Ensemble density functional theory for inhomogeneous fractional quantum Hall systems

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Abstract

The fractional quantum Hall effect (FQHE) occurs at certain magnetic field strengths $B^*(n)$ in a two-dimensional electron gas of density $n$ at strong magnetic fields perpendicular to the plane of the electron gas. At these magnetic fields strengths, the system is incompressible, i.e., there is a finite cost in energy for creating charge density fluctuations in the bulk, while the boundary of the electron gas has gapless modes of density waves. The bulk energy gap arises because of the strong electron-electron interactions. While there are very good models for infinite homogeneous systems and for the gapless excitations of the boundary of the electron gas, computational methods to accurately model finite, inhomogeneous systems with more than about ten electrons have not been available until very recently. We will here review an ensemble density functional approach to studying the ground state of large inhomogeneous spin polarized FQHE systems.
I. INTRODUCTION

The fractional quantum Hall effect (FQHE) is manifested in a two-dimensional electron gas (2DEG) in a strong magnetic field oriented perpendicular to the plane of the electrons [1]. The effect was discovered as a transport anomaly. This is still the ‘Hallmark’ of the effect, even though there are now a host of other phenomena associated with the effect which have been studied experimentally. In a transport measurement it is noted that at certain strengths \( B^* (n) \), which depend on the density \( n \) of the 2DEG, current can flow without any dissipation. That is, there is no voltage drop along the flow of the current. At the same time, the Hall voltage perpendicular to both the direction of the current and of the magnetic field is observed to attain a quantized value for a small, but finite, range of magnetic field or density, depending on which quantity is varied in the experiment. The effect is understood to be the result of an excitation gap in the spectrum of an infinite 2DEG at these magnetic fields, so that there is a finite cost in energy to be paid for making density fluctuations in the system. This means that the 2DEG is incompressible. In general, the magnetic field strengths \( B^* (n) \) at which the quantum Hall transport anomalies are observed are related to the density through the filling factor \( \nu = 2 \pi \ell_B^2 n \), with \( \ell_B = \sqrt{\hbar c/(eB)} \) the magnetic length. The quantum Hall effect was first discovered [2] at integer filling factors. In this integer quantum Hall effect, the energy gap is nothing but the kinetic energy gap \( \hbar \omega_c = \hbar eB/(m^* c) \). Later, the fractional quantum Hall effect was discovered [3] at certain rational filling factors of the form \( \nu = p/q \), with \( p \) and \( q \) relative primes, and \( q \) odd. In the FQHE, the excitation gap is a consequence of the strong electron-electron interactions.

Our understanding of the origin of the FQHE started with Laughlin’s seminal paper of 1983 [4], which dealt with the simplest fractions \( \nu = 1/m \), with \( m \) an odd integer. At these values of \( \nu \), there are on the average \( m \) magnetic flux quanta \( \Phi_0 = \hbar c/e \) per electron. In that paper, Laughlin constructed a variational wavefunction for spin-polarized systems in strong magnetic fields, strong enough that the splitting \( \hbar \omega_c \) between the magnetic subbands, or Landau levels, can be taken to be infinite. The wavefunction can then be constructed from
single-particle states entirely within the lowest Landau level. Laughlin wrote the variational wavefunction as

\[ \Psi_m \propto \prod_{i,j} (z_i - z_j)^m \exp \left[ -\frac{1}{4} \sum_k |z_k|^2 \right] \]

(1)

where \( m \) is an odd integer, and \( z_j = x_j + iy_j \) is the coordinate of the \( j \)th electron in complex notation. This wavefunction is an eigenstate of angular momentum. Laughlin went on to demonstrate that the system having the wavefunction Eq. (1) is an incompressible liquid with \( \nu = 1/m \), \( m \) odd, and with an energy gap to excitations, and that the elementary excitations are fractionally charged quasi-holes or quasi-particles of charge \( e^* = \pm e/m \). The origin of the energy gap can be understood in the so-called pseudo-potential representation of the electron-electron interactions. Here, the electron-electron interaction \( V(r_i - r_j) \) between electrons \( i \) and \( j \) is decomposed into strengths \( V_\ell \) in relative angular momentum channels \( \ell = 0, 1, 2, \ldots \), of the two electrons. For any realistic interaction \( V(r_i - r_j) \), it turns out that \( V_0 > V_1 > V_2 > \ldots \). Consider the case \( \nu = 1/3 \). In this case, the lowest angular momentum pseudo-potential that enters into the \( m = 3 \) Laughlin description is \( V_1 \), the interaction energy of two electrons of unit relative angular momentum (in units of \( \hbar \)). (Even relative angular momenta are not permissible for spin-polarized electron wavefunctions, since they have to be anti-symmetric under interchange of electron coordinates.) The Laughlin wavefunction is a very cleverly constructed highly correlated state which completely excludes unit relative angular momentum between any two electrons, and is furthermore the only state which satisfies this property at \( \nu = 1/3 \). Therefore, any excited state must contain some electrons with unit relative angular momentum. The energy gap is due to the cost of this, and hence is of order \( V_1 \). Note that because of the nature of the correlations between the electrons, which are contained in the factors \((z_i - z_j)^m\), the Laughlin wavefunction cannot be expressed as a single Slater determinant of single-particle states in the lowest Landau level. Figure depicts the exchange-correlation energy per particle for infinite, homogeneous FQHE systems vs. filling factor. The cusps at filling factors \( \nu = 1/3, 2/5, 3/5 \), and \( \nu = 2/3 \) have been included to scale, and these filling factors marked by vertical lines for clarity.
Note that these cusps are barely visible on this scale, yet they are responsible for all the physics of the FQHE!

More modern theories of the FQHE are based on the so-called composite fermions. This idea was originated by Jain, [6] who noted that the \( m = 3 \) Laughlin wavefunction can be written as \( \prod (z_i - z_j)^2 \Psi_1 \), where \( \Psi_1 = \prod (z_i - z_j) \exp \left[ -\frac{1}{4} \sum |z_k|^2 \right] \) is the Slater determinant wavefunction of a filled lowest Landau level. Because of constraints on the Hilbert space, \( \Psi_1 \) is an exact eigenstate of an interacting electron system at \( \nu = 1 \). Although \( \Psi_1 \) need not in general be the ground state of the interacting system, it is if the Landau level splitting \( \hbar \omega_c \) is much greater than the scale of the Coulomb interaction, \( e^2/(\varepsilon_0 \ell_B) \), and if the external potential is sufficiently well behaved [8], e.g., it is caused by a uniform positive background charge density, and we will assume that these conditions are satisfied. Multiplication by the Jastrow factor \( \prod (z_i - z_j)^2 \) makes the total wavefunction \( \Psi_3 \) vanish as the cube of the separation of two electrons when they approach each other, rather than linearly. In the two-dimensional world of the FQHE, a zero of the wavefunction at a fixed point \( z_0 \) produces a phase factor of \( 2\pi \) when an electron adiabatically encircles \( z_0 \). This is equivalent to adding a flux-tube containing a single flux quantum \( \Phi_0 \) at \( z_0 \). This is purely an Aharonov-Bohm phase – no magnetic field is added anywhere except at \( z_0 \), where the wavefunction vanishes.

Therefore, the FQHE at \( m = 3 \) can be interpreted as a system of electrons at \( \nu = 1 \), but with two flux quanta added to the position of each electron. These composite objects, electrons plus an integer number of flux quanta, are called composite fermions. So one can say that the fractional quantum Hall effect at \( \nu = 1/3 \) is an integer quantum Hall effect (\( \nu = 1 \)) of composite fermions. This generation of FQHE states from composite fermions was subsequently generalized to all FQHE fractions. One way of studying FQHE systems of electrons theoretically is to perform a singular gauge transformation [7], which is a gauge transformation in which an odd number of flux quanta is added to the position of each electron. The transformed wavefunction is thus a wavefunction for composite fermions. In a Lagrangian formulation, a term has to be added to the Lagrangian to ensure that the flux tubes indeed are located at the electrons. The resulting term in the Lagrangian is called the
Chern-Simons term, and is well known from earlier topological field theories.

II. FINITE SYSTEMS

We have outlined above how the electron-electron interactions in an infinite, homogeneous system produce the excitation gap. It is important to note that these gaps are only for excitations in the bulk of the system. When a system is bounded there must be gapless excitations located at the boundaries of the system. The following simple argument, due to MacDonald [8], demonstrates this point. Consider a finite system in which the chemical potential $\mu$ lies in the bulk ‘charge gap’, i.e., we have to pay the price of the energy gap to introduce particles to the bulk of the system. Now imagine that the chemical potential is increased an infinitesimal amount $\delta \mu$, and consider the resulting change in the current density. In the bulk, the current density cannot change since $\delta \mu$ is infinitesimal and cannot overcome the energy gap in the bulk. It follows that if there is a change in the current density as a response to $\delta \mu$, this must be located at the edges of the system. Current conservation also requires that if there is a resulting change in the current along the edge, this change must be constant along the edge. We can relate the change in current $\delta I$ to the change in orbital magnetization through

$$\delta I = \frac{c}{A} \delta M, \quad (2)$$

where $A$ is the total area of the system. This relation is nothing but the equation for the magnetic moment of a current loop. But we can write $\delta M$ in terms of $\delta \mu$ using a Maxwell relation:

$$\delta M = \frac{\partial M}{\partial \mu} \bigg|_B \delta \mu = \frac{\partial N}{\partial B} \bigg|_\mu \delta \mu, \quad (3)$$

where $N$ is the total number of electrons. By combining Eqs. (2) and (3) we arrive at

$$\frac{\delta I}{\delta \mu} = c \frac{\partial n}{\partial B} \bigg|_\mu. \quad (4)$$
Since $\partial n/\partial B$ is non-zero, it follows that $\delta I/\delta \mu$ is non-zero, and we conclude that there must be gapless excitations of the system, and that these excitations must localized to the edges. Since all experimental systems are finite and inhomogeneous, the low-energy properties probed by experiments must be determined by the gapless edge excitations. Advances in semiconductor nanofabrication technologies have lead to the possibility of manufacturing systems which are extremely inhomogeneous, and in practice dominated by edges. As an example, recent experiments have even been performed on tiny quantum dots, with about 30 electrons on them \cite{9,10}. In order to accurately understand the experiments and inhomogeneous FQHE systems in general, we must have a way of accurately calculating their properties. Certain aspects of inhomogeneous FQHE systems have been studied by different techniques. For example, field theories can be constructed to study the low-energy limit of the gapless edge excitations \cite{11}. Composite fermion methods have been used in a Hartree approximation to study finite FQHE systems \cite{12,13}. In this approach, the Chern-Simons term, arising from the singular gauge transformation, and the electron-electron interaction are treated in a self-consistent Hartree approximation. The hope is then that the most important aspects of the electron-electron correlations are included in this approximation. Near $\nu = 1$, at which the Slater determinant $\Psi_1$ is the exact ground state, it makes sense to use the Hartree-Fock approximation, and the stability of a quantum dot at $\nu = 1$ as a function of confining potential has been studied in this approximation \cite{14,15}. The edge structure has also been studied using semiclassical methods \cite{16,17}, in which the electron-electron interaction is included at the Hartree level and it is furthermore assumed that all potentials vary on a length scale much larger than $\ell_B$. Beenakker \cite{16}, and Chklovskii, Shklovskii and Glazman \cite{17} demonstrated that the edge of an integer quantum Hall system, in which the correlation energies between the electrons can be ignored, consists of a sequence of compressible and incompressible strips. Imagine going from the bulk of an integer quantum Hall effect, with $\nu$ filled Landau levels in the bulk (so that the chemical potential lies above the energy of these $\nu$ Landau levels), toward an edge. There is an external potential confining the system, and this potential rises toward the edge, causing the Landau levels to bend upward near the
edge. The compressible strips occur where the chemical potential crosses a Landau level. There are then both empty and occupied single-particle states available, and the electron gas can screen the external potential perfectly. Eventually this Landau level bends upward, rising above the chemical potential. There are then no more empty single particle states, and changing the electron density would involve a cost of energy of the order of $\hbar \omega_c$, the spacing between the Landau levels. Thus, an incompressible strip forms. Here, the electrons cannot screen the external potential. Further out on the edge, the chemical potential crosses the next lower Landau level, and a new compressible strip forms. Thus, whenever the chemical potential lies between two Landau levels, the electron gas is incompressible, and the electron density is constant, while the total potential varies. On the other hand, whenever the chemical potential crosses a Landau level, the electron gas can screen perfectly the external potential, and the electron density varies while the total potential remains constant. The width of the incompressible strips is then determined by the length over which the confining potential varies an amount equal to the energy gap $\hbar \omega_c$. The origin of the compressible and incompressible strips are the energy gaps, which are the kinetic energy gaps $\hbar \omega_c$ in the case of the integer quantum Hall effect. But it is easy to heuristically generalize the argument to include the energy gaps causing the FQHE \cite{17}. The conclusion is then that there should be compressible and incompressible strips, with the density of the incompressible strips fixed at the density of an FQHE fraction. The width of each incompressible strip is then fixed by the length over which the confining potential varies an amount equal to the energy gap of the FQHE fraction corresponding to the density of that strip.

Finite, inhomogeneous systems have also been studied by direct numerical diagonalizations \cite{18}. At the present, numerical diagonalizations are limited to systems with of the order of 10 electrons.

It is highly desirable to have a computational approach which accurately includes electron-electron correlations and can handle inhomogeneous systems with on the order of $10^2$–$10^3$ electrons. One such approach which is in principle valid for any interacting electron system is the density functional theory (DFT) \cite{19-21}. There have been some attempts
to apply density functional theory to the FQHE. Ferconi and Vignale [22] applied current
density functional theory [23] to small, parabolically confined quantum Hall systems and
showed that the current density functional theory gave good results for the ground state
energy and spin polarization near $\nu = 1$. However, the energy gaps due to correlation effects
were not included in that calculation. Ferconi, Geller and Vignale [24] also recently studied
FQHE systems within the spirit of the DFT using an extended Thomas-Fermi approxima-
tion at low, but non-zero, temperatures. In this, the kinetic energy was treated as a local
functional, as in the standard Thomas-Fermi approximation, while the exchange-correlation
energy was included in a local density approximation (LDA). This extended Thomas-Fermi
approximation is valid in the limit of very slowly varying confining potential. Ferconi, Geller
and Vignale focused on the incompressible and compressible strips at an edge of an FQHE
system, and obtained results in agreement with the predictions by Chklovskii, Shklovskii,
and Glazman [17].

We have developed for the fractional quantum Hall effect an ensemble DFT scheme
within the local density approximation, and have applied it to spin-polarized circularly
symmetric quantum dots [25]. In our approach, the kinetic energy is treated exactly, and the
density represented by Kohn-Sham orbitals. The results are in good agreement with results
obtained by semiclassical [16,17,24], Hartree-Fock [14,15] (for cases where the correlations
do not play a major role), and exact diagonalization methods [26]. Our calculations show
that the exchange and correlation effects of the FQHE are very well represented by the LDA
and that our approach provides a computational scheme to model large inhomogeneous
FQHE systems. We note that there exist previous formal DFTs for strongly correlated
systems, in particular for high-temperature superconductors [27], and DFT calculations of
high-$T_c$ materials [28] and transition-metal oxides [29]. However, ours are, to the best of
our knowledge, the first practical LDA-DFT calculations of a strongly correlated system in
strong magnetic fields, and demonstrate the usefulness of the LDA-DFT in studying large
inhomogeneous FQHE systems.
III. ENSEMBLE DENSITY FUNCTIONAL THEORY APPROACH

In typical DFT calculations of systems of $N_{\text{el}}$ electrons, the standard Kohn-Sham (KS) scheme \cite{30} is implemented, in which the particle density $n(r)$ is expressed in terms of a Slater determinant of $N \geq N_{\text{el}}$ KS orbitals, $\psi_\alpha(r)$. These obey an effective single-particle Schrödinger equation $H_{\text{eff}} \psi_\alpha = \epsilon_\alpha \psi_\alpha$, which is solved self-consistently by occupying the $N_{\text{el}}$ KS orbitals with the lowest eigenvalues $\epsilon_\alpha$, and iterating. This scheme works well in practice for systems for which the true electron density can be represented by a single Slater determinant of single-particle wavefunctions. However, when the KS orbitals are degenerate at the Fermi energy (which we identify with the largest $\epsilon_\alpha$ of the occupied orbitals) there is an ambiguity in how to occupy these degenerate orbitals. There exists an extension of DFT which is formally able to deal with this situation. This extension is called ensemble DFT \cite{20,21}, and in it, the density of the system is represented by an ensemble of Slater determinants of KS orbitals. However, while it can be shown using ensemble DFT that such a representation of the density is rigorous, it cannot be shown how the degenerate KS orbitals at the Fermi energy should be occupied, i.e., there has not been available a practical computational scheme for ensemble density functional theory.

We argued above that the Laughlin wavefunction cannot be represented as a Slater determinant of single-particle wavefunctions. Therefore, one may suspect that the density of a general FQHE system cannot be represented by a single Slater determinant. We will now argue that this is indeed the case. Consider a FQHE system in the $xy$-plane with the magnetic field along the $\hat{z}$-axis. A circularly symmetric external potential $V_{\text{ext}}(r) = V_{\text{ext}}(r)$ (due, e.g., to a uniform positive background charge density) confines the systems such that the density is fixed with a local filling of $\nu = 1/3$ up to an edge at $r_0$ ($r_0 \gg \ell_B$) where the density falls to zero within a distance of order $\ell_B$. That such systems exist is well demonstrated by the excellent agreement between the Laughlin wavefunction and experiments, and by many numerical calculations \cite{31,26}. Due to the circular symmetry we can label single-particle orbitals by angular momentum $m$, and by a Landau level index
$n \geq 0$. The orbitals $\psi_{m,n}(r)$ are centered on circles of radii $r_m \approx \sqrt{2m\ell_B}$ with Gaussian fall-offs for $r \ll r_m$ and $r \gg r_m$. The single-particle orbitals with $n = 0$ are then in the bulk all degenerate, and the degeneracy is not lifted by electron-electron interactions since the system is homogeneous in the bulk. Only the orbital $\psi_{0,0}$ is non-zero at the origin – all others vanish at $r = 0$. In order to obtain a constant density at $\nu = 1/3$ even at the center of the system, all single-particle orbitals in the bulk with $n = 0$ must have occupancies 1/3. If the Fermi energy lay above the energies of the bulk orbitals, they would all be filled and one would have $\nu = 1$. Therefore, to get occupancies 1/3 the Fermi energy must lie at the degenerate energy $\epsilon_{m0}$ of these orbitals. Thus, in applying DFT to the FQHE we can expect a huge degeneracy of KS orbitals at the Fermi energy, and they must all have fractional occupancies. Consequently, the particle density cannot be expressed in terms of a single Slater determinant. Instead, the density has to be constructed from an ensemble of Slater determinants, i.e., the orbitals at the Fermi energy are assigned fractional occupation numbers, just as the Laughlin wavefunction for $\nu = 1/3$ is not a single Slater determinant, but a highly correlated state with average occupancies of 1/3 of single-particle states. Therefore, one might expect from the outset that one has to use ensemble density functional theory – the standard Kohn-Sham scheme may not converge.

Although ensemble DFT has been developed formally, there are in practice few examples of applications and calculations using ensemble DFT for ground state calculations. A significant aspect of our work is that we have developed an ensemble scheme which is practical and useful for the study of the FQHE. In ensemble DFT, any physical density $n(r)$ can be represented by $n(r) = \sum_{mn} f_{mn} |\psi_{mn}(r)|^2$, where $f_{mn}$ are occupation numbers satisfying $0 \leq f_{mn} \leq 1$, and the orbitals $\psi_{mn}$ satisfy the equation

$$\left\{ \frac{1}{2m^*} \left[ \frac{\hbar^2}{2m^*} \nabla \times A(r) \right]^2 + V_{\text{ext}}(r) + V_{\text{H}}(r) + V_{\text{xc}}(r, B) \right\} \psi_{m,n}(r) = \epsilon_{mn} \psi_{mn}(r), \quad (5)$$

where $\nabla \times A(r) = B(r)$. In equation (5), $V_{\text{H}}(r)$ is the Hartree interaction of the 2D electrons, and, as usual, $V_{\text{xc}}(r, B)$ is the exchange-correlation potential, defined as a functional derivative of the exchange-correlation energy $E_{\text{xc}}[n(r), B]$ of the system with respect to den-
sity: $V_{xc}(\mathbf{r}, \mathbf{B}) = \frac{\delta E_{xc}[n(\mathbf{r}), \mathbf{B}]}{\delta n(\mathbf{r})}|_{\mathbf{B}}$. (We will hereafter not explicitly indicate the parametric dependence of $V_{xc}$ and $E_{xc}$ on $\mathbf{B}$.) For the case of the FQHE, we know that the exchange-correlation potential will be crucial, as it contains all the effects of the electron correlations which cause the FQHE in the first place, and a major part of the DFT application is to come up with an accurate model of $E_{xc}$ and so of $V_{xc}$. Leaving this question aside for a moment, and assuming that we have succeeded in doing so, the practical question is then how to determine the KS orbitals and their occupancies in the presence of degeneracies. We devised an empirical scheme, which means that after a lot of trial and error we made some educated guesses that work. Our scheme produces a set of occupancies for the KS orbitals which satisfy some minimum requirements, namely (a) the scheme converges to physical densities (to the best of our knowledge) for FQHE systems, (b) it reproduces finite temperature DFT distributions at finite temperatures, and (c) it reproduces the standard Kohn-Sham scheme for systems whose densities can be represented by a single Slater determinant.

In our scheme, we start with input occupancies and single-particle orbitals and iterate the system $N_{eq}$ times using the KS scheme. The number $N_{eq}$ is chosen large enough (about 20–30 in practical calculations) that the density is close to the final density after $N_{eq}$ iterations. If the density of the system could be represented by a single Slater determinant of the KS orbitals, we would now essentially be done. However, in this system there are now in general many degenerate or near-degenerate orbitals at the Fermi energy. After each iteration, the Kohn-Sham scheme chooses to occupy the $N_{el}$ orbitals with the lowest eigenvalues, corresponding to making a distinct Slater determinant of these orbitals. But there will be small fluctuations in the density between each iteration, which cause a different subset of these (near) degenerate orbitals to be occupied after each iteration. This corresponds to constructing different Slater determinants after each iteration, and the occupation numbers $f_{mn}$ of these orbital are zero or unity more or less at random after each iteration. This means that the computations will never converge. However, the average occupancies, i.e., the occupancies averaged over many iterations, become well defined and approach a definite
value, e.g., 1/3 for orbitals localized in a region where the local filling factor is close to \( \nu = 1/3 \). Therefore, we use these average occupancies to construct an ensemble by accumulating running average occupancies \( \langle f_{mn} \rangle \) after the initial \( N_{\text{eq}} \) iterations

\[
\langle f_{mn} \rangle = \frac{1}{(N_{\text{it}} - N_{\text{eq}})} \sum_{i=N_{\text{eq}}+1}^{N_{\text{it}}} f_{mn,i},
\]

where \( f_{mn,i} \) is the occupation number (0 or 1) of orbital \( \psi_{mn} \) after the \( i \)th iteration, and use these to calculate densities. Thus, our algorithm essentially picks a different (near) degenerate Slater determinant after each iteration, and these determinants are all weighted equally in the ensemble. It is clear that this scheme reduces to the KS scheme for which the density can be represented by a single Slater determinant of KS orbitals (for which the KS scheme picks only the one Slater determinant which gives the ground state density) for \( N_{\text{eq}} \) large enough. We have numerically verified that a finite-temperature version of our scheme converges to a thermal ensemble at finite temperatures down to temperatures of the order of \( 10^{-3} \hbar \omega_c/k_B \). We have also performed some Monte Carlo simulations about the ensemble obtained by our scheme. In these simulations, we used a Metropolis algorithm to randomly change the occupation numbers about our converged solution, keeping the chemical potential fixed. The free energy of the new set of occupation numbers was calculated self-consistently. If the free energy decreased, this set was kept, and if the free energy increased, the set was kept if a random number was smaller than \( \exp \left[ -\Delta F/k_B T^* \right] \), where \( \Delta F \) is the change in free energy, and \( T^* \) a fictitious temperature. The results were that to within numerical accuracy our ensemble DFT scheme gives the lowest free energy. As a condition for convergence, we typically demanded that the difference between the input and output ensemble densities, \( n_{\text{in}}(r) \) and \( n_{\text{out}}(r) \), of one iteration should satisfy

\[
\frac{1}{N_{\text{el}}} \int_0^{\infty} |n_{\text{in}}(r) - n_{\text{out}}(r)| r \, dr < 10^{-3}.
\]

Practical density functional theory calculations hinge on the availability of good approximations for the exchange-correlation potential \( V_{\text{xc}} \), which enters in the effective Schrödinger equation for the KS orbitals. The simplest, and probably the most commonly used, approx-
imation is the local density approximation (LDA). In this approximation, the exchange-correlation energy is assumed to be a local function of density, so that the total exchange-correlation energy consists of contributions from the local density of the system. Thus, in this approximation one writes $E_{xc}/N = \int dr \epsilon_{xc}(\nu) n(r)$, where $\epsilon_{xc}(\nu)$ is the exchange-correlation energy per particle in a homogeneous system of constant density $n = \nu/(2\pi\ell_B^2)$ and filling factor $\nu$. In other words, in the LDA one assumes that the system is locally homogeneous, i.e., the system can locally be approximated to have the energy per particle of an infinite, homogeneous system of the local density. This approximation obviously makes sense if the density of the system varies on a very long length scale, while it could be questionable for systems in which the density varies on some microscopic length scale. However, experience has shown that the LDA often works surprisingly well, even for systems in which the electron density is strongly inhomogeneous [19]. In fact, the first application of LDA-DFT was to calculate the work function of simple metals [32], so these were systems which were terminated with densities varying on the scale of a Bohr radius! Nevertheless, the LDA-DFT gave quite good results, vastly superior to those of the Hartree- or Hartree-Fock approximation.

In the FQHE, the length scale of exchange-correlation interactions and density fluctuations is given by the magnetic length $\ell_B$ due to the Gaussian fall-off of any single-particle basis in which the interacting Hamiltonian is expanded. The densities are relatively smooth on this length scale, which gives us additional hope that the LDA will work well for the FQHE, too. In addition, the cusps in the exchange-correlation energy will suppress density fluctuations, so in this sense one can actually expect the basic physics of the FQHE to make the LDA a good approximation.

In conventional LDA-DFT calculation, the exchange-correlation energy $\epsilon_{xc}$ is obtained by interpolating between the exchange-correlation energies per particle of systems with vanishing and infinite densities, respectively, for which exact results are known. Analogously, following Rasolt and Perrot [33], we obtain our exchange-correlation energy by interpolating between two limits for which the result is known very accurately. In our case, the two limits are $B \to \infty$, and $B \to 0$, respectively, and we stitch them together using a Padé approx-
Thus, we write for the exchange-correlation energy per particle of a uniform electron gas in a constant magnetic field

\[ \epsilon_{xc}(\nu) = \frac{\epsilon_{xc}^{\text{FQHE}}(\nu) + \nu^A \epsilon_{xc}^{\text{TC}}(n(\nu))}{1 + \nu^A}. \]  

(8)

Here, \( \epsilon_{xc}^{\text{TC}} \) is the zero-magnetic field result for a 2DEG obtained by Tanatar and Ceperley [34]. The term \( \epsilon_{xc}^{\text{FQHE}}(\nu) \) is the \( B \to \infty \) limit, which is the exchange-correlation energy of the FQHE in a system for which only single-particle states in the lowest Landau level are occupied. This contribution consists of two terms. The first one is a smooth interpolation formula \( \epsilon_{xc}^{\text{LWM}}(\nu) \) due to Levesque, Weiss and MacDonald [35] between ground state energies at some rational fillings. The second one, \( \epsilon_{xc}^{C}(\nu) \), is all-important for the study of the FQHE. This term contains the cusps in the ground state energy which cause the FQHE. Here we have used a simple model which captures the essential physics. We model \( \epsilon_{xc}^{C}(\nu) \) by constructing it to be zero at values of \( \nu = p/q \) which display the FQHE. Near \( \nu = p/q \), \( \epsilon_{xc}^{C}(\nu) \) is linear and has at \( \nu = p/q \) a discontinuity in the slope related to the chemical potential gap \( \Delta \mu = q(|\Delta_p| + |\Delta_h|) \). Here \( \Delta_p,h \) are the quasiparticle (hole) creation energies which can be obtained from the literature [30,37] at fractions \( \nu = p/q \). Farther away from \( \nu = p/q \), \( \epsilon_{xc}^{C}(\nu) \) decays to zero. Finally, in the LDA \( V_{xc}(r) \) is obtained from \( \epsilon_{xc}(\nu) \) as \( V_{xc}(r) = \left. \frac{\partial \epsilon_{xc}(\nu)}{\partial \nu} \right|_{\nu(\nu)} \) at constant \( B \). In our calculations, we restrict ourselves to include only the cusps at \( \nu = 1/3, 2/5, 3/5 \) and \( \nu = 2/3 \), which are the strongest fractions. These are some of the fractions of the form \( \nu = \frac{p}{(2p\pm1)} \) generated by the so-called \( V_1 \)-model, in which only the pseudo-potential \( V_1 \) is included.

A technical difficulty arises in the LDA: the discontinuities in \( V_{xc}(r) \) in the LDA give rise to a numerical instability. The reason is that an arbitrarily small fluctuation in charge density close to an FQHE fraction gives rise to a finite change in energy. Imagine that the local filling factor \( \nu(r) \) in some neighborhood of a point \( r \) is very close to, but less than, say, 1/3 after one iteration. In this neighborhood, the local exchange-correlation potential will then form a potential well with sharp barriers at the points around \( r \) where \( \nu(r) = 1/3 \). During the next iteration, charge will then be poured into this well. As a result, the local filling
factor will after this iteration exceed 1/3, and in this neighborhood \( V_{xc} \) now forms a potential barrier of finite height. So in the next iteration, charge is removed from this neighborhood, and so on. We can see that this leads to serious convergence problems. To overcome this, we made the compressibility of the system finite, but very small, corresponding to a finite, but very large, curvature instead of a point-like cusp in \( \epsilon_{xc} \) at the FQHE fractions. In other words, instead of having a step-like discontinuity \( \Delta \mu \) in the chemical potential, it rises smoothly an amount \( \Delta \mu \) over an interval \( \gamma \) in the filling factor. What we found worked very well in practice was to have the discontinuity in chemical potential occur over an interval of filling factor \( \gamma \) of magnitude \( 10^{-3} \). This corresponds to a sound velocity of about \( 10^6 \) m/s in the electron gas, which is three orders of magnitude larger than the Fermi velocity of a 2D electron gas at densities typical for the FQHE. In general, the finite compressibility does not lead to any spurious physical effects so long as the energy of density fluctuations on a size of the order of the systems size is larger than any other relevant energy in the problem. The only noticeable effect is that incompressible plateaus, at which the density would be perfectly constant were the compressibility zero, will have density fluctuations on a scale of \( \gamma \). Figure 2 depicts \( V_{xc} \) used in our calculations as a function of filling factor.

IV. APPLICATIONS TO QUANTUM DOTS

We have self-consistently solved the KS equations Eqs. (5) for a spin-polarized quantum dot in a parabolic external potential, \( V_{ext}(r) = \frac{1}{2}m^*\Omega^2r^2 \), by expanding the KS orbitals \( \psi_{mn}(r) = e^{im\phi}\varphi_{mn}(r) \) in the eigenstates of \( H_0 = \frac{1}{2m^*}(\mathbf{p} + \frac{e}{c}A(r))^2 \). We use the cylindrical gauge, \( A(r) = \frac{1}{2}Br\hat{\phi} \), and include the four lowest Landau levels \( (n = 0, \ldots, 3) \). We chose the static dielectric constant \( \epsilon_0 = 13.6 \), appropriate for GaAs, and a confining potential of strength \( \hbar\Omega = 1.6 \) meV.

The use of our LDA-DFT scheme is illustrated by a study of the edge reconstruction of the quantum dot as a function of magnetic field strength. As is known from Hartree-Fock and exact diagonalizations [4, 15, 26, 12, 13], for strong confinement the quantum dot forms
a maximum density droplet in which the density is uniform at $\nu = 1$ in the interior, and falls off rapidly to zero at $r \approx \sqrt{2N}\ell_B = r_0$. As the magnetic field strength increases, a “lump” of density breaks off, leaving a “hole” or deficit at about $r = r_0$. This effect is due to the short-ranged attractive exchange interaction: it is energetically favorable to have a lump of density break off so that the system can take advantage of the exchange energy in the lump. As $B$ is further increased, the correlations will cause incompressible strips with densities $\nu = p/q$ to appear \cite{16,17,38,24} on the edges, and incompressible droplets to form in the bulk at densities $\nu = p/q$. Figure 3 depicts various stages of edge reconstruction obtained by us as the magnetic field strength is increased. The value of $B$ for which the exchange lump appears compares very well with the value found by De Chamon and Wen \cite{15} in Hartree-Fock and numerical diagonalizations. At higher fields still, incompressible strips appear at the edges, and incompressible droplets are formed in the bulk. In figure 4 we show occupancies for the KS orbitals for a finite-temperature calculation with $N_{el} = 40$, $B = 4.45$ T, and $T = 0.003 e^2/(\epsilon_0\ell_B k_B)$. The diamonds depict the converged ensemble occupancies for the KS single-particle states using our ensemble scheme. At this finite temperature, we calculated the thermal occupancies of the KS orbitals after each iteration, and these ‘instantaneous’ thermal occupancies were then averaged using our ensemble scheme. The temperature was sufficiently low that the ‘instantaneous’ thermal occupancies were essentially 0 or 1 before convergence. The continuous curve shows the ‘instantaneous’ thermal occupancies obtained after a particular iteration after convergence has been achieved. This figures then clearly shows that our ensemble occupancies (in this case at a low, but nonzero, temperature) converged to the thermal occupancies. Note that this particular temperature is so low that no standard finite-temperature scheme could be used to achieve convergence.

Figure 5 depicts the eigenvalues of the KS orbitals for $N_{el} = 40$, and $B = 4.45$ T. The dashed line indicates the chemical potential of the system. This figure then shows that all KS orbitals in the bulk are in fact degenerate. It may at first seem paradoxical that the eigenvalues are degenerate on an incompressible strip, since, according to the picture
by Chklovskii, Shklovskii, and Glazman [17], on such a strip the density is constant, while
the total potential varies (since the electrons cannot screen the external potential). If the
total potential varies, then ought not the the eigenvalues of the KS orbitals localized on
that strip vary, too, since these then in general are subjected to different potential energies?
The problem with this argument as applied to DFT is that it ignores the effect of the
exchange-correlation potential. As the external and Hartree potentials vary across the strip,
the exchange-correlation potential varies across its discontinuity so as to completely screen
out the external and Hartree potentials. The discontinuity in $V_{xc}$ does not mean that this
potential is fixed at the lower limit of its discontinuity while the density is fixed at an
incompressible strip. What it does mean, is that $V_{xc}$ is free to achieve any value across its
discontinuity so as to completely screen out the external and Hartree potentials. In this
way, it is perhaps better to think of incompressibility as the limit of a finite compressibility
approaching zero. A strip can then remain incompressible with constant density so long as
$V_{xc}$ can screen the external and Hartree potentials, so the width of the incompressible strip
is given by the distance over which the external plus Hartree potentials varies an amount
given by the energy gap associated with the density at that strip. Also, all bulk KS states
are degenerate at the chemical potential. When a single particle is added, the chemical
potential simply increases a small amount, and all KS orbitals are again degenerate at the
chemical potential. We also would like to emphasize that incompressible regions that appear
in these calculations are not due to the presence of a uniform positive background density
which tends to fix the bulk density at the value of the background density.

There is also another edge effect caused by correlations. For particular, stiff confining
potentials, so-called composite edges [39,26] can appear. These can be thought of as particle-
hole conjugates of uniform incompressible droplets. Consider a droplet with a bulk density
corresponding to $\nu = 1/3$, falling off to zero at the edge. A incompressible droplet with a
bulk density of $\nu = 2/3$ is obtained by particle-hole conjugation. However, at the edge, the
density will first rise to $\nu = 1$ (since the density of the $\nu = 1/3$ droplet drops to zero), and
then eventually drop to zero. Note that this argument is based on particle-hole conjugation,
which is an exact symmetry of the lowest Landau level \([40]\), and it is unclear if composite edges exist in real systems, which do not strictly obey particle-hole symmetry.

Figure 6 depicts the particle density (inset) for a system where the confining potential is supplied by a uniform positive background charge density \( n_+ = 2/(6\pi \ell_B^2) \) (so that the corresponding filling factor is \( \nu_+ = 2/3 \)) for \( r < r_0 \), and falling linearly to zero over a distance \( a \) for \( a > r_0 \), where \( r_0 \) is fixed by charge neutrality. Thus, the parameter \( a \) is a convenient parameter with which one can control the stiffness of the confining potential \([15]\). From this figure, we see that for \( a = 0 \), the system forms a composite edge, even though our system does not obey particle-hole symmetry. We therefore conclude that such edges can exist in real systems. As \( a \) is increased, the edge undergoes an instability and reconstruction, and eventually forms incompressible strips.

V. CONCLUSION AND SUMMARY

In conclusion, we have showed that ensemble density functional theory can be applied to the FQHE. This opens the door to doing realistic calculations for large systems. We believe that our results are also significant in that they are the first LDA-DFT calculations of a strongly correlated system in a strong magnetic field, and they are (to the best of our knowledge) the first practical ensemble DFT calculations. There are, however, still many issues that need to be resolved, and new directions to go. For example, our calculations were of a spin-polarized system. As is well known \([8]\), the spin degree of freedom is very important, even for magnetic fields of the order of 10 T. The reason is that the effective \( g \)-factor in GaAs is very small, so small that the ratio between the Zeeman splitting and the cyclotron energy is about 2\%. This leads to the possibility of FQHE ground states which are not spin-polarized. It also gives rise to so-called charge–spin–texture excitations near \( \nu = 1/m, \ m = 1, 3, \ldots \). These excitations are lower in energy than a simple singlet particle-hole pair, and believed to be responsible for the observed \([41]\) rapid destruction of the spin polarization near \( \nu = 1 \). Correctly including the spin degree of freedom to account for this
involves a DFT for Heisenberg spins. We are presently, together with J. Kinaret (Chalmers
University of Technology) developing such a theory.

The authors would like to thank M. Ferconi, M. Geller and G. Vignale for helpful dis-
cussions and for sharing their results prior to publications, and K. Burke and E.K.U Gross
for useful comments about the DFT. O.H. would like to thank Chalmers Institute of Tech-
nology, where part of the numerical work was done. This work was supported by the NSF
through grant DMR93-01433.
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FIGURES

FIG. 1. The ground state energy $\epsilon_{xc}$ per particle of an infinite, homogeneous, spin-polarized FQHE system is depicted as a function of filling factor. The cusps at $\nu = 1/3, 2/5, 3/5$, and $\nu = 2/3$ are included (these filling factors are indicated by vertical lines for clarity).

FIG. 2. Exchange-correlation potential $V_{xc}$ as function of filling factor in units of $e^2/(\epsilon_0 \ell_B)$ for $0 \leq \nu \leq 1$. The increase in $V_{xc}$ at an FQHE filling occurs over a range of filling factor of 0.004.

FIG. 3. Edge reconstruction of a quantum dot as the magnetic field strength is increased. Plotted here is the local filling factor $\nu(r)$ for a parabolic quantum dot with $\hbar \Omega = 1.6$ meV and 40 electrons. For magnetic field strengths $B < 2.5$ T the dot forms a maximum density droplet, and for $B \approx 3.0$ T, an exchange hole is formed. For stronger magnetic fields, incompressible regions form, separated by compressible strips.

FIG. 4. Ensemble (diamonds) and ‘instantaneous’ (solid line) thermal occupancies for $N_{el} = 40$, $B = 4.45$T, and $T = 0.003 \frac{e^2}{(\epsilon_0 \ell_B k_B)}$ after convergence.

FIG. 5. Eigenvalues of the lowest-Landau level Kohn-Sham orbitals for $N_{el} = 40$ and $B = 4.45$ T as a function of angular momentum quantum number. The chemical potential is indicated by the dashed line.

FIG. 6. Local filling factor $\nu(r)$ as a function of $r$ (in units of $\ell_B$) for a system of 45 electrons in a magnetic field of $B = 5.0$ T. The confining potential is due to a positive background charge density at $\nu_+ = 2/3$ in the bulk, and falling linearly to zero within a distance $a$ near the edge. For a stiff edge ($a = 0$), the system forms a composite edge with $\nu(r)$ rising towards unity near the edge. As $a$ increases, the edge becomes softer and undergoes a reconstruction to a sequence of incompressible strips.
Exchange–correlation energy

\[ \varepsilon_{xc} \left[ \frac{e^2}{l_B \varepsilon_0} \right] \]

\[ \text{Filling factor } \nu(r) \]
$v(r)$ vs. $r$ [\(l_B\)]

- $B = 2.5$ T
- $B = 3.1$ T
- $B = 4.3$ T
Ensemble and thermal occupancies

$B=4.45 \, T, \, N_{el}=40, \, \hbar \Omega=1.6 \, \text{meV}, \, T=0.003 \, e^2/\varepsilon_0 l_B k_B$
Energy \( \frac{e^2}{\varepsilon_0 B} \)

Angular momentum quantum number \( m \)
