

Failure of the Weizsäcker kinetic energy functional for one-, two-, and three-electron distribution functions

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Abstract Further progress in pair-density functional theory (sometimes called 2-DFT) hinges on the development of computationally facile and quantitatively accurate models for the kinetic energy functional. In this paper we perform computational tests for two of the simplest models, the generalized Weizsäcker kinetic energy functional and its spin-resolved extension. Both of these models perform very poorly for atoms. The higher-order Weizsäcker functionals (based on the three-electron distribution function) perform better, but are still not successful. This suggests that an alternative approach for designing kinetic energy functionals of the pair density is needed.

Keywords Kinetic energy functionals · Pair density functional theory · Weizsäcker functional

1 Motivation

One of the biggest disadvantages of density-functional theory (DFT) is the inability to systematically improve results. If a given density functional approximation (e.g., the famous B3LYP [1–4]) fails to work, it is impossible to systematically improve the results without breaking with the fundamental spirit of DFT and resorting to ab initio-flavored approaches to the quantum many-body problem. (For example, one can systematically improve the results using Görling-Levy perturbation theory,

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but in doing so one incurs all of the computational costs and convergence issues associated with Møller-Plesset theory [5,6].) It is possible to construct hierarchies of density functional approximations (e.g., the Jacob's ladder of functionals [7–9]) that improve results *on average*. For a given system, however, there is no guarantee that the results will improve with the increasing complexity and computational cost of the density-functional approximation. Moreover, if the accuracy of none of the approximations suffices, further improvement of the results seems to require an approach based on many-electron correlated wavefunctions [10–13]. Finally, it is possible that there is not much room for further improvement in density-functional approximations. Recent work on functionals proves that the exact exchange-correlation functional has a discontinuous dependence on the Kohn-Sham orbitals [14,15]. (Similarly, the correlation functional in first-order density matrix functional theory must also have a discontinuous dependence on the orbitals.) Insofar as it seems very difficult to design explicit exchange-correlation functionals that are discontinuous, but continuous functionals will always produce physically absurd results in some systems, one may question whether how much improvement in density-functional approximations is possible.

In the mid-1990's, Ziesche proposed an alternative to Görling-Levy perturbation functional for improving density functional approximations [16,17]. Instead of considering a wavefunction-based correction strategy for systematically improving density-functional approximations, he considered an approach based on higher-order electron distribution functions and, specifically, the electron pair density. By including information from higher-order electron distribution functions, one may systematically approach the exact result [18,19]. At the top of the hierarchy, the N -electron distribution function is merely the square of the exact ground-state wavefunction for the system and the exact functional is known. For the pair density (2-density) and higher-order electron distribution functions (k -densities), the potential-energy portion of the electronic energy can be computed exactly, and the only term that needs to be approximated is the kinetic energy functional. Unlike the situation in density-functional theory and first-order density matrix functional theory, there is no evidence that the approximate functionals in k -density functional theory (for $k > 1$) need to be discontinuous.

The development of k -density functional theories and, especially, pair density functional theory is an active area of research [16–55]. Numerical results are scant, largely because of the theoretical difficulties attendant to this approach. In addition, most of the practical proposals require six-dimensional numerical integration of highly peaked (even singular) integrands, and therefore are not amenable to off-the-shelf black-box implementations.

The k -electron distribution function (k -density) can be defined in either the spin-averaged,

$$\rho_k(\mathbf{R}_1, \dots, \mathbf{R}_k) = \left\langle \Psi \left| \sum_{i_1 \neq i_2 \neq \dots \neq i_k} \delta(\mathbf{r}_{i_1} - \mathbf{R}_1) \cdots \delta(\mathbf{r}_{i_k} - \mathbf{R}_k) \right| \Psi \right\rangle \quad (1)$$

or spin-resolved

$$\rho_k^{\sigma_1 \dots \sigma_k}(\mathbf{R}_1, \dots, \mathbf{R}_k) = \left\langle \Psi \left| \sum_{i_1 \neq i_2 \neq \dots \neq i_k} |\sigma_1(i_1) \dots \sigma_k(i_k)\rangle (\delta(\mathbf{r}_{i_1} - \mathbf{R}_1) \dots \delta(\mathbf{r}_{i_k} - \mathbf{R}_k)) \langle \sigma_1(i_1) \dots \sigma_k(i_k) | \Psi \right\rangle \right. \quad (2)$$

form. In both cases, for $k > 1$, the exact interaction energy with the external potential and the exact electron-electron repulsion energy can be computed, and it is only the kinetic energy that needs to be approximated. For a given approximate kinetic energy functional, $\tilde{T}[\rho_k]$, the ground-state energy is then computed by the variational procedure,

$$E_{g.s.} = \min_{\{\rho_k | \rho_k \text{ is } N\text{-representable}\}} \left(\tilde{T}[\rho_k] + V_{ext}[\rho_k] + V_{ee}[\rho_k] \right) \quad (3)$$

Notice that the minimization has to be restricted to k -densities that are N -representable. The N -representability problem is a major difficulty in k -DFT; the necessary and sufficient conditions for N -representability are known on a lattice [41] and in real space [32], but they are not known in a useful form. There has been much work on necessary conditions for N -representability [19, 20, 27, 28, 38–42, 52, 54]. Partly because the N -representability problem seems so intractable, most of the work in k -DFT concentrates on the development of kinetic-energy functionals. (If the kinetic-energy functional is defined appropriately, the N -representability constraints can be shifted from the minimization principle into the functional [29, 30, 56]. That is, one can consider “ N -representability of the functional” [57–60] instead of “ N -representability of the k -density” [28, 32, 41].)

There is very little numerical evidence for the quality of kinetic-energy functionals [49, 50]. In particular, there do not seem to be numerical implementations of even the simplest possible functional form, the Weizsäcker-style functional, [18, 23–25, 33, 61]

$$T_w^{(k)}[\rho_k] = \frac{(N-k)!}{2(N-1)!} \int \int \dots \int \left| \nabla_{\mathbf{r}_1} \sqrt{\rho_k(\mathbf{r}_1, \dots, \mathbf{r}_k)} \right|^2 d\mathbf{r}_1 \dots d\mathbf{r}_k, \quad (4)$$

or one of its spin-resolved analogues, e.g., [18]

$$\begin{aligned} T_{w,s}^{(k)}[\rho_k^{\sigma_1 \sigma_2 \dots \sigma_k}] &= \frac{(N_\alpha - k)!}{2(N_\alpha - 1)!} \int \int \dots \int \left| \nabla_{\mathbf{r}_1} \sqrt{\rho_k^{\alpha \alpha \dots \alpha}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k)} \right|^2 d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_k \\ &+ \frac{(N_\beta - k)!}{2(N_\beta - 1)!} \int \int \dots \int \left| \nabla_{\mathbf{r}_1} \sqrt{\rho_k^{\beta \beta \dots \beta}(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_k)} \right|^2 d\mathbf{r}_1 d\mathbf{r}_2 \dots d\mathbf{r}_k \end{aligned} \quad (5)$$

The goal of this paper is to test the quality of these two simple functionals. Among the various spin-resolved Weizsäcker forms proposed in ref. [18], we chose Eq. (5) because it seems to give the best results.

The Weizsäcker functionals have appealing theoretical properties. All Weizsäcker functionals can be derived from considerations of the Fisher information [53, 62, 63];

there is also a derivation based on the quasiprobability distribution functions [64]. The spin-averaged Weizsäcker functionals (Eq. 4) are an increasing sequence of lower bounds to the true kinetic energy that becomes exact when $k = N$. The spin-resolved Weizsäcker functionals are also an increasing sequence of lower bounds for the kinetic energy; results are exact for the σ -spin component of the kinetic energy when $k = N_\sigma$. In wavefunction-based theories, a sequence of approximations that is exact for increasing numbers of electrons (e.g., CCSD ($k = 2$), CCSDT ($k = 3$), ...) rapidly converges towards the exact energy. One might expect, then, that the Weizsäcker kinetic energy bounds rapidly converge towards the true kinetic energy. The purpose of this paper is to show that this is not the case. This is shown in the next section. Following those results, we will speculate about the reasons for our disappointing findings and propose directions for future research.

2 Computational tests of k -Weizsäcker kinetic energy functionals

We evaluated the k -densities from the reoptimized Clementi-Roetti Hartree-Fock wavefunctions of Koga et al. [65,66]. We then evaluated the Weizsäcker kinetic energy functionals in Eqs. (4) and (5) using numerical integration methods; in problematic cases we used several different numerical integration algorithms to obtain an estimate on the integration error. Our results are accurate to four digits in most cases. For the higher-dimensional integrals ($k = 3$) of the larger atoms we are less confident in our results because different numerical integration techniques sometimes gave differing results. The number of digits in Tables 1 and 2 reflects our estimated uncertainties in the integration errors. Especially for large atoms and the $k = 3$ functionals, our estimates may be too optimistic. We are confident that the trends we report are correct.

The underlying reason for these numerical difficulties is that the integrands in Eq. (4) have singularities and near-singularities; this is most clear when they are rewritten as

$$T_w^{(3)}[\rho_3] = \frac{1}{2(N-1)(N-2)} \int \int \int \frac{|\nabla_{\mathbf{r}_1} \rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)|^2}{4\rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)} d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \quad (6)$$

For such strongly peaked functions, numerical integration methods converge poorly. However, even in the worst cases, our conclusions are not altered: because the errors are small compared to the total kinetic energy, they do not effect the qualitative trends.

In Table 1 presents the atomic kinetic energies computed using the Weizsäcker functionals for He-Ne and higher-atomic number elements from the first three main-group columns of the periodic table (Groups 1, 2, and 13). In agreement with theoretical predictions, the Weizsäcker functionals are lower bounds to the true kinetic energy and they are exact when the order of the functional is equal to the total number of electrons (spin-averaged functional) or the number of electrons of a given spin (spin-resolved functional). The spin-resolved functionals are much tighter lower bounds, but they still are not accurate. The errors are massive (several Hartrees) and they deteriorate rapidly with increasing electron number. The general trend is clear from Fig. 1 (alkaline earths). The failure of the Weizsäcker bounds to converge rapidly to the true kinetic energy can be characterized as follows: the percentage of the Hartree-Fock

Table 1 Results from the generalized Weizsäcker kinetic energy functionals, in Hartrees, for selected atoms

Atoms	$T_w^{(1)}$	$T_w^{(2)}$	$T_w^{(3)}$	$T_{w,s}^{(1)}$	$T_{w,s}^{(2)}$	$T_{w,s}^{(3)}$	Hartree-Fock
He	2.86168	2.86168	—	2.86168	—	—	2.8616799
Li	7.1948	7.23861	7.38568	7.23984	7.43273	—	7.4327257
Be	13.662	13.7127	14.573	13.662	13.898	—	14.5730211
B	21.985	22.0787	22.2825	22.0572	23.4816	24.5292	24.5290583
C	32.0674	32.2223	32.5006	32.2604	34.3106	35.3447	37.6886164
N	43.8028	44.0282	44.3807	44.1732	46.9322	48.0525	54.4009314
O	57.6913	57.9683	58.3223	58.1464	61.1564	66.1228	74.8093948
F	73.316	73.6661	74.1236	73.6478	77.0231	81.9227	99.4093436
Ne	90.6143	90.6643	91.4291	90.6143	92.3258	99.7039	128.5470893
Na	110.509	111.046	111.797	110.562	115.024	121.241	161.8589059
Mg	132.599	133.224	134.085	132.599	137.608	143.724	199.6146304
Al	156.791	157.508	158.297	156.818	162.574	169.636	241.8766997
K	345.148	346.486	347.507	345.186	355.197	365.724	599.1646995
Ca	384.08	385.53	387.534	384.08	394.778	406.	676.7580985
Ga	939.62	942.479	945.97	939.653	959.922	982.668	1923.2609442

The k -densities of the reoptimized Clementi-Roetti wavefunctions of Koga et al. [65] are used to evaluate the spin-averaged Weizsäcker functionals, $T_w^{(k)}[\rho_k]$, (Eq. 4) and the spin-resolved Weizsäcker functionals, $T_{w,s}^{(k)}[\sigma_1 \dots \sigma_k, \rho_k]$ (Eq. 5). The — entries refer to cases where the functional is undefined. In all these cases, generalizing the functional definition would reproduce the Hartree-Fock value in the last column

Table 2 Results from the generalized Weizsäcker kinetic energy functionals, in Hartrees, for selected isoelectronic atomic series

Atoms	$T_w^{(1)}$	$T_w^{(2)}$	$T_w^{(3)}$	$T_{w,s}^{(1)}$	$T_{w,s}^{(2)}$	$T_{w,s}^{(3)}$	Hartree-Fock
Be	13.6601	13.7106	13.8959	13.6601	14.5713	—	14.572855
B ⁺	22.2872	22.3957	22.7771	22.2872	24.2376	—	24.237358
C ²⁺	33.0613	33.2478	33.8879	33.0613	36.4089	—	36.408167
N ³⁺	45.9816	46.2655	47.2273	45.9816	51.0828	—	51.081823
O ⁴⁺	61.0466	61.4476	62.7937	61.0466	68.2579	—	68.257209
F ⁵⁺	78.2581	78.7956	80.5888	78.2581	87.9345	—	87.934406
Ne ⁶⁺	97.6095	98.3046	100.612	97.6095	110.111	—	110.11053
Si ¹⁰⁺	196.467	197.988	202.961	196.467	223.826	—	223.82185
K ¹⁵⁺	368.256	371.252	380.979	368.256	422.212	—	422.21645
Cr ²⁰⁺	593.661	598.628	614.679	593.661	683.107	—	683.10648
Cu ²⁵⁺	872.641	880.063	904.007	872.641	1006.49	—	1006.5046
B	21.9846	22.0784	22.2819	22.0569	23.4814	24.5288	24.528752
C ⁺	32.5439	32.7184	33.0817	32.7055	35.2783	37.2954	37.292134
N ²⁺	45.239	45.484	46.0095	45.5178	49.5057	52.7429	52.815497
O ³⁺	60.0679	60.4588	61.2438	60.4912	66.2951	71.0701	71.094284
F ⁴⁺	77.0323	77.5797	78.6521	77.6275	85.546	92.1264	92.126286
Ne ⁵⁺	96.1258	96.8369	98.2549	96.9202	107.248	115.901	115.91027
P ¹⁰⁺	223.607	225.496	229.078	225.806	252.933	276.098	276.09476
Ca ¹⁵⁺	404.397	408.005	414.778	408.681	460.472	505.033	505.03896
Mn ²⁰⁺	638.507	644.396	655.379	645.556	729.95	802.764	802.73882
Zn ²⁵⁺	925.894	934.596	950.774	936.387	1061.14	1169.17	1169.19

Table 2 continued

Atoms	$T_w^{(1)}$	$T_w^{(2)}$	$T_w^{(3)}$	$T_{w,s}^{(1)}$	$T_{w,s}^{(2)}$	$T_{w,s}^{(3)}$	Hartree-Fock
Mg	132.584	133.208	133.697	132.584	137.624	143.856	199.61330
Al ⁺	156.908	157.69	158.565	156.908	163.164	170.362	241.67309
Si ²⁺	183.418	184.374	185.528	183.418	191.047	200.572	287.9984
P ³⁺	212.092	213.244	214.486	212.092	221.216	231.817	338.56931
S ⁴⁺	242.95	244.312	245.885	242.95	253.716	266.992	393.37760
Cl ⁵⁺	275.982	277.577	279.041	275.982	288.516	303.688	452.42601
Ar ⁺⁶	311.166	313.006	315.31	311.166	325.595	343.71	515.68668
Ti ⁺¹⁰	473.657	476.676	480.553	473.657	497.036	527.066	811.05743
Co ⁺¹⁵	725.513	730.396	736.208	725.513	763.137	810.724	1275.3289
Ge ⁺²⁰	1031.51	1038.69	1047.2	1031.51	1086.82	1157.7	1845.2010
Al	156.78	157.496	158.39	156.808	162.551	169.322	241.86967
Si ⁺	183.203	184.084	184.967	183.255	190.264	197.408	288.56642
P ⁺²	211.786	212.845	213.804	211.868	220.252	229.919	339.6366
S ⁺³	242.537	243.795	245.046	242.652	252.557	264.476	395.07063
Cl ⁺⁴	275.451	276.923	278.528	275.605	287.141	300.258	454.8561
Ar ⁺⁵	310.52	312.226	314.22	310.718	324.043	340.326	518.998851
V ⁺¹⁰	518.283	521.411	524.973	518.773	542.876	572.986	904.77131
Ni ⁺¹⁵	780.088	785.051	790.99	780.989	819.021	866.408	1398.9843
As ⁺²⁰	1095.95	1103.19	1111.39	1097.38	1152.71	1222.06	2001.5808

The k -densities of the Clementi-Roetti Hartree-Fock wavefunctions [67] are used to evaluate the spin-averaged Weizsäcker functionals, $T_w^{(k)}[\rho_k]$, (Eq. 4) and the spin-resolved Weizsäcker functionals, $T_{w,s}^{(k)}[\rho_k^{\sigma_1 \dots \sigma_k}]$ (Eq. 5). The – entries refer to cases where the functional is undefined

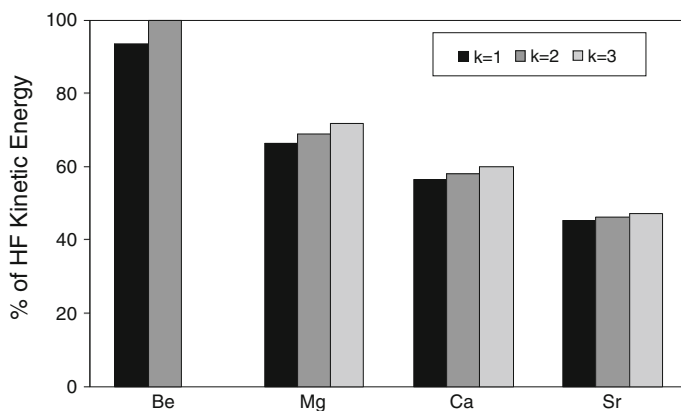


Fig. 1 The percentage of the Hartree-Fock kinetic energy that is obtained from the spin-resolved Weizsäcker kinetic-energy functionals, $T_{w,s}^{(k)}[\rho_k^{\sigma_1 \dots \sigma_k}]$ (Eq. 5) in the alkaline earth atoms

energy that is recovered does not diminish as k increases. That is, we have a problem of nondecreasing returns: the correction we obtain from increasing k does not decrease (significantly, if at all) as k increases. This is not what is usually observed in quantum chemistry, where a law of diminishing returns indicates that increasing k (e.g., from CCSD to CCSDT to CCSDTQ) provides successively smaller corrections to the energy. Because of this, we do not believe the Weizsäcker bounds are likely to be practically useful. Examination of the smaller atoms in Table 1 reveals that even the final correction (from $k = N - 1$ to $k = N$) is not at all negligible. Since evaluating the Weizsäcker functional for $k > 4$ is highly impractical, this limits the utility of this functional to systems with very few electrons.

We also investigated the Be, B, Mg, and Al isoelectronic series, as shown in Table 2. Not only does the absolute accuracy of the Weizsäcker functionals deteriorate rapidly with increasing Z , the relative accuracy decreases. For the isoelectronic series, we used the Hartree-Fock wavefunctions of Clementi and Roetti [67].

3 Discussion

Can we dismiss these results as inappropriate tests of the Weizsäcker functionals for the k -density? For example, it is dangerous to test conventional density functionals ($k = 1$) for the noninteracting kinetic energy and exchange energy using data from Hartree-Fock because of the small, yet subtle, differences between the definitions of the various energy terms in Hartree-Fock and conventional DFT. The same is true here: the values of the exact kinetic energy functionals for a Slater-determinantal k -density [29,30] might differ from the Hartree-Fock kinetic energy. (E.g., among all wavefunctions with a given 2-density, there might be one with a lower kinetic energy than the Hartree-Fock kinetic energy [30].) The variational principle for the energy dictates that the difference between the value of the exact kinetic energy functional and the Hartree-Fock kinetic energy is less than the quantum chemical electron correlation

energy.¹ Since the errors in the Weizsäcker functionals are enormously larger than the possible error in the Hartree-Fock approximation to the k -DFT kinetic energy, this theoretical subtlety does not affect the interpretation of our results.

Why are the Weizsäcker kinetic-energy functionals so poor? Consider that Eqs. (4) and (5) are derived, implicitly, from a reconstruction of the k -electron reduced density matrix from the k -density. For example, Eq. (4) may be derived by assuming that the spin-averaged k -electron reduced density matrix is [18]

$$\Gamma_k(\mathbf{r}_1, \dots, \mathbf{r}_k; \mathbf{r}'_1, \dots, \mathbf{r}'_k) = \left(\sqrt{\rho_k(\mathbf{r}_1, \dots, \mathbf{r}_k)} \right) \left(\sqrt{\rho_k(\mathbf{r}'_1, \dots, \mathbf{r}'_k)} \right). \quad (7)$$

The exact k -electron reduced density matrix can be written in terms of the natural k -bitals as [68, 69]

$$\Gamma_k(\mathbf{r}_1, \dots, \mathbf{r}_k; \mathbf{r}'_1, \dots, \mathbf{r}'_k) = \sum_i n_i^{(k)} \phi_i^{(k)}(\mathbf{r}_1, \dots, \mathbf{r}_k) \left(\phi_i^{(k)}(\mathbf{r}'_1, \dots, \mathbf{r}'_k) \right)^*. \quad (8)$$

An N -representability constraint on Γ_k restricts the occupation numbers of the natural k -bitals

$$0 \leq n_i^{(k)} \leq \frac{2N!}{k!(N-k+1)!}. \quad (9)$$

For $k < N$, there must be more than one occupied k -bital. The expression in Eq. (7) is not an N -representable Γ_k , and so it does not give an acceptable kinetic energy functional. In particular, for $k < N$, the density matrix ansatz in Eq. (7) strongly violates Fermi statistics (though it is perfectly satisfactory for bosonic systems). As is usually the case, failure to impose adequate N -representability conditions on the k -electron density matrix results in a very weak lower bound on the energy. Because the violation of N -representability in Eq. (9) reduces very slowly with increasing k , and is still “large” even for $k = N - 1$, the k -Weizsäcker family of functionals converges very slowly to the correct result.

Where do we go from here? The negative result in this paper suggests that while the Weizsäcker family of kinetic energy bounds may have theoretical utility, they are not useful for practical computations. Other functionals should be pursued. For Slater determinantal k -densities like those used here, March and Santamaria derived an exact functional, [70] which is, in spin-resolved form, [18]

¹ In fact, the difference between the value of the exact kinetic energy functional and the Hartree-Fock kinetic energy is probably much less than the quantum chemical correlation energy.

$$\begin{aligned}
T_{\text{MS}}^{(2)}[\rho_2^{\sigma_1\sigma_2}] = & - \int \int \frac{|\nabla_{\mathbf{r}_1} (\rho_2^{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2) - \rho_1^\alpha(\mathbf{r}_1) \rho_1^\alpha(\mathbf{r}_2))|^2}{8 (\rho_2^{\alpha\alpha}(\mathbf{r}_1, \mathbf{r}_2) - \rho_1^\alpha(\mathbf{r}_1) \rho_1^\alpha(\mathbf{r}_2))} d\mathbf{r}_1 d\mathbf{r}_2 \\
& - \int \int \frac{|\nabla_{\mathbf{r}_1} (\rho_2^{\beta\beta}(\mathbf{r}_1, \mathbf{r}_2) - \rho_1^\beta(\mathbf{r}_1) \rho_1^\beta(\mathbf{r}_2))|^2}{8 (\rho_2^{\beta\beta}(\mathbf{r}_1, \mathbf{r}_2) - \rho_1^\beta(\mathbf{r}_1) \rho_1^\beta(\mathbf{r}_2))} d\mathbf{r}_1 d\mathbf{r}_2 \quad (10)
\end{aligned}$$

This functional would give exact results for all the systems considered in this paper. The problem with the functional is that the integrand is often singular in real systems, leading to extreme numerical difficulties and possible lack of convergence. The March-Santamaria functional can be extended, with some difficulty, to $k > 2$. [18] Because the March-Santamaria functional is exact for a single Slater determinant, to test it we should use correlated wavefunctions. Those tests will be reported separately. [71]

An alternative approach, first proposed by Ayers and Levy, is more closely aligned with the spirit of a hierarchy of k -density functional theories. [31] In that approach, one starts with the noninteracting kinetic energy from Kohn-Sham DFT, $T_s[\rho]$, and then corrects it based on the differences between the pair density from the Kohn-Sham Slater determinant, $\rho_{2,s}(\mathbf{r}_1, \mathbf{r}_2)$, and the true pair density, obtaining a functional of the form [31]

$$T_{\text{AL}}^{(2)}[\rho_2] = T_s[\rho[\rho_2]] + T_c[\rho_{2,s}; \rho_2]. \quad (11)$$

This could be extended to $k = 3$ by replacing the Kohn-Sham calculation with Gonis-type theory for the pair density. [21, 22] Given the difficulties we encountered with the Weizsäcker family of functionals, we are skeptical that any truly explicit form for the kinetic energy functional will give satisfactory results. Based on this hunch, we are current writing a computer program that will allow us to explore approaches based on Eq. (11).

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