Exchange-correlation vector potentials and vorticity-dependent exchange-correlation energy densities in two-dimensional systems

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(Dated: October 25, 2018)

Abstract

We present a new approach how to calculate the scalar exchange-correlation potentials and the vector exchange-correlation potentials from current-carrying ground states of two-dimensional quantum dots. From these exchange-correlation potentials we derive exchange-correlation energy densities and examine their vorticity (or current) dependence. Compared with parameterizations of current-induced effects in literature we find an increased significance of corrections due to paramagnetic current densities.

PACS numbers: 71.15.Mb, 73.21.-b, 71.10.Ca
I. INTRODUCTION

Current-spin density functional theory (CSDFT)\(^1\,2\) is a powerful tool to calculate ground state (GS) properties of interacting electron systems. In contrast to spin-density functional theory (SDFT)\(^3\,4\) and density-functional theory (DFT)\(^5\,6\), CSDFT takes into account the coupling of the magnetic field to both, the spin density and the magnetic current density. However, CSDFT calculations require the exchange correlation (XC) energy as an input which is a functional of the spin densities \(n_\sigma(r)\) and the paramagnetic current density \(j_p(r)\). In the local vorticity spin-density approximation (LVSDA) the XC functional can be approximately calculated using XC energy densities from homogeneous systems which depend on the density parameter \(r_s\), the polarization \(\xi\) and the vorticity \(v\) (or alternatively the local filling factor \(f\)). Having investigated the XC energy density for two-dimensional (2D) systems with vanishing current density in a previous work\(^7\) the focus of this paper is on current-induced effects on the XC energy density. The relation \(v = -eB_{\text{hom}}/m^*\) allows to link the vorticity \(v = \nabla \times j_p(r)\) to homogeneous systems with a fictitious magnetic field \(B_{\text{hom}}\). This property is used by the current- or vorticity-induced corrections of XC energy densities in literature. They are parameterized as function of \(B_{\text{hom}}\) or the local filling factor \(f = 2\pi nl_B^2\). The local filling factor defines the number of occupied Landau levels of a 2D system in a magnetic field \(B\). \(l_B = \sqrt{1/(e|B_{\text{hom}}|)}\) is the magnetic length corresponding to \(B_{\text{hom}}\) (\(\hbar = 1\) throughout this paper).

CSDFT calculations for 2D systems (for quantum dots (QDs) see e.g. Refs. \([8,9,10]\)) have made use of current-density dependent XC energy densities based on interpolations provided by Levesque, Weis, and MacDonald (LWM)\(^11\) or Fano and Ortolani (FO)\(^12\). Both parameterizations are based on the assumption that the coupling of the magnetic field to the currents is only relevant for high \(B\). For these strong magnetic fields the considered system is in the lowest Landau level as the inter-Landau level spacings increases with growing \(B\) and the Zeeman energy and exchange effects favor spin polarization.

For this regime Laughlin\(^13\) postulated the relation

\[
\varepsilon_{\text{XC}}(f = m^{-1}) = \frac{e^2}{l_B\sqrt{2m}} \int_0^{\infty} dx \left[ g_f(xl_B) - 1 \right] \tag{1}
\]

for filling factors \(f = m^{-1} < 1\) (\(m\) is an odd number). For discrete filling factors \(f = \frac{1}{3}, \frac{1}{5}\) Levesque, Weis, and MacDonald (LWM)\(^11\) calculate the XC energy density by using the pair correlation function \(g_f(r)\) of a classical plasma with a density \(n = f/(2\pi l_B^2)\) and statistical
methods\textsuperscript{14} Interpolation delivers a continuous expression for the dependence of the XC energy density on the filling factor $f$ which is valid for $f < 1$

$$\varepsilon_{XC}^{\text{LWM}}(r_s, f)/\text{Ry} = -0.782133 \frac{2\sqrt{2}}{r_s} \left( 1 - 0.211 f^{0.74} + 0.012 f^{1.7} \right).$$ \hspace*{1cm} (2)

Fano and Ortolani (FO)\textsuperscript{12} pursue an alternative concept to parameterize current corrections for $\varepsilon_{XC}$: They follow the particle-hole symmetry for electrons in the lowest Landau level at large magnetic fields and establish an interpolation which exactly reproduces the well-known analytical result for filling factor $f = 1$ (see Ref. \textsuperscript{13})

$$\varepsilon_{XC}^{\text{FO}}(r_s, f)/\text{Ry} = \frac{2\sqrt{2}}{f^{3/2}r_s} \left[ -\sqrt{\frac{\pi}{8}} f^2 - 0.782133 f^{3/2} (1 - f)^{3/2} \right.$$
$$\left. + 0.683 f^2 (1 - f)^2 - 0.806 f^{5/2} (1 - f)^{5/2} \right].$$ \hspace*{1cm} (3)

In spite of concerns that the exact XC energy density might be irregular and not differentiable,\textsuperscript{16} the parameterizations (2) or (3) are used in a number of papers\textsuperscript{8,9,10,17} assuming that they reproduce an important part of current-induced XC effects. However, the LWM and the FO parameterization are only correct in the high density limit, i.e. for $r_s \to 0$.\textsuperscript{17}

To obtain XC energy densities $\varepsilon_{XC}(r_s, \xi, f)$ these current-dependent corrections are combined with XC energy densities $\varepsilon_{XC}^{\text{TC}/\text{LWM}/\text{FO}}(r_s, \xi)$ from systems without current-density by an interpolation established by Rasolt and Perrot\textsuperscript{18}

$$\varepsilon_{XC}(r_s, \xi, f) = \frac{\varepsilon_{XC}^{\text{LWM}/\text{FO}}(r_s, f) + f^p \varepsilon_{XC}^{\text{TC}/\text{AMGB}/\text{ISI}}(r_s, \xi)}{1 + f^p}. \hspace*{1cm} (4)$$

For large filling factors $f$ (i.e. for small magnetic fields $B_{\text{hom}}$) the Padé approximation yields the well-known result of local spin density approximation (LSDA), $\varepsilon_{XC}^{\text{TC}/\text{AMGB}/\text{ISI}}(r_s, \xi)$. For this quantity the interpolation by Tanatar and Ceperley (TC)\textsuperscript{19} is the most frequently used approach. However, recently new parameterizations were proposed by Attaccalite, Moroni, Gori-Giorgi, and Bachelet (AMGB)\textsuperscript{20} and Seidl (ISI=interaction strength interpolation)\textsuperscript{21}. In the limit of high effective magnetic fields or $f < 1$ Eq. (4) takes into account corrections due to paramagnetic currents. Usually the exponent is chosen to be $p = 4$ (see Ref. \textsuperscript{18}). However, results seem to be almost insensitive with respect a variation of $p$.\textsuperscript{17,18} The usage of the interpolation (4) is justified by an improvement of CSDFT results compared with benchmark calculations from ED and Quantum-Monte-Carlo.\textsuperscript{8,17}
It is also reported that results do not significantly depend on whether the LWM or the FO parameterization is applied.\textsuperscript{17} Even working with corrections which take into account discontinuities in the derivative of the XC energy density with respect to $f$ in the fractional quantum Hall regime (see Ref. \textsuperscript{22}) or an additional dependence on the polarization (see Refs. \textsuperscript{23,24}) do not further improve the CSDFT results.\textsuperscript{17}

The present paper is a natural extension of our previous publication\textsuperscript{7} where we presented 2D XC energy densities for systems without paramagnetic current density which were extracted from exact GS densities and energies provided by exact diagonalization (ED)\textsuperscript{25}. Here we want to focus on the current-induced effects on XC energy densities. Analogous to Ref. \textsuperscript{7}, the extraction of XC energy densities is performed in two steps: After briefly introducing CSDFT in Sec. II and the properties of the QD Hamiltonian in Sec. III we present the first step of the method, i.e. the calculation of scalar and vector XC potentials from exact QD GSs together with results (Sec. IV). In the following Section we introduce the second step which comprises the concept how to obtain XC energy densities from scalar and vector XC potentials. The results are compared with the current-dependent XC energy densities discussed above. Sec. VI gives a summary of the paper.

II. CURRENT-SPIN-DENSITY FUNCTIONAL THEORY AND LOCAL VORTICITY (SPIN-)DENSITY APPROXIMATION

In this Section we sketch the basics of CSDFT and LVSDA. The DFT formalism was originally established by Hohenberg, Kohn, and Sham\textsuperscript{5,6} and generalized to spin-polarized systems\textsuperscript{3} and current-carrying systems\textsuperscript{1,2} by including the coupling of the polarization to an applied magnetic field and to the paramagnetic current density. Accordingly, the Hohenberg-Kohn (HK) theorem has to be modified with respect to the spin degrees of freedom\textsuperscript{3} and to the paramagnetic current density\textsuperscript{1,2}. For the most general case, it states that two different non-degenerate GS wavefunctions $|\Psi\rangle$ and $|\Psi'\rangle$ always yield different combinations $(n_\sigma(r), j_\mu(r)) \neq (n'_\sigma(r), j'_\mu(r))$ of spin densities and paramagnetic current densities. This is sufficient to establish a functional of the total energy with the usual functional properties

$$E_{V_0,\sigma}[n_\sigma, j_\mu] = F_{HK}[n_\sigma, j_\mu] + \frac{\epsilon^2}{2m^*} \sum_\sigma \int d\mathbf{r} n_\sigma(\mathbf{r}) A^2(\mathbf{r}) + \sum_\sigma \int d\mathbf{r} j_\mu(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) + \epsilon \int d\mathbf{r} n_\sigma(\mathbf{r}) + \frac{\epsilon^2}{2m^*} \sum_\sigma \int d\mathbf{r} n_\sigma(\mathbf{r}) A^2(\mathbf{r})$$

(5)
and the universal HK functional

\[ F_{HK}[n_\sigma,j_p] = \langle \Psi[n_\sigma,j_p]|T + W|\Psi[n_\sigma,j_p]\rangle. \] \hspace{1cm} (6)

However, in contrast to the original HK theorem, the uniqueness of the potentials is lost in CSDFT, because it is possible that two different combinations of spin-dependent potentials and vector potential yield the same GS wavefunction. Thus, the one-to-one map between GS densities and XC potentials is destroyed. The consequence is that there might be discontinuities in the functional derivatives of the HK functional or the XC energy functional with respect to the densities.\textsuperscript{26} Capelle and Vignale\textsuperscript{26} conclude that this problem also affects the extraction of exact XC potentials from given GS densities. However, in the case of axially symmetric, parabolic quantum dots it is possible to restore the uniqueness as we will see in Section IV.

For practical purposes the variational scheme has to be mapped to the Kohn-Sham (KS) system, i.e. an effective single-particle system with the same GS densities as the interacting system. The spin-degree of freedom is considered in the KS equations\textsuperscript{3} by assuming the total spin \( S_z \) in \( z \)-direction to be a good quantum number

\[
\left[ \frac{1}{2m^*} \left\{ \nabla + e \left[ A(r) + A_{XC}(r) \right] \right\} \right]^2 + \frac{e^2}{2m^*} \left\{ A^2(r) - \left[ A(r) + A_{XC}(r) \right]^2 \right\}
+ V_\sigma(r) + V_H(r) + V_{XC,\sigma}(r) \right] \varphi_{j,\sigma}(r) = \varepsilon_{j,\sigma} \varphi_{j,\sigma}(r) \] \hspace{1cm} (7)

with the spin \( \sigma = \pm \) in \( z \)-direction and the KS energies \( \varepsilon_{j,\sigma} \) in increasing order. For a system containing \( N \) particles the spin densities and the paramagnetic current density are given by

\[
n_\sigma(r) = \sum_j \gamma_{j,\sigma} |\varphi_{j,\sigma}(r)|^2 \] \hspace{1cm} (8)

\[
j_p(r) = \sum_{j,\sigma} \gamma_{j,\sigma} [\varphi_{j,\sigma}^*(r) \nabla \varphi_{j,\sigma}(r) - \left( \nabla \varphi_{j,\sigma}^*(r) \right) \varphi_{j,\sigma}(r)] \] \hspace{1cm} (9)

with \( \gamma_{j,\sigma} \) being occupation numbers of the KS levels in the GS (\( \sum_{j} \gamma_{j,\sigma} = N_\sigma \) and \( N_+ + N_- = N \)). Then the GS density and polarization are

\[
n(r) = n_+(r) + n_-(r) \] \hspace{1cm} (10)

\[
\xi(r) = \frac{n_+(r) - n_-(r)}{n(r)} \] \hspace{1cm} (11)

The XC potentials

\[
V_{XC,\sigma}([n_\sigma,j_p], r) = \frac{\delta E_{XC}[n_\sigma,j_p]}{\delta n_{\sigma}(r)} \] \hspace{1cm} (12)
\[ eA_{XC,\sigma}(\[n_{\sigma},j_{p}\], r) = \frac{\delta E_{XC}[n_{\sigma},j_{p}]}{\delta j_{p}(r)} \]  \tag{13} 

are defined as functional derivatives of the XC energy functional

\[ E_{XC}[n_{\sigma},j_{p}] = F_{HK}[n_{\sigma},j_{p}] - \frac{1}{2} \frac{e^2}{4\pi\varepsilon\varepsilon_0} \int dr \int dr' \frac{n(r)n(r')}{|r-r'|} - T_{S}[n_{\sigma},j_{p}], \]  \tag{14} 

\((T_{S}[n_{\sigma},j_{p}]\) denotes the kinetic energy functional of the KS system.) The total GS energy \(E_0\) of the interacting system can be calculated from

\[ E_0 = \sum_{j,\sigma} \gamma_{j,\sigma} \varepsilon_{j,\sigma} - \frac{1}{2} \frac{e^2}{4\pi\varepsilon\varepsilon_0} \int dr \int dr' \frac{n(r)n(r')}{|r-r'|} - \sum_{\sigma} \int dr V_{XC,\sigma}([n_{\sigma},j_{p}], r)n_{\sigma}(r) \]

\[-e\int dr j_{p}(r) \cdot A_{XC}(r) + E_{XC}[n_{\sigma},j_{p}]. \]  \tag{15} 

Concerning the XC potentials we apply the LVSDA

\[ E_{XC}[n_{\sigma},v] \approx \int dr n(r)\varepsilon_{XC}(n_{\sigma}(r), v(r)). \]  \tag{16} 

Using the vorticity \(v(r) = \nabla \times \frac{j_{p}(r)}{n(r)}\) instead of the paramagnetic current density is a consequence of the gauge invariance of CSDFT and appropriate for local density approximations. The most important parameterizations of the XC energy density used in 2D calculations were introduced in Sec. I.

III. QUANTUM DOT HAMILTONIAN AND GROUND STATE DENSITIES

We consider a two-dimensional QD with an axially symmetric parabolic confinement potential of strength \(\omega_0\) in a magnetic field \(\mathbf{B} = (0, 0, B)\). The Hamiltonian for \(N\) particles in real-space representation (with \(r = (x, y)\), \(p = (p_x, p_y)\), angular momentum in \(z\)-direction \(l_z = xp_y - yp_x = \frac{1}{\hbar^2}\frac{\partial}{\partial x}\), and vector potential \(\mathbf{A}(r) = \frac{B}{2}(-y, x)\)) reads

\[ H = \sum_{j=1}^{N} \left( \frac{1}{2m^*} p_j^2 + eA_{XC}(r_j) \right)^2 + \frac{1}{2} \omega_0^2 r_j^2 \]  \tag{17} 

or

\[ H = \sum_{j=1}^{N} \left( \frac{p_j^2}{2m^*} + \frac{1}{2} m^* \omega_0^2 r_j^2 + \frac{\omega_c^2}{2} l_z^2 \right) + \frac{1}{2} \sum_{j,k=1}^{N} \frac{e^2}{4\pi\varepsilon\varepsilon_0|\mathbf{r}_j - \mathbf{r}_k|}. \]  \tag{18} 

Here \(e\) is the electron charge, \(m^* = 0.067 m_e\) and \(\varepsilon = 12.4\) are the effective mass and the screening constant of the host semiconductor (assumed to be GaAs), \(\omega_c = \frac{eB}{mc}\) is the cyclotron frequency, and \(\omega_h = \sqrt{\omega_0^2 + \omega_c^2/4}\) is the hybrid frequency.
The reference densities and energies for the investigation of XC energy densities are calculated by ED techniques which provide results of high accuracy. Note that the (spin-)density and the current density of all eigenstates of the angular momentum operator are functions of radius $r$ but not of the angle $\varphi$. Moreover, the current density is always of the form $j_p(r) = j_{p,\varphi}(r) \mathbf{e}_\varphi$ whereas the radial component vanishes. Therefore, the relevant quantities provided by ED are the spin-densities $n_\sigma(r)$ and the azimuthal component $j_{p,\varphi}(r)$ of the paramagnetic current density (or the $z$-component $v$ of the vorticity) of the GS and its energy $E_0$.

The many-particle Hamiltonian also shows an interesting scaling property which plays an important role in the context of the HK theorem. It is revealed if we rewrite (18) as a function of $\omega_0$, $\omega_c$, and $N$ and separate the angular momentum contribution. This concept is similar to the modification of the Hamiltonian of a (natural) atom in Ref. [26]:

$$H(\omega_0, \omega_c, N) = \sum_{j=1}^{N} \left( \frac{1}{2} m^* \frac{d}{dr} \left( r \frac{d}{dr} \right) j_j^2 + \frac{1}{2} m^* \left( \omega_0^2 + \frac{\omega_c^2}{4} \right) j_j^2 \right) + \frac{1}{2} \sum_{j,k=1}^{N} \frac{e^2}{4 \pi \varepsilon_0 |r_j - r_k|} + \sum_{j,k=1}^{N} \frac{\omega_c l_j}{2}$$

We identify the first part of (19) as a Hamiltonian of a QD in zero magnetic field with the confinement frequency $\sqrt{\omega_0^2 + \omega_c^2/4}$. The sum over all single-particle angular momenta in the last term yields the total angular momentum. As a result we can map the spectra and wave functions of QDs in the magnetic field to QDs in zero magnetic field.

The KS Hamiltonian of axially symmetric 2D QDs reads

$$H_{S,\sigma} = -\frac{1}{2m^*} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right] + \frac{1}{2} m^* \omega_0^2 r^2 + V_H(r) + V_{XC,\sigma}(\{n_\sigma, v\}, r)$$

Obviously, the KS Hamiltonian shows the same scaling properties as the original Hamiltonian

$$H_{S,\sigma}(\omega_0, \omega_c, N) = H_{S,\sigma}(\sqrt{\omega_0^2 + \omega_c^2/4}, 0, N) + \frac{\omega_c}{2} L.$$ 

Therefore, the XC effects do not depend on the strength of the external magnetic field. We can restrict our studies to systems without magnetic field. However, without magnetic field we can apply the original HK theorem to the Hamiltonian (17) what guarantees the uniqueness of the wavefunction and of the external potential. For the KS system the uniqueness of the (XC) potentials in quantum dots is explicitly investigated in the following Section.
IV. SCALAR AND VECTOR XC POTENTIALS

A review of the literature on the numerical inversion of KS equations, i.e. the calculation of XC potentials from GS densities can be found in Ref. [7]. However, in this paper we will focus on an unpolarized and on a fully polarized system for which we can analytically calculate the scalar XC potential and the XC vector potential. Before we present our results for \( V_{XC} \) and \( A_{XC} \) we will discuss the problem of uniqueness of XC potentials in CSDFT in the next paragraph.

A. Uniqueness of XC (vector) potentials

Because of Eqs. (19) and (21) we can assume the single-particle states \( |\varphi_{j,\sigma}\rangle \) (\( j \) is a combination of radial and angular momentum quantum number) of the KS Slater determinant

\[
|\Psi\rangle = |\varphi_{1,\downarrow}\rangle \ldots |\varphi_{N,\downarrow}\rangle |\varphi_{1,\uparrow}\rangle \ldots |\varphi_{N,\uparrow}\rangle
\]

(22)

to be eigenfunctions of the KS Hamiltonian (20) at \( B = 0 \)

\[
H_{KS} = -\frac{1}{2m^*} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \varphi^2} \right] + \frac{1}{2m^*} \omega_0^2 r^2 + \frac{\partial}{\partial \varphi} \frac{e A_{XC,\varphi}(r)}{im^*} r + V_H(r) + \sum_\sigma V_{XC,\sigma}(r) |\sigma\rangle \langle \sigma|.
\]

(23)

with the potentials \((V_{XC,\sigma}, A_{XC,\varphi})\)

\[
H_{KS}|\varphi_{j,\sigma}\rangle = \varepsilon_{j,\sigma}|\varphi_{j,\sigma}\rangle.
\]

(24)

Due to the axial symmetry of the system the wavefunctions \( |\varphi_{j,\sigma}\rangle \) are also eigenfunctions of the angular momentum operator \( l|\varphi_{j,\sigma}\rangle = l_{j,\sigma}|\varphi_{j,\sigma}\rangle \).

Now let us assume that there is a KS Hamiltonian \( H'_{KS} \) with the potentials \((V'_{XC,\sigma}, A'_{XC,\varphi}) \neq (V_{XC,\sigma} + e_\sigma, A_{XC,\varphi})\) so that the KS single-particle wavefunctions are also eigenfunctions of \( H'_{KS} \)

\[
H'_{KS}|\varphi_{j,\sigma}\rangle = \varepsilon'_{j,\sigma}|\varphi_{j,\sigma}\rangle.
\]

(25)

Subtracting Eq. (24) from Eq. (25) delivers the constraint

\[
\Delta V_{XC,\sigma}(r) + l_{j,\sigma} \frac{e}{m^*} \frac{\Delta A_{XC,\varphi}(r)}{r} - \varepsilon'_{j,\sigma} + \varepsilon_{j,\sigma} = 0
\]

(26)
for the potential differences \( \Delta V_{XC,\sigma}(r) = V_{XC,\sigma}^{\prime}(r) - V_{XC,\sigma}(r) \) and \( \Delta A_{XC,\phi}(r) = A_{XC,\phi}^{\prime}(r) - A_{XC,\phi}(r) \). Eq. (26) has to be fulfilled for all wavefunctions \( |\varphi_{j,\sigma}\rangle \).

If at least two states with different angular momenta \( l_{j,\sigma} \neq l_{j',\sigma} \) are occupied we can conclude from

\[
\begin{align*}
    l_{j',\sigma} \left( \Delta V_{XC,\sigma}(r) + l_{j,\sigma} \frac{e}{m^*} \frac{\Delta A_{XC,\phi}(r)}{r} - \varepsilon_{j,\sigma} + \varepsilon_{j',\sigma} \right) \\
    -l_{j,\sigma} \left( \Delta V_{XC,\sigma}(r) + l_{j',\sigma} \frac{e}{m^*} \frac{\Delta A_{XC,\phi}(r)}{r} - \varepsilon_{j',\sigma} + \varepsilon_{j,\sigma} \right) = 0,
\end{align*}
\]

that the scalar potentials agree up to a constant \( \Delta V_{XC,\sigma}(r) = \text{const} \). Thus, \( \Delta A_{XC,\phi}(r) = \text{const} \cdot r \) immediately follows. As a consequence of finite XC vector potentials at \( B = 0 \) we derive \( \Delta A_{XC,\phi}(r) = 0 \). If there are also occupied states in the other spin direction we obtain \( \Delta V_{XC,-\sigma}(r) = \text{const} \). This result is in contradiction to \( (V_{XC,\sigma}^{\prime}, A_{XC,\phi}^{\prime}) \neq (V_{XC,\sigma} + c_{\sigma}, A_{XC,\phi}) \) and the uniqueness of XC potentials is proven.

The assumption of at least two occupied states with different angular momenta \( l_{j,\sigma} \neq l_{j',\sigma} \) in one spin direction is correct for the configurations considered in this paper. All other cases are more or less pathological:

- For \( N_\uparrow = N_\downarrow = 1 \) uniqueness cannot be proven except for the the case \( l_{1\uparrow} = l_{1\downarrow} = 0 \) (i.e. conventional DFT without paramagnetic current densities and vanishing \( A_{XC} \)).

- In the case of \( N \geq 2, l_{1\downarrow} = \ldots = l_{N_\downarrow} \) and \( l_{1\uparrow} = \ldots = l_{N_\uparrow} \), uniqueness cannot be guaranteed either. However, such a configuration should not be a GS in particular for larger particle numbers.

In general the XC potentials are overdetermined by Eq. (26). Therefore, the crucial aspect is the existence of appropriate XC potentials but not their uniqueness.

### B. Results for XC (vector) potentials

From the discussion of the uniqueness of XC potentials presented above immediately follows that we can analytically calculate the scalar and the vector potentials if we are able to derive the exact KS wavefunctions from \( (n_\sigma(r), j_\rho(r)) \). This can be accomplished for special systems.

The simplest conceivable configuration is the fully polarized two-electron \( \nu = 1 \)-quantum-Hall-droplet (QHD) with quantum numbers \( L = -1, S = 1, \) and \( S_z = -1 \). In particular the
confinement energy $\omega_h = 2/3\text{Ry}$ allows for a completely analytical solution.\textsuperscript{27} (For the rest of this subsection we denote energies in Ry and lengths in effective Bohr radii $a_0$.) According to Taut\textsuperscript{27} the separation of center-of-mass and relative motion delivers the GS wavefunction

$$\Psi(\mathbf{r}_1, \mathbf{r}_1) = \varphi_{\text{CM}}(|\mathbf{r}_1 + \mathbf{r}_2|/2)\varphi_{\text{rel}}(|\mathbf{r}_1 - \mathbf{r}_2|)$$

$$= C_{\text{CM}} e^{-R^2/3} C_{\text{rel}} r (1 + r/3) e^{-r^2/12}$$

(28)

($R = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$) and GS energy $8/3$. The constants are $C_{\text{CM}} = \sqrt{2/3\pi}$ and $C_{\text{rel}} = 1/\sqrt{2\pi (9\sqrt{6\pi} + 42)}$.

Using these results we can analytically calculate the GS density $n(r)$, the azimuthal component of the paramagnetic current density $j_{p,\varphi}(r)$, and the ($z$-component of the) vorticity

$$v(r) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{j_{p,\varphi}(r)}{n(r)} \right).$$

(29)

Now we are interested in the effective potentials which exactly reproduce the GS density combination $(n(r), j_{p,\varphi}(r))$. In this context we make use of the scaling relations (19) and (21) and restrict ourselves to the case $B = 0$.

Labeling states and occupation numbers by three indices which characterize the radial quantum number, the angular momentum and the spin state, the GS of the (spin-down) $\nu = 1$-QHD in the KS system is given by $\gamma_{0,0,-1} = \gamma_{0,-1,-1} = 1$. Then the relations between KS wavefunctions $\phi_{j,l,\sigma}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} R_{j,l}(\mathbf{r})$ and density (Fig. I(a))

$$n(\mathbf{r}) = \sum_{j,l,\sigma} \gamma_{j,l,\sigma} \phi_{j,l,\sigma}^{*}(\mathbf{r}) \phi_{j,l,\sigma}(\mathbf{r})$$

(30)

and paramagnetic current density (Fig. I(b))

$$j_{p,\varphi}(\mathbf{r}) = \frac{2\text{Ry}}{r} \sum_{j,l,\sigma} \gamma_{j,l,\sigma} l \phi_{j,l,\sigma}^{*}(\mathbf{r}) \phi_{j,l,\sigma}(\mathbf{r})$$

(31)

allow for the calculation of the vorticity (Fig. I(c)) and of the exact KS orbitals

$$R_{0,1}(\mathbf{r}) = \sqrt{\frac{\pi}{\text{Ry}}} r j_{p,\varphi}(r)$$

(32)

and

$$R_{0,0}(\mathbf{r}) = \sqrt{2\pi n(r) - R_{0,1}^2(\mathbf{r})}.$$  

(33)

The radial KS wavefunctions $R_{0,0}(\mathbf{r})$ und $R_{0,1}(\mathbf{r})$ are depicted in Fig. I(d).
Consequently, we can calculate the effective scalar single-particle potential up to a constant \( \varepsilon_{0,0,-1} \) (which is a KS energy) by inverting the KS Schrödinger equation for \( \phi_{0,0,-1}(r) \) (see Fig. II(e))

\[
V_{\text{eff}}(r) = r^2/9 + V_H(r) + V_{\text{XC}}(r) - \varepsilon_{0,0,-1} = \frac{\left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) \right] R_{0,0}(r)}{R_{0,0}(r)}.
\]  

(34)

In particular the KS equation for states with \( l = 0 \) only involves the scalar potential, but not the XC vector potential. As for given density \( n(r) \) the Hartree-potential \( V_H(r) \) (Fig. II(f)) is also known we can derive the exact scalar XC potential (Fig. II(g))

\[
V_{\text{XC}}(r) = \varepsilon_{0,0,-1} - r^2/9 - V_H(r) + \frac{\left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) \right] R_{0,0}(r)}{R_{0,0}(r)}
\]  

(35)

up to the gauge constant \( \varepsilon_{0,0,-1} \).

Finally we can find an approach to the XC vector potential (Fig. II(h)) by exploiting the KS equation for \( \phi_{0,-1,-1}(r) \). After solving the KS equation for \( A_{\text{XC},\phi}(r) \) and substituting the scalar XC potential we obtain

\[
e A_{\text{XC},\phi}(r) = \frac{1}{\text{Ry}} \frac{r}{2} \left( \frac{1}{r^2} - \frac{\left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) \right] R_{0,1}(r)}{R_{0,1}(r)} + \frac{\left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) \right] R_{0,0}(r)}{R_{0,0}(r)} + \varepsilon_{0,0,-1} - \varepsilon_{0,-1,-1} \right).
\]  

(36)

The singularity in the term \( 1/r^2 \) is eliminated by the second one as both terms together represent the kinetic energy density of the state \( \phi_{0,-1,-1}(r) \) which is finite at \( r = 0 \).

Now let us focus on the asymptotic of all relevant quantities. In the limit of large radii the asymptotic expansions of the densities and the vorticity are

\[
\lim_{r \to \infty} n(r) \to \frac{2\pi}{3} C_{CM}^2 C_{rel}^2 r^4 e^{-r^2/3}
\]  

(37)

\[
\lim_{r \to \infty} j_{\rho,\phi}(r) \to \frac{4\pi C_{CM}^2 C_{rel}^3 e^{-r^2/3}}{3(1/\text{Ry})}
\]  

(38)

\[
\lim_{r \to \infty} v(r) \to \text{Ry} \left( -24/r^4 + 54/r^5 \right)
\]  

(39)

Thus, the results for the radial wavefunctions \( R_{0,0}(r) \) and \( R_{0,1}(r) \) are

\[
\lim_{r \to \infty} R_{0,0}(r) \to 2\sqrt{2\pi} C_{CM} C_{rel} r e^{-r^2/6}
\]  

(40)

\[
\lim_{r \to \infty} R_{0,1}(r) \to \frac{2\pi C_{CM} C_{rel} r^2 e^{-r^2/6}}{\sqrt{3}}
\]  

(41)

The effective potential is parabolic in the limit of large \( r \)

\[
\lim_{r \to \infty} V_{\text{eff}}(r) \to \frac{1}{9} r^2 - \frac{4}{3} + \frac{3}{2r} + \frac{3}{4r^2}.
\]  

(42)
With the Hartree potential converging to zero

\[ \lim_{r \to \infty} V_H(r) \to \frac{4}{r} \]  

we assume that the XC potential vanishes in the limit \( r \to \infty \). This is achieved by a gauge constant \( \varepsilon_{0,0,-1} = 4/3 \)

\[ \lim_{r \to \infty} V_{XC}(r) \to -\frac{5}{2r} + \frac{3}{4r^2}. \]  

The asymptotic of the XC vector potential gives a constraint for \( \varepsilon_{0,-1,-1} = 2 \) if we do not want \( A_{XC,\varphi}(r) \) to diverge in the limit of large radii. (This is a reasonable requirement as we work at \( B = 0 \). A contribution \( A_{XC,\varphi}(r) = \frac{B'}{2} r \) would correspond to an external magnetic field \( B' = (0, 0, B') \).)

\[ \lim_{r \to \infty} A_{XC,\varphi}(r) \to \frac{1}{R_y} \left( -\frac{1}{4} - \frac{7}{8r} \right). \]  

Thus, the XC potentials \((V_{XC}(r), A_{XC,\varphi}(r))\) are uniquely determined.

Besides this fully analytic approach it is also possible to perform the calculation of XC potentials starting with GS densities from ED. Using numerical data for the densities allows us to study the dependence of the XC vector potential on the strength of the external confinement potential. In Fig. 2 we show the scalar XC potentials (up to a constant) and the XC vector potentials for \( \omega_0 \) in the range between 3 meV and 100 meV. In the context of the XC vector potentials we find a pronounced sensitivity to the precision of the densities at the edge of the dot. Because the \( A_{XC,\varphi}(r) \) is calculated as a difference of two (large) effective potentials, numerical errors are growing at the edge of the dot although 16 Landau levels were used in ED. However, the results from the bulk part of the QD are reliable and show a continuous dependence on the strength of \( \omega_0 \).

The second system for which we study scalar and vector XC potentials is the unpolarized four-electron system \((\nu = 2\text{-QHD})\) with \( S = 0, L = -2 \). In this case all GS densities are provided by ED using 335259 Slater determinants (see Fig. 3 for GS (paramagnetic current) densities at \( \omega_0 = 3 \text{ meV} \)). Concerning the mathematical structure of the KS equations it is similar to the \( \nu = 1 \) two-electron droplet: the \( \nu = 2 \) four-electron droplet can be regarded as a combination of two \( \nu = 1 \) two-electron droplets with different spin polarizations. Therefore the inversion of KS equations is completely analogous to Eqs. (30)-(36) if we use half of the GS density and paramagnetic density of the four-electron \( \nu = 2\text{-QHD} \).
Fig. 4 shows the results for scalar XC potentials (up to a constant) and vector XC potentials as a function of the strength of the confinement potential. Concerning the precision of the vector potentials we can repeat the same arguments as for the two-electron system, i.e. only the values from the bulk part of the QD are reliable. Similar to the \( \nu = 1 \)-droplet we find again a continuous dependence on \( \omega_0 \). Another aspect is the size of the amplitude of the XC vector potential which is even larger than for the two electron system (see Fig. 2). This represents a strong hint that current-induced corrections are for the \( \nu = 2 \)-QHD at least as important as for the \( \nu = 1 \)-QHD. This aspect is not considered in calculations relying on an interpolation of the type of Eq. (4) which neglects the influence of higher Landau levels.

V. VORTICITY-DEPENDENT XC ENERGY DENSITIES

In this Section we will deal with the vorticity dependence of XC energy densities extracted from the XC scalar and vector potentials above. The two parts comprise the methodology and the results for the four-electron \( \nu = 2 \) system.

A. Calculation of XC energy densities

The steps for extracting XC energy densities from XC potentials are analogous to Ref. 7, but generalized with respect to the vorticity dependence. Eqs. (12) and (13) provide the general relation between XC functional and XC potentials. To construct a relation between XC potentials and XC energy densities we apply the LVSDA (16) and obtain

\[
e A_{XC,\phi}(r) = -\frac{1}{n(r)} \frac{\partial}{\partial r} \left( n(r) \frac{\partial \varepsilon_{XC}}{\partial v}(r) \right) \quad (46)
\]

\[
V_{XC,\sigma}(r) = \varepsilon_{XC}(r) + n(r) \frac{\partial \varepsilon_{XC}}{\partial n_\sigma}(r) - e A_{XC,\phi}(r) \frac{j_{p,\phi}(r)}{n(r)}. \quad (47)
\]

We solve for \( \frac{\partial \varepsilon_{XC}}{\partial v}(r) \) and \( \frac{\partial \varepsilon_{XC}}{\partial n_\sigma}(r) \)

\[
\frac{\partial \varepsilon_{XC}}{\partial v}(r) = \frac{1}{n(r)} \left[ \int \frac{\partial^2 \varepsilon_{XC}}{\partial (r')^2} n(r') e A_{XC,\phi}(r') \right] \quad (48)
\]

\[
\frac{\partial \varepsilon_{XC}}{\partial n_\sigma}(r) = \frac{1}{n(r)} \left( \varepsilon_{XC}(r) + V_{XC,\sigma}(r) + e A_{XC,\phi}(r) \frac{j_{p,\phi}(r)}{n(r)} \right) \quad (49)
\]

considering the (physical) boundary condition

\[
\lim_{r \to \infty} n(r) \frac{\partial \varepsilon_{XC}}{\partial v}(r) = 0. \quad (50)
\]
The results are substituted in the derivative of the XC energy density as a function of the radius
\[
\frac{\partial \varepsilon_{XC}(r)}{\partial r} = \sum_{\sigma} \frac{\partial \varepsilon_{XC}}{\partial n_{\sigma}} \frac{\partial n_{\sigma}}{\partial r} + \frac{\partial \varepsilon_{XC}}{\partial v} \frac{\partial v}{\partial r}.
\] (51)

After some transformations we arrive at a linear differential equation (DEQ)
\[
\frac{\partial \varepsilon_{XC}(r)}{\partial r} + \frac{\partial \log n}{\partial r} \varepsilon_{XC}(r) = I(r)
\] (52)

with the inhomogeneity
\[
I(r) = \frac{1}{n(r)} \sum_{\sigma} (V_{XC,\sigma}(r) + c_{\sigma}) \frac{\partial n_{\sigma}}{\partial r}(r) + eA_{XC,\varphi}(r) \frac{\partial \log n}{\partial r}(r)
\]
\[+ \frac{1}{n(r)} \frac{\partial v}{\partial r}(r) \left[ \int_{r}^{\infty} dr' n(r') eA_{XC,\varphi}(r') \right].
\] (53)

which contains all the information about the dependence on the spin densities and the vorticity. In Eq. (53) we take into account that the gauge constants \(c_{\sigma}\) of the scalar potentials are not known from the previous step. They will be calculated later. The solution of the homogeneous part of DEQ (52) is given by \(\varepsilon_{XC}^{\text{hom}}(r) = \alpha/n(r)\), a special solution can be calculated using the ansatz \(\varepsilon_{XC}^{\text{spec}}(r) = \beta(r)/n(r)\). The function \(\beta(r)\) follows from an elementary DEQ
\[
\frac{\partial \beta}{\partial r}(r) = n(r)I(r),
\] (54)

whose solution is
\[
\beta(r) = \int_{0}^{r} dr' n(r')I(r') - \beta(0).
\] (55)

Thus the general solution of DEQ (52) is
\[
\varepsilon_{XC}(r) = \varepsilon_{XC}^{\text{hom}}(r) + \varepsilon_{XC}^{\text{spec}}(r) = \frac{\alpha - \beta(0)}{n(r)} + \frac{1}{n(r)} \int_{0}^{r} dr' n(r')I(r').
\] (56)

After substituting the inhomogeneity the result reads
\[
\varepsilon_{XC}(r) = \frac{\alpha - \beta(0) - n_{\sigma}(0) \sum_{\sigma} c_{\sigma} + \sum_{\sigma} c_{\sigma} \frac{n_{\sigma}(r)}{n(r)} + \frac{1}{n(r)} \int_{0}^{r} dr' \left\{ \sum_{\sigma} V_{XC,\sigma}(r') \frac{\partial n_{\sigma}}{\partial r'}(r') + eA_{XC,\varphi}(r') \frac{\partial \log n}{\partial r'}(r') + \frac{\partial v}{\partial r'}(r') \left[ \int_{r'}^{\infty} dr'' n(r'') eA_{XC,\varphi}(r'') \right] \right\} \right. \]
\[+ eA_{XC,\varphi}(r') j_{p,\varphi}(r') \frac{\partial \log n}{\partial r'}(r') + \frac{\partial v}{\partial r'}(r') \left[ \int_{r'}^{\infty} dr'' n(r'') eA_{XC,\varphi}(r'') \right] \].
\] (57)

With the modulus of the XC energy being finite in LVSDA
\[
|E_{XC}[n_{\sigma}, v]| \approx \left| \int dr n(r)\varepsilon_{XC}(r) \right| = \int dr n(r)|\varepsilon_{XC}(r)| < \infty
\] (58)
we choose $\alpha - \beta(0) - n_\sigma(0) \sum_\sigma c_\sigma = 0$ thus avoiding any divergent contributions. Consequently the analytical solution of (52) satisfying the physical boundary conditions is

$$\varepsilon_{\text{XC}}(r) = \sum_\sigma c_\sigma n_\sigma(r) + \frac{1}{n(r)} \int_0^r \left\{ \sum_\sigma V_{\text{XC},\sigma}(r') \frac{\partial n_\sigma}{\partial r'}(r') + e A_{\text{XC},\sigma}(r') j_{p,\sigma}(r') \frac{\partial \log n}{\partial r'}(r') \right\} + \frac{\partial v}{\partial r'}(r') \left[ \int_{r'}^\infty \log n(r'') e A_{\text{XC},\sigma}(r'') \right] \right\}.$$  \hspace{1cm} (59)

The last step is the calculation of the gauge constants $c_\sigma$ of the scalar potentials. One condition which has not been used yet is the agreement of the DFT GS energy and the exact GS energy. If we eliminate $V_{\text{XC},\sigma}(r)$ in Eq. (15) and write it in a modified form

$$E_{\text{GZ}} = \sum_{j,\sigma} \gamma_{j,\sigma} \int \text{dr} \varphi_{j,\sigma}^*(r) \left( \frac{1}{2m^*} (p + e A(r))^2 + V_\sigma(r) \right) \varphi_{j,\sigma}(r) + \frac{1}{2} \int \text{dr} V_\text{Hi}(r)n(r) + E_{\text{XC}}[n_\sigma, v]$$  \hspace{1cm} (60)

we can calculate the (exact!) XC energy $E_{\text{XC}}[n_\sigma, v]$ for GS densities: the KS wavefunctions are known from the selfconsistent solution of the KS equations. Thus the expectation values $\int \text{dr} \varphi_{j,\sigma}^*(r) \left( \frac{1}{2m^*} (p + e A(r))^2 + V_\sigma(r) \right) \varphi_{j,\sigma}(r)$ of the non-interacting system can be calculated. The Coulomb energy and the GS-energy are uniquely determined by the interacting system. On the other hand the XC energy in LVSDA is given by

$$E_{\text{XC}}[n_\sigma, v] \approx \int \text{dr} n(r) \varepsilon_{\text{XC}}(r)$$

$$= \sum_\sigma c_\sigma N_\sigma + \int_{r=0}^\infty \text{dr} \int_0^r \left\{ \sum_\sigma V_{\text{XC},\sigma}(r') \frac{\partial n_\sigma}{\partial r'}(r') + e A_{\text{XC},\sigma}(r') \times \right.$$  \hspace{1cm} \left. \times j_{p,\sigma}(r') \frac{\partial \log n}{\partial r'}(r') + \frac{\partial v}{\partial r'}(r') \left[ \int_{r'}^\infty \log n(r'') e A_{\text{XC},\sigma}(r'') \right] \right\}$$  \hspace{1cm} (61)

what makes $\sum_\sigma c_\sigma N_\sigma$ accessible. In the case of unpolarized systems $c := c_\uparrow = c_\downarrow$, and for full polarization the constant $c_\sigma$ of the unoccupied spin direction is irrelevant (as the corresponding $N_\sigma = 0$). Consequently, the results for the XC energy density are unique. For partially polarized systems uniqueness of the results can be achieved by additionally demanding asymptotic agreement of $V_{\text{XC},\sigma}(r)$ for finite systems$^{26}$

$$\lim_{r \to \infty} V_{\text{XC},\uparrow}(r) = \lim_{r \to \infty} V_{\text{XC},\downarrow}(r).$$  \hspace{1cm} (62)

As a result of the inversion of the LVSDA formalism we obtain the XC energy density as a function of the radius. After eliminating the radius using the spin densities $n_\sigma(r)$ and vorticity $v(r)$ or alternatively $r_\sigma(r), \xi(r), v(r)$ we arrive at the representation of the XC energy density as a function of $(r_\sigma, \xi, v)$. 

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B. Results for vorticity-dependent XC energy densities

In this Section we summarize the numerical results for the extracted XC energy densities. Because of the high contribution of self-interaction in the two-electron system only the four-electron $\nu = 2$-QHD can be used for the derivation of vorticity-dependent XC energy densities. After solving the DEQ (52) for different confinement energies $\omega_0$ we get a set of $\varepsilon_{XC}$ for different $r_s$, $\nu$, and $\xi = 0$ (no polarization). The results for different vorticities are shown in Fig. 5 as a function of $r_s$ together with the pure TC parameterization, TC combined with LWM, and TC combined with FO. Whereas the LWM and FO parameterizations do not deviate very much from the pure TC data which does not consider any current-induced effects, the extracted XC energy densities exhibit a pronounced dependence on the vorticity. In particular, the curve of extracted $\varepsilon_{XC}$ starts for small $r_s$ below the reference curves, crosses it and finally lies above it. Moreover, the crossing wanders to larger $r_s$ if we decrease the vorticity (see Fig. 5(a)-(f)).

Although the interpretation of these large deviations from the standard parameterizations is difficult as the data set is very small our results give rise to the question if the vorticity dependence of XC energy densities can be treated in the frame of LVSDA. There might be also non-local effects from paramagnetic currents which cannot be considered in this approach. However, in any case it is necessary to reexamine the vorticity-dependence of $\varepsilon_{XC}$ with focus on Landau level mixing and arbitrary densities.

VI. SUMMARY

In this paper we presented a new approach to study scalar XC potentials and XC vector potentials of current-carrying ground states in axially symmetric, parabolic quantum dots. Starting from exact ground states densities and paramagnetic current densities we analytically calculated the XC potentials of the two-electron $\nu = 1$-droplet and the four-electron $\nu = 2$-droplet and studied them as a function of the strength of the confinement potential. In both systems the XC vector potentials are of the same order of magnitude which shows the importance of this current-induced effect even for higher filling factors. This result is not taken into account in the interpolation introduced by Rasolt and Perrot.

The second step involved the extraction of vorticity-dependent XC energy densities.
The effect of the vorticity is far more pronounced than predicted by Rasolt and Perrot\textsuperscript{18}, Levesque, Weis, and MacDonald\textsuperscript{11} and Fano and Ortolani\textsuperscript{12}. A possible reason for this behavior is the assumption that the influence of current densities is only relevant for strong magnetic fields when the local filling factor $f$ is less than one. This is the restriction which enters the derivations of the parameterizations in literature. However, our results point out that a new approach to current- or vorticity-dependent XC energy densities is required which also comprise the effects of Landau level mixing.

VII. ACKNOWLEDGEMENT

A. W. thanks the the RRZE Erlangen and the DFG (Ro 522/19-1).

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FIG. 1: Analytical results for the two-electron $\nu = 1$-QHD with confinement energy $2/3$ Ry.
Figs. (a)-(h) depict the GS density, the paramagnetic GS density, the vorticity, the radial KS wavefunctions, the effective scalar potential, the Hartree potential, the scalar XC potential, and the XC vector potential.

FIG. 2: Scalar XC potentials (a) and (c) and XC vector potentials (b) and (d) of the two-electron $\nu = 1$-QHD as a function of the strength of the confinement potential. In (a) and (b) the results for $\omega_0 = 3$ meV - 10 meV (stepsize 1 meV) are shown, in (c) and (d) results for $\omega_0 = 10$ meV - 100 meV (stepsize 10 meV). The arrows indicate curves corresponding to increasing confinement potentials.

FIG. 3: GS density (a) and GS paramagnetic current density (b) of a four-electron $\nu = 2$-QHD with confinement energy 3 meV.
FIG. 4: Scalar XC potentials (a) and (c) and XC vector potentials (b) and (d) of the four-electron \( \nu = 2\)-QHD as a function of the strength of the confinement potential. In (a) and (b) the results for \( \omega_0 = 3 \text{meV} - 10 \text{meV} \) (stepsize 1 meV) are shown, in (c) and (d) results for \( \omega_0 = 10 \text{meV} - 100 \text{meV} \) (stepsize 10 meV). The arrows indicate curves corresponding to increasing confinement potentials.

FIG. 5: Vorticity-dependent XC energy densities extracted from the four-electron \( \nu = 2\)-QHD. (a)-(f) show the XC energy densities as a function of \( r_s \) for different vorticities.
Fig. 1, Wensauer, PRB (2 columns)
Fig. 2, Wensauer, PRB
Fig. 3, Wensauer, PRB
Fig. 4, Wensauer, PRB
Fig. 5, Wensauer, PRB (2 columns)