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Search for antiferromagnetism in homogeneous electron systems

K. Capelle[a] and L.N. Oliveira

Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970 São Carlos, SP, Brazil

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Abstract. We present numerical and analytical evidence for the absence of a second-order phase transition of homogeneous electron systems into an antiferromagnetic state. Our results are based on numerical data extending from the extreme high-density regime ($r_s \to 0$) to the extreme low-density regime ($r_s = 100$). The particle-particle interaction is treated within the random-phase approximation, augmented by various types of local-field corrections. The latter turn out to be crucial for a correct description of the screening of spin-density waves. Our results indicate the absence of a second-order transition of the three-dimensional homogeneous electron gas, the two-dimensional homogeneous electron gas, and laterally homogeneous electron layers, into a collinear antiferromagnetic state.

PACS. 71.10.Ca Electron gas, Fermi gas – 75.50.Ee Antiferromagnetics – 75.30.Fv Spin-density waves

1 Introduction

The interacting homogeneous electron gas is one of the most widely studied model systems of condensed matter physics. Its importance arises from the fact that it is simultaneously one of the simplest models for many-body phenomena in extended systems, serving, thus, as a test ground for approximations and concepts, and the basic ingredient for the local-density approximation to density-functional theory, the most widely used method for electronic structure calculations. In the present paper we investigate the antiferromagnetic properties of interacting three-dimensional and two-dimensional homogeneous electron gases, and also study laterally homogeneous electron layers.

The main motivation for this work arises from the observation that, in spite of many efforts, no conclusive proof for either the presence or the absence of antiferromagnetism (AFM) in the homogeneous electron gas exists to date. Our approach to the problem is of a perturbative nature, based on evaluating the stability criterium for antiferromagnetism with a screened particle-particle interaction. Screening is described within the random-phase approximation, augmented by various local-field corrections. Any perturbative approach is subject to bias in the selection of diagrams which are taken into account at any given density. An unbiased approach, such as a Quantum Monte Carlo (QMC) simulation, would be of great value in finally settling the question, and we hope that our work stimulates detailed QMC investigations of antiferromagnetic states. As long as such QMC calculations are not available, however, the results presented below are, to the best of our knowledge, the strongest yet reported in the literature. Furthermore, note that even in the thoroughly studied case of the phase diagram of the homogeneous electron gas in three dimensions, very recently new phases, not accounted for by the standard QMC calculations, have been predicted theoretically [1,2]. In this situation a perturbative study of the possibility of antiferromagnetic phases, not based on QMC, can contribute to a clarification of the actual nature of the phase diagram.

Another widely used many-body technique for which the results of the present investigation are relevant is density-functional theory (DFT). Recent DFT calculations for antiferromagnetic systems have encountered various difficulties [3–5]. In response, a novel DFT approach to antiferromagnetic systems has been developed [6]. Since the homogeneous electron gas is simultaneously the basic ingredient for the most popular approximation to conventional DFT (the local-density approximation), and the natural first test case for any novel DFT, an analysis of its antiferromagnetic properties is clearly desirable.

Previous perturbative explorations of the possibility of AFM phases in homogeneous electron systems were mostly based on a series of papers by Overhauser [7–10], in which it was proved that, within the Hartree-Fock approximation, an AFM phase always has lower energy than the paramagnetic phase. This instability towards AFM of the homogeneous electron gas produces a spin-density wave (SDW) similar to that observed, *e.g.*, in chromium [11].

Overhauser further argued that the instability may persist if certain correlations beyond Hartree-Fock are included [10]. Several lines of attack have been pursued in order to include such correlations: For three-dimensions Fedders and Martin [12] and Hamann and Overhauser [13] showed that going beyond the Hartree-Fock approximation by introducing screening into the description

[a] e-mail: capelle@if.sc.usp.br

of the paramagnetic state tends to eliminate the instability and makes antiferromagnetism unfavorable. The conclusion of Fedders and Martin is based on six data points in the metallic density regime ($r_s = 1, 2 \ldots 6$, where r_s is the standard density parameter), obtained using Thomas-Fermi screening of the Hartree-Fock approximation, and a rough estimate of the changes brought about by going beyond Thomas-Fermi screening *via* the random-phase approximation (RPA). The Thomas-Fermi approximation and the RPA, however, are not at all reliable at metallic and low densities.

Perdew and Datta performed density-functional calculations for the three-dimensional homogeneous electron gas [14] and found evidence for a charge-density wave, but not for AFM. Due to the necessary approximations for the density dependence of the coefficients of the involved gradients of the spin-densities, however, it is not clear if these calculations are valid in the metallic density regime. Furthermore, certain types of AFM states, such as those in which the resulting SDW has a very short wavelength, cannot be excluded conclusively on the basis of these calculations.

Although the results of Fedders and Martin and of Perdew and Datta thus indicate absence of various types of SDW states for certain densities of the homogeneous electron gas, they are not conclusive in the metallic density regime. They also do not extend to two-dimensional or layered systems. Furthermore, several other, mostly perturbative, calculations [10,15–18] did predict AFM within various approximations, but differ vastly in the value obtained for the critical density at which AFM sets in.

In order to clarify this situation, in the present work we reexamine and extend the work of Overhauser and of Fedders and Martin (FM). We consider a wide range of densities, from extremely low ($r_s = 100$) all the way to extremely high densities ($r_s \to 0$) and base our description of screening not on the Thomas-Fermi approximation, but on the random-phase approximation, augmented, in the metallic and low-density regimes, by the inclusion of local-field corrections. We begin by considering three-dimensional electron gases and then extend the same methodology to two-dimensional and layered systems.

2 Three-dimensional electron gas

In the following Section 2.1 we summarize the conclusions which emerge from a critical reexamination of the procedure and the results of Fedders and Martin. We point out limitations of their approach and briefly report how their treatment can be improved and what results follow from such improvements. In Section 2.2 we then proceed to a more reliable description of screening, based on local-field corrections to the RPA, and search for instabilities at metallic and lower densities.

2.1 Stability criterium for antiferromagnetism

Fedders and Martin derived the following Stoner-like criterium for the stability of antiferromagnetism in the homogeneous electron gas [12]:

$$\int \frac{\mathrm{d}^3 p'}{(2\pi)^3} V(\mathbf{p}-\mathbf{p}') \frac{f\left(E\left(\mathbf{p}'+\frac{\mathbf{q}}{2}\right)\right) - f\left(E\left(\mathbf{p}'-\frac{\mathbf{q}}{2}\right)\right)}{E\left(\mathbf{p}'+\frac{\mathbf{q}}{2}\right) - E\left(\mathbf{p}'-\frac{\mathbf{q}}{2}\right) - \omega} =: R(\mathbf{p},\mathbf{q},\omega) \leq -1, \quad (1)$$

where

$$f(E) = \frac{1}{1+\mathrm{e}^{(E-\mu)/k_\mathrm{B}T}} \quad (2)$$

is the usual Fermi function with temperature T, Boltzman constant k_B and chemical potential μ. The function $E(\mathbf{p})$ denotes the single-particle energies appearing in the single-particle Green's function. A solution to this integral equation corresponds to a pole in the $m_z m_z$ correlation function, where m_z is the z-component of the spin magnetization. (Consult Refs. [12,19,20] for a more detailed discussion of Eq. (1)). The FM criterium (1) does neglect non-collinear spin configurations (such as spin spirals) and the competition and coupling between spin-density waves and charge-density waves. It also does not apply to first-order phase transitions, since it is based on considering stability with respect to small fluctuations.

Within these limitations, Fedders and Martin proceeded by noting that the SDW ground state is characterized by the parameters $\omega = 0$, $\mathbf{p} = 0$ and $\mathbf{q} = 2\mathbf{k}_\mathrm{F}$, where $\mathbf{k}_\mathrm{F}$ is the Fermi momentum [8,9]. The first two of these parameters simply characterize the lowest energy stationary AFM state. The value $\mathbf{q} = 2\mathbf{k}_\mathrm{F}$ reflects the nesting of the Fermi surface, which is crucially important for the stability of antiferromagnetism both in Overhauser's calculation and in realistic materials such as chromium [11]. The task is thus to evaluate the integral $R(0, 2\mathbf{k}_\mathrm{F}, 0)$ and see whether it ever becomes equal to -1, the point at which the instability sets in. To this end one needs to make a choice for the particle-particle interaction $V(\mathbf{p})$ appearing in equation (1). The simplest choice for $V(\mathbf{p})$ is the bare interaction

$$V_0(\mathbf{p}) = \frac{4\pi e^2}{\mathbf{p}^2}, \quad (3)$$

which corresponds to the Hartree-Fock approximation for the two-particle Green's function. This choice always leads to an instability towards AFM [12], in complete accordance with Overhauser's earlier calculations. Following the procedure developed by Fedders and Martin, the Hartree-Fock approximation can be improved upon by screening the bare interaction. In the original work the Thomas-Fermi approximation

$$V_\mathrm{TF}(\mathbf{p}) = \frac{4\pi e^2}{\mathbf{p}^2 + \xi_\mathrm{TF}^2}, \quad (4)$$

where ξ_TF is the Thomas-Fermi screening momentum, was employed for this purpose. Fedders and Martin then made two further approximations in order to be able to evaluate equation (1). The first of these consists in

replacing the Fermi functions by step functions (*i.e.*, by their zero-temperature limit). The second approximation is to replace the energies $E(\mathbf{p})$, which should be those corresponding to the approximation chosen for the Green's function (*i.e.*, in the present case the Hartree-Fock single-particle energies), by the free-particle energies $E(\mathbf{p}) = \mathbf{p}^2/(2m)$. On the basis of these calculations FM concluded that there is no AFM in the three-dimensional homogeneous electron gas at the metallic densities $r_\mathrm{s} = 1...6$.

We have repeated the FM analysis for the density interval $r_\mathrm{s} = 1..100$ and also included Fermi-liquid corrections (which result in an improved description of screening as compared to the Thomas-Fermi approximation) and exchange-corrections to the single-particle energies (thereby undoing the second of the approximations just mentioned). Our essential conclusions can be summarized as follows: (i) Within the Thomas-Fermi approximation and for $r_\mathrm{s} = 1...6$ we confirm the numerical results of FM. We have also obtained an approximate analytical solution to the FM integral equation, which agrees to within a few percent with the numerical data in the range of high and metallic densities. (ii) Fermi-liquid and exchange corrections make the situation for AFM more unfavorable, not less so, *i.e.*, the criterium is violated by a larger margin if the particle-particle interaction is treated in a more reliable fashion. (iii) Contrary to the expectations of FM [12], the exchange corrections to the single-particle energies are not negligible, but yield changes of the uncorrected values on the 10% level. Qualitatively, however, they do not change any previous conclusion. (iv) The FM criterium for the stability of AFM phases can be generalized to include non-collinear SDW states and the competition with (and coupling to) charge-density wave instabilities. These results will be discussed in more detail in a future publication [20].

2.2 Random-phase approximation and local-field factors

In the present work we are mainly concerned with the metallic and low-density regime, in which the Thomas-Fermi approximation is notoriously unreliable. Although the inclusion of Fermi-liquid and exchange corrections improves this situation somewhat, a reliable treatment of metallic and low-density systems requires a more elaborate approach. Fedders and Martin already indicated a possible direction for further improvements, namely a description of screening based on many-body techniques, such as the RPA. However, they limited their treatment of the RPA to giving a rough estimate, without providing numerical results. Furthermore the RPA, too, is unreliable at metallic and at low densities. One can, however, extend the validity of the RPA description of screening into the metallic and even well into the low-density regime by introducing local-field factors in the expression for the RPA dielectric constant.

Within the RPA the potential $V(\mathbf{p})$ is

$$V_\mathrm{RPA}(\mathbf{p}) = \frac{V_0(\mathbf{p})}{\epsilon_\mathrm{RPA}(\mathbf{p})}, \tag{5}$$

where static RPA dielectric function $\epsilon_\mathrm{RPA}(\mathbf{p})$ is given by

$$\epsilon_\mathrm{RPA}(\mathbf{p}) = 1 - \frac{4\pi e^2}{\mathbf{p}^2}\chi(\mathbf{p}), \tag{6}$$

and $\chi(\mathbf{p})$ is the $\omega = 0$ limit of the Lindhard function, *i.e.*, the response function of the non-interacting homogeneous electron gas. The inclusion of local-field corrections is accomplished *via*

$$\epsilon_\mathrm{LFF}(\mathbf{p}) = 1 - \frac{V_0(\mathbf{p})\chi(\mathbf{p})}{1 + V_0(\mathbf{p})\mathcal{G}(\mathbf{p})\chi(\mathbf{p})}. \tag{7}$$

A large variety of approximations for the local-field factor (LFF) $\mathcal{G}(\mathbf{p})$ are available. In a first step we employed the Hubbard form,

$$\mathcal{G}(\mathbf{p}) = \frac{p^2}{2(p^2 + k_\mathrm{F}^2)}, \tag{8}$$

where $p = |\mathbf{p}|$. The Hubbard approximation for the local-field factor in many cases already provides substantial improvement over the RPA. However, a large number of alternative expressions for $\mathcal{G}(\mathbf{p})$ exist, which, in particular at low densities, improve on the Hubbard expression. Probably the simplest of these is the form [19,21]

$$\mathcal{G}(\mathbf{p}) = \frac{p^2}{2(p^2 + k_\mathrm{F}^2 + \xi_\mathrm{TF}^2)}. \tag{9}$$

More sophisticated improvements on the Hubbard approximation are contained, *e.g.*, in the recent work of Gold and Calmels [22,23], and of Sato, Iyetomi and Ichimaru [18,24], where parametrizations for the local-field correction over a wide range of densities are provided.

The parametrization of Gold and Calmels employs a sum-rule-based version of the self-consistent approach of Singwi, Tosi, Land and Sjölander [25], and has been shown to be very accurate up to $r_\mathrm{s} \approx 20$, reasonably accurate for higher values of r_s, and to satisfy various exact properties of the exact local-field factor [23]. The proposed expression for $\mathcal{G}$ is [23]

$$\mathcal{G}(x) = r_\mathrm{s}^{3/4}\frac{0.846x^2}{2.188C_{13}(r_\mathrm{s}) + x^2C_{23}(r_\mathrm{s})}, \tag{10}$$

where x is a dimensionless momentum variable and the functions $C_{13}(r_\mathrm{s})$ and $C_{23}(r_\mathrm{s})$ are numerically known [23,26].

The parametrization of Sato and Ichimaru [18], on the other hand, is specifically designed to incorporate the second-order exchange diagram [27], which is an important non-RPA contribution to the correlation energy. These authors provide the expression

$$G(x) = \left(\frac{x^2}{4} + 0.0057x^4\right)\left(0.79 + 0.21\tanh\left(\frac{4 - x^2}{0.45}\right)\right), \tag{11}$$

for $0 \le x = k/k_\mathrm{F} \le 2$.

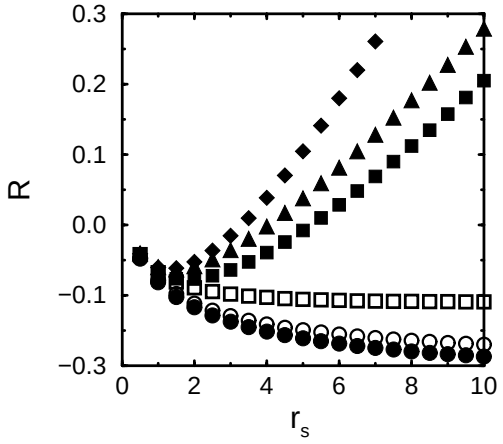

Fig. 1. Value of the integral (1) for low and intermediate (metallic) values of r_s. $R = -1$ would indicate an instability towards antiferromagnetism. The empty circles correspond to simple Thomas-Fermi screening, full circles to the static RPA, and the triangles to the RPA including local-field corrections in the Hubbard form. Open squares are obtained with equation (9). Filled squares are results from using the Sato-Ichimaru parametrization. Diamonds, finally, correspond to the RPA with local-field corrections in the Gold form.

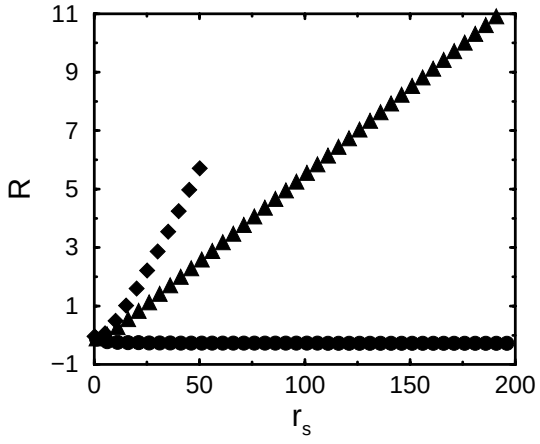

Fig. 2. Extension of Figure 1 to high values of r_s, *i.e.* to low densities. The local-field correction in the Gold form (diamonds) is only available for $r_s \leq 50$. The local-field factor of Sato and Ichimaru leads to values almost indistinguishable from those obtained with the Hubbard approximation (triangles) on this scale. Similarly, the Thomas-Fermi results and those obtained with the local-field factor (9) are virtually indistinguishable from the RPA results (filled circles) on this scale. Consequently, only results obtained with the RPA and the approximations of Gold and Hubbard are plotted. Obviously, the RPA and the Thomas-Fermi approximation are not only quantitatively but also qualitatively wrong at large r_s, *i.e.*, at low densities.

The integral resulting if the bare potential, screened by a dielectric constant including any of these four local-field corrections, is substituted in equation (1), must be evaluated numerically. Results are listed in Table 1 for some representative values of the densities and, for many more densities, plotted in Figures 1 and 2. For comparison we have also included values obtained with Thomas-Fermi screening and the uncorrected RPA in the table and the figures.

Several conclusions can be drawn from these data: (i) In agreement with the results obtained by Fedders and Martin, Thomas-Fermi screening yields values which are fairly close to satisfying the stability criterium, but not close enough. (ii) RPA screening yields values which are slightly closer to AFM than pure Thomas-Fermi screening. This is, however, an artifact of the RPA, which is removed by the more reliable local-field corrected approximations. (iii) Local-field factors drastically modify the behaviour of the integral at low and metallic densities, where they improve most upon the RPA. This shows that previous approximations, including in particular those of Fedders and Martin, which were based on the RPA or on Thomas-Fermi screening, are not reliable in the density regimes they were applied to. (iv) Different parametrizations of the local-field factor show considerable quantitative, but almost no qualitative differences among each other, while they show both quantitative and qualitative differences with the uncorrected RPA. (v) There is no sign of antiferromagnetism in the entire investigated density interval, within any of the employed approximation schemes.

A critical assessment of the validity of the resulting claim that there is no AFM in the three-dimensional interacting electron gas at any density is postphoned until Section 5. The next two sections are devoted to the two-dimensional electron gas and thin laterally homogeneous electron films. In both of these systems screening is weaker than in three dimensions, so that an instability would seem more likely.

3 Two-dimensional electron gas

There exist two fundamentally distinct conceptions of a two-dimensional interacting electron gas. In the first of these the particles are considered to be constrained to move in a plane, while the basic equations (such as Maxwell's and Schrödinger's equations) retain their familiar three-dimensional form. In particular, the Coulomb potential, resulting from the Green's function of the three-dimensional Laplace equation, is still given by $1/r$. Such systems will below be called quasi-two-dimensional systems. In the second conception of a two-dimensional electron gas the entire physics is assumed to be two-dimensional. The Coulomb potential, arising from the solution to the two-dimensional Laplace equation, is then logarithmic [28]. Strictly speaking, only the second case deserves to be called a 'two-dimensional electron gas'. What is observed in nature, however, is closer to the first case: The two-dimensional electron gases of semiconductor physics [29], electrons on liquid helium [29], or weakly coupled layered systems, such as in the high-temperature superconductors [30], transition metal dichalcogenides [31] and organic conductors [32] are typical examples of *quasi*-two-dimensional systems. In this paper we will exclusively

Table 1. The values of $-100R(r_s)$ in three dimensions for some representative densities. $-100R(r_s)$ must be larger or equal 100, in order for an instability towards AFM to exist. The first row gives the density parameter, the second the results of the Thomas-Fermi approximation for screening. The third row contains the results for q-dependent screening (the static RPA). The fourth to seventh rows contain results including local-field corrections to the RPA. Row four is based on the form for the local-field factor (LFF) given by Hubbard, row five on equation (9), row six employs that of Gold and Camels (which is only available for $r_s \leq 50$) and row seven that of Sato and Ichimaru. As is obvious from the data in this Table, the criterium for AFM is not satisfied in any of these approximations, for any listed density. Note that the data listed in this Table are only representative values. A much larger number of densities is plotted in Figures 1 and 2.

r_s	0.2	0.5	1	2	3	4	5	6	10	100
$-100R(r_s)_{\mathrm{TF}}$	6.1	9.7	13	16	18	19	20	21	22	25
$-100R(r_s)_{\mathrm{RPA}}$	6.2	9.8	13	17	19	20	21	22	24	27
$-100R(r_s)_{\mathrm{RPA+HLFF}}$	6.0	9.0	11	11	8.6	5.2	1.2	−3.1	−23	−550
$-100R(r_s)_{\mathrm{RPA+SLFF}}$	6.0	9.2	12	14	15	15	16	16	16	16
$-100R(r_s)_{\mathrm{RPA+GLFF}}$	6.0	9.1	11	10	6.5	1.2	−5.4	−13	−48	-
$-100R(r_s)_{\mathrm{RPA+ILFF}}$	6.1	9.3	12	13	11	8.9	5.8	2.1	−15	−580

deal with this type of two-dimensional systems. The two-dimensional Fourier transform of the $1/r$ Coulomb potential then yields

$$V_0(\mathbf{p}) = \frac{2\pi e^2}{p}. \tag{12}$$

The density of the two-dimensional electron gas is determined by the density parameter r_s, which is defined, in two dimensions, according to

$$r_s = \frac{1}{a_0\sqrt{n\pi}} = \frac{1}{\tilde{\alpha} k_F a_0}, \tag{13}$$

where n is the two-dimensional density, $a_0 = \hbar^2/(me^2)$ is the Bohr radius, $\tilde{\alpha} = 1/\sqrt{2}$, and k_F is the radius of the Fermi circle.

Of course, the Mermin-Wagner theorem [33] excludes the existence of long-range magnetic order in strictly two-dimensional systems at nonzero temperature [34–40]. The present investigation aims specifically at the zero temperature case, where the Mermin-Wagner theorem does not apply.

The Fedders and Martin criterium, equation (1), is easily adapted to the two-dimensional case. Employing planar polar coordinates and performing one of the integrals we find that at zero temperature

$$R = \frac{\tilde{\alpha} r_s}{8\pi^2 e^2}\left[\int_{\pi/2}^{3\pi/2}\int_0^{-2k_F\cos\varphi} - \int_0^{\pi/2}\int_0^{2k_F\cos\varphi} - \int_{3\pi/2}^{2\pi}\int_0^{2k_F\cos\varphi}\right]\frac{V(k)}{\cos\varphi}\,\mathrm{d}\varphi\mathrm{d}k. \tag{14}$$

Within the Thomas-Fermi approximation the two-dimensional screened potential is given by

$$v(\mathbf{k}) = \frac{2\pi e^2}{k+\xi}, \tag{15}$$

where $\xi = 2/a_0$ and $a_0 = \hbar^2/(me^2)$ is the Bohr radius. If this potential is substituted in (14) one finds that the k integral can be done analytically. The result is

$$R(r_s) = \frac{\tilde{\alpha} r_s}{4\pi}\left[\int_{\pi/2}^{3\pi/2}\mathrm{d}\varphi\frac{\log\left|1-\frac{2k_F\cos\varphi}{\xi}\right|}{\cos\varphi} - \int_0^{\pi/2}\mathrm{d}\varphi\frac{\log\left|1+\frac{2k_F\cos\varphi}{\xi}\right|}{\cos\varphi} - \int_{3\pi/2}^{2\pi}\mathrm{d}\varphi\frac{\log\left|1+\frac{2k_F\cos\varphi}{\xi}\right|}{\cos\varphi}\right]. \tag{16}$$

The remaining φ integrals must, in general, be evaluated numerically.

3.1 Unscreened interaction

We first consider the Hartree-Fock approximation, *i.e.*, no screening. For three-dimensional systems the corresponding calculation leads to a rederivation of Overhauser's result that the homogeneous electron gas, within the Hartree-Fock approximation, is unstable towards AFM [12]. Since Overhauser himself proved his theorem only in one [8] and three [9] dimensions, it is interesting to check whether the instability can also be found in two dimensions.

In fact, the desired result follows directly from equation (16). In the limit $\xi \to 0$ all three logarithms tend towards positive infinity. In the second and third integral, which are subtracted, the integration limits are such that $\cos\varphi$ is always positive. In the first integral, which enters (16) with a positive sign, the limits are such that the contribution of $\cos\varphi$ is always negative. Hence, for $\xi \to 0$ all three terms are negative and

$$\lim_{\xi\to 0} R(r_s) = -\infty \tag{17}$$

for all nonzero r_s, *i.e.*, for all finite densities. It follows that the two-dimensional homogeneous electron gas in the Hartree-Fock approximation is always unstable towards AFM.

Table 2. Values of $-100R(r_s)$ in two dimensions for a number of selected densities. $-100R(r_s)$ must be larger or equal 100 in order to have an instability towards antiferromagnetism. As discussed in the main text, the values for Thomas-Fermi screening and RPA screening are identical. Thus only one row of data, the second, is given for both approximations. The third and fourth rows contain results including local-field corrections to the (static) RPA. Row three is based on the expression given by Sato and Ichimaru, while row four employs the two-dimensional local-field parametrization of Gold and Calmels. Note that the data listed in this Table are only representative values. A much larger number of densities is plotted in Figures 3 and 4.

r_s	0.2	0.5	1	2	3	4	5	6	10	100
$-100R(r_s)_{\mathrm{RPA}}$	21	30	37	42	44	45	46	47	48	50
$-100R(r_s)_{\mathrm{RPA+ILFF}}$	20	25	22	3.9	−20	−47	−76	−110	−230	−3100
$-100R(r_s)_{\mathrm{RPA+GLFF}}$	20	22	13	−28	−84	−150	−220	−300	−650	−13000

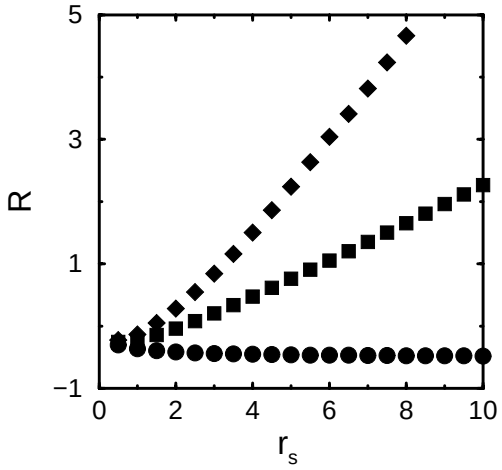

Fig. 3. Value of the integral (14) for low and intermediate values of r_s. The filled circles correspond to simple Thomas-Fermi screening *and* wave-vector dependent screening. Filled squares correspond to the static RPA including two-dimensional local-field corrections in the Ichimaru-Sato form. Diamonds correspond to two-dimensional local-field corrections in the Gold-Calmels form.

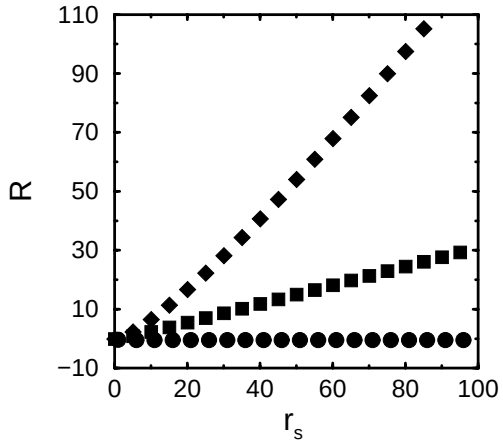

Fig. 4. Extension of Figure 3 to high values of r_s, *i.e.* to low densities. We have extended these calculations to $r_s = 200$ without finding any qualitative change in the behaviour of the curves. The data between $r_s = 100$ and $r_s = 200$ are not included in this curve in order to keep the values obtained from Thomas-Fermi screening (the filled circles) visible on the same scale.

3.2 Screened interaction

In order to go beyond the Hartee-Fock approximation we now numerically evaluate the integral (16), with the Thomas-Fermi value for ξ, as a function of the density parameter r_s. The results are listed, for some representative densities, in the second row of Table 2 and plotted, for many more densities, in Figures 3 and 4 (represented by the filled circles). Obviously, the criterium $R = -1$ is not satisfied in the entire density interval. Qualitatively, this is the same result obtained in three dimensions: Screening the interaction eliminates the antiferromagnetic phase found in the Hartree-Fock approximation. The logical next step would be the corresponding calculation for wave-vector dependent screening. For this one needs as input the RPA expression for the two-dimensional dielectric function. However, in the range of wave vectors needed for evaluation of equation (14), namely $k \in (0, 2k_F)$, the RPA for the two-dimensional dielectric function is identical with the Thomas-Fermi expression [29,41,42]. This result is related to the counterintuitive fact that Thomas-Fermi screening in two dimensions is independent of the density [29]. The Thomas-Fermi data in Table 2 and Figures 3 and 4 thus already represent the values obtained from the static RPA.

In the same way as in three dimensions one can now include local-field corrections in order to improve the results for low densities. The screened potential then becomes

$$V_{\mathrm{LFF}}(\mathbf{p}) = \frac{V_0(\mathbf{p})}{\epsilon_{\mathrm{LFF}}(\mathbf{p})}. \tag{18}$$

The necessary approximations for the two-dimensional dielectric constant are obtained from

$$\epsilon_{\mathrm{LFF}}(\mathbf{p}) = 1 - \frac{1 - \epsilon_{\mathrm{RPA}}(\mathbf{p})}{1 + \mathcal{G}(\mathbf{p})\,[1 - \epsilon_{\mathrm{RPA}}(\mathbf{p})]}, \tag{19}$$

which follows from the definition of the local-field factor and the RPA. The two-dimensional RPA is known from the literature [29,41,42], and the two-dimensional local-field factor $\mathcal{G}(\mathbf{p})$ has been parametrized by various workers. In the numerical calculations based on equation (18) we employed two such parametrizations.

One is the sum-rule-based two-dimensional parametrization of Gold and Calmels [23]. Here $\mathcal{G}$ takes the form

$$\mathcal{G}(x) = r_{\rm s}^{2/3} \frac{1.402x}{\sqrt{2.644 C_{12}^2(r_{\rm s}) + x^2 C_{22}^2(r_{\rm s})}}, \qquad (20)$$

where the functions $C_{12}(r_{\rm s})$ and $C_{22}(r_{\rm s})$ are numerically known [23,26].

The other parametrization for the two-dimensional local-field factor used in the present work is that given by Sato and Ichimaru [18] and further discussed by Iyetomi and Ichimaru [24]. Their explicit expression for $\mathcal{G}$ is

$$\mathcal{G}(x) = \left(\frac{x}{\pi} + 0.009x^4 - 0.00038x^6\right) \times \left(0.965 + 0.035 \tanh\left[\frac{4-x^2}{0.078}\right]\right), \qquad (21)$$

where $0 \le x = k/k_{\rm F} \le 2$. This expression incorporates the second-order exchange correction [43,44], which has been found to be crucially important in two dimensions [18,24,43,44].

Results obtained on the basis of these two parametrizations for $\mathcal{G}(q)$ by numerically evaluating the double integral (14) for densities ranging from $r_{\rm s} = 0.2$ to $r_{\rm s} = 100$, are listed in the third and fourth row of Table 2 and plotted in Figures 3 and 4. The different parametrizations for $\mathcal{G}(q)$ are seen to differ quantitatively, in particular at low densities, but to display the same qualitative behaviour. The net result of these calculations is that, whatever the approximation scheme, and at any investigated density, the AFM stability criterium is violated.

The resulting conclusion that AFM does not exist for two dimensional densities from $r_{\rm s} = 0.2$ to $r_{\rm s} = 100$ is in disagreement with a result obtained by Bergman and Rice [45]. These authors use an integral equation of the same type as that of Fedders and Martin and solve it approximately by neglecting higher-order terms in the irreducible particle-hole interaction and assuming a certain form for the Green's functions. They predict an AFM state at $r_{\rm s} \ge 2.9$ for, *e.g.*, two-dimensional inversion layers on Si [100] surfaces. However, as these authors themselves point out, their result has to be viewed with caution, since by predicting AFM in three dimensions at $r_{\rm s} = 4.3$ their approximations contradict the conclusion of a number of other authors [12,13,45].

In another work, Ichimaru and coworkers [18,24] found indications for a possible instability of two-dimensional electron systems towards SDW states at $r_{\rm s} = 1.89$. (Note that this value is not compatible with the Bergman-Rice estimate $r_{\rm s} \ge 2.9$.) Their result is based on an approximation to density-functional theory, with the exchange-correlation functional expressed in terms of the local-field factor (21). From the above it follows that we cannot confirm their finding. While at present we do not have an explanation for the discrepancy between their result and ours, we offer the following tentative remarks on this issue: It follows from our data that although the local-field factors of Gold and Calmels, equation (20), and of Ichimaru and coworkers, equation (21), are both unfavorable for AFM, the latter is less so than the former. It is thus more likely to find spurious AFM in an approximate calculation based on equation (21). Apart from this, the discrepancy may arise from the fact that these authors consider only the spin-susceptibility, while the Fedders and Martin criterium arises from an analysis of the full $m_z m_z$ correlation function. Alternatively, it may indicate that inclusion of only the second-order exchange energy in the local-field factor (21), important as it is, is not enough to guarantee consistent results.

A detailed evaluation of the data summarized in Table 2 and Figures 3 and 4 can be summarized as follows: (i) Use of an unscreened interaction shows that Overhauser's instability persists in a two-dimensional electron gas, at any density. (ii) This instability disappears if the interaction is screened, regardless of which approximation scheme is used for screening. (iii) The net effect of the local-field corrections in two dimensions is essentially the same as in three dimensions: the RPA results are drastically changed at low densities, and the AFM criterium is even more strongly violated than in the RPA. (iv) Comparing the tendency towards AFM in two and three dimensions we find that the two-dimensional electron gas violates the criterium by a smaller margin than the three-dimensional one (*i.e.*, is less stable) at large densities, while it violates it by a larger margin (is more stable) at low densities.

4 Laterally homogeneous thin films

Quasi-two-dimensional systems, in which the Coulomb interaction retains its three-dimensional form, only roughly approximate realistic layered systems or thin films. However, as long as their width is small compared to their other two dimensions, such structures can be treated in a very similar way as the quasi-two-dimensional systems. The two-dimensional potential is simply modified according to

$$V(\mathbf{p}) = \frac{1}{\epsilon(\mathbf{p})} \frac{2\pi e^2}{p} F_b(\mathbf{p}), \qquad (22)$$

where $\epsilon(\mathbf{p})$ is the dielectric constant of the layer. $F_b(\mathbf{p})$ is the so called form factor and b measures the inverse width of the layer [46]. The effective layer width is approximately $3/b$. A simple analytical approximation for this form factor is available [46,47], namely

$$F_b(\mathbf{p}) = \frac{1 + \frac{9}{8}\frac{p}{b} + \frac{3}{8}\frac{p^2}{b^2}}{\left(1 + \frac{p}{b}\right)^3}. \qquad (23)$$

This approximation describes well the nearly two-dimensional electron gases of semiconductor physics [29,47,48]. The present expression for this factor is somewhat simpler than that given in the original references because for the present purposes we do not need to distinguish the dielectric constants of the adjacent metal and semiconductor, as is required in semiconductor physics [29]. It is now a simple matter to introduce this model potential in equation (14) and perform the resulting

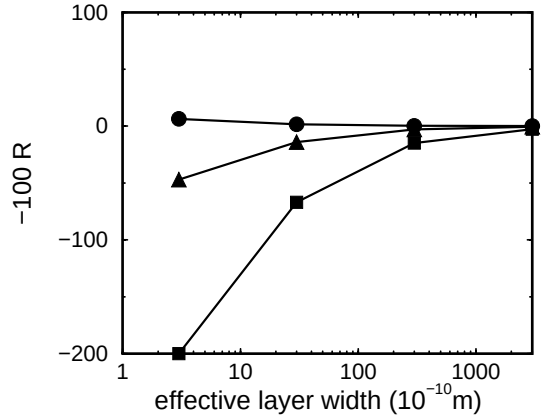

Fig. 5. Antiferromagnetism criterium in a homogeneous electron layer as a function of the effective width of the layer. Screening is treated within the static RPA including the two-dimensional local-field correction of Gold and Calmels [23] and the finite width is taken into account through the form factor defined in equation (23). Squares denote data for $r_s = 6$, triangles those for $r_s = 3$ and circles correspond to $r_s = 0.5$. The effective layer width is taken to be 3 Å, 30 Å, 300 Å and 3000 Å, respectively and is displayed on a logarithmic scale. The solid lines are only guides for the eye.

double integral numerically for various approximations for screening. Results for four different values of the effective layer width are listed in Table 3 for the uncorrected RPA, and in Table 4 for the RPA with the Gold-Calmels local-field correction. The following conclusions can be drawn from detailed analysis of these data:

(i) There is no antiferromagnetism in thin films of homogeneous electron gases for any investigated value of the density and the effective layer width, and for any employed approximation for the dielectric constant.

(ii) For high densities both local-field factors are in quantitative and qualitative agreement with each other and with the RPA. For lower densities the local-field factors still yield results which agree at least qualitatively with each other, while, as expected, the RPA results differ drastically.

(iii) For small and intermediate densities the AFM criterium is violated more strongly as the system becomes more two dimensional. For large densities the situation is exactly reversed, so that AFM becomes less unfavorable for thinner layers. This behaviour is demonstrated in Figure 5, in which the value of $-100R$ is plotted as a function of the effective layer width for several values of the density parameter r_s. The data recorded in Table 4 and plotted in Figure 5 were obtained on the basis of the Gold-Calmels parametrization for the two-dimensional local-field factor. If the Ichimaru-Sato local-field parametrization is used instead of that of Gold and Calmels the quantitative details are slightly different, but the overall behaviour of the curves remains the same.

Conclusion (iii), on the effect of two-dimensionality on AFM, is in agreement with the findings of Section 3, which were obtained by direct comparison of the results from the two-dimensional calculation with those obtained in three-dimensions. Note, however, that whereas the limit of zero layer width of the potential (22) is the correct potential for a two-dimensional system, the limit of infinite layer width is not that of a three-dimensional system, because the approximations made in deriving the form factor (23) break down in this limit. While the data obtained for thin films should thus be reliable, as long as the effective width is not too large, extrapolation to three dimensions, starting from a two-dimensional potential is, evidently, not justified.

5 Loopholes

The results obtained so far seem to rule out antiferromagnetism in the homogeneous electron gas. Overhauser's theorem, obtained in the Hartree-Fock approximation, that the homogeneous electron gas is antiferromagnetic for any density would then be merely an artifact of the Hartree-Fock approximation. In fact, this is not the case. There are two loopholes in the treatment given here (and also in most previous works on the same subject [12–14,45]). These loopholes can be summarized under the headings of 'first-order transitions' (or 'antiferromagnetically modified screening') and 'non-collinearity'.

We first turn to a discussion of first-order transitions. Overhauser already argued [10] that in order to analyze the energetic stability of an AFM state one should take into account that the screening itself is modified in that state. In other words, it should be taken into account that the nature of the correlations leading to screening beyond Hartree-Fock depends on the presence or absence of AFM. Of course, this effect is difficult to account for on the basis of the models for screening discussed above. For second-order phase transitions this is not necessary, because the order parameter for antiferromagnetism is vanishingly small at the critical temperature. Consequently, a small AFM fluctuation, appearing spontaneously in the system, will find itself in a hostile environment, dominated by normal-state screening, and thus energetically unfavorable for AFM. Such fluctuations will disappear.

On the other hand, if the order parameter is finite at the critical temperature, as is the case for first-order transitions, an AFM fluctuation can locally lead to a state with finite order parameter and considerably modified screening. In a suitable density and temperature regime such a fluctuation may thus stabilize itself and induce a phase transition into an AFM state. As Fedders and Martin already pointed out [12], the normal (paramagnetic) state would then be only metastable at those values of temperature and density. Of course, this argument should not be taken as implying that such a metastability necessarily exists, the point to make is merely that it cannot be conclusively excluded on the basis of results obtained from the stability criterium of FM.

The second loophole, associated with non-collinearity, arises from the fact that the AFM stability criterium, equation (1), is derived solely from the $m_z m_z$ correlation function and thus not applicable to non-collinear states,

Table 3. Criterium for antiferromagnetism in a homogeneous electron film of finite width, evaluated within the static RPA. The effective width of the layer varies from 3 Å to 3000 Å. The value of $-100R(r_s)$ must be larger than 100, in order for AFM to exist. For comparison purposes we have also included, in the second row, the corresponding values from Table 2 for strictly two-dimensional systems.

r_s	0.2	0.5	1	2	3	4	5	6	10	100
$-100R(r_s)$, 2 dim	21	30	37	42	44	45	46	47	48	50
$-100R(r_s)$, 3 Å	4.8	9.2	14	21	25	28	31	33	37	48
$-100R(r_s)$, 30 Å	1.1	2.3	3.8	6.2	8.1	9.7	11	12	16	39
$-100R(r_s)$, 300 Å	0.20	0.43	0.75	1.3	1.7	2.2	2.5	2.9	4.1	17
$-100R(r_s)$, 3000 Å	0.032	0.070	0.12	0.21	0.30	0.38	0.46	0.53	0.78	4.2

Table 4. Criterium for antiferromagnetism in a homogeneous electron film of finite width, evaluated within the static RPA and the two-dimensional local-field correction of Gold and Calmels. The effective width of the layer varies from 3 Å to 3000 Å. The value of $-100R(r_s)$ must be larger than 100, in order for AFM to exist. For comparison purposes we have also included, in the second row, the corresponding values from Table 2 for strictly two-dimensional systems.

r_s	0.2	0.5	1	2	3	4	5	6	10	100
$-100R(r_s)$, 2 dim	20	22	13	−28	−84	−150	−220	−300	−650	−13000
$-100R(r_s)$, 3 Å	4.3	6.3	4.2	−15	−47	−90	−142	−200	−480	−12000
$-100R(r_s)$, 30 Å	0.98	1.5	1.0	−4.3	−14	−29	−47	−67	−186	−9111
$-100R(r_s)$, 300 Å	0.18	0.28	0.19	−0.88	−3.0	−6.0	−10	−15	−42	−3200
$-100R(r_s)$, 3000 Å	0.028	0.045	0.031	−0.15	−0.51	−1.0	−1.7	−2.6	−7.6	−660

which would require consideration of m_x and m_y, in addition to m_z. The criterium is thus not adequate to investigate non-collinear spin configurations. However, we regard such non-collinear states in homogeneous electron systems as highly unlikely because, although they cannot be excluded on the basis of a study of only the $m_z m_z$ correlation function, they are expected to leave at least some traces in that function. We have found no such traces (such as values of R close to -1), at any density.

If a non-collinear spin configuration and/or a first-order transition should exist in the homogeneous electron gas, many-body calculations considering only stability with respect to small fluctuations, and taking into account only collinear magnetism, are inconclusive. Clearly, the same applies to the corresponding phenomena in real (inhomogeneous) systems. One method which is applicable to homogeneous and inhomogeneous systems, and is capable of handling both non-collinear spin configurations and first-order transitions, is the recently developed novel density-functional approach to spin-density waves [6]. Detailed results obtained with this approach will be reported in a future publication.

6 Summary

Our main conclusions concerning the Fedders and Martin criterium are summarized at the end of Section 2.1, while our findings based on the local-field corrected RPA for three-dimensional, two-dimensional, and layered electron gases are summarized at the ends of Sections 2.2, 3.2, and 4, respectively. The central result of these investigations is that there is almost certainly no antiferromagnetic state in homogeneous electron systems at any density, the caveat 'almost certainly' referring to the possibility of first-order transitions from a metastable state, and non-collinear spin configurations, which cannot be excluded conclusively.

From the absence of conventional AFM in the three-dimensional homogeneous electron gas, the two-dimensional homogeneous electron gas, and thin laterally homogeneous films, it follows that existence of AFM is tightly tied to inhomogeneities. As viable mechanisms for second-order transitions into an AFM state in realistic systems thus remain only those explicitly related to inhomogeneity, such as band structure effects, magnetic impurities, spin-orbit coupling, etc.

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