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Density functional theory of the fractional quantum Hall effect

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A conceptual difficulty in formulating the density functional theory of the fractional quantum Hall effect is that while in the standard approach the Kohn-Sham orbitals are either occupied or unoccupied, the physics of the fractional quantum Hall effect calls for fractionally occupied Kohn-Sham orbitals. This has necessitated averaging over an ensemble of Slater determinants to obtain meaningful results. We develop an alternative approach in which we express and minimize the grand canonical potential in terms of the composite fermion variables, which provides a natural resolution of the fractional-occupation problem because the fully occupied orbitals of composite fermions automatically correspond to fractionally occupied orbitals of electrons. We demonstrate the quantitative validity of our approach by evaluating the density profile of fractional Hall edge as a function of temperature and the distance from the delta dopant layer and showing that it reproduces edge reconstruction in the expected parameter region.

The density functional theory (DFT) is a powerful tool for treating many particle ground states. A quantitatively reliable DFT of the fractional quantum Hall (FQH) effect would obviously be extremely useful for elucidating the fundamental physics of FQH systems with spatially varying density, whether induced by an external potential or generated spontaneously, which are not readily amenable to many of the theoretical methods used in the field. However, the problem is nontrivial^{1,2} because the solution is not close to a single Slater determinant in which some of the Kohn-Sham orbitals are fully occupied and the others empty, but instead entails fractional occupation of Kohn-Sham orbitals, as demanded by the physics of the FQH effect (FQHE). Theoretically, fractionally occupied orbitals arise because all single particle orbitals of electrons are degenerate in the absence of interaction, and interaction produces a strongly correlated state in a nonperturbative fashion. A possible way to obtain on-average fractionally filled Kohn-Sham orbitals is through ensemble averaging. In the first application of DFT to the FQHE, Ferconi, Geller and Vignale¹ averaged over a thermal ensemble to achieve fractional fillings and obtained the density profile at the edge for a sufficiently smooth confinement potential. In another approach, Heinonen, Lubin and Johnson² performed an average over the ensemble of Slater determinants obtained in successive steps of the iterative scheme for solving the Kohn-Sham equations, and also generalized their approach to include the spin degree of freedom^{3,4}.

We present in this work a formulation of the DFT of FQHE in terms of composite fermions rather than electrons. This provides a natural solution to the fractional-occupation problem because occupied orbitals of composite fermions, as obtained in the DFT formulation, automatically correspond to fractionally filled Kohn-Sham orbitals of electrons. We minimize, in a local density approximation, the thermodynamic potential expressed as a functional of the CF density in various CF Landau levels, using an exchange correlation functional for composite fermions deduced from microscopic calculations and an

entropy functional that properly incorporates the physics of strong correlations. To test the quantitative validity of our approach, we determine the density profile of the FQHE edge and find, in agreement with previous exact diagonalization studies, that the edge undergoes a reconstruction when the delta-dopant layer containing the positive neutralizing charge is farther than a critical distance. We further find that, for general fractions, edge reconstruction extends much deeper into the interior of the sample than previously suspected, and determine the temperatures where it is washed out by thermal fluctuations. As another application, we calculate how the periodic potential produced by a Wigner crystal (WC) in a nearby layer affects the density of composite fermions at $\nu \approx 1/2$.

The objective is to minimize the grand potential

$$\Omega[\rho] = \mathcal{E}_{xc}[\rho] + \mathcal{E}_H[\rho] + \int d^2\mathbf{r} \rho(\mathbf{r})(V(\mathbf{r}) - \mu) - k_B T S \quad (1)$$

expressed in terms of the electron density $\rho(\mathbf{r})$, which is related to the local filling factor as $\rho(\mathbf{r}) = \nu(\mathbf{r})/2\pi l^2$, where $l = \sqrt{\hbar c/eB}$ is the magnetic length. Here E_{xc} and E_H are the exchange-correlation and Hartree energies, $V(\mathbf{r})$ is the potential energy due to interaction with an external charge distribution, μ is the chemical potential, T is the temperature, and S is the entropy. To express $\Omega[\rho]$ in terms of composite fermions, let us recall some relevant facts about composite fermions^{5,6}. The density of composite fermions is the same as that of electrons, but composite fermions experience an effective magnetic field $B^* = B - 2\rho\phi_0$ ($\phi_0 = hc/e$), form Landau-like levels [called Λ levels (Λ LS)], and their filling factor ν^* is related to the electron filling factor by the equation $\nu = \nu^*/(2\nu^* \pm 1)$. (We specialize, for simplicity, to composite fermions carrying two flux quanta.) Because we will deal with non-uniform densities, we define $\nu^*(\mathbf{r}) = \sum_j \nu_j^*(\mathbf{r})$, where $\nu_j^*(\mathbf{r})$ is the local filling factor of the j th Λ L. The effective CF cyclotron energy is given by the relation $\hbar\omega_c^* = \hbar \frac{eB^*}{m^*c} = \hbar \frac{eB}{(2\nu^* \pm 1)m^*c} \equiv \frac{\alpha}{2\nu^* \pm 1} \frac{e^2}{\epsilon l}$

where the last equality is motivated from dimensional arguments^{6,7}, and has also been tested in calculations that identify the CF cyclotron energy to the energy required to excite a far separated CF particle-hole pair⁸. Explicit calculation yields $\alpha = 0.33$ for a system with zero thickness^{6,7}, which is what we shall assume below.

We first determine the exchange correlation function by making the local density approximation, which is valid when the variation in the density is sufficiently slow that we can consider it to be locally constant. In other words, we assume that the variations in density are negligible on the scale of the CF magnetic length $l^* = \sqrt{\hbar c/e|B^*|}$. We write

$$\mathcal{E}_{\text{xc}} = \int d^2\mathbf{r} \rho(\mathbf{r}) E_{\text{xc}}[\rho(\mathbf{r})] \quad (2)$$

where $E_{\text{xc}}[\rho(\mathbf{r})]$ is the exchange-correlation energy per particle for a system with *uniform* density. For a uniform system, E_{xc} is precisely the energy that is usually obtained in numerical calculations (because the total energy includes electron-background and background-background terms which cancel the Hartree part of the interaction energy of electrons). It is possible to obtain, in the CF theory, the thermodynamic limits for the energies at the discrete value of fillings $\nu = n/(2n \pm 1)$, where the electronic ground states are accurately represented as $\nu^* = n$ filled ALs of composite fermions^{9,10}. From explicit calculation with the microscopic theory of composite fermions, the exchange-correlation energy per *electron* at $\nu = n/(2n \pm 1)$ is given very accurately by¹¹

$$E_{\text{xc}} \left[\nu = \frac{n}{2n \pm 1} \right] = a \frac{n}{2n \pm 1} + b \quad (3)$$

with $a = -0.324$ and $b = -0.303$. (We express all energies and also $k_B T$ in units of $e^2/\epsilon l$, which is $\sim 150\text{K}$ at $B = 9\text{T}$ for parameters appropriate for GaAs.) The energy as a function of continuous ν has downward cusps at $\nu = n/(2n \pm 1)$. Rather than attempting a microscopic calculation for the full curve of energy vs. filling factor, which can be performed assuming that the composite fermions in the partially filled AL form a crystal¹², we will make a model that is more natural from the DFT point of view and sufficient for current purposes. We will interpret the exchange-correlation energy of electrons as a sum of exchange-correlation and kinetic energies for composite fermions:

$$E_{\text{xc}}[\nu] = E_{\text{xc}}^*[\nu] + E_{\text{K}}^*[\nu] \quad (4)$$

where we follow the usual convention that all quantities marked by an asterisk $*$ refer to composite fermions. We shall further assume that composite fermions themselves are weakly correlated, i.e., E_{xc}^* is smooth and all cusps arise from E_{K}^* . In terms of the CF cyclotron energy $\hbar\omega_c^*$, E_{K}^* at the special fillings $\nu = n/(2n \pm 1)$ is given by $E_{\text{K}}^* \left[\nu = \frac{n}{2n \pm 1} \right] = \frac{n}{2} \hbar\omega_c^* = \frac{\alpha}{2} \frac{n}{2n \pm 1}$. This leads us to the final form of E_{xc} for arbitrary ν that we use in our

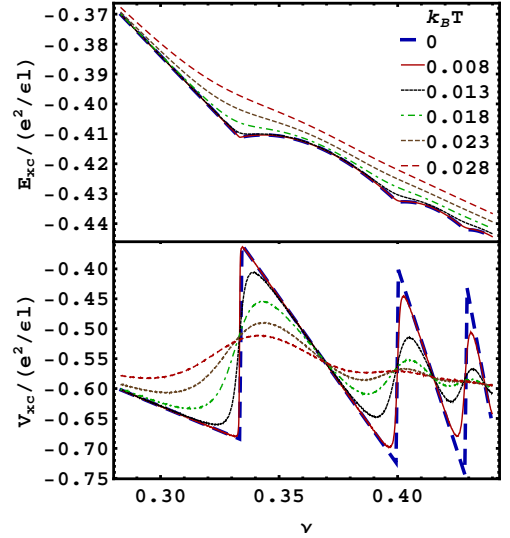


FIG. 1. Exchange-correlation energy $E_{\text{xc}}(\nu)$ (Eq. 5) and potential $V_{\text{xc}}(\nu) = E_{\text{xc}} + \nu \partial E_{\text{xc}} / \partial \nu$ as a function of the filling factor ν for several temperatures.

calculations below:

$$E_{\text{xc}}[\nu] = a\nu + b - \frac{\alpha}{2} \nu + E_{\text{K}}^*[\nu] \quad (5)$$

At $T = 0$, the average kinetic energy per CF for a general filling $\nu = \nu^*/(2\nu^* \pm 1)$ with $n = \text{int}(\nu^*)$ is given by

$$E_{\text{K}}^*[\nu] = \left(2n + 1 - \frac{n(n+1)}{\nu^*} \right) |1 - 2\nu| \frac{\alpha}{2} \quad (6)$$

where $\nu^* = |\frac{\nu}{1-2\nu}|$. At finite T , the CF kinetic energy per particle can be evaluated numerically as $E_{\text{K}}^* = \frac{1}{\nu^*} \sum_j (j + 1/2) \hbar\omega_c^* \nu_j^*$ with $\nu^* = \sum_j \nu_j^*$ and $\nu_j^* = (e^{\frac{(j+1/2)\hbar\omega_c^* - \mu}{k_B T}} + 1)^{-1}$. The resulting E_{xc} is plotted in Fig. 1 along with $V_{\text{xc}} = \delta \mathcal{E}_{\text{xc}} / \delta \nu(\mathbf{r}) = E_{\text{xc}} + \nu \partial E_{\text{xc}} / \partial \nu$. In the limit of $T = 0$, E_{xc} has cusps and V_{xc} discontinuities at $\nu = n/(2n \pm 1)$. We note that, for simplicity, we have not incorporated into our model the physics of the $\nu = n/(4n \pm 1)$ incompressible states at $\nu < 1/3$ described in terms of composite fermions carrying four flux quanta.

To obtain an expression for the entropy, we need the knowledge of the excitation spectrum of the strongly correlated FQH state. As detailed calculations have shown¹³, the counting of excited states is consistent with the model of weakly interacting composite fermions for temperatures small compared to the CF Fermi energy $E_{\text{F}}^* \sim 0.1e^2/\epsilon l$. We note that the degeneracy of the CF ALs is determined by the effective magnetic field, which in turn depends on density and thus position. As a result, a sum over all single CF energy levels is written as

$$\sum_{i,\gamma} = \sum_i \int \frac{d^2\mathbf{r}}{2\pi(l^*)^2} = \sum_i \frac{1}{2\pi l^2} \int d^2\mathbf{r} |1 - 2\nu(\mathbf{r})| \quad (7)$$

where i is the AL index and γ labels single CF states within a AL. The entropy of composite fermions is thus

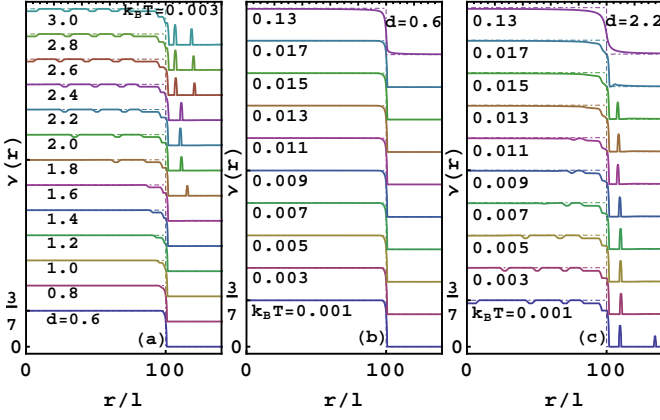


FIG. 2. (a) Evolution of the 3/7 edge as a function of the setback distance d for a small temperature $k_B T = 0.003$. The $\nu(r)$ for successive d are vertically displaced for clarity. Edge reconstruction is seen to occur at $d \approx 1.6$. (b-c) Evolution of the 3/7 edge as a function of temperature for two values of d . For $d = 2.2$ the edge structure melts at $k_B T \approx 0.017$. $k_B T$ is quoted in units of $e^2/\epsilon l$.

given by

$$S[\{\nu_i^*\}] = -\frac{1}{2\pi l^2} \int d^2 \mathbf{r} |1 - 2\nu(\mathbf{r})| \sum_i \{ \nu_i^*(\mathbf{r}) \ln[\nu_i^*(\mathbf{r})] + (1 - \nu_i^*(\mathbf{r})) \ln[1 - \nu_i^*(\mathbf{r})] \} \quad (8)$$

For FQH states corresponding to filled Λ Ls ($\nu_i = 1$ or 0) the entropy vanishes as it should.

In terms of $\nu_j^*(\mathbf{r})$, the thermodynamic potential is rewritten as (with \mathcal{E} representing the total energies and E representing the energies per particle)

$$\Omega[\nu_j^*(\mathbf{r})] = \mathcal{E}_K^* + \mathcal{E}_H + \mathcal{E}_{xc}^* + \int \frac{d^2 \mathbf{r}}{2\pi l^2} \nu(\mathbf{r}) V(\mathbf{r}) - \mu \left(\int \frac{d^2 \mathbf{r}}{2\pi l^2} \nu(\mathbf{r}) - N \right) - k_B T S[\{\nu_j^*(\mathbf{r})\}] \quad (9)$$

where under local density approximation, we have

$$\mathcal{E}_K^*[\{\nu_j^*\}] = \frac{\alpha}{2\pi l^2} \int d^2 \mathbf{r} |1 - 2\nu(\mathbf{r})|^2 \sum_i \nu_j^*(\mathbf{r}) \left(j + \frac{1}{2} \right), \quad (10)$$

$$\mathcal{E}_{xc}^*[\nu(\mathbf{r})] = \frac{1}{2\pi l^2} \int d^2 \mathbf{r} \left[\left(a - \frac{\alpha}{2} \right) \nu(\mathbf{r}) + b \right] \nu(\mathbf{r}), \quad (11)$$

and the entropy is given in Eq. 8. Eq. 10 reduces to Eq. 6 in the limit of zero temperature, when all Λ Ls other than the topmost one are fully occupied, but we allow occupation of higher Λ Ls, as appropriate at finite temperatures. The term μN , where N is the number of electrons, has no effect on the self-consistency equations. The electron density (or filling factor) is given by

$$\rho(\mathbf{r}) = \frac{\nu(\mathbf{r})}{2\pi l^2} = \frac{1}{2\pi l^2} \frac{\sum_j \nu_j^*(\mathbf{r})}{2 \sum_j \nu_j^*(\mathbf{r}) \pm 1} \quad (12)$$

Using $\delta\nu(\mathbf{r})/\delta\nu_i^*(\mathbf{r}') = (1 - 2\nu(\mathbf{r}))|1 - 2\nu(\mathbf{r})|\delta(\mathbf{r} - \mathbf{r}')$ we minimize Eq. 9 with respect to $\nu_j^*(\mathbf{r})$. This results in the condition

$$\nu_j^*(\mathbf{r}) = \frac{1}{\exp[\epsilon_j^*(\mathbf{r})/k_B T] + 1} \quad (13)$$

where $\epsilon_j^*(\mathbf{r})$, the local self-consistent energy of the j th Λ L, is given by

$$\epsilon_j^* = |1 - 2\nu(\mathbf{r})|(\epsilon_{1j}^* + 2k_B T s^*) + (1 - 2\nu(\mathbf{r}))(\epsilon_2^* - \mu) \quad (14)$$

$$\epsilon_{1j}^* = \left(j + \frac{1}{2} \right) \alpha - 4\alpha |1 - 2\nu(\mathbf{r})| \sum_i \left(i + \frac{1}{2} \right) \nu_i^*(\mathbf{r}) \quad (15)$$

$$\epsilon_2^* = \frac{1}{2\pi l^2} \int \frac{\nu(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^2 \mathbf{r}' + V(\mathbf{r}) + 2 \left(a - \frac{\alpha}{2} \right) \nu(\mathbf{r}) + b \quad (16)$$

$$s^* = - \sum_i \{ \nu_i^*(\mathbf{r}) \ln[\nu_i^*(\mathbf{r})] + (1 - \nu_i^*(\mathbf{r})) \ln[1 - \nu_i^*(\mathbf{r})] \} \quad (17)$$

The solution $\nu_j^*(\mathbf{r})$ is obtained by demanding self-consistency of Eq. 13. From the knowledge of $\nu_j^*(\mathbf{r})$, the electron density and the free energy Ω can be readily evaluated. The self-consistent Λ L energies $\epsilon_j^*(\mathbf{r})$ are very complicated functions of various parameters, and display a non-trivial dependence on the position.

To obtain the self-consistent solution we begin with an initial choice for $\nu_j^*(\mathbf{r})$ that tracks the neutralizing charge and calculate the new values according to Eq. 13 fixing the chemical potential to ensure the correct total charge. A new choice is then obtained by mixing the input and output values, and the procedure is iterated until self-consistency is achieved. See Supplemental Material (SM)¹⁴ for further details. To ensure smoothness on the scale of l^* , which is expected on physical grounds and also assumed in local density approximation, we average the local filling factor $\nu_j^*(\mathbf{r})$ over a length l_{ave} at each step of our self-consistency loop. In our calculations shown below, we use $l_{\text{ave}} = l^*$ (which depends on the local filling factor). As mentioned above, in the limit $T \rightarrow 0$ the local CF filling factor $\nu_j^*(\mathbf{r})$ approaches either 0 or 1 in each Λ L, depending on whether the self-consistent Λ L energy $\epsilon_j^*(\mathbf{r})$ is positive or negative. This produces a fractional value for the local $\nu(\mathbf{r})$, as appropriate for the physics of the problem.

As a first application of the above formalism, we consider the behavior at the edge of a FQH state. Following the typical experimental geometry, we shall model the positively charged background as a uniformly charged δ -doped disk at a set-back distance d from the plane containing the electrons. This corresponds to

$$V(\mathbf{r}) = -e^2 \int d^2 \mathbf{r}' \frac{\rho_b(\mathbf{r}')}{\sqrt{|\mathbf{r} - \mathbf{r}'|^2 + d^2}} \quad (18)$$

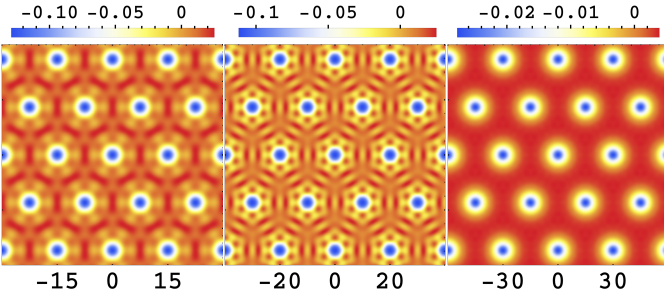


FIG. 3. Change in the density of the CF Fermi sea due to the presence of a WC of lattice constant c in a nearby layer at a distance d . The three panels, from left to right, have $(d, c) = (3, 15), (3, 20), (6, 30)$. The color represents $\Delta\nu(\mathbf{r})$ according to scale shown on top. All lengths are in units of l .

Exact diagonalization studies on small systems^{15–18} at $\nu = 1/3$ have found that an edge excitation mode becomes soft when d becomes larger than a critical value $\sim 1.5l$ (recall $l \approx 8\text{nm}$ for $B = 9\text{T}$), which is interpreted in terms of an edge reconstruction¹⁹. The systems were too small to shed light on the nature of the reconstructed edge, or to study this physics at more general fillings of the type $\nu = n/(2n \pm 1)$ which are expected to have much more complex edges. As seen in SM¹⁴, our DFT method shows that for the $1/3$ state edge reconstruction occurs at $d = 1.5$ at small T , which is a strong confirmation of the quantitative validity of our approach. We illustrate the power of our approach by taking the example of the edge of $3/7$ FQH state. Fig. 2(a) displays the evolution of the edge at a low temperature as a function of d . Edge reconstruction is seen at $d \sim 1.6l$. Incompressible stripes of $\nu = 2/5$ and $\nu = 1/3$ are seen to emerge except for very small d , with a stripe pattern alternating between $3/7$ and $2/5$ extending deep into the interior at large d at low T . We note that the alternating stripe pattern is qualitatively distinct from that seen in integer quantum Hall effect²⁰. The reason is because the densities for nearby FQH states are very close, and thus the stripe formation does not entail a high Hartree cost. Figs. 2(b) and (c) and S2¹⁴ display the evolution of the $3/7$ edge as a function of T . Edge reconstruction is absent at small d , while for $d = 2.2$, it is washed out by $k_B T = 0.017$, which is much smaller than the CF Fermi energy $E_F^* \sim 0.1$. Fig. S3 depicts the spatial dependence of $\epsilon_j^*(\mathbf{r})$ for several choices of parameters. We note that significant experimental progress has been made toward imaging the quantum Hall edges to explore compressible and incompressible stripes as well as edge reconstruction (see Refs.^{21–24} and references therein).

As a second application of our DFT method, we consider the geometry investigated in the recent experiment of Deng *et al.*²⁵, where they study commensurability oscillations of composite fermions near filling factor $\nu = 1/2$ in the presence of a periodic potential produced by a Wigner crystal in a nearby layer at a distance d . Analogous commensurability oscillations have been observed in an antidot superlattice²⁶ and also in the presence of a one

dimensional periodic potential^{27–31}. We ask here how the presence of a nearby WC affects the density of composite fermions in the vicinity of $\nu = 1/2$, where composite fermions form a compressible CF Fermi sea⁷. The above method is not convenient in this regime, as we have a very large number of occupied Λ Is. We therefore work directly with Eq. 1, setting $T = 0$. We further neglect the physics of incompressibility, which should be valid for $\nu \approx 1/2$, and approximate the exchange-correlation energy as $E_{xc} = a\nu + b$ (from Eq. 3). Minimization with respect to the electron density gives

$$2a\nu(\mathbf{r}) + b + \frac{1}{2\pi} \int d^2\mathbf{r}' \frac{\nu(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + V(\mathbf{r}) = \mu \quad (19)$$

where we measure energies in units of $e^2/\epsilon l$ and length in units of l . The potential due to the WC is modeled through Eq. 18 with $\rho_b = -\sum_{\mathbf{R}} (2\pi)^{-1} e^{-|\mathbf{r}-\mathbf{R}|^2/2}$, corresponding to a Gaussian electron at each site \mathbf{R} of a triangular lattice with lattice constant c . Fourier transformation gives the deviation of filling factor from its uniform value as:

$$\Delta\nu(\mathbf{r}) = -\frac{4\pi}{\sqrt{3}c^2} \sum_{\mathbf{K} \neq 0} \frac{e^{-|\mathbf{K}|d - \frac{|\mathbf{K}|^2}{2}} + i\mathbf{K} \cdot \mathbf{r}}{1 + 2a|\mathbf{K}|} \quad (20)$$

where the reciprocal lattice vectors are given by $\mathbf{K} = s_1\mathbf{K}_1 + s_2\mathbf{K}_2$ with $\mathbf{K}_1 = (2\pi/c, -2\pi/\sqrt{3}c)$, $\mathbf{K}_2 = (0, 4\pi/\sqrt{3}c)$, and s_1, s_2 are integers. $\Delta\nu(\mathbf{r})$ is independent of the unperturbed filling factor (provided we are in the compressible region near $\nu = 1/2$). The parameters b, μ and the potential due to the uniform neutralizing background only couple to $\mathbf{K} = 0$ and thus play no role in $\Delta\nu(\mathbf{r})$. Figs. 3 and S4 (in Supplemental Material¹⁴) show $\Delta\nu(\mathbf{r})$ for several values of d and c . An injected composite fermion sees the sum of the external and the Hartree potentials $V_H(\mathbf{r}) + V(\mathbf{r}) = \mu - 2a\nu(\mathbf{r}) - b$, and is thus attracted to high density regions. Complex patterns can appear, often dominated by values of $|\mathbf{K}| \approx -1/2a \approx 3/2$ where the denominator becomes small, as seen in the left two panels of Fig. 3. In such situations, the potential experienced by an injected composite fermion is complicated and may not produce clearly identifiable geometric resonances. However, for large d and large c these additional patterns are suppressed by the numerator and the density $\Delta\nu(\mathbf{r})$ closely reflects a hexagonal lattice as seen in the right panel of Fig. 3, thus allowing standard commensurability oscillations. This is consistent with the experiments of Deng *et al.*²⁵, where they observe commensurability oscillations for relatively large values of d and c ($d \approx 6.5$ and $20 < c < 60$).

We have assumed in our calculations a fully spin polarized system, as appropriate for sufficiently high magnetic fields. It would be interesting to extend our approach to include spin and explore the possibility of spin textures at the edge^{3,4,32,33}. Zhang, Hu and Yang have investigated precisely the model studied above by careful exact diagonalization studies³³ and concluded that edge reconstruction of the $1/3$ state does not involve spin reversal

unless the magnetic field is very small (<1.0 T for GaAs). This is not surprising because, as stressed by Karlhede *et al.*³², the energetics of spin textures at the edge is closely related to that of skyrmions³⁴, and calculations have shown that skyrmions at $1/3$ become viable only at very low Zeeman energies³⁵. We note that the Chern-Simons mean field theory of composite fermions^{7,36} has also been used to treat the effect of an external periodic potential on the state in the vicinity of half filling^{37,38}; see SM for a comparison with our approach.

In summary, we have presented a new formulation of the density functional theory of the FQHE that offers a natural way of producing fractionally occupied Kohn-Sham orbitals of electrons. We have introduced an exchange correlation energy that is consistent with microscopic calculations, and an entropy that incorporates the physics of strong correlations. We have applied our DFT to study the physics of the FQH edge as well as to the CF Fermi sea exposed to a periodic potential.

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