

Generalization of homogeneous coordinate scaling in density-functional theory

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A generalization of homogeneous coordinate scaling for wave functions [$\phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) = \alpha^{m/2}\phi_i(\beta^p\mathbf{r})$, $(\alpha, \beta) \in \mathbb{R}^+$, $(m, p) \in \mathbb{R}$] and electron densities [$n_{\alpha\beta mp}(\mathbf{r}) = \alpha^m n(\beta^p\mathbf{r})$] is introduced. It is shown that, under such a scaling, the Kohn-Sham (KS) noninteracting kinetic energy $T_s[n]$ scales as $T_s[n_{\alpha\beta mp}] = \alpha^m T_s[n]/\beta^p$, which leads to the integral, or generalized virial, expression $T_s[n] = 1/(m-p) \int \delta T_s[n]/\delta n(\mathbf{r}) [mn(\mathbf{r}) + p\mathbf{r} \cdot \nabla n(\mathbf{r})] d^3r$. For $m=3$ and $p=2$ the general expression yields the well-known relation $T_s[n] = 1/2 \int \delta T_s[n]/\delta n(\mathbf{r}) [3n(\mathbf{r}) + \mathbf{r} \cdot \nabla n(\mathbf{r})] d^3r$. The general virial also reduces to the new integral expression $T_s[n] = - \int \delta T_s[n]/\delta n(\mathbf{r}) \mathbf{r} \cdot \nabla n(\mathbf{r}) d^3r$, as well as to the controversial one, $T_s[n] = - \int \delta T_s[n]/\delta n(\mathbf{r}) n(\mathbf{r}) d^3r$, due to the scaling of $T_s[n]$ under $n_{amp}(\mathbf{r}) = \alpha^m n(\alpha^p\mathbf{r})$ and its invariance for $m=p$. The validity of the controversial expression is further discussed and the first-degree homogeneous character of $T_s[n]$ under density scaling established. The scaling properties of the KS potential and eigenvalues are also analyzed. Examples of numerical tests that confirmed all the integral expressions for $T_s[n]$ and its scaling properties, as well as the scaling of the KS potential and eigenvalues, are provided.

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I. INTRODUCTION

The investigation of the scaling properties of functionals is very useful to understand their structure and to approximate those explicitly unknown functionals of the density, such as the kinetic energy functional of noninteracting systems ($T_s[n]$) and the exchange-correlation functional ($E_{xc}[n]$) in Kohn-Sham (KS) density-functional theory (DFT) [1–23]. Both functionals are approximated in the so-called orbital-free methods [24] while only $E_{xc}[n]$ needs to be approximated in KS-DFT [25,26].

Since the introduction by Sham [3] of the number of particle conserving scaling $n_\alpha(\mathbf{r}) = \alpha^3 n(\alpha\mathbf{r})$, the scaling properties of density functionals have been intensively studied [6,27]. Scalings of the density that do not conserve the number of electrons have been also investigated. Notably, Liu and Parr [17] started the discussion on the consequences of density scaling $n_\alpha(\mathbf{r}) = \alpha n(\alpha\mathbf{r})$, and Perdew and co-workers studied the scaling $n_\alpha(\mathbf{r}) = \alpha^2 n(\alpha^{1/3}\mathbf{r})$.

Naturally, one wonders if all the possibilities for the scaling of wave functions and densities have been exhausted. On that account, in this work we introduce a generalization of homogeneous scaling of the KS wave functions and electron densities, and investigate the properties of the noninteracting kinetic-energy functional under such a scaling. The generalization contains completely new, as well as all previously defined, homogeneous coordinate and density scaling. It also introduces more degrees of freedom by scaling the coordinates and the amplitude of the functions separately.

As explained below, the generalization of homogeneous scaling proposed here not only leads to new integral relations for $T_s[n]$ but also to a well-established one. However, it also yields the controversial result that $T_s[n]$ scales linearly under density scaling, which we prove true using completely different routes from that of Liu and Parr [17], whose demonstration has been proved incorrect [28].

We continue by providing a background on KS-DFT in Sec. II, with emphasis on the definition of $T_s[n]$ and including all the necessary information related to general scaling. In Sec. III we discuss in detail the noninteracting kinetic-energy functional for the scaled density, which leads to a redefinition of $T_s[n]$ addressed in Sec. IV. The study of the scaling properties of $T_s[n]$ and its functional derivative is carried out in Sec. V, and in Sec. VI the integral or virial relations for $T_s[n]$ are found via parametric derivatives. Numerical evidence of the validity of the integral relations are provided in Sec. VII, followed by a discussion on the issue of linear scaling of $T_s[n]$ under density scaling in Sec. VIII. Finally, concluding remarks are made in Sec. IX.

II. GENERAL ASPECTS

A. The Kohn-Sham problem

We say that $\{\phi\}$ is a KS set [26] for the density

$$n(\mathbf{r}) = \sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 \quad (1)$$

if it is a set of N_s orthonormal wave functions in the Hilbert space that, given the occupation numbers n_i ($i = 1, \dots, N_s$), minimizes the kinetic-energy functional

$$T_s[n] = \min_{\{\phi\}_{\perp \rightarrow n}} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3r \quad (2)$$

of a noninteracting system of density $n(\mathbf{r})$. That is according to Levy's constrained search [29,30], which via Lagrange multipliers translates to the unconstrained search

$$T_s[n] = \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3r + \int v([n], \mathbf{r}) \left[\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n(\mathbf{r}) \right] d^3r - \sum_{i=1}^{N_s} n_i \epsilon_i[n] \left[\int |\phi_i(\mathbf{r})|^2 d^3r - 1 \right] \right\}, \quad (3)$$

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where v is the local Lagrange multiplier that ensures the wave functions reproduce a given density (KS potential) and ϵ_i are the Lagrange multipliers that keep the wave functions normalized to 1 (KS eigenvalues). This is the equation that links a given density to a set of KS wave functions, eigenvalues, and potential.

Equating to zero the functional derivatives with respect to the wave functions of the expression in curly brackets in Eq. (3) yields the KS equations [26]

$$-\frac{1}{2}\nabla^2\phi_i(\mathbf{r}) + v([n],\mathbf{r})\phi_i(\mathbf{r}) = \epsilon_i[n]\phi_i(\mathbf{r}). \quad (4)$$

Notice that the Hermitian character of the operator in this equation guarantees the orthogonality of the wave functions, and therefore the orthogonalization is automatically enforced by the constraint on the normalization.

After repartitioning the total energy of the interacting system to include the noninteracting kinetic-energy functional $T_s[n]$ and the classical electron-electron repulsion or Hartree functional $E_H[n]$, the KS potential is found to be [26]

$$v([n],\mathbf{r}) = \frac{\delta E_H[n]}{\delta n(\mathbf{r})} + \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})} + v_{\text{ext}}(\mathbf{r}), \quad (5)$$

with $E_{xc}[n]$ being the exchange-correlation energy-density functional and $v_{\text{ext}}(\mathbf{r})$ the external potential.

On the other hand, if the KS potential and number of electrons N_e were given, then, assuming that we know the explicit form of the noninteracting kinetic-energy functional in terms of the density, one could find the ground-state density by solving the Euler-Lagrange equation [26]

$$\frac{\delta}{\delta n(\mathbf{r})} \left\{ T_s[n] + \int v([n],\mathbf{r})n(\mathbf{r}) - \mu \left[\int n(\mathbf{r}) - N_e \right] \right\} = 0, \quad (6)$$

where μ is the Lagrange multiplier that fixes the integral of the density to the number of electrons.

B. Scaling of wave functions and the electron density

A generalization of the homogeneous coordinate scaling in DFT can be realized by defining a new set of scaled KS wave functions according to

$$\phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) = \alpha^{m/2}\phi_i(\beta^p\mathbf{r}), \quad (7)$$

where α and β are positive real numbers, and m and p are any real numbers. This scaling represents a uniform contraction or expansion of wave functions in space controlled by β and p , in conjunction with a change of amplitude controlled by α and m .

The scaling in Eq. (7) defines a one-to-one mapping between the scaled wave functions and the original ones, clearly spanning the same Hilbert space and conserving the orthogonality, but changing the normalization of the wave functions to

$$\int |\phi_{\alpha\beta mp}^{(i)}(\mathbf{r})|^2 d^3r = \frac{\alpha^m}{\beta^{3p}}. \quad (8)$$

By construction the corresponding electron density [Eq. (1)] scales as

$$n_{\alpha\beta mp}(\mathbf{r}) = \alpha^m n(\beta^p\mathbf{r}). \quad (9)$$

In principle the number of electrons N_e , seen as the integral of the density, is not conserved under general homogeneous

scaling; in fact it becomes $N_{e\alpha\beta mp} = \alpha^m N_e / \beta^{3p}$. But the apparent change in the number of electrons does not come from a change in the occupation numbers but rather from the new norm of the scaled KS wave functions. Indeed, the relation $\sum_{i=1}^{N_s} n_i = N_e$ holds for any scaling.

The associate inverse homogeneous scaling is given by

$$n(\mathbf{r}) = \alpha^{-m} n_{\alpha\beta mp}(\beta^{-p}\mathbf{r}), \quad (10)$$

which can be written as

$$n(\mathbf{r}) = \alpha^{-m} \int n_{\alpha\beta mp}(\mathbf{r}') \delta(\mathbf{r}' - \beta^{-p}\mathbf{r}) d^3r' \quad (11)$$

and leads to the following expression for the functional derivative of the density with respect to the scale density:

$$\frac{\delta n(\mathbf{r})}{\delta n_{\alpha\beta mp}(\mathbf{r}')} = \alpha^{-m} \delta(\mathbf{r}' - \beta^{-p}\mathbf{r}). \quad (12)$$

In defining the general scaling given by Eq. (9) we consider not only new scalings but also particular scalings previously investigated by different authors. Notably, Eq. (9) contains the particle conservation homogeneous scaling introduced by Sham, $n_\alpha(\mathbf{r}) = \alpha^3 n(\alpha\mathbf{r})$ [2,3], the density scaling of Liu and Parr, $n_\alpha(\mathbf{r}) = \alpha n(\mathbf{r})$ [16,17,19], and the scaling of Perdew and co-workers, $n_\alpha(\mathbf{r}) = \alpha^2 n(\alpha^{1/3}\mathbf{r})$ [22].

C. Homogeneous scaling of functionals

Similar to the case of homogeneous coordinates scaling [1], if a functional of the density scales as

$$F[n_{\alpha\beta mp}] = \frac{\alpha^k}{\beta^l} F[n], \quad (13)$$

then it is a homogeneous functional of degree k in α and degree l in β . For the functional derivative of such a homogeneous functional we have

$$\frac{\delta F[n_{\alpha\beta mp}]}{\delta n_{\alpha\beta mp}(\mathbf{r})} = \frac{\alpha^k}{\beta^l} \int \frac{\delta F[n]}{\delta n(\mathbf{r}')} \bigg|_{n_{\alpha\beta mp}(\mathbf{r}')} \frac{\delta n(\mathbf{r}')}{\delta n_{\alpha\beta mp}(\mathbf{r})} d^3r', \quad (14)$$

which becomes

$$\frac{\delta F[n_{\alpha\beta mp}]}{\delta n_{\alpha\beta mp}(\mathbf{r})} = \frac{\alpha^{k-m}}{\beta^{l-3p}} \frac{\delta F[n]}{\delta n(\mathbf{r}')} \bigg|_{\mathbf{r}'=\beta^p\mathbf{r}}, \quad (15)$$

by Eq. (12).

III. KINETIC-ENERGY FUNCTIONAL FOR THE SCALED DENSITY

It is necessary to find the functional minimized by the scaled wave functions to be able to study its scaling properties. A path to such a functional is provided by the knowledge of the KS equations the scaled wave functions are solutions of.

Notice that we could have worked with an alternative functional that does not include explicitly the constraint on

the norm of the wave functions, such as

$$\min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r \right. \\ \left. + \int v([n], \mathbf{r}) \left[\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n(\mathbf{r}) \right] d^3 r \right. \\ \left. - \sum_{i=1}^{N_s} n_i \epsilon_i[n] \int |\phi_i(\mathbf{r})|^2 d^3 r \right\}, \quad (16)$$

which is a functional, often used in papers and textbooks (see Eq. 7.2.4 in Yang and Parr, for example [1]), that reaches its minimum at the same KS set as $T_s[n]$. Instead, we strictly follow the definition of $T_s[n]$ given by Levy's constrained search, explicitly taking into account all the constraints.

In Sec. II A we established the link between the Lagrange multiplier version of Levy's constrained search and the KS equations. Now we proceed to find the KS equations satisfied by the scaled wave functions, and from those equations we get the noninteracting kinetic-energy functional for the scaled density.

A. KS equations for the scaled wave functions

The KS equations of interest can be found by introducing the change of variable $\mathbf{r} = \beta^p \mathbf{r}'$ and multiplying by $\alpha^{m/2}$ in Eq. (4) to obtain

$$\left(-\frac{1}{2} \nabla^2 + \beta^{2p} v([n], \beta^p \mathbf{r}') \right) \alpha^{m/2} \phi_i(\beta^p \mathbf{r}') \\ = \beta^{2p} \epsilon_i[n] \alpha^{m/2} \phi_i(\beta^p \mathbf{r}'), \quad (17)$$

which by Eq. (7) reduces to

$$\left(-\frac{1}{2} \nabla^2 + v([n_{\alpha\beta mp}], \mathbf{r}) \right) \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) = \epsilon_i[\alpha\beta mp] \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}), \quad (18)$$

with

$$v([n_{\alpha\beta mp}], \mathbf{r}) = \beta^{2p} v([n], \beta^p \mathbf{r}) \quad (19)$$

and

$$\epsilon_i[\alpha\beta mp] = \beta^{2p} \epsilon_i[n]. \quad (20)$$

Consequently, if the original wave functions are the solutions of the KS equations in Eq. (4) then the scaled wave functions are the solutions of the KS equations in Eq. (18) with eigenvalues and potential defined by Eqs. (19) and (20), respectively.

B. T_s for the scaled density

It has been proven that the scaled wave functions are normalized to $\alpha^{m/2}/\beta^{3p/2}$ and that they are the solutions of the KS equations defined by Eq. (18). That indicates that the scaled wave functions must minimize the kinetic energy of a noninteracting system of electron density equal to the scaled density [Eq. (9)]; that is,

$$\{\phi_{\alpha\beta mp}[n_{\alpha\beta mp}]\} \\ = \arg \min_{\{\phi\} \rightarrow n_{\alpha\beta mp}} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r \quad (21)$$

and

$$T_s[n_{\alpha\beta mp}] = \min_{\{\phi\} \rightarrow n_{\alpha\beta mp}} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r, \quad (22)$$

with the minimization search performed over *sets of orthogonal wave functions normalized to $\alpha^{m/2}/\beta^{3p/2}$* .

The free search version of Eq. (22) is

$$T_s[n_{\alpha\beta mp}] \\ = \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r \right. \\ \left. + \int v([n_{\alpha\beta mp}], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n_{\alpha\beta mp}(\mathbf{r}) \right) d^3 r \right. \\ \left. - \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \left(\int |\phi_i(\mathbf{r})|^2 d^3 r - \frac{\alpha^m}{\beta^{3p}} \right) \right\}, \quad (23)$$

and equating to zero the functional derivative with respect to the wave functions of the expression in curly brackets we get back Eq. (18).

IV. GENERAL FORM OF $T_s[n]$

The evaluation of $T_s[n]$ at the scaled density must lead to the minimization expression in terms of Lagrange multipliers in Eq. (23). But if we evaluate Eq. (3) at the scaled density we do not get Eq. (23) as expected. The reason is that the value for the constraint on the squared norm is kept fixed to 1 when it should change to α^m/β^{3p} . Hence, the constraint on the norm should be generalized. For that purpose we integrate Eq. (1), assume that all the wave functions have the same norm, use the fact that $\sum_i n_i = N_e$, and extract the following expression for the squared norm of the wave functions:

$$\int |\phi_i(\mathbf{r})|^2 d^3 r = \frac{\int n(\mathbf{r}) d^3 r}{N_e}, \quad (24)$$

which yields a norm of 1 and $\alpha^{m/2}/\beta^{3p/2}$ for the unscaled and scaled densities, respectively.

Taking into account the general normalization for the wave functions introduced by Eq. (24), the free minimization in terms of Lagrange multipliers becomes

$$T_s[n] = \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r \right. \\ \left. + \int v([n], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n(\mathbf{r}) \right) d^3 r \right. \\ \left. - \sum_{i=1}^{N_s} n_i \epsilon_i[n] \left(\int |\phi_i(\mathbf{r})|^2 d^3 r - \frac{\int n(\mathbf{r}) d^3 r}{N_e} \right) \right\}, \quad (25)$$

which, as it can be easily verified, yields Eq. (3) for the unscaled density and Eq. (23) for the scaled density. Therefore, as also shown in Sec. III B, the meaning of the symbol \perp in Levy's constraint search must be modified to read *orthogonal and normalized to $(\int n/N_e)^{1/2}$* .

It also important to notice that the functional derivative of $T_s[n]$, defined by Eq. (25), with respect to the density is

$$\frac{\delta T_s[n]}{\delta n(\mathbf{r})} = -v(\mathbf{r}) + \frac{\sum_{i=1}^{N_s} n_i \epsilon_i[n]}{N_e}, \quad (26)$$

which by comparison with Eq. (6) defines the Lagrange multiplier μ as

$$\mu = \frac{\sum_{i=1}^{N_s} n_i \epsilon_i[n]}{N_e}. \quad (27)$$

V. SCALING OF $T_s[n]$ AND $\delta T_s[n]/\delta n$

A. Scaling of $T_s[n]$ via KS equations

The scaling of $T_s[n]$ under general homogeneous scaling of the coordinates can be investigated in different ways, probably the most straightforward being a direct integration of the KS equations [Eq. (18)] after multiplying it by $n_i \phi_{\alpha\beta mp}^{(i)*}$, and adding up the first N_s lowest energy states. Such a procedure yields

$$\begin{aligned} & -\frac{1}{2} \sum_{i=1}^{N_s} \int n_i \phi_{\alpha\beta mp}^{(i)*}(\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) d^3 r \\ & + \int v([n_{\alpha\beta mp}], \mathbf{r}) n_{\alpha\beta mp}(\mathbf{r}) d^3 r \\ & = \sum_{i=1}^{N_s} n_i \epsilon_i[\alpha\beta mp] \int |\phi_{\alpha\beta mp}^{(i)}(\mathbf{r})|^2 d^3 r, \end{aligned} \quad (28)$$

where the first term on the left-hand side of this expression is the noninteracting kinetic energy for the scaled density; hence,

$$\begin{aligned} T_s[n_{\alpha\beta mp}] & = -\frac{1}{2} \sum_{i=1}^{N_s} \int n_i \phi_{\alpha\beta mp}^{(i)*}(\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) d^3 r \quad (29) \\ & = \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \int |\phi_{\alpha\beta mp}^{(i)}(\mathbf{r})|^2 d^3 r \\ & \quad - \int v([n_{\alpha\beta mp}], \mathbf{r}) n_{\alpha\beta mp}(\mathbf{r}) d^3 r, \end{aligned} \quad (30)$$

which, by Eqs. (7)–(9), (19), and (20), reduces to

$$\begin{aligned} T_s[n_{\alpha\beta mp}] & = \sum_{i=1}^{N_s} n_i \beta^{2p} \epsilon_i[n] \frac{\lambda^m}{\beta^{3p}} - \int \beta^{2p} v([n], \beta^p \mathbf{r}) \lambda^m n(\beta^p \mathbf{r}) d^3 r \\ & = \frac{\lambda^m}{\beta^p} \sum_{i=1}^{N_s} n_i \epsilon_i[n] - \frac{\lambda^m}{\beta^p} \int v([n], \beta^p \mathbf{r}) n(\beta^p \mathbf{r}) \beta^{3p} d^3 r. \end{aligned} \quad (31)$$

After changing the integration variable ($\beta^p \mathbf{r} \rightarrow \mathbf{r}$) and simplifying terms, Eq. (31) becomes

$$T_s[n_{\alpha\beta mp}] = \frac{\lambda^m}{\beta^p} \left(\sum_{i=1}^{N_s} n_i \epsilon_i[n] - \int v([n], \mathbf{r}) n(\mathbf{r}) d^3 r \right), \quad (32)$$

but we also know that

$$T_s[n] = \sum_{i=1}^{N_s} n_i \epsilon_i[n] - \int v([n], \mathbf{r}) n(\mathbf{r}) d^3 r, \quad (33)$$

and therefore

$$T_s[n_{\alpha\beta mp}] = \frac{\lambda^m}{\beta^p} T_s[n], \quad (34)$$

proving that $T_s[n]$ scales homogeneously with degree m in α and p in β .

B. Scaling of $T_s[n]$ via Lagrange multipliers

Another way of carrying out an investigation of the scaling of $T_s[n]$ is by using Levy's constrained search directly (see Appendixes A and B), but the investigation using Lagrange multipliers we describe next, although longer, is more tractable.

Let us proceed by introducing the change of variable $\mathbf{r} = \beta^p \mathbf{r}'$ and multiplying both sides of Eq. (25) by α^m to get

$$\begin{aligned} \alpha^m T_s[n] & = \beta^p \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \alpha^{m/2} \phi_i^*(\beta^p \mathbf{r}') \nabla_{\beta^p \mathbf{r}'}^2 \phi_i(\beta^p \mathbf{r}') d^3 r' \right. \\ & \quad + \int \beta^{2p} v([n], \beta^p \mathbf{r}') \left(\sum_{i=1}^{N_s} n_i |\alpha^{m/2} \phi_i(\beta^p \mathbf{r}')|^2 - \alpha^m n(\beta^p \mathbf{r}') \right) d^3 r' \\ & \quad \left. - \sum_{i=1}^{N_s} n_i \beta^{2p} \epsilon_i \left(\int |\alpha^{m/2} \phi_i(\beta^p \mathbf{r}')|^2 d^3 r' - \frac{\alpha^m \int n(\mathbf{r}') d^3 r'}{\beta^{3p}} \right) \right\}, \end{aligned} \quad (35)$$

which, by Eqs. (7) and (9) and taking into account that the scaled and unscaled wave functions span the same Hilbert space, becomes

$$\begin{aligned} \frac{\alpha^m}{\beta^p} T_s[n] & = \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r + \int v([n_{\alpha\beta mp}], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n_{\alpha\beta mp}(\mathbf{r}) \right) d^3 r \right. \\ & \quad \left. - \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \left(\int |\phi_i(\mathbf{r})|^2 d^3 r - \frac{\int n_{\alpha\beta mp}(\mathbf{r}) d^3 r}{N_e} \right) \right\}, \end{aligned} \quad (36)$$

where $v([n_{\alpha\beta mp}], \mathbf{r})$ and $\epsilon_i[n_{\alpha\beta mp}]$ are defined by Eqs. (19) and (20), respectively.

The right-hand side of Eq. (36) is a search for a set of orthogonal wave functions $\{\phi\}$ normalized to $(\int n_{\alpha\beta mp}(\mathbf{r})d^3r/N_e)^{1/2}$ that yields the scaled density $n_{\alpha\beta mp}(\mathbf{r})$ and minimizes the kinetic energy, that is, $T_s[n_{\alpha\beta mp}]$, and once more we get Eq. (34).

The same result should be obtained by evaluating $T_s[n]$ at the scaled density. In fact that is the case, as we prove next. We start by noticing that for the noninteracting kinetic energy Eq. (25) evaluated at the scaled density Eq. (9) we have

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3r \right. \\ &+ \int v([n_{\alpha\beta mp}], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n_{\alpha\beta mp}(\mathbf{r}) \right) d^3r \\ &\left. - \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \left(\int |\phi_i(\mathbf{r})|^2 d^3r - \frac{\int n_{\alpha\beta mp}(\mathbf{r}) d^3r}{N_e} \right) \right\}; \end{aligned} \quad (37)$$

but the search could be done also over the scaled wave functions that yield the scaled density because they belong to the same Hilbert space as the unscaled wave functions

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= \min_{\{\phi_{\alpha\beta mp}\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_{\alpha\beta mp}^{(i)*}(\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) d^3r \right. \\ &+ \int v([n_{\alpha\beta mp}], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_{\alpha\beta mp}^{(i)}(\mathbf{r})|^2 - n_{\alpha\beta mp}(\mathbf{r}) \right) d^3r \\ &- \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \left(\int |\phi_{\alpha\beta mp}^{(i)}(\mathbf{r})|^2 d^3r \right. \\ &\left. \left. - \frac{\int n_{\alpha\beta mp}(\mathbf{r}) d^3r}{N_e} \right) \right\}. \end{aligned} \quad (38)$$

Replacing the scaled wave functions and density [Eqs. (7) and (9)] into the expression above, one gets

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \alpha^{m/2} \phi_i^*(\beta^p \mathbf{r}) \nabla^2 \alpha^{m/2} \phi_i(\beta^p \mathbf{r}) d^3r \right. \\ &+ \int v([n_{\alpha\beta mp}], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\alpha^{m/2} \phi_i(\beta^p \mathbf{r})|^2 - \alpha^m n(\beta^p \mathbf{r}) \right) d^3r \\ &- \sum_{i=1}^{N_s} n_i \epsilon_i[n_{\alpha\beta mp}] \left(\int |\alpha^{m/2} \phi_i(\beta^p \mathbf{r})|^2 d^3r \right. \\ &\left. \left. - \frac{\alpha^m \int n(\mathbf{r}) d^3r}{\beta^{3p} N_e} \right) \right\}, \end{aligned} \quad (39)$$

which after the change of variable $\beta^p \mathbf{r} \rightarrow \mathbf{r}$ takes the form

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= \alpha^m \min_{\{\phi\}} \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3r \right. \\ &+ \frac{\int v([n_{\alpha\beta mp}], \mathbf{r}/\beta^p)}{\beta^{2p}} \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n(\mathbf{r}) \right) d^3r \\ &\left. - \sum_{i=1}^{N_s} n_i \frac{\epsilon_i[n_{\alpha\beta mp}]}{\beta^{2p}} \left(\int |\phi_i(\mathbf{r})|^2 d^3r - \frac{\int n(\mathbf{r}) d^3r}{N_e} \right) \right\}, \end{aligned} \quad (40)$$

but the minimization here is performed by a search over all orthogonal sets of wave functions normalized to $(\int n(\mathbf{r})d^3r/N_e)^{1/2}$ that yields the unscaled density, which is the definition of $T_s[n]$ and therefore we obtain Eq. (34) once again. We also obtain the scaling expressions for the potential and eigenvalues given by Eqs. (19) and (20), respectively.

C. Scaling of $T_s[n]$ via wave functions

Equation (29) establishes the fact that, if the wave functions are solutions of the KS equations in Eq. (18), then, after all, the kinetic energy for the scale density can be calculated using only the scaled wave functions. Indeed, using Eq. (21) we can write

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_{\alpha\beta mp}^{(i)*} [n_{\alpha\beta mp}](\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)} \\ &[n_{\alpha\beta mp}](\mathbf{r}) d^3r, \end{aligned} \quad (41)$$

because all the rest of the terms in either Eq. (23) or Eq. (25) are zero, given that those scaled wave functions minimize the kinetic energy and obey all the constraints.

Consequently, by replacing Eq. (7) into Eq. (29), one must get the same scaling relation for $T_s[n_{\alpha\beta mp}]$ as in Eq. (34), which is readily proven true.

D. Scaling of $\delta T_s[n]/\delta n$

According to Eqs. (15) and (34) the scaling of the functional derivative of $T_s[n_{\alpha\beta mp}]$ is given by

$$\frac{\delta T_s[n_{\alpha\beta mp}]}{\delta n_{\alpha\beta mp}(\mathbf{r})} = \beta^{2p} \frac{\delta T_s[n]}{\delta n(\mathbf{r}')} \Big|_{\mathbf{r}'=\beta^p \mathbf{r}}, \quad (42)$$

which only depends on the parameters that scale the coordinates, in contrast to the scaling dependency of the kinetic energy functional on all the scaling parameters.

VI. PARAMETRIC DERIVATIVES OF $T_s[n_{\alpha\beta mp}]$

A. Derivative of $T_s[n_{\alpha\beta mp}]$ with respect to α

Taking the derivative of $T_s[n_{\alpha\beta mp}]$ [Eq. (34)] with respect to α we get

$$T_s[n] = \frac{\beta^p}{m\alpha^{m-1}} \int \frac{\delta T_s[n_{\alpha\beta mp}]}{\delta n_{\alpha\beta mp}(\mathbf{r})} \frac{\delta n_{\alpha\beta mp}(\mathbf{r})}{\delta \alpha} d^3r; \quad (43)$$

using Eqs. (9) and (42), and changing the integration variable to $\beta^p \mathbf{r}$, we have

$$T_s[n] = \int \frac{\delta T_s[n]}{\delta n(\mathbf{r})} n(\mathbf{r}) d^3 r, \quad (44)$$

which does not depend on any of the scaling parameters and was first published by Liu and Parr [17] but obtained through a faulty derivation [28]. For a detailed discussion of this issue see Sec. VIII.

B. Derivative of $T_s[n_{\alpha\beta mp}]$ with respect to β

We can also find the derivative of $T_s[n_{\alpha\beta mp}]$ [Eq. (34)] with respect to β , which leads to

$$T_s[n] = -\frac{p\beta^{p-1}}{\alpha^m} \int \frac{\delta T_s[n_{\alpha\beta mp}]}{\delta n_{\alpha\beta mp}(\mathbf{r})} \frac{\delta n_{\alpha\beta mp}(\mathbf{r})}{\delta \beta} d^3 r, \quad (45)$$

and by using Eqs. (9) and (42) again and changing the integration variable we get

$$T_s[n] = -\int \frac{\delta T_s[n]}{\delta n(\mathbf{r})} \mathbf{r} \cdot \nabla n(\mathbf{r}) d^3 r, \quad (46)$$

which, as Eq. (44), does not depend on any of the scaling parameters.

C. The case $\beta = \alpha$

But the most interesting case yet is when we couple α and β ($\beta = \alpha$) and take the derivative with respect to α . In this case $n_{\alpha\beta mp} \equiv n_{\alpha mp} = \alpha^m n(\alpha^p \mathbf{r})$, the parametric derivative of $T_s[n_{\alpha mp}]$ is

$$T_s[n] = \frac{\alpha^{p-m+1}}{(m-p)} \int \frac{\delta T_s[n_{\alpha mp}]}{\delta n_{\alpha mp}(\mathbf{r})} \frac{\delta n_{\alpha mp}(\mathbf{r})}{\delta \alpha} d^3 r, \quad (47)$$

and using Eq. (42) once more we get the general virial relation

$$T_s[n] = \frac{1}{m-p} \int \frac{\delta T_s[n]}{\delta n(\mathbf{r})} [mn(\mathbf{r}) + p\mathbf{r} \cdot \nabla n(\mathbf{r})] d^3 r, \quad (48)$$

which only depends on the exponents.

The first thing to notice is that if $m = p$ the noninteracting kinetic-energy functional $T_s[n]$ is left invariant and we get

$$\int \frac{\delta T_s[n]}{\delta n(\mathbf{r})} [n(\mathbf{r}) + \mathbf{r} \cdot \nabla n(\mathbf{r})] d^3 r = 0, \quad (49)$$

which in combination with Eq. (48), and for any m and p , yields also Eqs. (44) and (46). Therefore, both expressions can be obtained as a consequence of the scaling of $T_s[n]$ under $n_{\alpha mp}(\mathbf{r}) = \alpha^m n(\alpha^p \mathbf{r})$ and its invariance for

$$n_\alpha(\mathbf{r}) = \alpha^m n(\alpha^m \mathbf{r}). \quad (50)$$

Second, for $m = 3$ and $p = 1$ (fixed number of electrons) we get the very well known virial expression [4–8,23]

$$T_s[n] = \frac{1}{2} \int \frac{\delta T_s[n]}{\delta n(\mathbf{r})} [3n(\mathbf{r}) + \mathbf{r} \cdot \nabla n(\mathbf{r})] d^3 r, \quad (51)$$

which can also be directly obtained by repeating a similar analysis for $\alpha^m = \beta^{3p}$.

The fact that Eq. (44) comes also from the same general expression as Eq. (51) further supports the validity of the first.

Of course, all the virials found obey the scaling property of $T_s[n_{\alpha\beta mp}]$. Indeed, a substitution of the scaled density into each of the integral relations also leads to Eq. (34).

D. Consequences for the total energy and μ

Multiplying the KS equations [Eq. (4)] by $n_i \phi_i^*(\mathbf{r})$, integrating, and adding up over the N_s lower eigenvalue states allows us to write the total energy of the KS noninteracting system as

$$\epsilon[n] = T_s[n] + \int v([n], \mathbf{r}) n(\mathbf{r}) d^3 r = \sum_{i=1}^{N_s} n_i \epsilon_i. \quad (52)$$

On the other hand, multiplying by the density $n(\mathbf{r})$ the minimization equation for the KS noninteracting problem in terms of the density [Eq. (6)], integrating, and using Eq. (44), we get

$$T_s[n] + \int v([n], \mathbf{r}) n(\mathbf{r}) d^3 r = \mu N_e, \quad (53)$$

which compared with Eq. (52) defines once more μ as in Eq. (27), and the total noninteracting ground-state energy as

$$\epsilon[n] = \mu N_e. \quad (54)$$

Equation (54) is not only a direct consequence of Eq. (44), but it was also obtained by Lindgren and Salomonson as a consequence of the extension of the search domains for wave functions and densities [31,32].

VII. NUMERICAL TESTS

A. Kinetic-energy functional

Even when we do not know the explicit general form of the kinetic-energy-density functional or its first functional derivative, we can still test the kinetic-energy integral relations numerically by noticing that, for the functional derivative of the kinetic-energy functional at the ground state, one has from Eq. (6) that

$$\frac{\delta T_s[n]}{\delta n(\mathbf{r})} = \mu - v([n], \mathbf{r}), \quad (55)$$

which in conjunction with Eq. (27) can be replaced into Eqs. (44), (46), and (51) to test their validity. Proceeding as described one gets

$$T_s[n] = \sum_{i=1}^{N_s} n_i \epsilon_i[n] - \int v([n], \mathbf{r}) n(\mathbf{r}) d^3 r \quad (56)$$

from Eq. (44),

$$T_s[n] = \int \left(v([n], \mathbf{r}) - \frac{\sum_{i=1}^{N_s} n_i \epsilon_i[n]}{N_e} \right) \mathbf{r} \cdot \nabla n(\mathbf{r}) d^3 r \quad (57)$$

from Eq. (46), and

$$T_s[n] = -\frac{1}{2} \int v([n], \mathbf{r}) [3n(\mathbf{r}) + \mathbf{r} \cdot \nabla n(\mathbf{r})] d^3 r \quad (58)$$

from Eq. (51).

Using this method we have tested the different integral relations for $T_s[n]$ in a number of DFT calculations for atoms, for both the Perdew and Wang (PW92) local density

TABLE I. Noninteracting kinetic energy for He, Li, Na, and Ca at the ground state calculated using the wave functions [Eq. (3)] and the integral relations [Eqs. (56)–(58)]. All in Hartree.

$T_s[n]$	He		Li	
	PW92	PBE	PW92	PBE
Eq. (3)	2.767389	2.855948	7.237015	7.401883
Eq. (56)	2.767389	2.855948	7.237015	7.401883
Eq. (57)	2.767389	2.855948	7.237015	7.401884
Eq. (58)	2.767389	2.855948	7.237015	7.401883
	Na		Ca	
Eq. (3)	160.894848	161.835704	674.654934	676.671267
Eq. (56)	160.894849	161.835705	674.654933	676.671266
Eq. (57)	160.894853	161.835709	674.654953	676.671287
Eq. (58)	160.894848	161.835704	674.654934	676.671268

approximation (LDA) and the Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) [33,34], with very good results. Table I shows the values of $T_s[n]$ calculated using the different virial expressions for He, Li, Na, and Ca as examples.

B. Scaling of the KS potential, eigenvalues, and total energy

Numerical tests for different atoms also confirmed the scaling properties of the ground-state KS potential and eigenvalues. As an example, Fig. 1 shows the left- and right-hand sides of Eq. (19) for He, Li, Na, and Ca, in the local density (PW92) [33] and generalized gradient (PBE) [34] approximations. The left-hand side of Eq. (19) was calculated by inverting the KS equations for the highest occupied *scaled* S -wave function and its eigenvalue.

VIII. LINEAR SCALING OF $T_s[\alpha n]$

We have provided analytical demonstrations and numerical evidence of the homogeneous scaling properties of the noninteracting kinetic-energy functional under general homogeneous coordinate scaling, including the case of density scaling which leads to Eq. (44). However, that relation has been controversial since Liu and Parr's [17] attempt to prove it was first supposedly shown incorrect by Chan and Handy [19].

One of Chan and Hardy's [19], as well as Gál's [28], arguments is that if $T_s[\alpha n] = \alpha T_s[n]$ then $T_s[n] = T_{vW}[n]$, where $T_{vW}[n]$ is the von Weizsäcker [35] kinetic-energy functional which is exact for one-state, up to two electrons, systems. The line of reasoning is the following. Assume that we have a density which integrates to $N_e > 2$, using $\alpha = 1/N_e$; from Eq. (34) ($m = 1, p = 0$) we get

$$T_s[n/N_e] = T_s[n]/N_e. \quad (59)$$

But $\int n/N_e = 1$, so we have a one-electron system, meaning that $T_s[n/N_e] = T_{vW}[n/N_e] = T_{vW}[n]/N_e$, and therefore $T_s[n] = T_{vW}[n]$. But the problem with this argument is that even when the $1/N_e$ -scaled density integrates to 1, it is still the sum over more than one wave function, in contrast with the one- or two-electron density which only contains one state; i.e., the scaled density cannot have a shape that corresponds with that of a one- or two-electron density. The number of fermions

determines the shape of the density while its normalization is essentially arbitrary (i.e., as a probability density it could be normalized to 1 instead of to the number of particles). Therefore, the kinetic energy of the scaled density cannot be the von Weizsäcker functional. But let us prove that analytically once again.

Multiplying Eq. (3) by α we can write

$$\begin{aligned} \alpha T_s[n] = \min_{\{\phi\}} & \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \alpha^{1/2} \phi_i^*(\mathbf{r}) \nabla^2 \alpha^{1/2} \phi_i(\mathbf{r}) d^3r \right. \\ & + \int v([n], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\alpha^{1/2} \phi_i(\mathbf{r})|^2 - \alpha n(\mathbf{r}) \right) d^3r \\ & \left. - \sum_{i=1}^{N_s} n_i \epsilon_i \left(\int |\alpha^{1/2} \phi_i(\mathbf{r})|^2 d^3r - \alpha \right) \right\}. \quad (60) \end{aligned}$$

Introducing the scaled wave functions and density as $\phi_\alpha^{(i)}(\mathbf{r}) = \alpha^{1/2} \phi_i(\mathbf{r})$ and $n_\alpha(\mathbf{r}) = \alpha n(\mathbf{r})$, respectively, Eq. (60) becomes

$$\begin{aligned} \alpha T_s[n] = \min_{\{\phi_\alpha\}} & \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_\alpha^{(i)*}(\mathbf{r}) \nabla^2 \phi_\alpha^{(i)}(\mathbf{r}) d^3r \right. \\ & + \int v([n], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_\alpha^{(i)}(\mathbf{r})|^2 - n_\alpha(\mathbf{r}) \right) d^3r \\ & \left. - \sum_{i=1}^{N_s} n_i \epsilon_i \left(\int |\phi_\alpha^{(i)}(\mathbf{r})|^2 d^3r - \alpha \right) \right\}, \quad (61) \end{aligned}$$

and using the fact that the original and scaled wave functions span the same space we can write

$$\begin{aligned} \alpha T_s[n] = \min_{\{\phi\}} & \left\{ -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3r \right. \\ & + \int v([n], \mathbf{r}) \left(\sum_{i=1}^{N_s} n_i |\phi_i(\mathbf{r})|^2 - n_\alpha(\mathbf{r}) \right) d^3r \\ & \left. - \sum_{i=1}^{N_s} n_i \epsilon_i \left(\int |\phi_i(\mathbf{r})|^2 d^3r - \alpha \right) \right\}. \quad (62) \end{aligned}$$

The right-hand side of this equation delivers the minimum value of the noninteracting kinetic energy, constrained to sets of orthogonal wave functions $\{\phi\}$ normalized to $\alpha^{1/2}$ that yield the scaled density n_α . That is precisely $T_s[n_\alpha]$; therefore, $\alpha T_s[n] = T_s[n_\alpha]$ and consequently, in general, $T_s[n/N_e] \neq T_{vW}[n/N_e]$. Notice that only the norm of the wave functions changes; the occupation numbers do not change at all. Besides, the KS potential is also left intact, showing that the physics has not changed.

Chan and Handy [17] also performed numerical tests to study the scaling of $T_s[n]$ under density scaling. But those tests changed the number of states, which, in light of what has been shown in this paper and particularly in this section, is erroneous.

Another numerical study of the scaling of $T_s[n]$ under density scaling was undertaken by Borgoo, Teale, and Tozer [36],

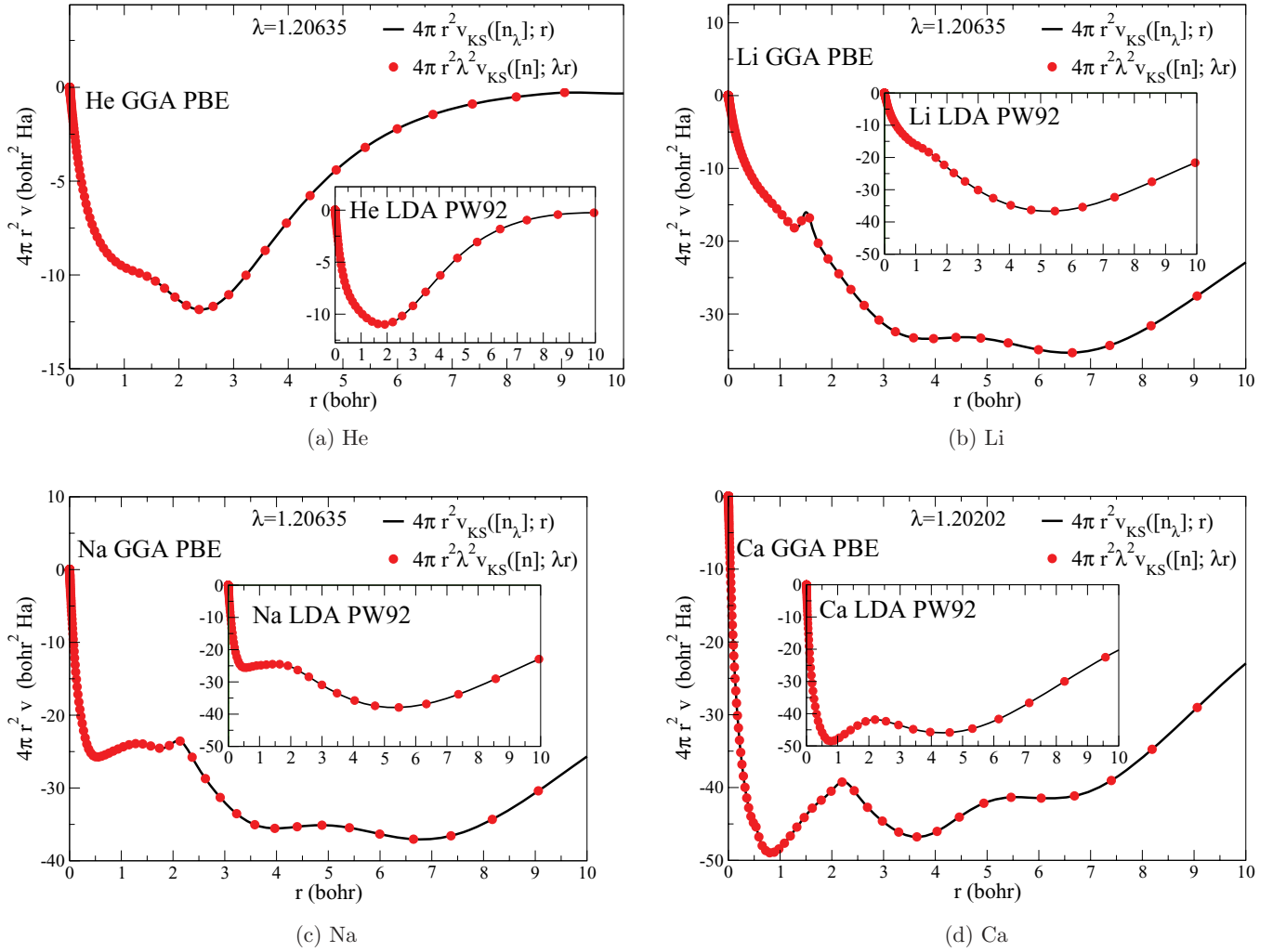


FIG. 1. (Color online) Scaling of the Kohn-Sham potential of (a) He, (b) Li, (c) Na, and (d) Ca calculated using PBE-GGA and PW92-LDA for the exchange-correlation functional. Left- (dots) and right-hand sides (line) of Eq. (19) with $\beta^p \equiv \lambda$.

who essentially investigated the behavior of

$$k = \frac{\int [\mu - v([n], \mathbf{r})] n(\mathbf{r}) d^3 r}{T_s[n]} \quad (63)$$

for exact densities assuming that μ was the chemical potential. However, that is a mistake, because as we have shown in Secs. VID and IV, the Lagrange multiplier μ is the average noninteracting total energy per electron [Eqs. (27) and (54)]. They also made the mistake of allowing the number of states to change during the calculations for closed-subshell atoms.

Nonetheless, Gál [28] proved that the demonstration of Liu and Parr was incorrect by using the fact that wave functions and densities do not form a one-to-one map in general, which renders inappropriate the applicability of the chain rule for functional derivation.

It may be possible to correct the errors in Liu and Parr's demonstration in light of new developments, which account for the necessary extensions of the domains of wave functions and densities, that allow to take unconstrained functional derivatives when using Lagrange multipliers and the chain rule for functional differentiation [31,32,37]. But that goes beyond

this work, which avoids the use of the chain rule for functional differentiation, and proves, without using the chain rule for functional derivatives at all, that $T_s[n]$ does scale linearly under density scaling.

IX. REMARKS

We have introduced a generalization of homogeneous coordinate scaling [Eqs. (7) and (9)] and demonstrated that, although one can easily find its corresponding noninteracting kinetic-energy functional $T_s[n_{\alpha\beta mp}]$ via variable substitution in the $T_s[n]$ functional and KS equations, a modification of the constrained search is in order to get the same expression for $T_s[n_{\alpha\beta mp}]$ by direct evaluation of $T_s[n]$ at the scaled density. The modification defines the norm of the wave functions directly from the density for a given number of electrons [Eq. (24)]. It is a natural generalization of Levy's constrained search (Sec. IV) that brings consistency between results obtained using variable substitution in $T_s[n]$ and KS equations and those obtained from the evaluation of $T_s[n]$ at the scaled density.

Consequently, it is shown that, using variable substitution in the KS equations, variable substitution into $T_s[n]$, or the evaluation of $T_s[n]$ at the scaled density, $T_s[n]$ scales homogeneously [Eq. (34)] under the generalized scaling [Eqs. (7) and (9)].

Also, a general integral relation or virial for the kinetic energy of the KS noninteracting kinetic energy [Eq. (48)] was found via parametric derivatives. The general virial for $T_s[n]$ contains as a particular case a well-known and widely accepted integral expression [Eq. (51)] and reduces to two expressions [Eqs. (44) and (46)] due to the invariance of $T_s[n]$ under a specific scaling [Eq. (50)]. In addition, numerical calculations of all the virial expressions for $T_s[n]$ for different atoms confirmed their validity, reasserting at the same time the homogeneous scaling of $T_s[n]$.

Furthermore, the linear homogeneous scaling of $T_s[n]$ under density scaling was discussed in more detail, including the reasons why analytical work and numerical tests performed by other authors were at fault.

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APPENDIX A: THIRD PROOF OF $T_s[n_{\alpha\beta mp}] = \alpha^m T_s[n]/\beta^p$

Multiply Eq. (2) by α^m and introduce the change of variable $\mathbf{r} = \beta^p \mathbf{r}'$ in its right-hand side to get

$$\alpha^m T_s[n] = \beta^p \min_{\{\phi\}_\perp \rightarrow n} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \times \int \alpha^{m/2} \phi_i^*(\beta^p \mathbf{r}) \nabla^2 \alpha^{m/2} \phi_i(\beta^p \mathbf{r}) d^3 r, \quad (\text{A1})$$

which by Eq. (7) reduces to

$$\alpha^m T_s[n] = \beta^p \min_{\{\phi\}_\perp \rightarrow n} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_{\alpha\beta mp}^{(i)*}(\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) d^3 r. \quad (\text{A2})$$

Notice that this is a minimization of the average of the kinetic energy for the scaled wave functions over all the orthonormal sets of unscaled wave functions that yield the unscaled density. That is the same as performing the search over sets of orthogonal wave functions normalized to $\alpha^{m/2}/\beta^{3p/2}$ that yield the scaled density and evaluating the kinetic energy at those wave functions. Therefore, we can write

$$\frac{\alpha^m}{\beta^p} T_s[n] = \min_{\{\phi\}_\perp \rightarrow n_{\alpha\beta mp}} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d^3 r, \quad (\text{A3})$$

which proves again Eq. (34).

APPENDIX B: FOURTH PROOF OF $T_s[n_{\alpha\beta mp}] = \alpha^m T_s[n]/\beta^p$

Another way to analyze the scaling of $T_s[n]$ is by returning to Eq. (22) and realizing that it represents a search that selects wave functions scaled as in Eq. (7) to calculate the kinetic energy. That is the same as selecting the wave functions that yield the unscaled density and scaling them afterward to calculate the kinetic energy. Therefore,

$$T_s[n_{\alpha\beta mp}] = \min_{\{\phi\}_\perp \rightarrow n} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_{\alpha\beta mp}^{(i)*}(\mathbf{r}) \nabla^2 \phi_{\alpha\beta mp}^{(i)}(\mathbf{r}) d^3 r, \quad (\text{B1})$$

which by Eq. (7) becomes

$$T_s[n_{\alpha\beta mp}] = \frac{\alpha^m}{\beta^p} \min_{\{\phi\}_\perp \rightarrow n} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \times \int \phi_i^*(\beta^p \mathbf{r}) \nabla_{\beta^p \mathbf{r}}^2 \phi_i^{(i)}(\beta^p \mathbf{r}) \beta^{3p} d^3 r, \quad (\text{B2})$$

and by changing the integration variable ($\beta^p \mathbf{r} \rightarrow \mathbf{r}$) yields

$$\begin{aligned} T_s[n_{\alpha\beta mp}] &= \frac{\alpha^m}{\beta^p} \min_{\{\phi\}_\perp \rightarrow n} -\frac{1}{2} \sum_{i=1}^{N_s} n_i \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i^{(i)}(\mathbf{r}) d^3 r \\ &= \frac{\alpha^m}{\beta^p} T_s[n]. \end{aligned} \quad (\text{B3})$$

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