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Spin correlations in electron liquids: Analytical results for the local-field correction in two and three dimensions

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Abstract. We study the spin correlations in two- and three-dimensional electron liquids within the sum-rule version of the self-consistent field approach of Singwi, Tosi, Land, and Sjölander. Analytic expressions for the spin-antisymmetric static structure factor and the corresponding local-field correction are obtained with density dependent coefficients. We calculate the spin-dependent pair-correlation functions, paramagnon dispersion, and static spin-response function within the present model, and discuss the spin-density wave instabilities in double-layer electron systems.

PACS. 71.10.-w Theories and models of many electron systems – 71.45.Gm Exchange, correlation, dielectric and magnetic functions, plasmons – 73.20.Dx Electron states in low-dimensional structures (superlattices, quantum well structures and mutlilayers)

1 Introduction

The study of exchange and correlation effects in homogeneous quantum electron liquids is a subject of continuing interest. The electron system interacting *via* the $1/r$ Coulomb potential offers a suitable model for metals and doped semiconductors. It is also important as a testing ground for various many-body theories. Advances in technology have made it possible to manufacture lower dimensional systems (quantum-wells and wires) with many interesting experimental results, which in turn stimulate further theoretical work. The random-phase approximation [1] (RPA) has been very successful in describing the dielectric properties of the interacting electron system in the high density limit. In particular, the static structure factor, the pair-correlation function, the plasmon dispersion relation, and ground-state energy are widely investigated. As the density of the electron liquid is lowered the exchange and correlation effects become very important, eventually driving the system into a crystal phase. A physically motivated approximation scheme to take the correlations into account is provided by Singwi *et al.* [2] (STLS) in terms of the local-field factors. The local-fields take the repulsion hole around an electron into account to describe the correlation effects. Although semi-classical in its origin, the conceptual simplicity and ease with which one can implement it computationally, have led to numerous applications of the method [3] with varying success. A major drawback of the STLS approach has been that the compressibility sum-rule is not satisfied, namely the compressibility evaluated directly from the ground-state energy is not equal to that calculated using the long-wavelength limit of the local-field correction [4]. This was later corrected in a related approach by Vashishta and Singwi [5].

A sum-rule version of the STLS approximation, which uses the exact limiting behavior of the local-field corrections, is formulated by Gold [6] for a charged Bose gas at zero temperature. In subsequent work, Gold and Calmels [7,8] extended the sum-rule approach to treat electron liquids (fermions), in various dimensions. In this paper we study the response of two-dimensional (2D) and three-dimensional (3D) electron systems to a weak external magnetic field, namely the wave vector- and frequency-dependent paramagnetic susceptibility, within the sum-rule version of the STLS approach developed for density response by Gold and Calmels [7]. Since our study is a natural extension of that of Gold and Calmels [7] to the spin response, our results are largely complementary to theirs. Despite its shortcoming alluded above (and also discussed later) we use the STLS method, firstly to extend the Gold and Calmels [7] approach to study the spin response within the same approximation. Our aim is to develop a simple parametrization for the spin-antisymmetric local-field factor much as it is done for the spin-symmetric part. We also provide a theoretical basis from which the formulation of Gold and Calmels [7] follow naturally. We assume that the electron systems are embedded in a uniform positive background to maintain charge neutrality, and they interact *via* the $1/r$ Coulomb potential in both two- and three-dimensions.

The spin correlations in a 3D electron system within the self-consistent field approximation (or STLS) was first studied by Lobo *et al.* [9]. Diagrammatic approaches

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employing the ladder sums were utilized to treat accurately the short-range part of the Coulomb interaction [10,11]. In 2D, Moudgil *et al.* [12] used the dynamic and static local-fields to study the spin correlations. There has been many unifying attempts to construct the local-field corrections for 3D and 2D electron systems, incorporating their small and large wave vector limiting behavior [13–17]. The enhancement of the paramagnetic susceptibility (spin-response function) of an interacting electron system over its Pauli value is due to short-range Coulomb and exchange effects. We investigate the correlation effects within the sum-rule version of the STLS approach. The density and spin-density responses are combined to determine the spin-dependent pair-correlation functions in the system. The dispersion relation for collective excitations of spin fluctuations (paramagnons) is obtained. We find that the 2D and 3D electron liquids show a paramagnetic instability at low densities, as predicted by the full STLS calculations [9,12] and other approaches [18]. We also explore the possibility of spin-density wave instability in double layer electron systems, using the results obtained in the present work. Finally, we mention that it has already been shown [19] that the spin correlations can be treated within the Gold-Calmels method [6–8], for a short-range potential.

The rest of this paper is organized as follows. In Section 2 we outline the method of sum-rule version of STLS in application to spin-density response. We obtain the self-consistent spin-antisymmetric structure factor and local-field correction for 3D and 2D electron gases in Sections 3 and 4, respectively. The finite width effects in 2D electron systems is investigated in Section 5, and the collective spin excitations within our model is discussed in Section 6. In Section 7 we study the spin-density wave instabilities in double-layer systems. Finally, we give a general discussion of our results in Section 8. We conclude with a brief summary.

2 Theory and model

In the many-body description of homogeneous electron liquids, the wave vector- and frequency-dependent density and spin-density response functions play a central role. They characterize the response of the system to external longitudinal fields, and are expressed in the form

$$\chi^{\rm d}(q,\omega) = \frac{\chi_0(q,\omega)}{1 - v_q[1 - G_{\rm s}(q)]\,\chi_0(q,\omega)}\,, \qquad (1)$$

and

$$\chi^{\rm s}(q,\omega) = \frac{\chi_0(q,\omega)}{1 + v_q G_{\rm a}(q)\,\chi_0(q,\omega)}\,, \qquad (2)$$

where $\chi_0(q,\omega)$ is the free-electron polarizability [20] taken as a reference, v_q is the bare Coulomb potential (for the D-dimensional electron gas), and $G_{\rm s}(q)$ and $G_{\rm a}(q)$ are the spin-symmetric and spin-antisymmetric static local-field corrections describing the many-body exchange and correlation effects. The above expressions for $\chi^{\rm d}(q,\omega)$ and $\chi^{\rm s}(q,\omega)$ may be regarded as defining relations, provided the local-fields $G_{\rm s}$ and $G_{\rm a}$ are accurately calculated. The fluctuation-dissipation theorem enables us to write the static structure factor $S_{\rm s}(q)$, and the magnetic structure factor $S_{\rm a}(q)$, in terms of the response functions, *viz.*,

$$S_{\rm s,a}(q) = -\frac{1}{n\pi}\int_0^\infty {\rm d}\omega\,\chi^{\rm d,s}(q,i\omega)\,, \qquad (3)$$

where the frequency integration is to be performed along the imaginary axis to better capture the collective mode contributions.

In the following we outline the basic steps of obtaining closed-form expressions for the structure factors and local-field corrections in a D-dimensional ($D = 2$ or 3) electron liquid. Our approach is largely based on the generalized mean spherical approximation [13,21]. In the MSA, the free-electron gas response function $\chi_0(q,\omega)$ reduces to a simple form

$$\chi_0^{\rm MSA}(q,\omega) = \frac{2n\epsilon_q}{\omega^2 - [\epsilon_q/S_0(q)]^2}\,, \qquad (4)$$

where $\epsilon_q = q^2/2m$ is the free-particle energy, and $S_0(q)$ is the static structure factor for the noninteracting electron gas (*i.e.* the result of the Hartree-Fock approximation). Note that $\chi_0^{\rm MSA}$ differs from the exact expression provided by the Lindhard function $\chi_0(q,\omega)$. In $\chi_0^{\rm MSA}$ the particle-hole pair continuum is approximated by a collective mode with energy $\epsilon_q/S_0(q)$, much the same as Feynman excitation spectrum for bosons. If we now replace $\chi_0(q,\omega)$ by $\chi_0^{\rm MSA}(q,\omega)$ in equations (1, 2), we obtain the generalized MSA (including the local-field corrections) to the density and spin-density responses in an interacting electron system. Performing the frequency integral of equation (3) we obtain the static structure factors

$$S_{\rm s}(q) = \frac{\epsilon_q}{\left[[\epsilon_q/S_0(q)]^2 + v_q[1 - G_{\rm s}(q)]2n\epsilon_q\right]^{1/2}}\,, \qquad (5)$$

and

$$S_{\rm a}(q) = \frac{\epsilon_q}{\left[[\epsilon_q/S_0(q)]^2 - v_q G_{\rm a}(q)2n\epsilon_q\right]^{1/2}}\,. \qquad (6)$$

The above equations provide closed form expressions for the static structure factors in terms of the local-field corrections, and were first obtained by Iwamoto *et al.* [13] in a related work. Gold and Calmels [7] postulated the form of equation (5) in their STLS based self-consistent calculation of the spin-symmetric structure factor and the local-field correction. Here, we concentrate on the spin-density response and develop a similar self-consistent scheme to calculate the spin-antisymmetric structure factor $S_{\rm a}(q)$ and corresponding local-field factor $G_{\rm a}(q)$, in order to complement the earlier work of Gold and Calmels [7].

The density and spin-density response function of equations (1, 2) also define the effective potentials, in the mean-field approximation, such that $\psi^{\rm s}(q) = v_q[1 - G(q)]$, and $\psi^{\rm a}(q) = v_q G_{\rm a}(q)$. $G_{\rm s}(q)$ and $G_{\rm a}(q)$ are the static local-field factors arising from the short-range Coulomb correlations

and the exchange-correlation effects for the density and spin-density responses, respectively. In the approximation scheme of Singwi *et al.* [2] they are given, respectively, as [2,9]

$$G_{\rm s,a}(q) = \frac{1}{n}\int \frac{{\rm d}^D k}{(2\pi)^D}\,\frac{\mathbf{k}\cdot\mathbf{q}}{q^2}\frac{v_k}{v_q}\left[1 - S_{\rm s,a}(q-k)\right], \qquad (7)$$

where n is the electron density, and $D = 2, 3$ is the dimensionality. The integral expressions for $G_{\rm s}(q)$ and $G_{\rm a}(q)$ follow from the assumption that the two-particle distribution function may be decoupled as a product of two one-particle distribution functions multiplied by the pair-correlation function. More precisely, the $G_{\rm s}(q)$ and $G_{\rm a}(q)$ are reduced to become functionals of the sum and difference between the correlation functions of pairs of particles with parallel and antiparallel spins [2,9]. In the sum-rule version of the STLS scheme as introduced by Gold [6] and Gold and Calmels [7] the long- and short-wavelength limits of the local-field factors $G_{\rm s}(q)$ and $G_{\rm a}(q)$ are utilized to simplify the full integral expressions, and parametric representations are obtained. When the local-field factors are absent (*i.e.* set equal to zero), the response functions reduce to their familiar forms in the random-phase approximation (RPA) and Hartree-Fock (HF) approximation, respectively.

A major shortcoming of the present STLS approximation in the study of spin correlations is that the spin-susceptibility calculated from the ground-state energy (assumed to be known as a function of spin-polarization parameter or magnetization) will differ that calculated using the long-wavelength limit of $G_{\rm a}(q)$. This has been rectified from a theoretical standpoint, analogous to the case of density response, by Vashishta and Singwi [22]. To make connection with the earlier calculations [7] of $G_{\rm s}(q)$ within the same approximation, we shall ignore this inconsistency as was done in other applications [7,9,12].

3 Three-dimensional electron gas

We first consider the specific model of a 3D electron gas. It consists of electrons interacting *via* the Coulomb potential (in Fourier space) $v_q = 4\pi e^2/\epsilon_0 q^2$, in the presence of a neutralizing uniform background. The density parameter $r_{\rm s} = (4\pi n a_{\rm B}/3)^{-1/3}$, given in terms of the number density n, and the Bohr radius $a_{\rm B} = \epsilon_0/me^2$ (where ϵ_0 is the dielectric constant of the background), completely characterizes the system at zero temperature. The Fermi momentum $k_{\rm F}$ is related to the electron density through $n = k_{\rm F}^3/3\pi^2$. We adopt a new screening wave number $q_{\rm s} = 12^{1/4}/(r_{\rm s}^{3/4} a_{\rm B})$, introduced by Gold and Calmels [7], to scale the momentum and length variables in the subsequent calculations. In these units, the model spin-antisymmetric static structure factor takes the form

$$S_{\rm a}(x) = \left[[S_0(x)]^{-2} - \frac{G_{\rm a}(x)}{x^4}\right]^{-1/2}, \qquad (8)$$

Table 1. The parameters $C_1^{\rm 3D}$ and $C_2^{\rm 3D}$ for the local-field correction in a 3D electron gas for various values of $r_{\rm s}$.

$r_{\rm s}$	$C_1^{\rm 3D}(r_{\rm s})$	$C_2^{\rm 3D}(r_{\rm s})$
0.01	0.4977	14.12
0.1	0.4778	4.313
0.5	0.4028	1.668
1	0.3331	1.003
2	0.2424	0.5417
3	0.1877	0.3570
4	0.1518	0.2599
5	0.1267	0.2019
6	0.1084	0.1646
7	0.09457	0.1402
8	0.08404	0.1261

where $x = q/q_{\rm s}$, and $S_0(x)$ is the familiar HF static structure factor. For the spin-antisymmetric local-field correction we choose the following Hubbard approximation type parametrized expression

$$G_{\rm a}(x) = \frac{C_1^{\rm 3D}(r_{\rm s})\,x^2}{C_2^{\rm 3D}(r_{\rm s}) + x^2}, \qquad (9)$$

where the coefficients $C_i^{\rm 3D}(r_{\rm s})$ $(i = 1, 2)$ are to be determined from the small and large q behavior of $G_{\rm a}(x)$ given in the STLS approximation. More specifically, we have

$$\frac{C_1^{\rm 3D}(r_{\rm s})}{C_2^{\rm 3D}(r_{\rm s})} = \frac{8 r_{\rm s}^{3/4}}{3\pi 12^{1/4}}\int_0^\infty {\rm d}x\,[1 - S_{\rm a}(x)], \qquad (10)$$

and

$$C_1^{\rm 3D}(r_{\rm s}) = \frac{8 r_{\rm s}^{3/4}}{\pi 12^{1/4}}\int_0^\infty {\rm d}x\,x^2[1 - S_{\rm a}(x)]. \qquad (11)$$

These coupled integral equations are solved for the parameters $C_i^{\rm 3D}(r_{\rm s})$ at each $r_{\rm s}$. They are much easier to solve than the full STLS equations as noted by Gold and Calmels [7] who investigated the density response in electron liquids using a similar scheme.

We summarize our results in Table 1, for the coefficients $C_i^{\rm 3D}(r_{\rm s})$, tabulating them for various $r_{\rm s}$ values. In contrast to the density-response case, the above set of equations for the spin-density response fail to provide self-consistent solutions beyond $r_{\rm s} \simeq 8$. This may be taken as a signal for a spin-density related instability developing in the system. A similar kind of instability was also encountered in the solution of full STLS equations which may be related to the transition to paramagnetic phase as found by Misawa [23] and Rajagopal and Kimball [18]. We discuss the physical meaning of this numerical instability in Section 8.

Once the $r_{\rm s}$-dependent coefficients in the parametrized model of the spin-antisymmetric local-field factor $G_{\rm a}(x)$ are determined, we can investigate various physical quantities of interest. We first display the spin-density structure factor $S_{\rm a}(q)$ for a 3D electron gas in Figure 1. Unlike

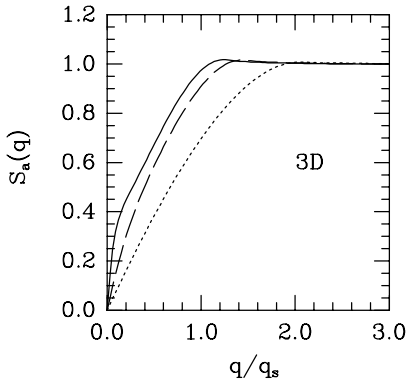

Fig. 1. The spin-antisymmetric static structure factor $S_a(q)$, within the sum-rule version of the STLS approach for a 3D electron gas, at $r_s = 1$ (dotted line), $r_s = 4$ (dashed line), and $r_s = 7$ (solid line).

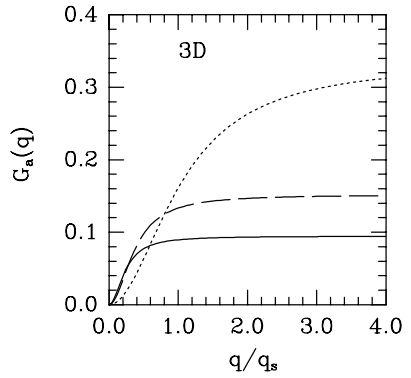

Fig. 2. The spin-antisymmetric static local-field correction $G_a(q)$, within the sum-rule version of the STLS approach for a 3D electron gas, at $r_s = 1$ (dotted line), $r_s = 4$ (dashed line), and $r_s = 7$ (solid line).

its spin-symmetric counterpart $S_s(q)$, $S_a(q)$ exhibits a slight peak around $q \simeq 2k_F$ with increasing r_s. The corresponding local-field factor $G_a(q)$ is shown in Figure 2. As the density is lowered, the magnitude of $G_a(q)$ decreases, and it retains a constant value for $q \gtrsim q_s$. Similar behavior in $G_a(q)$ was also found in the calculations of Iwamoto *et al.* [13].

From the knowledge of $S_a(q)$, one can determine the spin-antisymmetric pair-correlation function by the Fourier transform

$$g_a(r) = \frac{1}{n} \int \frac{d^3q}{(2\pi)^3} \, e^{-i\mathbf{q}\cdot\mathbf{r}} \, [S_a(q) - 1] \,, \qquad (12)$$

and in particular, its value at zero separation ($r = 0$) is easily calculated. We find that $g_a(0) = -C_1^{3D}(r_s)$. Combining this result with the spin-symmetric pair-correlation function $g_s(r)$, calculated within the same approximation [7] we can deduce the spin-dependent pair correlation functions

$$g_{\uparrow\uparrow}(r) = g_s(r) + g_a(r), \quad \text{and} \quad g_{\uparrow\downarrow}(r) = g_s(r) - g_a(r). \qquad (13)$$

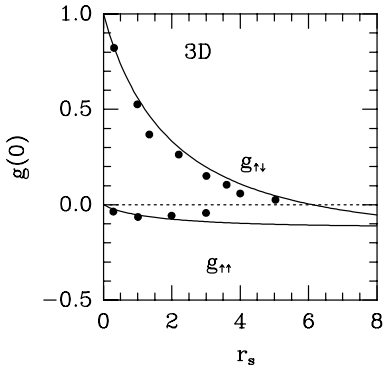

Fig. 3. The spin-dependent pair-correlation functions $g_{\uparrow\uparrow}(0)$, and $g_{\uparrow\downarrow}(0)$ at zero separation obtained from $g_s(0)$ and $g_a(0)$, as a function of r_s for a 3D electron gas. The solid circles are from the full STLS calculation of reference [9].

$g_s(r)$ gives the probability of finding an electron at r, if another electron is located at the origin, irrespective of their spins. For some applications, the decomposition of $g_s(r)$ into $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$ is quite useful. In Figure 3 we show $g_{\uparrow\uparrow}(0)$ and $g_{\uparrow\downarrow}(0)$ combining our results and those of Gold and Calmels [7], as a function of r_s. $g_{\uparrow\downarrow}(0)$ satisfies the positive definiteness requirement up to $r_s \sim 6$, as in the original STLS calculation [9]. $g_{\uparrow\uparrow}(0)$, on the other hand, is slightly negative, indicating that the short-range correlations for parallel spins are overestimated in the STLS approximation. Technically, the local-field corrections take Pauli exchange-hole into account but neglect the Coulomb-hole contribution. In extended versions of the theory it is possible to improve this situation by incorporating the screening function into the self-consistent scheme [2]. The sum-rule version reproduces the original STLS results [9] of $g_{\uparrow\uparrow}(0)$ and $g_{\uparrow\downarrow}(0)$ quite well.

4 Two-dimensional electron gas

In a 2D electron gas within the same model, we assume that the bare Coulomb potential is still given by e^2/r in configuration space, which has a Fourier transform $v_q = 2\pi e^2/q$. The RPA parameter in this case is defined as $r_s = (\pi n a_B^2)^{-2}$, where n denotes the areal density of the electrons. Using the relation $n = k_F^2/2\pi$ (we assume a single-valley), the scaling parameter becomes $q_s = 2/(r_s^{2/3} a_B)$. The model spin-density structure factor is expressed as

$$S_a(x) = \left[[S_0(x)]^{-2} - \frac{G_a(x)}{x^3} \right]^{-1/2} , \qquad (14)$$

in which the noninteracting structure factor $S_0(q)$ appropriate for a 2D electron gas is used. Similar arguments as in the 3D case leads us to propose a parametrized spin-antisymmetric local-field factor of the form

$$G_a(x) = \frac{C_1^{2D}(r_s)\, x}{[[C_2^{2D}(r_s)]^2 + x^2]^{1/2}} \,. \qquad (15)$$

Table 2. The parameters C_1^{2D} and C_2^{2D} for the local-field correction in a strictly 2D electron gas for various values of r_s.

r_s	$C_1^{2D}(r_s)$	$C_2^{2D}(r_s)$
0.01	0.4948	3.837
0.1	0.4517	1.666
0.5	0.3168	0.7479
1	0.2242	0.4550
1.5	0.1711	0.3220
2	0.1373	0.2468
2.5	0.1142	0.1996
2.8	0.1036	0.1796

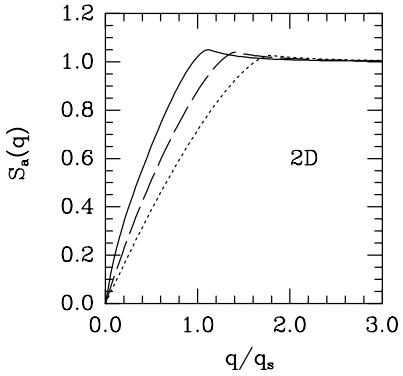

Fig. 4. The spin-antisymmetric static structure factor $S_a(q)$, within the sum-rule version of the STLS approach for a 2D electron gas, at $r_s = 0.5$ (dotted line), $r_s = 1$ (dashed line), and $r_s = 2$ (solid line).

The coefficients $C_i^{2D}(r_s)$ are now determined by the nonlinear equations

$$\frac{C_1^{2D}(r_s)}{C_2^{2D}(r_s)} = r_s^{2/3} \int_0^\infty \mathrm{d}x\,[1 - S_a(x)]\,, \qquad (16)$$

and

$$C_1^{2D}(r_s) = 2r_s^{2/3} \int_0^\infty \mathrm{d}x\, x[1 - S_a(x)]\,. \qquad (17)$$

The results of our self-consistent calculations are displayed in Table 2. We find that beyond $r_s \gtrsim 3$, it becomes very difficult to obtain a solution. Similar difficulties were encountered in the full STLS calculations [12] for $r_s > 4$. The spin-antisymmetric static structure factor and the local-field correction in a 2D electron liquid are illustrated in Figures 4 and 5, respectively. Our results are in good agreement with the full STLS calculations [12] of the same quantities. In particular the peak structure in $S_a(q)$ is well reproduced. The spin dependent pair-correlation functions at the origin are shown in Figure 6. As in the 3D case, the spin-antisymmetric pair-correlation function in our model is given by $g_a(0) = -C_1^{2D}(r_s)$. Combining this result with the earlier findings of Gold and Calmels [7] yields $g_{\uparrow\uparrow}(0)$ and $g_{\uparrow\downarrow}(0)$ shown in Figure 6. We find good agreement with the full STLS calculations of Moudgil *et al.* [12] for

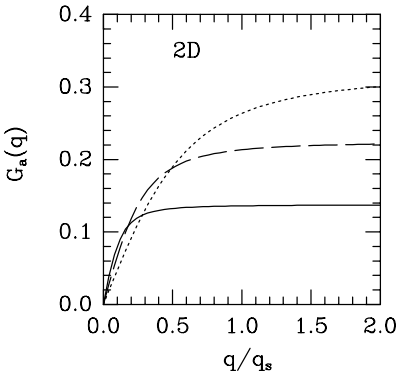

Fig. 5. The spin-antisymmetric static local-field correction $G_a(q)$, within the sum-rule version of the STLS approach for a 2D electron gas, at $r_s = 0.5$ (dotted line), $r_s = 1$ (dashed line), and $r_s = 2$ (solid line).

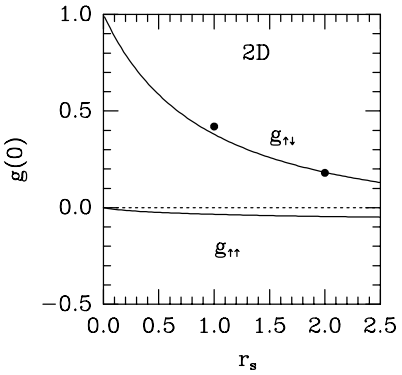

Fig. 6. The spin-dependent pair-correlation functions $g_{\uparrow\uparrow}(0)$, and $g_{\uparrow\downarrow}(0)$ at zero separation obtained from $g_s(0)$ and $g_a(0)$, as a function of r_s for a 2D electron gas. The solid circles are from the full STLS calculation of reference [12].

the correlation function $g_{\uparrow\downarrow}(0)$. Sato and Ichimaru [24] considered second-order exchange processes in the spin-dependent correlations for 2D electron systems and gave a parametrized expression for the spin-antisymmetric local-field factor. Calculations of higher-order spin correlations (and the associated local-field corrections) incorporating nonlinear effects using density-functional theoretical methods were recently performed by Iyetomi and Ichimaru [25].

5 Two-dimensional electron gas with finite width effects

The model of a 2D electron gas has found a wealth of applications both from fundamental and practical points of view [26]. Electrons confined in the interface of GaAs/GaAlAs is a striking example, in which several key experiments reveal interesting physical phenomena. Among the various models, describing the finite extension of electrons in the perpendicular direction, the infinite quantum-well of width L is widely used. As a result, the interaction potential is given by $v_q = 2\pi e^2 F(q)/\epsilon_0 q$,

Table 3. The parameters C_1^{2D} and C_2^{2D} for the local-field correction in a quantum-well of width $L = a_B$, and a heterojunction for various values of r_s.

	quantum-well		heterojunction	
r_s	$C_1^{2D}(r_s, L)$	$C_2^{2D}(r_s, L)$	$C_1^{2D}(r_s, b)$	$C_2^{2D}(r_s, b)$
0.01	0.5000	40.76	0.4998	11.67
0.1	0.4969	4.294	0.4952	3.660
0.5	0.4273	1.242	0.4592	1.635
1	0.3174	0.7016	0.4048	1.096
1.5	0.2369	0.4727	0.3513	0.8302
2	0.1838	0.3479	0.3030	0.6618
2.5	0.1480	0.2722	0.2614	0.5448
2.8	0.1319	0.2406	0.2398	0.4909

where the form factor is

$$F(q) = \frac{1}{4\pi^2 + x^2} \left[3x + \frac{8\pi^2}{x} - \frac{32\pi^4}{x^2} \frac{1 - e^{-x}}{4\pi^2 + x^2} \right], \quad (18)$$

with $x = qL$. In the case of semiconductor heterojunctions, the finite width effects are described by a variational parameter in the ground-state wave function [27]. For vanishing depletion density the width parameter is given by $b = (33\pi n/2a_B)^{1/3}$. The form factor modifying the bare Coulomb interaction reads

$$F(q) = \frac{1}{(1+x)^3} \left[1 + \frac{9x}{8} + \frac{3x^2}{8} \right], \quad (19)$$

where $x = q/b$. For both quantum-well and heterojunction cases, the first integral equation determining the coefficients is modified to

$$\frac{C_1^{2D}(r_s)}{C_2^{2D}(r_s)} = r_s^{2/3} \int_0^\infty dx \, [1 - S_a(x)] \, F(x), \quad (20)$$

whereas the second equation for $C_2^{2D}(r_s)$ remains unchanged. The form factor also enters the spin-antisymmetric structure factor $S_a(x)$, and introduces a slight modification. Our results for the infinite quantum-well with width $L = a_B$ ($a_B \simeq 100$ Å for GaAs) and the heterojunction with variational parameter b are listed in Table 3. As noted by Gold and Calmels [7], the quantity $q_s/b = 2/(33/2)^{1/3}$ is independent of r_s, and therefore the coefficients $C_i^{2D}(r_s)$ for heterojunctions are universal, depending solely on r_s. We observe that the finite extension of the 2D electron gas in the perpendicular direction has very little effect on the coefficient $C_1^{2D}(r_s)$ (compare with the results in Tab. 2). However, the coefficient $C_2^{2D}(r_s)$ is affected quite significantly. In general the coefficients $C_i^{2D}(r_s)$ increase with finite width, small r_s values being modified the most. The full STLS equations are solved recently for a quasi-two-dimensional electron gas (heterojunction) by Bulutay and Tomak [28]. They found some differences between their results and those of Gold and Calmels [7], which presumably may be accounted for by the respective treatment of depletion charge density and ionized acceptors in the well-acting region, in these works.

6 Collective spin excitations

Collective excitations in an electron gas, may be studied as complex poles of the density and spin-density response functions $\chi^{d,s}(q,\omega)$, or as peaks of the dynamic structure factor $S(q,\omega)$. The calculation of the collective spin modes is similar to that of density excitations [20]. Using the spin-density response function in our model, we find for the collective spin excitations (paramagnons)

$$\omega_q^2 = [\epsilon_q / S_0(q)]^2 - 2n\epsilon_q v_q G_a(q). \quad (21)$$

Note that the boson-like χ_0^{MSA} is used in obtaining the above expression. Gold and Calmels [7] in their discussion of the plasmon modes within the same model, employed the Lindhard expression $\chi_0(q,\omega)$. In Figure 7a we show the dispersion ω_q of the paramagnon peak in a 3D electron gas. The influence of spin-antisymmetric local-field factor $G_a(x)$ is to harden the spin collective mode ω_q, than its value evaluated within the Feynman approximation $\epsilon_q/S_0(q)$. Both dispersion laws show a linear behavior in q. Similar results are found for a 2D electron liquid as illustrated in Figure 7b. The spin-density excitations, for instance, in a 2D electron gas was measured by Pinczuk *et al.* [29], and recently in dilute electron bilayers by Plaut *et al.* [30] using inelastic light scattering experiments. We do not attempt a direct comparison with the experimental results, since they are mostly performed at very small wave vectors q for the local-field corrections to be distinctly significant. A more precise calculation would use the Lindhard form of $\chi_0(q,\omega)$, in which case the damping of the collective modes could also be studied.

7 Spin instabilities in layered structures

The existence of a charge-density wave (CDW) instability in double-layer electron systems is predicted at a critical layer separation [31]. Such instabilities are induced by the exchange-correlation effects in both Fermi and Bose liquids [32]. Similar behavior originating from spin-density fluctuations are largely ignored. Intersubband spin-density excitations and the phase transitions they induce have been gaining attention with recent experimental [33] and theoretical efforts [34] in the context of double-layer quantum Hall systems. We briefly explore the conditions under which a spin-density wave (SDW) instability evolves in a double-layer electron system. The static spin susceptibility may be written as [35]

$$\chi_\pm^s(q) = \frac{\chi_0(q)}{1 + [v_q G_a(q) \pm v_q e^{-qd}]\chi_0(q)}, \quad (22)$$

in which the interlayer Coulomb interaction, $v_q e^{-qd}$, is used, but the interlayer correlation effects are ignored. As in the density response in double-layer systems, intralayer spin correlation effects are expected to dominate the spin response. For more refined calculations it would be possible to extend the formalism set out in Section 2,

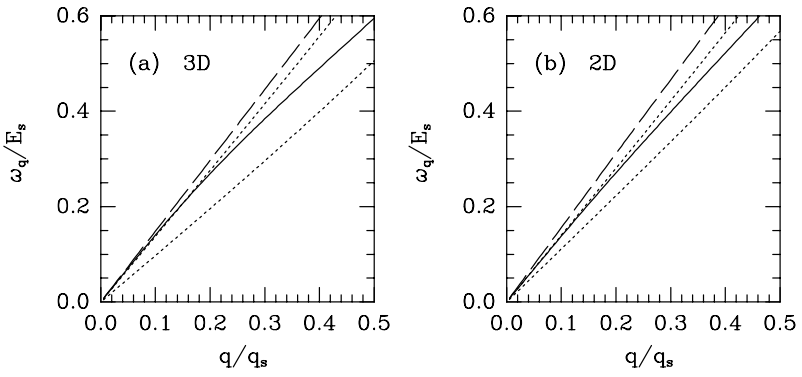

Fig. 7. The collective spin excitation energies (in units of $E_s = q_s^2/2m$) (a) in a 3D electron gas, at $r_s = 1$ (dashed line) and $r_s = 4$ (solid line); and (b) in a 2D electron gas at $r_s = 0.5$ (dashed line) and $r_s = 1$ (solid line). The dotted lines in both cases indicate the Feynman spectrum $\epsilon_q/S(q)$.

for multicomponent systems and calculate both the intralayer and interlayer local-field factors self-consistently. The above expression for $\chi^s_\pm(q)$ is obtained by diagonalizing the spin response matrix for a double-layer system. A SDW instability is identified when $1/\chi^s_-(q = q_c \geq 0) = 0$, for some wave number q_c. More explicitly, we have the condition for a singular behavior in static spin susceptibility

$$x_c = r_s^{2/3} \left[e^{-x_c d q_s} - G_a(x_c)\right] \chi_0(x_c)/\rho_F \,, \qquad (23)$$

where $x_c = q_c/q_s$, and $\rho_F = m/\pi$ is the 2D density of states at the Fermi level. Our equation (23) is the SDW counterpart of Gold and Calmels'equation (53) [7] for CDW instability. It differs from the CDW condition, in the sense that a critical layer distance d_c cannot be found. d_c was defined such that for $d < d_c$ the double-layer electron system exhibits instability. It appears that within the present formalism SDW instabilities are predicted to occur for any distance d, since we can find a solution of equation (23) for all values of d. Taking the finite width effects into account in the 2D electron layers would not change this situation. We note, however, that this may be due to the approximations involved.

8 Discussion

In this work we have solved the self-consistent equations for $S_a(q)$ and $G_a(q)$ within the sum-rule version of the STLS scheme. The STLS approximation provides a reasonable improvement over the RPA for small densities. Despite the fact that the pair-correlation function becomes negative for small values of r as r_s increases, it has been found that the STLS ground-state energies are in good agreement with the Monte Carlo simulation results [36] in the range $1 < r_s < 20$. The sum-rule version of the STLS approach as developed by Gold and Calmels [7] has the facility of reproducing most of the full STLS results with analytical expressions for the static structure factor and local-field correction. We have rederived the model $S_s(q)$ and $S_a(q)$ introduced by Gold and Calmels [7], within the generalized MSA. The analytical form of $S_s(q)$ describes the transition between the exchange effects for small r_s and correlation effects for large r_s quite well as noted by Gold and Calmels [7]. They attribute this to the local-field factor being essentially a q-integral between zero and $2k_F$. In the case of spin-density response, the self-consistent calculations of $S_a(q)$ and $G_a(q)$ are plagued by numerical problems beyond a certain r_s value. This is not a shortcoming of the sum-rule version, since similar instabilities are also encountered in the full STLS calculations [12]. Moudgil *et al.* [12] ascribe this to an instability developing in the paramagnetic phase. We believe that the numerical instabilities associated with the spin correlations mainly come from the underlying Hartree-Fock (HF) nature of the STLS. In contrast to the description of density correlations which takes the RPA as reference (*i.e.*, $G_s(q) = 0$ form), the spin-response is basically built on the HF approximation. This is evident when we set $G_a(q) = 0$ in equation (2). It is known that the HF approximation, even for the density-response leads to unphysical instabilities which are removed at the level of RPA or higher order approximations. Divergence in the spin-response of a 2D electron gas was also found by Yarlagadda and Giuliani [37] in various approximations. More elaborate theories of spin correlations in 3D seem to indicate the existence of instability at a much lower density (*i.e.*, high r_s) [14,38]. When the spin-symmetric and spin-antisymmetric local-field corrections are constructed [13,15] using the exact ground-state properties [36] of 3D and 2D electron gas, no such unstable behavior is observed. We believe that the instability predicted by the STLS needs to be explored (and possibly be overcome) by theories that go beyond the present mean-field approach. The present status of the electron correlations, with particular emphasis on the most up-to-date Monte Carlo simulations [39], was reviewed by Senatore and March [40]. The inadequacy of the STLS approximation (and similar schemes) in not being able to describe the spin-dependent correlations was recognized earlier and various improved schemes were formulated [41]. In particular, the treatment of Utsumi and Ichimaru [42] introduces parametrized expressions satisfying the spin-susceptibility sum-rule and the restrictions on the short-range correlations demanded by the Pauli principle.

That the numerical instabilities encountered in spin correlations within the present approach would somewhat limit its applicability. In ordinary metals (bulk) the relevant density regime $1 < r_s < 10$, and in doped semiconductors in two and three-dimensions, $0.1 < r_s < 3$, make

the results of our calculations applicable to most experimental situations. It has also been argued [43] that the correlation effects are important in white dwarf stars for $0.001 < r_s < 0.01$.

A simplified attempt to go beyond the RPA has been provided by the Hubbard approximation (HA) in which only the exchange effects are taken into account by considering the Pauli hole around each electron. The corresponding local-field factors in the HA may be obtained by substituting the HF static structure factors in equation (7). This prescription yields the same $G_s(q)$ and $G_a(q)$, a result not substantiated by the STLS calculations.

The effects of disorder may be incorporated into the present approximation in a phenomenological way. The noninteracting susceptibility including the phenomenological relaxation-time τ, within a number-conserving scheme is given by [44]

$$\chi_0(q,\omega;1/\tau) = \frac{(\omega+i/\tau)\chi_0(q,\omega+i/\tau)}{\omega+(i/\tau)\chi_0(q,\omega+i/\tau)/\chi_0(q,0)} = \frac{2n\epsilon_q}{\omega(\omega+i/\tau)-[\epsilon_q/S_0(q)]^2}, \quad (24)$$

where the last equality holds when we use $\chi_0^{\rm MSA}$ in our model. In the limit $\tau \to \infty$, we recover the collision-free expression for $\chi_0^{\rm MSA}(q,\omega;1/\tau \to 0)$. The spin-antisymmetric static structure factor is calculated to be

$$S_a(q) = (2/\pi)\epsilon_q I(\Delta),$$

where

$$I(\Delta) = 2\begin{cases} \frac{1}{\sqrt{\Delta}}\left[\frac{\pi}{2} - \tan^{-1}\left(\frac{1/\tau}{\sqrt{\Delta}}\right)\right] & \text{for} \quad \Delta > 0, \\ \tau & \text{for} \quad \Delta = 0, \\ \frac{1}{\sqrt{-\Delta}}\tanh^{-1}\left(\frac{1/\tau}{\sqrt{-\Delta}}\right) & \text{for} \quad \Delta < 0, \end{cases} \quad (25)$$

and $\Delta = 4([\epsilon_q/S_0(q)]^2 - 2nv_qG_a(q)\epsilon_q) - 1/\tau^2$. A similar expression for the spin-symmetric static structure factor $S_s(q)$ in the presence of collisional broadening is straightforward to obtain. Equation (25) was earlier considered for a charged Bose gas [45]. It could be interesting to solve the self-consistent equation for the structure factor and local-field correction with finite τ, to investigate the effects of disorder. We point out that the STLS form of the local-fields $G_{s,a}(q)$ may also be modified to take the disorder effects into account. Studies along these lines are largely unexplored.

As a further application of the present work, we calculate the static spin susceptibility $\chi^s(q)$. In this connection, we may either use the MSA or Lindhard expressions for the noninteracting system $\chi_0(q)$. As an illustration we show in Figure 8 the static spin susceptibility $\chi^s(q)$ for a 2D electron gas at $r_s = 1$. The results indicated by solid and dotted lines are evaluated using the MSA and Lindhard forms of $\chi_0(q)$, respectively. In both curves the same $G_a(q)$ is used. The dashed line shows the spin susceptibility given by Iwamoto's model [15]. Here, the spin-antisymmetric local-field factor is constructed using

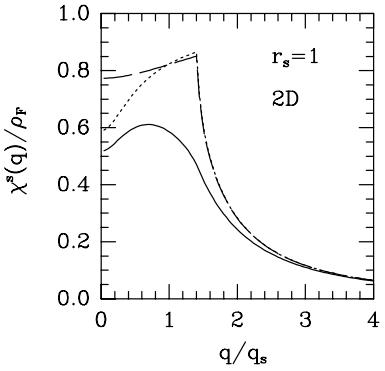

Fig. 8. The static spin response $\chi^s(q)$ as a function of q, for $r_s = 1$ in a 2D electron gas. Solid and dotted lines are calculated within the present model and $\chi_0^{\rm MSA}$ and Lindhard functions, respectively. The dashed line is from reference [15].

the Monte Carlo correlation energies. We observe that for large q, all models have similar behavior. They differ in their prediction of the long-wavelength limit.

The sum-rule version of the STLS approximation is also employed to study the exchange-correlation effects in quasi-one-dimensional (Q1D) electron systems by Calmels and Gold [8]. The self-consistent calculations of spin-symmetric static structure factor and local-field correction $G_s(q)$, were used to obtain ground state energy. Extending our work to investigate the spin-antisymmetric structure should be possible. This would again complement the work of Calmels and Gold [8] in the description of spin dependent ground state correlations in Q1D electron systems. In Q1D systems, the Coulomb interaction is further characterized a quantum wire width parameter, similar to the Q2D systems, having a finite quantum well width. The STLS nature of the present approximation is expected to reveal spin instabilities around $r_s \sim 1$.

9 Summary

In summary, we have studied the spin-density correlations in 2D and 3D electron liquids using the sum-rule version of the STLS approximation. Our approach and results are complementary to the recent investigation of density correlations in the same systems by Gold and Calmels [7]. Within the sum-rule version of STLS, the spin-antisymmetric static structure factor and the local-field correction are calculated in terms of r_s-dependent coefficients, in closed-form. They can be used along with the spin-symmetric counterparts obtained by Gold and Calmels [7] in more complex calculations and as input to other theoretical approaches. Our calculations predict a paramagnetic instability in electron liquids for lower densities as in the full STLS method. A heuristic explanation is given for this behavior. Collective spin excitations are calculated. SDW instabilities in double-layer electron systems are investigated. Our results indicate that a SDW would be present for all layer separations. It would be interesting to develop calculational schemes that combines

the simplicity of the present approach and the sum-rule requirements demanded by microscopic considerations.

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