

Exchange-energy functionals for finite two-dimensional systems

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(Dated: January 7, 2014)

Implicit and explicit density functionals for the exchange energy in finite two-dimensional systems are developed following the approach of Becke and Roussel [Phys. Rev. A **39**, 3761 (1989)]. Excellent agreement for the exchange-hole potentials and exchange energies is found when compared with the exact-exchange reference data for the two-dimensional uniform electron gas and few-electron quantum dots, respectively. Thereby, this work significantly improves the availability of approximate density functionals for dealing with electrons in quasi-two-dimensional structures, which have various applications in semiconductor nanotechnology.

I. INTRODUCTION

Since the advent of density-functional theory (DFT)¹ much effort went in the development of approximate functionals for the exchange and correlation energies. Most of this work focused on three-dimensional (3D) systems, where considerable advances beyond the commonly used local (spin) density approximation (L(S)DA) were achieved by generalized gradient approximations, orbital functionals, and hybrid functionals.² For two-dimensional (2D) and low-dimensional systems in general, such efforts have been relatively scarce, partly due to the lack of direct applications before the rapid developments in semiconductor technology in the early 1980s. Presently, the variety of relevant low-dimensional systems is very large, including, e.g., modulated semiconductor layers and surfaces, quantum-Hall systems, spintronic devices, and quantum dots (QDs). The research of electronic, optical, and magnetic properties of low-dimensional structures form already a significant contribution to condensed-matter and materials physics.

Semiconductor QDs are finite quasi-2D electron systems confined typically in GaAs/AlGaAs heterostructures.³ Due to their controllability in size, shape, and number of confined electrons, they have an increasing number of potential applications in quantum-information technology. Within the DFT approach, QDs are most commonly treated using the 2D-LSDA exchange functional derived in 1977 by Rajagopal and Kimball,⁴ which is then combined with the 2D-LSDA correlation parametrized first by Tanatar and Ceperley⁵ and later, for the complete range of collinear spin polarization, by Attaccalite and co-workers.⁶ Despite the relatively good performance of LSDA with respect to, e.g., quantum Monte Carlo calculations,⁷ there is lack of accurate 2D density functionals. Moreover, previous studies have shown that functionals developed for 3D systems perform poorly when applied to 2D systems.^{8,9,10} The exact-exchange functional employed within the optimized effective potential method, which automatically conforms to various dimensionalities, seems an appealing alterna-

tive, and it has recently been applied to QDs.¹¹ In that method, however, the development of approximations for the correlation energies compatible with exact-exchange energies remains a complicated problem.

In this work we present an *ab initio* derivation of new exchange functionals for finite 2D systems in the framework proposed by Becke and Roussel.¹² We calculate the cylindrical average of the exchange hole for a single-electron wave function of a 2D harmonic oscillator, and use it as a basis of an averaged exchange hole for a generic N -electron system. By utilizing the short-range behavior of the exchange hole we are able to derive one implicit and one explicit density functional for the exchange energy. Both functionals lead to accurate exchange-hole potentials and exchange energies when compared with the reference data of the 2D electron gas (2DEG) and few-electron QDs. The new exchange-energy functionals constitute a natural basis for developing corresponding correlation-energy functionals.

II. FORMALISM

Within the Kohn-Sham (KS) method of spin-DFT,¹³ the ground state energy and spin densities $\rho_{\uparrow}(\mathbf{r})$ and $\rho_{\downarrow}(\mathbf{r})$ of a system of $N = N_{\uparrow} + N_{\downarrow}$ interacting electrons are determined. The total energy, which is minimized to obtain the ground-state energy, is written as a functional of the spin densities (in Hartree atomic units)

$$E_v[\rho_{\uparrow}, \rho_{\downarrow}] = T_s[\rho_{\uparrow}, \rho_{\downarrow}] + E_H[\rho] + E_{xc}[\rho_{\uparrow}, \rho_{\downarrow}] + \sum_{\sigma=\uparrow,\downarrow} \int d\mathbf{r} v_{\sigma}(\mathbf{r}) \rho_{\sigma}(\mathbf{r}), \quad (1)$$

where $T_s[\rho_{\uparrow}, \rho_{\downarrow}]$ is the KS kinetic energy functional, $v_{\sigma}(\mathbf{r})$ is the external (local) scalar potential acting upon the interacting system, $E_H[\rho]$ is the classical electrostatic or Hartree energy of the total charge density $\rho(\mathbf{r}) = \rho_{\uparrow}(\mathbf{r}) + \rho_{\downarrow}(\mathbf{r})$, and $E_{xc}[\rho_{\uparrow}, \rho_{\downarrow}]$ is the exchange-correlation energy functional. The latter can be further decomposed into

the exchange and correlation parts as

$$E_{xc}[\rho_\uparrow, \rho_\downarrow] = E_x[\rho_\uparrow, \rho_\downarrow] + E_c[\rho_\uparrow, \rho_\downarrow]. \quad (2)$$

The exchange-energy functional can be expressed as

$$E_x[\rho_\uparrow, \rho_\downarrow] = -\frac{1}{2} \sum_{\sigma=\uparrow, \downarrow} \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{\rho_\sigma(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|} h_x^\sigma(\mathbf{r}_1, \mathbf{r}_2), \quad (3)$$

where, within the restriction that the noninteracting ground state is nondegenerate and hence takes the form of a single Slater determinant, the exchange-hole (or Fermi-hole) function h_x^σ is given by

$$h_x^\sigma(\mathbf{r}_1, \mathbf{r}_2) = \frac{|\sum_{k=1}^{N_\sigma} \psi_{k,\sigma}^*(\mathbf{r}_1) \psi_{k,\sigma}(\mathbf{r}_2)|^2}{\rho_\sigma(\mathbf{r}_1)}. \quad (4)$$

The sum in the numerator is the one-body spin-density matrix of the Slater determinant constructed from the KS orbitals, $\psi_{k,\sigma}$. The exchange-hole function as defined here is always positive. Moreover, integrating this function over $\mathbf{r}_2$ yields

$$\int d\mathbf{r}_2 h_x^\sigma(\mathbf{r}_1, \mathbf{r}_2) = 1. \quad (5)$$

This exact property reflects the fact that around an electron with spin σ at $\mathbf{r}_1$, other electrons of the same spin are less likely to be found as a consequence of the Pauli principle. From Eq. (3) it is clear that to evaluate the exchange energy in 2D, we just need to know the *cylindrical* average w.r.t. $\mathbf{s} = \mathbf{r}_2 - \mathbf{r}_1$ of the exchange-hole around $\mathbf{r}_1$. Expressing the exchange-hole by its Taylor expansion

$$h_x^\sigma(\mathbf{r}_1, \mathbf{r}_2 = \mathbf{r}_1 + \mathbf{s}) = \exp(\mathbf{s} \cdot \nabla') h_x^\sigma(\mathbf{r}_1, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_1}, \quad (6)$$

the cylindrical average is defined as

$$\bar{h}_x^\sigma(\mathbf{r}_1, s) = \frac{1}{2\pi} \int_0^{2\pi} d\phi_s \exp(\mathbf{s} \cdot \nabla') h_x^\sigma(\mathbf{r}_1, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_1}. \quad (7)$$

The short-range behavior with respect to s is then obtained as

$$\begin{aligned} \bar{h}_x^\sigma(\mathbf{r}_1, s) &= \rho_\sigma(\mathbf{r}_1) + \frac{s^2}{4} \nabla'^2 h_x^\sigma(\mathbf{r}_1, \mathbf{r}')|_{\mathbf{r}'=\mathbf{r}_1} + \dots \\ &= \rho_\sigma(\mathbf{r}_1) + s^2 C_x^\sigma(\mathbf{r}_1) + \dots, \end{aligned} \quad (8)$$

where C_x^σ is the so-called local curvature of the exchange hole around the given reference point $\mathbf{r}_1$. This function can be expressed as^{12,14,15}

$$C_x^\sigma = \frac{1}{4} \left[\nabla^2 \rho_\sigma - 2\tau_\sigma + \frac{1}{2} \frac{(\nabla \rho_\sigma)^2}{\rho_\sigma} + 2 \frac{\mathbf{j}_{p,\sigma}^2}{\rho_\sigma} \right], \quad (9)$$

where

$$\tau_\sigma = \sum_{k=1}^{N_\sigma} |\nabla \psi_{k,\sigma}|^2 \quad (10)$$

is (twice) the spin-dependent kinetic-energy density, and

$$\mathbf{j}_{p,\sigma} = \frac{1}{2i} \sum_{k=1}^{N_\sigma} [\psi_{k,\sigma}^* (\nabla \psi_{k,\sigma}) - (\nabla \psi_{k,\sigma}^*) \psi_{k,\sigma}] \quad (11)$$

is the spin-dependent paramagnetic current density. Both τ_σ and $\mathbf{j}_{p,\sigma}$ depend explicitly on the KS orbitals. Thus the expression in Eq. (9) has an implicit dependence on the spin-densities ρ_σ . Now, once we can provide an approximation for $\bar{h}_x^\sigma(\mathbf{r}_1, s)$ satisfying the normalization condition of Eq. (5), we can compute the exchange-hole potential

$$U_x^\sigma(\mathbf{r}_1) = -2\pi \int_0^\infty ds \bar{h}_x^\sigma(\mathbf{r}_1, s), \quad (12)$$

and finally the exchange energy

$$E_x[\rho_\uparrow, \rho_\downarrow] = \frac{1}{2} \sum_\sigma \int d\mathbf{r}_1 \rho_\sigma(\mathbf{r}_1) U_x^\sigma(\mathbf{r}_1). \quad (13)$$

III. EXCHANGE-ENERGY FUNCTIONAL

A. Model

As the basis of our exchange model we consider the ground state single-electron wave function of a 2D harmonic oscillator

$$\psi_\sigma(\mathbf{r}) = \frac{\alpha}{\sqrt{\pi}} \exp\left[-\frac{\alpha^2 r^2}{2}\right], \quad (14)$$

which is normalized for each $\alpha \neq 0$. We point out that the harmonic (parabolic) approximation for the confining potential is the most common choice when modeling QDs fabricated in semiconductor heterostructures.³ The exact exchange-hole function (4) for the single-particle case becomes $h_x^\sigma(\mathbf{r}_1, \mathbf{r}_2) = \psi_\sigma^*(\mathbf{r}_2) \psi_\sigma(\mathbf{r}_2) = \rho_\sigma(\mathbf{r}_2)$. Setting $\mathbf{r}_1 = \mathbf{r}$ and $\mathbf{r}_2 = \mathbf{r} + \mathbf{s}$, we calculate the cylindrical average as

$$\begin{aligned} \bar{h}_x^\sigma(\mathbf{r}, s) &= \frac{1}{2\pi} \int_0^{2\pi} d\phi_s \rho_\sigma(\mathbf{r} + \mathbf{s}) \\ &= \frac{\alpha^2}{2\pi^2} \exp[-\alpha^2 (r^2 + s^2)] \times \\ &\quad \times \int_0^{2\pi} d\phi_s \exp[-2\alpha^2 r s \cos(\phi)] \\ &= \frac{\alpha^2}{\pi} \exp[-\alpha^2 (r^2 + s^2)] I_0(2\alpha^2 r s), \end{aligned} \quad (15)$$

where $I_0(x)$ is the zeroth order modified Bessel function of the first kind (note that $I_0(0) = 1$). Performing the integral in Eq. (12) yields

$$U_x^\sigma(r) = -|\alpha| \sqrt{\pi} \exp[-\alpha^2 r^2/2] I_0(\alpha^2 r^2/2) \quad (16)$$

for the exchange-hole potential. Since the modified Bessel function has the limit property $I_0(x) \rightarrow \exp(x)/\sqrt{2\pi x}$, when $x \rightarrow +\infty$ with $x \in \mathbb{R}$, we immediately find $\lim_{r \rightarrow \infty} U_x^\sigma(r) = -1/r$.

B. Implicit density functional

At this point, we adopt the strategy of Becke and Rous-
sel¹² and elevate expression (15) as a general model for
the averaged exchange hole of a generic N -electron 2D
system. In order to locally reproduce the short-range
behavior of the exchange hole, we replace α^2 and r^2 by
functions of r , respectively, i.e., $\alpha^2 \rightarrow a(r)$ and $r^2 \rightarrow b(r)$.
Now we can rewrite Eq. (15) as

$$\bar{h}_x^\sigma(a, b; s) = \frac{a}{\pi} \exp[-a(b + s^2)] I_0(2a\sqrt{b}s). \quad (17)$$

This model satisfies, through its original definitions,
 $\bar{h}_x^\sigma(a, b; s) \geq 0$ and the unit normalization condition of
Eq. (5). From the second-order term in the Taylor ex-
pansion in Eq. (8) we obtain

$$(y - 1) \exp(y) = \frac{C_x^\sigma}{\pi \rho_\sigma^2}, \quad (18)$$

where $y := ab$. The zeroth-order term gives

$$a = \pi \rho_\sigma \exp(y), \quad (19)$$

and hence we get

$$b = \frac{y}{\pi \rho_\sigma} \exp(-y). \quad (20)$$

As the result, Eqs. (18)-(20) determine, together with
Eqs. (17), (12) and (13), an implicit density functional.
This completes the derivation of our first approximation
to the exchange-energy functional.

C. Explicit density functional

We now show that one can also derive an explicit
density functional. For that purpose, we consider the
2DEG where the derivatives in Eq. (9) are zero, i.e.,
 $\nabla^2 \rho_\sigma = 0$ and $\nabla \rho_\sigma = 0$, and we take the known ex-
pression for the kinetic-energy density of the 2DEG,¹⁶
 $\tau_\sigma = 2\pi \rho_\sigma^2 + \mathbf{j}_{p,\sigma}^2 / \rho_\sigma$. Note that the current-dependent
term in Eq. (9) cancels the current-contribution to the
kinetic energy, leading to the expected result that the
exchange energy of a uniform electron gas does not de-
pend on the current density.²² These simplifications lead
to $y = 0$, $b = 0$, and $a = \pi \rho_\sigma$, so that the averaged
exchange-hole function becomes

$$\bar{h}_x^\sigma(s) = \rho_\sigma \exp[-\pi \rho_\sigma s^2], \quad (21)$$

and the exchange-hole potential is now given by $U_x^\sigma[\rho_\sigma] =$
 $-\pi \rho_\sigma^{1/2}$, which is an explicit functional of the spin-
density. Defining the 2D density parameter $r_s = 1/\sqrt{\pi \rho}$,
where $\rho = \rho_\uparrow + \rho_\downarrow$ is the total density, and the polar-
ization $\xi = (\rho_\uparrow - \rho_\downarrow)/\rho$, the total exchange energy per
particle becomes

$$\epsilon_x[r_s, \xi] = -\frac{\sqrt{\pi}}{4\sqrt{2}r_s} \left[(1 + \xi)^{3/2} + (1 - \xi)^{3/2} \right]. \quad (22)$$

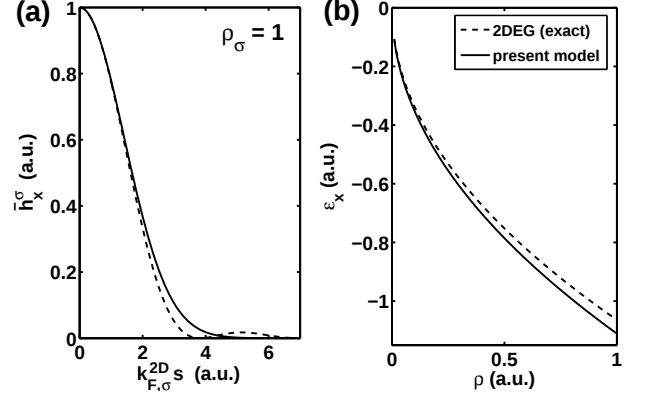


FIG. 1: Exchange hole (a) and the exchange energy per particle (b) for two-dimensional electron gas ($\xi = 0$) in the exact expression (dashed line) and in the present model (solid line).

This expression can be compared with the exact 2DEG
result⁴ widely applied to finite systems in terms of the
LSDA,

$$\epsilon_x^{2DEG}[r_s, \xi] = -\frac{2\sqrt{2}}{3\pi r_s} \left[(1 + \xi)^{3/2} + (1 - \xi)^{3/2} \right]. \quad (23)$$

Interestingly, the only difference between these two ex-
pressions for ϵ_x is in the prefactor, which is about $\sim 4.4\%$
smaller in the latter. Concluding, Eq. (22) can be used as
an explicit density functional in the LSDA fashion when
applied to inhomogeneous systems.

IV. NUMERICAL RESULTS

A. Two-dimensional electron gas

Besides the exchange energies, it is interesting to com-
pare the averaged exchange hole given in Eq. (21) with
the exact exchange hole of the 2DEG. Following the
derivation of Gori-Giorgi and co-workers¹⁷ for the pair-
distribution functions of the 2DEG, we find

$$\bar{h}_{x,\sigma}^{2DEG}(s) = 4\rho_\sigma \frac{J_1^2(k_{F,\sigma}^{2D} s)}{(k_{F,\sigma}^{2D})^2}, \quad (24)$$

where $k_{F,\sigma}^{2D} = (4\pi\rho_\sigma)^{1/2}$ is the Fermi momentum (for spin
 σ) in 2D, and J_1 is the ordinary Bessel function of the first
order. In Fig. 1(a) we compare the exchange holes with a
fixed spin-density $\rho_\sigma = 1$ between our model (solid line)
and the exact 2DEG result (dashed line) and find a good
qualitative agreement. Figure 1(b) demonstrates the dif-
ferences in the exchange energies (per particle) given in
Eqs. (22) and (23) as a function of the total density (for
 $\xi = 0$).

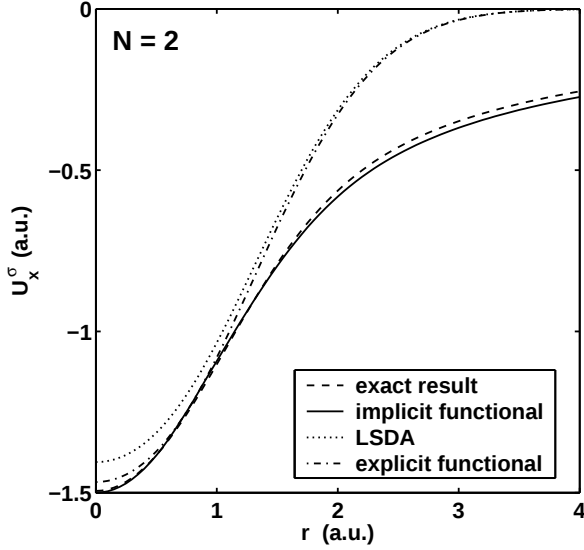


FIG. 2: Exchange-hole potential of a two-electron quantum dot calculated exactly (dashed line) and using the implicit density functional of Sec. IIIB (solid line), standard LSDA (dotted line), and the explicit density functional of Sec. IIIC (dash-dotted line). The analytic density and orbitals are used as input for the model and LSDA.

B. Few-electron quantum dots

Next, we consider the smallest nontrivial QD consisting of two electrons. The Hamiltonian is given by

$$H = \sum_{j=1}^2 \left(-\frac{1}{2} \nabla_j^2 + \frac{1}{2} \omega_0^2 r_j^2 \right) + \frac{1}{|\mathbf{r}_2 - \mathbf{r}_1|}, \quad (25)$$

where we set the strength of the harmonic confinement to $\omega_0 = 1$. In this case the ground-state (singlet) wave function is known analytically,¹⁸ and the total density can be expressed as¹⁹

$$\rho(r) = \frac{4}{\pi(\sqrt{2\pi} + 3)} \left\{ e^{-r^2} (1 + r^2/2) + \frac{1}{2} \sqrt{\pi} e^{-3r^2/2} \times \left[I_0(r^2/2) + r^2 I_0(r^2/2) + r^2 I_1(r^2/2) \right] \right\}. \quad (26)$$

The exact (spin) exchange-hole potential is simply

$$U_{N=2}^{x,\sigma}(\mathbf{r}) = - \int d\mathbf{r}' \frac{\rho_{\sigma}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (27)$$

In Fig. 2 we compare the exact exchange-hole potential (dashed line) to the result of our implicit density functional (solid line) and find an excellent agreement. We note that in the range $0.75 \lesssim r \lesssim 0.85$ the parameter y is not solvable from Eq. (18). Therefore, we set y to zero in this region. This corresponds to the 2DEG result discussed above, i.e., we perform a well-valid LSDA-type approximation in this small regime. The dash-dotted line shows the result of our explicit density functional which

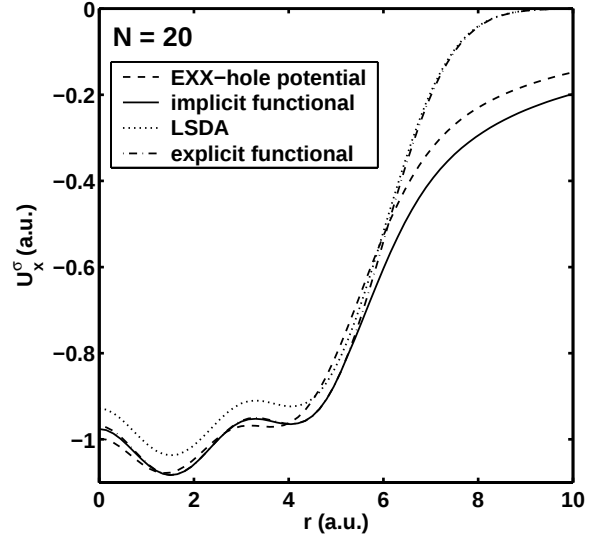


FIG. 3: Similar to Fig. 2 but for 20 electrons. The exact-exchange result was calculated using the KLI approximation. Self-consistent (correlation included) density and orbitals from the standard LSDA are used as input for our functionals and LSDA exchange.

TABLE I: Exchange energies for different number of electrons calculated using the exact exchange, the implicit density functional of Sec. IIIB, standard LSDA, and the the explicit density functional of Sec. IIIC. For $N > 2$ the EXX result was calculated within the KLI approximation, and as input for our functionals and LSDA exchange we used the self-consistent density and orbitals from the standard LSDA.

N	EXX	Implicit functional	LSDA	Explicit functional
2	-1.0839	-1.0836	-0.983	-1.026
6	-2.229	-2.284	-2.130	-2.223
12	-4.890	-5.059	-4.763	-4.972
20	-8.781	-9.124	-8.632	-9.012

is identical to the implicit functional in the 2DEG limit. This density functional has the wrong asymptotic behavior, but it is considerably closer to the exact result than that of the standard LSDA of Eq. (23) (dotted line).

In Fig. 3 we show the exchange-hole potentials for a 20-electron QD with $\omega_0 = 0.42168$, corresponding to a typical confinement of 5 meV in the effective-mass approximation when modeling QDs in GaAs.³ The exact-exchange (EXX) result (dashed line) is calculated in the Krieger-Li-Iafrate (KLI) approach²⁰ within spin-DFT implemented in the *octopus* real-space code.²¹ Again, we find a very good agreement between the EXX and the results of our implicit density functional (solid line). Also, the explicit functional (dash-dotted line) reproduces the EXX curve at small r by a good accuracy, whereas the LSDA curve (dotted line) lies considerably above the EXX result in this regime. However, as seen in Table I the LSDA exchange energy is rather accurate. This is

due to the fact that the difference in the EXX and LSDA curves at small r is compensated at $5 \lesssim r \lesssim 6$, where the LSDA curve lies below the EXX one. In smaller QDs instead, the table shows that our exchange-energy functionals are superior to the LSDA also in terms of the exchange energies, i.e., not only in terms of the exchange-hole potentials.

V. CONCLUSIONS

To conclude, we have provided new exchange functionals for finite two-dimensional systems that, until now, have lacked accurate functionals beyond the local density approximations. We have presented *ab initio* derivation of both implicit and explicit exchange functionals that significantly improve the exchange-hole potentials

and exchange energies of few-electron two-dimensional quantum dots. Our results also suggest that accurate approximations for the correlation energy functional can be developed analogously.

Acknowledgments

We thank S. Kurth, A. Castro, and R. Hammerling for useful discussions and help in the numerical calculations. This work was supported by the Deutsche Forschungsgemeinschaft, the EU's Sixth Framework Programme through the Nanoquanta Network of Excellence (No. NMP4-CT-2004-500198), the Academy of Finland, and the Finnish Academy of Science and Letters through the Viljo, Yrjö and Kalle Väisälä Foundation.

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²² A uniform current in a homogeneous electron gas can be viewed as being generated by a transformation to a moving Galilei frame. Since the electron-electron Coulomb interaction is the same in any Galilei frame, the exchange energy cannot depend on the Galilei frame and, hence, must be current-independent.