Density-functional theory of quantum wires and dots in a strong magnetic field

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Abstract

We study the competition between the exchange and the direct Coulomb interaction near the edge of a two-dimensional electron gas in a strong magnetic field using density-functional theory in a local approximation for the exchange-energy functional. Exchange is shown to play a significant role in reducing the spatial extent of the compressible edge channel regions obtained from an electrostatic description. The transition from the incompressible edge channels of the Hartree-Fock picture to the broad, compressible strips predicted by electrostatics occurs within a narrow and experimentally accessible range of confinement strengths.

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I. INTRODUCTION

The concept of current-carrying edge channels accounts for the magnetotransport properties of a two-dimensional electron gas (2DEG) in a high magnetic field, both in the integer and fractional quantum Hall regime. Although the initial theoretical studies have used a noninteracting picture of edge channels, a considerable effort has recently been devoted to understand the effects of electron-electron interactions in the integer quantum Hall regime.

At present there are two incompatible pictures for the electronic ground state of edge channels in the integer quantum Hall regime. In the Hartree-Fock approximation the ground state wave function is a single Slater determinant, which corresponds to occupation numbers zero and one. In this description the edge state is incompressible and the electron density drops rapidly at the edges, on a length scale which is typically of the order of the magnetic length. Although the Hartree-Fock approximation is widely used for the description of quantum dots and wires, it has been challenged on the grounds that it does not take the global electrostatics into account properly. In the electrostatic description given in Ref. a more gradual variation of the electron density at the edge is found energetically favorable. Here the typical length scale for the density drop at the edge is of the order of the depletion length, which is much larger than the magnetic length. In this picture the electrons at the edge can screen the electrostatic confinement potential by a slow density variation and the edge states are therefore compressible. However, this description completely neglects the exchange interaction.

A transition from incompressible to compressible edge states was already qualitatively discussed in Ref. where a spontaneous transition from an unpolarized (i.e. equal occupation for both spin levels) to a polarized (different occupation for different spin levels) Hartree-Fock ground state was found for a critical confinement strength. It was speculated that a development to the electrostatic regime takes place as the confinement strength is decreased. More recently the transition between smoothly and abruptly varying density distributions has been studied by Chamon and Wen. On the basis of few particle exact
solutions they predict formation of compressible edge states when the strength of the confinement potential is reduced beyond a certain point. Their approach is difficult to extend to quantum wires or dots with a large number of electrons.

In the present work we interpolate between the different regimes of applicability of both Hartree-Fock and electrostatic pictures by extending the Thomas-Fermi approach used in Ref. 8 to a Thomas-Fermi-Dirac like treatment of the exchange effects in strong magnetic fields. First results of the present approach have been published in Ref. 10. Very recently Ferconi and Vignale 11 have studied the ground state energies and densities of a quantum dot in an arbitrary magnetic field, taking into account exchange-correlation effects by employing a Kohn-Sham scheme of current-density functional theory 12. For small quantum dots (2 or 3 electrons) their method yields an accuracy better than 3% when compared with exact results. For a larger number of electrons and high magnetic fields we find that the Kohn-Sham formalism encounters serious problems.

In Sec. II we describe our implementation of density-functional theory in strong magnetic fields as applied to quantum wires and derive expressions for the density profile and single-particle potentials of the ground state. In Sec. III we present results of the numerical calculations and we investigate both the accuracy of our theory and the relation with possible experiments. Two experimentally relevant applications are studied in Sec. IV: the influence of a plane of constant potential parallel to the 2DEG on the electronic ground state and the ground state properties of a quantum dot in a strong magnetic field. Section V summarizes our conclusions.

II. DENSITY-FUNCTIONAL THEORY IN STRONG MAGNETIC FIELDS

A. The system

Let us consider first a quantum wire of the strictly two dimensional electron gas along the y axis in the xy plane (Fig. II). Perpendicular to the plane a strong uniform magnetic
field is applied. Also present is a uniform positive background charge which ensures global neutrality. We use periodic boundary conditions in the $y$-direction and adopt the Landau gauge so that $\mathbf{A}_0 = B_0 x \hat{y}$ and $\mathbf{B}_0 = B_0 \hat{z}$. In the high magnetic field limit considered here only the lowest (spin-up and spin-down) Landau levels are occupied.

The wire is confined in the $x$ direction by a parabolic confinement potential:

$$V_c(x) = \alpha \frac{e}{4\pi \epsilon_0 l_B} x^2,$$

where $\epsilon = \epsilon_0 \epsilon_r$ is the dielectric constant and $\alpha$ is a dimensionless parameter. We will ignore here the difference between the ‘bare’ magnetic length $l_B = \sqrt{\hbar/eB_0}$ and the magnetic length $l$ which is renormalized by the parabolic confinement potential:

$$l = l_B \sqrt{\frac{\omega_c^2}{\omega_c^2 + \omega_0^2}},$$

where $\omega_c = eB_0/m^*$ is the cyclotron frequency with $m^*$ the effective electron mass and $\omega_0$ characterizes the parabolic confinement potential $\frac{1}{2} m^* \omega_0^2 x^2$. Since we treat the problem numerically, the assumption of a parabolic form for the confinement is not essential: It is chosen here because it is widely used in the literature. All lengths will be given in units of $l_B$ throughout the paper unless otherwise indicated.

B. Theory

We use density-functional theory in strong magnetic fields to find the electronic ground state of the system. Without a magnetic field, the total energy of the system would be a functional of the electron density only. However, a magnetic field, apart from giving rise to Zeeman splitting, causes orbital currents to flow in the electron gas, even when the system is in thermodynamic equilibrium. As a consequence, the total energy is now a functional of the density $n(\mathbf{r})$, the spin density $\mathbf{s}(\mathbf{r})$ and the paramagnetic current density $\mathbf{j}_p(\mathbf{r})$.

We do not take into account correlation effects, which means that we operate strictly in the integer quantum Hall regime, since correlation is responsible for the energy gaps that
cause the fractional quantization. Due to the fact that the correlation part of the energy is disregarded and exchange does not depend on the current density the total energy functional depends only on the total and the spin density or equivalently, since the spin-quantization axis is well defined by the strong magnetic field, on the density of spin up and spin down electrons.

In the Kohn-Sham scheme of density-functional theory the ground state densities \( n^\sigma \) of the interacting electron system are expressed in terms of a set of \( M^\sigma \) Kohn-Sham orbitals \( \phi_i^\sigma(\mathbf{r}) \):

\[
n^\sigma(\mathbf{r}) = \sum_{i=1}^{M^\sigma} |\phi_i^\sigma(\mathbf{r})|^2,
\]

where \( \sigma = \uparrow, \downarrow \) denotes up or down spin respectively and \( M^\sigma \) is the number of electrons with spin \( \sigma \). These orbitals satisfy the Kohn-Sham equations:

\[
\left\{ -\frac{\hbar^2}{2m^*} \nabla^2 + V_{\text{eff}}^\sigma(\mathbf{r}) \right\} \phi_i^\sigma(\mathbf{r}) = \epsilon_i^\sigma \phi_i^\sigma(\mathbf{r}),
\]

with \( V_{\text{eff}}^\sigma(\mathbf{r}) \) the effective one-particle potential:

\[
V_{\text{eff}}^\sigma(\mathbf{r}) = V_c(\mathbf{r}) + V_H([n]; \mathbf{r}) + V_x^\sigma([n^\uparrow, n^\downarrow]; \mathbf{r}),
\]

where \( V_H \) is the Hartree potential and \( V_x^\sigma \) the exchange potential. Here we have disregarded the exchange-correlation vector potential \( A_{\text{xc}} \) which gives only a very small contribution to the total energy. The Kohn-Sham ground state wave function is a Slater determinant of the \( M^\sigma \) lowest Kohn-Sham orbitals:

\[
\Phi^\sigma(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_{M^\sigma}) = \frac{1}{\sqrt{M^\sigma}} \det \{ \phi_i^\sigma(\mathbf{r}_i) \}.
\]

It can be shown (see Sec. III B) that in the limit of high magnetic fields the mixing between Landau level wave functions vanishes. Consider, e.g., the case of a single occupied, spin resolved Landau level. For large magnetic fields the Kohn-Sham ground state wave function, Eq. (6), reduces to a Slater determinant of lowest Landau level wave functions with integer filling. As a consequence the scheme cannot describe fractional filling in the
extreme quantum limit we are interested in. The reason for the failure of this procedure is the fact that the crucial assumption of the Kohn-Sham scheme, namely that the interacting $v$-representable densities are also non-interacting $v$-representable, breaks down in the high magnetic field limit.

It is not possible to extend the Kohn-Sham scheme to fractional filling since in that case the effective potential, $V_{\text{eff}}^\sigma (r)$, is no longer a unique functional of the total and spin density. However, at sufficiently high magnetic fields the basis wave functions are known to be just Landau level wave functions. We may then use a variational scheme which allows fractional filling and in which $E[n^\uparrow, n^\downarrow]$ is a unique functional of the total and spin density.

The equilibrium density distribution $n(x) = n^\uparrow(x) + n^\downarrow(x)$ which minimizes the total energy $E$ of the system can be found by solving:

$$\frac{\delta E[n^\uparrow, n^\downarrow]}{\delta n^\uparrow (x)} = \frac{\delta E[n^\uparrow, n^\downarrow]}{\delta n^\downarrow (x)} = \mu,$$

where $\mu$ is the chemical potential and the total energy of the quantum wire is given by:

$$E[n^\uparrow, n^\downarrow] = T[n] + E_c[n] + E_H[n] + E_Z[n^\uparrow, n^\downarrow] + E_x[n^\uparrow, n^\downarrow].$$

The total energy, Eq. (8), consists of five contributions: The first term on the right hand side is the kinetic energy which we define as a functional of the total density:

$$T[n] = \sum_{N\sigma} \int_{-\infty}^{\infty} dx \ n_N^\sigma (x) \ (N + \frac{1}{2})\hbar \omega_c,$$

where $N$ labels the Landau levels. The densities $n_N^\sigma (x)$ are the partial densities for a given spin direction $\sigma$ and Landau level $N$. The total electron density is found by summing over all occupied Landau levels and over spin directions: $n(x) = \sum_{N\sigma} n_N^\sigma (x)$ and is for sufficiently high magnetic fields given by:

$$n(x) = \sum_{\sigma, NX} \nu_{NX}^\sigma |\psi_{NX}(x, y)|^2,$$

where $X \equiv k_y l_B^2$ is the quantum number of an electron with momentum $k_y$, $\psi_{NX}(x, y) \sim \phi_{NX}(x) \exp (iX y/l_B^2)$ are the single particle bulk Landau level wave functions and $\nu_{NX}^\sigma$ is the
local filling factor for electrons with spin \( \sigma \) in Landau level \( N \). For well behaved confinement potentials the partial densities can be deduced from the total densities \( n^\uparrow \) and \( n^\downarrow \). For these potentials the total filling factor for a given spin direction, \( \nu^\sigma(x) \), lying between \( N_{\text{max}} - 1 \) and \( N_{\text{max}} \), always consists of \( N_{\text{max}} - 1 \) completely filled Landau levels and a partially filled one. This means that the kinetic energy (and also the exchange energy, see Eqs. \( (15) \) and \( (16) \)) is still a functional of the total and not the partial densities.

The second contribution is the confinement energy which is given by:

\[
E_c[n] = \int_{-\infty}^{\infty} dx \, n(x) \, eV_c(x). \tag{11}
\]

The electrostatic Hartree energy is:

\[
E_H[n] = \int_{-\infty}^{\infty} dx \, n(x) \, eV_H[n], \tag{12}
\]

where the Hartree potential, \( V_H[n] \), is itself a functional of the total density. For the strictly two dimensional electron gas (See Ref. \( 14 \) for the case of a quasi-two dimensional electron gas) it is given by:

\[
V_H[n] = -\frac{e}{2\pi\ell_B} \int_{-\infty}^{\infty} dx' \, n(x') \ln |x - x'|. \tag{13}
\]

The fourth term denotes the Zeeman energy:

\[
E_Z[n^\uparrow, n^\downarrow] = \frac{1}{2} g\mu_B B_0 \int_{-\infty}^{\infty} dx \left\{ n^\uparrow(x) - n^\downarrow(x) \right\}, \tag{14}
\]

where \( g \) is the bare Landé factor.

Our only concern left is the explicit form of the last term in Eq. \( (8) \), which is the exchange-energy functional. In the local density approximation (LDA) it reads:

\[
E_x[n^\uparrow, n^\downarrow] = \int_{-\infty}^{\infty} dx \left\{ n^\uparrow(x) \, \epsilon_x(n^\uparrow(x)) + n^\downarrow(x) \, \epsilon_x(n^\downarrow(x)) \right\}. \tag{15}
\]

Here \( \epsilon_x \) denotes the one-particle exchange energy of the homogeneous 2DEG with ground state densities \( n^\uparrow \) and \( n^\downarrow \), which is magnetic field dependent: In the absence of a magnetic field, it is proportional to \( \sqrt{n} \) (Ref. \( 13 \)), but in the magnetic quantum limit considered here, the local exchange energy per electron is:
\[ \varepsilon_x(n^\sigma(x)) = -\frac{e^2}{4\pi\ell_B} \sum_{N,N'} c_{NN'} n^\sigma_{N'}(x), \]  
(16)

where the coefficients \( c_{NN'} \) describe the exchange coupling between Landau levels \( N \) and \( N' \). They can be found by calculating the exchange energy per particle of an extended \( N \) Landau level system. For two occupied levels, e.g., they are \( c_{00} = \sqrt{2\pi^3} \), \( c_{01} = c_{10} = \sqrt{\pi^3}/2 \) and \( c_{11} = \sqrt{9\pi^3}/8 \).

The local density approximation is clearly only justified when the density variations are small on a characteristic length scale, which in our case is the magnetic length. In practice, however, it often turns out to be a useful and accurate tool even in cases in which this condition is not met.

Because we expect the results for higher Landau levels to be qualitatively the same, we will in the following restrict ourselves to the magnetic quantum limit, for which only the lowest Landau level is occupied. In the space of the lowest (spin-polarized) Landau level, the kinetic energy per particle is constant and may be disregarded. The validity of this approximation is discussed in Sec. III B. The density is in this case given by:

\[ n(x) = \frac{1}{2\sqrt{\pi^3}} \sum_\sigma \int_{-\infty}^{\infty} dX \nu^\sigma(X) e^{-(x-X)^2}, \]  
(17)

where we have replaced the sum over \( X \) in Eq. (10) by an integral and substituted the lowest Landau level wave functions. This relation shows that in the extreme quantum limit there exists a one to one correspondence between the density and the filling factor which enables us to use the latter as the variational function in the determination of the ground state of the system (see Sec. III A).

The exchange energy per electron in the lowest Landau level \( (N = N' = 0) \) reduces to:

\[ \varepsilon_x(n^\sigma) = -\sqrt{2\pi^3} \frac{e^2}{4\pi\ell_B} n^\sigma(x), \]  
(18)

i.e. the one-particle exchange energy for a given spin direction is just proportional to the corresponding electron density.

On substituting Eqs. (13), (17) and (18) in Eq. (8) for the total energy and performing the functional derivatives, Eqs. (7) become:
\[
\frac{\delta E[n^\uparrow, n^\downarrow]}{\delta n^\uparrow(x)} = eV_c(x) + eV_H[n] + 2\epsilon_x[n^\uparrow] + \frac{1}{2} g \mu_B B_0 = \mu,
\]
\[
\frac{\delta E[n^\uparrow, n^\downarrow]}{\delta n^\downarrow(x)} = eV_c(x) + eV_H[n] + 2\epsilon_x[n^\downarrow] - \frac{1}{2} g \mu_B B_0 = \mu.
\]

The numerical treatment of these coupled equations and the results will be presented in the next section.

III. CALCULATION OF THE GROUND STATE PROPERTIES

A. Results

As described above we obtain the ground state occupation numbers by numerically minimizing the total energy with respect to the filling factors, while keeping the total number of electrons constant. We discretize the filling factor and impose the boundary conditions: \(0 \leq \nu^\sigma \leq 1\). The numerical algorithm that minimizes the total energy uses a sequential quadratic programming method and is very stable. Numerical integration of the singular integrand in Eq. (13) requires some care. By sampling the integrand equidistantly and symmetrically around the divergence, \(x = x'\), and by sampling enough points to avoid oscillatory behavior in the resulting integral. An advantage of the present numerical scheme is that it can be very easy generalized to different confinement potentials. It should be noted, however, that the choice of confinement potential is not completely arbitrary. For e.g. a hard wall potential there is a stronger mixing with higher Landau levels near the edges and for such a confinement Eqs. (17) and (18) may be no longer accurate.

With the approach outlined above we can obtain, to a very good approximation, both the electrostatic solution (by neglecting the exchange term) and the Hartree-Fock solution as calculated by Dempsey et al.\(^8\) (by forcing the filling factors to be integer valued). Therefore we expect our approach to give a good description of the intermediate regime between these two extremes.

In Fig. 2 ground state occupation numbers obtained with different methods are plotted as a function of the confinement strength \(\alpha\). Fig. 2(a) shows the purely electrostatic solution,
the Hartree-Fock solution is plotted in Fig. 2(b) and the solution including exchange in the local density approximation is shown in Fig. 2(c). The small incompressible regions found in the electrostatic solution are caused by Zeeman splitting.

The calculations were performed using a magnetic field of 7.2 T which for filling factor \( \nu = 2 \) in the bulk corresponds to a zero-field bulk density of \( 3.5 \times 10^{11} \text{ cm}^{-2} \). For GaAs the static dielectric constant \( \epsilon_r = 12.5 \) and the bare Landé factor \( |g| = 0.44 \). The filling factors are plotted for a constant number of electrons and confinement strengths \( \alpha = 0.035, 0.041 \) and 0.047 respectively. Converted to energy level spacings of a parabolic confinement potential of the form: \( \frac{1}{2} m^* \omega_0^2 x^2 \) these values correspond to \( \hbar \omega_0 = 3.4 \text{ meV}, 3.8 \text{ meV} \) and 4.1 meV respectively.

As can be seen from Fig. 2(c) the effect of exchange on the electrostatic solution is a reduction of the compressible regions because it favors integer filling. However, a comparison with Fig. 2(b) shows that for soft confinement potentials the Hartree-Fock approximation no longer holds, i.e. the electrostatic interaction overcomes the tendency of exchange to form an incompressible ground state. Note, however, that the solution for \( \alpha = 0.047 \) in Fig. 2(c) is almost identical to the corresponding Hartree-Fock solution shown in Fig. 2(b), which shows that for confinement potentials that are strong enough the solution is forced into the integer filling regime, in agreement with the qualitative picture given in Ref. 8. Note that this transition from incompressible to compressible state is a genuine correlation effect since it corresponds to the mixing of different single-determinant configurations, in spite of our exchange-only potential.

It is clear from Fig. 2(c) that the width of the incompressible region is of the same order of magnitude as the width of the outermost compressible strip, even for the relatively wide strips we consider here (approximately 420 nm for a magnetic field of 7.2 T). This in contrast to the electrostatic description of edge states shown in Fig. 2(a), where the width of the incompressible region is always much smaller than that of the compressible one. However, for soft confinement potentials the solution including exchange does not deviate dramatically from the purely electrostatic one, which obviously implies that the Hartree-Fock approach
breaks down in this regime. Only a strong confinement potential can cause incompressible edge channels, although in Fig. 2(c) the confinement is still not strong enough to reduce the splitting to that of the bare Zeeman splitting. In the case of even harder confinement ($\alpha \approx 0.073$, \textit{i.e.} $\hbar \omega_0 \approx 5.3$ meV) we find that the splitting indeed reduces to this minimum value (not shown).

Note that the entire range from the electrostatic to the (unpolarized) Hartree-Fock regime can be realized in realistic confinement potentials with $\hbar \omega_0$ ranging from 3.4 meV to 5.3 meV. Confinement potentials with level spacings of a few meV have been realized\textsuperscript{17,18} so it should be possible to test these results by experiments. A possible method to stiffen the confinement experimentally is fabricating the 2DEG closer to the surface of the AlGaAs/GaAs heterostructure.

In essence, our method to include exchange is using an position dependent $g$-factor that depends on the local density. A simple approximation to this method would be to use the enhanced $g$-factor corresponding to a single occupied spin level.\textsuperscript{19} This method does increase the width of the incompressible strip but in general does not reproduce the qualitative and quantitative features obtained with our method.\textsuperscript{20}

In Fig. 3 the calculated one-particle potentials in the wire are plotted for both spin directions. These potentials correspond to the ground state density distribution of Fig. 2(c) with $\alpha = 0.035$ which is also included in the figure. Fig. 3(a) shows the electrostatic potential, which consists of the Hartree and confinement potential. Also plotted are the exchange potential and the total potential for the majority-spin electrons, \textit{i.e.} electrons occupying the lowest spin level. In Fig. 3(b) the same can be seen for the minority-spin electrons. In the figures the constant Zeeman term has been omitted for simplicity so that the total potential is just the sum of the electrostatic and exchange potential.

Fig. 3(a) shows that for a majority spin electron the energetically most favourable position is near the edges. This is because these electrons are forced by exchange to form an electrostatically unfavourable density profile in which no screening of the confinement potential is possible, \textit{i.e.} the density of majority spin electrons is constant in the bulk of
The wire. This in contrast to the minority spin electrons, for which the potential in the bulk is flat. This is due to the fact that these electrons still have the freedom to form a density distribution which can screen the external potential without being influenced much by the exchange interaction.

The typical voltage drop from the edge to the middle of the wire has experimentally realistic values of \( \approx 300 \text{ mV} \) for the bare confinement potential and \( \approx 30 \text{ mV} \) for the selfconsistent potential.

We also performed calculations of the widths of compressible and incompressible regions as a function of the confinement strength. The results are visible in Fig. 4 where the widths of the outermost incompressible region (I) and innermost compressible region (C) have been plotted as a function of \( \alpha \). If no incompressible strip is present in the middle of the wire, C is defined as half the width of the total compressible middle region (see inset). In the figure the points do not always lie on the smooth curve which serves as a guide for the eye. This is due to the spacing between sampling points (0.2 \( l_B \)), which imposes a upper bound on the accuracy of the calculated widths.

The compressible strip shrinks rapidly as the confinement is increased but if the width has reached a value of roughly a few magnetic lengths, the further decrease becomes very slow and in practice we always find a small but finite compressible region. It is clear, however, that a Hartree-Fock treatment should give good results for hard confinements where small compressible regions exist. We recover the spin-polarizing transition of Ref. 8 since the incompressible strip between spin-up and spin-down channels (I in Fig. 4) drops to zero at a certain critical value of the confinement strength (neglecting Zeeman splitting). Both the value for the critical confinement strength and the overall shape of the curve agree well with the results of Ref. 8.

An important consequence of exchange on the distribution of electrons for experiments is the increased separation between the compressible regions. This causes a strong decrease in inter-edge channel scattering because of the reduced overlap of the edge-channel wave functions, which leads to an increase in the spin-flip equilibration length of the edge chan-
nels. This in contrast to the assumption of an edge channel separation of the order of one magnetic length in Ref. 21. Using a typical edge channel separation of a few magnetic lengths in accordance with the present results, Khaetskii’s theory would give a much longer equilibration length.

The exchange enhanced channel separation has also consequences for the two-terminal magnetoconductance of a narrow channel or point contact. In Ref. 7, Chklovskii et al. discuss the conductance for these systems in the framework of their electrostatic description of the channels. They obtain conductance quantization but, due to the small width of the incompressible regions, the calculated plateau widths are much smaller than those experimentally observed. They attribute this discrepancy between theory and experiment to the presence of disorder. However, we propose as an alternative explanation the electronic exchange interaction which we find to strongly enhance the width of the insulating strips.

B. Accuracy

In this subsection we study the accuracy of our theory and how our present results are altered if we take into account realistic features which do not change the qualitative results but are important to describe experimental situations.

First we investigate the validity of Eq. (17) for high magnetic fields where mixing with higher Landau levels was disregarded. To this end we use a parabolic confinement $\frac{1}{2}m^*\omega_0^2x^2$ and a density distribution of the form: $n(x) = \frac{1}{2\pi l_B}\theta(x - W/2)\theta(x + W/2)$, where $W$ is the width of the wire. The 2DEG in the presence of the uniform magnetic field and parabolic confinement potential is our unperturbed system and we treat the Hartree potential as a perturbation. The energy levels of the unperturbed system are $E_{nk} = \left(n + \frac{1}{2}\right)\hbar\Omega + \hbar^2k_y^2/2M$, where $\Omega = \sqrt{\omega_c^2 + \omega_0^2}$ is the renormalized cyclotron frequency and $M$ is the renormalized electron mass: $M = m^*(1 + \omega_c^2/\omega_0^2)$. The wave functions are the bulk Landau level wave functions with effective magnetic length $l = l_B\sqrt{\omega_0^2/(\omega_c^2 + \omega_0^2)}$. According to first order perturbation theory, the ground state wave function, $|\psi\rangle$, of the electron at the edge, with
quantum number $X = W/2$, is approximately:

$$|\psi\rangle = |\psi_0\rangle + \frac{\langle \psi_1 | eV_H | \psi_0 \rangle}{E_0 - E_1} |\psi_1\rangle,$$

where we have used the Hartree potential as the perturbation. A straightforward calculation of the coefficient of $|\psi_1\rangle$ (which of course depends on $W$) shows that for $20 \, l_B \leq W \leq 40 \, l_B$, a magnetic field of 5 T and a typical value of $\hbar \omega_0 = 3$ meV for the parabolic confinement, the mixing with the first Landau level wave function is approximately 10% and that this value decreases as $1/\sqrt{B_0}$ with increasing magnetic field. We have to conclude that the dip in the electrostatic, i.e. Hartree and confinement, potential at the edges which is responsible for the spin-polarizing transition and ultimately for the compressible edge state, cannot be compensated by mixing with higher Landau levels, i.e. that our approximation is allowed in the high magnetic field limit considered here. By performing a similar calculation it is possible to show that the mixing due to the exchange-correlation potential used by Ferconi and Vignale is only a few percent.

Another approximation which gives rise to quantitative deviations from our theory is the assumption that the electron gas is strictly two dimensional. In reality the electron wave functions also extend in the $z$-direction and a form factor $F(q)$ in the Coulomb interaction, $V(q) = e^2 F(q)/2\epsilon|q|$, takes this effect into account. Calculations of edge channel splitting including a form factor in the Hartree-Fock approximation have already been calculated by Rijkels and Bauer. By comparison with Ref. 14 we estimate the values of $\alpha$ to decrease by about 0.004 if a form factor would be included into our calculations. This shifts the range of $\hbar \omega_0$ in which both the electrostatic and the Hartree-Fock regime are unreliable to lower energies, i.e. to 3.2 meV-5.1 meV.

### IV. APPLICATIONS

The present theory can be easily generalized to a variety of systems. In the next subsections we consider two special cases, which are experimentally relevant.
A. Back gate

As a first application we have carried out calculations for a system like the one considered in Sec. IIA, but now in the presence of an infinite plane of constant potential at a distance $d$ from the 2DEG, which may represent a real back gate or a plane of not fully depleted donors parallel to the 2DEG. This gate can be easily included into the calculations by adding the potential of a mirror charge distribution of opposite sign located at a distance $2d$ from the electron gas:

$$V_{bg}(x) = \frac{e}{2\pi \epsilon l_B} \int_{-\infty}^{\infty} dx' n(x') \ln \sqrt{(x - x')^2 + (2d)^2}. \quad (21)$$

In Fig. 5 we have plotted the solutions that minimize the total energy of the system including the back gate as a function of the distance $d$ to the wire for a given number of electrons and a fixed confinement potential.

It is clear from the figure that moving the back gate closer to the 2DEG has the effect of reducing the width of the compressible regions. This is to be expected because the back gate screens the long-range Coulomb interaction in the electron gas, thus effectively reducing the importance of the direct interaction relative to the exchange interaction and thereby forcing the solution for small distances $d$ into the Hartree-Fock regime.

It should be noted that the description of the back gate given here does not apply for a quantum wire defined by a depletion gate. In that case the back gate would also screen the charge on the depletion gates, thus increasingly altering the confinement potential as the back gate is moved closer to the 2DEG. In that case a fully self-consistent calculation is necessary. Furthermore, for our results to be correct, the distance from the gate to the 2DEG should not be too small since in that case also the short-range exchange interaction would be influenced by the gate.
B. Ground state of a quantum dot

A system that is very similar to the strip previously considered is a quantum dot in a high magnetic field, especially when the number of electrons in the dot is large. There are two main differences. In the first place we use the symmetric gauge to describe the dot. In this gauge the wave functions in the lowest Landau level, labeled by the quantum number of angular momentum, are

\[ \phi_m(z) = \frac{1}{\sqrt{2\pi m!}} e^{-|z|^2/2} \]

where \( z = \frac{x+iy}{\sqrt{2}} \). The second difference is that because the system is finite the filling factor \( \nu \) is no longer labeled by the continuous variable \( X \) but by the discrete quantum number \( m \). As a consequence the radial symmetric density is now given by:

\[ n(r) = \frac{1}{2\pi} \sum_{m,\sigma} \nu_m^\sigma \exp \left( - \frac{r^2}{2} \right) \left( \frac{r^2}{2} \right)^m, \]

where \( \nu_m^\sigma \) is the filling factor for a given angular momentum \( m \) and spin direction \( \sigma \). We impose as boundary conditions that \( 0 \leq \nu_m^\sigma \leq 1 \) and that the total charge in one spin level \( \sum_m \nu_m^\sigma \) is an integer. Due to the circular symmetry of the dot the Hartree potential is in this case given by:

\[ V_H(r) = -\frac{e}{4\pi\epsilon_0 B} \int_0^{2\pi} d\phi \int_0^\infty dr' \frac{r'n(r')}{\sqrt{r^2 + r'^2 - 2rr'\cos\phi}}. \]

An analysis analogous to the one presented in Sec. IIIB shows that for high magnetic fields (approximately 5 T) the mixing with higher Landau levels due to the Hartree potential and the exchange-correlation potentials used in Ref. 11 is only a few percent. As a consequence, fractional occupation numbers are essential, which cannot be described by the Kohn-Sham scheme of Ref. 11.

We have calculated the ground state of a dot consisting of 40 electrons using a parabolic confinement potential \( V_c(r) = \alpha \frac{e^2}{4\pi\epsilon_0 B} r^2 \) with varying strength \( \alpha \) in a magnetic field of 5.0 T. To find the ground state for a given magnetic field we vary the distribution of electrons among the occupied spin levels while keeping the total number of electrons constant. The results are plotted in Fig. 6. The ground states are similar to those of the strip except for the fact...
that the middle region is wider. This is due to the fact that the wave functions are centered
around the radii \( r_m = \sqrt{2m l_B} \), where \( m \) is the angular momentum index, and not around
equidistant points like in the strip.

In Ref. [17] a selfconsistent calculation was performed for the density profile of a quantum
dot containing 39 electrons using a modified Hartree form for the electrostatic electron-
electron interaction:

\[
V_{ee}(r, r') = -\frac{e}{4\pi \ell l} \left\{ \frac{1}{\sqrt{|r - r'|^2 + \langle \delta z \rangle^2}} - \frac{1}{\sqrt{|r - r'|^2 + 4d^2}} \right\},
\]  

(24)

thus taking into account the finite \( \langle \delta z \rangle \) of the wave functions and a back gate at
distance \( d \). Again we want to extend these calculations to include exchange but we must
keep in mind that a finite \( \langle \delta z \rangle \) also reduces the exchange interaction by a form factor:

\[
F(\langle \delta z \rangle) = \exp \left( \frac{1}{2} \langle \delta z \rangle^2 \right) \text{Erfc} \left( \frac{\langle \delta z \rangle}{\sqrt{2}} \right),
\]

(25)

where \( \langle \delta z \rangle \) is given in units of the magnetic length and \( \text{Erfc}(x) = 1 - \text{Erf}(x) \) denotes the
complementary error function. A calculation using interaction Eq. (24) and the local ex-
change contribution reduced by the form factor Eq. (25) gives a ground state which differs
from that of McEuen et al. in the sense that the widths of the incompressible (compressible)
regions are larger (smaller) in our solution.

We have calculated the addition spectrum of dots consisting of 37 and 38 electrons in
order to determine the effect of exchange on the inter-level transitions that are responsible
for the oscillatory behavior of the addition energy. Here we take into account the fact that
the magnetic length is renormalised by the magnetic field, Eq. (B), in order to compare
the energies at different magnetic fields. The addition energy \( \Delta E(N) \) needed for adding an
extra electron to a dot of \( N \) electrons is:

\[
\Delta E(N) = E(N + 1) - E(N),
\]

(26)

where \( E(N) \) is the total energy given by Eq. (8). The results are depicted in Fig. 7. It
should be mentioned that our results are very close to the Hartree-Fock solutions. This is
due to the fact that the combination of the back gate and exchange force the solution into the integer filling regime.

The inset of Fig. 7 shows the energy dependence of different dot configurations with magnetic field for a dot containing 39 electrons. The ground state is formed by the configuration with lowest energy. The numbers in the inset represent the number of electrons in the majority (i.e. lowest) spin level for the indicated curve. As the magnetic field increases, the degeneracy of the spin levels is increased and at certain magnetic fields an electron can jump from the upper to the lower level, causing the kinks in the ground state energy. When all electrons are in the lowest spin level no transitions can occur and the curves for both the total and addition energy are smooth.

Recent calculations\textsuperscript{9} and measurements\textsuperscript{22} indicate that at higher magnetic fields than the ones shown in Fig. 7 an edge reconstruction occurs, resulting in an extra kink in the curve for the addition energy in the regime where only one spin level is occupied. Performing a calculation with filling factors that are restricted to integer values, we are able to reproduce this feature. However, for the small confinement strength $\alpha$ at which this transition occurs, the fractional-filling solution is not so well converged. In spite of the fact that we find evidence for the edge reconstruction, the numerical accuracy of our solution does not allow decisive conclusions.

In comparison with the results obtained in Ref. 17 the oscillations found in our calculations have a larger period and amplitude by a factor of approximately 1.5. The increase in amplitude of the oscillations can be qualitatively understood in terms of the capacitance model for the island proposed by Evans \textit{et al.}\textsuperscript{23} and is due to the increase of the width of the incompressible strip in the picture including exchange. This results in a decrease of the capacitance between the inner and outer compressible regions where the extra electron can be added and hence in an increase in the peak-to-peak amplitude. The larger period can be explained in a similar fashion: Exchange effects reduce the widths of the compressible strips and thus the capacitances $C_1$ and $C_2$ between the respective compressible strips and the back gate which results in an increased period of the oscillations compared to the elec-
trostatic treatment of McEuen et al.. Compared with their experimental data, the period of the oscillations found in our calculations is about 0.3 T too large whereas their calculations give a period which is 0.25 T too small. However, these values depend sensitively on the calculated ground state density since the total energy, with a typical value around 1 eV, has to be calculated with an absolute accuracy of at least 0.1 meV in order to resolve the oscillations and therefore small numerical deviations from the true ground state would drastically influence the addition energies.

V. SUMMARY AND CONCLUDING REMARKS

We have used density-functional theory in strong magnetic fields to investigate the effects of the electron-electron interaction on edge states in the integer quantum Hall regime. We have included exchange in the local density approximation. In this approximation smooth density distributions corresponding to fractional filling at the edges can be treated, which is beyond a Hartree-Fock treatment of edge channels. To describe fractional occupation could otherwise only be achieved by exact diagonalization or configuration interaction calculations. We have found that the width of the edge channels is strongly reduced due to exchange effects and that the width of the incompressible strips is of the order of several magnetic lengths, which should have a strong influence on the spin-flip equilibration length and the two-terminal conductance of a point contact. We predict a range of confinement potentials $h\omega_0=3.2$ meV-5.1 meV in which the entire regime from electrostatic to Hartree-Fock is covered. Furthermore we have calculated ground state properties of the system in the presence of a back gate parallel to the quantum wire. We established an increasingly important role for the exchange interaction as the back gate is closed in on the 2DEG. As a second application we have calculated the ground state of a quantum dot in a strong magnetic field. We found that the results are similar to those found for the quantum wire. We compared addition energies for the dot with the selfconsistent calculations of McEuen et al. and found that the oscillations in the addition energies have larger amplitudes and
periods in our calculations.

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FIGURES

FIG. 1. Schematic picture of the system, consisting of a strip of 2DEG in a uniform magnetic field. The wire is confined by a parabolic potential in the $x$-direction. For details see text.

FIG. 2. Electronic ground state filling factors, (a) ignoring exchange and including exchange in (b) the Hartree-Fock approximation and (c) the local density approximation. The filling factors are plotted for confinement strengths $\alpha = 0.047$ (solid line), 0.041 (dashed line) and 0.035 (dashed-dotted line). Calculated for a magnetic field of 7.2 T.

FIG. 3. One-particle potentials and density distribution for the ground state of Fig. 2(c) with $\alpha = 0.035$ for (a) majority-spin electrons and (b) minority-spin electrons. Plotted are the electrostatic potential consisting of the confinement and the Hartree potential (dashed line), the exchange potential (dashed-dotted line) and the total potential excluding the Zeeman term (solid line). In the regions where the exchange potential is zero the total and Hartree potential coincide. The potentials are offset for clarity and are given in units of $\frac{e}{4\pi\epsilon l_B}$.

FIG. 4. Width of innermost compressible region (C) and outermost incompressible region (I) (see inset), plotted as a function of the confinement strength $\alpha$. The solid lines are drawn as a guide for the eye.

FIG. 5. Occupation of the system in the presence of the back gate at a distance $d = \infty$ (dashed-dotted line), $d = 20l_B$ (dashed line) and $d = 10l_B$. The confinement strength $\alpha = 0.035$ and $B = 7.2$ T. (solid line).

FIG. 6. Occupation numbers of a quantum dot consisting of 40 electrons for confinement strengths $\alpha = 0.09$ (solid line), 0.08 (dashed line) and 0.07 (dashed-dotted line). The discrete filling factors are positioned at the radii $r_{nm}$ and have been connected by lines for clarity.
FIG. 7. Addition energy for quantum dots of 37 and 38 electrons as a function of magnetic field. The calculation was performed for a confinement strength $\hbar \omega_0 = 1.6$ meV, $d = 100$ nm and $\langle \delta z \rangle = 10$ nm. The inset shows the ground state energies of the different possible configurations of the dot as a function of magnetic field. The numbers represent the number of electrons in the lowest spin level. Only odd numbers are indicated.
2DEG
(c) Position (in units of mag. length)
(b) **Position (in units of mag. length)**
