Spin susceptibility in a two-dimensional electron gas

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The problem of the many-body enhancement of the static spin susceptibility at long wavelengths and its relation to the quasiparticle effective mass is investigated for a normal electron gas in two-dimensional space as a function of the electronic density. We start from a discussion of the results of the simple Hartree-Fock approximation for various interaction potentials and proceed to develop a complete theory. We find that the effects of the electron-electron interaction are significantly larger than in the familiar three-dimensional case. Our approach is based on a new self-consistent scheme which goes beyond the simple random-phase approximation by explicitly allowing for charge- and spin-fluctuation-induced vertex corrections of the Hubbard type. We show that when the latter are neglected, the many-body enhancement of the spin susceptibility can be cast in a remarkably simple and elegant analytic form.

I. INTRODUCTION

The enhancement of the paramagnetic spin susceptibility χ_S of an electron gas (EG) due to the electron-electron interaction is a classic many-body problem. Pioneering work on the subject goes all the way back to Bloch, Wigner, and Sampson, and Seitz.[1] The challenging aspect of this problem is the fact that at metallic densities the concomitant effects of exchange and correlation are both large but opposite in sign and eventually lead to a value for χ_S sensibly larger than the free-electron Pauli value. Both for the three-dimensional (3D) and the two-dimensional (2D) case within the Hartree-Fock (HF) approximation, in which only the exchange contribution is retained, χ_S actually diverges for values of the parameter r_s, the average electron distance in Bohr radii, respectively equal to $(9\pi/4)^{1/3} \approx 6.03$ and $\pi/2^{1/2} \approx 2.22$. The situation is further complicated by the appearance of the more exotic instabilities of the spin-density-wave type.[2,3] At metallic densities the effect of the correlations is to rid the spin susceptibility of these instabilities. Ultimately the correct many-body enhancement results from a delicate balance of the two contributions.

The value of χ_S is physically accessible through a number of different experimental techniques. The situation is particularly favorable since the effects of the electron-phonon interaction can in general be safely neglected. This makes the spin-susceptibility problem an especially valuable testing ground for many-body theories.

For the case of a 3D EG there are reported data from conduction-spin-resonance, spin-wave, Knight-shift, and total-susceptibility measurements.[4] Several theoretical methods have been employed for the solution of this problem for the 3D EG.[3,5-9] In general it is believed that there exists a reasonably good agreement between theory and experiment, although Fig. 6 of Ref. 4 may raise some doubts since the various theories arguably seem to cover all the conceivable (as well the inconceivable), experimental results. More specifically there exists a theoretical "consensus curve" of χ_S versus r_s, which not only appears to be supported by the experimental results, but has been reproduced within a few percent via a variety of diverse many-body techniques, ranging from self-consistent-field approaches,[3,9] microscopic Landau Fermi-liquid analyses,[6,7] to full fledged perturbative-theoretic calculations.[5,7,8] In all cases the amount of analytic and numerical work necessary to reach the final answer is considerable.

The major problem with the familiar three-dimensional metals is that for obvious reasons the density dependence of the many-body enhancement of χ_S can only be approximately measured by looking at different materials. This makes it difficult to clearly discern the sought phenomenon amid band-structure effects whose relevance varies from metal to metal.

For the case of a 2D EG the study of the many-body enhancement of the static paramagnetic spin susceptibility has a decisive advantage in that currently available quasi-two-dimensional electronic systems, notably the Si-inversion-layer structures, are characterized by the rather interesting possibility of varying the carrier density and other intrinsic parameters within the same sample.[10] This offers the remarkable possibility of measuring χ_S for a range of density values while keeping constant other uninteresting (albeit not necessarily irrelevant) factors.

In this case an experimental determination of χ_S can be achieved by concomitantly measuring, by magnetotransport techniques, both the quasiparticle effective mass[11,12] and the anomalous Landé g factor.[13,14]

The purpose of the present paper is to provide a theory of the many-body enhancement of the static paramagnetic spin susceptibility in a normal 2D EG at long wavelengths and discuss the density dependence of this remarkable phenomenon as well as its relation to the quasiparticle mass renormalization.

A natural starting point for our analysis is provided by a discussion of the Hartree-Fock theory, which sets the stage for a more complete and reliable approach. As it will be shown however, the inclusion of correlation effects is necessary. Janak was the first to attempt the study of the effects of screening in his study of the effects of the electronic interactions on the Landé g factor.[15] His theory suffered, however, from serious shortcomings and was limited to a static approach to screening. Work along similar lines can be found in Refs. 16–18.

The effect of correlations can more satisfactorily be included by employing, as a first approximation, an approach due to Hamann and Overhauser and based on the dynamically screened exchange approximation.[3] It is quite satisfying, although hitherto unnoticed, that in this case the many-body enhancement of the spin susceptibility can be cast in a simple and elegant analytic form.

In order to go beyond this useful, but necessarily simplified, approach we then proceed to develop a complete theory based on the Landau theory of the Fermi liquids and a new self-consistent scheme in which the effects of charge- and spin-fluctuation-induced vertex corrections are accounted for following the procedure first suggested, in its most elementary form, by Hubbard.[19] An extensive investigation of the relevance of these corrections in realistic situations has been discussed elsewhere.[20]

The present paper is structured as follows: In Sec. II we discuss several interesting results concerning the application of the Hartree-Fock theory to the case of various interaction potentials; in Sec. III we develop the formalism for the dynamically screened exchange approach and relate the many-body enhancement for the spin susceptibility to the quasiparticle effective mass; in Sec. IV we introduce the generalized Hubbard many-body local fields which account for charge- and spin-fluctuation-induced vertex corrections; in Sec. V we develop a general theory for the spin susceptibility by relating such a quantity to the quasiparticle effective interaction; finally, in Sec. VI we discuss our results and provide some conclusions.

II. HARTREE-FOCK THEORY

We start at first with an analysis of the Hartree-Fock (HF) theory. Within this approximate scheme one can readily obtain the static spin susceptibility $\chi_S(\mathbf{q},\omega)$ by following the procedure of Wolff.[21] One finds that $\chi_S(\mathbf{q},0)$ can be expressed as

$$\chi_S(\mathbf{q},0)=2\mu_B^2\sum_{\mathbf{p}}\frac{n_{\mathbf{p}-\mathbf{q}/2}-n_{\mathbf{p}+\mathbf{q}/2}}{E_{\mathbf{p}+\mathbf{q}/2}-E_{\mathbf{p}-\mathbf{q}/2}}u(\mathbf{p}), \tag{1}$$

where μ_B is the Bohr magneton, $n_{\mathbf{p}}$ is the momentum-space occupation number, and $E_{\mathbf{p}}$, the quasiparticle energy, is given by the familiar expression

$$E_{\mathbf{p}}=\frac{p^2}{2m}-\sum_{|\mathbf{p}'|<p_F}v(\mathbf{p}-\mathbf{p}'). \tag{2}$$

In Eq. (1) $u(\mathbf{p})$ is the solution of the integral equation

$$u(\mathbf{k})=1+\sum_{\mathbf{p}}\frac{n_{\mathbf{p}-\mathbf{q}/2}-n_{\mathbf{p}+\mathbf{q}/2}}{E_{\mathbf{p}+\mathbf{q}/2}-E_{\mathbf{p}-\mathbf{q}/2}}v(\mathbf{k}-\mathbf{p})u(\mathbf{p}), \tag{3}$$

$v(\mathbf{q})$ being the Fourier transform of the appropriate interaction potential. In the long-wavelength limit this equation is easily solved to give for χ_S the static value of the susceptibility, $\chi_S(\mathbf{q}\to 0,0)$, the following expression,

$$\frac{\chi_S}{\chi_P}=\frac{m^*}{m}u(p_F), \tag{4}$$

In Eq. (4) χ_P is the Pauli susceptibility given by $\mu_B^2N(0)$, where $N(0)=m/\pi\hbar^2$ is the density of states for a noninteracting electron gas in two dimensions. In Eq. (4) m^* is the quasiparticle effective mass defined in terms of the derivative of the quasiparticle energy evaluated at the Fermi wave vector p_F via the relation

$$v_{\mathrm{qp}}=\frac{p_F}{m^*}=\left(\frac{\partial E(\mathbf{p})}{\partial p}\right)_{p_F}. \tag{5}$$

For illustrative purposes we will first examine the simple case of a short-range (local) interaction which we model here via a delta-function potential so that $v(\mathbf{q})=C$, where C is a constant. In this case there is no correction to the bare mass and the susceptibility can be readily expressed in analytic form as follows:

$$\frac{\chi_S^{(\delta)}(z)}{\chi_P}=\frac{[1-(1-z^{-2})^{1/2}\Theta(1-z^{-2})]}{1-\frac{C}{2\mu_B^2}[1-(1-z^{-2})^{1/2}\Theta(1-z^{-2})]}, \tag{6}$$

where $z=q/2p_F$. It is clear that in this case the ratio is independent of the electronic density. In Fig. 1 we plot $\chi_S^{(\delta)}$ as a function of z for different values of the interaction strength C. We note that for $z<1$, $\chi_S^{(\delta)}$ is a constant

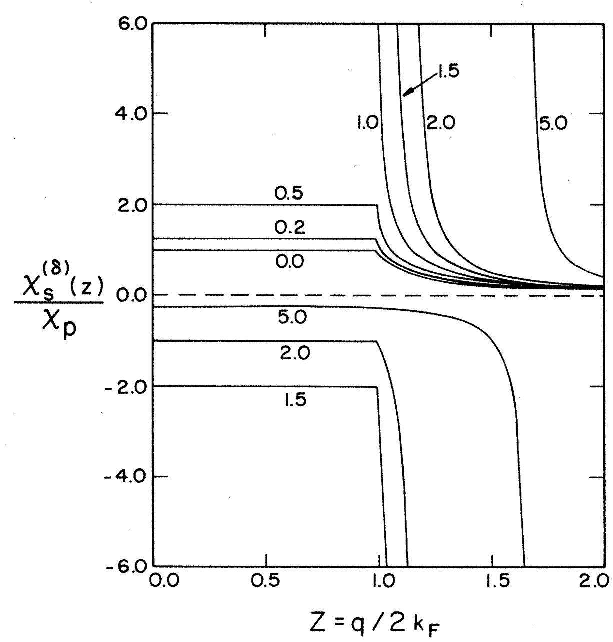

FIG. 1. Enhanced spin susceptibility $\chi_S^{(\delta)}(z)/\chi_P$ vs $z=q/2p_F$, given by Eq. (6) in text, for a delta-function interaction of strength C. The curves are for different values of $C/(2\mu_B^2)$.

whose value diverges as C tends to the critical value $2\mu_B^2$. For C larger than this value $\chi_S^{(\delta)}$ changes sign and decreases in magnitude. For $z>1$ the situation is more interesting. For C less than $2\mu_B^2$, $\chi_S^{(\delta)}$ is a monotonically decreasing function of z. When C exceeds this value, however, $\chi_S^{(\delta)}$ becomes negative (a sign of incipient ferromagnetic instability), and displays a singularity for $z=[1-(1-2\mu_B^2/C)^2]^{-1/2}$. This behavior is quialitatively not dissimilar from the one encountered in the 3D case first discussed by Wolff.[21]

We will consider next the case of a screened interaction potential which we write in the general form

$$v(\mathbf{q})=\frac{2\pi e^2}{q+2\alpha p_F}=\frac{2\pi e^2}{q+\dfrac{2^{3/2}\alpha}{r_s a_B}}, \tag{7}$$

where, as mentioned above, r_s is the mean electronic separation measured in units of the Bohr radius a_B, and is related to the electronic density via the relation $r_s=(\pi a_B{}^2 n)^{-1/2}$. In Eq. (7) α is a positive adjustable parameter which controls the range of the interaction. In the long-wavelength limit, using Eqs. (1), (3), and (5), one can obtain the following simple analytic formula for the HF susceptibility for this case:

$$\frac{\chi_S}{\chi_P}=\frac{m^*}{m}\left\{1-\frac{m^*}{m}\left[\frac{r_s}{2^{1/2}\pi}\frac{\Theta(\alpha^2-1)}{(\alpha^2-1)^{1/2}}\left[\frac{\pi}{2}-\tan^{-1}\frac{1}{(\alpha^2-1)^{1/2}}\right]-\frac{r_s}{2^{3/2}\pi}\frac{\Theta(1-\alpha^2)}{(1-\alpha^2)^{1/2}}\ln\left|\frac{1-(1-\alpha^2)^{1/2}}{1+(1-\alpha^2)^{1/2}}\right|\right]\right\}^{-1}, \tag{8}$$

where $\Theta(x)$ is the familiar step function and the effective mass m^* can be explicitly obtained from Eqs. (2), (5), and (7) and is given by

$$\frac{m}{m^*}=1-\frac{2^{1/2}r_s}{\pi}+\frac{\alpha r_s}{2^{1/2}}-\frac{(2\alpha^2-1)r_s}{2^{1/2}\pi}\frac{\Theta(\alpha^2-1)}{(\alpha^2-1)^{1/2}}\left[\frac{\pi}{2}-\tan^{-1}\frac{1}{(\alpha^2-1)^{1/2}}\right]$$
$$+\frac{(2\alpha^2-1)r_s}{2^{3/2}\pi}\frac{\Theta(1-\alpha^2)}{(1-\alpha^2)^{1/2}}\ln\left|\frac{1-(1-\alpha^2)^{1/2}}{1+(1-\alpha^2)^{1/2}}\right|. \tag{9}$$

A noteworthy feature of Eq. (8) is the manifest possibility of a polarization instability signaled by a diverging spin response. This situation can be realized when the denominator of Eq. (8) vanishes. This in turn occurs when, for a given α, r_s acquires the following critical value

$$r_s^*=2^{1/2}\left[\frac{2}{\pi}-\alpha+\frac{2\alpha^2}{\pi}\frac{\Theta(\alpha^2-1)}{(\alpha^2-1)^{1/2}}\left[\frac{\pi}{2}-\tan^{-1}\frac{1}{(\alpha^2-1)^{1/2}}\right]-\frac{\alpha^2}{\pi}\frac{\Theta(1-\alpha^2)}{(1-\alpha^2)^{1/2}}\ln\left|\frac{1-(1-\alpha^2)^{1/2}}{1+(1-\alpha^2)^{1/2}}\right|\right]^{-1}. \tag{10}$$

A plot of the above expression is displayed in Fig. 2. The critical value r_s^* increases almost linearly with α.

A specific case of interest is that of Thomas-Fermi screening, characterized by the condition $\alpha=r_s/2^{1/2}$. In this case, at variance with the corresponding 3D situation, the screening length is independent of the electron density. As can be readily verified, for this choice of α, the divergence does not occur and the spin susceptibility is a well-behaved simple monotonic function of r_s^*, which is displayed in Fig. 3 by the curve labeled TF. Notice that in this case the many-body enhancement of the spin response is rather small.

Finally for $\alpha=0$ one recovers the HF result for the Coulomb interaction. In this case, upon making use of Eqs. (8) and (9), one readily obtains the following expression for the HF spin susceptibility:

$$\frac{\chi_S}{\chi_P}=\frac{1}{1-\dfrac{\pi r_s}{2^{1/2}}}. \tag{11}$$

Care must be taken in this limit since the ratio m/m^* diverges here logarithmically for vanishing α, i.e.,

$$\frac{m}{m^*}\sim-\frac{r_s}{2^{1/2}\pi}\ln\frac{\alpha}{2} \quad \text{as } \alpha\to 0. \tag{12}$$

As shown in Eq. (11) above, a differential instability occurs for Coulomb interactions at $r_s^*=\pi/2^{1/2}\approx 2.22$. This is displayed by the curve labeled HF in Fig. 3. It should be mentioned at this point, however, that within HF such an instability is preempted by a sudden transition to a ferromagnetic ground state. As is readily found,

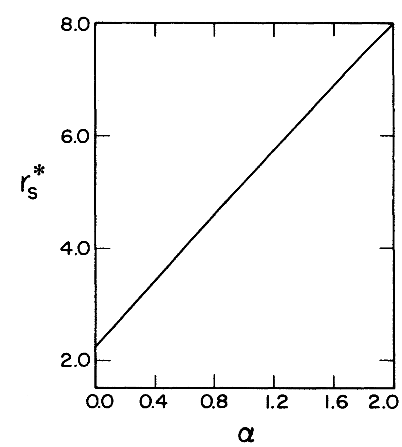

FIG. 2. Plot of r_s^* the critical value of the average electronic separation, given by Eq. (10) in text, vs the screening parameter α. The curve displays the divergence condition of spin susceptibility in the Hartree-Fock approximation with screened interaction.

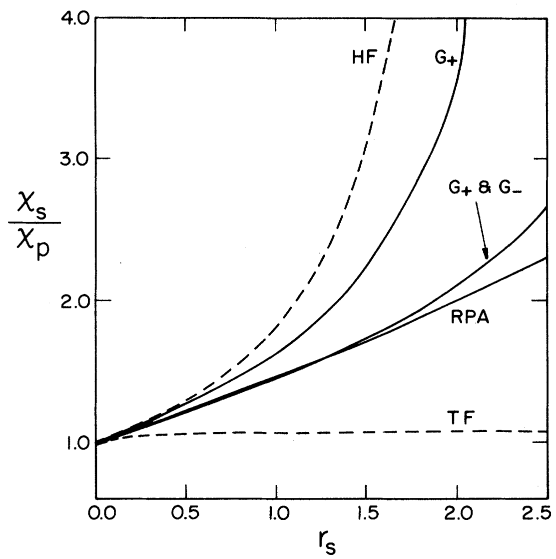

FIG. 3. Plot of the many-body susceptibility enhancement χ_S/χ_P vs the density parameter r_s. The solid curves labeled G_+ & G_-, G_+, and RPA correspond to the following three cases: (i) our full theory, (ii) no spin fluctuations, and (iii) no vertex corrections, respectively. The dashed curves labeled HF and TF correspond, respectively, to Hartree-Fock approximation and Hartree-Fock approximation with Thomas-Fermi screening. The meaning of these curves is explained in the text.

such a phenomenon is characterized by the Bloch condition $r_s \geq 3\pi 2^{1/2}/16(2^{1/2}-1) \approx 2.01$.

As well-known correlations do in general change the nature of the ground state and make the ferromagnetic phase energetically unfavorable, it is interesting to mention, however, how such a situation is drastically modified by the presence of a large quantizing magnetic field when a number of Landau levels are completely filled. In this case the energy separation between the Landau levels will in general lead to a quenching of the correlations, thereby restoring the (at times perhaps more interesting) HF scenario.[22]

III. GENERALIZED HARTREE-FOCK THEORY: THE HAMANN-OVERHAUSER APPROACH

In this section we will derive a simple formula for the susceptibility based on the dynamically screened exchange approach of Hamann and Overhauser which is known to lead to the correct result for the spin problem in 3D.[3] Here, and in what follows, we will focus our analysis on the case of the Coulomb interaction. The gist of the approach is as follows. One starts with the derivation of a suitable pseudo-Hamiltonian in which only the quasiparticle degrees of freedom of the electron gas appear explicitly. As first discussed in Ref. 3 this can be achieved by introducing an appropriate canonical transformation designed to eliminate, (more appropriately average out), the collective part of the spectrum of the system. Such a pseudo-Hamiltonian can be written as

$$H_{\mathrm{qp}} = \sum_{\mathbf{p},\sigma} E_{\mathbf{p}} :a^\dagger_{\mathbf{p},\sigma} a_{\mathbf{p},\sigma}: + \tfrac{1}{2} \sum_{\mathbf{p},\mathbf{p}',\mathbf{q},\sigma,\sigma'} \mathrm{Re}[\Lambda_C(\mathbf{q},\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}-\mathbf{q}})] :a^\dagger_{\mathbf{p}-\mathbf{q},\sigma} a^\dagger_{\mathbf{p}'+\mathbf{q},\sigma'} a_{\mathbf{p}',\sigma'} a_{\mathbf{p},\sigma}:, \tag{13}$$

where we have used a normal product representation, and $a^\dagger_{\mathbf{p},\sigma}$ ($a_{\mathbf{p},\sigma}$) is a creation (destruction) operator of a quasiparticle of momentum $\mathbf{p}$ and spin $\sigma = \pm 1$, and $\epsilon_{\mathbf{p}} = p^2/2m$. In Eq. (13) $E_{\mathbf{p}}$, the quasiparticle energy, is given by

$$E_{\mathbf{p}} = \epsilon_{\mathbf{p}} - \sum_{\mathbf{q}} \left[n_{\mathbf{p}-\mathbf{q}} \mathrm{Re}[\Lambda_C(\mathbf{q},\epsilon_{\mathbf{p}}-\epsilon_{\mathbf{p}-\mathbf{q}})] + \frac{1}{\pi} \mathrm{P} \int_0^\infty d\omega \frac{|\mathrm{Im}[\Lambda_C(\mathbf{q},\omega)]|}{\omega - \epsilon_{\mathbf{p}} + \epsilon_{\mathbf{p}-\mathbf{q}}} \right], \tag{14}$$

where the symbol P mandates that the principal value of the integral must be taken. In Eqs. (13) and (14) $\Lambda_C(\mathbf{q},\omega)$ is an effective potential which is defined in terms of $\chi_C(\mathbf{q},\omega)$, the full momentum- and frequency-dependent charge response function of the system, as follows:

$$\Lambda_C(\mathbf{q},\omega) = v(\mathbf{q})[1 + v(\mathbf{q})\chi_C(\mathbf{q},\omega)]. \tag{15}$$

Within the present approximation the function $\chi_C(\mathbf{q},\omega)$ can be written as

$$\chi_C(\mathbf{q},\omega) = \frac{\chi_0(\mathbf{q},\omega)}{1 - v(\mathbf{q})\chi_0(\mathbf{q},\omega)}, \tag{16}$$

where $\chi_0(\mathbf{q},\omega)$ is the familiar Lindhard function for a 2D EG.[23] It should be emphasized here that the expression for the quasiparticle energy $E_{\mathbf{p}}$ of Eq. (14) is appropriate for an *unpolarized* electron system. Moreover, in Eq. (14) the second term is the dynamically screened exchange, whereas the third one represents the appropriate contribution of the corresponding Coulomb hole. As should be clear from Eqs. (14)–(16), the present approximation is equivalent to the familiar random-phase approximation (RPA).[24,25]

The next step consists of studying the response of the quasiparticle gas to an externally applied sinusoidal magnetic field $H_0 \cos \mathbf{q}\cdot\mathbf{x}$. This can be achieved by adding to H_{qp} the suitably transformed coupling term H_{int} given by

$$H_{\mathrm{int}} = \tfrac{1}{2}\mu_B H_0 \sum_{\mathbf{k},\sigma} (S_z)_{\sigma\sigma} :a^\dagger_{\mathbf{k}+\mathbf{q},\sigma} a_{\mathbf{k},\sigma}: + \mathrm{H.c.}, \tag{17}$$

where H.c. stands for Hermitian conjugate, $(S_z)_{\uparrow\uparrow(\downarrow\downarrow)} = \pm 1$. Then, to do the equivalent of solving the HF equation, the total Hamiltonian given by $H_{\mathrm{qp}} + H_{\mathrm{int}}$ is again canonically transformed so as to remove the off-diagonal terms in the single quasiparticle operators. The transformed Hamiltonian is given by

$$H_{\mathrm{total}} = e^{-T}(H_{\mathrm{qp}} + H_{\mathrm{int}})e^{T}, \tag{18}$$

where the appropriate form of the operator T can be surmised from the HF analysis to be

$$T=\frac{1}{2}\sum_{\mathbf{k},\sigma} C(\mathbf{k})(S_z)_{\sigma\sigma}\, :a^{\dagger}_{\mathbf{k}+\mathbf{q}/2,\sigma}a_{\mathbf{k}-\mathbf{q}/2,\sigma}: -\text{H.c.}\ . \quad (19)$$

Then, upon requiring that the off-diagonal one-particle terms vanish, and upon defining

$$u(\mathbf{k})=(E_{\mathbf{k}+\mathbf{q}/2}-E_{\mathbf{k}-\mathbf{q}/2})C(\mathbf{k}), \quad (20)$$

one can see that $\chi_S(\mathbf{q},0)$ is given again by the HF expression of Eq. (4). In this case, however, $u(\mathbf{k})$ is determined by the following integral equation:

$$u(\mathbf{k})=1+\frac{1}{2}\sum_{\mathbf{p}}\left[\frac{n_{\mathbf{p}-\mathbf{q}/2}-n_{\mathbf{p}+\mathbf{q}/2}}{E_{\mathbf{p}+\mathbf{q}/2}-E_{\mathbf{p}-\mathbf{q}/2}}[\Lambda_C(\mathbf{k}-\mathbf{p},\epsilon_{\mathbf{p}+\mathbf{q}/2}-\epsilon_{\mathbf{k}+\mathbf{q}/2})+\Lambda_C(\mathbf{p}-\mathbf{k},\epsilon_{\mathbf{k}-\mathbf{q}/2}-\epsilon_{\mathbf{p}-\mathbf{q}/2})]u(\mathbf{p})\right]. \quad (21)$$

It is easily seen that if $\Lambda_C(\mathbf{q},\omega)$ is replaced by the screened potential $v(\mathbf{q})$, then one simply recovers the HF susceptibilities of the previous section.

In the limit of small $\mathbf{q}$ we have found that, interestingly enough, the integral equation (21) for $u(\mathbf{p})$ can be solved exactly. In this limit the many-body enhancement of the susceptibility can then be cast in the following elegant and suggestive form:

$$\frac{\chi_S}{\chi_P}=\frac{\dfrac{m^*}{m}}{1-\dfrac{m^*}{m}f_{2,3}(r_s)}, \quad (22)$$

where the functions $f_{2,3}(r_s)$ depend only on the density parameter r_s and the dimensionality of the system. For the 3D EG case, $f_3(r_s)$ is given by the following single quadrature,

$$f_3(r_s)=\int_0^1 dz\frac{1}{1+(18\pi^4)^{1/3}r_s^{-1}z+\dfrac{1-z}{2z^{1/2}}\ln\left|\dfrac{1+z^{1/2}}{1-z^{1/2}}\right|}. \quad (23)$$

For a 2D EG, instead, $f_2(r_s)$ can be written in a closed analytic form and is identical to that obtained from Eq. (8) for the case of Thomas-Fermi screening, i.e.,

$$f_2(r_s)=\frac{r_s}{8^{1/2}\pi}\left[\frac{2\Theta(r_s^2-2)}{(r_s^2/2-1)^{1/2}}\left[\frac{\pi}{2}-\tan^{-1}\frac{1}{(r_s^2/2-1)^{1/2}}\right]-\frac{\Theta(2-r_s^2)}{(1-r_s^2/2)^{1/2}}\ln\left|\frac{1-(1-r_s^2/2)^{1/2}}{1+(1-r_s^2/2)^{1/2}}\right|\right]. \quad (24)$$

A plot of both $f_3(r_s)$ and $f_2(r_s)$ is provided in Fig. 4. Both these curves are proportional to $-r_s\ln r_s$ in the limit of small r_s. It should be noted that the r_s dependence of $f_2(r_s)$ is more pronounced. The resulting values for χ_S/χ_P in three dimensions can be readily shown to reproduce the results of Ref. 3, i.e., the "consensus curve". A plot of the susceptibility ratio χ_S/χ_P for the case of a 2D EG is shown in Fig. 3 by the curve labeled RPA.[25] This curve was obtained using Eqs. (22) and (23) and the appropriate value of the effective mass ratio m^*/m as calculated from Eqs. (5) and (14).[20,26] Notice the large enhancement over the result of the Thomas-Fermi screened potential. It should be stressed here that for large r_s the many-body corrections are comparatively significantly larger in two dimensions.

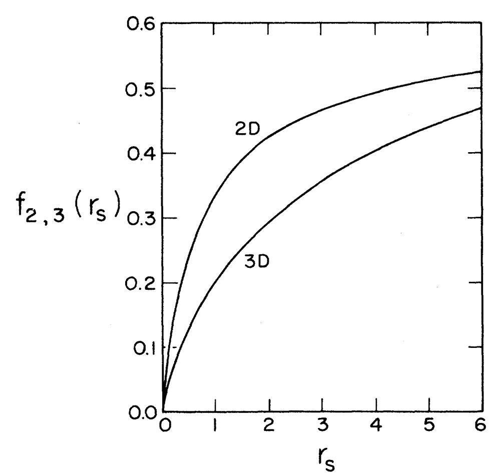

FIG. 4. Plot of $f_{2,3}$, Eqs. (20) and (21) in the text, vs the density parameter r_s. Notice that $f_2(r_s)$ is larger than its 3D counterpart and leads to a more pronounced many-body enhancement. Both functions behave as $-r_s\ln r_s$ for small r_s.

It is interesting to notice here that the perhaps surprising result of Eq. (24) (i.e., the fact that the RPA result basically displays the same structure as the Thomas-Fermi theory) is peculiar to the 2D situation and can be traced to the fact that in such a case the static Lindhard response function $\chi_0(\mathbf{q},0)$ is independent of the wave vector $\mathbf{q}$ for $q<2p_F$.

IV. HUBBARD VERTEX CORRECTIONS

In order to go beyond the dynamically screened exchange theory, we discuss here an approximate approach which allows one to account for the effects of charge- and spin-fluctuation-induced vertex corrections.

As originally suggested by Hubbard[19] and later exploited,[27] and generalized by several other authors,[28,29] it is possible to include some of the short-range effects of exchange and correlation by introducing suitable many-body local fields $G_+(\mathbf{q},\omega)$ and $G_-(\mathbf{q},\omega)$. For the sake of the present analysis it will suffice to define here these quantities through their relation to the full momentum- and frequency-dependent charge and spin susceptibilities of the system. A complete discussion of such a procedure can be found in Ref. 26. We have

$$\chi_C(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1-v(\mathbf{q})[1-G_+(\mathbf{q},\omega)]\chi_0(\mathbf{q},\omega)}, \tag{25}$$

and

$$\chi_S(\mathbf{q},\omega)=-\mu_B^2\frac{\chi_0(\mathbf{q},\omega)}{1+v(\mathbf{q})G_-(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)}. \tag{26}$$

Clearly the fields $G_+(\mathbf{q},\omega)$ and $G_-(\mathbf{q},\omega)$, respectively, account for charge- and spin-fluctuation-induced vertex corrections. In Eqs. (25) and (26) the quantity $\chi_0(\mathbf{q},\omega)$ differs from the usual Lindhard[30] function in that in its evaluation the expression for the momentum-space (bare) occupation number $n_\mathbf{p}$ appropriate to the interacting system must, in principle, be used.[26]

The many-body local fields not only enter the response functions, but can be shown also to modify in a significant fashion the effective potentials appearing in the theory.[31,26] For instance, in order to account for charge-fluctuation-induced vertex corrections, the expression for Λ_C of Eq. (15) must be modified as follows:

$$\Lambda_C(\mathbf{q},\omega)=v(\mathbf{q})\{1+v(\mathbf{q})[1-G_+(\mathbf{q},\omega)]^2\chi_C(\mathbf{q},\omega)\}. \tag{27}$$

The physical processes associated with $G_-(\mathbf{q},\omega)$ necessitate here further discussion. The inclusion of G_- in the theory accounts for the effects of spin fluctuations and leads to extra terms in the quasiparticle energy. For instance, for an unpolarized state, Eq. (14) is in this case modified to read[26]

$$E_\mathbf{p}=\epsilon_\mathbf{p}-\sum_\mathbf{q}\left[n_{\mathbf{p}-\mathbf{q}}\mathrm{Re}[\Lambda_C(\mathbf{q},\epsilon_\mathbf{p}-\epsilon_{\mathbf{p}-\mathbf{q}})+3\Lambda_S(\mathbf{q},\epsilon_\mathbf{p}-\epsilon_{\mathbf{p}-\mathbf{q}})]+\frac{1}{\pi}\mathrm{P}\int_0^\infty d\omega\frac{|\mathrm{Im}[\Lambda_C(\mathbf{q},\omega)]|+3|\mathrm{Im}[\Lambda_S(\mathbf{q},\omega)]|}{\omega-\epsilon_\mathbf{p}+\epsilon_{\mathbf{p}-\mathbf{q}}}\right], \tag{28}$$

where Λ_C is defined in Eq. (27) and the new effective potential Λ_S is defined in terms of the full momentum- and frequency-dependent spin response $\chi_S(\mathbf{q},\omega)$ as follows:

$$\Lambda_S(\mathbf{q},\omega)=-\mu_B^{-2}[v(\mathbf{q})G_-(\mathbf{q},\omega)]^2\chi_S(\mathbf{q},\omega). \tag{29}$$

The exact expressions for $G_+(\mathbf{q},\omega)$ and $G_-(\mathbf{q},\omega)$ are not known in general, so appeal must be made to approximate procedures. A possible way to tackle the problem is to investigate the exact asymptotic behaviors of these functions and then, as is customarily done, assume for them simple analytic formulas designed to interpolate between the known regimes. We find that suitable formulas for the 2D EG case are given by

$$G_\pm(\mathbf{q})=\frac{G_\pm(\infty)q}{\{q^2+[\beta_\pm G_\pm(\infty)p_F]^2\}^{1/2}}, \tag{30}$$

where for the sake of simplicity we have neglected the frequency dependence of these functions. In Eq. (30) the quantities $G_\pm(\infty)$ and $\beta_\pm$ are density dependent and are related to the limiting values of the functions $G_+(\mathbf{q},\omega)$ and $G_-(\mathbf{q},\omega)$, respectively, for large and small wave vectors $\mathbf{q}$.

The exact large-wave-vector limits of the many-body local fields in a 2D EG have been analyzed in Ref. 32. There it was shown how the appropriate limiting values of $G_+(\mathbf{q},\omega)$ and $G_-(\mathbf{q},\omega)$ can be expressed in terms of $g(0)$, the value at the origin of the pair correlation function of the system. $g(0)$ is a function of the electronic density and its theoretical value can be approximately obtained via direct perturbative or numerical approaches.[33,34]

The coefficient β_+ can be simply obtained from the compressibility sum rule which relates the static charge susceptibility, Eq. (25), to E, the total ground-state energy of the electronic system, a quantity which has been the object of several detailed investigations and is therefore approximately known.[35–37] For a more detailed analysis the reader is referred to Ref. 26.

Finally, once β_+ is known β_- can be determined through a self-consistent procedure that will be discussed in detail in the next section.

V. SPIN SUSCEPTIBILITY

Making use of the results of the previous section, we can now proceed to the evaluation of the many-body enhancement of the spin susceptibility.

The first possible improvement upon the calculation contained in Sec. III is the inclusion of the effect of charge-fluctuation-induced vertex corrections described by the function G_+. The procedure employed to obtain the susceptibility in this case is identical to that of Sec. III in which these corrections were neglected. As is readily found, the susceptibility ratio in this case is still determined by the effective mass ratio m^*/m and the function $u(\mathbf{k})$ through Eqs. (4) and (21). In this situation, however, in Eq. (21) and (14) the modified expression for the effective potential $\Lambda_C(\mathbf{q},\omega)$ of Eq. (27) must be used. The results of such a calculation are displayed in Fig. 3 by the curve labeled G_+. It should be noticed that the inclusion of the many-body local field G_+ leads to a rather large enhancement of χ_S/χ_P as compared to the RPA calculation. An analysis of the effective mass for this case can be found in Ref. 26.

To carry the susceptibility analysis further, the effects of the processes associated with the spin-fluctuation-induced vertex corrections will be considered next. In this case the procedure employed above lands into difficulty in view of the fact that spin fluctuations in the electron gas will couple directly to any externally applied magnetic field, so that an alternative method of deriving the spin susceptibility must be used. A possible way to proceed is to make use of the Landau theory of the Fermi liquid.[38]

Within such a framework the static spin susceptibility χ_S can be obtained in terms of the quasiparticle interaction function as follows:

$$\frac{\chi_P}{\chi_S}=\frac{m}{m^*}+\frac{m}{\pi}\int_0^{2\pi}\frac{d\phi}{2\pi}f_a, \tag{31}$$

where the antisymmetrized interaction function f_a is given by

$$f_a\equiv\tfrac{1}{2}(f^{\uparrow\uparrow}-f^{\uparrow\downarrow}), \tag{32}$$

and $f^{\sigma\sigma'}$ can be obtained from the quasiparticle energy $E_{\mathbf{p}}^{\sigma}$ via a functional derivative with respect to the occupation number $n_{\mathbf{p}}^{\sigma}$ as follows:

$$f^{\sigma\sigma'}\equiv\frac{\delta E_{\mathbf{p}}^{\sigma}}{\delta n_{\mathbf{k}}^{\sigma'}}. \tag{33}$$

In order to perform the functional derivative of Eq. (33), the expression for the quasiparticle energy in a system with arbitrary polarization must be found. By following the procedure outlined in Refs. 3 and 26 a generalization of Eq. (14) to the polarized state can be obtained.[39] The enhancement of the spin susceptibility is then calculated by a straightforward application of Eqs. (31) and (33). The result can be cast in the following form:[39]

$$\frac{\chi_P}{\chi_S}=\frac{m}{m^*}-m\int_0^{2\pi}\frac{d\phi}{(2\pi)^2}[\Lambda_C(\mathbf{k}_F-\mathbf{p}_F,0)-\Lambda_S(\mathbf{k}_F-\mathbf{p}_F,0)]$$
$$+\frac{2}{\pi(a_0p_F)^2}\int_0^{\infty}dz\frac{1}{z^2}\int_0^{\infty}du[Q_-(\mathbf{q},i\omega)Q_+(\mathbf{q},i\omega)P_+(z,u)+Q_-(\mathbf{q},i\omega)^2P_-(z,u)], \tag{34}$$

where ϕ is the angle between a fixed vector $\mathbf{p}_F$ and a variable vector $\mathbf{k}_F$, both of which lie on the Fermi surface, and we have introduced the variables $z=q/2p_F$ and $u=\omega m/qp_F$. In Eq. (34) the functions $Q_\pm$ and $P_\pm$ are defined as follows:

$$Q_+(\mathbf{q},\omega)=\frac{1-G_+(\mathbf{q},\omega)}{1-v(\mathbf{q})\chi_0(\mathbf{q},\omega)[1-G_+(\mathbf{q},\omega)]}, \tag{35}$$

$$Q_-(\mathbf{q},\omega)=\frac{G_-(\mathbf{q},\omega)}{1+v(\mathbf{q})\chi_0(\mathbf{q},\omega)G_-(\mathbf{q},\omega)}, \tag{36}$$

and

$$P_\pm(z,u)=\frac{[(z^2-u^2-1)^2+(2zu)^2]^{1/2}\pm(z^2-u^2-1)}{[(z^2-u^2-1)^2+(2zu)^2]}. \tag{37}$$

It should be pointed out here that in formulating a complete theory for the spin susceptibility with the inclusion of the effects of spin fluctuations, particular care must be taken to also allow for *transverse* spin fluctuations. In deriving the expression of Eq. (34), this has been done by treating longitudinal and transverse spin fluctuations on the same footing, so that, for the sake of simplicity, only one many-body local field (i.e., G_-) is used here to describe the phenomenon.[39]

We have made use of Eqs. (30) and (34) – (37) to evaluate the spin susceptibility. The necessary effective-mass ratio has also been determined by using Eq. (28) for the quasiparticle energy. A crucial input of the present analysis is represented by the many-body local field $G_\pm(\mathbf{q},\omega)$ discussed in the previous section. As explained there, we have made use of the interpolation formulas of Eq. (30), which, in turn, depend on the choice of the density-dependent quantities $\beta_\pm$ and $g(0)$. We have chosen for $g(0)$ the theoretical value obtained in Ref. 34. As far as β_+ is concerned, as mentioned above, we have determined this parameter as a function of the electronic density from the total ground-state energy E via the compressibility sum rule. For E we have used the approximate interpolation formula proposed by Jonson,[35] which was obtained by implementing for the case of a 2D EG the classic numerical method of Singwi, Tosi, Land, and Sjolander.[40] Figure 5 displays the appropriate values of β_+ for a 2D EG as a function of the density parameter r_s.

Furthermore, and most importantly, we have determined the coefficient β_- via the following self-consistent procedure. Once the value of β_+ has been established, one starts with a trial value for β_- and proceeds to evaluate the corresponding m^* and χ_S/χ_P, respectively, from Eqs. (5) and (34). Then, by equating such a value to $\chi_S(\mathbf{q}\to 0,0)$, as given by Eq. (26), a new β_- is then determined from the relation

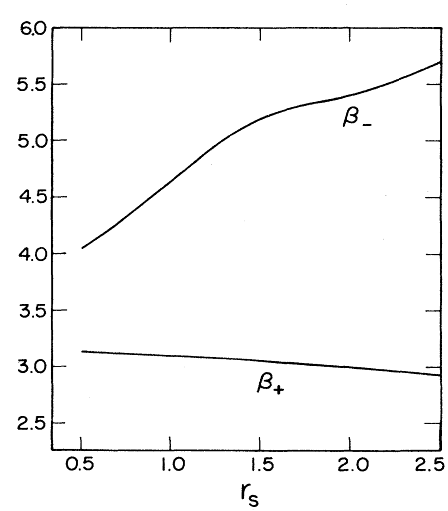

FIG. 5. Theoretical self-consistent results for the coefficients β_+ and β_-, defined in Eq. (30) in text, vs the density parameter

$$\frac{\chi_S(\mathbf{q}\rightarrow 0,0)}{\chi_P}=\frac{1}{1-\frac{2^{1/2}r_s}{\beta_-}} . \tag{38}$$

which is readily obtained from Eq. (26) if one makes use of the familiar Lindhard function for $\chi_0(\mathbf{q},\omega)$. This value for β_- becomes then the starting input for a new iteration. This procedure is repeated until convergence is reached. The appropriate self-consistent values for β_+ and β_- obtained in this way are plotted in Fig. 5 as a function of the density parameter r_s. It is important to realize that once β_+ and β_- are determined, our theory is free of arbitrary parameters. A plot of the susceptibility enhancement for this last case, representing our new full theory, is finally shown by the solid curve labeled G_+ & G_- in Fig. 3.

VI. DISCUSSION AND CONCLUSIONS

We have theoretically investigated the problem of the many-body enhancement of the paramagnetic spin susceptibility in a 2D EG. We have studied in detail the implications of the HF theory for the cases of local and screened interactions, in which case the problem has a simple analytic solution given by Eqs. (8) and (9) of Sec. I.

We have accounted for correlation effects beyond HF by a number of methods of increasing sophistication and physical significance. We have first evaluated the spin-response ratio χ_S/χ_P, by solving exactly in the long-wavelength limit an integral equation first introduced by Hamann and Overhauser,[3] and based on a generalization of the original Wolff HF theory formulation.[21] Our results, notably Eqs. (22)–(24), are extremely simple and allow a direct and straightforward calculation of χ_S. In fact, once the effective mass is known, in the 3D EG case we reduce the problem to a single quadrature and easily recover the established result of the "consensus curve".[3,4] We find that for the case of a 2D EG our result has a simple analytic form and formally coincides with that obtained within the HF approximation making use of the Thomas-Fermi screened potential, the only difference stemming from the different value attained by the quasiparticle effective mass. It is also interesting to notice in this respect that the result for χ_S/χ_P of Eqs. (22) and (24) has the same structure of the simple Thomas-Fermi formula of Eq. (8), so that it formally coincides with the result first obtained by Janak.[15]

We have analyzed the effect on the susceptibility of both charge- and spin-fluctuation-induced vertex corrections which we have accounted for by means of the many-body fields G_+ and G_-, which we have here approximated by suitable interpolation formulas in the spirit of Hubbard.

The results of our study are summarized in Fig. 3, where the curve labeled G_+ & G_- represents our new result for the many-body enhancement of the spin susceptibility in a 2D EG. An important conclusion which can be drawn from our study is that the final value of χ_S results from a subtle balance between various competing effects and that the simple RPA,[25,3] although providing a reasonable starting point, does not account for the full extent of the many-body physics inherent in the phenomenon at hand. It should also be stressed, however, that it is not enough to go beyond the RPA just by introducing, as is customary, the symmetric local field G_+ while altogether neglecting the effects of the spin fluctuations: in general, such a procedure tends to make things worse. We have arrived at the conclusion that the concomitant effects of both charge- and spin-fluctuations-induced vertex corrections must be accounted for in a satisfactory approach.

It must be stressed here that, in general, for large values of the density parameter r_s the many-body corrections are comparatively significantly larger in two dimensions than in three dimensions.

It must also be remarked that the results are sensibly dependent on the specific values used for $g(0)$ which enters the many-body fields, as well as the particular approximate interpolation formulas used for the latter. In particular, the choice of Eq. (30) as suitable expressions for $G_\pm$ was motivated only by natural requirements of simplicity and adherence to the spirit of Hubbard's original diagrammatic analysis of Ref. 19. In order to check the ultimate validity of the present theoretical approach, we have investigated the importance of our specific choice of Eq. (30) by making use of more complicated, yet still frequency-independent, reasonable forms of $G_\pm$. We have concluded that in spite of possible small changes in the actual numerical values, the results and conclusions reported above remain valid, although further rigorous studies on the importance of the frequency and wave-vector dependence of the many-body local fields in an electron gas are still needed.

Finally, although the present work is strictly concerned with the simple electron-gas model, we expect that a similar qualitative behavior will characterize the spin susceptibility of electrons and holes in layered electronic systems and superlattices. In particular, the present approach can be generalized to the more realistic case of electrons in quasi-two-dimensional semiconducting heterostructures and more specifically to inversion layers. As it turns out, the inclusion of the specific physical features and parameters related to the structure, such as the finite-thickness effects, the image potentials, the various background dielectric constants, the valley degeneracy, and band mass, is of crucial importance in such cases. Work on this particularly interesting problem is reported elsewhere.[20]

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