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Effects of Thickness on the Spin Susceptibility of the Two Dimensional Electron Gas

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Using available quantum Monte Carlo predictions for a strictly 2D electron gas, we estimate the spin susceptibility of electrons in actual devices taking into account the effect of the finite transverse thickness and finding very good agreement with experiments. A weak disorder, as found in very clean devices and/or at densities not too low, just brings about a minor enhancement of the susceptibility.

Spin fluctuations are believed to play an important role in the two dimensional electron gas (2DEG), near the apparent metal-insulator transition observed at low temperature in clean devices, with lowering the density [1]. Indeed, it has been found that the application of an in-plane magnetic field, which polarizes the electron spin, suppresses the metallic conductivity [1,2]. This, together with earlier suggestions that metallic behavior in 2D should be accompanied by a tendency toward a ferromagnetic instability [3], has recently prompted a number of experimental investigations of the spin susceptibility χ_s of the 2DEG [4–11], which is generally found to increase [12] in an appreciable manner when decreasing the density n. Similar behavior is found also on the theoretical side for a strictly 2DEG, according to the most recent (and most accurate) quantum Monte Carlo (QMC) results [13]. However, the susceptibilities measured in different devices differ among each other and, with one exception [10], do not agree with theory [13]. Evidently, the details of the devices play a role in determining the properties of the 2DEG and should be accounted for by theory, as we shall show below. In particular, in experiments the electron gas (EG) (i) has a finite transverse thickness, (ii) suffers scattering by a number of sources (scattering which in fact determines its mobility), and depending on the system, (iii) occupies one or two degenerate valleys. In this Letter we address points (i) and (ii) for one-valley systems, exploiting the available QMC data. We find that taking into account the finite thickness of the specific device quantitatively brings into agreement theory and experiment and reconciles measurements on different systems, whereas the details of the scattering sources play a minor role. Furthermore, we offer some comments on the effect of (iii) valley degeneracy.

At zero temperature and at given number density n, the state of the 2DEG can be specified by the spin polarization $\zeta = (n_\uparrow - n_\downarrow)/n$. The spin susceptibility $\chi_s = (\partial \zeta / \partial B)_{B=0}$, which measures the ratio of the induced spin polarization to an in-plane applied weak magnetic field B, is readily shown to be inversely proportional to the derivative

$[\partial^2 E(\zeta)/\partial \zeta^2]_{\zeta=0}$, involving the EG internal energy $E(\zeta)$. In fact, minimization of the energy per particle $E(\zeta) + \zeta g_b \mu_B B/2$ with respect to ζ yields the condition $E'(\zeta) = -g_b \mu_B B/2$ from which $(\partial \zeta / \partial B)_{B=0} = -(g_b \mu_B/2)/E''(0)$ immediately follows. An estimate of the spin susceptibility can be thus obtained from the knowledge of the internal energy $E(\zeta)$.

The effect of thickness on the 2DEG can be cast, in the simplest approximation, in terms of a device specific form factor $F(q)$ modifying in Fourier space the 2D electron-electron interaction $v(q) = 2\pi e^2/\epsilon q$ into $\tilde{v}(q) = v(q)F(q)$ [14]. Rather than performing new simulations for each device we have estimated the effects of thickness on $E(\zeta)$ and hence on χ_s in a straightforward manner resorting to perturbation theory. In fact, to the lowest order in $\Delta v(r) = \tilde{v}(r) - v(r)$, one has for the energy per particle $E(\zeta) = E_{2D}(\zeta) + \Delta(\zeta)$,

$$\Delta(\zeta) = \frac{n}{2} \int d\mathbf{r} \Delta v(r)[g_{2D}(\zeta; r) - 1], \qquad (1)$$

with $E_{2D}(\zeta)$ and $g_{2D}(\zeta; r)$ the known energy [13] and pair correlation function [15], respectively, of the strictly 2D electron gas. The accuracy of the energy estimates obtained in such a manner has been checked *a posteriori* performing selected simulations with the interaction $\tilde{v}(r)$ [16]. We have computed the effect of thickness in two cases, for a GaAs heterojunction-insulated gate field-effect transistor (HIGFET) [9] and for an AlAs quantum well (QW) [10]. In the first case the form factor is [17]

$$F(q) = \left[1 + \frac{9}{8} \frac{q}{b} + \frac{3}{8} \frac{q^2}{b^2} \right] \left[1 + \frac{q}{b} \right]^{-3}, \qquad (2)$$

with $b^3 = 48\pi m_b e^2 n^*/\epsilon \hbar^2$ and $n^* = n_d + \frac{11}{32} n$. Here, n_d is the depletion charge density in the device [18], $m_b = 0.067 m_e$ the band electron mass, and $\epsilon = 12.9$ the average background dielectric constant. For the AlAs QW, on the other hand, the form factor can be written as [19]

$$F(q) = \frac{1}{4\pi^2 + q^2a^2}\left(3qa + \frac{8\pi^2}{qa} - \frac{32\pi^4}{q^2a^2}\frac{1 - e^{-qa}}{4\pi^2 + q^2a^2}\right),$$

$$(3)$$

with $a = 45$ Å the width of the well [10]. Once $F(q)$ is known, it is a simple matter to evaluate $\Delta(\zeta)$, using Eq. (1), from which the enhancement χ_s/χ_P of the spin susceptibility χ_s on its independent-particle or Pauli value χ_P is immediately obtained as $E_0''(0)/E''(0)$, with $E_0(\zeta) = E_F(1 + \zeta^2)/2$ the energy per particle of noninteracting Fermions in 2D and E_F the Fermi energy. Thus

$$\chi_s/\chi_P = E_F/E''(0). \qquad (4)$$

Our main findings [20] are summarized in Fig. 1, which shows a number of calculations and measurements of χ_s/χ_P. This quantity is plotted against the 2D coupling parameter $r_s = U/E_F = 1/\sqrt{\pi n}a_B$ to get rid of uninteresting details of different materials which simply determine the effective Bohr radius $a_B = \hbar^2\epsilon/m_be^2$ through the dielectric constant ϵ and band mass m_b; above, $U = e^2\sqrt{\pi n}/\epsilon$ denotes a rough estimate of the potential energy per particle and $E_F = \hbar^2\pi n/m_b$.

The QMC prediction for the strictly 2D case [13] (thick solid line) is between 30% and 50% off the experimental values for GaAs (thick dashed line). The key result of this Letter is that this significant discrepancy is quantitatively explained as an effect of finite thickness, as clearly shown
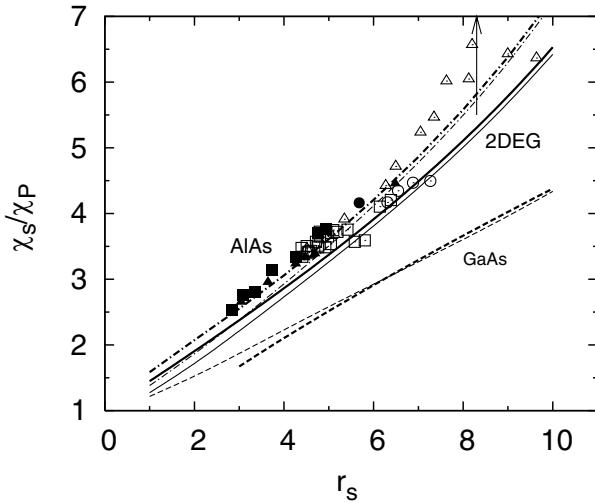

FIG. 1. Spin susceptibility in the 2DEG. The thick full curve is the QMC prediction for a strictly 2D system [13]. Experimental results are given by the thick dashed curve for a GaAs HIGFET [9] and by various symbols, corresponding to different samples, for AlAs QW's [10]. The thin dashed and full curves add the thickness effect onto the QMC prediction [13] for GaAs and AlAs, respectively. Finally, the thick and thin dot-dashed curves provide the QMC prediction without and with inclusion of thickness for AlAs, as obtained from the polarization field B_P [see Eq. (5) in the text]. The arrow indicates the location of the MIT transition in AlAs.

by the thin dotted line, obtained via Eqs. (1), (2), and (4). This conclusion is further strengthened by our explicit estimate of the effect of weak disorder, due to background doping in the GaAs HIGFET [9], which turns out to be negligible (see below). We emphasize that the parameters entering the form factor of Eq. (2) reflect our knowledge of the real sample [18], and they are not adjusted to achieve a particular value of the spin susceptibility.

In view of the interest for a possible ferromagnetic instability in low-density 2D electron systems, the question arises as to whether thickness, which noticeably changes the spin susceptibility, also alters the stability range of the polarized fluid ($26 \lesssim r_s \lesssim 35$) predicted by QMC calculations in the strictly 2D case [13]. Figure 2 shows that this stability window is only slightly shrunk (by $\lesssim 2$ in r_s) and the ferromagnetic instability pushed at slightly higher r_s.

For the AlAs device the situation is somewhat different. In order to engineer a one-valley 2DEG with isotropic mass, the electrons are confined in a very narrow QW, thus reducing the importance of finite thickness effects, but also boosting the possible influence of well width fluctuations [10]. The spin susceptibility, measured with either the tilted field or the polarization field methods (filled and empty symbols in Fig. 1, respectively), turns out to be fairly close to the strictly 2D QMC value. As expected, the tiny width of the QW does not affect this value significantly, as shown by the thick and the thin full curves in Fig. 1. Therefore, the small discrepancy between the QMC prediction (with or without finite thickness) and the experimental result points to a possible role of disorder.

A convenient parameter to measure the importance of the transverse electron spread $\Delta z = \sqrt{\langle z^2\rangle - \langle z\rangle^2}$ on the 2D motion is the ratio $t = \Delta z/r_sa_B$. In the HIGFET [18] $t = (\sqrt{3}/b)/(r_sa_B) \simeq 0.680/r_s^{1/3}$, while for the AlAs QW $t = \sqrt{(1 - 6/\pi^2)/12}a/(r_sa_B) \simeq 0.323/r_s$. We find that at a given t, the form factors of Eqs. (2) and (3) are very close to each other, yielding values of the susceptibility that
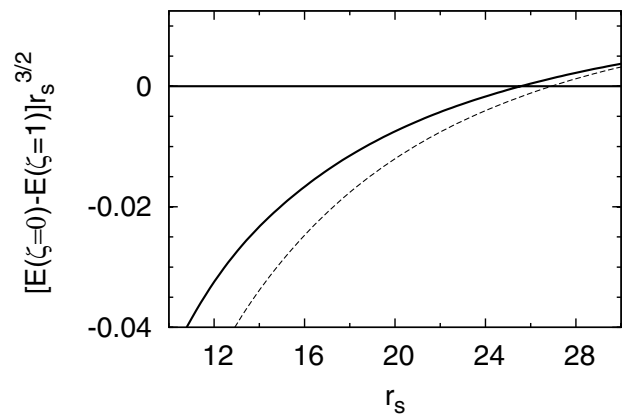

FIG. 2. Difference of QMC energies of unpolarized and polarized phases for the strictly 2DEG (solid line, Ry) and with the thickness of the GaAs HIGFET (dashed line, Ry*).

differ at most by 3% (at $t = 0.316$, $r_s = 10$). We should note that Eq. (2) is for a hard-wall QW. Changing to a well with a depth of as little as 140 meV, to mimic the AlAs device more closely, increases the EG thickness t by about 25%, with negligible effects on the susceptibility on the whole r_s range.

Before discussing our estimates of the effect of disorder, it is worth to briefly comment on the two different techniques used to measure χ_s/χ_P. Within the Landau-Fermi liquid theory, the susceptibility enhancement can be expressed in terms of the quasiparticle parameters g^* and m^* as $\chi_s/\chi_P = g^* m^*/g_b m_b$, where m_b and g_b are the mass and g factor entering the Hamiltonian describing the interacting electrons, which for electrons in a device coincide with the band mass and g factor. One of the experimental techniques employed to estimate χ_s is the tilted field method of Fang and Stiles [21], which allows the determination of $g^* m^*$ from the analysis of the minima in the Shubnikov–de Haas oscillations. The experimental results in Fig. 1 for the HIGFET and part of those for the QW's (full symbols) were obtained with this technique. An alternative manner to extract $g^* m^*$ from experiments has been suggested by Okamoto [4]. If the interacting electrons can be replaced by independent particles with effective parameters (m^* and g^*), then the (in-plane) magnetic field necessary to induce full spin polarization satisfies $\mu_B g^* B_P = 2E_F^* = \hbar^2 2\pi n/m^*$, which gives $\chi_s/\chi_P = 2E_F/g_b \mu_B B_P$. However, the (in-plane) polarization field must also satisfy the exact condition $g_b \mu_B B_P = 2E'(1)$, which combined with the above, yields

$$\chi_s/\chi_P = E_F/E'(1). \qquad (5)$$

The experimental results for the AlAs QW's obtained with both techniques are consistent with each other, due to the spread in the data. On the other hand, this is not the case with QMC calculations [13] for which Eq. (5) yields an appreciable overestimate of the susceptibility enhancement. While the correct definition of the spin susceptibility is the one of Eq. (4), in comparing measured and calculated values of χ_s/χ_P, it is appropriate to refer to theoretical estimates consistent with the adopted experimental determination. In particular, for low density, where only polarization field data are available (say r_s larger than about 6), the theoretical value to be considered is the dash-dotted lines, calculated using Eq. (5).

We now turn to the discussion of the disorder effects. A realistic description of these devices needs the inclusion of the different scattering sources that determine the mobility at zero temperature. The GaAs HIGFET [9] is a very clean device with no intentional doping and with a concentration of background impurities of $\approx 5 \times 10^{12}$ cm^{-3}, which is indeed a very low value [22]. Such a concentration was obtained through a best fit of the measured mobility [24], as a function of the electron density, computed using Born approximation [25]. We estimate the gross effect of such

weak disorder on the spin susceptibility by means of perturbation theory, describing the disorder in terms of an external one-body potential $u(\mathbf{r})$, coupling to the electron density, with known first and second moment ensemble averages [26]. As usual, we assume a vanishing first moment. The first nonvanishing contribution to the energy reads:

$$\Delta_d(\zeta) = \frac{1}{2n} \int \frac{d\mathbf{q}}{(2\pi)^2} \chi_{n,n}(q, \zeta) \frac{\langle u(\mathbf{q})^2 \rangle}{A}, \qquad (6)$$

with $u(\mathbf{q})$ the 2D Fourier transform of the one-body potential and $\langle \cdots \rangle$ denoting the ensemble average over disorder configurations per unit area. Above, $\chi_{n,n}(q, \zeta)$ is the density-density response function (in Fourier space) at polarization ζ for the strictly 2DEG [25].

In Fig. 3 we show our results for the GaAs HIGFET, using Eq. (6) to estimate the effect of disorder in a density range in which $\Delta_d(\zeta)$ is much smaller (less than 1%) than the unperturbed 2DEG energy . The effect of disorder is to enhance the spin susceptibility, contrary to that of transverse thickness. However, in the experimental density range ($3 \lesssim r_s \lesssim 8$) such an effect is negligible.

The mobility in AlAs QW's is roughly 2 orders of magnitude smaller than in the GaAs HIGFET, as the scattering sources are more effective. We were able to reproduce the measured mobilities [10], using Born approximation [25,27], only up to $r_s \lesssim 4$. In this density range the additional enhancement of χ_s due to disorder remains $\lesssim 10\%$, yielding a good agreement between the prediction of Eq. (4), with $E(\zeta) = E_{2D}(\zeta) + \Delta(\zeta) + \Delta_d(\zeta)$, and the available results of the tilted field experiments. Our findings suggest that, far from the metal-insulator transition, occurring at $r_s^c = 8.3$ in AlAs QW's and at $r_s^c = 12.4$ in the GaAs HIGFET, disorder effects yield a small enhancement
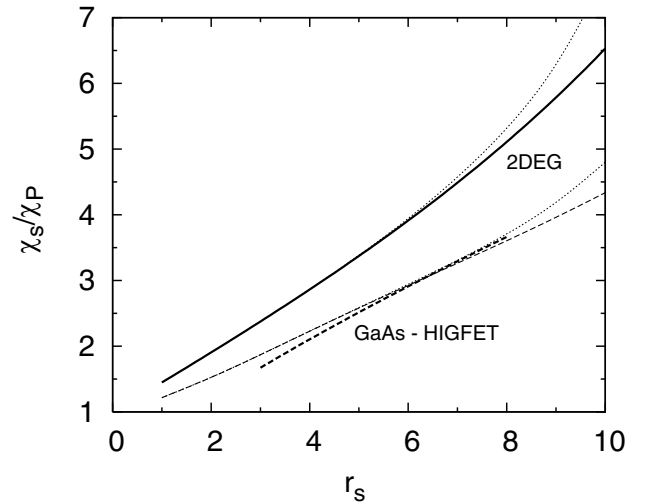

FIG. 3. Effect of a weak disorder appropriate to the GaAs HIGFET on the spin susceptibility. Upper and lower dotted curves are for the strictly 2DEG and for a 2DEG with the GaAs HIGFET thickness. Other curves as in Fig. 1.

of χ_s, which is either negligible as in GaAs or helps in reducing the small residual discrepancy between QMC calculations and experiments. However, to obtain indications valid at larger r_s and/or stronger disorder, an approach that takes into account disorder and electron-electron interaction on the same footing is required.

We finally comment on the two-valley electron systems, realized in Si metal-oxide-semiconductor field-effect transistors (MOSFETs) [4–7] and in wide AlAs QW [11]. In particular, Shkolnikov *et al.* [11], tuning the valley population, have shown that valley degeneracy brings about a depression of the spin susceptibility, in sharp qualitative contrast with the enhancement predicted by Hartree-Fock theory. A first estimate of the spin susceptibility of a two-valley symmetric EG can be simply obtained from previous QMC studies of the energy of four- [28] and two-component [29] electrons performed with the same level of accuracy, assuming a quadratic dispersion of the energy $E(\zeta)$ with ζ [30]. Such an estimate clearly shows the qualitative effect observed in Ref. [11]. A detailed comparison with either the Si MOSFET [4–7] or the anisotropic-mass AlAs QW [11] devices along the lines of the present calculation would require QMC input which is presently not available. We are currently performing extensive simulations of the strictly 2D two-valley system with finite polarization to obtain an accurate theoretical prediction of χ_s in such a system.

In conclusion, we have shown that a realistic description of actual devices, starting from the 2DEG model and including specific features of the systems, enables us to reproduce the spin susceptibility without any adjustable parameters. In GaAs HIGFET [9] the thickness plays a crucial role, while the weak disorder provides only a negligibly small enhancement. In the AlAs QW's case [10] the 2DEG spin susceptibility is directly comparable with experiments. A residual small discrepancy is likely due to the influence of QW's width fluctuations.

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[1] E. Abrahams, S. V. Kravchenko, and M. P. Sarachik, Rev. Mod. Phys. **73**, 251 (2001); S. V. Kravchenko and M. P. Sarachik, Rep. Prog. Phys. **67**, 1 (2004), and references therein.

[2] V. T. Dolgopolov, G. V. Kravchenko, A. A. Shashkin, and S. V. Kravchenko, Phys. Rev. B **46**, 13303 (1992).

[3] C. Castellani, C. Di Castro, and P. A. Lee, Phys. Rev. B **57**, R9381 1998; see, also, C. Castellani, C. Di Castro, P. A. Lee, M. Ma, S. Sorella, and E. Tabet, Phys. Rev. B **33**, 6169 (1986); D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. **66**, 261 (1994).

[4] T. Okamoto, K. Hosoya, S. Kawaji, and A. Yagi, Phys. Rev. Lett. **82**, 3875 (1999).

[5] A. A. Shashkin, S. V. Kravchenko, V. T. Dolgopolov, and T. M. Klapwijk, Phys. Rev. Lett. **87**, 086801 (2001).

[6] V. M. Pudalov, M. E. Gershenson, H. Kojima, N. Butch, E. M. Dizhur, G. Brunthaler, A. Prinz, and G. Bauer, Phys. Rev. Lett. **88**, 196404 (2002).

[7] S. A. Vitkalov, M. P. Sarachik, and T. M. Klapwijk, Phys. Rev. B **65**, 201106(R) (2002).

[8] E. Tutuc, S. Melinte, and M. Shayegan, Phys. Rev. Lett. **88**, 36805 (2002); E. Tutuc *et al.*, Phys. Rev. B **67**, 241309(R) (2003).

[9] J. Zhu, H. L. Stormer, L. N. Pfeiffer, K. W. Baldwin, and K. W. West, Phys. Rev. Lett. **90**, 56805 (2003).

[10] K. Vakili, Y. P. Shkolnikov, E. Tutuc, E. P. De Poortere, and M. Shayegan, Phys. Rev. Lett. **92**, 226401 (2004).

[11] Y. P. Shkolnikov, K. Vakili, E. P. De Poortere, and M. Shayegan, Phys. Rev. Lett. **92**, 246804 (2004).

[12] The results of Ref. [8] show a decrease of χ_s with n, but see Refs. [8,9] for an explanation.

[13] C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G B. Bachelet, Phys. Rev. Lett. **88**, 256601 (2002).

[14] T. Ando, A. B. Fowler, and Frank Stern, Rev. Mod. Phys. **54**, 437 (1982).

[15] P. Gori-Giorgi, S. Moroni, and G. B. Bachelet, Phys. Rev. B **70**, 115102 (2004).

[16] We have performed simulations with interaction $\tilde{v}(r)$, with parameters corresponding to the HIGFET [9], at $r_s = 5$ and $\zeta = 0, 1$, and determined $\Delta = E(\zeta) - E_{2D}(\zeta)$; we find a fractional difference from the first order estimate of Eq. (1) of only a few percent.

[17] F. C. Zhang and S. Das Sarma, Phys. Rev. B **33**, 2903R (1986), and references therein.

[18] For the considered HIGFET the depletion is negligible [H. Stormer (private communication)] and we set $n_d = 0$.

[19] A. Gold, Phys. Rev. B **35**, 723 (1987).

[20] A brief account of these results has been given at the 2004 APS March Meeting, presentation W11.015 [S. De Palo, G. Senatore, M. Botti, and S. Moroni, Bull. Am. Phys. Soc. **49**, 1303 (2004)].

[21] F. F. Fang and P. J. Stiles, Phys. Rev. **174**, 823 (1968).

[22] We refer the reader to [23] for the description of disorder in GaAs Heterostructures and to [19] for QW's, noting that Eq. (3c) of [19] has misprints.

[23] See, e.g., A. Gold, Appl. Phys. Lett. **54**, 2100 (1989).

[24] Jun Zhu, Ph.D. thesis, Columbia University, 2003.

[25] S. De Palo and G. Senatore (to be published).

[26] Evidently, one has to calculate the EG properties for a given configuration of disorder and then average the properties on disorder configurations (ensemble average).

[27] We include disorder parameters for the real device [K. Vakili (private communication)], adjusting only the parameters for the QW width fluctuations (roughness scattering), to obtain agreement with the measured mobility.

[28] S. Conti and G. Senatore, Europhys. Lett. **36**, 695 (1996).

[29] F. Rapisarda and G. Senatore, Aust. J. Phys. **49**, 161 (1996).

[30] Evidently, if $E_{1v}(\zeta)$ and $E_{2v}(\zeta)$ are the energy of the two-component (spin degeneracy) and four-component (spin and valley degeneracy) systems, we set $E_{2v}(\zeta) \approx E_{2v}(0) + [E_{2v}(1) - E_{2v}(0)]\zeta^2$ and exploit the fact that for symmetric valleys $E_{2v}(1) = E_{1v}(0)$.