Exact exchange: A pathway for a density functional theory of the integer quantum Hall effect

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Abstract – It is shown here that the exact-exchange (EE) formalism provides a natural and rigororous approach for a density functional theory (DFT) of the integer quantum Hall effect (IQHE). Application of a novel EE method to a quasi–two-dimensional electron gas (q2DEG) subjected to a perpendicular magnetic field leads to the following main findings. i) the microscopic exchange energy functional of the IQHE has been obtained, whose main feature being that it minimizes with a discontinuous derivative at every integer filling factor \( \nu \); ii) an analytical solution is found for the magnetic-field dependent EE potential, in the one-subband regime; iii) as a consequence of i), the EE potential display sharp discontinuities at every integer \( \nu \); and iv) the widely used local spin density approximation (LSDA) is strongly violated for filling factors close to integer values.

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Introduction. – Density functional theory (DFT) is one of the most used computational tools for the theoretical study of inhomogeneous interacting systems such as atoms, molecules, and solids [1]. In its Kohn-Sham (KS) implementation, the real interacting electronic system is rigorously mapped into an auxiliary non-interacting system, where all the interactions are included in an effective single-particle potential, the spin-dependent KS potential \( v_{\sigma}^{KS}(r) \). The crucial ingredient of this potential is its exchange-correlation (xc) contribution, that is obtained from the xc energy functional \( E_{xc}[\rho(r)] \), with \( \rho(r) = \rho_\uparrow(r) + \rho_\downarrow(r) \) being the electronic density. While it is usually stated that \( E_{xc} \) is unknown, this is not fully correct: \( E_{xc} \) can be split in its exchange (\( E_x \)) and correlation (\( E_c \)) contributions, being only the latter the one that is really unknown. From the exact Fock expression for \( E_x \) one may obtain the corresponding exact-exchange (EE) local potential, to be used in the KS effective single-particle equations [2,3]. Along the years, many advantages of the EE formalism have been addressed. To quote just a few: correct asymptotic behavior of \( v_{\sigma}^{KS}(r) \) for atoms and molecules [2], and for solid surfaces [4], complete cancellation of the self-interaction error between the Hartree energy and conventional density-based approximations for the exchange energy [3], and considerable improvement of the KS gaps of semiconductors [5]. The EE method also provides a natural solution to the hard problem that represent electronic systems of reduced dimensionality. Differently from the usual functionals based on local density approximations, in the EE scheme \( E_x \) is an explicit functional of the KS orbitals, thus dimensionality of the system is automatically and rigorously included. A good example of this is the great improvement achieved in the computation of many-body effects on the electronic properties of quasi–two-dimensional electron gases (q2DEG) using either the EE formalism [6,7] or the more elaborate optimized effective potential (OEP) method, where correlation effects are also computed through an orbital-dependent \( E_c \) energy functional [8,9].

Possible generalizations of the DFT formalism to the high magnetic field regime of the fractional quantum Hall effect (FQHE) have been proposed by Ferconi, Geller and Vignale [10] and by Heinonen, Lubin, and Johnson [11]. The inherent fractional filling factors \( \nu \) needed for the
Kohn-Sham formulation. — Within the KS formulation of DFT, the 3D spin(σ)-dependent KS orbitals of the present system in the Landau gauge may be factorized as

\[ \Psi_{i,n,k}^{\text{KS}}(x,y,z) = \phi_n(x)e^{ik_y\lambda^x(z)}e^{ik_z\lambda^z(z)} \sqrt{L}, \]

where

\[ \phi_n(x) = \exp \left[ -(x-I_0)^2 \right] \right]^{1/2} + H_n \left( \frac{x-I_0}{\lambda} \right), \]

and the \( \lambda^x(z) \)s are the self-consistent solutions of the effective one-dimensional KS equations

\[ \left[ -\frac{1}{2} \frac{\partial^2}{\partial z^2} + v_{\text{KS}}^\sigma(z) \right] \lambda^x_{\sigma}(z) = \gamma^x_{\sigma}(\nu) \lambda^x_{\sigma}(z), \]

in effective atomic units (effective Bohr radius \( a_0^e = e^2/c^2\), and effective Hartree \( Ha^* = m^*e^4/\lambda^2 \)).

The 3D eigenvalues associated with \( \Psi_{i,n,k}^{\text{KS}}(x,y,z) \) are given by \( \varepsilon^\sigma_{i,n}(\nu) = \gamma^x_{\sigma}(\nu) + (n + 1/2)\hbar c/Ha^* - |g|\mu_B B\sigma/2Ha^* \). Here \( \omega_c = eB/m^* \) is the cyclotron frequency, and the last term is the Zeeman coupling, with \( s(1) = +1 \), and \( s(-1) = -1 \). The set of energy levels \( \varepsilon^\sigma_{i,n}(\nu) \) are the Landau levels (LL) of the q2DEG. Each LL is represented by a Gaussian density of states (DOS) of half-width \( \Gamma \) (see fig. 1), that represents the disorder effects from charged impurities, interface defects, etc. [33,34]. \( H_n(x) \) are the \( n \)-th Hermite polynomials, and \( n (= 0, 1, 2, \ldots) \) is the orbital quantum number index. \( k \) is the one-dimensional wave vector label that distinguishes states within a given LL, each with a degeneracy \( N_\nu \). \( A \) is the area of the q2DEG in the \( x-y \) plane, \( B \) is the magnetic field strength in the \( z \)-direction, and \( \Phi_0 = \Phi_0 \) is the magnetic flux number. \( l_B = \sqrt{\hbar c/eB/a_0^e} \) is the magnetic length. \( \nu = N/N_\nu \) is the dimensionless filling factor, with \( N \) being the total number of electrons. The \( \lambda^x_{\sigma}(z) \) are the self-consistent KS eigenfunctions for electrons in subband \( i (= 1, 2, \ldots) \), spin \( \sigma \) (=1,1) and eigenvalue \( \gamma^x_{\sigma}(\nu) \). The spin-dependent KS potential is the sum of three contributions: \( v_{\text{KS}}^\sigma = v_{\text{ext}}^\sigma + v_{\text{H}}^\sigma + v_{\text{xc}}^\sigma \). \( v_{\text{ext}}^\sigma \) represents the epitaxial potential plus the external fields (in the present case the electric field generated by the delta-doping layers). \( v_{\text{H}}^\sigma \) is the classical Hartree potential. \( v_{\text{xc}}^\sigma \) is the local exchange-correlation (xc) potential to be defined below.

The xc potential can be further split in the form

\[ v_{\text{xc}}^\sigma(z) = v_{\text{xc}}^\uparrow(z) + v_{\text{xc}}^\downarrow(z). \]

In the following we shall consider only its exchange contribution, assuming that correlation effects are negligible for \( \nu \)'s around integer values (IQHE), since the phase-space blocking situation of a set of full Landau levels precludes the existence of low-energy correlation-induced effects. In other words, as the number of electrons on the LL’s is close to its full occupation, only a few Slater determinants would contribute to the wave function, thus the exchange energy dominates over the correlation effects. This amounts to the “exact-exchange” characterization of the present computational approach.
Exact exchange at finite magnetic field. – The exact 3D Fock expression for the exchange energy is given by
\[ E_x = - \sum_{a,b,\sigma} f_{a}^\sigma f_{b}^\sigma \times \int d^3r \int d^3r' \Psi_a^\sigma(r)^* \Psi_b^\sigma(r')^* \Psi_a^\sigma(r) \Psi_b^\sigma(r') \frac{2}{|r - r'|}, \tag{3} \]
with \( f_a^\sigma, f_b^\sigma \) being the finite temperature weights, taking values between 0 and 1. Substituting the eigenfunctions \( \Psi_{i,n,k}(r) \) in eq. (3) and using the quasi-2D Fourier representation of the Coulomb interaction [34], we obtain
\[ E_x = - \sum_{n,m} n_{1,2D}^{n,m} \int d\nu \int d\nu' \sum_{\sigma} \langle \nu | \Psi_{n,m}^{\sigma} | \nu' \rangle \langle \nu' | \Psi_{n,m}^{\sigma} | \nu \rangle \frac{2}{|\nu - \nu'|}. \tag{4} \]
Here \( n_{1,2D}^{n,m} = \frac{f_{1}^{\sigma} f_{2}^{\sigma}}{2eB} \int d\nu \int d\nu' \sum_{\sigma} \langle \nu | \Psi_{n,m}^{\sigma} | \nu' \rangle \langle \nu' | \Psi_{n,m}^{\sigma} | \nu \rangle \frac{2}{|\nu - \nu'|} \)
\[ I_x^{n,m}(\nu - \nu') = \frac{n_c!}{n_c!} \frac{I_x^{n,m}(\nu - \nu')}{n_c!} \times \left[ \frac{I_x^{n,m}(\nu - \nu')}{n_c!} \right]^{2} \left( e^{-z|z'-z'|/l_B} \right), \tag{5} \]
as given elsewhere [16]. Here \( I_x^{n,m}(x) \) are the generalized Laguerre polynomials, and \( n^c = \min(n,m), n^{x} = \max(n,m) \). We emphasize that eq. (4) is valid for all values of \( \nu \), either integer or fractional, which results from an “ensemble average” defined as follows. While in a perfect crystal the degenerate states within a LL can be labeled by \( k \) and a delta-Dirac DOS, an average over an ensemble of impurities and defects breaks this degeneracy, yielding the Gaussian DOS used above. This allows us to convert sums over the occupied \( k \) states into the integral defined in \( n_{1,2D}^{n,m} \).

When only the first subband \( i = 1 \) is occupied, eq. (4) simplifies drastically to
\[ e_x(\nu) = \frac{-1}{2eB} \sum_{\sigma} \langle \rho_\sigma | S^{\nu}_{1} | \rho_\sigma \rangle \langle \rho_\sigma | S^{\nu}_{1} | \rho_\sigma \rangle \tag{6} \]
with \( e_x = E_x/N \) being the exchange energy per particle, \( \langle \rho_\sigma | S^{\nu}_{1} | \rho_\sigma \rangle \) representing integrals over \( z \) and \( z' \) of the densities \( \rho_\sigma(z) \) and \( \rho_\sigma(z') \) times \( S^{\nu}_{1}(z - z') \), and
\[ S^{\nu}_{1}(z - z') = \sum_{n,m} n_{1,2D}^{n,m} n_{1,2D}^{m,n} I_n^{m}(z - z'). \tag{7} \]

Here we have used that \( \rho_\sigma(z) = N_\sigma |\lambda^\nu_1(z)|^2 = \nu_\sigma N_\sigma \times |\lambda^\nu_1(z)|^2 \), and that \( \nu_\sigma = \sum_{n} n_{1,2D}^{n,m} \) is the spin-dependent filling factor. Since \( \int \rho_\sigma(z) dz = \nu_\sigma N_\sigma \), this allows us to define \( \nu_\sigma N_\sigma / A^* = (\pi \tau_2^\nu)^{-1} \), with \( \tau_2^\nu \) being the 2D dimensionless parameter that characterizes the electronic in-plane density, and \( A^* \) is the area in units of \( a_0^2 \). Using these relations, one obtains \( \nu = 2(l_B/r_0)^2 \). This one-subband (1S) regime is quite relevant both from the experimental and theoretical viewpoints. Real q2DEG are easily driven to this regime by a suitable modulated or delta-doping design, bias application, or by changing the width \( d \) of the quantum well, barrier height, etc. [34]. From the theoretical side, it was realized already some time ago the considerable simplification one gets in the EE defining equations at zero-magnetic field, when restricted to this regime [6–9,35,36].

In ref. [19] an analytical expression for the exchange energy of a 3D electron gas subjected to a magnetic field is given, for \( n = 0, 1 \). The physical situation is however quite different: the energy spectrum along \( z \) is a free-particle continuum, instead of our discrete spectrum \( \gamma^\nu_i \); besides, the value of \( n \) is not restricted to any particular value in eq. (6).

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\footnote{See for example eq. (10.93) in ref. [37].}
results to be presented below were obtained by using the full expression for $S^o_{\sigma}(t)$ in eq. (7); nonetheless the approximated eq. (9) is quite useful to understand the full numerical results.

Next, we obtain the spin-dependent EE potential from $v_\sigma^e(z) = \delta(N_{e\sigma}/\delta \rho_\sigma(z))$ for the 1S case, which reads

$$v_\sigma^e(z) = -\frac{1}{l_B N_0 \epsilon_0^2} \int dz' \rho_\sigma(z') S_1^o(z-z') - \frac{1}{2 l_B N_0} \int dz \int dz' \rho_\sigma(z) \rho_\sigma(z') \times \frac{\partial \left( S_1^o(z-z')/\nu_\sigma^2 \right)}{\partial \gamma_1^\sigma}, \quad (10)$$

where the first (second) term comes from the explicit (implicit) dependence of $E_\Sigma$ on $\rho_\sigma(z)$. This implicit dependence is easy of understand: by changing $\rho_\sigma(z)$, a change in $v_{\Sigma}(z)$ and $v_\sigma^e(z)$ is induced through the self-consistent solution of the KS equation, that in turn affects $\gamma_1^\sigma$. After some cumbersome calculations, eq. (10) becomes

$$v_\sigma^e(z) = u_\sigma^e(z) + \Delta v_\sigma^e, \quad (11)$$

with $u_\sigma^e(z)$ being the first term in eq. (10), $\Delta v_\sigma^e = \gamma_1^\sigma e \int S_1^o(z)^2 u_\sigma^e(z) dz$, and $\gamma_1^\sigma = -\langle \rho_\sigma | S_1^o/\rho_\sigma \rangle / (\nu_\sigma^2 N_0 l_B)$. It remains to define

$$S_2^o(t) = \sum_{n,m} \left( \frac{\partial n_{m,\sigma}^{2D}}{\partial \gamma_1^\sigma} \right) n_{m,\sigma}^{2D} I_n^m(t) \sum_n \left( \frac{\partial n_{n,\sigma}^{2D}}{\partial \gamma_1^\sigma} \right). \quad (12)$$

Equations (6) and (11) are the main results of this paper. Notice that eq. (11) is not invariant under a constant shift $v_\sigma^e(z) \to v_\sigma^e(z) + C$, since here we consider the grand-canonical ensemble. That is, for given values of the external parameters $\nu$, $r_s$, and $T$, the chemical potential $\mu$ is fixed. A rigid shift in $v_\sigma^e(z)$ will induce then a rigid shift in the KS eigenvalues $\gamma_1^\sigma$, that at constant $\mu$ will modify the occupation factors $n_{m,\sigma}^{2D}$, leading to a change in $v_\sigma^e(z)$. In other words, $v_\sigma^e(z)$ is fully determined by eq. (11), and then no floating constant should be fixed by imposing asymptotic boundary conditions, as is usual for similar closed systems [35,38]. Naturally, the KS equations must be solved numerically and self-consistently: for each $\nu$, both $\nu_{\Sigma}(z)$ and $v_\sigma^e(z)$ determine and are determined by the solutions $\lambda_1^\sigma(z)$ and $\gamma_1^\sigma$, which yields the self-consistent loop. The following set of GaAs material parameters have been used in the numerical calculations: $m^* = 0.067 m_0$, ($m_0$ being the bare electronic mass), $\epsilon = 12.85$, $g = -0.44$, $T = 340 \text{ mK}$, and $\Gamma(B) = 0.150 \sqrt{B} \text{ meV}$. The GaAs-AlxGa1-xAs conduction band barrier height has been taken as 228 meV, which corresponds to $x \simeq 0.3$.

Results and discussion. – In the following we analyze the dependence upon $\nu$ of $e_\Sigma(\nu)$, and $v_\sigma^e(z)$. First, fig. 2 shows the results for the exchange energy $e_\Sigma(\nu)$, as given by eq. (6). $e_\Sigma(\nu)$ approaches a constant asymptotic value in the limit of large $\nu$ (small $B$ limit). This is easy to understand: as $B \to 0$, at fixed density, electrons redistribute among an increasing number of LL’s, such that the overlap of many Gaussian DOS reaches asymptotically the constant DOS of a q2DEG in the zero-field limit.

The oscillations of $e_\Sigma(\nu)$ are however its more interesting feature: At every integer value of $\nu$, $e_\Sigma(\nu)$ minimizes locally in a non-analytical way, yielding an inverted "cusp". Besides, at each odd $\nu (= \nu')$, $e_\Sigma(\nu)$ has a local minimum while $e_\Sigma(\nu')$ exhibits a local maximum, with the sum of both resulting in a weaker local minimum in $e_\Sigma(\nu)$, due to a partial cancellation between the two opposite behaviours. An equivalent situation happens at each even $\nu (= \nu')$, but with the roles of $e_\Sigma(\nu')$ and $e_\Sigma(\nu)$ exchanged. The qualitative behaviour of $e_\Sigma(\nu)$ and $e_\Sigma(\nu')$ around each $\nu'$ and $\nu''$ is easy to understand. For example, at each $\nu''$, the relative spin-polarization displayed in the upper panel of fig. 2 attains its possible maximum value $\Delta\nu/\nu = 1/\nu''$, and this optimizes the spin-up exchange energy gain. However, for $e_\Sigma(\nu)$ this is the worst possible configuration, and then it exhibits a local maximum. For each $\nu''$, on the other side, $\Delta\nu/\nu = 0$ as corresponds to a spin-compensated situation, and this optimizes the gain of the spin-down exchange energy, but delivers the smallest energy gain in $e_\Sigma(\nu)$, that displays thus a local maximum. Besides these qualitative considerations, one can obtain the same results analytically, starting directly from eq. (6) and expanding around every $\nu'$ and $\nu''$. Proceeding this way, we have found that both $e_\Sigma(\nu')$ and $e_\Sigma(\nu')$ depart linearly from each integer $\nu$, and these analytical linear approximations are represented by the crossing straight lines displayed at $\nu' = 2$, and $\nu'' = 3$. 

Fig. 2: (Colour online) (a) Spin-dependent filling factors $\nu$, (left scale) and relative spin polarization $\Delta \nu/\nu$ (right scale) for increasing values of the total filling factor $\nu$, $\Delta \nu = \nu_1 - \nu$. (b) Exchange energy per particle $e_\Sigma(\nu)$ vs. $\nu$, at fixed density $r_s = 2.5$. $e_\Sigma(\nu)$ and $e_\Sigma(\nu')$ are also shown. The straight lines at $\nu = 2$ and $\nu = 3$ represents the analytical approximations associated with the slope discontinuities of $e_\Sigma(\nu)$ and $e_\Sigma(\nu')$, respectively. The x-LSDA results are also shown for comparison.
The x-LSDA results are also shown in fig. 2. The exchange energy per particle is obtained from the corresponding expression for the spin-polarized homogeneous interacting 3D electron gas [37]. For large \( \nu \) (small \( B \)), the x-LSDA overestimates the EE energy, but this is not a general trend. For bigger densities (smaller \( r_s \)), we have found that it underestimates the EE energy (not shown). Interestingly, the x-LSDA displays small oscillations with non-analytical cusps around odd \( \nu \), where the spin polarization (fig. 2(a)) is maximum.

The remarkable behavior of \( v_{x}^\uparrow(z) \) and \( v_{x}^\downarrow(z) \) as a function of \( z \) and for several values of \( \nu \) is displayed in fig. 3. The crucial feature to note from fig. 3 is the abrupt jump (a rigid upward shift) of \( v_{x}^\uparrow(z) \) and \( v_{x}^\downarrow(z) \) when \( \nu \) crosses an integer value. After the jump, and as the filling continues, both \( v_{x}^\uparrow(z) \) and \( v_{x}^\downarrow(z) \) somehow follow the opposite behavior, and start to move down continuously. As shown in the upper panel, for \( \nu = 2.99 \) both EE potentials are again close to their value at \( \nu = 1.99 \), just before the jump. It should be noted here, however, that only for \( p_\sigma \to 0 \), the difference \( v_{x}^\uparrow(z)[\nu = [\nu] + p_\sigma] - v_{x}^\downarrow(z)[\nu = [\nu] - p_\sigma] \) becomes a constant. For finite (not infinitesimal) \( p_\sigma \), the potentials at filling factors smaller and greater than \( [\nu] \) differ by a \( z \)-dependent function, as can be seen in fig. 3.

The discontinuity in \( v_{x}^\sigma(z) \) at integer values of \( \nu \) can be traced back to a discontinuity in \( S_2^{[\nu,\sigma]}(t) \), that in turn induces a discontinuity in \( \eta_{[\nu]}^{[\nu,\sigma]} \). To explain this, we should return to the general expression for \( S_2^{[\nu,\sigma]}(t) \) in eq. (12), and assume that for \( \nu \) close to an integer value (either even or odd) essentially only one (per spin) of the occupation factors \( n_0^{2D} \) contributes to the derivative with respect to \( \gamma_1^\nu \). This situation is schematically depicted in fig. 4, for fillings close to \( \nu = 2 \) (left panel) and close to \( \nu = 3 \) (right panel).

Expressed in a different way, the assumption amounts to the approximation \( \partial n_{[\nu]}^{2D}/\partial \gamma_1^\nu \approx \delta_{n_{[\nu]}^{[\nu,\sigma]}} (\partial n_{[\nu]}^{2D}/\partial \gamma_1^\nu) \). Referring to the situation displayed in fig. 4, for \( \nu \approx 1.99 \), \([\nu] = [\nu] = 0\), and these are the only two LL that contribute to \( S_2^{[\nu,\sigma]}(t) \) in eq. (12) (one for each spin); for \( \nu \approx 2.01 \) instead, \([\nu] = [\nu] = 1\), and only for them the occupation factors change when \( \gamma_1^\nu \) changes.

Proceeding in this way, eq. (12) may be simplified to

\[
S_2^{[\nu,\sigma]}(t) \approx \sum_n n_{n,\sigma}^{2D} I_n^{[\nu,\sigma]}(t). \tag{13}
\]

We emphasize here that eq. (13) is valid only for \( \nu \) close to integer values, while eq. (12) is valid for arbitrary filling factors. Application of eq. (13) to the filling factors displayed in fig. 4 leads to the same result in all cases. For the discontinuity in \( S_2^{[\nu,\sigma]} \) we obtain thus

\[
\Delta S_2^{[\nu,\sigma]}(t) \equiv \Delta S_2^{[\nu,\sigma]+p_\sigma}(t) - S_2^{[\nu,\sigma]-p_\sigma}(t)
\]

\[
= \sum_{n=0}^{|\nu|-1} \left( I_n^{[\nu,\sigma]}(t) - I_n^{[\nu,\sigma]-1}(t) \right) < 0, \tag{14}
\]

and the negative sign is justified below for a few simple cases. From this, one obtains the discontinuity in \( \eta_{[\nu]}^{[\nu,\sigma]} \),

\[
\Delta \eta_{[\nu]}^{[\nu,\sigma]} \equiv \eta_{[\nu]}^{[\nu]+p_\sigma} - \eta_{[\nu]}^{[\nu]-p_\sigma} = \frac{\langle \rho_{\sigma} \Delta S_2^{[\nu,\sigma]} \rangle_{\gamma_1^\nu} \rho_{\sigma}}{\nu_2^2 (N_\sigma)^2 I_B} > 0,
\]

\[
= \frac{1}{r_s \sqrt{\nu^2/2}} \int dz dz' (\lambda_1^\nu(z) \lambda_1^\nu(z'))^2 \Delta S_2^{[\nu,\sigma]}(z-z'), \tag{15}
\]

with a positive sign, in agreement with the full numerical results displayed in fig. 3.

The simplest case to analyze is the discontinuity at \( \nu = 1 \). In this case, \([\nu] = 1\), \([\nu] = 0\) and eq. (14) reduces to

\[
\Delta S_2^{[\nu]}(t) = I_0^{[\nu]}(t) - I_0^{[\nu]}(t), \tag{16}
\]
which admits a simple physical interpretation. $I_{10}^{0}(t)$ is proportional to the exchange energy among electrons in the filled ground-state LL (intra-LL exchange interaction), while $I_{10}^{1}(t)$ is proportional to the exchange interaction among electrons in the ground and first-excited LL’s (inter-LL exchange interaction). Since usually intra-LL interactions are stronger than inter-LL ones, $I_{10}^{0}(t) > I_{10}^{1}(t)$ for all values of $t$, one gets the negative sign of $\Delta S_{2}^{[\nu]}(t)$, that in turn leads to the abrupt positive jump in $v_{x}^{\nu}(z)$ displayed in fig. 3 at $\nu = 1$. The next simple case is the discontinuity at $\nu = 2$. Here $[\nu_{1}^{\nu}] = [\nu_{1}] = 1$, with the result that $\Delta S_{2}^{[\nu]}(t) = \Delta S_{2}^{[\nu]}(1) = I_{0}^{1}(t) - I_{0}^{0}(t)$, the same as above. This implies that the discontinuities in $v_{x}^{\nu}(z)$ and $v_{x}^{\nu}(z)$ are the same at $\nu = 2$, as observed in fig. 3 and as expected from physical grounds. Note, however, that since $\Delta S_{2}^{[\nu]}$ scales as $\nu^{-1/2}$ at fixed $r_{s}$ (see eq. (15)), the discontinuity at $\nu = 2$ in $v_{x}^{\nu}(z)$ and $v_{x}^{\nu}(z)$ is approximately a factor $1/\sqrt{2}$ smaller than the discontinuity in $v_{x}^{\nu}(z)$ at $\nu = 1$. The next interesting case is $\nu = 3$. Here $[\nu_{2}] = 2$ and $[\nu_{1}] = 1$, and then

$$\Delta S_{2}^{[\nu]}(t) = I_{0}^{2}(t) + I_{0}^{1}(t) - I_{0}^{0}(t) - I_{1}^{1}(t),$$

while $\Delta S_{2}^{[\nu]}(t)$ is once again given by eq. (16). When replaced in eq. (15), this leads to discontinuities of different sizes for $v_{x}^{\nu}(z)$ and $v_{x}^{\nu}(z)$ at $\nu = 3$, as can be barely appreciated from the upper panels in fig. 5; we also provide there a comparison between the EE and the x-LSDA potentials. The difference between the x-LSDA exchange potentials is indistinguishable on the scale of the drawing for $\nu = 2.99$ and $\nu = 3.01$, as expected. It is also worth of note the drastically different asymptotic behavior of both types of exchange potentials: the well-known exponential decay of x-LSDA should be contrasted with the much slower and physically correct $-1/z$ decay of the EE potentials. In the lower panel of fig. 5 we give a global view of the x-LSDA exchange potential as a function of $z$ and $\nu$. Being just proportional to $(\rho_{s}(z))^{3/2}$, the same has no discontinuities at integer values of $\nu$, showing instead changes in the slope as $\nu$ crosses integer values. This is also easily grasped from the projection in the $\nu$-$z$ plane. The much faster decay of the x-LSDA exchange potential is evident from the strong narrowing of the central segment, whose darkness is proportional to the deepness of the potential.

In retrospective, it is important to realize that the discontinuity originates from the $\eta_{x}^{\nu}$ term, which comes from the implicit derivative of the exchange energy with respect to the density. This is the term that includes the in-plane density $(\nu_{s}N_{s}/A^{*})$ dependence of the exchange energy. The inclusion of the implicit derivative is also important to recover the correct strict-2D limit at zero magnetic field.

The six lowest LL eigenvalues $\epsilon_{n}(\nu)(\equiv \epsilon_{n}^{\nu}(\nu))$ are shown in fig. 6, both in the EE and x-LSDA approaches. The discontinuities that the EE $v_{x}^{\nu}(z)$ and $v_{x}^{\nu}(z)$ have at integer values of $\nu$ induces an abrupt change of all the LL energies, and of the chemical potential $\mu$. These numerical self-consistent results fully validate the strong renormalization of the LL electronic structure schematically displayed in fig. 4. Focusing first in the situation at $\nu \approx 2$, the “doublet” LL ordering $\{\nu_{s} = n\}$ is easily observed from fig. 6, and is schematically shown in the left panel of fig. 4. The LL ordering changes however drastically for $\nu \approx 3$, since now the “doublet” structure is built with $\{d_{n}^{\nu} = n_{0} + 1\}$ pairs of LL, as shown schematically in the right panel of fig. 4. How does the $q$-DAP passes from one configuration close to even $\nu$ to the case close to odd $\nu$? The answer is in the evolution of $v_{x}^{\nu}(z)$ and $v_{x}^{\nu}(z)$ for $2.01 \leq \nu \leq 2.99$ displayed in the upper panel of fig. 3. It is seen there how the continuous downward shift of $v_{x}^{\nu}(z)$ is larger than the one for $v_{x}^{\nu}(z)$, being the net result a global downward shift of the spin-up LL relative to the spin-down LL. And this is precisely the situation schematically depicted in fig. 4, restricted however to the two limiting values $\nu = 2.01, 2.99$. Once again, these qualitative considerations are validated by inspection of how the self-consistent

\[This will be presented elsewhere.\]
LL eigenvalues $\varepsilon^n_\nu(\nu)$ evolve in fig. 6 in this filling factor window.

The x-LSDA eigenvalues displayed in the right panel of fig. 6 behaves in a quite different way. First, since the x-LSDA exchange potentials are continuous functions of $\nu$, no discontinuities are present in the corresponding eigenvalues. Second, the chemical potential $\mu$ still have however some broadened discontinuities, either proportional to the “cyclotron gap” $h\omega_c$ at $\nu = \text{even}$, or proportional to the “spin-gap” $\varepsilon^\uparrow_\nu(\nu) - \varepsilon^\downarrow_\nu(\nu)$ at $\nu = \text{odd}$. For instance, $h\omega_c \simeq 0.16$ and 0.08 for $\nu = 2$ and 4, respectively, in reasonable agreement with the jump in $\mu$ at these filling factors. Third, note that the jump in $\mu$ at $\nu = 4$ (cyclotron gap) is bigger than the jump at $\nu = 3$ (spin-gap).

Conclusions. – The exact-exchange energy functional of the integer quantum Hall effect (IQHE) has been found. It minimizes locally with discontinuities in the derivative at each integer filling factor $\nu$. In the one-subband regime, where only the ground-state subband of the quasi-two-dimensional electron gas is occupied, an explicit analytical expression has been found for the associated spin-dependent exact-exchange potential. Its striking feature is that it jumps abruptly by a positive constant every time $\nu$ passes through an integer value. This is in analogy to the discontinuities in finite systems and solids when the total number of electrons $N$ passes through integer values, but in our case the novelty is that the discontinuities are induced by the magnetic field, at fixed density. The size of the jump is the same for spin-compensated situations at each $\nu = \text{even}$. For $\nu = \text{odd}$, the discontinuities are different, being the jump bigger for the exact-exchange potential of the majority spin-component. Strong differences are found regarding the standard x-LSDA for filling factors close to integer values.

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REFERENCES


