Edge structure of fractional quantum Hall systems from density-functional theory

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We use the Hohenberg-Kohn formulation of density functional theory (DFT) to study the density profile at the edge of a confined two-dimensional electron gas in the fractional quantum Hall regime. The strong correlation effects present in this system are accounted for in our DFT approach and lead to the appearance of incompressible strips at fractional filling factors for smooth confining potentials.

The structure of the edge states[1] in the integral and fractional quantum Hall regimes of the two-dimensional electron gas[2] is believed, by many, to control the transport properties of a broad class of two-dimensional systems in the presence of a strong perpendicular magnetic field, such as Hall bars, quantum wires, and quantum dots. Particular interest has recently been focused on the question of how the edge structure of a confined quantum Hall fluid is affected by a change in the *smoothness* of the confining potential.[3–8] The latter is characterized by the variation in the confining potential over a magnetic length $l \equiv (\hbar c/eB)^{1/2}$, divided by an appropriate energy gap of the system. If this ratio is small, the potential is said to be smooth, or slowly varying. In the case of sharp edges the correct description appears to be one in terms of one or more chiral Luttinger liquids.[3] For a sufficiently smooth confining potential, however, the edge is believed to separate into narrow incompressible and wide compressible regions,[4–6] and in this case conventional edge state theory may not apply. In both cases, the distribution of the electronic density in the edge region offers a straightforward signature of the regime a particular sample is in. The possibility of directly measuring edge channels has been recently demonstrated[9] in the integral regime, and this gives hope that soon a similar measurement could be performed in the fractional regime.

Several calculations have been made recently of the edge structure in the integral and fractional quantum Hall regimes,[7] and of the transition between sharp and smooth confinement.[8] If the system is sufficiently large, then exact diagonalization techniques are not applicable, and one has to resort to some alternative methods. One possible way to investigate the edge structure in the fractional regime is to use composite fermions[10] in a mean-field approximation,[8] which provides a useful single-particle description of the edge. An alternative approach, which we take in this paper, is the density-functional theory (DFT), originally formulated by Hohenberg, Kohn and Sham,[11] and later extended by Vignale and Rasolt[12] to systems in strong magnetic fields. In this work, we use the finite-temperature generalization of the Hohenberg-Kohn formulation. The fundamental advantage of the DFT approach is that it is, in principle, an *exact* theory of the ground-state density distribution. Its central statement is that the exact equilibrium density distribution can be obtained by minimizing the energy (or the grand-canonical potential) which can, in turn, be expressed as a unique functional of the density. In general, the exact form of the energy functional is not known. In the case of smoothly confined quantum Hall fluids, however, the existence of a small parameter, namely, the ratio of the magnetic length $l \sim 100$ Å to the characteristic confinement length (i.e., the length over which the density varies significantly) $a \sim 1000$ Å, creates a rather unique situation. For such slowly varying densities, a local density approximation[13] (LDA) provides an excellent representation of the true energy functional. This representation becomes exact in the limit of infinitely slowly varying density, i.e., when $l/a \to 0$.

In this paper, we present results of an ongoing investigation of the edge structure in the fractional quantum Hall regime as a function of the smoothness of the confining potential. The inclusion of correlation effects is essential for a proper description of the system. We demonstrate that, for smooth confinement, a picture in terms of compressible and incompressible regions is also valid in the fractional regime. The analog of the cyclotron gap, which is responsible for the formation of the incompressible regions in the integral regime, is provided in the fractional regime by the gap in the exchange-correlation scalar potential at certain filling factors, the filling factor ν being defined as $\nu = 2\pi l^2 n$, where n is the two-dimensional number density.

We emphasize that, in contrast to previous studies of the edge structure problem, which employed the Thomas-Fermi or the Hartree-Fock approximation, our DFT approach includes the effects of exchange and, more importantly, correlation. To the best of our knowledge, this is the first application of DFT to include also the effects of incompressibilities at fractional filling factors in a quantum Hall fluid.

For simplicity we consider a system of spinless fermions, the method being generalizable to electrons with spin. Although our interest in this paper focuses on the properties of the ground state, we find it convenient to approach the ground-state regime as the zero-temperature limit of the finite-temperature density-functional formalism.[14] An advantage of this formalism is that it offers a simple way to obtain a smoothly varying density in a *partially* filled Landau level. We now derive the set of self-consistent equations that we use to describe the edge structure. The grand-canonical potential Ω of the system may be written as a functional of the density

$\rho(\mathbf{r})$ as[15]

$$\Omega[\rho] = T_s[\rho] + E_H[\rho] + \int d\mathbf{r}\ [V(\mathbf{r}) - \mu]\rho(\mathbf{r}) + F_{\mathrm{xc}}[\rho] - TS_s[\rho], \quad (1)$$

where $T_s[\rho]$ is the kinetic energy of the noninteracting two-dimensional electron gas of density ρ, $S_s[\rho]$ is the noninteracting entropy,

$$E_H[\rho] \equiv \frac{e^2}{2\epsilon}\int d\mathbf{r}\ d\mathbf{r}'\ \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} \quad (2)$$

is the Hartree energy with ϵ denoting the dielectric constant of the host semiconductor, $V(\mathbf{r})$ is an external confining potential, μ is the chemical potential, $F_{\mathrm{xc}}[\rho]$ is the remaining exchange-correlation contribution to the free energy in the presence of the magnetic field B, and T is the temperature. In the $T \to 0$ limit, $F_{\mathrm{xc}}[\rho]$ reduces to the usual exchange-correlation energy $E_{\mathrm{xc}}[\rho]$. An essential feature of E_{xc} for a uniform Hall fluid is the existence of cusps at certain fractional filling factors that lead to incompressible states and a quantized Hall conductance at these filling factors. We shall show that by including this strong-correlation effect in DFT leads to the appearance of incompressible strips at fractional filling factors for smooth confining potentials.

The density may be written as a sum of contributions coming from the various Landau levels ρ_n according to

$$\rho(\mathbf{r}) = \frac{1}{2\pi l^2}\sum_{n=0}^{\infty}\ \rho_n(\mathbf{r}). \quad (3)$$

To obtain the finite-temperature density profile, we minimize the grand-canonical potential with respect to the $\rho_n(\mathbf{r})$. The noninteracting kinetic energy and entropy functionals are

$$T_s[\rho] = \frac{1}{2\pi l^2}\sum_{n=0}^{\infty}\ \int d\mathbf{r}\ \rho_n(\mathbf{r})\ \left(n+\frac{1}{2}\right)\hbar\omega_c, \quad (4)$$

and

$$S_s[\rho] = -\frac{1}{2\pi l^2}\sum_{n=0}^{\infty}\ \int d\mathbf{r}\ \{\rho_n(\mathbf{r})\ln\rho_n(\mathbf{r}) + [1-\rho_n(\mathbf{r})]\ln[1-\rho_n(\mathbf{r})]\}, \quad (5)$$

respectively. Here $\omega_c = eB/m^*c$ is the cyclotron frequency. The chemical potential is determined by the normalization condition $N = \int d\mathbf{r}\ \rho(\mathbf{r})$, where N is the number of electrons. The minimization yields

$$\mu = \left(n+\frac{1}{2}\right)\hbar\omega_c + V_H(\mathbf{r}) + V(\mathbf{r}) + V_{\mathrm{xc}}(\mathbf{r}) + k_BT\ \ln\left[\frac{\rho_n(\mathbf{r})}{1-\rho_n(\mathbf{r})}\right], \quad (6)$$

where the Hartree potential V_H is given by

$$V_H(\mathbf{r}) = \frac{e^2}{\epsilon}\int d\mathbf{r}'\ \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \quad (7)$$

and where

$$V_{\mathrm{xc}}(\mathbf{r}) \equiv \frac{\delta F_{\mathrm{xc}}[\rho]}{\delta\rho(\mathbf{r})} \quad (8)$$

is the exchange-correlation scalar potential. From Eq. (6) it follows that

$$\rho(\mathbf{r}) = \frac{1}{2\pi l^2}\sum_n f\left[\hbar\omega_c\left(n+\frac{1}{2}\right) + V_{\mathrm{eff}}(\mathbf{r}) - \mu\right], \quad (9)$$

where f is the Fermi distribution function, and

$$V_{\mathrm{eff}}(\mathbf{r}) = V(\mathbf{r}) + V_H(\mathbf{r}) + V_{\mathrm{xc}}(\mathbf{r}) \quad (10)$$

is an effective potential that includes exchange-correlation effects. In the strong magnetic-field regime, the kinetic energy is accurately described by the local density approximation (4), and this makes our approach equivalent to the solution of the Kohn-Sham equations,[12] with the advantage that our scheme, being less computationally intensive, allows us to investigate larger systems.

In order to proceed with the calculation we need a form for the exchange-correlation potential, which contains gaps at the fractional filling factors associated with the formation of an incompressible liquid. We have used an approximation given by MacDonald[16] for the lowest Landau level, at zero temperature, which exhibits particle-hole symmetry. The use of the zero-temperature form for V_{xc} is justified since we are interested precisely in this limit. The approximation consists of a smooth part and a superimposed oscillatory part, and uses a mapping to composite fermions to give gaps at the filling factors $\nu = p/(2p+1)$, with p an integer. The gaps agree with the known calculated values at filling factors 1/3 and 2/5. A plot of V_{xc} is presented in Fig. 1.

In the low-temperature limit, Eq. (6) becomes

$$\mu_k(\rho(\mathbf{r})) + V_{\mathrm{eff}}(\mathbf{r}) = \mu, \quad (11)$$

where $\mu_k(\rho) = ([\nu]+\frac{1}{2})\hbar\omega_c$ is the zero-temperature chemical potential of the noninteracting electron gas, and $[\nu]$ is the integral part of $2\pi l^2\rho$. μ_k exhibits discontinuities at integral filling factors, and V_{xc} (in the limit $T \to 0$) is discontinuous at the filling factors of the fractional quantum Hall effect. When the density reaches one of the filling factors associated with a gap, μ_k or V_{xc} on the left-hand side of Eq. (11) changes by the discontinuity there. This implies that the density resists crossing that filling factor; instead it develops an incompressible region, where a constant density is maintained, up to a width W such that the difference in the classical potential $V(\mathbf{r})+V_H(\mathbf{r})$ evaluated at the end points of the incompressible region exactly compensates for the discontinuity in μ_k or V_{xc}. Incompressible regions at integer filling factors are due to discontinuities in μ_k, while those at fractional filling factor are associated with the discontinuities in V_{xc}. In both cases, a simple estimate of the width of an incompressible region, obtained by balancing the discontinuity against the change in the classical potential, yields[6]

$$W \propto \left(\frac{\Delta_i}{|\rho'|}\right)^{1/2}, \quad (12)$$

where Δ_i is the gap at that filling factor, and ρ' is the

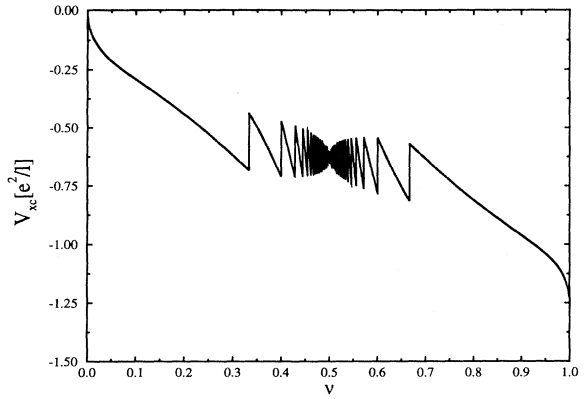

FIG. 1. Exchange-correlation potential as function of the filling factor. The energies are in units of $e^2/\epsilon l$, from Ref. 16.

slope of the classical density profile there. From this formula we see that large gaps and slowly varying density profiles are the necessary condition for the occurrence of incompressible regions of appreciable size.

We present here results for a quantum dot whose confining potential is generated by a positively charged background in the shape of a truncated cone. A section of the positive charge background is shown in Fig. 2. Given the rotational symmetry of the system about an axis parallel to the external magnetic field, the density profile is assumed to depend on the radial coordinate only. The advantage arising from having a positive charge background as a confining potential is in having a simple way to control the density in the bulk of the dot. The smoothness of the potential can be adjusted by changing the slope with which the positive charge density goes to zero, by changing the parameters L and w defined in Fig. 2. We have also performed calculations for Hall bars, and for a parabolic confining potential, obtaining similar results as those in this paper. The density profile is obtained by solving self-consistently the set of equations (9) and (10). All the results we present for the edge structures considered in the fractional regime have been obtained at a temperature of $0.07e^2/\epsilon l$, which is sufficiently low for the fractional incompressible strips to be observed, the relevant gaps being about $0.3e^2/\epsilon l$. We start from a temperature of $0.5e^2/\epsilon l$, and then anneal to low temperature, maintaining self-consistency at each temperature step. Calculations performed at different temperatures have been seen to affect only the size of the incompressible regions, provided that the temperature is low enough for their formation and high enough to avoid instabilities. We have not noticed any appreciable contribution coming from higher Landau levels, and this shows that the only energy scales of the problem are $e^2/\epsilon l$ and k_BT. It was not possible, in our numerical calculations, to anneal below the temperature of $\approx 0.07e^2/\epsilon l$. Numerical instabilities prevent the achievement of self-consistency below this temperature. It is not clear at present whether or not these numerical instabilities can be associated with a real physical phenomenon, such as the formation of charge-density waves, which are in fact expected to occur as the temperature goes to zero,[17] and the consequent breakdown of our assumptions concerning the slow variation of the density.

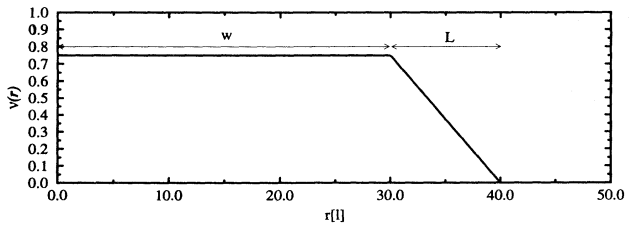

FIG. 2. Filling factor of disk of the positive charge background as a function of the radial coordinate r. Linear distances are expressed in units of the magnetic length. L is the length over which the density goes to zero with a slope w/L, while w is the size of the bulk region.

The $\nu = 2/3$ edge state has received much attention recently, and several theories of its structure and excitation spectrum have been proposed. One is in terms of two branches of excitations.[3] In particular, MacDonald[3] described it as consisting of a $\nu = 1/3$ droplet of holes in a $\nu = 1$ droplet of electrons, which suggests that there may be a reconstructed edge where the filling factor goes first from 2/3 to 1, and then from 1 to 0. Another picture is characterized by having an incompressible region at filling factor 1/3 that separates two compressible regions, one between the 2/3 state and the 1/3 state, and the other between 1/3 and 0.

We plot in Fig. 3 the density profile for the case of a filling factor 2/3 in the bulk with a sharp confinement given by a disk of positive charge ($w = 40l$, $L = 0$.) The figure shows that there are no incompressible regions, which means that in this situation the Beenakker[5] and Chang[4] picture does not hold. This is also consistent with the qualitative formula (12), since in this case ρ' is very large. Numerical calculations done by Johnson and MacDonald,[7] and by Meir,[7] seem to indicate that a $\nu = 1$ droplet may appear at the edge of the system. The possibility of such a composite edge is a direct consequence of the higher hierarchical character of the $\nu = 2/3$ state relative to that of, for example, the $\nu = 1/3$ state. Since the density functional contains information only about the magnitude of the cusps, but not about their "hierarchical" status (that is, the nature of the underlying wave function), we do not expect our approach to be able to reproduce the composite edge. However, enhancement of the density at the edge of the systems could be expected on the basis of fairly general energetic arguments, since the local exchange-correlation energy favors a larger filling factor. The fact that we do not see this enhancement in our calculations may be attributed to the effect

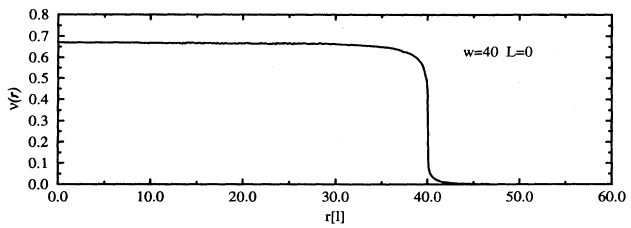

FIG. 3. Self-consistent filling-factor profile for the case $w = 40$, and $L = 0$, for a filling factor 2/3 in the bulk. The distances here, as well as in the other figures, are given in units of the magnetic length, and $T = 0.07e^2/\epsilon l$.

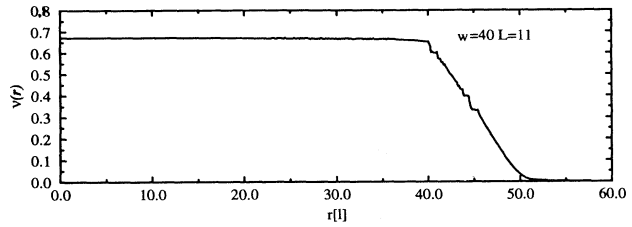

FIG. 4. Self-consistent filling-factor profile for the case $w = 40$, and $L = 11$, for a filling factor 2/3 in the bulk. $T = 0.07e^2/\epsilon l$.

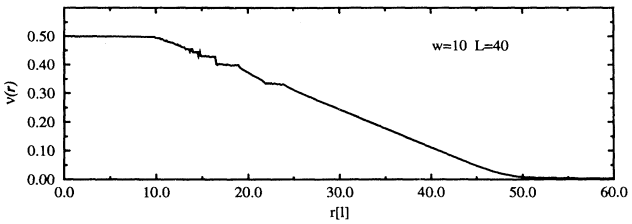

FIG. 5. Self-consistent filling-factor profile for the case $w = 10$, and $L = 40$, for a filling factor 2/3 in the bulk. $T = 0.07e^2/\epsilon l$.

of the finite temperature. Numerical calculations done by Chklovskii,[8] for the 2/3 state in a channel, also produce no rise in the filling factor.

In Fig. 4 we present results for the 2/3 edge for a smoother potential ($w = 40$, $L = 11$). Incompressible regions start to appear, beginning with the fractional filling factors associated with the larger gaps in V_{xc}. In Fig. 5 the confining potential is made even smoother ($w = 10$, $L = 40$) and the result is that more incompressible regions have appeared, and the widths of the main ones have increased. Qualitatively the widths of the incompressible regions appear to conform fairly well to the behavior prescribed by Eq. (12). We have observed analogous results to those shown for filling factor 2/3, for different values of the filling factor in the bulk.

We have found that in the fractional quantum Hall regime, in the case of sharp confinement, the density goes to zero from the value in the bulk without presenting additional incompressible strips at intermediate filling factors or without edge reconstructions. In making the confining potential smoother, incompressible regions start to appear beginning with the filling factors having larger gaps in V_{xc}, and then including the others when the confining potential becomes smooth enough. Nevertheless, the widths of the incompressible regions are always smaller than the compressible ones. We have recently received a preprint by Heinonen *et al.*,[18] where they make a study analogous to ours using the Kohn-Sham formulation of DFT.

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[1] R. B. Laughlin, Phys. Rev. B **23**, 5632 (1981); B. I. Halperin, *ibid.* **25**, 2185 (1982); C. W. Beenakker and H. van Houten, in *Solid State Physics,* edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1991), Vol. 44, p. 1, and references therein.

[2] K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett. **45**, 494 (1980).

[3] A. H. MacDonald, Phys. Rev. Lett. **64**, 222 (1990); X.-G. Wen, Phys. Rev. B **41**, 12 838 (1990).

[4] A. M. Chang, Solid State Commun. **74**, 871 (1990).

[5] C. W. L. Beenakker, Phys. Rev. Lett. **64**, 216 (1990).

[6] D. B. Chklovskii, B. I. Shklovskii, and L. I. Glazman, Phys. Rev. B **46**, 4026 (1992).

[7] M. D. Johnson and A. H. MacDonald, Phys. Rev. Lett. **67**, 2060 (1991); J. Dempsey, B. Y. Gelfand, and B. I. Halperin, *ibid.* **70**, 3639 (1993); Y. Meir, *ibid.* **72**, 2624 (1994); K. Lier and R. R. Gerhardts, Phys. Rev. B **50**, 7757 (1994).

[8] C. de Chamon and X. G. Wen, Phys. Rev. B **49**, 8227 (1994); L. Brey, *ibid.* **50**, 11 861 (1994); D. B. Chklovskii, *ibid.* **51**, 9895 (1995).

[9] R. J. F. Haren, F. A. P. Blom, and J. H. Wolter, Phys. Rev. Lett. **74**, 1198 (1995).

[10] J. K. Jain, Phys. Rev. Lett. **63**, 199 (1989).

[11] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1965); W. Kohn and L. Sham, *ibid.* **140**, A1133 (1965).

[12] G. Vignale and M. Rasolt, Phys. Rev. Lett. **59**, 2360 (1987); for a more recent review, see, for example, G. Vignale, in *Density Functional Theory*, Vol. 337 of *NATO Advanced Study Institute Series B: Physics*, edited by E. K. U. Gross and R. M. Dreizler (Plenum Press, New York, 1995), p. 485.

[13] M. Ferconi and G. Vignale, Phys. Rev. B **50**, 14 722 (1994).

[14] N. D. Mermin, Phys. Rev. **137**, A1441 (1965).

[15] We have omitted in Eq. (1) the dependence of $\Omega[\rho]$ on the current (Ref. 12), which is irrelevant in the slowly varying limit considered here. Also, the $T_s[\rho]$ we use here includes the magnetic field.

[16] A. H. MacDonald (unpublished).

[17] H. Fukuyama, P. M. Platzman, and P. W. Anderson, Phys. Rev. B **19**, 5211 (1979).

[18] O. Heinonen, M. I. Lubin, and M.D. Johnson (unpublished).