Constraints of reduced density-matrix functional theory for the two-dimensional homogeneous electron gas

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Reduced density-matrix functional theory (RDMFT) has become an appealing alternative to density-functional theory to describe electronic properties of highly-correlated systems. Here we derive exact conditions for the suitability of RDMFT to describe the two-dimensional homogeneous electron gas, which is the base system for, e.g., semiconductor quantum dots and quantum Hall devices. Following the method of Cioslowski and Pernal [J. Chem. Phys. 111, 3396 (1999)] we focus on the properties of power functionals of the form \( f(n, n') = (nn')^\alpha \) for the scaling function in the exchange-correlation energy. We show that in order to have stable and analytic solutions, and for \( f \) to satisfy the homogeneous scaling constraint, the power is restricted to \( 1/4 \leq \alpha \leq 3/4 \). Applying a reasonable ansatz for the momentum distribution and the lower bound for the exchange-correlation energy tightens the physical regime further to \( 0.64 \lesssim \alpha \lesssim 0.75 \).

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I. INTRODUCTION

Reduced density-matrix functional theory (RDMFT) is an appealing method to tackle the many-particle problem through the one-body reduced density matrix (1-RDM), which is obtained by integrating out all but two spatial coordinates in the many-body wave function. Computationally, RDMFT is significantly more demanding than the more common density-functional theory (DFT) whose key quantity is the single-particle density, i.e., the diagonal of the 1-RDM. On the other hand, RDMFT has been shown to improve considerably from the present capabilities of DFT, especially when applied to strongly correlated systems. As briefly reviewed below, the development of energy functionals of the 1-RDM is still at a relatively early stage. In connection with this process, exact and general constraints of RDMFT have been studied in the case of the three-dimensional homogeneous electron gas (3DEG) which, as shown by Cioslowski and Pernal, provides a natural framework to obtain constraints to the 1-RDM functionals. More recently, the practical performance of different functionals for the 3DEG – including the physically appealing power functional – has been examined by Lathiotakis et al.

Until now, developments of RDMFT in two dimensions (2D) have been very scarce despite the large variety of strongly correlated 2D many-electron systems such as semiconductor quantum dots, quantum Hall devices, and Aharonov-Bohm interferometers. In these systems the movement of particles is essentially restricted to a plane, so that the quantum mechanical degrees of freedom have been frozen in the third (off-plane) direction. Experience within DFT has shown that 2D functionals (where, e.g., the density scaling is different from that in 3D) are needed to capture the physical properties of semiconductor quantum dots. In RDMFT, however, the only work that addresses 2D systems have been done by Harju and Tölo, who tested several 1-RDM (and also 2-RDM) functionals for quantum Hall droplets at high magnetic fields. In this paper we aim at bridging the gap between the methodological potential of RDMFT and the interest in 2D systems in the condensed matter community. In particular, we use the homogeneous 2D electron gas (2DEG) as the playground to obtain exact constraints to the 1-RDM functionals applied in 2D. In the derivation we apply the procedure of Cioslowski and Pernal mentioned above. The existence of a stable solution and the homogeneous scaling constraint bring the first density-independent restrictions to the scaling parameter. Further density-dependent constraints are introduced through the bounds on the natural orbitals and on the exchange-correlation (xc) energy. Finally we show that, apart from the possibility for border-minima solutions, the Müller and Goedecker-Umrigar functionals of the scaling \( f(n, n') = (nn')^{1/2} \) are not valid for the 2DEG of any density, and that the power functional with \( f(n, n') = (nn')^\alpha \) is applicable only at \( 0.64 \lesssim \alpha \lesssim 0.75 \).

II. REDUCED DENSITY-MATRIX FUNCTIONAL THEORY

In a system of \( N \) interacting electrons the total energy of the ground state can be expressed as a sum of the kinetic, external, and electron-electron (\( e-e \)) interaction energy, i.e.,

\[ E_{\text{tot}}[\Psi] = T[\Psi] + E_{\text{ext}}[\Psi] + E_{\text{int}}[\Psi], \]

where the total energy is a functional of the \( N \)-electron ground-state wave function \( \Psi \). According to Gilbert’s theorem, there is a one-to-one correspondence between \( \Psi \) and the one-body reduced density matrix (1-RDM),

\[ \gamma(r, r') = \Psi^*(r')\Psi(r) = \sum_{i=1}^{\infty} n_i \varphi_i^*(r')\varphi_i(r), \]
where \( \varphi_i \) are natural orbitals and \( n_i \) the corresponding occupation numbers, which have values \( 0 \leq n_i \leq 1 \) and sum up to \( N \). In Eq. (1), the two first terms have simple expressions as functionals of \( \gamma \), i.e.,

\[
T[\gamma] = \int d\mathbf{r} \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \left[ -\frac{1}{2} \nabla^2 \right] \gamma(\mathbf{r}, \mathbf{r}')
\]

and

\[
E_{\text{ext}}[\gamma] = \int d\mathbf{r} \int d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') V_{\text{ext}}(\mathbf{r}, \mathbf{r}') \gamma(\mathbf{r}, \mathbf{r}').
\]

In contrast, the e-e interaction term in Eq. (1) has a more complex expression,

\[
E_{\text{int}}[\gamma] = \int d\mathbf{r} \int d\mathbf{r}' \rho_2(\mathbf{r}, \mathbf{r}') \nabla^2 \gamma(\mathbf{r}, \mathbf{r}'),
\]

where the minimization is performed over all normalized and antisymmetric \( \Psi \) that yield \( \gamma \). Here the pair density is defined by

\[
\rho_2(\mathbf{r}, \mathbf{r}') = N(N - 1) \int \cdots \int d\mathbf{r}_3 \cdots d\mathbf{r}_N \Psi^*(\mathbf{r}, \mathbf{r}', \mathbf{r}_3, \ldots, \mathbf{r}_N) \Psi(\mathbf{r}, \mathbf{r}', \mathbf{r}_3, \ldots, \mathbf{r}_N),
\]

which can be rarely calculated in practice.

Now, practical use of RDMFT requires approximations on \( E_{\text{int}}[\gamma] \) given in Eq. (5). At this stage, it is useful to partition the term as

\[
E_{\text{int}}[\gamma] = E_H[\gamma] + E_{xc}[\gamma],
\]

where

\[
E_H[\gamma] = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \gamma(\mathbf{r}, \mathbf{r}') \gamma(\mathbf{r}', \mathbf{r})
\]

is the Hartree energy corresponding to the classical electrostatic energy calculated from the diagonal of \( \gamma \), i.e., the single-particle density \( \rho(\mathbf{r}) = \gamma(\mathbf{r}, \mathbf{r}) \). The second term in Eq. (7) is the xc energy. It is important to note that this is not the same as the xc energy in the conventional DFT. The difference is due to the exact expression of the kinetic energy in RDMFT [Eq. (3)] in contrast with the approximate DFT expression employing the Kohn-Sham orbitals.

The simplest approximation for \( E_{xc} \) is given by the Hartree-Fock (HF) term

\[
E_{xc}^{\text{HF}}[\gamma] = -\frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \gamma(\mathbf{r}, \mathbf{r}') \gamma(\mathbf{r}', \mathbf{r})
\]

\[
= -\frac{1}{2} \sum_{i,j} n_i n_j \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}) \varphi_i(\mathbf{r})
\]

\[
\times \frac{\varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}) \varphi_i(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|},
\]

which corresponds to the exchange energy of RDMFT. Most further approximations in RDMFT have emerged from this expression with an aim to account for the correlation energy which is omitted in the HF term. These functionals can be expressed in a form

\[
E_{xc}[\gamma] = \frac{1}{2} \sum_{i,j} \int d\mathbf{r} \int d\mathbf{r}' \gamma(\mathbf{r}, \mathbf{r}') \gamma(\mathbf{r}', \mathbf{r})
\]

\[
\times f(n_i, n_j) \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}) \varphi_i(\mathbf{r})
\]

\[
\times \frac{\varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}) \varphi_j(\mathbf{r}) \varphi_i(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|},
\]

where the difference from the HF expression is embedded in the function \( f(n_i, n_j) \).

Various approximations for \( f(n_i, n_j) \) have been introduced, many of them based on a form \( f(n_i, n_j) = (n_i n_j)^\alpha \), where \( \alpha = 1 \) corresponds to the HF case. One of the first approximations is the Müller functional with \( \alpha = 1/2 \) (Ref. 16). The factor is the same in the Goedecker-Unrigh functional, which removes the orbital self-interaction. Further hierarchical corrections, where \( f(n_i, n_j) \) depends on the orbital occupancies, have been introduced by Gritsenko et al.\textsuperscript{18} They are commonly known as BBC1, BBC2, and BBC3 functionals according to corrections to the Buijse-Baerends functional.\textsuperscript{19}

More recently, the so-called power functional was introduced by Sharma et al.\textsuperscript{14} In that functional \( \alpha \) is introduced as a mixing parameter between the HF and Müller approximations, i.e., \( 1/2 \leq \alpha \leq 1 \). It was found that the optimal \( \alpha \) varies between 0.525 (stretched H2) and 0.65 (solids), and the best overall fit for the 3D homogeneous electron gas was found at \( \alpha = 0.55 \ldots 0.58 \) (Ref. 10). In 2D, RDMFT has been applied to quantum Hall droplets by Tölo and Harju\textsuperscript{15} who found that in in many cases the power functional yields reasonable results with \( \alpha \sim 0.65 \ldots 0.7 \), but also clear limitations of the functional were found.

\section{III. Two-Dimensional Homogeneous Electron Gas}

In 2DEG we can consider a positive background charge compensating for the electrostatic (Hartree) energy, so that the total energy [Eq. (1)] consists of the kinetic and xc components alone, i.e.,

\[
E_{\text{tot}}^{2\text{DEG}}[\gamma] = T[\gamma] + E_{xc}[\gamma],
\]

where

\[
T[\gamma] = -\frac{1}{2} \sum_{\sigma=\uparrow, \downarrow} \sum_{p} n_\sigma(k_p) \int d\mathbf{r} \varphi_{p\sigma}^*(\mathbf{r}) \nabla^2 \varphi_{p\sigma}(\mathbf{r})
\]

and, similar to Eq. (10),

\[
E_{xc}[\gamma] = -\frac{1}{2} \sum_{\sigma=\uparrow, \downarrow} \sum_{p,q} \int d\mathbf{r} \int d\mathbf{r}' f(n_{\sigma}(k_p), n_{\sigma}(k_q))
\]

\[
\times \frac{\varphi_{p\sigma}^*(\mathbf{r}) \varphi_{q\sigma}^*(\mathbf{r}) \varphi_{q\sigma}(\mathbf{r}) \varphi_{p\sigma}(\mathbf{r})}{|\mathbf{r} - \mathbf{r}'|},
\]
where we have introduced $k_p$ as the wave vector of the pth spin-dependent natural orbital. In the 2DEG it can be now expressed as a plane wave,

$$\varphi_{p\sigma}(r) = A^{-1/2} \exp(\mathrm{i} k_p \cdot r) \chi_p(\sigma),$$

where $A$ is the area and $\chi$ is the spin component. Now, it is straightforward to calculate the integrals in Eqs. (12) and (13) yielding, respectively, $-|k_p|^2$ and $2\pi A^{-1}|k_p - k_q|^{-1}$. The summation over plane waves can be replaced by an integration,

$$\sum_p \rightarrow (4\pi^2)^{-1} A \int dk.$$  \hfill(15)

As a result of these replacements, we can express the total energy of the 2DEG as a functional of the momentum distribution,

$$E_{\text{tot}}^{2\text{DEG}}[n_{\uparrow}, n_{\downarrow}] = \frac{A}{8\pi^2} \sum_{\sigma = \uparrow, \downarrow} \int dk \, n_\sigma(k) |k|^2 - \frac{A}{16\pi^2} \sum_{\sigma = \uparrow, \downarrow} \int dk \int dk' \frac{f(n_{\sigma}(k), n_{\sigma}(k'))}{|k - k'|}.$$  \hfill(16)

The normalization constraint is given by an integral

$$N_\sigma = A \int \frac{dk}{4\pi^2} k n_\sigma(k) = A \rho_\sigma,$$

where $\rho_\sigma$ is the spin density (per area). We can define the area energy density per spin simply by

$$\epsilon_{\sigma}[n_{\sigma}] = E_{\text{tot}}^{2\text{DEG}}[n_{\sigma}] / A = t_\sigma[n_{\sigma}] + \epsilon_{\text{xc}}[n_{\sigma}],$$

where $t_\sigma$ and $\epsilon_{\text{xc}}$ are the kinetic and xc energy densities per spin, respectively.

For brevity, we omit the spin index $\sigma$ in the following. Thus, it should be noted that in the rest of the paper $n$, $\rho$, $t$, and $\epsilon_{\text{xc}}$ refer to quantities per spin-particle (with spin $\sigma$). With this notation, particular care is needed for the formula of the lower bound on the xc energy [Eq. (19) below], which is conventionally considered for the spin-unpolarized 2DEG with $\rho_{\text{tot}} = \rho_\uparrow + \rho_\downarrow = 2\rho$.

We can now seek for a stationary value for the functional $\epsilon[n]$ with respect to variations in $n$, so that the normalization in Eq. (17) is satisfied. The normalization constraint introduces a Lagrange multiplier $\mu$ in the variational (Euler-Lagrange) equation written as

$$\frac{de}{dn} - \mu \frac{d\rho}{dn} = 0,$$

leading to

$$\frac{1}{2} |k|^2 - \frac{1}{2\pi} \int dk' \frac{\partial}{\partial n(k')} f(n(k), n(k')) |k - k'| = \mu. \hfill(20)$$

It is important to note that in this paper we concentrate on analytic solutions of Eq. (19). Thus, we exclude the possibility for partial or full border minima, where $n(k)$ is equal to 0 or 1 – as allowed by the $N$-representability condition – but Eq. (19) is not satisfied.2

### A. General constraints

Next we examine a set of constraints for the solutions of Eqs. (18)-(20). First, the (ground-state) solutions have to be stable upon normalization. Hence, for a uniform scaling with a constant, positive $\lambda \neq 1$ we require

$$\epsilon(\lambda^2 n(\lambda k)) > \epsilon(n(k)),$$

so that the first derivative with respect to $\lambda$ at $\lambda = 1$ is zero,

$$\left. \frac{\partial}{\partial \lambda} \epsilon[\lambda^2 n(\lambda k)] \right|_{\lambda=1} = 0,$$  \hfill(22)

and the second derivative is positive,

$$\left. \frac{\partial^2}{\partial \lambda^2} \epsilon[\lambda^2 n(\lambda k)] \right|_{\lambda=1} > 0.$$  \hfill(23)

As the second constraint, the function $f(n(k), n(k'))$ has to satisfy the homogeneous scaling $\hat{f}$

$$f(\lambda^2 n(\lambda k), \lambda^2 n(\lambda k')) = \lambda^{2\beta} f(n(k), n(k')),$$  \hfill(24)

for all $n(k)$ and $n(k')$. The kinetic-energy density scales as $t(\lambda^2 n(\lambda k)) = \lambda^2 t(n(k))$, and, from Eq. (24) we find that the xc energy scales as $\epsilon_{\text{xc}}(\lambda^2 n(\lambda k)) = \lambda^{2\beta - 1} \epsilon_{\text{xc}}(n(k))$. Now, Eq. (22) leads to

$$t(\rho) = \frac{2\beta - 3}{2\beta - 1} \epsilon(\rho),$$  \hfill(25)

and with Eq. (18) to

$$\epsilon_{\text{xc}}(\rho) = \frac{2}{2\beta - 1} \epsilon(\rho).$$  \hfill(26)

By definition, the kinetic-energy density must be positive, $t > 0$, and the xc energy must be non-positive, $\epsilon_{\text{xc}} \leq 0$. It is then straightforward to show with Eqs. (23), (24), and (26) that both these conditions are satisfied when

$$\frac{1}{2} < \beta < \frac{3}{2}.$$  \hfill(27)

The range is slightly larger than in 3D, where the corresponding result is $2/3 < \beta_{3D} < 4/3$ (Ref. 6).

From Eq. (24) we may immediately conclude that in the case of a power functional, $f(n_i, n_j) = (n_i n_j)^\alpha$, the power $\alpha$ is restricted to

$$\frac{1}{4} < \alpha < \frac{3}{4}.$$  \hfill(28)

Hence, e.g., the Müller functional with $\alpha = 1/2$ (see the next section) satisfies the stability and homogeneous scaling constraints. It is important to note, however, that there are further restrictions for the density $\rho$, which in fact appear to be prohibitive to the Müller functional. These limitations arise from (i) how the specific
form of the momentum distribution satisfies the condition $0 \leq n(k) \leq 1$, and from (ii) the universal lower bound for $\varepsilon_{xc}$. The latter condition corresponds to the 2D counterpart of the Lieb-Oxford bound, whose existence was rigorously proven by Lieb, Solovej, and Yngvason. Recently, however, the tightest form for this bound was suggested through nonrigorous but physical arguments. The bound was found to correspond to the 2D counterpart of the Lieb-Oxford bound whose existence was rigorously proven by Lieb, Solovej, and Yngvason. Recently, however, the tightest form for this bound was suggested through nonrigorous but physical arguments. The bound was found to correspond to the 2D counterpart of the Lieb-Oxford bound

\[ 2 \varepsilon_{xc} \geq -C (2\rho)^{3/2}, \]  

where $C = 1.96$ (Ref. 23). The factor of two on both sides of Eq. (29) results from the per-spin notation (see above).

### B. Limits of the Müller functional

We examine the constraints of the Müller functional,

\[ f(n(k), n(k')) = (n(k)n(k'))^{1/2}, \]  

which in fact coincides with the Goedecker-Umrigar functional in the case of the 2DEG, since the self-interaction terms vanish for plane-wave orbitals. Now we have $\beta = 1$ and use an ansatz

\[ n(k) = \rho \eta(k), \]  

where $\eta$ is independent of the density and satisfies the normalization

\[ \int dk \eta(k) = 4\pi^2. \]  

We can solve the variational equation (29) that becomes,

\[ \frac{1}{2} |k|^2 \eta(k)^{1/2} - \frac{1}{4\pi} \int dk' \frac{\eta(k')^{1/2}}{|k-k'|} = \mu \eta(k)^{1/2}. \]  

Substituting $\eta(k) = \phi(k)^2$ and taking the Fourier transform yields

\[ -\frac{1}{2} \nabla^2 \phi(r) - \frac{1}{2} \phi(r) \frac{1}{|r|} = \mu \phi(r), \]  

which has a simple solution,

\[ \phi(r) = \sqrt{8\pi} e^{-|r|} \]  

with $\mu = -1/2$. Taking an inverse Fourier transform leads to

\[ \eta(k) = 8\pi (1 + |k|^2)^{-3}, \]  

and finally, according to Eq. (31) the momentum distribution of the Müller functional in the 2DEG reads

\[ n(k) = 8\pi \rho (1 + |k|^2)^{-3}. \]  

Now we go back to constraints (i) and (ii) mentioned at the end of the previous section. First, from the requirement $0 \leq n(k) \leq 1$ it follows that $\rho \leq (8\pi)^{-1}$ for the spin-density. In terms of the commonly used density parameter $r_s$ (Wigner-Seitz radius) for the spin-unpolarized 2DEG the condition reads

\[ r_s \equiv (2\pi \rho)^{-1/2} \geq 2. \]  

To obtain the second constraint (ii) we first employ Eqs. (23) and (24) and find $t = \rho/2$, $\varepsilon_{xc} = -\rho$, and $\epsilon = -\rho/2$. Thus, again for the spin-unpolarized 2DEG, we get from Eq. (29) another condition

\[ r_s \leq \frac{C}{\sqrt{\pi}} \approx 1.1. \]  

We can immediately see that conditions (35) and (39) are exclusive. Thus, the Müller functional is not valid for the 2DEG of any density, apart from the possibility of border-minima solutions (see the end of Sec. III).

### C. Limits of the power functional

Finally we examine the limits of the power functional

\[ f(n(k), n(k')) = (n(k)n(k'))^{\beta/2} = (n(k)n(k'))^{\alpha}. \]  

In contrast with the Müller functional with $\beta = 1$ we cannot analytically solve the variational equation (29) in order to obtain the exact momentum distribution. However, we may try to find a reasonable ansatz for the momentum distribution. First, we examine how the Euler-Lagrange equation (19) scales with the density and separate the density-dependent part from $n(k)$ as

\[ n(k) = \rho^{1/(2\beta-1)} \eta \left( \rho^{1/2} \frac{|k|}{\pi \epsilon} \right), \]  

where $\eta$ is independent of the density. Following the strategy of Cioslowski and Pernal we choose a parametrized trial function for $\eta$ similar to that of the Müller functional [Eq. (31)],

\[ \overline{\eta}(k) = D (1 + \zeta |k|^2)^{-3/2} \]  

where $D = 4\pi \zeta (3\beta^{-1} - 1)$ is the normalization constant obtained from Eq. (32). The parameter $\zeta$ is now solved such that the total energy density, which has a form

\[ \epsilon(\rho) = I_{\epsilon} \rho^{\frac{3\beta}{2(-2\beta+1)}} \]  

is minimized. As pointed out in Ref. 8 this forms an upper bound to the integral

\[ I_{\epsilon} = \frac{1}{8\pi^2} \int dk |\eta(k)||k|^2 - \frac{1}{16\pi^3} \int dk \int dk' \frac{f(\eta(k), \eta(k'))}{|k-k'|}, \]  

where

\[ f(\eta(k), \eta(k')) \]
which is independent of the density, and has the absolute, stable minimum for the unknown exact momentum distribution. Thus, we have an inequality $I_0 \leq I_\gamma$, where

$$I_\gamma = \min_\xi \left\{ \frac{\beta}{2\zeta(3-2\beta)} - 4^{\beta/2} - \frac{3\zeta}{\beta} \left( \frac{3\zeta}{\beta} - \zeta \right)^\beta F(\zeta) \right\}$$

with an integral

$$F(\zeta) = \int dk \int dk' \frac{(1 + \zeta|k|^2)^{-3/2}(1 + \zeta|k'|^2)^{-3/2}}{|k - k'|}.$$  \hfill (45)

The integral is similar to the Hartree energy integral with a “density” distribution $(1 + \zeta|k|^2)^{-3/2}$. In the lack of an analytic solution (although we do not preclude its possible existence), we solve $F(\zeta)$ numerically by taking a Fourier transform and using the convolution theorem implemented in the octopus code. \textsuperscript{23} We find $F(\zeta) = \gamma \zeta^{-3/2}$ with $\gamma \approx 19.74$. After rewriting Eq. (45) and differentiating with respect to $\zeta$ we obtain the minimum at

$$\zeta_m(\beta) = \left[ \frac{a}{b(\beta - 3/2)} \right]^{-1/\beta} \hfill (46)$$

with $a(\beta) = (6\beta - 1 - 4)^{-1}$ and $b(\beta) = 4^{\beta/2} - 3(3\beta - 1)^{\beta/2}$. Thus, $I_\gamma = a\zeta_m^{-1} - b\zeta_m^{-3/2}$ is obtained by inserting $\zeta_m$ to Eq. (45).

Let us now consider the constraints (i) and (ii) for the allowed values of $a(k)$ and $\epsilon_{xc}$, respectively (see the end of Sec. IIIA). First, from Eqs. (41) and (42) we obtain

$$0 \leq \bar{n}(k) = \rho^{1/(2\beta - 1)}D(1 + \zeta_m|k|^2)^{-3/\beta} \leq 1 \hfill (47)$$

leading to

$$\rho \leq D^{1-2\beta} = \left[ 4\pi\zeta_m(3\beta - 1) \right]^{1-2\beta}. \hfill (48)$$

Secondly, from Eqs. (43), (20), and (29) we obtain

$$\frac{4I_\gamma}{2\beta - 1} \rho^{3\beta/2 - 1 + 1} \geq -C(2\rho)^{3/2}, \hfill (49)$$

yielding another condition for the density,

$$\rho \geq \left[ 2^{-1}C^2I_\gamma(2\beta - 1)^{2\beta/3} \right]^{1/3}. \hfill (50)$$

Combining Eqs. (48) and (50) leads to a single constraint for $\beta$ which has a simple form,

$$\beta \geq \frac{3}{2\pi(C/\gamma)^{2/3} + 1} \approx 1.28. \hfill (51)$$

Now, keeping in mind the physical limits of $\beta$ given in Eq. (27), we get a condition $1.28 \lesssim \beta \leq 1.5$. Correspondingly, the power functional satisfies the stability (in terms of the analyticity of the minimum) and homogeneous scaling constraints and constraints (i) and (ii), when the power is restricted to

$$0.64 \lesssim \alpha \lesssim 0.75. \hfill (52)$$

It should be noted, however, that the lower limit, for example, is valid only for a single density, i.e., the one that satisfies the equality conditions in both Eqs. (18) and (50). At larger $\alpha$, the range for allowed densities increases as visualized in Fig. 1. The maximum possible density, for which an admissible power exists, corresponds to a maximum value $r_s \approx 15$ for the density parameter. This density range is too low for the most 2D applications in, e.g., quantum dot and quantum Hall physics dealing with desities in the range $0.1 \lesssim r_s \lesssim 10$.

Despite the strict conditions for $\alpha$ and the corresponding densities, it is interesting to note that the optimal power for 2D quantum Hall droplets was found to be $0.65 \ldots 0.7$ (Ref. 13), which coincides with the allowed range obtained here. However, it is important to bear in mind that our analysis for the 2DEG does not include (i) the possibility for border minima, and (ii) the evaluation of the accuracy of the power functional in comparison with the exact xc energy of the 2DEG known through quantum Monte Carlo calculations. \textsuperscript{25,26} These issues will be addressed in future works. We also point out that the validity of our ansatz momentum distribution in Eq. (11) could be further evaluated.

\section{Summary}

In summary, we have examined the constraints of reduced density-matrix functionals in the description of the homogeneous two-dimensional electron gas, which is the base for a large spectrum of applications in low-dimensional physics, e.g., in the quantum Hall regime.
As our main result, we have found that the power of the scaling function \( f(n, n') = (nn')^\alpha \) is physically limited to \( 0.64 \lesssim \alpha \lesssim 0.75 \). The result has been preceded by a thorough analysis of how \( \alpha \) is restricted and affected by (i) the existence of stable solutions with analytic minima, (ii) the homogeneous scaling constraint for \( f(n, n') \), (iii) the allowed values for \( n(k) \), and (iv) the lower bound of the exchange-correlation energy. Yet another issue to be addressed in the future is the possibility for border-minima solutions as well as the practical accuracy of the power functional in comparison with exact results when applied—within the constraints addressed here—to different systems, first and foremost to the two-dimensional electron gas of different densities.

In general, we hope that our analysis serves as a useful guideline in the development of density-matrix functionals in two dimensions.

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1 P.-O. Löwdin, Phys. Rev. 97, 1474 (1955).
2 T. L. Gilbert, Phys. Rev. B 12, 2111 (1975).
3 For a review, see, e.g., R. M. Dreizler and E. K. U. Gross, Density Functional Theory (Springer, Berlin, 1990); U. von Barth, Phys. Scr. T109, 9 (2004).
4 For recent works, see, e.g., D. R. Rohr, J. Toulouse, and K. Pernal, Phys. Rev. A 82, 052502 (2010); K. J. H. Giesbertz, E. J. Baerends, and O. V. Gritsenko, Phys. Rev. Lett. 101, 033004 (2008).
5 M. Levy, Density Matrices and Density Functionals, (Reidel, Dordrecht, 1987).
6 J. Cioslowski and K. Pernal, J. Chem. Phys. 111, 3396 (1999).
7 J. Cioslowski and K. Pernal, Phys. Rev. A 61, 034503 (2000).
8 S. Sharma, J. K. Dewhurst, N. N. Lathirotakis, and E. K. U. Gross, Phys. Rev. B 78, 201103(R) (2008).
9 N. N. Lathirotakis, N. Helbig, and E. K. U. Gross, Phys. Rev. B 75, 195120 (2007).
10 N. N. Lathirotakis, S. Sharma, J. K. Dewhurst, F. G. Eich, M. A. L. Marques, and E. K. U. Gross, Phys. Rev. A 79, 040501(R) (2009).
11 See, e.g., M. C. Rogge, E. Räsänen, and R. J. Haug, Phys. Rev. Lett. 105, 046802 (2010).
12 For recent works, see, e.g., E. Räsänen, S. Pittalis, and C. R. Proetto, Phys. Rev. B 81, 195103 (2010); S. Pittalis and E. Räsänen, Phys. Rev. B 82, 165123 (2010); ibid 82, 195124 (2010); S. Pittalis, E. Räsänen, J. G. Vilhena, and M. A. L. Marques, Phys. Rev. A 79, 012503 (2009).
13 L. A. Constantin, Phys. Rev. B 78, 155106 (2008).
14 L. A. Constantin, J. P. Perdew, and J. M. Pitarke, Phys. Rev. Lett. 101, 016406 (2008).
15 E. Tööö and A. Harju, Phys. Rev. B 81, 075321 (2010).
16 A. M. K. Müller, Phys. Lett. A 105, 446 (1984).
17 S. Goedecker and C. J. Umrigar, Phys. Rev. Lett. 81, 866 (1998).
18 O. Gritsenko, K. Pernal, and E. J. Baerends, J. Chem. Phys. 122, 204102 (2005).
19 M. A. Buïjse, Ph.D. Thesis, Vrije Universiteit Amsterdam, 1991.
20 P. Gori-Giorgi, S. Moroni, and G. B. Bachelet, Phys. Rev. B 70, 115102 (2004).
21 E. H. Lieb, Phys. Lett. 70A, 444 (1979); E. H. Lieb and S. Oxford, Int. J. Quantum Chem. 19, 427 (1981).
22 E. H. Lieb, J. P. Solovej, and J. Yngvason, Phys. Rev. B 51, 10646 (1995).
23 E. Räsänen, S. Pittalis, K. Capelle, and C. R. Proetto, Phys. Rev. Lett. 102, 206406 (2009).
24 M. A. L. Marques, A. Castro, G. F. Bertsch, A. Rubio, Comput. Phys. Commun. 151, 60 (2003); A. Castro, H. Appel, M. Oliveira, C. A. Rozzi, X. Andrade, F. Lorenzen, M. A. L. Marques, E. K. U. Gross, and A. Rubio, Phys. Stat. Sol. (b) 243, 2465 (2006).
25 B. Tanatar, D. M. Ceperley, Phys. Rev. B 39, 5005 (1989).
26 C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. Lett. 88, 256601 (2002).