Ensemble Density Functional Theory of the Fractional Quantum Hall Effect

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We develop an ensemble density functional theory for the fractional quantum Hall effect using a local density approximation. Model calculations for edge reconstructions of a spin-polarized quantum dot give results in good agreement with semiclassical and Hartree-Fock calculations, and with small system numerical diagonalizations. This establishes the usefulness of density functional theory to study the fractional quantum Hall effect, which opens up the possibility of studying inhomogeneous systems with many more electrons than has heretofore been possible.

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The fractional quantum Hall effect (FQHE) is manifested in a two-dimensional electron gas (2DEG) in a strong magnetic field perpendicular to the plane of the electrons [1]. The effect is due to the electron-electron interactions, which cause a downward cusp in ground state energy as a function of filling factor $\nu = 2\pi\ell_B^2 n$ at certain rational fillings $\nu = p/q$. Here $\ell_B = \sqrt{\hbar c/eB}$ is the magnetic length, B the magnetic field strength, and n the electron density. These downward cusps give rise to an energy gap, and so for these values of ν, the ground state of the system is an incompressible liquid. Experimentally, FQHE systems are accessible in strip geometries, Corobino geometries, and more recently in quantum dots [2,3], with as few as $\approx$50 electrons, as well as wide-well heterojunctions and double layer systems. Theoretically, different aspects of FQHE systems can be modeled by Laughlin's wave function [4], by Hartree-Fock [5,6] or composite fermion Hartree [7,8]; by semiclassical methods [9–11], by field theoretical approaches [12], which also exist for the edge excitations on the boundary of FQHE systems [13], and by exact numerical diagonalizations. 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 treats inhomogeneous systems with 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) [14–16].

We have developed an ensemble DFT scheme within the local density approximation (LDA) for the fractional quantum Hall effect, and applied it to spin-polarized circularly symmetric quantum dots [17]. The results are in good agreement with results obtained by semiclassical [9–11], Hartree-Fock [5,6] (for cases where the correlations do not play a major role) or exact diagonalization methods [18]. Our calculations show that the exchange and correlation effects 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 [19], and DFT calculations of high-T_c materials [20] and transition-metal oxides [21]. Ferconi, Geller, and Vignale [11] have also recently studied FQHE systems within the DFT using an extended Thomas-Fermi approximation, including a LDA for the exchange-correlation energy. However, ours are, to the best of our knowledge, the first practical DFT-LDA calculations of a strongly correlated system in strong magnetic fields, and demonstrate the usefulness of the DFT-LDA in studying large inhomogeneous FQHE systems.

In typical DFT calculations of systems of $N_{\rm el}$ electrons, the standard Kohn-Sham (KS) scheme [22] is implemented, in which the particle density $n(\mathbf{r})$ is expressed in terms of a Slater determinant of $N \geq N_{\rm el}$ KS orbitals $\psi_\alpha(\mathbf{r})$. These obey an effective single-particle Schrödinger equation $H_{\rm eff}\psi_\alpha = \epsilon_\alpha\psi_\alpha$, which is solved self-consistently by occupying the $N_{\rm el}$ KS orbitals with the lowest eigenvalues ϵ_α (we identify the Fermi energy of the system with the largest ϵ_α of the occupied orbitals), and iterating. This scheme works well in practice for systems which are noninteracting v representable [15,16], i.e., systems for which the true electron density can be represented by a single Slater determinant of single-particle wave functions. However, when the KS orbitals are degenerate at the Fermi energy there is an ambiguity in how to occupy these degenerate orbitals. This is the case for the FQHE, as we now demonstrate. Consider a FQHE system in the x-y plane with the magnetic field along the $\hat{z}$ axis. A circularly symmetric external potential $V_{\rm ext}(\mathbf{r}) = V_{\rm ext}(r)$ (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 ℓ_B. That such systems exist is well demonstrated by the excellent agreement between the Laughlin wave function and experiments, and by many numerical calculations [18,23]. Because of the circular symmetry, we can label single-particle orbitals by angular momentum m and by a "band" or Landau level index $n \geq 0$. The orbitals $\psi_{m,n}(\mathbf{r})$ are centered on circles of radii $r_m \approx \sqrt{2m}\,\ell_B$ with Gaussian falloffs for $r \ll r_m$

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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. 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 lies 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 ϵ_{m0} of these orbitals. Thus in applying DFT to the FQHE, we can expect a huge degeneracy of KS orbitals at the Fermi energy. 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 wave function is not a single Slater determinant, but a highly correlated state with average occupancies of $1/3$ of single-particle states. This is generally known as *ensemble* density functional theory [15,16].

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 $n(\mathbf{r})$ can be represented by $n(\mathbf{r}) = \sum_{mn} f_{mn}|\psi_{mn}(\mathbf{r})|^2$, where f_{mn} are occupation numbers satisfying $0 \leq f_{mn} \leq 1$, and the orbitals ψ_{mn} satisfy the equation

$$\left(\frac{1}{2m^*}\left[\mathbf{p} + \frac{e}{c}\mathbf{A}(\mathbf{r})\right]^2 + V_{\mathrm{ext}}(\mathbf{r}) + V_H(\mathbf{r}) + V_{\mathrm{xc}}(\mathbf{r},\mathbf{B})\right) \times \psi_{(m,n)}(\mathbf{r}) = \epsilon_{mn}\psi_{mn}(\mathbf{r}), \quad (1)$$

where $\nabla \times \mathbf{A}(\mathbf{r}) = \mathbf{B}(\mathbf{r})$. In Eq. (1), $V_H(\mathbf{r})$ is the Hartree interaction of the 2D electrons, and $V_{\mathrm{xc}}(\mathbf{r},\mathbf{B})$ is the exchange-correlation potential, defined as a functional derivative of the exchange-correlation energy $E_{\mathrm{xc}}[n(\mathbf{r}),\mathbf{B}]$ of the system with respect to density: $V_{\mathrm{xc}}(\mathbf{r},\mathbf{B}) = \delta E_{\mathrm{xc}}[n(\mathbf{r}),\mathbf{B}]/\delta n(\mathbf{r})|_{\mathbf{B}}$. We will hereafter not explicitly indicate the parametric dependence of V_{xc} and E_{xc} on $\mathbf{B}$. The question is then how to determine these orbitals and their occupancies in the presence of degeneracies. Here we have devised a scheme to obtain a set of occupancies which (a) converges to physical densities (to the best of our knowledge) for FQHE systems, and (b) reproduces finite temperature DFT as well as the standard KS scheme for noninteracting v-representable systems. This scheme may be of much more general applicability to general systems which are not noninteracting v representable other than the FQHE. 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. Were the system noninteracting v representable, 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, and small fluctuations in the density between iterations cause the KS scheme to occupy a different subset of these orbitals at each iteration. This corresponds to constructing different Slater determinants at each iteration. While the occupation numbers f_{mn} of these orbitals are zero or unity more or less at random at each iteration, the *average* occupancies, i.e., the occupancies averaged over many iterations, become well defined and approach the value, say, $1/3$ for orbitals localized in a region where the local filling factor is close to $\nu = 1/3$. We use this to construct an ensemble by accumulating running average occupancies f_{mn} after the initial N_{eq} iterations 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 reproduces the results of the KS scheme for noninteracting v-representable systems (for which the KS scheme picks only the one Slater determinant which gives the ground state density) for N_{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 preliminary Monte Carlo simulations about the ensemble obtained by our scheme. The results are that to within numerical accuracy our scheme gives the lowest energy.

In the LDA, the exchange-correlation energy is assumed to be a local function of density, $E_{\mathrm{xc}}/N = \int d\mathbf{r}\,\epsilon_{\mathrm{xc}}(\nu)n(\mathbf{r})$, where $\epsilon_{\mathrm{xc}}(\nu)$ is the exchange-correlation energy per particle in a *homogeneous* system of constant density $n = \nu/2\pi\ell_B^2$ and filling factor ν. Experience has shown that the LDA often works surprisingly well, even for systems in which the electron density is strongly inhomogeneous [14]. In the FQHE, the length scale of exchange-correlation interactions and density fluctuations is given by the magnetic length ℓ_B due to the Gaussian falloff 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 also. For the exchange-correlation energy per particle of a uniform electron gas in a constant magnetic field, we use the Padé approximant [24] $\{\epsilon_{\mathrm{xc}}(\nu) = \epsilon_{\mathrm{xc}}^L(\nu) + \nu^4\epsilon_{\mathrm{xc}}^{TC}[n(\nu)]\}/1 + \nu^4$ where $\epsilon_{\mathrm{xc}}^{TC}$ is the zero-magnetic-field result [25]. The term $\epsilon_{\mathrm{xc}}^L(\nu)$ consists of two terms. The first one is a smooth interpolation formula [26] $\epsilon_{\mathrm{xc}}^{LWM}(\nu)$ between ground state energies at some rational fillings. The second one, $\epsilon_{\mathrm{xc}}^C(\nu)$, 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 $\epsilon_{\rm xc}^C(\nu)$ by constructing it to be zero at values of $\nu = p/q$ which display the FQHE. Near $\nu = p/q$, $\epsilon_{\rm xc}^C(\nu)$ 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 [27,28] at fractions $\nu = p/q$. Farther away from $\nu = p/q$, $\epsilon_{\rm xc}^C(\nu)$ decays to zero. Finally, in the LDA, $V_{\rm xc}(r)$ is obtained from $\epsilon_{\rm xc}(\nu)$ as $V_{\rm xc}(r) = \partial[\nu\epsilon_{\rm xc}(\nu)]/\partial\nu|_{\nu=\nu(r)}$ 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.

A technical difficulty arises in the LDA: The discontinuities in $V_{\rm xc}(r)$ in the LDA give rise to a numerical instability. The reason is that an arbitrarily small fluctuation in charge density close to a FQHE fraction gives rise to a finite change in energy. To overcome this problem, we made the compressibility of the system finite, but very small, corresponding to a finite, but very large, curvature instead of a pointlike cusp in $\epsilon_{\rm xc}$ at the FQHE fractions. What we found that worked very well in practice was to have the discontinuity in chemical potential occur over an interval of filling factor 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. Figure 1 depicts $V_{\rm xc}$, used in our calculations as a function of filling factor.

We have self-consistently solved the KS equation [Eq. (1)] for a spin-polarized quantum dot in a parabolic external potential, $V_{\rm ext}(r) = \frac{1}{2}m^*\Omega^2 r^2$ by expanding the KS orbitals $\psi_{mn}(\mathbf{r}) = e^{im\phi}\varphi_{mn}(r)$ in the eigenstates of $H_0 = (1/2m^*)[\mathbf{p} - (e/c)\mathbf{A}(\mathbf{r})]^2$ in the cylindrical gauge, $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\hat{B}r\phi$, including the four lowest Landau levels ($n = 0, \ldots, 3$). We chose $\epsilon_0 = 13.6$, appropriate for GaAs, and a confining potential of strength [2] $\hbar\Omega = 1.6$ meV. In particular, we have used our DFT-LDA scheme to study the edge reconstruction of the quantum dot as a function of magnetic field strength. As is known from Hartree-Fock and exact diagonalizations [5–8,18], 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 [9–11,29] on the edges and incompressible droplets to form in the bulk at densities $\nu = p/q$. Figure 2 depicts various stages of edge reconstruction obtained by us as the magnetic field strength is increased. The value of Ω for which the exchange lump appears compares very well with the value found by De Chamon and Wen [6] in Hartree-Fock and numerical diagonalizations. At higher fields still, the incompressible strips appear at the edges, and incompressible droplets are formed in the bulk. We would like to point out that the total potential $V_{\rm xc} + V_H + V_{\rm ext}$ is constant on an incompressible strip, due to the correlations included in $V_{\rm xc}$. Consequently, the KS eigenvalues of states localized at an incompressible strip are degenerate. We emphasize that incompressible regions that appear in our calculations are not due to the presence of a uniform positive background density, which

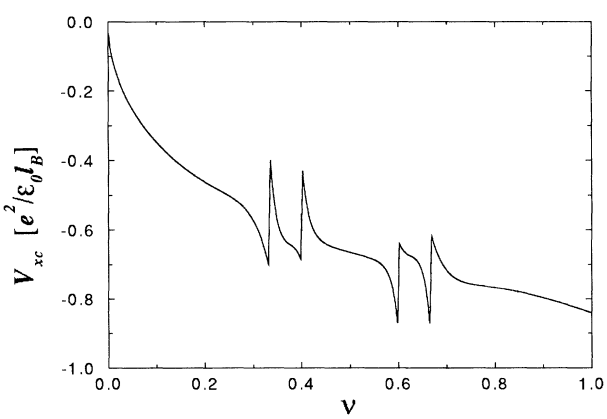

FIG. 1. Exchange-correlation potential $V_{\rm xc}$ as a function of filling factor in units of $e^2/\epsilon_0\ell_B$ for $0 \le \nu \le 1$. The increase in $V_{\rm xc}$ at a FQHE filling occurs over a range of a filling factor of 0.004.

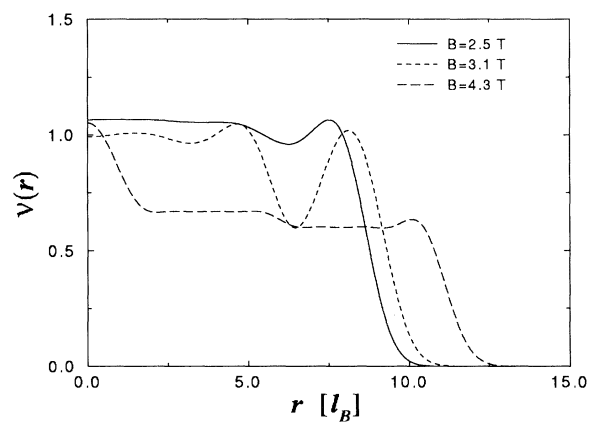

FIG. 2. Edge reconstruction of a quantum dot as the magnetic field strength is increased. Plotted here is the local filling factor $\nu(r)$ for a parabolic quantum dot with $\hbar\Omega = 1.6$ meV and 40 electrons. For magnetic field strengths $B < 2.5$ T, the dot forms a maximum density droplet, and for $B \approx 3.0$ T, an exchange hole is formed. For stronger magnetic fields, incompressible regions form, separated by compressible strips.

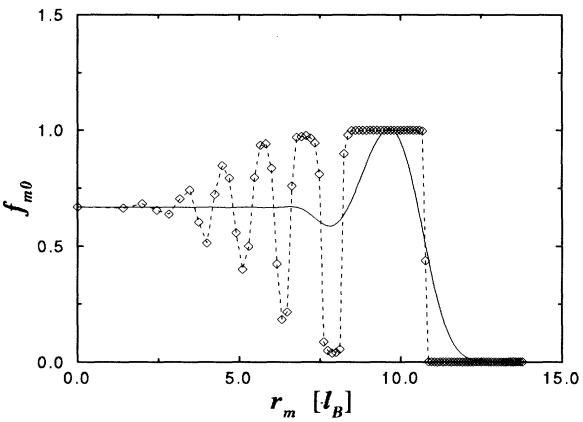

FIG. 3. Occupancies f_{m0} vs orbital centers r_m for a composite edge of a system of 45 electrons (diamonds). Here $B = 5.0$ T. Near the edge, the occupancies rise to unity. The full line shows the corresponding local filling factor.

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 [18,30] 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. An 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 [31], and it is unclear if composite edges exist in real systems which do not strictly obey particle-hole symmetry.

Figure 3 depicts the occupations of the Kohn-Sham orbitals and the particle density (inset) for a system where the confining potential is supplied by a uniform positive background charge density $n_+ = 2/6\pi\ell_B^2$ for $r < r_0$, where r_0 is fixed by charge neutrality. From this figure, we see that for this choice of potential 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. We have also verified the stability of all our incompressible regions by adding or subtracting a particle from the system.

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