

## The self-consistent calculation of exchange enhanced odd integer quantized Hall plateaus within Thomas–Fermi–Dirac approximation

G. Bilgeç<sup>a,\*</sup>, H. Üstünel Toffoli<sup>b</sup>, A. Siddiki<sup>c</sup>, I. Sokmen<sup>a</sup>

<sup>a</sup> Dokuz Eylül University, Physics Department, Faculty of Arts and Sciences, 35160 Izmir, Turkey

<sup>b</sup> Middle East Technical University, Physics Department, Ankara 06531, Turkey

<sup>c</sup> Mugla University, Physics Department, Faculty of Arts and Sciences, 48170-Kötekli, Mugla, Turkey

### ARTICLE INFO

#### Article history:

Received 26 August 2009

Received in revised form

11 November 2009

Accepted 13 November 2009

Available online 24 November 2009

#### Keywords:

Landé  $g$  factor

Quantum Hall effect

Spin-splitting

DFT

### ABSTRACT

We study the emergent role of many-body effects on a two-dimensional electron gas (2DEG) within the Thomas–Fermi–Dirac–Poisson approximation, including both the exchange and correlation interactions in the presence of a strong perpendicular magnetic field. It is shown that the indirect interactions widen the odd-integer incompressible strips spatially, whereas the even-integer filling factors almost remain unaffected.

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Since the discovery of quantum Hall effect [1] much effort has been devoted to understand the peculiar transport properties of the low dimensional systems in the presence of (Landau) quantizing strong magnetic fields. In the single particle, non-interacting electron picture, the twofold degenerate Landau states are split only due to the Zeeman effect. The Coulomb interaction enriched generalization of the single particle picture introduces the compressible and incompressible fluids as a consequence of the energy gaps. Namely if the Fermi energy is pinned one of the spin-split Landau levels, due to high density of states, a metal-like compressible state is formed, otherwise a quasi-insulating incompressible state exists. Since the semi-conducting materials in which the experiments are performed, have a reduced  $g^*$ -factor (i.e.  $\approx -0.44$  for GaAs) it was quite surprising to observe odd integer quantized Hall plateaus, which is a direct indication of spin resolved transport. Soon after the experimental observations, the spin effects were attributed to indirect interactions that enhances the effective  $g^*$ -factor. These many-body effects were left untouched in the pioneering work of Chklovskii et al. [2], which ended in a considerably large discrepancy between their non-self-consistent theoretical predictions and experiments considering high-resolution images of Hall samples [3–5] demonstrating that the strip widths are several times larger than the model.

As evidenced by these measurements, the single-particle picture is not sufficient to describe the behavior of the system. In the presence of exchange and correlation effects, which stem from many-body interactions, the spin gap in a two-dimensional electron system (2DES) is expected to be enhanced compared to the single particle Zeeman energy [6]. A strong evidence of enhanced spin splitting as obtained in several theoretical treatments [6–8] is the enlargement of incompressible strips, visible as plateaus in the spatial filling factor profile. This enhancement is expected to be much more pronounced in odd integer Hall plateaus [7] due to polarization effects. Inclusion of the Coulomb interaction *beyond* the classical Hartree approximation, i.e. both the exchange and correlation interactions, is possible within the direct diagonalization techniques [9], prohibitively demanding for the systems under investigation [10] or quantum Monte-Carlo techniques [11]. Another affordable yet accurate alternative for studying exchange and correlation effects is the density functional theory formalism (DFT) [11–13]. The most common treatment of exchange and correlation in DFT of spin-polarized systems is the so-called local spin density approximation (LSDA) [14]. The goal of the present paper is to illustrate the effect of addition of exchange and correlation on the spin gap through an LSDA-corrected self-consistent Thomas–Fermi–Dirac Poisson approximation (TFPA) [15–18]. To be clear with LSDA, we note that the exchange part is exact, however, we use the Tanatar–Ceperley parameterizations to describe the correlation part, of course other parameterizations are also possible [19]. The Attacalite parametrization is shown to be in good agreement

\* Corresponding author. Tel.: +90 2324128666; fax: +90 2324534188.  
E-mail address: gonul.bilgec@deu.edu.tr (G. Bilgeç).

with the previous ones, at least for the systems under consideration [20].

In a single Landau level the spin degrees of freedom is manifested by the separation of the Landau levels energetically, which is due to many-body effects and results in quantum Hall ferromagnetism. Here we describe the effects of many-body correlations energetically within the Thomas–Fermi–Dirac approximation. Our single particle based calculation scheme is valid only if the total potential landscape varies slowly on the length scale of the extend of the wave-function, i.e. Thomas–Fermi approximation. The inclusion of the exchange (and correlation) potentials do not violate the above assumption, known as the Dirac approximation. However, to be more precise one has to include the finite extend of the wave functions to the calculation scheme, which then will be Hartree–Fock approximation (without correlations). The Thomas–Fermi–Dirac approach describes the energetics of the electronic system quite reasonably, since the exchange part is exact, in contrast, the correlation part is not covered properly. Since, in our work we do not consider the fractional quantized Hall effect regime and correlation energy is small compared to the exchange we, therefore, neglect the corrections arising from correlation effects.

We investigate the exchange and correlation interactions in a two-dimensional electron gas confined in a GaAs/AlGaAs heterojunction, under the conditions of integer quantized Hall effect. Spin-split incompressible strips (ISs) with integer filling factor are first studied using an empirical effective  $g^*$  factor [10] then a simplified density functional approach is utilized to obtain quantitative results. We consider a two-dimensional electron gas (2DEG) with translation invariance in the  $y$ -direction and an electron density  $n_{el}(x)$  confined to the interval  $-d < x < d$ , in the plane  $z = 0$ .

The Coulomb interaction between electrons is separated into a classical Hartree and an exchange-correlation potential. The effective potential is then

$$V(x) = V_H(x) + V_{bg}(x) + V_Z + V_x(x) + V_c(x). \quad (1)$$

The first term in Eq. (1) is the Hartree potential, obtained at each step of the self-consistent TFPA calculations through the solution of the Poisson equation,

$$V_H(x) = \frac{2e^2}{\bar{\kappa}} \int_{-d}^{+d} dx' n_{el}(x') K(x, x'), \quad (2)$$

where  $-e$  is the electron charge,  $\bar{\kappa} = 12.4$  is the average background dielectric constant of GaAs and  $K(x, x')$  is the kernel satisfying the given boundary conditions,  $V(-d) = V(d) = 0$ . In our study, we use the kernel and background potential from Refs. [2,17,18,21]

$$K(x, x') = \ln \left| \frac{\sqrt{(d^2 - x^2)(d^2 - x'^2)} + d^2 - x'x}{(x - x')d} \right|. \quad (3)$$

The background term  $V_{bg}(x)$  in Eq. (1) describes the external electrostatic confinement potential composed of gates and donors modelled by a smooth functional form,

$$V_{bg}(x) = -E_{bg}^0 \sqrt{1 - (x/d)^2}, \quad E_{bg}^0 = 2\pi e^2 n_0 d / \bar{\kappa}, \quad (4)$$

where  $E_{bg}^0$  is the depth of the potential in a positive background charge density  $en_0$ . The third term is the Zeeman energy and reads  $V_Z = g^* \sigma \mu_B B$ , where  $g^*$  is the effective Landé- $g$  factor,  $\mu_B = e\hbar/2m_e$  is the Bohr magneton and  $\sigma = \pm \frac{1}{2}$  is the spin. The last two terms in Eq. (1) are, respectively, the exchange and correlation potentials in LSDA. In the present work, we use the Tanatar and Ceperley parametrization [11] with polarization dependent exchange and correlation potentials. In this parametrization,

$V_x(x)$  acts differently on the two spin channels while  $V_c(x)$  has a unified form for both channels.

The solution of the TFPA involves the self-consistent determination of the effective potential given in Eq. (1) for a density

$$n_{el}(x) = \int dE D(E) f(E + V(x) - \mu^*), \quad (5)$$

obtained in the approximation of a slowly varying potential valid in the case in consideration where the magnetic length is larger than the characteristic length of the potential. Here,  $f(\epsilon)$  is the Fermi function,  $D(E)$  and  $\mu^*$  are the density of states (DOS) and the constant equilibrium electrochemical potential, respectively.

In order to motivate the importance of  $g^*$ -factor enhancement, we present a preliminary calculation of the first incompressible strip (IS-1) width that in the presence of only the Zeeman term, ignoring exchange and correlation. In Fig. 1, we show the width of IS-1 while increasing the value of  $g^*$  factor as a free parameter. The width increases significantly until it reaches a value of approximately 4. For  $g^*$  factors larger than this value the self consistency implies an electrostatic stability which prevents formation of larger incompressible strips (thick solid line). However, in lower magnetic fields, the smaller incompressible strip width of IS-1 width grows approximately linearly without reaching saturation (thin broken line). This result clearly demonstrates the importance of electrostatic equilibrium, i.e. the compensation of indirect Coulomb interaction by direct Coulomb interaction. Since we do not include explicitly the exchange interaction, instead we included the 'expected' effect of the indirect interaction and saw that large odd integer incompressible strip does not become wider after a certain value of 'guessed'  $g^*$  and is balanced by electrostatics.

The effect is even more striking when the IS widths are calculated in the presence and absence of exchange and correlation and compared, where we fixed the value of  $g^*$ . In Fig. 2, we present the local filling factor  $\nu(x)$  for the bulk and experimentally determined  $g^*$  factor of 5.2 [10]. The figure concludes that, the inclusion of the indirect interactions spatially enlarges the IS-1 beyond the empirically estimated value of  $g^*$ , which we attribute to the incomplete treatment of correlation effects within our simplified DFT approach.

The filling factor calculated in the presence of the LSDA for a magnetic field of  $B = 7.1$  T is displayed in Fig. 3(a). At this value of the magnetic field (chosen so as to give a single, wide incompressible strip) the increase in the strip width in the

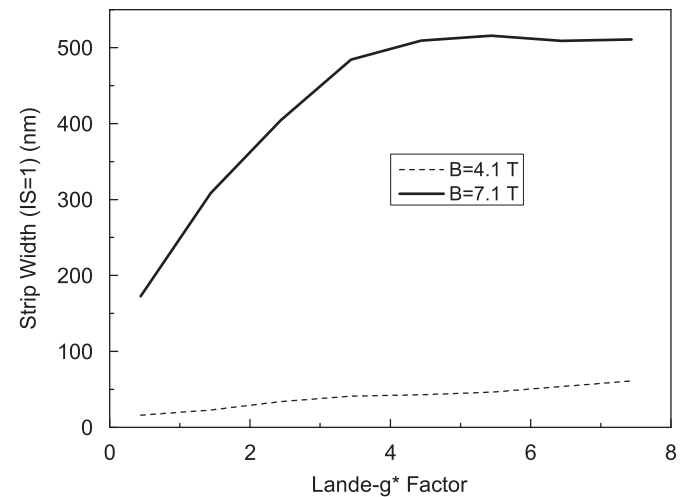
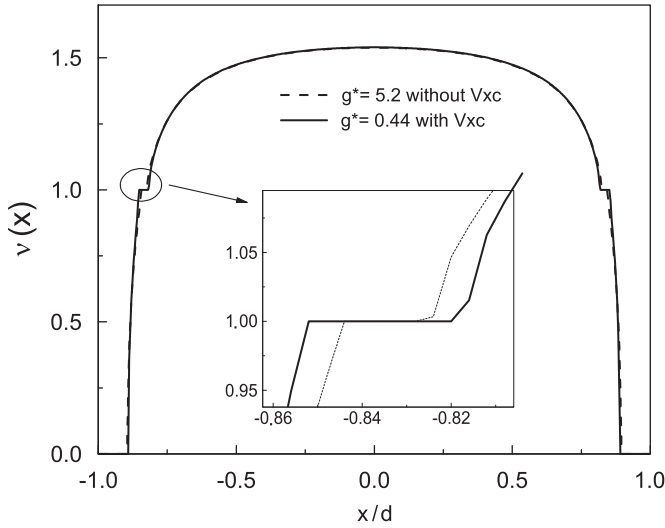
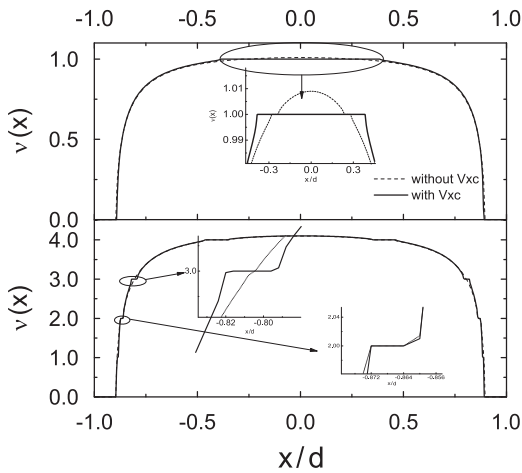


Fig. 1. The width of the first incompressible strip ( $\nu = 1$ ) without the exchange and correlation as a function of bulk Lande- $g^*$  factor at  $T = 0.05$  K, in a sample of width  $3 \mu\text{m}$ , and for magnetic fields  $B = 4.1$  T (dotted line)  $B = 7.1$  T (solid line).



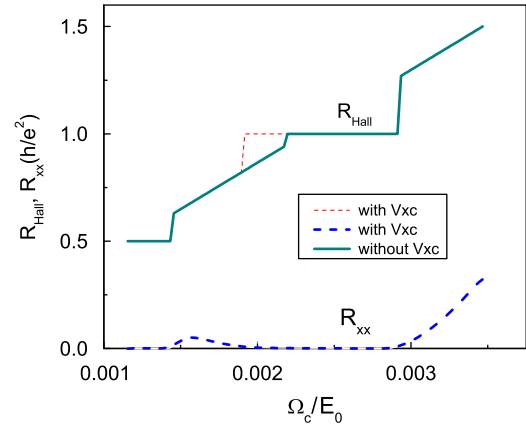
**Fig. 2.** The spatial variation of filling factor obtained from experimental effective Landé- $g^*$  factor [10] ignoring  $V_{xc}$  (dashed line) and bulk Landé- $g^*$  factor including  $V_{xc}$  (solid line). Calculations are performed at default temperature and at  $B = 4.7$  T.



**Fig. 3.** Electronic ground state filling factors, neglecting  $V_{xc}$  (dashed line) and including  $V_{xc}$  (solid line) calculated for a sample width of  $2d = 3 \mu\text{m}$ , at temperature  $T = 0.05$  K and for magnetic fields: (a)  $B = 1.8$  T, (b)  $B = 7.1$  T.

presence of  $V_{xc}$  is clearly seen. As the magnetic field is lowered to yield more ISs, the odd-integer strips (IS-1 and IS-3 in Fig. 3(b)) continue to be enhanced while those corresponding to even integers (IS-2 and IS-4 in Fig. 3(b)) remain mostly unchanged. This behavior is due to the nearly full spin polarization for the odd-integer ISs. Since the exchange-correlation effect often grows with increasing polarization, its effect is more pronounced for the fully polarized odd-integer ISs. On the other hand, the even-integer, spin-compromised ISs are effected only to a small extent. Our calculation shows that, even considering the effect of indirect interaction in a naive way, one can obtain well developed odd integer incompressible strips and the ferromagnetic state of the quantized Hall effect. The findings are in agreement with the literature, however, our calculation scheme is simpler. Moreover we can include (i) geometric effects (sample size and effects arising from confinement potential) and (ii) temperature effects without making further assumptions.

At a final step we show our transport results obtained within a local version of Ohm's law [22] where the local conductivity



**Fig. 4.** Calculated Hall and longitudinal resistances versus scaled magnetic field  $\hbar\omega_c/E_0$ , ignoring  $V_{xc}$  (solid line) and including  $V_{xc}$  (dashed line). Sample width of  $2d = 3 \mu\text{m}$  and for a magnetic field of  $B = 7.1$  T, at default temperature.

tensor entities are assumed to take a simple analytical form [10],  $\sigma_l(x) = (e^2/h)(v(x) - [v(x)])^2$  and  $\sigma_H(x) = (e^2/h)v(x)$ . The global resistances are obtained by utilizing the equation of continuity and translation invariance in the presence of a fixed imposed external current. Fig. 4 presents the calculated resistances with and without including indirect interactions. One can clearly observe that, the existence of  $V_{xc}$  enlarges the  $v = 1$  Hall plateau drastically, which is exactly the case in the experiments [5].

The transport results are preliminary, however, our self-consistent scheme allows us to describe the ferromagnetic state(s) of the quantized Hall effect within a simplified and fundamental approach, i.e. Thomas-Fermi-Dirac-Poisson approximation together with the local version of Ohm's law. The above method is so to say a zeroth order approximation, however, we obtained the odd integer quantized Hall plateaus without any localization effects and the many-body effects are included at a basic level. The main achievement of this work is manifested in Fig. 4: Namely odd integer quantization of the Hall resistance and the vanishing longitudinal resistance, due to exchange interaction within a self-consistent scheme, including temperature and size effects.

We have calculated the filling factor profile of 2DESs in the presence of a strong magnetic field using the self-consistent TFPA. The exchange-correlation potential, included within the Tanatar-Ceperley parametrization of LSDA is observed to enhance the IS widths at integer filling. Our method provides a fully self-consistent calculation scheme to obtain even and odd integer quantized Hall plateaus, displaying clear differences in width enhancement due to spin polarization. The results indicate that the enhancement effect is much more pronounced in odd-integer fillings due to the possibility of polarization while the even-integer, spin-compromised plateaus are hardly affected. The distinguishing part of this work relies on the fact that, without any complicated numerical (e.g. parallel computing) or analytical (e.g. localization) methods we can obtain the odd integer quantized Hall plateaus in a good qualitative agreement with the experiments.

The authors acknowledges, the Feza-Gursey Institute for supporting the III. Nano-electronic symposium, where this work has been conducted partially and would like to acknowledge the Scientific and Technical Research Council of Turkey (TUBITAK) for supporting under Grant no 109T083. We also would like to thank Esa Räsänen for his critical reading of the manuscript and for fruitful discussions.

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