of r_s, where the volume per electron is given by $\Omega_0 = 4\pi(r_s a_0)^3/3$ with a_0 being the Bohr radius, the transition from the paramagnetic state to the fully spin-polarized state is expected to occur at $r_s \equiv r_s^c = 75 \pm 5$ and the Wigner solid at $r_s = 100 \pm 20$.[1] The theoretical description of the strong electron correlations in these low-density régimes poses a major challenge in both of these cases.

Our present attention is focused on the spin-spin correlations in the intermediate- to low-density paramagnetic state. We have carried out a microscopic calculation of the wave number and frequency dependent spin response function $\chi_\sigma(\mathbf{q},\omega)$.

A well known phenomenological description of $\chi_\sigma(\mathbf{q},\omega)$ is provided by the Stoner model.[2] Within the Hubbard lattice model,[3]

$$\chi_\sigma(\mathbf{q},\omega) = \frac{\chi^0(\mathbf{q},\omega)}{1 - \bar{I}\chi^0(\mathbf{q},\omega)/\chi^0(0,0)}, \quad (1)$$

where

$$\chi^0(0,0) \equiv \lim_{\mathbf{q}\to 0} \chi^0(\mathbf{q},0) = \frac{m k_F}{\hbar^2 \pi^2}. \quad (2)$$

The function $\chi^0(\mathbf{q},\omega)$ is the Lindhard function[4] and corresponds to the spin-spin correlation function for a system of noninteracting electrons. The spin contribution to an experimentally measured susceptibility is given by

$$\chi_{\text{spin}} = \mu_B^2 \lim_{\mathbf{q}\to 0} \chi_\sigma(\mathbf{q},\omega = 0), \quad (3)$$

where μ_B is the Bohr magneton.

An essential feature of Eq. (1) is that all many-body interaction effects have been compressed into a single phenomenological parameter $\bar{I}$. This is strictly correct only within the Hartree-Fock approximation for the limiting case of short-range interparticle forces as modeled by contact interactions $V(\mathbf{r}-\mathbf{r}') \propto I\delta(\mathbf{r}-\mathbf{r}')$. For small

$\mathbf{q}/k_F$ and $\hbar\omega/E_F$ it is expected that Eq. (1) can provide a useful phenomenological description of spin-spin correlations in the paramagnetic phase. This has been the basis, for example, of the description of paramagnons in ^{3}He and nearly ferromagnetic metals such as Pd.[5,6] However, the ability of the Stoner model to describe quantitatively $\chi_\sigma(\mathbf{q},\omega)$ for an electron gas over a wide range of momentum, frequency, and density is certainly not obvious *a priori*, and our microscopic calculation of $\chi_\sigma(\mathbf{q},\omega)$ can shed independent light on its validity.

The outline of the remainder of this paper is as follows. In Sec. II we describe a first principles microscopic calculation of $\chi_\sigma(\mathbf{q},\omega)$ based directly on many-body methods.[7] The effective electron-electron interactions are described by a static random-phase-approximation (RPA) screened interaction with a local-field correction. The resulting integral equations are then solved numerically without further approximation. In Sec. III we discuss our results for the dynamical spin structure factor at small $\mathbf{q},\omega$,

$$S_\sigma(\mathbf{q},\omega) = \frac{2\hbar}{n}\Im m\chi_\sigma(\mathbf{q},\omega), \tag{4}$$

in terms of paramagnons and discuss the validity of the Stoner model. Section IV contains a summary of the results.

II. THEORY

The exact expression for the spin-spin susceptibility is[7]

$$\chi_\sigma(\mathbf{q},\omega) = -2\sum_{\mathbf{k}}\int\frac{d\nu}{2\pi i}G_{\mathbf{k}}(\nu)G_{\mathbf{k}+\mathbf{q}}(\nu+\omega)L_\sigma(\mathbf{k}\nu,\mathbf{q}\omega). \tag{5}$$

The vertex function L_σ is defined as

$$L_\sigma(\mathbf{k}\nu,\mathbf{q}\omega) = 1+\sum_{\mathbf{k}'}\int\frac{d\nu'}{2\pi i}\gamma^I_{\mathbf{k}\nu,\mathbf{k}'\nu'}(\mathbf{q}\omega)G_{\mathbf{k}'}(\nu') \times G_{\mathbf{k}'+\mathbf{q}}(\nu'+\omega)L_\sigma(\mathbf{k}'\nu',\mathbf{q}\omega), \tag{6}$$

where G is the single particle propagator and γ^I is the difference between the spin parallel and antiparallel electron-hole scattering function.

If the scattering function γ^I is taken to be a static effective interaction V_{eff}, then the equation becomes a sum of ladder graphs. The frequency integrals can be done analytically in this case and the vertex function L_σ then satisfies the integral equation

$$L_\sigma(\mathbf{k};\mathbf{q},\omega) = 1-\sum_{\mathbf{p}}V_{\text{eff}}(|\mathbf{k}-\mathbf{p}|) \times\frac{n_{\mathbf{p}-\mathbf{q}/2}-n_{\mathbf{p}+\mathbf{q}/2}}{\hbar\omega-\epsilon_{\mathbf{p},\mathbf{q}}+i\eta}L_\sigma(\mathbf{p};\mathbf{q},\omega). \tag{7}$$

The spin susceptibility $\chi_\sigma(\mathbf{q},\omega)$ is then given by

$$\chi_\sigma(\mathbf{q},\omega) = -2\sum_{\mathbf{k}}\frac{n_{\mathbf{k}-\mathbf{q}/2}-n_{\mathbf{k}+\mathbf{q}/2}}{\hbar\omega-\epsilon_{\mathbf{k},\mathbf{q}}+i\eta}L_\sigma(\mathbf{k};\mathbf{q},\omega), \tag{8}$$

where $n_{\mathbf{p}}$ is the Fermi-Dirac distribution,

$$\epsilon_{\mathbf{k},\mathbf{q}} = \epsilon^0_{\mathbf{k}+\mathbf{q}/2}+\Sigma_{\mathbf{k}+\mathbf{q}/2}-\epsilon^0_{\mathbf{k}-\mathbf{q}/2}-\Sigma_{\mathbf{k}-\mathbf{q}/2}\ , \tag{9}$$

$\epsilon^0_{\mathbf{p}}$ is the kinetic energy for free particles, and

$$\Sigma_{\mathbf{p}} = -\sum_{|\mathbf{k}|<k_F}V_{\text{eff}}(|\mathbf{p}-\mathbf{k}|) \tag{10}$$

is the self-energy. This forms a closed set of equations in the spirit of a self-consistent Hartree-Fock-like approximation.

The numerically exact solution of these equations was obtained by Szymański *et al.*,[8] who calculated the screened response function $\chi_{\text{sc}}(\mathbf{q},\omega)$ in the case of bare Coulomb interactions over a wide range of densities. A related integral equation was numerically solved at high density by Hamann and Overhauser[9] for the case of zero ω using an approximate form for the self-energy which is valid for small $\mathbf{q}$.

It should be emphasized that the procedure indicated above which uses the same V_{eff} in the expressions for both L_σ and Σ [Eqs. (7) and (10)] is consistent for the calculation of $\chi_\sigma(\mathbf{q},\omega)$ but should not be used to calculate $\chi_{\text{sc}}(\mathbf{q},\omega)$ except in the case of bare Coulomb interactions.[7,10] The essential reason for this is that the general four-point scattering function for parallel spins as deduced from Eq. (10) is

$$\gamma^{\uparrow\uparrow} = -V_{\text{eff}}+F, \tag{11}$$

where F is a complicated functional which does not need to be specified here. The corresponding function for antiparallel spins is

$$\gamma^{\uparrow\downarrow} = F. \tag{12}$$

The scattering function γ^I entering Eq. (7) is

$$\gamma^I = \gamma^{\uparrow\uparrow}-\gamma^{\uparrow\downarrow} = -V_{\text{eff}}. \tag{13}$$

We emphasize that this major simplifying feature applies rigorously to $\chi_\sigma(\mathbf{q},\omega)$ but does not apply to $\chi_{\text{sc}}(\mathbf{q},\omega)$.

We now consider how to specify $V_{\text{eff}}(\mathbf{q})$. In Ref. 8, Eq. (7) was solved with the bare Coulomb interaction. Neglect of screening overestimates the importance of the exchange terms to the RPA. In this case the ferromagnetic transition occurs at an electron density of $r_s = \pi[9\pi/4]^{\frac{1}{3}} = 6.03$. At the other extreme, if $V_{\text{eff}}(\mathbf{q})$ is approximated by static screening of either the Thomas-Fermi form or the static RPA form then the ferromagnetic transition does not occur at all no matter how small the electron density is made. For electron liquid densities $r_s \gtrsim 5$, exchange and correlation effects become increasingly important. The large depletion of density in the vicinity of each electron diminishes the efficiency of screening in the particle-hole channel. We can approximate the effect of this by introducing a local field surrounding each electron $[1-G(\mathbf{q})]$ which modifies its interaction with other electrons (see, for example, Ref. 11). The RPA expression for the screened interaction between electrons

$$V(\mathbf{q}) = \frac{4\pi e^2/\mathbf{q}^2}{1+[4\pi e^2/\mathbf{q}^2]\chi^0(\mathbf{q},\omega=0)} \tag{14}$$

is replaced by the effective screened interaction,

$$V_{\text{eff}}(\mathbf{q}) = \frac{4\pi e^2/\mathbf{q}^2}{1+[4\pi e^2/\mathbf{q}^2][1-G(\mathbf{q})]\chi^0(\mathbf{q},\omega=0)} \ . \tag{15}$$

The local field $[1-G(\mathbf{q})]$ is small compared with unity for $\mathbf{q}/k_F \gtrsim 1$, reflecting the depletion of density around each electron for distances smaller than the average interparticle spacing.

Here we determine $G(\mathbf{q})$ from the Monte Carlo numerical simulation calculations of Ceperley and Alder.[1] We write

$$G(\mathbf{q}) = \frac{2}{3}\frac{\mathbf{q}^2}{\mathbf{q}^2+q_s^2} \ . \tag{16}$$

The parameter q_s is determined by the requirement that the compressibility[10] agrees with the value obtained from Ref. 1. The large $\mathbf{q}$ behavior $G(\mathbf{q})$ should be determined by the requirement[12]

$$\lim_{\mathbf{q}\to\infty} G(\mathbf{q}) = \tfrac{2}{3}[1-g(\mathbf{r}=0)] \ , \tag{17}$$

where $g(\mathbf{r})$ is the pair correlation function. At the low densities with which we are working $g(\mathbf{r}=0)$ can be set equal to zero[1] so that Eq. (16) has the correct limiting behavior.

We have solved Eq. (7) exactly following the numerical procedure described in detail in Ref. 8. We determined the spin-spin susceptibility $\chi_\sigma(\mathbf{q},\omega)$ from Eq. (8) and used Eq. (4) to determine the spin structure factor $S_\sigma(\mathbf{q},\omega)$.

A. Static aspects

While in the present calculation our interest is centered on the dynamic spin-spin correlations at finite $\mathbf{q}$ and ω, it is useful to make two observations about the static properties of our model.

First, in the limit of small $\mathbf{q}$ Eq. (7) can be solved analytically for $\omega=0$ and has the solution

$$\lim_{\mathbf{q}\to 0}\frac{\chi_\sigma(\mathbf{q},0)}{\chi^0(\mathbf{q},0)} = \left[1-\frac{m}{8\pi^2\hbar^2k_F^3}\int_0^{2k_F} dp\, p^3 V^{\text{eff}}(\mathbf{p})\right]^{-1} . \tag{18}$$

Analysis of the long wavelength limit of $\chi_\sigma(\mathbf{q},0)$ formally determines the small $\mathbf{q}$ structure to be

$$\chi_\sigma(\mathbf{q},\omega=0)-\chi_\sigma(\mathbf{q}\to 0,\omega=0) = -b\mathbf{q}^2+\cdots \ . \tag{19}$$

The derivation of this result follows the same lines as the derivation of the self-consistent Hartree-Fock response functions,[13] but a detailed examination shows that the coefficient b has a weak logarithmic divergence, even though the interparticle interaction is screened. This singularity arises from electron-hole scattering across the Fermi surface with momentum transfer $2k_F$. The underlying physical reason is the sharp Fermi surface and the change in the character of screening and correlations when the scattering wave vector no longer spans the Fermi surface. It has the same origin as the nonanalytic structure in $\chi_\sigma(\mathbf{q},\omega=0)$ found by Geldart and Rasolt.[14] Even in the case of dynamically screened interactions, the long wavelength structure of the susceptibility was found to be

$$\chi_\sigma(\mathbf{q},\omega=0)-\chi^0(0,0) = -b'\mathbf{q}^2-b''\mathbf{q}^2\ln|\mathbf{q}|+\cdots \ , \tag{20}$$

where both b' and b'' are finite. However, $b''/b' \ll 1$ so the nonanalytic $\mathbf{q}^2\ln|\mathbf{q}|$ contribution is much smaller than the regular $\mathbf{q}^2$ term and is not of practical importance. The nonanalytic variation of $\chi_\sigma(\mathbf{q})$ at small $\mathbf{q}$ is also weak in the present work and will not be further discussed.

The second observation is that our model predicts a divergence in $\chi_\sigma(\mathbf{q}=0)$ at density $r_s^c = 58$ [see Eq. (18)]. Quader, Bedell, and Brown[15] found, using the induced interaction model to determine Landau parameters, that in the small $\mathbf{q}$ limit the buildup of spin fluctuations in the particle-hole cross channel could suppress a second-order phase transition to the ferromagnetic phase altogether. Quader's results were for a system with finite range interactions and it is not clear for our Coulombic system whether this mechanism would still suppress the instability. It is even less clear that the mechanism would significantly influence the paramagnon peaks occurring at finite $\mathbf{q}$ and ω. In ^{3}He the paramagnon peaks are known to persist [although the mechanism for this is thought to be associated mainly with an enhancement of $\chi_\sigma(\mathbf{q})$ due to an increase in the effective mass].

III. RESULTS AND DISCUSSION

In the present calculation we are not interested in determining the phase diagram for the system, but rather the dynamic spin-spin correlations at finite $\mathbf{q}$ and ω well inside the paramagnetic phase. We now present results deduced from our full numerical solution of Eq. (7).

Figure 1 shows the spin structure factor $S_\sigma(\mathbf{q},\omega)$ at $r_s = 20$, 40, and 55 for $\mathbf{q}/k_F = 0.1$. Also shown is the corresponding curve for the noninteracting case. Even for $r_s = 20$ there is already a large peak on the low-energy side of the central peak for the noninteracting case. This peak can be identified with the paramagnon. As r_s increases the paramagnon peak becomes sharper and higher, and moves towards $\omega = 0$. It is interesting that the paramagnon peak is observable at comparatively high densities which are well above the density for the ferromagnetic transition. This suggests that the system exhibits dynamical ferromagnetic trends long before any actual transition point is reached (see also Fig. 5). Figure 1(b) shows $S_\sigma(\mathbf{q},\omega)$ for $\mathbf{q}/k_F = 0.25$, 0.5, and 0.75 at $r_s = 55$.

The dispersion of the paramagnon peak as a function of $\mathbf{q}$ is shown in Fig. 2 for $r_s = 55$. The gradient of the dispersion is very flat and the peak rapidly approaches $\omega = 0$ as $\mathbf{q}$ goes towards zero. It is interesting to note that it is only at very small values of $\mathbf{q}/k_F$ that the curve can display the linear behavior predicted by the Stoner model.

The most important features of the $\mathbf{q}$ and ω dependence of the dynamic $\chi_\sigma(\mathbf{q},\omega)$ can be represented in terms of a complex function $\bar{I}(\mathbf{q},\omega)$ which is defined by

$$\chi_\sigma(\mathbf{q},\omega) \equiv \frac{\chi^0(\mathbf{q},\omega)}{1-\bar{I}(\mathbf{q},\omega)\chi^0(\mathbf{q},\omega)/\chi^0(0,0)} \,. \tag{21}$$

In the Stoner model it is assumed that $\bar{I}(\mathbf{q},\omega)$ is real and independent of $\mathbf{q}$ and ω. It is interesting to determine the extent to which this approximation is valid. From the numerical results for $\chi_\sigma(\mathbf{q},\omega)$ we can obtain the real and imaginary part of $\bar{I}(\mathbf{q},\omega)$. In the regime of well developed paramagnons we find $\Im m\bar{I}(\mathbf{q},\omega)$ to be very small and $\Re e\bar{I}(\mathbf{q},\omega)$ to be essentially independent of frequency (see Fig. 3). This is consistent with the Stoner model. For larger $\mathbf{q}$ and ω, $\bar{I}(\mathbf{q},\omega)$ shows significant structure and the description of $\chi_\sigma(\mathbf{q},\omega)$ in terms of the Stoner model would not be valid.

In Fig. 4(a) we plot the static spin susceptibility $\chi_\sigma(\mathbf{q})$ for $r_s = 55$. Shown for comparison is $\chi_\sigma^{\text{Stoner}}(\mathbf{q})$ given by Eq. (1), with the parameter $\bar{I}$ adjusted so that $\chi_\sigma(\mathbf{q}) \equiv$ $\chi_\sigma^{\text{Stoner}}(\mathbf{q})$ for $\mathbf{q}=0$. We see that $\chi_\sigma^{\text{Stoner}}(\mathbf{q})$ is a remarkably good approximation to $\chi_\sigma(\mathbf{q})$ if the correct value of $\bar{I}$ is used.

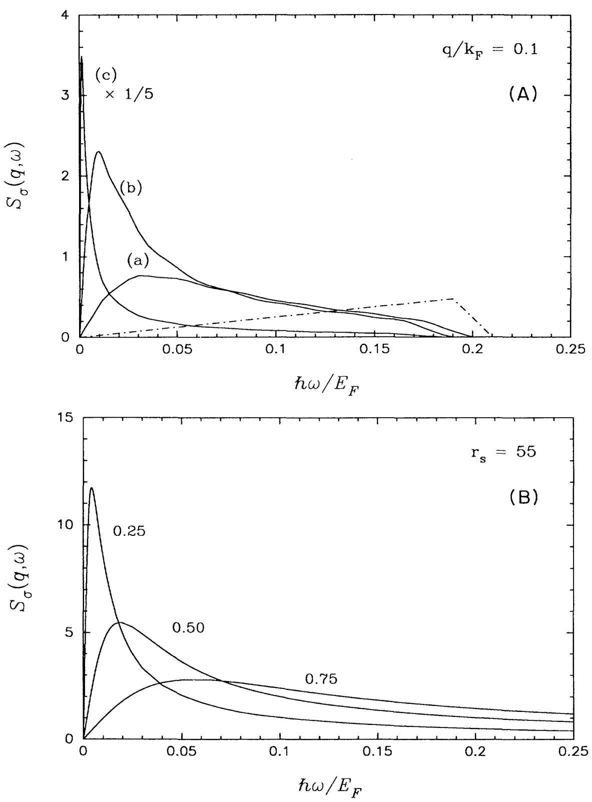

FIG. 1. (a) The spin structure factor $S_\sigma(\mathbf{q},\omega)$ as a function of ω for $\mathbf{q}/k_F = 0.1$. The labels on the curves correspond to $r_s = 20$ (a), $r_s = 40$ (b), and $r_s = 55$ (c). The dotted line is the corresponding curve for the noninteracting case. (b) $S_\sigma(\mathbf{q},\omega)$ for $\mathbf{q}/k_F = 0.25$, 0.5, and 0.75 at $r_s = 55$.

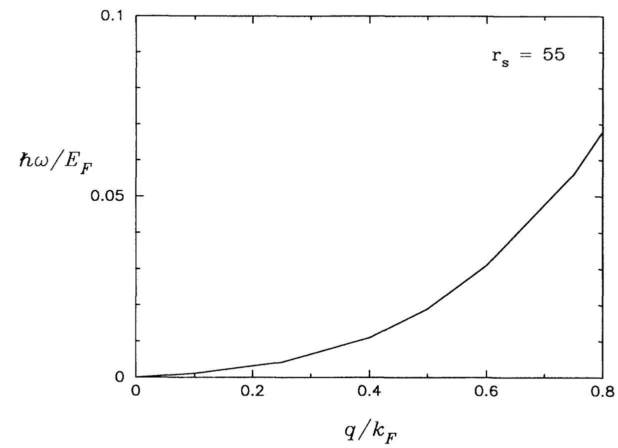

FIG. 2. The dispersion of the paramagnon peak as a function of $\mathbf{q}$ for $r_s = 55$.

We can represent the wave number dependence of $\chi_\sigma(\mathbf{q},\omega=0)$ in terms of the real function $\bar{I}(\mathbf{q})$

$$\chi_\sigma(\mathbf{q},0) \equiv \frac{\chi^0(\mathbf{q},0)}{1-\bar{I}(\mathbf{q})\chi^0(\mathbf{q},0)/\chi^0(0,0)} \,. \tag{22}$$

Figure 4(b) confirms that $\chi_\sigma^{\text{Stoner}}(\mathbf{q})$ is a remarkably good approximation to $\chi_\sigma(\mathbf{q})$. For $|\mathbf{q}| \lesssim 2k_F$ we see that $\bar{I}(\mathbf{q})$ is almost flat, but there is a peak centered around $|\mathbf{q}| \approx 2k_F$. This peak reflects the tendency of the electron gas to sustain *short-range* spin correlations induced by exchange and correlation, an effect which is beyond the scope of the original Stoner model to treat. The maximum of $\chi_\sigma(\mathbf{q})$ itself is at $\mathbf{q}=0$ so any instability is directed towards a ferromagnetically ordered state rather than, for example,

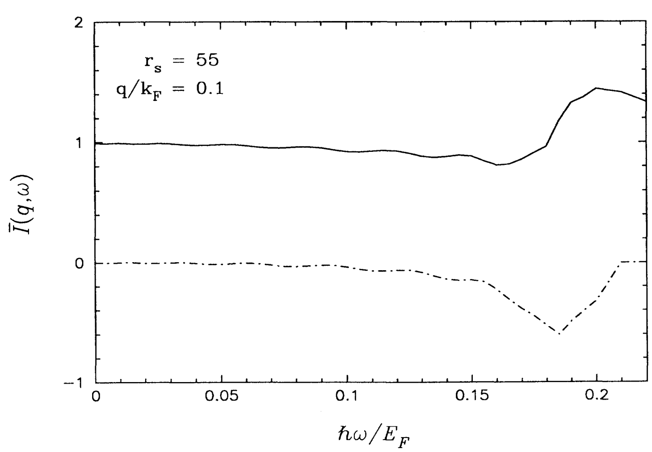

FIG. 3. The function $\bar{I}(\mathbf{q},\omega)$ defined in Eq. (21) as a function of ω for $\mathbf{q}/k_F = 0.1$ and $r_s = 55$. The solid line is the real part and the dotted line the imaginary part. The position of the paramagnon peak is at $\hbar\omega/E_F \approx 0.001$ [see Fig. 1(a)].

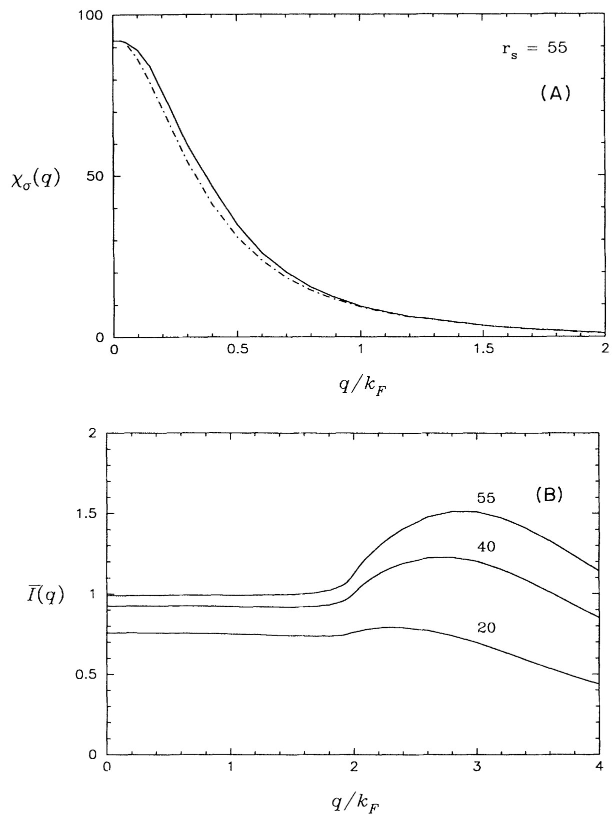

FIG. 4. (a) The static spin susceptibility $\chi_\sigma(\mathbf{q})$ for $r_s = 55$ normalized to the noninteracting $\chi_\sigma^0(\mathbf{q}=0)$. The dotted line is $\chi_\sigma^{\rm Stoner}(\mathbf{q})$ (see text). (b) $\bar{I}(\mathbf{q})$, defined by Eq. (22), for density $r_s = 20$, 40, and 55.

a spin density wave state. At large $\mathbf{q}$, $\bar{I}(\mathbf{q})$ decreases, falling off as $1/\mathbf{q}^2$.[16]

Setting $\bar{I} = \lim_{\mathbf{q}\to 0} \bar{I}(\mathbf{q}, \omega = 0)$, Eq. (18) provides us with a straightforward analytic expression for the Stoner parameter,

$$\bar{I} = \frac{m}{8\pi^2\hbar^2 k_F^3} \int_0^{2k_F} dp\, p^3 V^{\rm eff}(\mathbf{p}). \tag{23}$$

We note in Fig. 5 that $\bar{I}$ as a function of decreasing density initially increases rapidly and then more slowly approaches the critical value $\bar{I} = 1$. Thus $\chi_\sigma(\mathbf{q}, \omega)$ is enhanced over the noninteracting value for a wide range of densities. This is the underlying cause of the persistence of the paramagnon peak to densities so far away from any spin ordered phase. To make this point clear we note that in Fig. 5 $\bar{I}$ at $r_s/r_s^c = 0.6$ is 10% less than the critical value $\bar{I} = 1$. This corresponds to a density five times larger than the critical value.

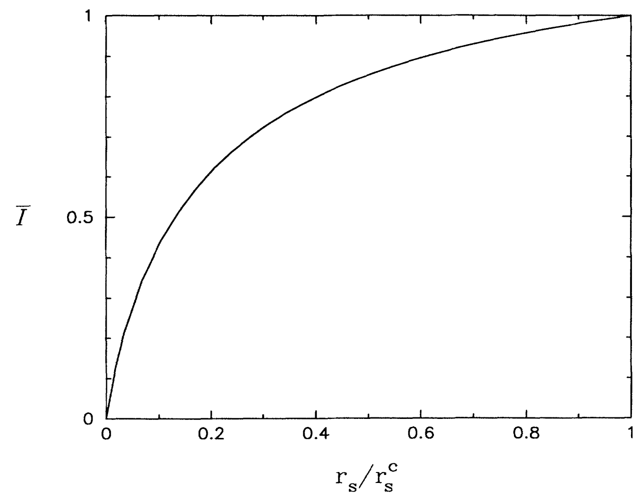

FIG. 5. The Stoner parameter $\bar{I}$ as a function of r_s/r_s^c, where $r_s^c = 58$ identifies the density at which our $\chi_\sigma(\mathbf{q})$ diverges.

IV. CONCLUSION

We have presented a parameter-free microscopic study of paramagnetic fluctuations in the electron liquid throughout the paramagnetic region of phase space. Our results confirm the phenomenological Stoner model prediction of the appearance of a paramagnon peak in the spin structure factor $S_\sigma(\mathbf{q}, \omega)$ for momentum transfers $|\,\mathbf{q}\,| \lesssim k_F$. The peak moves towards $\omega = 0$ as the transition is approached. We determine the Stoner parameter $\bar{I}(r_s)$ as a function of density by using our calculated value of $\chi_\sigma(\mathbf{q})$ at $\mathbf{q} = 0$ in the Stoner expression. With this $\bar{I}(r_s)$ the Stoner model is found to give a good representation of our $\chi_\sigma(\mathbf{q}, \omega)$ for $\mathbf{q} \lesssim 2k_F$ and $\hbar\omega \lesssim 8\epsilon_F$. We also find strong short-range spin correlations which become particularly important at low densities. These lead to a wave number dependent $\bar{I}(\mathbf{q})$ with strong $\mathbf{q}$ dependence for $|\,\mathbf{q}\,| \gtrsim 2k_F$. This dependence is absent in the Stoner model.

An interesting prediction from our results is that the paramagnon peak persists up to unexpectedly high densities where one would not *a priori* expect spin alignment effects. This is clearly seen in the density dependence of the susceptibility enhancement factor $[1 - \bar{I}(r_s)]^{-1}$.

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