

# Orbital-free density functional theory: Differences and similarities between electronic and nuclear systems

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Orbital-free density functional theory (OF-DFT) has been used when studying atoms, molecules, and solids. In nuclear physics, applications of OF-DFT have been quite scarce so far, as DFT has been widely applied to the study of many nuclear properties mostly within the Kohn–Sham (KS) scheme. There are many realizations of nuclear KS-DFT, but computations become very demanding for heavy systems, such as superheavy nuclei and the inner crust of neutron stars, and it is hard to describe exotic nuclear shapes using a finite basis made with a limited number of orbitals. These bottlenecks could, in principle, be overcome by an orbital-free formulation of DFT. This work is a first step towards the realistic application of OF-DFT to nuclei. In particular, we have implemented possible choices for an orbital-free kinetic energy and solved the associated Schrödinger equation either with simple potentials or with simplified nuclear density functionals. While the former choice sheds light on the differences between electronic and nuclear systems, the latter choice allows us to discuss the practical applications to nuclei as well as open questions.  
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Subject Index D10, D11

## 1. Introduction

Orbital-free density functional theory (OF-DFT) was introduced in Ref. [1], in which an interesting remark was made, related to the original Hohenberg–Kohn (HK) theorem [2]. This HK theorem sets an exact one-to-one correspondence between the energy  $E$  of an interacting fermion system and that of a fictitious, non-interacting fermion system ( $E_f$ ) with the same density  $\rho$ . If  $\rho$  is, in turn, expressed in terms of orbitals like  $\rho = \sum_j |\phi_j|^2$  we have the usual Kohn–Sham (KS) formulation of DFT [3]. The Kohn–Sham form of the energy density functional (EDF) is

$$E_f = E_{KS} = \sum_j \int d^3r \phi_j^*(\mathbf{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 \right) \phi_j(\mathbf{r}) + \int d^3r \mathcal{V}_{KS}[\rho], \quad (1)$$

where the first term is the kinetic energy with a mass  $m$  and the second term includes all interactions (for electronic systems, this means Hartree energy, exchange-correlation energy, and interaction with the external potential).

In Ref. [1], the authors noted that one can actually map the interacting fermion system onto a non-interacting *boson* system. In fact, in the proof of the HK theorem, no special role is played

by the statistics of the particles (as well as by their mass). Therefore, one could write the energy of the system as

$$E_b = E_{\text{OF-DFT}} = \frac{\hbar^2}{2m} \int d^3r (\nabla \sqrt{\rho})^2 + \int d^3r \mathcal{V}[\rho], \quad (2)$$

where the first term is now the boson kinetic energy. The second term could be, at least in principle, related to the KS interaction energy by adding the KS kinetic energy and subtracting the boson kinetic energy (one should remember here that the KS kinetic energy, although written in terms of orbitals, must be a functional of  $\rho$  as every property of the system at hand is).

Either from Eqs. (1) or (2), one can minimize the energy using the variational principle with a fixed number of particles. From Eq. (1) one easily obtains the famous Kohn–Sham set of equations,

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + v_{\text{KS}} \right) \phi_j(\mathbf{r}) = \varepsilon_j \phi_j(\mathbf{r}), \quad (3)$$

where the effective KS potential is  $v_{\text{KS}} \equiv \frac{\delta}{\delta \rho} \int d^3r \mathcal{V}[\rho] = \frac{\partial \mathcal{V}}{\partial \rho}$  and  $\varepsilon_j$  are the Lagrange multipliers associated with the normalization of the single orbitals, which are interpreted as eigenenergies of those orbitals. On the other hand, if one starts from Eq. (2) and applies

$$\frac{\delta}{\delta \rho} \left( E - \mu \int d^3r \rho \right) = 0, \quad (4)$$

one easily arrives at

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + \frac{\partial \mathcal{V}}{\partial \rho} \right) \sqrt{\rho} = \mu \sqrt{\rho}, \quad (5)$$

which is the basic (Euler) equation of OF-DFT. We shall simply write  $v = \frac{\partial \mathcal{V}}{\partial \rho}$  in what follows.

The practical advantage of the latter equation (5) over the conventional KS equations (3) is clear. Instead of solving  $N$  equations for  $N$  orbitals, one has to solve only *one* equation. All particles lie on a single orbital and this must have a simple shape, like that of an  $\ell = 0$  orbital in a spherical potential, etc. This has motivated a series of applications for atoms, molecules, and solids; see, e.g., Refs. [4–6] for useful papers that review many of these applications. Even public software is available [7]. The time-dependent (TD) extension of OF-DFT is discussed in Ref. [8] and references therein.

In the case of nuclear systems, the advantages brought by OF-DFT can be even stronger. Many finite nuclei have intrinsic deformed shapes, so that Kohn–Sham levels have little degeneracy and the set of equations can be very large. Superheavy nuclei, or nucleons in the inner crust of neutron stars, are still a big challenge for conventional nuclear DFT and the same can be said for time-dependent calculations. OF-DFT can be very instrumental in all these cases, and others. Some nuclei are known to exhibit shape coexistence, and a description in terms of orbitals calls for a superposition of orbitals associated with different shapes that are non-orthogonal. A prospective OF-DFT description would be simpler to implement and to interpret.

Despite these motivations, to the best of our knowledge the only modern application of OF-DFT to finite nuclei is in Ref. [9], where an orbital-free formulation is proposed as an alternative to KS for the global fit of masses but no details are provided. Therefore, our purpose in the present work is to start to fill this gap. In particular, the scope of the paper is to explore different prescriptions for the orbital-free kinetic energy, and see how they perform for simple nuclei. One of the key questions that we have in mind is if there are basic differences between electronic and

nuclear systems due to the long-range or short-range character of the underlying interaction. Ultimately, we would like to assess to what extent OF-DFT is useful for nuclear systems.

Notice that OF-DFT bears some resemblance to what have, in the nuclear physics context, been called the Thomas–Fermi (TF) or extended TF (ETF) approximations [10–17]. In Ref. [10], it was demonstrated that the ETF approximation provides a good description of the ground-state energy but it yields an incorrect tail for the density distribution (see also Ref. [18]). A simple recipe was considered in Ref. [10] to cure this problem by changing the coefficient of the von Weizsäcker correction term in the kinetic energy within the ETF approximation. An equivalent recipe for the von Weizsäcker correction, but in a slightly different context, was adopted in Ref. [17]. In this paper, we also address the question of the density distributions and the capability of OF-DFT to reproduce its asymptotic tail.

The paper is organized as follows. In Sect. 2, some possible choices of the OF-DFT ansatz, together with the relationship with ETF, are discussed. In Sect. 3, we present our first, exploratory results aimed at showing analogies and differences between nuclear and Coulomb systems. In Sect. 4, we move to applications based on a realistic, albeit simplified, nuclear interaction and discuss the issue of the shell structure. Our conclusions are drawn in Sect. 5.

## 2. The OF-DFT kinetic energy

We go back to Eq. (2), i.e.,

$$E = \frac{\hbar^2}{2m} \int d^3r (\nabla \sqrt{\rho})^2 + \int d^3r \mathcal{V}[\rho] \equiv T + V.$$

Let us assume that we have an ansatz for  $V$  and focus on how to start from the boson kinetic energy  $T$  and best approximate the fermion kinetic energy, keeping a density-dependent (and not orbital-dependent) form.

The mere replacement of the fermion kinetic energy with the boson one is named after von Weizsäcker (vW). In this case,

$$T = T_{\text{vW}} \equiv \frac{\hbar^2}{2m} \int d^3r (\nabla \sqrt{\rho})^2. \quad (6)$$

This expression is obviously exact for a single fermion, or two fermions in a spin-singlet state. In Coulomb systems, it provides a rigorous lower bound to the exact kinetic energy (cf. Sect. 1a of Ref. [6]). A sort of complementary choice is the kinetic energy given by the TF approximation, which takes care of the Pauli principle and is exact in a uniform system, but is approximate for finite systems. In this case,

$$T_{\text{TF}} = \frac{\hbar^2}{2m} \int d^3r \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3}. \quad (7)$$

This form of the kinetic energy is close to another rigorous lower bound, as shown by Lieb [19]. The TF approximation is known to have shortcomings in the nuclear case, and in particular not to provide the correct asymptotic form of the nuclear densities [10,11].

In the Coulomb case, there exist some pragmatic prescriptions for mixing vW and TF. One possibility is

$$T_{\text{TF,vW},\beta} = T_{\text{TF}} + \beta T_{\text{vW}}, \quad (8)$$

even though one may also introduce another factor in front of the first term. This equation is motivated by a conjecture, again by Lieb [20], namely that the exact kinetic energy  $T$  should obey  $T < T_{\text{vW}} + T_{\text{TF}}$ . Popular choices for  $\beta$  are  $\beta = \frac{1}{5}$  and  $\frac{1}{9}$ . One could use the response

**Table 1.** Values of the total energy and of the r.m.s. radius of  $^{16}\text{O}$ , calculated either with the potential (13) (this result is labeled as exact) or with different prescriptions for the kinetic energy as defined by Eq. (8).

	$E$ (MeV)	$\sqrt{\langle r^2 \rangle}$ (fm)
exact	-142.27	2.575
OF-DFT ( $\beta = 1/9$ )	-140.85	2.500
OF-DFT ( $\beta = 1/5$ )	-135.19	2.562
OF-DFT ( $\beta = 1$ )	-96.31	3.120

function of the uniform free electron gas  $\chi_0$  and write the kinetic energy of the slightly perturbed gas: the second-order expansion in  $\nabla\rho$  is equivalent to  $\beta = \frac{1}{9}$  in Eq. (8). The choice of  $\beta = \frac{1}{9}$  can also be obtained with the semi-classical approximation to the kinetic energy, while  $\beta = 1$  is the original value derived by von Weizsäcker.  $\beta = \frac{1}{5}$  was obtained from empirical fits.

Another possible choice is

$$T = \int d^3r \tau_{\text{TF}} F(\mathbf{r}), \quad (9)$$

where  $F$  is the so-called enhancement factor. We mention this choice because it has been adopted in Ref. [9]; the corresponding expression for  $F$  is provided in the [appendix](#) below. We have tested this choice, and checked that we obtain results that lead to the same qualitative conclusions obtained with our simpler prescription (8). Notice that, if one adopts

$$F = \left( 1 + \beta \frac{\tau_{\text{vW}}}{\tau_{\text{TF}}} \right), \quad (10)$$

then one goes back to Eq. (8).

In what follows, we are going to display the results obtained by solving the Euler equation (5) in spherical symmetry. The explicit form of the equation in this case is provided in the [appendix](#).

### 3. Results for simple potential models

In this section, we use simple systems of non-interacting fermions in a given potential. The model Hamiltonian for such systems reads

$$H = \sum_i \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i) \right). \quad (11)$$

The total energy for this Hamiltonian is obviously

$$E = \sum_{i:\text{occ}} \epsilon_i, \quad (12)$$

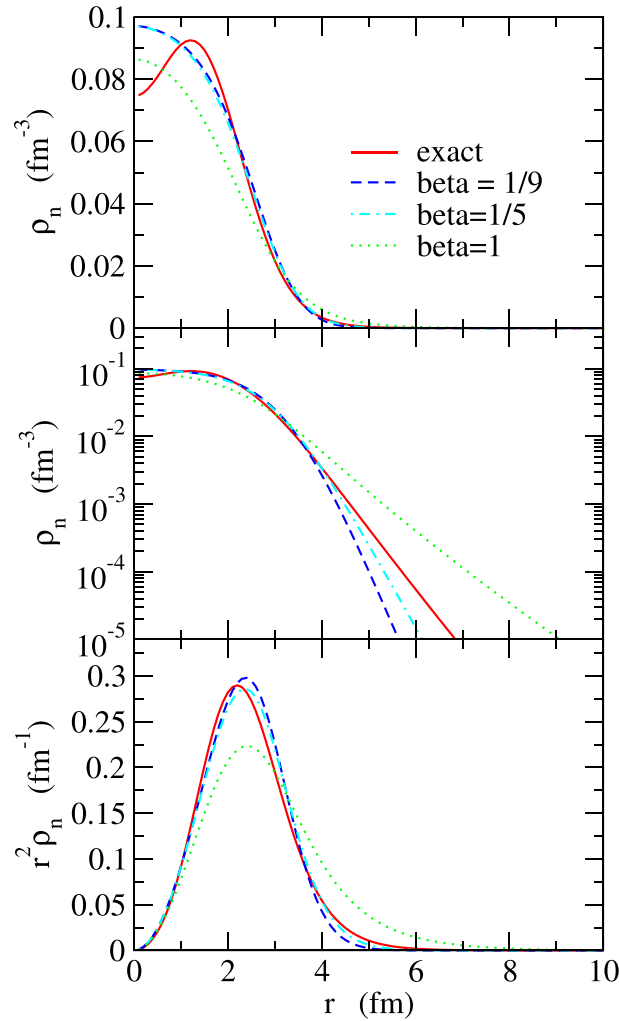
i.e., the sum of the eigenenergies for the occupied orbits.

#### 3.1. Nuclear systems

Let us first consider a system with 8 neutrons in a Woods–Saxon potential given by

$$V(r) = -\frac{V_0}{1 + \exp[(r - R_0)/a]}, \quad (13)$$

with  $V_0 = 50$  MeV,  $R_0 = 1.2 \times 16^{1/3}$  fm, and  $a = 0.65$  fm, mimicking the  $^{16}\text{O}$  nucleus. For simplicity, the spin–orbit interaction is ignored. The single-particle energies  $\epsilon$  with this potential are  $-32.6$  and  $-16.8$  MeV for the 1s and 1p states, respectively. The total energies and the root-mean-square (r.m.s.) radii for several values of  $\beta$  are summarized in Table 1. The corresponding



**Fig. 1.** Density distributions as a function of the radius  $r$  for a system with 8 neutrons in a Woods–Saxon potential given by Eq. (13). The top and middle panels show the density distributions on linear and logarithmic scales, respectively, while the bottom panel shows the densities on a linear scale multiplied by  $r^2$ . In each panel, the solid line denotes the exact density, while the dashed, dot-dashed, and dotted lines show the densities from orbital-free DFT with  $\beta = 1/5$ ,  $1/9$ , and  $1$ , respectively.

density distributions are shown in Fig. 1. These results indicate that  $\beta = 1/9$  is slightly better for the total energy while  $\beta = 1/5$  is slightly better for the r.m.s. radius. Both choices can be reasonable although not highly accurate, while  $\beta = 1$  should be discarded. This overall conclusion is confirmed by looking at the density distributions. In particular, the exponential tail shown in the middle panel indicates that the tail is not well reproduced with  $\beta = 1/9$  and  $1$ , as has been discussed in Ref. [10], while  $\beta = 1/5$  significantly improves the tail. This consideration may be important when applying OF-DFT to, e.g., nuclear reactions.

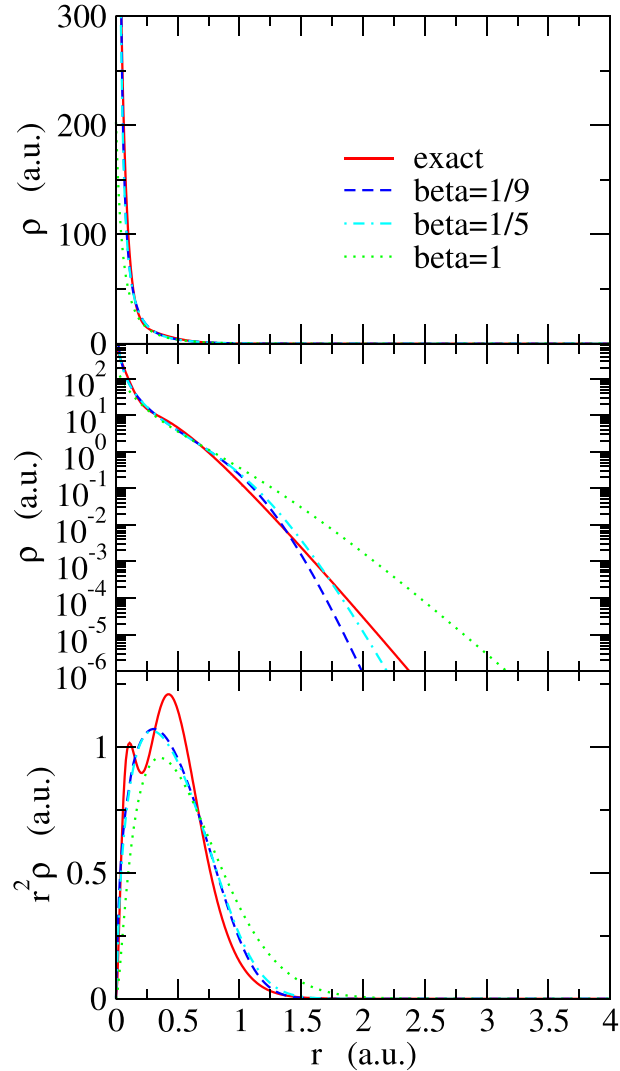
### 3.2. Coulomb systems

We next consider a system of 10 electrons in the attractive Coulomb potential

$$V(r) = -\frac{10e^2}{r}. \quad (14)$$

**Table 2.** Values of the total energy and of the r.m.s. radius of the 10 electrons bound by the Coulomb potential (14). The exact result is compared with different prescriptions for the kinetic energy as defined by Eq. (8).

method	$E$ (Ha)	$\sqrt{\langle r^2 \rangle}$ (a.u.)
exact	-200.0	0.27
OF-DFT ( $\beta = 1/9$ )	-208.6	0.30
OF-DFT ( $\beta = 1/5$ )	-196.1	0.32
OF-DFT ( $\beta = 1$ )	-142.0	0.48



**Fig. 2.** Same as Fig. 1, but for a system with 10 electrons in a Coulomb potential given by Eq. (14).

We use atomic units in this subsection. The eigenenergies of this potential are  $\epsilon = -50.0$  (Ha) for the 1s orbital and  $-12.5$  (Ha) for the 2p and 2s orbitals. The results are shown in Table 2 and Fig. 2.

From Table 2, one can see that there is not a big difference between the results obtained with  $\beta = 1/5$  and  $1/9$ , while  $\beta = 1$  does not perform well, as was the case for the nuclear system that we have just discussed. The same qualitative conclusion as in the nuclear case can be obtained

for the tail of the density distributions: while the deviation is large for  $\beta = 1$  and  $1/9$ , the choice of  $\beta = 1/5$  significantly improves the surface behavior of the density distribution. However, we notice that the central density is considerably larger in the Coulomb case, and the deviation of the tail appears only at much smaller densities (relative to the central density) as compared to the nuclear case. The wrong tail in the density distribution would thus be much less relevant here as compared with the nuclear case.

#### 4. Towards realistic models

In a first attempt towards realistic nuclear OF-DFT calculations, we have solved the self-consistent equations associated with the potential part of a Skyrme EDF for a few spherical nuclei. In fact, we have used the simple force introduced in Ref. [21], i.e.,

$$v_{NN}(\mathbf{r}, \mathbf{r}') = \left[ t_0 + \frac{t_3}{6} \rho \left( \frac{\mathbf{r} + \mathbf{r}'}{2} \right)^\alpha \right] \delta(\mathbf{r} - \mathbf{r}'), \quad (15)$$

with which the potential part of the energy functional in Eq. (1) reads

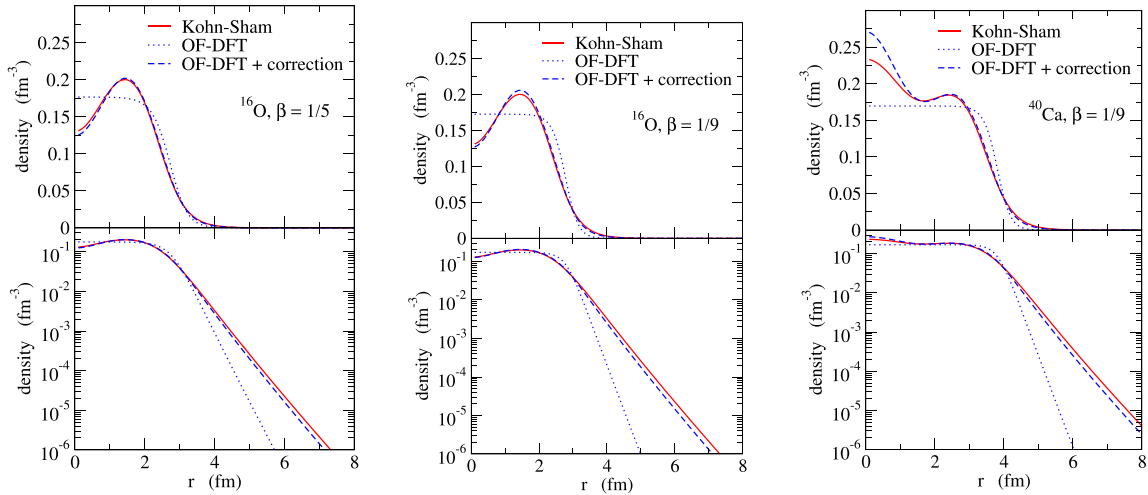
$$\mathcal{V}_{KS}[\rho] = \frac{3}{8} t_0 \rho(\mathbf{r})^2 + \frac{t_3}{16} \rho(\mathbf{r})^{\alpha+2}. \quad (16)$$

We have used the same values for the parameters  $t_0$ ,  $t_3$ , and  $\alpha$  as those in Ref. [21]. This is a semi-realistic choice and is not as accurate as a standard, complete Skyrme EDF; still, we can learn about shell effects.

In fact, a criticism that has been raised against OF-DFT is that shell effects may be somehow missing. A discussion of shell effects, for the Coulomb case, can be found in, e.g., Ref. [22] and references therein. Similar discussions can be found for the nuclear case in several ETF works. For instance, in the density distributions, oscillations associated with the occupancies of different orbitals do not show up, at least with simplified effective potentials. Ideally, the exact OF-DFT should reproduce the exact density, including the oscillations. This means that, most likely, the exact OF-EDF will include a potential with more, or higher-order, derivative terms than those that we can build at present.

At the moment, we have not had yet built sophisticated new OF-EDFs and this is not doable within a short-range perspective. Even though the Strutinsky shell correction method can be applied to the ground-state energies [12–16,22], we would like to take into account the shell effect on the density distributions as well. For this purpose, we have found a simple prescription that allows the shell-effects to be recovered with little cost, on top of OF-DFT. As has been done in Refs. [23–25] for the Coulomb case and in Ref. [18] for the nuclear case, we have implemented the following procedure. After arriving at a converged OF result, we have included the resultant effective potential in the Kohn–Sham equation and carried out just one further iteration.

The results of this procedure are shown in Fig. 3. It can be easily seen that just one iteration of the Kohn–Sham equations using the converged potential from the OF Euler equation is enough to produce density distributions that are similar to the ones obtained from the full iterative Kohn–Sham procedure. This holds true as far as we consider shell effects, i.e., the oscillations in the inner region, but also as far as the tail is considered. In Fig. 3, we emphasize the two complementary aspects by displaying densities on both linear and logarithmic scales. Our conclusion is quite general and is demonstrated by using two different nuclei and the two reasonable choices for  $\beta$ , namely  $\beta = 1/5$  and  $1/9$ .



**Fig. 3.** A comparison of the density distributions obtained with a simplified Skyrme EDF. The left, middle, and right panels show the density distributions for  $^{16}\text{O}$  from OF-DFT with  $\beta = 1/5$ , those for  $^{16}\text{O}$  with  $\beta = 1/9$ , and those for  $^{40}\text{Ca}$  with  $\beta = 1/9$ , respectively. The upper and lower panels show the density distributions on linear and logarithmic scales, respectively. In each panel, the solid and dotted lines show the density obtained with the Kohn–Sham method and the OF-DFT, respectively. The dashed lines show the densities with OF-DFT, but with the correction based on the last iteration using the Kohn–Sham method after convergence is achieved with OF-DFT, as discussed in the text.

## 5. Conclusion

In this paper, we have made a first attempt to seriously answer the question of whether OF-DFT can be applied to nuclear systems with some chance of success. OF-DFT has been applied to Coulomb systems by different groups and in different ways. Nuclei are characterized by a different basic interaction, which is short-range rather than long-range; at the same time, nuclear DFT is more demanding from the computational viewpoint and the study of superheavy isotopes, or of the crust of neutron stars, would benefit from OF-DFT. Nuclei with shape coexistence, which are not easy to describe using a limited basis of single-particle orbitals, are a further motivation to explore OF-DFT for nuclei.

We have found that OF-DFT provides reasonable results for magic nuclei, once the kinetic energy has been approximated with Eq. (8) in a similar way as for electronic systems. A careful look into the density distributions reveals that the tails are not well reproduced in both the nuclear and electronic cases, even though the long-range character of the Coulomb force does indeed play a role and washes out the discrepancies between the exact results and those with reasonable values of  $\beta$ , more than in the nuclear case. One of the interesting results of our work is that density distributions can also be markedly improved by just one last KS iteration, after the OF-DFT procedure has reached convergence.

Fine-tuning of the OF functionals is now in order. This is among our perspectives but, at the same time, one should develop the formalism to go beyond the simple EDFs that depend on the local number density only. OF versions of EDFs that depend on density gradients, higher-order derivatives, or other generalized densities (spin–orbit densities, pairing densities, etc.) should be investigated. We plan to go along this line, by comparing different formulations (for instance, spin polarization vs spin–orbit density). Another possible direction towards this goal may be to use deep learning techniques, as has been advocated in Ref. [26].



Last but not least, we should go beyond the spherical approximation and formulate OF-DFT for deformed nuclei. In this case, the way to optimize the energy may be re-discussed (see, e.g., Ref. [27]). Moreover, it was argued in Ref. [10] that the ETF approximation “fails to give reasonable deformation energies due to a drastic overestimation of the surface energy contributions” (see Sect. 3.3 in Ref. [10]). It would be interesting to see how well the deformation energy is described with the prescription of a single KS iteration after convergence of OF-DFT.

More generally, past ETF studies of nuclear systems have not been able to go beyond some level of accuracy. The broad and novel perspective that we wish to highlight goes beyond ETF, with a more flexible form of the kinetic energy, and uses state-of-the-art methods like Bayesian inference or machine learning [28,29] to improve over ETF.

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### A. Euler equation and total energy in the spherical case

In this appendix, we derive the Euler equation associated with the OF-DFT kinetic energy in the form of Eq. (8) and a generic potential part. We also specialize the result to the case of spherical symmetry.

The EDF with  $T$  given by Eq. (8) reads

$$E = \beta \frac{\hbar^2}{2m} \int d^3r (\nabla \sqrt{\rho})^2 + \alpha \frac{\hbar^2}{2m} \int d^3r \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} + V[\rho]. \quad (\text{A1})$$

The variation of the first term is

$$\frac{\delta T_{\text{vW}}}{\delta \rho} = \frac{\partial \sqrt{\rho}}{\partial \rho} \frac{\delta T_{\text{vW}}}{\delta \sqrt{\rho}} = \frac{1}{2\sqrt{\rho}} \left( -\nabla \frac{\partial T_{\text{vW}}}{\partial \nabla \rho} \right) = -\frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}}, \quad (\text{A2})$$

while for the second term it is

$$\frac{\delta T_{\text{TF}}}{\delta \rho} = \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \rho^{2/3}. \quad (\text{A3})$$

Then, the Euler equation becomes

$$\left[ -\beta \frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{\rho}}{\sqrt{\rho}} + \alpha \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \rho^{2/3} + \frac{\delta V}{\delta \rho} \right] = \mu. \quad (\text{A4})$$

By multiplying both sides of this equation by  $\sqrt{\rho}/\beta$ , one obtains

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{\alpha}{\beta} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \rho^{2/3} + \frac{1}{\beta} \frac{\delta V}{\delta \rho} \right] \sqrt{\rho} = \frac{\mu}{\beta} \sqrt{\rho}. \quad (\text{A5})$$

In general, using a spherical basis, we can write

$$\sqrt{\rho} \equiv \Phi = \sum_{lm} \frac{\phi_{lm}}{r} Y_{lm}. \quad (\text{A6})$$

In the spherical case, only  $\phi_{00}$  is to be considered. From the previous equation (A5), we easily obtain the reduced Schrödinger equation in the form

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + \frac{\alpha}{\beta} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \rho^{2/3} + \frac{1}{\beta} \frac{\delta V}{\delta \rho} \right] \phi = \frac{\mu}{\beta} \phi. \quad (\text{A7})$$

The total energy can be written in a useful form by exploiting the fact that

$$\nabla \sqrt{\rho} = \frac{1}{2\sqrt{\rho}} \nabla \rho = \frac{1}{2\rho} \frac{\partial \rho}{\partial r} \mathbf{e}_r.$$

In this way,

$$\begin{aligned} E &= \beta \frac{\hbar^2}{2m} \int d^3r \frac{1}{4\rho} \left( \frac{\partial \rho}{\partial r} \right)^2 + \alpha \frac{\hbar^2}{2m} \int d^3r \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} + \int d^3r \frac{\delta V}{\delta \rho} \rho \\ &= \beta \frac{\hbar^2}{2m} \int dr 4\pi r^2 \frac{1}{4\rho} \left( \frac{\partial \rho}{\partial r} \right)^2 + \alpha \frac{\hbar^2}{2m} \int dr 4\pi r^2 \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} + \int dr 4\pi r^2 \frac{\delta V}{\delta \rho} \rho. \end{aligned} \tag{A8}$$

For the sake of completeness, we also report here the Euler equation and its reduction to the spherical case, in the specific case of the kinetic energy given by Eq. (9) with the enhancement factor proposed in Ref. [9], namely

$$F = \frac{1 + (1 + \kappa)X + 9\kappa X^2}{1 + \kappa X} \tag{A9}$$

and

$$X = \frac{5}{27} \frac{|\nabla \sqrt{\rho}|^2}{(3\pi^2)^{2/3} \rho^{5/3}}. \tag{A10}$$

In this case, the Euler equation becomes

$$\left[ -\frac{\hbar^2}{2m} \frac{F'}{9} \nabla^2 + \frac{\hbar^2}{2m} (3\pi^2)^{2/3} \rho^{2/3} (F - F'X) + \frac{\delta V}{\delta \rho} \right] \sqrt{\rho} = \mu \sqrt{\rho}. \tag{A11}$$

In the spherical case, we easily arrive at

$$\frac{d^2 \phi}{dr^2} = \left[ (3\pi^2)^{2/3} \rho^{2/3} \frac{9(F - F'X)}{F'} + \frac{2m}{\hbar^2} \frac{9}{F'} \frac{\delta V}{\delta \rho} - \frac{2m}{\hbar^2} \frac{9}{F'} \mu \right] \phi. \tag{A12}$$

The total energy reads

$$E = \frac{\hbar^2}{2m} \int d^3r \frac{3}{5} (3\pi^2)^{2/3} \rho^{5/3} F + \int d^3r \frac{\delta V}{\delta \rho} \rho \tag{A13}$$

and we could also write

$$E = \mu - \frac{2}{5} \frac{\hbar^2}{2m} \int d^3r (F - F'X) (3\pi^2)^{2/3} \rho^{5/3}. \tag{A14}$$

The second term can be interpreted as a rearrangement energy.

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