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Nonlocal symmetrized kinetic-energy density functional: Application to simple surfaces

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We study the properties of a nonlocal kinetic-energy functional, which includes a nonspherical average of the density through a symmetrization procedure. We demonstrate that this functional can be used successfully for both localized and extended systems. In particular, when applied to metallic jellium surfaces, the density profiles, surface energies, work functions, and image plane positions compare very favorably to those obtained using the exact Kohn-Sham method. [S0163-1829(98)08208-3]

I. INTRODUCTION

Although in density-functional theory (DFT),[1–5] the kinetic energy $T_S[n]$ of a noninteracting electron system can be evaluated exactly using a set of one-electron wave functions (the Kohn-Sham orbitals),[6] the development and application of functionals $T_S[n]$, which depend explicitly on the density, are of a wide interest. The use of such *orbital-free* functionals significantly reduces the computational effort in ground-state calculations and in first-principles molecular-dynamics simulations of complex systems.[7–9] On the other hand, the development of kinetic-energy functionals is undoubtedly of formal interest, due to the challenge of describing a number of quantum properties using the density directly as the basic variable. Moreover, the ideas employed in this development can also be useful for the construction of exchange-correlation functionals $E_{\mathrm{XC}}[n]$, which are not known exactly but are, in any case, needed in every DFT calculation.

Focusing on the discussion of the kinetic-energy functionals, there are approximations that give good total energies (and, in some cases, well-behaved density profiles) when applied to specific electron systems, but tend to fail in applications to problems with different structure. This is the case of the widely used semilocal functional (based on density gradients terms) TF(λ)W, which consists in a Thomas-Fermi functional plus a Weizsäcker term multiplied by a prefactor λ. The optimum parameter λ depends very sensitively on the system under consideration,[10,11] and, moreover, the obtained density profiles for any system do not show any quantum oscillations. This lack of universality also arises in more recent models by Wang and Teter,[12] Perrot,[13] and Foley and Madden,[14] developed only for extended systems where a mean density can be defined. On the other hand, nonlocal functionals, like the weighted-density approximation (WDA) by Alonso and Girifalco[15] and the averaged-density approximation (ADA) by Chacón, Alvarellos, and Tarazona,[16] although in principle can be used in any system, cannot be applied successfully to extended systems due to technical reasons (the weight functions have a very long range).[17] As a consequence, the development of a universal explicit kinetic-energy functional remains as an open question.

All the nonlocal models mentioned above are based on an averaging using a weight function with spherical symmetry. In a previous paper,[18] we developed a symmetrized ADA (sADA) functional, that uses a nonspherical average of the density, making possible a better description of the collective effects of electronic systems. In particular, when applied to atoms, we obtain not only accurate ground energies, but also density profiles with a clear shell structure and with spin-polarized ground states for group-V b atoms. In order to check the universality of the model, in this work we present the application of the functional to a very different inhomogeneous electron system, the jellium surface. The jellium surface is a clear example of a simple model in which the DFT provides an easy way to handle a description of the physical properties of interest.[19–21]

The outline of the paper is as follows. In Sec. II we summarize the construction of the sADA functional. In Sec. III, we present and compare the ground-state properties (surface energies, work functions, and density profiles) obtained with the sADA functional. Section IV contains the discussion of these properties for the stabilized jellium model. As a final test of the capabilities of the functional, in Sec. V we study the density induced in linear order by a weak external field. Conclusions are presented in Sec. VI.

II. THEORY. SCALING FACTOR

The sADA kinetic-energy functional is given by[18]

$$T_S[n]=T_W[n]+T_{nl}[n]=\tfrac{1}{8}\int\frac{|\nabla n(\mathbf{r})|^2}{n(\mathbf{r})}d\mathbf{r}+\int n(\mathbf{r})\{\tfrac{8}{5}t_s[\tilde{n}(\mathbf{r})]-\tfrac{3}{5}t_s[n(\mathbf{r})]\}d\mathbf{r},\qquad(1)$$

(atomic units are used throughout this paper) where $t_s(n_0)=3(3\pi^2n_0)^{2/3}/10$ is the kinetic energy per particle of an homogeneous electron gas of density n_0 and $T_W[n]$ is the Weizsäcker term.[22] $\tilde{n}(\mathbf{r})$ is an averaged density calculated using a universal weight function $\omega(\rho)$ through the expression

TABLE I. Total energies and, between brackets, chemical potentials for several closed-shell atoms (in atomic units) obtained through the Kohn-Sham method and the sADA kinetic-energy functionals using $\beta=-\frac{1}{2}$ and $\frac{1}{2}$ in the scaling function of Eq. (3).

Atom	Kohn-Sham	sADA ($\beta=-\frac{1}{2}$)	sADA ($\beta=\frac{1}{2}$)
He	-2.834 (-0.570)	-2.848 (-0.155)	-2.679 (-0.150)
Ne	-128.23 (-0.497)	-128.70 (-0.087)	-126.57 (-0.127)
Ar	-525.93 (-0.382)	-521.62 (-0.072)	-516.64 (-0.130)
Kr	-2750.1 (-0.309)	-2742.7 (-0.153)	-2721.1 (-0.130)
Be	-14.446 (-0.411)	-14.786 (-0.034)	-14.139 (-0.126)
Mg	-199.13 (-0.350)	-198.43 (-0.027)	-195.71 (-0.129)
Ca	-675.73 (-0.282)	-671.15 (-0.105)	-665.11 (-0.127)
Sr	-3129.4 (-0.263)	-3120.8 (-0.148)	-3096.8 (-0.129)

$$\tilde{n}(\mathbf{r})=\int n(\mathbf{r}')[2\zeta(\mathbf{r},\mathbf{r}')]^3\omega(2\zeta(\mathbf{r},\mathbf{r}')|\mathbf{r}-\mathbf{r}'|)d\mathbf{r}', \quad (2)$$

which includes a symmetric function $\zeta(\mathbf{r},\mathbf{r}')$ of the densities at $\mathbf{r}$ and $\mathbf{r}'$. The weight function $\omega(\rho)$ is obtained by requiring that the functional correctly describes the energy and Lindhard's linear response[23] of the homogeneous electron gas. In the nonsymmetrized ADA functional[16] $\zeta(\mathbf{r},\mathbf{r}')=k_F(\mathbf{r})$, with the local Fermi momentum $k_F(\mathbf{r})=[3\pi^2 n(\mathbf{r})]^{1/3}$; that means that average (2) is spherically symmetric about the point $\mathbf{r}$. As commented upon in Sec. II, the long-ranged weight function of this model yields numerical problems in extended systems. Within the nonsymmetrized scheme, this limitation can be avoided averaging not the density, but the Fermi momentum (AFMA functional),[17] obtaining a nonlocal functional which gives good results for the jellium surface problem. However, both the ADA and AFMA functionals give no shell structure for atoms.

As shown in the original paper,[18] the sADA functional solves the long-range problem of the weight function, and gives a clear shell structure in atomic systems when the symmetric scaling factor

$$\zeta(\mathbf{r},\mathbf{r}')=\frac{1}{2^{1/\beta}}[k_F(\mathbf{r})^\beta+k_F(\mathbf{r}')^\beta]^{1/\beta} \quad (3)$$

is used. We found that the free parameter β must lie in the interval $[-1,1]$, and its values do not drastically affect the main results obtained with functional (1). In that paper we chose $\beta=-\frac{1}{2}$ for empirical reasons: this value gives the best fitting of the Kohn-Sham ground-state energies of light atoms. Nevertheless, as shown in Table I, the total energies become worse by only about 2%, and the chemical potentials (and the first ionization energies) are, in general, closer to the Kohn-Sham values, when a value $\beta=+\frac{1}{2}$ is used in Eq. (3) instead of $\beta=-\frac{1}{2}$. Further, as can be seen in Fig. 1, density profiles preserve the clear shell structure of the atoms. Moreover, another achievement of the sADA functional, the spin polarization of atoms such N and P, is maintained. We can conclude that, at least for localized systems, the general trends of the results obtained with the functional do not depend too much on the specific value of β.

This independence is not the case for extended systems. For a metallic surface, with the jellium edge at $z=0$, a negative value of β implies that the weight function has an unphysical behavior. Specifically, Fig. 2(a) shows that the weight function centered inside the bulk has a peak in the vacuum region: as a consequence, the averaged density $\tilde{n}(z)$ well inside the metal receives a spurious contribution from the density far outside the bulk. On the other hand, in Fig. 2(b) we can observe that the weight function centered at $z'\gg 0$ has a very long range inside the bulk, and $\tilde{n}(z)$ does not go to zero when $z\rightarrow+\infty$ [see Fig. 2(c)]. These unphysical behaviors disappear for $\beta>0$.[24] Since our aim is to use the same kinetic-energy density functional for any electron system, we conclude that the β value in the scaling factor (3) must be positive. We take $\beta=\frac{1}{2}$, an intermediate value between the geometric ($\beta=0$) and the arithmetic ($\beta=1$) means. The scaling factor $\zeta(\mathbf{r},\mathbf{r}')$ will simply be

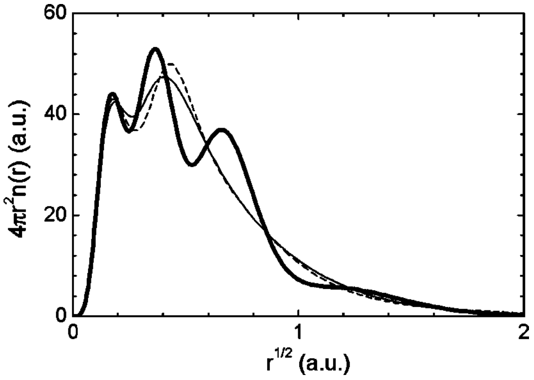

FIG. 1. Radial density $4\pi r^2 n(\mathbf{r})$ for the Kr atom. Thick solid line: Kohn-Sham; solid line: sADA functional ($\beta=+\frac{1}{2}$); dashed line: sADA functional ($\beta=-\frac{1}{2}$).

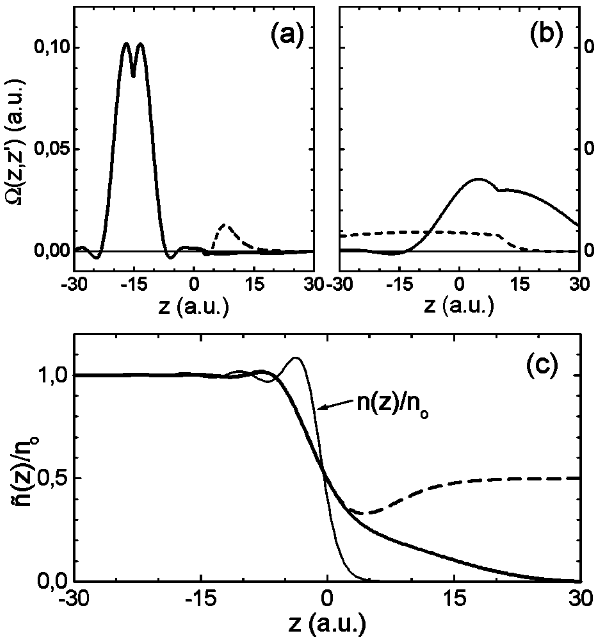

FIG. 2. Projected weight functions $\Omega(z,z')=2\zeta(z,z')\omega(2\zeta(z,z')|z-z'|)$ [panel (a): $z'=-15$ a.u.; panel (b): $z'=10$ a.u.] and averaged densities $\tilde{n}(z)/n_o$ [panel (c)] for a jellium surface ($r_s=4$ a.u.). Thick solid line: $\beta=+\frac{1}{2}$; dashed line: $\beta=-\frac{1}{2}$. Note that the averaged density $\tilde{n}(z)$ is given by $\tilde{n}(z)=\int n(z')\Omega(z,z')dz'$.

TABLE II. Surface energies (in erg cm^{-2}) and, between brackets, work functions (in eV) for jellium surfaces, obtained with the Kohn-Sham method and the kinetic-energy functionals quoted in the text.

r_s (a_o)	KS	sADA	AFMA	TF(1/4)W	SGA4
2	-1087	-1033	-1271	-640	-1090
	(3.88)	(3.83)	(3.70)	(3.78)	(3.54)
3	189	164	154	270	153
	(3.50)	(3.47)	(3.41)	(3.26)	(3.24)
4	155	143	143	172	132
	(3.09)	(3.05)	(3.03)	(2.86)	(2.89)
5	97	91	90	98	81
	(2.70)	(2.71)	(2.69)	(2.52)	(2.60)
6	59	58	56	58	50
	(2.42)	(2.43)	(2.41)	(2.26)	(2.35)

$$\zeta(\mathbf{r},\mathbf{r}') = \tfrac{1}{4}[\sqrt{k_F(\mathbf{r})} + \sqrt{k_F(\mathbf{r}')}]^2. \tag{4}$$

This choice guarantees accurate results not only for localized systems (see Table I) but also, as we will see in Sec. III, for extended ones. So, in this paper, we will study the influence in the description of the jellium surfaces due to the use of the symmetrization procedure given by Eq. (4).

III. RESULTS

In this section, our aim is to compare our sADA functional with the exact Kohn-Sham (KS) results, and with the non-symmetrized AFMA functional. We will also compare with the TF($\lambda = \frac{1}{4}$)W functional proposed by Chizmeshya and Zaremba[11] (the λ value was fitted empirically to give the best energies for the jellium surface problem) and with the square gradient approximation of fourth-order (SGA4).[25] We must remark the empirical character of the TF($\lambda = 1/4$)W approximation and the fact that the SGA4 functional does not give good ground energies in localized systems.[18,26]

To obtain the ground-state properties of a jellium surface, we minimized the total energy functional $E[n]$, solving the Euler-Lagrange equation

$$\frac{\delta E[n]}{\delta n(z)} = \mu. \tag{5}$$

In every calculation in this section we will use the local-density approximation (LDA) of Dirac and Wigner[27] for the exchange-correlation functional. To solve Eq. (5), we transform the equation into a Schrödinger-like one by means of the substitution[28] $\Psi(z) = n(z)^{1/2}$ and, in order to speed up the convergence of the iteration procedure, we treat the classical electrostatic term of the functional derivative of $E[n]$ using the integral scheme proposed by Manninen *et al.*[29]

In Table II we compare the exact KS surface energies in the range of metallic densities ($r_s = 2a_o \sim 6a_o$) with those obtained with the sADA functional, the nonlocal AFMA functional, and the TF($\lambda = \frac{1}{4}$)W and SGA4 functionals. We minimized the last functional using a conjugate gradient method.[30] Using the nonlocal functionals we obtain an overall agreement respect to the KS energies. However, this is lost by the TF($\lambda = \frac{1}{4}$)W model for high densities, and by the SGA4 functional for low ones. As can be seen in Table II, and was commented upon in Sec. I, energy values are generally good when using kinetic-energy functionals that depend explicitly on the density.

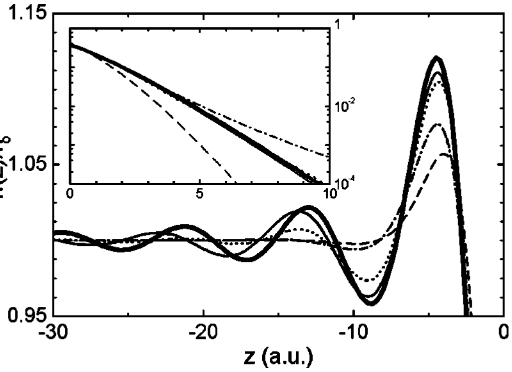

FIG. 3. Electronic density profile for a jellium surface ($r_s = 5a_o$) using several kinetic-energy density functionals. Thick solid line: Kohn-Sham; solid line: sADA; dotted line: AFMA; dashed line: TF($\lambda = \frac{1}{4}$)W; dot-dashed line: SGA4.

The quality of the sADA functional is manifested more clearly when comparing the density profiles. In Fig. 3 we can see that the density which minimizes the total energy shows Friedel oscillations (but a little shifted respect to the KS profile); moreover, there is no difference between the two profiles in the surface and vacuum regions. When the AFMA functional is used, the Friedel oscillations are quickly damped, and the density close to the surface is described slightly worse. The semilocal functionals, TF($\lambda = \frac{1}{4}$)W and SGA4, give densities with no Friedel oscillations at all and there is no agreement with the KS profiles in the vacuum region. Finally, as is well known, the density profile which minimizes the energy including the SGA4 functional, has a power-law decay rather than an exponential one.[19]

The work function Φ is directly related to the density behavior in the vacuum region through the equality[19]

$$n(z) \propto \exp[-(8\Phi)^{1/2} z]. \tag{6}$$

As we show in Table II, the coincidence in the vacuum between the KS profiles and those obtained with the nonlocal functionals sADA and AFMA translates into an excellent agreement of the work functions given by these functionals (except in the limit of high metallic densities for the AFMA nonlocal model). This concordance is lost when using the semilocal functionals. Moreover, although the decay of the density profiles obtained with the semilocal functionals are not well behaved, the corresponding work functions are rather good because Eq. (6) is not verified by these functionals.

IV. STABILIZED JELLIUM MODEL

In their seminal articles,[20] Lang and Kohn emphasized a clear limitation of the jellium model: the surface energies for high-density metals are negative and, therefore, the bulk metal is mechanically unstable. Preserving the simplicity of the jellium model, this defect can be solved by means of the stabilized jellium model,[31,32] where a constant (structureless pseudopotential) is added to the external potential in the bulk

TABLE III. Surface energies σ_T (in erg cm^{-2}) and work functions Φ (in eV) for alkaline metals, using the stabilized jellium model, obtained with the Kohn-Sham (KS) method and the sADA and SGA4 functionals.

		σ_T			Φ		
Metal	r_s (a_o)	KS	sADA	SGA4	KS	sADA	SGA4
Li	3.28	302	262	252	3.36	3.33	2.99
Na	3.99	171	155	143	2.93	2.91	2.69
K	4.96	89	83	74	2.48	2.48	2.36
Rb	5.23	74	71	63	2.38	2.37	2.25

region, in order to simulate the effect arising from the crystalline ionic array in the metal.

As an additional test for the sADA functional, in Table III we present the surface energy and the work function for the alkali metals. We compare these results with the exact Kohn-Sham ones,[33] and with those obtained by us after a complete minimization of the total energy using the SGA4 functional. The $E_{\mathrm{XC}}[n]$ functional used in the calculations is the LDA proposal by Perdew and Zunger,[34] which was used in the above quoted works.

We see that the good results obtained with the sADA functional are maintained in this more realistic description of the metallic surface. However we must comment that the good results for the SGA4 functional quoted in Ref. 31 are accidental. These authors use a parametrized form for the density profile and, as consequence, the minimization of the total energy is not complete. This partial minimization overestimates both the surface energy and the work function.[31,35]

V. LINEAR INDUCED DENSITY

We would like to finish our tests on the quality of the sADA kinetic-energy functional with a very hard one: the calculation of the density induced by a weak static external electric field $\delta\mathbf{E}$ acting normally to the jellium surface. Writing this external field as $\delta\mathbf{E}=-2\pi\sigma\mathbf{e}_z$, where σ is the net surface charge density induced by the external field, the linear induced density can be expressed as

$$\delta n(z)=\sigma n_1(z)+o(\sigma^2). \tag{7}$$

Further, the centroid of this induced charge

$$z_1=\int_{-\infty}^{+\infty} z n_1(z)dz \tag{8}$$

defines the image plane position.[20] The dynamical sum rule[36] allows us to write z_1 only in terms of the values of the induced density outside the metal,

$$z_1=\int_{0}^{+\infty} z n_1(z)dz. \tag{9}$$

Since this sum rule is classical, it must be satisfied by any explicit kinetic-energy functional, and we have checked, as an additional test for the convergence of our calculations, that the centroids obtained using both equations coincide in all the calculations we have made.

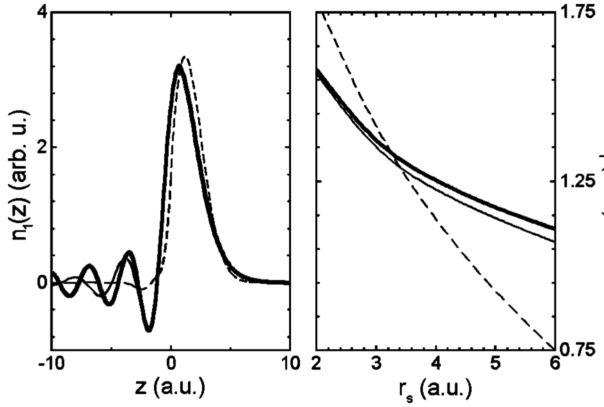

FIG. 4. Left panel: induced density $n_1(z)$ for a jellium surface ($r_s=2a_o$); right panel: image plane position z_1 in terms of r_s. Thick solid line: Kohn-Sham; solid line: sADA; dashed line, TF($\lambda=\frac{1}{4}$)W.

Note that this calculation is a first test to check the quality of the static linear-response function given by the functional in a nonhomogeneous electron system. We saw in Sec. II that the density profiles obtained are extremely accurate. On the other hand, any ADA functional exactly reproduces the linear-response function of the noninteracting homogeneous electron gas. For both reasons we expect to obtain a good linear induced density when the sADA functional is used for jellium surfaces.

The left panel of Fig. 4 presents the *exact* Kohn-Sham-induced density $n_1(z)$, the one obtained with sADA and the one corresponding to the TF($\lambda=\frac{1}{4}$)W functional. The result of the last functional has the maximum displaced with respect to the exact peak, and has no Friedel oscillations. The $n_1(z)$ density given by our nonlocal functional reproduces almost exactly that main peak and the behavior in the vacuum region ($z>0$). Inside the metal, the induced density shows well-defined Friedel oscillations but, as in the ground-state density, shifted when compared to the Kohn-Sham ones. The latter shift has no influence on the value of the image plane position because the dynamical sum rule imposes that $\int_{-\infty}^{0} z n_1(z)dz$ be zero for any functional. In the right panel of Fig. 4 we can clearly see this: there is an excellent agreement between the exact centroids and those given by the sADA functional, because the $z>0$ values of $n_1(z)$ are almost the same in both calculations. On the other hand, for the TF($\lambda=\frac{1}{4}$)W functional, even if the density profile seems quite good indeed, the small differences in $n_1(z)$ for $z>0$ give only a qualitative description of the dependence of z_1 on the bulk density, as already shown by Chizmeshya and Zaremba.[11]

VI. CONCLUSIONS

In this paper we discussed some properties of the sADA kinetic-energy functional. In the first place, we can conclude that the sADA kinetic-energy functional, with $\beta=\frac{1}{2}$, is a universal functional, i.e., that gives good results, when compared to the Kohn-Sham method, for localized (atoms) and inhomogeneous extended systems (jellium surfaces). We have confirmed that the nonspherical averaging procedure given by Eqs. (2) and (3) is essential in the improvement of the kinetic-energy functional, specifically when discussing the structure of the density profiles. We must remark that the sADA functional is a *continuous* density functional, i.e., it has no derivative discontinuities (in the sense of Perdew and Levy[37]). Thus it cannot describe, for instance, the steplike evolution of the ionization energy with the number of electrons for a fixed nuclear charge. This does not prevent an accurate kinetic functional, such as the one presented here, which describes almost exactly the density both in the inner (K shell) and in the outer region of an atom, from giving structured atomic profiles.[18]

When the sADA kinetic-energy functional is applied to jellium surfaces, we obtained excellent results for the ground-state properties: surface energies, work functions, and density profiles. Moreover, the results for the linear induced density, directly related to the linear response of the functional, are very good. This is in agreement with the accurate linear-response matrix obtained with the sADA functional in one-dimensional electron systems.[38]

Because the symmetrization procedure considerably improves the description of the nonlocality of the kinetic energy, we guess that the long standing puzzle of the asymptotic limit of the image potential in surfaces[39] may be solved by the symmetrization of the WDA exchange-correlation functional.[15,40,41] This symmetrization is in progress, in order to clarify if it is the way to obtain the correct asymptotic behavior of the image potential.

Finally, in Sec. I we commented that one of the motivations for the development of a $T_S[n]$ functional is the simplification of *orbital-free* DFT calculations in complex systems. Although our sADA model is easier to apply than the Kohn-Sham method in molecular-dynamics simulations, its own complexity makes it more difficult to apply than other kinetic functionals. For instance, the functionals developed specifically for solids by Wang and Teter[12] and Perrot[13] are much simpler than the sADA. Nevertheless, the sADA functional, with some simplifications suggested by the structure of the problem at hand, could be easier to apply, and could achieve similar results to the ones obtained with those functionals.

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