First-degree homogeneous *N*-particle noninteracting kinetic-energy density functionals

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It is known in density-functional theory that the noninteracting kinetic-energy density functional $T_s[\rho]$ is not first-degree homogeneous in density scaling. However, it is shown here that, for every particle number N, there is an N-particle noninteracting kinetic-energy density functional $T_N[\rho]$, that is, a density functional that gives the noninteracting kinetic energy for N-particle densities, which is of first-degree homogeneity in the density $\rho(\vec{r})$. This gives a powerful tool, a strong requirement, for constructing such functionals. A systematic procedure to obtain the real part of $T_N[\rho]$, the full $T_N[\rho]$ in one-dimension, for each N is also proposed. It is pointed out, further, that in the Euler-Lagrange equations that determine the one-particle orbitals that define $T_s[\rho]$, the Lagrange multiplier that forces the orbitals to yield $\rho(\vec{r})$ is not other than the first derivative of $T_s[\rho]$, $\delta T_s[\rho]/\delta\rho(\vec{r})$, which yields a natural derivation of the Kohn-Sham equations. Utilizing the same idea, it is shown for ground states how the Schrödinger equation can be derived from the basics of density-functional theory as well.

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I. INTRODUCTION

The ultimate goal of density-functional theory [1] is to determine ground-state properties of particle systems directly from the ground-state particle density without the use of wave functions. This would require the knowledge of the ground-state-energy density functional $E_v[\rho]$, which, for a given external potential $v(\vec{r})$, takes its minimum at the real ground-state N-particle density of the N-particle system [2], that is, for ground-state densities

$$\frac{\delta E_v[\rho]}{\delta_N \rho(\vec{r})} = 0, \tag{1}$$

or, resolving the constraint

$$\int \rho(\vec{r})\, d\vec{r} = N \tag{2}$$

on the functional differentiation (utilizing the formula of number-conserving functional differentiation [3], or by the usual method of Lagrange multipliers),

$$\frac{\delta E_v[\rho]}{\delta \rho(\vec{r})} = \mu, \tag{3}$$

where μ is determined by Eq. (2). A major part of $E_v[\rho]$ is the noninteracting kinetic-energy density functional $T_s[\rho]$, the concept of which is introduced into density-functional theory to get single-particle Schrödinger equations, the Kohn-Sham equations [4–6],

$$-\tfrac{1}{2}\nabla^2 u_i(\vec{r}) + \nu_{\mathrm{KS}}(\vec{r}) u_i(\vec{r}) = \varepsilon_i^{\mathrm{KS}} u_i(\vec{r}), \quad i = 1, \ldots, N \tag{4}$$

with

$$\nu_{\mathrm{KS}}(\vec{r}) = \frac{\delta(E_v[\rho] - T_s[\rho])}{\delta \rho(\vec{r})}, \tag{5}$$

for the determination of the ground-state density, instead of the direct use of Eq. (3), through

$$\rho(\vec{r}) = \sum_{i=1}^{N} u_i^*(\vec{r}) u_i(\vec{r}), \tag{6}$$

hereby treating a large part of the energy exactly, as

$$E_v = T_s[u_1, \ldots, u_N] + E_v[\rho] - T_s[\rho], \tag{7}$$

where

$$T_s[u_1, u_1^*, \ldots, u_N, u_N^*] = \int \sum_{i=1}^{N} u_i^*(\vec{r})(-\tfrac{1}{2}\nabla^2) u_i(\vec{r})\, d\vec{r}. \tag{8}$$

Though the Kohn-Sham method eliminates the problem of the lack of knowledge of $T_s[\rho]$, investigating T_s as a functional of $\rho(\vec{r})$ is of great importance as the introduction of orbitals $u_i(\vec{r})$ means a step backward on the road to using the particle density as the basic variable in determining ground-state properties, which gets more and more disadvantageous with increasing number of particles. To discover the properties of $T_s[\rho]$ and derive exact relations for it is essential to obtain adequate approximations for it. One of its substantial properties is its behavior under coordinate scaling namely, scaling of degree-two homogeneity in coordinate [7], from which

$$T_s[\rho] = -\frac{1}{2} \int \rho(\vec{r})\, \vec{r} \cdot \nabla \frac{\delta T_s[\rho]}{\delta \rho(\vec{r})}\, d\vec{r} \tag{9}$$

follows [8], giving the virial theorem of density-functional theory through Eq. (3).

Recently, the question of homogeneity of T_s in density scaling has attracted much attention, which was induced by a result of Liu and Parr [9], namely,

$$T_s[\rho]=\int \rho(\vec{r})\frac{\delta T_s[\rho]}{\delta\rho(\vec{r})}d\vec{r}, \tag{10}$$

that is, $T_s[\rho]$ is first-degree homogeneous in ρ. Equation (10), however, as was shown later [10], cannot be correct as this would mean that $T_s[\rho]$ is equal to the Weizsäcker functional [11]

$$T_W[\rho]=\frac{1}{8}\int\frac{|\nabla\rho(\vec{r})|^2}{\rho(\vec{r})}d\vec{r} \tag{11}$$

for all $\rho(\vec{r})$, not only for one-particle densities, for which Eq. (11) is an exact expression for $T_s[\rho]$. The source of the problem with the derivation of Eq. (10) in Ref. [9] has been pointed out to be the inappropriate handling of the complex wave-function–density–wave-function mapping of density-functional theory [12]; with this, the conclusion made to resolve the contradiction about Eq. (10) [10], that $T_s[\rho]$ does not have an unconstrained derivative [which is quite obvious, considering the definition given by Eq. (17), but note that the logic behind the proof of Ref. [9] could be applied to fractional particle-number generalizations of Eq. (17) as well], is avoided. Also, a proposed correction of Eq. (10), namely, replacing the unconstrained functional differentiation with number-conserving functional differentiation, has been proved to be wrong [3] as

$$\int \rho(\vec{r})\frac{\delta T_s[\rho]}{\delta_N\rho(\vec{r})}d\vec{r}=0, \tag{12}$$

like for any number-conserving functional derivative.

In this paper it will be shown that Eq. (10) can be true for N-particle noninteracting kinetic-energy density functionals, $T_N[\rho]$, which are exact expressions for $T_s[\rho]$ for N-particle systems, that is,

$$T_s[\rho_N]=T_N[\rho_N], \tag{13}$$

where ρ_N denotes N-particle densities; the Weizsäcker functional giving an example, being a one-particle noninteracting kinetic-energy density functional,

$$T_s[\rho_1]=T_W[\rho_1]. \tag{14}$$

For simplicity in notation, throughout spin is not taken into account; see Appendix B for the discussion of the case when multiple occupations of the Kohn-Sham orbitals are allowed.

II. NONINTERACTING KINETIC ENERGY AND ONE-PARTICLE EQUATIONS

The noninteracting kinetic energy of a Fermion system of density distribution $\rho(\vec{r})$ is defined in density-functional theory as [13,6]

$$T_s[\rho]=\min_{\psi_D\to\rho} T[\psi_D] \tag{15}$$

with

$$T[\psi]=\langle\psi|\sum_{i=1}^{N}-\tfrac{1}{2}\nabla_i^2|\psi\rangle. \tag{16}$$

ψ_D denotes normalized Slater determinants, that is,

$$T_s[\rho]=\min_{\{u_i\}\to\rho}\int\sum_{i=1}^{N}u_i^*(\vec{r})(-\tfrac{1}{2}\nabla^2)u_i(\vec{r})d\vec{r}, \tag{17}$$

$u_i(\vec{r})$ being normalized one-particle functions. Equation (15) defines a $\psi_D[\rho]$ mapping,

$$\rho\to\psi_D:\quad \rho[\psi_D]=\rho,\quad T[\psi_D]=T_s[\rho], \tag{18}$$

where

$$\rho[\psi]=\langle\psi|\hat{\rho}(\vec{r})|\psi\rangle. \tag{19}$$

For a given $\rho(\vec{r})$, thus, Eq. (18) gives the $\{u_i(\vec{r})\}_{i=1}^N$ from which $T_s[\rho]$ can be produced through Eq. (8), establishing a minimization problem with $u_i(\vec{r})$ as variational variables. One approach of this problem [6] (or see p. 151 of [1]) is to minimize $T_s[u_1,u_1^*,\ldots,u_N,u_N^*]$ with Eq. (6) and

$$\int u_i^*(\vec{r})u_j(\vec{r})d\vec{r}=\delta_{ij} \tag{20}$$

as constraints, getting the Euler-Lagrange equations

$$-\tfrac{1}{2}\nabla^2u_i(\vec{r})+\lambda_\rho(\vec{r})u_i(\vec{r})=\varepsilon_iu_i(\vec{r}),\quad i=1,\ldots,N, \tag{21}$$

in canonical form, for the minimizing $\{u_i(\vec{r})\}_{i=1}^N$, where λ_ρ is a Lagrange multiplier corresponding to the constraint Eq. (6) and ε_i are due to the normalization constraint, Eq. (20) with $j=i$. In Eq. (21), thus, λ_ρ is determined by Eq. (6), that is by $\rho(\vec{r})$, but Eq. (21) does not say anything more about it, though, of course, for v-representable densities, it must give $v_{KS}(\vec{r})$ of Eq. (4) within an additive constant.

With a different approach to the variational problem established by Eq. (18) for determining $\{u_i(\vec{r})\}_{i=1}^N$ for a given $\rho(\vec{r})$, however, λ_ρ can be identified. Instead of minimizing $T_s[u_1,u_1^*,\ldots,u_N,u_N^*]$, the minimization of

$$\Delta_{T_s}[u_1,u_1^*,\ldots,u_N,u_N^*]:=T_s[u_1,u_1^*,\ldots,u_N,u_N^*]-T_s[\rho[u_1,u_1^*,\ldots,u_N,u_N^*]] \tag{22}$$

also leads to the proper $\{u_i(\vec{r})\}_{i=1}^N$ for a $\rho(\vec{r})$ since

$$\Delta_{T_s}[u_1,u_1^*,\ldots,u_N,u_N^*]\geqslant 0 \tag{23}$$

for any normalized $u_i(\vec{r})$ $(i=1,\ldots,N)$ for any N, with equality for the $\{u_i(\vec{r})\}_{i=1}^N$ determined by Eq. (18). (Equation (23) holds by definition of $T_s[\rho]$: a set of $u_i(\vec{r})$ determines a $\rho(\vec{r})$, for which $T_s[\rho]$ gives the minimum of $T_s[\tilde{u}_1,\tilde{u}_1^*,\ldots,\tilde{u}_N,\tilde{u}_N^*]$.) Minimizing $\Delta_{T_s}[u_1,u_1^*,\ldots,u_N,u_N^*]$, with only orthonormalization constraints [Eq. (20)], gives all

$\{u_i(\vec{r})\}_{i=1}^N$ that correspond to some $\rho(\vec{r})$ of normalization N through the mapping Eq. (18). The corresponding Euler-Lagrange equations,

$$-\tfrac{1}{2}\nabla^2 u_i(\vec{r}) - \frac{\delta T_s[\rho]}{\delta\rho(\vec{r})} u_i(\vec{r}) = \varepsilon_i u_i(\vec{r}), \quad i=1,\ldots,N, \tag{24}$$

show that the functional derivative of $T_s[\rho]$ itself is what is responsible for the constraint of "fixed $\rho(\vec{r})$"; giving a $\rho(\vec{r})$, $\delta T_s[\rho]/\delta\rho(\vec{r})$ provides the corresponding $\{u_i(\vec{r})\}_{i=1}^N$ through Eq. (24). From Eq. (24) the Kohn-Sham equations (4) follow straight away for v-representable, ground-state densities through the Hohenberg-Kohn Euler-equation (3), that is,

$$\frac{\delta T_s[\rho]}{\delta\rho(\vec{r})} + v_{\mathrm{KS}}(\vec{r}) = \mu, \tag{25}$$

with

$$\varepsilon_i^{\mathrm{KS}} = \varepsilon_i + \mu, \tag{26}$$

giving a simple derivation of them. Equation (25) brings a new constraint, the given external potential $v(\vec{r})$, into Eq. (24) [as $v_{\mathrm{KS}}(\vec{r}) = v(\vec{r}) + v_j(\vec{r}) + v_{\mathrm{xc}}(\vec{r})$, $v_j(\vec{r})$ being the classical Coulomb part and $v_{\mathrm{xc}}(\vec{r})$ being the exchange-correlation part of the potential of the interaction between the particles of the given system (N,v)]; thus, while Eq. (24) gives $\{u_i(\vec{r})\}_{i=1}^N$ for any $\rho(\vec{r})$, the Kohn-Sham equations give $\{u_i(\vec{r})\}_{i=1}^N$ for the $\rho(\vec{r})$ that is determined by $v(\vec{r})$, therefore being usable to determine a $\rho(\vec{r})$. Also, from Eq. (24), Eq. (9), that is, the behavior of $T_s[\rho]$ under coordinate scaling, is derivable directly, just as the virial theorem of density-functional theory can be derived from the Kohn-Sham equations [14], by integrating their gradients multiplied by $\rho(\vec{r})\vec{r}$ and doing some algebraic manipulation. It is worth pointing out that the reason why the procedure leading to Eq. (21) cannot give λ_ρ explicitly is that by minimizing only $T_s[u_1, u_1^*, \ldots, u_N, u_N^*]$, available information [Eq. (23)], given by the definition of $T_s[\rho]$, is lost, while the second variational procedure utilizes the definition of $T_s[\rho]$ fully, this way relaxing the external constraint of "fixed $\rho(\vec{r})$," incorporating it into the Euler-Lagrange equations naturally. The case of Levy's generalization of the Hohenberg-Kohn functional is similar, as it is defined by

$$F[\rho] = \min_{\psi\to\rho}\{T[\psi] + V[\psi]\} \tag{27}$$

with

$$V[\psi] = \langle\psi|\sum_{i<j}\frac{1}{|\vec{r}_i - \vec{r}_j|}|\psi\rangle \tag{28}$$

and ψ denoting normalized antisymmetric wave functions; thus, with

$$\Delta_F[\psi] := T[\psi] + V[\psi] - F[\rho[\psi]], \tag{29}$$

$$\Delta_F[\psi] \geqslant 0 \tag{30}$$

(for similar reasons as in the case of $T_s[\rho]$). Minimizing $\Delta_F[\psi]$ for a given N under the normalization constraint on ψ,

$$\langle\psi|\psi\rangle = 1, \tag{31}$$

yields the ψ that is associated to a ρ by density-functional theory, through

$$\rho\to\psi: \quad \rho[\psi] = \rho, \quad T[\psi] + V[\psi] = F[\rho], \tag{32}$$

the Euler-Lagrange equation

$$\sum_{i=1}^N -\tfrac{1}{2}\nabla_i^2\psi + \sum_{i<j}\frac{1}{|\vec{r}_i - \vec{r}_j|}\psi - \sum_{i=1}^N \frac{\delta F[\rho]}{\delta\rho(\vec{r}_i)}\psi = E'_\rho\psi \tag{33}$$

arising for ψ, where the Lagrange multiplier E'_ρ is determined by the constraint (31). [See Appendix A for the derivation of Eq. (33).] Among the solutions of Eq. (33) that give (the given) $\rho(\vec{r}), \psi_\rho$, that one corresponds to $\rho(\vec{r})$ [by Eq. (32)] that has the least E'_ρ since

$$E'_\rho = T[\psi_\rho] + V[\psi_\rho] - \int \rho(\vec{r})\frac{\delta F[\rho]}{\delta\rho(\vec{r})}d\vec{r}, \tag{34}$$

the last term being constant for fixed $\rho(\vec{r})$. This least E'_ρ gives a functional of $\rho(\vec{r})$,

$$E'_0[\rho] = F[\rho] - \int \rho(\vec{r})\frac{\delta F[\rho]}{\delta\rho(\vec{r})}d\vec{r}. \tag{35}$$

For (ground-state) v-representable $\rho(\vec{r})$, Eq. (33) leads to the Schrödinger equation

$$\sum_{i=1}^N -\tfrac{1}{2}\nabla_i^2\psi + \sum_{i<j}\frac{1}{|\vec{r}_i - \vec{r}_j|}\psi + \sum_{i=1}^N v(\vec{r}_i)\psi = E\psi \tag{36}$$

through the Hohenberg-Kohn Euler-equation,

$$\frac{\delta F[\rho]}{\delta\rho(\vec{r})} + v(\vec{r}) = \mu, \tag{37}$$

with

$$E = E'_\rho + \mu N. \tag{38}$$

(For not ground-state v-representable densities ρ, if $F[\rho]$ is differentiable, $E'_0[\rho]$ is not the minimum E'_ρ, that is, none of the minimum states ψ_0 of Eq. (33) gives ρ ($\psi_0 \neq \psi_\rho$).) It is worth emphasizing that Eq. (33) could not have been obtained by minimizing just $T[\psi] + V[\psi]$, similarly to the case of $T_s[\rho]$. It is important to note that Eq. (33) itself is just a mathematical construction without any physics, and the Hohenberg-Kohn Euler-equation (the Hohenberg-Kohn theorems) is what brings physical meaning into it, making it a physical law: the Schrödinger equation. It has been shown for ground states, thus, how Schrödinger's quantum mechan-

ics and the Kohn-Sham quantum mechanics emerge from density-functional theory (with its energy density functional

$$E_\nu[\rho] \equiv F[\rho] + \int \rho(\vec{r})\nu(\vec{r})d\vec{r} = E_0'[\rho] + \mu N \tag{39}$$

and variational principle for $E_\nu[\rho]$ for the determination of the ground-state density), through the minimization of $\Delta_F[\psi]$ and $\Delta_{T_s}[u_1,\ldots,u_N]$ under normalization constraint, using the Hohenberg-Kohn Euler-equation as postulatum.

Turning to the N-particle noninteracting kinetic-energy density functionals, which are defined by Eq. (13) though, of course, not uniquely, it is easy to see that $T_N[\rho]$ can take the place of $T_s[\rho]$ in density-functional theory for N-particle systems. From the definition (13) it follows that [3]

$$\frac{\delta T_s[\rho_N]}{\delta_N \rho(\vec{r})} = \frac{\delta T_N[\rho_N]}{\delta_N \rho(\vec{r})}, \tag{40}$$

hence T_s can be replaced by T_N in Eq. (1), thus the Euler equation

$$\frac{\delta T_N[\rho]}{\delta \rho(\vec{r})} + \nu_{\mathrm{KS}}(\vec{r}) = \mu_N \tag{41}$$

arises for the determination of the ground-state ρ_N, where μ_N is determined by Eq. (2) but, of course, is not the μ of Eq. (25) (from Eq. (40), using the number-conserving functional-differentiation formula [3],

$$\frac{\delta T_N[\rho_N]}{\delta \rho(\vec{r})} - \frac{\delta T_s[\rho_N]}{\delta \rho(\vec{r})} = \frac{1}{N}\int \rho_N(\vec{r}')\left\{\frac{\delta T_N[\rho_N]}{\delta \rho(\vec{r}')} - \frac{\delta T_s[\rho_N]}{\delta \rho(\vec{r}')}\right\} d\vec{r}' = c, \tag{42}$$

with $\mu_N - \mu = c$ for ground states). With Eq. (41), then, the Kohn-Sham equations can be derived through minimizing

$$\Delta_{T_N}[u_1,u_1^*,\ldots,u_N,u_N^*] := T_s[u_1,u_1^*,\ldots,u_N,u_N^*] - T_N[\rho[u_1,u_1^*,\ldots,u_N,u_N^*]] \tag{43}$$

under normalization constraint on $u_i(\vec{r})$ $(i=1,\ldots,N)$, getting the Euler-Lagrange equations

$$-\tfrac{1}{2}\nabla^2 u_i(\vec{r}) - \frac{\delta T_N[\rho]}{\delta \rho(\vec{r})} u_i(\vec{r}) = \varepsilon_i^N u_i(\vec{r}), \quad i=1,\ldots,N \tag{44}$$

with, utilizing Eq. (41),

$$\varepsilon_i^{\mathrm{KS}} = \varepsilon_i^N + \mu_N, \tag{45}$$

and

$$\varepsilon_i^N = \varepsilon_i + \mu - \mu_N; \tag{46}$$

as, for normalized $\{u_i(\vec{r})\}_{i=1}^N$,

$$\Delta_{T_N}[u_1,u_1^*,\ldots,u_N,u_N^*] = \Delta_{T_s}[u_1,u_1^*,\ldots,u_N,u_N^*], \tag{47}$$

since

$$\rho[u_1,u_1^*,\ldots,u_N,u_N^*] = \rho_N(\vec{r}). \tag{48}$$

For Eq. (9)

$$T_N[\rho_N] = -\frac{1}{2}\int \rho_N(\vec{r})\vec{r}\,\nabla \frac{\delta T_N[\rho_N]}{\delta \rho(\vec{r})} d\vec{r} \tag{49}$$

arises, which is quite natural since coordinate scaling conserves the normalization of $\rho(\vec{r})$. From $T_N[\rho]$ $(N=1,2,\ldots)$, formally $T_s[\rho]$ can be constructed for integer $\int \rho(\vec{r})d\vec{r}$,

$$T_s[\rho] = \sum_{N=1}^{\infty} T_N[\rho]\delta_{N,\int\rho}. \tag{50}$$

From $T_s[\rho]$ a type of $T_N[\rho]$ may be constructed by fixing the explicit N's, that is, $\int \rho(\vec{r})d\vec{r}$, in $T_s[\rho]$, considering $T_s[\rho]$ as a two-variable functional,

$$T_s[\rho] = \tilde{T}_s\left[\rho, \int \rho\right], \tag{51}$$

thus

$$T_N[\rho] = \tilde{T}_s[\rho,N], \tag{52}$$

and its derivative

$$\frac{\delta T_N[\rho]}{\delta \rho(\vec{r})} = \left(\frac{\delta \tilde{T}_s[\rho,N]}{\delta \rho(\vec{r})}\right)_N, \tag{53}$$

emphasizing that the right side of Eq. (53) is not a number-conserving functional derivative but just a partial functional derivative (only the explicit N's in $T_s[\rho]$ (a variable of $\tilde{T}_s[\rho,N]$) are fixed, the variation of the remaining part is unconstrained). In the next two sections, it will be shown how a degree-one homogeneous $T_N[\rho]$ can be defined for arbitrary particle number N, for which

$$T_N[\rho] = \int \rho(\vec{r})\frac{\delta T_N[\rho]}{\delta \rho(\vec{r})} d\vec{r}, \tag{54}$$

consequently,

$$\sum_{i=1}^{N} \varepsilon_i^N = 0, \tag{55}$$

that is,

$$\sum_{i=1}^{N} \varepsilon_i^{\mathrm{KS}} = \mu_N N \tag{56}$$

(not μN). It is worth noting here that with the concept of N-particle noninteracting kinetic energy, the local tempera-

ture $\tau(\vec{r})$ [15,16], introduced by Ghosh, Berkowitz, and Parr [15] into density-functional theory, may be redefined as

$$T_N = \int \tfrac{3}{2}\rho(\vec{r}) k\tau(\vec{r}) d\vec{r},$$

giving a local temperature of degree-zero homogeneity with respect to density scaling in the case of degree-one homogeneous $T_N[\rho]$'s.

III. ORBITALS INCORPORATING THE "GIVEN DENSITY" CONSTRAINT

In the previous section it was pointed out that the given $\rho(\vec{r})$ constraint in the determination of the one-particle orbitals $u_i(\vec{r})$ from which $T_s[\rho]$ is constructed is secured in the Euler-Lagrange equations for $u_i(\vec{r})$ $(i=1,\ldots,N)$ by none other than $\delta T_s[\rho]/\delta\rho(\vec{r})$ itself. Since $\delta T_s[\rho]/\delta\rho(\vec{r})$ is not known and the lack of knowledge of $T_s[\rho]$ is why the determination of $u_i(\vec{r})$'s is a question, finding some other way to ensure the fixing of $\rho(\vec{r})$ in the construction of $T_s[\rho]$ is of great importance. A natural way arises straight away as one of the orbitals, the one corresponding to the lowest state of Eq. (24) therefore being choosable to be real and positive, can be expressed simply by the other $N-1$ orbitals from Eq. (6),

$$u_1(\vec{r}) = \left(\rho(\vec{r}) - \sum_{i=2}^{N} |u_i(\vec{r})|^2 \right)^{1/2}, \tag{57}$$

consequently, with the use of the first of the one-particle equations (24), using Eq. (57), $\delta T_s[\rho]/\delta\rho(\vec{r})$ can be eliminated, getting $N-1$ equations without unknown $\rho(\vec{r})$ dependence for $N-1$ variables. (This approach has been considered by several papers from various aspects on different levels [17–25], the work of Holas and March [24] giving a thorough general summary of the subject.) With the separation of $\rho(\vec{r})$ in $u_i(\vec{r})$,

$$u_i(\vec{r}) = \sqrt{\rho(\vec{r})}\,\phi_{i-1}(\vec{r}), \quad i=2,\ldots,N, \tag{58a}$$

and

$$u_1(\vec{r}) = \sqrt{\rho(\vec{r})}\,\phi_N(\vec{r}), \tag{58b}$$

the Weizsäcker functional appears as a natural component of $T_s[\rho]$,

$$T_s = T_W[\rho] + \int \tfrac{1}{2}\rho(\vec{r}) \sum_{i=1}^{N} |\nabla\phi_i(\vec{r})|^2 d\vec{r} \tag{59}$$

with

$$\phi_N(\vec{r}) = \left[1 - \sum_{i=1}^{N-1} |\phi_i(\vec{r})|^2 \right]^{1/2}. \tag{60}$$

In Eq. (59), with Eq. (60), the ρ constraint (6) is fully incorporated, so the functional $T_s[\rho,\phi_1,\ldots,\phi_{N-1}]$ obtained with Eqs. (59) and (60) has to be minimized in $\phi_i(\vec{r})$ with only orthonormalization constraint,

$$\int \rho(\vec{r})\,\phi_i^*(\vec{r})\,\phi_j(\vec{r})\,d\vec{r} = \delta_{ij}, \tag{61}$$

to get the Euler-Lagrange equations that determine $\phi_i(\vec{r})$ $(i=1,\ldots,N-1)$ for a given $\rho(\vec{r})$. The resulting $N-1$ coupled differential equations for $\{\phi_i(\vec{r})\}_{i=1}^{N-1}$, however, are quite complicated.

A great simplification of the problem can be achieved by writing $|\phi_i(\vec{r})|$'s as hyperspherical functions,

$$|\phi_j(\vec{r})| = \prod_{k=0}^{j-1} \sin\theta_k(\vec{r}) \cos\theta_j(\vec{r}), \quad j=1,\ldots,N-1 \tag{62a}$$

and

$$|\phi_N(\vec{r})| = \prod_{k=0}^{N-1} \sin\theta_k(\vec{r}), \tag{62b}$$

with

$$\theta_0(\vec{r}) = \frac{\pi}{2}, \tag{63}$$

as did Dawson and March [19] and Holas and March (for general N) [24] in one dimension, where $\phi_i(\vec{r})$'s are real functions. In three dimensions generally $\phi_j(\vec{r})$ $(j=1,\ldots,N-1)$ are complex, thus

$$\phi_j(\vec{r}) = |\phi_j(\vec{r})| e^{i\varphi_j(\vec{r})}, \tag{64}$$

with which

$$T_s = T_W[\rho] + \int \tfrac{1}{2}\rho(\vec{r}) \sum_{j=1}^{N} \left(|\nabla|\phi_j(\vec{r})|\|^2 + |\phi_j(\vec{r})|^2 |\nabla\varphi_j(\vec{r})|^2 \right) d\vec{r}, \tag{65}$$

where the second term in the brackets does not appear for real $\phi_j(\vec{r})$ $[\varphi_j(\vec{r})=0]$. With the transformation (62), the "real" part in T_s is given as

$$T^r = T_W[\rho] + \int \tfrac{1}{2}\rho(\vec{r}) \sum_{j=1}^{N-1} \prod_{k=0}^{j-1} \sin^2\theta_k(\vec{r}) |\vec{\nabla}\theta_j(\vec{r})|^2 d\vec{r}. \tag{66}$$

This expression can be obtained by mathematical induction, deriving the N-particle case from the $(N-1)$-particle case by writing

$$T^r[\rho] = \sum_{j=1}^{N} T_W[\rho_j] = T_W[\rho\cos^2\theta_1] + \sum_{j=2}^{N} T_W[\rho_j], \tag{67}$$

then applying the transformation

$$\rho \to \rho \sin^2\theta_1, \tag{68a}$$

$$\theta_j \to \theta_{j+1}, \quad j=1,\ldots,N-2 \tag{68b}$$

on the variables of the $(N-1)$-particle $T^r[\rho,\theta_1,\ldots,\theta_{N-2}]$ to get the second term in Eq. (67), and using the expression

$$T^r = T_W[\rho] + \int \tfrac{1}{2}\rho(\vec{r})|\vec{\nabla}\theta_1(\vec{r})|^2 d\vec{r} \tag{69}$$

of the two-particle case, thereby getting the recursion formula

$$T^r[\rho,\theta_1,\ldots,\theta_{N-1}] = T^r[\rho,\theta_1] + T_p^r[\rho\sin^2\theta_1,\theta_2,\ldots,\theta_{N-1}], \tag{70}$$

with $T_P = T - T_W$.

To get $T_s[\rho]$ for a given $\rho(\vec{r})$, then, the functional $T_s[\rho,\theta_1,\ldots,\theta_{N-1},\varphi_1,\ldots,\varphi_{N-1}]$ given by Eq. (65) with Eq. (62) has to be minimized in $\theta_j(\vec{r})$ $(j=1,\ldots,N-1)$ and $\varphi_j(\vec{r})$ $(j=1,\ldots,N-1)$ with the orthonormalization constraint (61) [with Eq. (64)],

$$\int \rho(\vec{r})|\phi_j(\vec{r})|^2 d\vec{r} = 1 \tag{71}$$

and

$$\int \rho(\vec{r})|\phi_j(\vec{r})||\phi_k(\vec{r})|\exp\{i[\varphi_k(\vec{r})-\varphi_j(\vec{r})]\}d\vec{r} = 0, \tag{72}$$

using Eq. (62). For the two-particle case, with

$$T_s[\rho,\theta_1,\varphi_1] = T_W[\rho] + \int \tfrac{1}{2}\rho(\vec{r})\{|\vec{\nabla}\theta_1(\vec{r})|^2 + \cos^2\theta_1(\vec{r})|\vec{\nabla}\varphi_1(\vec{r})|^2\}d\vec{r}, \tag{73}$$

$$\int \rho(\vec{r})\cos^2\theta_1(\vec{r})d\vec{r} = 1 \tag{74}$$

as the normalization constraint from Eq. (71), and

$$\int \rho(\vec{r})\sin 2\theta_1(\vec{r})\cos\varphi_1(\vec{r})d\vec{r} = 0 \tag{75a}$$

and

$$\int \rho(\vec{r})\sin 2\theta_1(\vec{r})\sin\varphi_1(\vec{r})d\vec{r} = 0 \tag{75b}$$

as the two real orthogonality constraints coming from the complex constraint (72), the resulting Euler-Lagrange equations are

$$\nabla^2\theta_1(\vec{r}) + \frac{\vec{\nabla}\rho(\vec{r})}{\rho(\vec{r})}\cdot\vec{\nabla}\theta_1(\vec{r}) - \tfrac{1}{2}\sin 2\theta_1(\vec{r})|\vec{\nabla}\varphi_1(\vec{r})|^2 = -\lambda_n\sin 2\theta_1(\vec{r}) + \lambda_o 2\cos 2\theta_1(\vec{r})\cos\varphi_1(\vec{r}) \tag{76}$$

and

$$\cos^2\theta_1(\vec{r})\nabla^2\varphi_1(\vec{r}) + \frac{\vec{\nabla}\rho(\vec{r})}{\rho(\vec{r})}\cdot\cos^2\theta_1(\vec{r})\vec{\nabla}\varphi_1(\vec{r}) - \sin 2\theta_1(\vec{r})\vec{\nabla}\theta_1(\vec{r})\cdot\nabla\varphi_1(\vec{r}) = -\lambda_o\sin 2\theta_1(\vec{r})\sin\varphi_1(\vec{r}), \tag{77}$$

with the Lagrange multipliers λ_n and λ_o corresponding to the constraints (74) and (75a), respectively. The other Lagrange multiplier corresponding to the orthogonality constraint (75) can be eliminated by the transformation

$$\lambda_a = \lambda_o\cos\varphi_0, \quad \lambda_b = \lambda_o\sin\varphi_0 \tag{78}$$

[where λ_a and λ_b are the original Lagrange multipliers associated with Eqs. (75a) and (75b), respectively] and setting $\varphi_0 = 0$, as the addition of an arbitrary constant to $\varphi_j(\vec{r})$'s is allowed by Eqs. (65) and (72). For one dimension, where $\varphi_j(\vec{r}) = 0$ $(j=1,\ldots,N-1)$ can be taken, Eqs. (76) and (77) reduce to the well-known equation [18,19]

$$\theta''(r) + \frac{\rho'(r)}{\rho(r)}\theta'(r) = \lambda\sin 2\theta(r). \tag{79}$$

It is worth pointing out that Eq. (65) takes its minimum at $\varphi_j(\vec{r})$ taking the value of an arbitrary constant, which allows real $\phi_j(\vec{r})$'s; and the normalization (71) does not give any restriction with this respect, as there is no $\varphi_j(\vec{r})$ in it; the only reason why $\varphi_j(\vec{r}) \neq 0$ in general, that is, $\phi_j(\vec{r})$ has to be complex, is the orthogonality constraint (72).

IV. HOMOGENEOUS *N*-PARTICLE NONINTERACTING KINETIC-ENERGY FUNCTIONALS

It has been shown that the noninteracting kinetic energy can be obtained for any given N-particle density $\rho_N(\vec{r})$ by the minimization of the functional $T_s[\rho,\phi_1,\ldots,\phi_{N-1}]$, defined by Eqs. (59) and (60), with respect to $\phi_i(\vec{r})$ $(i=1,\ldots,N-1)$ under normalization constraints [Eq. (61)]. The $\{\phi_i(\vec{r})\}_{i=1}^{N-1}$ that gives $T_s[\rho_N]$ can thus be determined from the corresponding $N-1$ Euler-Lagrange equations. These $N-1$ equations, however, give a $\{\phi_i(\vec{r})\}_{i=1}^{N-1}$ for any $\rho(\vec{r})$, not only for a $\rho_N(\vec{r})$, but these $\phi_i[\rho]$ $(i=1,\ldots,N-1)$ yield $T_s[\rho]$ only for $\rho_N(\vec{r})$'s, that is, in this way an N-particle noninteracting kinetic-energy density functional is defined,

$$T_N[\rho] := T_s[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]], \tag{80}$$

for the $N=1$ case having

$$T_1[\rho] \equiv T_W[\rho]. \tag{81}$$

An interesting question is whether this $T_N[\rho]$ has any degree of homogeneity in density scaling, like $T_W[\rho]$, which is of degree-one homogeneity. Examining the $N=2$ case in one dimension in the hyperspherical function representation of $\phi_i(\vec{r})$'s, it can be seen that $\rho(r)$ appears in the Euler-Lagrange equation (79) only in the form $\rho'(r)/\rho(r)$, which is of degree-zero homogeneity in $\rho(r)$, on the basis of which

the degree-one homogeneity of the emerging kinetic-energy functional, which is $T_2[\rho]=T_W[\rho]+\int\frac{1}{2}\rho(r)[\theta'(r)]^2dr$, has been concluded a few times in the literature, as $\theta(r)$ must be a functional of $\rho'(r)/\rho(r)$. However, $\theta(r)$ has a dependence on the Lagrange multiplier λ as well,

$$\theta=\theta\left[\frac{\rho'}{\rho},\lambda\right], \tag{82}$$

which ruins the degree-one homogeneity, since it would contradict with the constraint (74), which determines λ and which allows homogeneity of only degree minus one in $\rho(\vec{r})$ for $\cos^2\theta(\vec{r})$. The connection between the possible homogeneity properties of $T_2[\rho]$ and $\cos^2\theta(\vec{r})$ can be exhibited more directly, without concerning $\theta(r)$ itself, through the identity

$$[\vec{\nabla}\cos^2\theta(\vec{r})]^2=4[\vec{\nabla}\theta(\vec{r})]^2\cos^2\theta(\vec{r})[1-\cos^2\theta(\vec{r})]. \tag{83}$$

Equation (83) shows that $\cos^2\theta(\vec{r})$ has to be of degree-zero homogeneity to yield $[\nabla\theta(\vec{r})]^2$ of degree-zero homogeneity, that is, $T_2[\rho]$ of degree-one homogeneity. The normalization constraint, thus, leads to $T_N[\rho]$, which are not first-degree homogeneous, even more, not homogeneous at all, as can be seen from Eq. (83). However, Eq. (71) has to hold only for the given N, that is, for N-particle densities $\rho_N(\vec{r})$; for general $\rho(\vec{r})$ it can be modified in a way to yield Eq. (71) for $\rho_N(\vec{r})$. The most simple and, also, reasonable extension of Eq. (71) is

$$\int\rho(\vec{r})|\phi_j(\vec{r})|^2d\vec{r}=\frac{1}{N}\int\rho(\vec{r})d\vec{r}\quad(j=1,\ldots,N-1), \tag{84}$$

with N being the given N, that is, $N=\int\rho_N(\vec{r})d\vec{r}$, and for the above case, giving

$$\int\rho(\vec{r})\cos^2\theta_1(\vec{r})d\vec{r}=\tfrac{1}{2}\int\rho(\vec{r})d\vec{r}. \tag{84a}$$

Equation (84) can be considered as a natural generalization of the normalization (71), there being no reason to require the components $\rho(\vec{r})|\phi_j(\vec{r})|^2$ $(j=1,\ldots,N-1)$ of a $\rho(\vec{r})$ with $\int\rho(\vec{r})d\vec{r}\neq N$ to be normalized to 1. It can be seen immediately that this generalized normalization does not spoil the degree-zero homogeneous nature of $\phi_i[\rho]$'s, which emerges from the Euler-Lagrange equations, which contain $\rho(\vec{r})$ explicitly only in the form $\nabla\rho(\vec{r})/\rho(\vec{r})$.

The degree-one homogeneity of $T_N[\rho]$ defined with the normalization (84) can be proved explicitly for general (integer, greater than 1) N in the following way. The functional derivative of $T_N[\rho]$ can be expressed as

$$\begin{aligned}\frac{\delta T_N[\rho]}{\delta\rho(\vec{r})}&=\frac{\delta T_s[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]}{\delta\rho(\vec{r})}\\&=\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}\\&\quad+\sum_{i=1}^{N-1}\int\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r}')}\frac{\delta\phi_i(\vec{r}')}{\delta\rho(\vec{r})}d\vec{r}'.\end{aligned} \tag{85}$$

Note that while after the first equality sign in Eq. (85), there is a full functional derivative with respect to $\rho(\vec{r})$, after the second equality sign, a partial functional differentiation with respect to $\rho(\vec{r})$ appears (in the first term). [Throughout, when a differentiation with respect to $\rho(\vec{r})$ is a full one, the ρ dependence of the variables ϕ_i of the functional considered is displayed.] Following from the minimizational definition of $T_s[\rho]$, the partial functional derivatives of $T_s[\rho,\phi_1,\ldots,\phi_{N-1}]$ with respect to its variables $\phi_i(\vec{r})$ are related to the constraints (84) and (61) (with $i\neq j$),

$$\begin{aligned}C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]&=\int\rho(\vec{r})\phi_j^*(\vec{r})\phi_k(\vec{r})d\vec{r}-\frac{\int\rho(\vec{r})d\vec{r}}{N}\delta_{jk}\\&=0,\end{aligned} \tag{86}$$

by the Euler-Lagrange equations

$$\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r})}=\sum_{j\leqslant k}\lambda_{jk}\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r})}\quad(i=1,...,N-1), \tag{87}$$

with λ_{jk} being the Lagrange multipliers ensuring the fullfilment of the (orthonormalization) constraints. From the constraints themselves, being required for every $\rho(\vec{r})$, by differentiation with respect to $\rho(\vec{r})$,

$$\begin{aligned}0&=\frac{C_{jk}[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]}{\delta\rho(\vec{r})}\\&=\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}\\&\quad+\sum_{i=1}^{N-1}\int\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r}')}\frac{\delta\phi_i(\vec{r}')}{\delta\rho(\vec{r})}d\vec{r}'\end{aligned} \tag{88}$$

arises, that is, the partial functional derivative of a $C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]$ with respect to its variable $\rho(\vec{r})$ is

$$\begin{aligned}&\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}\\&=-\sum_{i=1}^{N-1}\int\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r}')}\frac{\delta\phi_i(\vec{r}')}{\delta\rho(\vec{r})}d\vec{r}'.\end{aligned} \tag{89}$$

With Eq. (87), Eq. (85) gives

$$\frac{\delta T_N[\rho]}{\delta\rho(\vec{r})}=\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}+\sum_{i=1}^{N-1}\int\sum_{j\leqslant k}\lambda_{jk}\times\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\phi_i(\vec{r}\,')}\frac{\delta\phi_i(\vec{r}\,')}{\delta\rho(\vec{r})}d\vec{r}\,', \quad (90)$$

which, with the use of Eq. (89), yields

$$\frac{\delta T_N[\rho]}{\delta\rho(\vec{r})}=\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}-\sum_{j\leqslant k}\lambda_{jk}\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}. \quad (91)$$

Since

$$\int\rho(\vec{r})\frac{C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}d\vec{r}=C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}], \quad (92)$$

that is, $C_{jk}[\rho,\phi_1,\ldots,\phi_{N-1}]$ are (partially) homogeneous of degree one in $\rho(\vec{r})$, and $C_{jk}[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]=0$, from Eq. (91)

$$\int\rho(\vec{r})\frac{\delta T_N[\rho]}{\delta\rho(\vec{r})}d\vec{r}=\int\rho(\vec{r})\frac{\delta T_s[\rho,\phi_1,\ldots,\phi_{N-1}]}{\delta\rho(\vec{r})}d\vec{r}=T_s[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]=T_N[\rho], \quad (93)$$

where the (partial) degree-one homogeneity of $T_s[\rho,\phi_1,\ldots,\phi_{N-1}]$ in $\rho(\vec{r})$, following from its construction, (59), has been used (in the second equality), and which means that $T_N[\rho]=T_s[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]$ itself is also of degree-one homogeneity in $\rho(\vec{r})$, not just partially but fully as well. Note that the key to this proof is the expression of the full derivative of $T_s[\rho,\phi_1[\rho],\ldots,\phi_{N-1}[\rho]]$ in terms of partial functional derivatives with respect to $\rho(\vec{r})$ of functionals, for which degree-one homogeneity in $\rho(\vec{r})$ follows from the explicit $\rho(\vec{r})$ dependence in their (known) form.

It has to be emphasized that this degree-one homogeneity of $T_N[\rho]$ ($N=1,2,\ldots$) of course does not mean that $T_s[\rho]$ itself is of degree-one homogeneity, as shown formally by Eq. (50) too. With this property of $T_N[\rho]$, a strong requirement is obtained, which can be used to construct density functionals that give the exact noninteracting kinetic energy for a given particle number. A method proposed by Gál and Nagy [26] gives an example for how the degree-one homogeneity in $\rho(\vec{r})$, together with the degree-two homogeneity in $\vec{r}$, that is, Eqs. (10) and (9), can be used to derive explicit analytical expressions for T_s as a functional of $\rho(\vec{r})$, if the noninteracting kinetic-energy density is assumed to be a function of $\rho(\vec{r})$ and its derivatives, yielding the Weizsäcker functional as a general component, in agreement with Eq. (59). Note that the $T_N[\rho]$'s of degree-one homogeneity constructed here can be considered as the generalizations of the Weizsäcker functional (which is $T_1[\rho]$) for arbitrary N, $T_W[\rho]$ itself being in accordance with the generalized normalization constraint (84) and not with Eq. (71), as it can be derived using $\rho(\vec{r})=u_1^*(\vec{r})u_1(\vec{r})$, which gives the normalization (71) only for $N=1$.

Finally, it is worth pointing out that, utilizing the recursive structure of $T^r[\rho,\theta_1,\ldots,\theta_{N-1}]$ [characterized by the formula Eq. (70)], with the knowledge of $T_N[\rho]$ for a given N considering the "real parts," to obtain $T_{N+1}[\rho]$, only one variational variable needs to be determined as a functional of $\rho(\vec{r})$ (that is, only one differential equation has to be solved), applying the transformation (68a) to the Pauli part (P) of $T_N[\rho]$, herewith having a systematic procedure to get $T_N[\rho]$ for every N; e.g., for the three-particle case (in one dimension),

$$T_3[\rho]=T_W[\rho]+\int\tfrac{1}{2}\rho(r)[\theta'(r)]^2dr+T_2^P[\rho\sin^2\theta], \quad (94)$$

with $T_2^P[\rho]=T_2[\rho]-T_W[\rho]$, for which the corresponding Euler-Lagrange equation that determines $\theta[\rho]$ is

$$\theta''(r)+\frac{\rho'(r)}{\rho(r)}\theta'(r)+\sin 2\theta(r)\left.\frac{\delta T_2^P[\rho]}{\delta\rho(r)}\right|_{\rho\sin^2\theta}=\lambda\sin 2\theta(r). \quad (95)$$

V. SUMMARY

In this study it has been shown that, in the Euler-Lagrange equations that determine the orbitals from which the noninteracting kinetic energy T_s is built, the Lagrange multiplier that forces the orbitals to yield a given density $\rho(\vec{r})$ can be identified with the first derivative of $T_s[\rho]$, giving a new, simple derivation of the Kohn-Sham equations; and on a similar basis, for ground states, the Schrödinger equation has also been shown to emerge from the Hohenberg-Kohn Euler-equation. After pointing out that $T_s[\rho]$ can be replaced in density-functional theory by N-particle noninteracting kinetic-energy density functionals, $T_N[\rho]$, that is, functionals of $\rho(\vec{r})$ that give T_s for N-particle densities, a natural definition for $T_N[\rho]$ has been given by (i) constructing T_s from $N-1$ functions $\phi_i(\vec{r})$ that incorporate the given $\rho(\vec{r})$ constraint and (ii) using the Euler-Lagrange equations resulting for the $\phi_i(\vec{r})$'s for the given N to define $\phi_i[\rho]$ ($i=1,\ldots,N-1$) for $\rho(\vec{r})$ of $\int\rho(\vec{r})d\vec{r}\neq N$ as well. The hyperspherical function representation of $\phi_i(\vec{r})$'s has been considered for complex $\phi_i(\vec{r})$'s, generalizing the earlier results for one dimension. Finally, the normalization constraints on $\phi_i(\vec{r})$'s have been generalized in a reasonable way to lead to $T_N[\rho]$ functionals of degree-one homogeneity, this property giving a powerful tool, being a strong requirement, to construct density functionals that give $T_s[\rho]$ for a given particle number. In addition, a systematic procedure has been presented by which the "real part" of $T_N[\rho]$ can be obtained for each N by the solution of uncoupled differential equations.

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APPENDIX A: DERIVATION OF EQ. (33)

Because of its third term, the derivation of Eq. (33) may need some explanation; the kinetic energy and the electron-electron repulsion energy terms arise similarly as in the derivation of the (ground-state) Schrödinger equation through the minimization of the usual energy wave-function functional, $E_v[\psi]$, of quantum mechanics.

The third term in Eq. (33) comes from the functional differentiation of $-F[\rho[\psi]]$ [in Eq. (29)] with respect to $\psi^*(\vec{r}_1,\ldots,\vec{r}_N)$, that is,

$$\sum_{i=1}^{N} \frac{\delta F[\rho]}{\delta \rho(\vec{r}_i)} \psi(\vec{r}_1,\ldots,\vec{r}_i,\ldots,\vec{r}_N) = \frac{\delta F[\rho[\psi]]}{\delta \psi^*(\vec{r}_1,\ldots,\vec{r}_N)}, \tag{A1}$$

where $\rho[\psi]$ is given by Eq. (19). Writing the ψ dependence of ρ in the generally used detailed form

$$\rho(\vec{r}) = N \int \cdots \int \psi^*(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)\psi(\vec{r},\vec{r}_2,\ldots,\vec{r}_N)d\vec{r}_2\cdots d\vec{r}_N, \tag{A2}$$

the origin of the summation over the electron indices is, however, hidden. To get to Eq. (A1) (through $\rho[\psi]$), formally that expression of ρ in terms of ψ has to be used in which the antisymmetric nature of Fermion wave functions is not utilized, which is

$$\rho(\vec{r}) = \sum_{i=1}^{N} \int \cdots \int \psi^*(\vec{r}_1,\ldots,\vec{r}_N)\psi(\vec{r}_1,\ldots,\vec{r}_N)d\vec{r}_1\cdots d\vec{r}_{i-1} \times d\vec{r}_{i+1}\cdots d\vec{r}_N\Big|_{\vec{r}_i=\vec{r}}, \tag{A3}$$

as in the case of the components of $E_v[\psi]$ to get the Schrödinger equation. With Eq. (A3), applying the chain rule of functional differentiation, Eq. (A1) follows straight away.

APPENDIX B: INCLUSION OF SPIN IN THE DERIVATION OF FIRST-DEGREE HOMOGENEITY

In this appendix the spin of the electrons will be incorporated into the derivation of the first-degree homogeneous *N*-particle noninteracting kinetic-energy density functionals. To give a wider view on the subject, the derivation this time will be based directly on the Kohn-Sham orbitals, proving that, with the generalized normalization proposed in Sec. IV, the Kohn-Sham orbitals can be taken as degree-half homogeneous functionals of the density $\rho(\vec{r})$.

Consider a system with two Kohn-Sham orbitals, that is,

$$\rho(\vec{r}) = n_1|u_1(\vec{r})|^2 + n_2|u_2(\vec{r})|^2, \tag{B1}$$

where n_1 and n_2 are the occupation numbers of the corresponding orbitals. From Eq. (B1) the lowest-lying orbital can be expressed as

$$u_1(\vec{r}) = \sqrt{\frac{\rho(\vec{r}) - n_2|u_2(\vec{r})|^2}{n_1}}. \tag{B2}$$

Following the procedure described in Sec. III, that is, inserting Eq. (B2) into the orbital equations (24) and then solving them for $u_2(\vec{r})$, yields $u_2(\vec{r})$ as a functional of $\rho(\vec{r})$, and also of $\varepsilon = \varepsilon_2 - \varepsilon_1$,

$$u_2(\vec{r}) = u_2[\rho,\varepsilon],$$

where $\varepsilon = \varepsilon[\rho]$ is determined by the normalization of $u_2(\vec{r})$. Now, to examine the behavior of $u_2[\rho] = u_2[\rho,\varepsilon[\rho]]$ under density scaling, multiply Eqs. (B2) and (24) with some $\sqrt{k}$,

$$\sqrt{k}u_1(\vec{r}) = \sqrt{\frac{k\rho(\vec{r}) - n_2|\sqrt{k}u_2(\vec{r})|^2}{n_1}} \tag{B3}$$

and

$$-\tfrac{1}{2}\nabla^2\sqrt{k}u_i(\vec{r}) - \frac{\delta T_s[\rho]}{\delta\rho(\vec{r})}\sqrt{k}u_i(\vec{r}) = \varepsilon_i\sqrt{k}u_i(\vec{r}), \tag{B4}$$

from which

$$\sqrt{k}u_2(\vec{r}) = u_2[k\rho,\varepsilon^{(k)}]. \tag{B5}$$

Taking the generalized normalization

$$\int |u_i(\vec{r})|^2 d\vec{r} = \frac{\int \rho(\vec{r})d\vec{r}}{N}, \quad i = 1,2 \tag{B6}$$

and multiplying it with k gives

$$\int |\sqrt{k}u_2(\vec{r})|^2 d\vec{r} = \frac{\int \rho(\vec{r})d\vec{r}}{N}, \tag{B7}$$

from which $\varepsilon^{(k)}$ in Eq. (B5) emerges as

$$\varepsilon^{(k)} = \varepsilon[k\rho], \tag{B8}$$

which, note, would not be the case if the traditional normalization constraint was used. Equations (B5) with (B8) give

$$\sqrt{k}u_2[\rho] = u_2[k\rho], \tag{B9}$$

that is, $u_2[\rho]$ is homogeneous of degree half. On the basis of Eq. (B2), the same can be said about $u_1[\rho]$ as well.

For systems with more than two Kohn-Sham orbitals, where

$$\rho(\vec{r}) = \sum_{i=1}^{m} n_i|u_i(\vec{r})|^2, \tag{B10}$$

the foregoing proof is trivially extendable, giving functionals $u_i[\rho]$ of degree-half homogeneity. From this result then the degree-one homogeneity of the *N*-particle noninteracting

kinetic-energy density functionals $T_N[\rho]$ constructed as described in Secs. III and IV follows straight away via

$$T_N = \int \sum_{i=1}^{m} n_i u_i^*(\vec{r})(-\tfrac{1}{2}\nabla^2)u_i(\vec{r})d\vec{r} \qquad \text{(B11)}$$

with

$$N = \sum_{i=1}^{m} n_i .$$

It is important to point out that $T_N[\rho]$ depends on the occupation structure of the orbitals; however, considering, for example, only Fermion systems with only the highest (occupied) orbitals allowed to be singly occupied, while the others being doubly occupied, the particle number N determines $T_N[\rho]$ without ambiguity of course. Note also that different occupation of a given number of orbitals does not necessarily lead to different $T_N[\rho]$, as in the case of one- and two-electron ground-state systems, where

$$T_1[\rho] \equiv T_2[\rho] \equiv T_W[\rho]. \qquad \text{(B12)}$$

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