QUASI-LOCAL DENSITY FUNCTIONAL THEORY 
AND ITS APPLICATION WITHIN EXTENDED 
THOMAS-FERMI APPROXIMATION

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Abstract

A generalization of the Density Functional Theory is proposed. The theory developed leads to single-particle equations of motion with a quasi-local mean-field operator, which contains a quasi-particle position-dependent effective mass and a spin-orbit potential. The energy density functional is constructed using the Extended Thomas-Fermi approximation. Within the framework of this approach the ground-state properties of the doubly magic nuclei are considered. The calculations have been performed using the finite-range Gogny D1S force. The results are compared with the exact Hartree-Fock calculations.

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The Hartree-Fock (HF) method is one of the most widely used approaches in nuclear physics. It is based on the concept of independent particle motion in the mean field produced by effective nucleon-nucleon forces which are generally non-local and density dependent. The resulting equations of motion contain the non-local single-particle potential (SPP) which is determined self-consistently. The comprehensive study of nuclear ground state properties within the HF method has been performed with the zero-range Skyrme-like forces \[1, 2\]. The status of this problem is not completely the same for finite range forces. The exact solution of the HF equations in this case is not an easy task, mainly due to the non-locality of the SPP. For example, the complete solution of the HF equations was carried out in Ref. \[3\] for a finite range effective force with a Gaussian formfactor using a harmonic oscillator basis. On the other hand, the M3Y effective force with a Yukawa formfactor was employed in Ref. \[4\] within the Campi and Bouyssy \[5\] local approximation for the single-particle density matrix.

Thus the problem of localization of the non-local SPP becomes actual. As it is known the non-local exchange Fock part of the SPP is determined using the non-local single-particle density matrix (DM in the following). If one approaches the DM in terms of only local quantities such as the particle density and kinetic-energy density, the corresponding HF exchange energy becomes a functional of these local quantities. The equations of motion obtained from the resulting local HF functional are second-order differential equations. It is important to note that they do not contain any integral operators which lead to difficulties in the general non-local case. For instance the Negele and Vautherin expansion of the DM \[6\] and its modification by Campi and Bouyssy \[5\] enables the HF energy to be expressed in the pointed functional form. Recently, another approach based on the Extended Thomas-Fermi method (ETF, see, for instance, Ref. \[7\]) has been proposed to this aim in Ref. \[8\].

An alternative, in a sense, approach to the mean field theory, which is widely used in applications to electron systems, is based on the Kohn-Sham (KS) \[9\] method within the framework of the Density Functional Theory (DFT). The original version of this theory was developed in the pioneering paper of Hohenberg and Kohn (HK) \[10\] where an energy functional depending only on the local particle density was considered (so we shall call it local DFT). Later on other versions of the DFT were proposed (see, for example, Refs. \[11, 12\]). In particular, the non-local extension of this theory was discussed by Gilbert in Ref. \[13\] where the functional dependence on the DM was included.

The main merit of the KS scheme consists of the following: it gives a way to obtain single-particle equations of motion for the local DFT. These equations contain the local mean-field potential that has to be determined self-consistently. Notice that in contrast to the approximate HF method, the DFT yields, in principle, the exact ground-state energies (and the referred quantities) of the many-body system. Concerning the single-particle spectrum only the last occupied level has the exact physical meaning of the chemical potential in the DFT which is just the particle separation energy.

There is one more important difference between the HF and KS methods that is revealed in the applications to nuclei. The radial-dependent effective mass and the spin-orbit potential are essential components of the HF approach in nuclear physics. These two quantities arise owing to the kinetic-energy density and spin density dependence of the HF energy functional. However, in the original KS method the effective mass is constant and equal to the physical mass and there is no spin-orbit potential because this method starts from a local energy density functional. At the same time at least the spin-orbit potential is necessary for the realistic description of nuclear properties. It is possible to introduce the kinetic-energy density and spin density dependence of the DFT energy functional formally. In this case, to derive the single-particle equations following the ideology of the KS method, one would assume that any kinetic-energy density and spin density can be produced by the many-particle wave function describing the non-interacting system in some external potential with a spin-orbit component. But, as opposed to the case of the local particle density (see Ref. \[14\]), this statement has not been proved.

To include the radial-dependent effective mass and the spin-orbit potential in the consid-
eration in a rigorous way, one would have to use the non-local extension of the DFT and to derive single-particle equations of motion directly from the energy functional of this theory. However the straightforward application of the standard variational principle to the non-local energy functional leads to serious difficulties in view of the specific properties of the pseudo-Hamiltonian obtained (see Ref. [13] for details).

The main goal of the present paper is to develop the modification of the non-local generalization of the DFT which would be free from the above-mentioned shortcomings of the non-local theory. To this aim we define an energy functional that depends on the DM produced by a determinant wave function (in what follows we call it by a Slater-determinant DM). Although this DM generally does not correspond to any interacting fermion system nevertheless, we will show that the minimum of this functional coincides with the exact ground-state energy of the interacting system under consideration. Applying the variational principle, we derive the single-particle equations of motion which, in contrast to the KS equations, contain a non-local SPP. This is described in the second part.

In the third part the quasi-local reduction of the DFT is developed. Within the quasi-local DFT the energy functional depends on the local particle densities as well as on the uncorrelated kinetic-energy and spin densities. The single-particle equations, which are obtained by the minimization of this functional, contain the local SPP, the uncorrelated radial-dependent effective mass and the spin-orbit potential.

In the fourth part we derive a semiclassical HF energy functional within the quasi-local scheme starting from the recently proposed expansion of the DM in the Extended Thomas Fermi method [8]. The explicit formulae for the energy functional, the SPP and the effective mass are obtained using the finite-range Gogny force [3], as described in the fifth part. The residual correlation term is taken phenomenologically. In the sixth section we apply our method to the description of the ground-state properties of some doubly-magic spherical nuclei. The main results are set out in the summary. In the Appendix 1 some auxiliary formulae for the SPP are given. In Appendix 2 we describe a simple method to take into account the two-body correction of the centre-of-mass motion to the binding energy.

2 THE NON-LOCAL GENERALIZATION OF THE DFT

Let us consider a system of $N$ interacting fermions. In the nuclear case we are interested in systems with two kinds of particles, namely neutrons and protons. Let $H$ be the non-relativistic many-particle Hamiltonian. The explicit form of this operator is not important here. One can associate it with the usual formulae:

$$H = T + \sum_{i \neq j} v_{ij}^{NN} + \sum_{i \neq j} v_{ij}^{Coul} + \cdots,$$

where

$$T = -\frac{\hbar^2}{2m} \Delta,$$

is the kinetic-energy operator, $v_{ij}^{NN}$ is the bare nucleon-nucleon (NN) strong two-particle interaction, $v_{ij}^{Coul}$ is the Coulomb force acting between protons and the dots note the many-particle interactions if needed.

The HK energy functional [10], which only depends on the local particle density $n$, can be defined within the framework of the constrained search method as follows (see, for example, [11, 12])

$$E_{HK}[n] = \inf_{\Psi \rightarrow n} <\Psi|H|\Psi>, $$

where $|\Psi>$ is an arbitrary normalized $N$-particle state. The short notation $\Psi \rightarrow n$ hereinafter means the many-to-one mapping of the wave function $\Psi(x_1, \ldots, x_N)$ to the local density $n(r)$ i.e.
it means that the following equalities are fulfilled
\[
\begin{align*}
  n(r) &= n_p(r) + n_n(r), \\
  n_q(r) &= \sum_{\sigma} \rho(x, x), \\
  \rho(x, x') &= N \int \Psi(x, x_2, \ldots, x_N) \Psi^*(x', x_2, \ldots, x_N) dx_2 \cdots dx_N,
\end{align*}
\]
where \( \rho(x, x') \) is the single-particle DM, \( x = \{r, \sigma, q\} \) includes the spatial \( r \) and spin \( \sigma \) variables and the index of nucleon type \( q = n, p \). The integration over \( x \) includes the summation over \( \sigma \) and \( q \).

The functional (3) depends on the total local density \( n(r) \). One can define other energy functionals which are dependent either on \( n_q(r) \) or even on \( \rho(x, x) \). The particular choice of functional dependence is determined by the task under consideration.

In the local DFT it is proved that the minimum of the functional \( E_{HK}[n] \) is just the true ground-state energy \( E_{GS} \) and is attained for the true ground-state density \( n_{GS} \). To obtain \( E_{GS} \) and \( n_{GS} \), one can use the KS method which yields single-particle equations similar to the HF equations.

The rigorous derivation of these equations is based on the following statement proved by Lieb [14]:

If \( n(r) \geq 0 \), \( \int n(r) dr = N \), \( \int (\nabla \sqrt{n(r)})^2 d\mathbf{r} < \infty \), then there exists \( N \)-particle Slater-determinant wave function \( \Psi_0 \) built up from an orthonormal set of \( N \) single-particle wave functions \( \varphi_i \):
\[
\Psi_0(x_1, \ldots, x_N) = (N!)^{-1/2} \det \{\varphi_i(x_j)\},
\]
such that \( \Psi_0 \to n(r) \). In other words there is a many-to-one mapping of \( N \)-particle Slater determinant wave functions onto the local density \( n(r) \).

This theorem enables one to define the kinetic-energy functional \( T_0[n] \) for a system of non-interacting particles:
\[
T_0[n] = \inf_{\Psi_{0} \to n} \langle \Psi_0 | T | \Psi_0 \rangle,
\]
and to divide the HK functional \( E_{HK}[n] \) into two parts:
\[
E_{HK}[n] = T_0[n] + W[n],
\]
where the energy functional \( W[n] \) contains the potential energy as well as the correlation part of the kinetic energy.

Because the density \( n \) is produced by some Slater-determinant wave function one has from Eqs. (5)-(7):
\[
n_q(r) = \sum_{i=1}^{N} \sum_{\sigma} |\varphi_i(r, \sigma, q)|^2.
\]

By the same reasoning the kinetic-energy functional of the non-interacting system (8) can be written as
\[
T_0[n] = \sum_{i=1}^{N} \frac{\hbar^2}{2m} \int |\nabla \varphi_i(r, \sigma, q)|^2 d\mathbf{r}.
\]

Notice that one could define the kinetic-energy functional on the basis of a more general set of \( N \)-particle wave functions:
\[
T[n] = \inf_{\Psi \to n} \langle \Psi | T | \Psi \rangle.
\]
However, this functional cannot be written in the form (11) and thus it is useless to derive KS equations.

Applying the variational principle to the functional \( E_{HK}[n] \) with functions \( \varphi_i, \varphi_i^* \) as functional variables, one obtains in accordance with Eqs. (4), (9)–(11) the following KS equations:
\[
h_{HK} \varphi_i = \varepsilon_i \varphi_i,
\]
with
\[ h_{HK} = -\frac{\hbar^2}{2m} \Delta + U(r), \] (14)
where \( U(r) = \delta W/\delta n \) is the local mean-field potential and \( \varepsilon_i \) are the Lagrange multipliers to ensure the normalization condition of the single-particle wave functions \( \varphi_i \).

Often the energy functional \( W[n] \) is divided into two parts: \( W[n] = E_H[n] + E_{XC}[n] \), where \( E_H[n] \) is the “direct” (Hartree) functional, while \( E_{XC}[n] \) is the exchange-correlation energy functional. Consequently, the mean field potential \( U \) is also divided into two parts. For the sake of simplicity we will not do this in the present paper.

Eq. (14) does not contain a radial dependent effective mass nor a spin-orbit potential which are essential ingredients of the model nuclear single-particle Hamiltonian. To include them we propose the following method based on a special version of the non-local extension of the DFT. Let us define the energy functional:
\[ \mathcal{E}_0[\rho_0] = \inf_{\Psi_0 \rightarrow \rho_0} < \Psi_0 | \tilde{H} | \Psi_0 >, \] (15)
where \( \Psi_0 \) is any Slater-determinant wave function of the form (7), \( \rho_0 \) is the single-particle DM produced by \( \Psi_0 \) according to Eq. (6) (i.e. Slater-determinant DM) and \( \tilde{H} \) is an effective many-body Hamiltonian which generally does not coincide with the microscopic Hamiltonian \( H \). In our approach the operator \( \tilde{H} \) plays the role of an arbitrary reference point, the choice of which will be discussed below. We have to note that at the present moment \( \tilde{H} \) is an arbitrary \( N \)-particle operator such that the matrix element in (15) exists.

The functional \( \mathcal{E}_0[\rho_0] \) has a form of the HF energy functional built up on the base of the effective Hamiltonian \( \tilde{H} \). So in what follows we shall refer to it also as the HF energy functional. Let us define the residual correlation energy \( E_{RC} \) as follows
\[ E_{RC}[\hat{n}] = E[\hat{n}] - E_0[\hat{n}], \] (16)
where \( \hat{n} = \{ n_p, n_n \} \) and
\[ E[\hat{n}] = \inf_{\Psi \rightarrow \hat{n}} < \Psi | H | \Psi >, \] (17)
\[ E_0[\hat{n}] = \inf_{\Psi_0 \rightarrow \hat{n}} < \Psi_0 | \tilde{H} | \Psi_0 >= \inf_{\rho_0 \rightarrow \hat{n}} \inf_{\Psi_0 \rightarrow \rho_0} < \Psi_0 | \tilde{H} | \Psi_0 >= \inf_{\rho_0 \rightarrow \hat{n}} \mathcal{E}_0[\rho_0]. \] (18)
The quantity \( E[\hat{n}] \) is the exact energy functional built up with the true microscopic Hamiltonian (1) on the set of any normalized wave functions \( \Psi \). The auxiliary functional \( E_0[\hat{n}] \) (as well as the kinetic-energy functional \( T_0[n] \) in the KS theory) is defined according to the Lieb theorem for any (not very ”bad”) local density \( \hat{n} \). The final energy functional of our version of the non-local DFT is defined as:
\[ \mathcal{E}[\rho_0] = \mathcal{E}_0[\rho_0] + E_{RC}[\hat{n}], \] (19)
where \( \rho_0 \) is related to \( \hat{n} \) through Eqs.(4)-(6). The functionals \( \mathcal{E}_0[\rho_0] \) and \( E_{RC}[\hat{n}] \) are defined by Eqs. (15) and (16). For the moment we shall not discuss if these functionals are known or not. The most important for us is that they are rigorously defined.

The main property of the functional \( \mathcal{E}[\rho_0] \) is expressed by the following equalities:
\[ \inf_{\rho_0} \mathcal{E}[\rho_0] = \inf_{\hat{n}} \inf_{\rho_0 \rightarrow \hat{n}} \mathcal{E}[\rho_0] = \inf_{\hat{n}} E[\hat{n}] = E_{GS}, \] (20)
where \( E_{GS} \) is the true ground state energy of the interacting system as in the case of the HK theory. To obtain the equations of motion we have to suppose that the choice of the Hamiltonian \( \tilde{H} \) in Eq. (15) ensures that the infimum of the functional \( \mathcal{E}[\rho_0] \) in (20) is a minimum. In addition, we use the general formula for the Slater-determinant DM \( \rho_0 \) under the variation which follows from Eqs. (6) and (7). Namely
\[ \rho_0(x, x') = \sum_{i=1}^{N} \varphi_i(x) \varphi_i^*(x'), \] (21)
where the sum is taken over the occupied states. Applying the variational principle to the functional $\mathcal{E}[\rho_0]$ defined by Eq. (19) and using the functions $\varphi_i, \varphi_i^*$ as functional variables according to Eq. (21) one will get the following set of single-particle equations:

$$\int h_0(x,x')\varphi_i(x')dx' + U_{RC}(x)\varphi_i(x) = \varepsilon_i\varphi_i(x),$$  \hspace{1cm} (22)

where we have defined the non-local Hamiltonian $h_0$ and the local potential $U_{RC}$ as follows:

$$h_0(x,x') = \frac{\delta \mathcal{E}_0[\rho_0]}{\delta \rho_0(x,x')}, \hspace{1cm} (23)$$

$$U_{RC}(x) = U_{RC}(r,q) = \frac{\delta \mathcal{E}_{RC}}{\delta n_q(r)}. \hspace{1cm} (24)$$

It is worthwhile noting that the occupation numbers of the Slater-determinant DM are fixed to be either 1 or 0. Thus, we avoid difficulties arising from the variation over the occupation numbers that appear in the theory developed in Ref. [13].

3 REDUCTION TO THE QUASI-LOCAL THEORY

The approach described above enables one to introduce a reduced energy functional $\mathcal{E}_0^{QL}$ which depends on the following set of local quantities: the local particle $n_q$, kinetic-energy $\tau_q$ and spin $J_q$ densities for neutrons and protons:

$$n_q(r) = \sum_\sigma \int dx' \delta(x-x')\rho_0(x,x'), \hspace{1cm} (25)$$

$$\tau_q(r) = \sum_\sigma \int dx' \delta(x-x')(\nabla x \nabla x')\rho_0(x,x'), \hspace{1cm} (26)$$

$$J_q(r) = i \sum_\sigma \int dx' \delta(r-r')\delta_{q,q'}[\langle \sigma | \sigma', \sigma \times \nabla r \rangle]\rho_0(x,x'), \hspace{1cm} (27)$$

where $\delta(x-x') = \delta(r-r')\delta_{\sigma,\sigma'}\delta_{q,q'}$, the quantities $\tau_q$ and $J_q$ are the uncorrelated neutron and proton kinetic-energy and spin densities respectively. Introducing the short notation $\rho_{QL} \equiv \{n_p, n_n, \tau_p, \tau_n, J_p, J_n\}$, let us define the quasi-local energy functional as follows:

$$\mathcal{E}_0^{QL}[\rho_{QL}] = \mathcal{E}_0[\rho_{QL}] + \mathcal{E}_{RC}[\hat{n}],$$  \hspace{1cm} (28)

where

$$\mathcal{E}_0^{QL}[\rho_{QL}] = \inf_{\rho_0 \rightarrow \rho_{QL}} \mathcal{E}_0[\rho_0]. \hspace{1cm} (29)$$

Notice, that the many-to-one mapping $\rho_0 \rightarrow \rho_{QL}$ is established according to Eqs. (25)-(27), and that the set $\hat{n} = \{n_p, n_n\}$ enters $\rho_{QL}$: $\hat{n} \in \rho_{QL}$.

From Eqs. (19), (20), (28) and (29) we have

$$\inf_{\rho_{QL}} \mathcal{E}_0^{QL}[\rho_{QL}] = E_{GS}. \hspace{1cm} (30)$$

Using Eq. (10) and the explicit expressions for the remaining local quantities:

$$\tau_q(r) = \sum_{i=1}^N \sum_\sigma |\nabla \varphi_i(r,\sigma,q)|^2, \hspace{1cm} (31)$$

$$J_q(r) = i \sum_{i=1}^N \sum_{\sigma,\sigma'} \varphi_i^*(r,\sigma',q)[\langle \sigma | \sigma', \sigma \times \nabla \rangle] \varphi_i(r,\sigma,q), \hspace{1cm} (32)$$
one can apply the variational principle to the energy functional $E_{QL}[\rho_{QL}]$ with $\varphi_i$, $\varphi_i^*$ as functional variables. The resulting single-particle equations are:

$$h_q \varphi_i = \varepsilon_i \varphi_i,$$

where

$$h_q = -\nabla \cdot \left( \frac{\hbar^2}{2m_q^*(r)} \nabla + U_q(r) - iW_q(r) \cdot [\nabla \times \sigma] \right),$$

and

$$\frac{\hbar^2}{2m_q^*(r)} = \frac{\delta E_{QL}}{\delta \tau_q(r)},$$

$$U_q(r) = \frac{\delta E_{QL}}{\delta n_q(r)},$$

$$W_q(r) = \frac{\delta E_{QL}}{\delta J_q(r)}.$$  

If the functional $E_{QL}$ were known, one would be able to calculate the exact ground state energy $E_0 = E_{GS}$ and exact local densities $n_q = n_{q,GS}$. The kinetic-energy density $\tau_q$ and spin density $J_q$ correspond to the system without correlations and do not coincide with the exact densities in our approach.

The following remark is in order. As was pointed in the Introduction, the energy functional dependence on the exact kinetic-energy and spin densities could be introduced, for example, by the above procedure of the quasi-local reduction being applied to the energy functional of the non-local theory developed in Ref. [13]. However, the mapping of the Slater-determinant wave functions $\Psi_0$ onto the exact kinetic-energy and spin densities is not defined, as opposed to the mapping onto the exact local density, i.e. Eqs. (31) and (32) are wrong for the exact densities. As a consequence, it is impossible to derive the single-particle equations such as (33). The use of the Slater-determinant DM ($\rho_0$ in our approach) enables us to avoid this problem.

4 EXTENDED THOMAS-FERMI APPROXIMATION IN THE QUASI-LOCAL DFT

Now we are turn to the discussion of the choice of the effective operator $\tilde{H}$. First, the energy functional $\mathcal{E}_0$ has to be well defined. While the functional $E[\tilde{n}]$ is always defined, this is not the case for the functionals $E_0[\rho_0]$ and $E_0[\tilde{n}]$. Indeed, the matrix element of the microscopic Hamiltonian with the bare nucleon-nucleon (NN) interactions over the Slater-determinant wave functions can diverge due to the short-range singularity of the force as it is happens in the standard many-body theory. Thus, we will use a Hamiltonian $\tilde{H}$ with an effective NN interaction whose matrix elements are well defined. Second, the local energy functional $E[\tilde{n}]$ obviously has the minimal property that is necessary to apply the variational principle; however, it can be not true for the non-local energy functional $\mathcal{E}^{\prime}[ho_0]$ (in spite of the fact that the equality (20) is always true). Hence one has to choose $\tilde{H}$ to ensure the minimal property of the energy functional $\mathcal{E}^{\prime}[ho_0]$. Notice that at least in one particular case, when $\tilde{H} = T$, this condition is fulfilled because we come to the usual KS theory. Indeed, if one sets $\tilde{H} = T$ then $m_q^* = m$, $W_q = 0$, and Eq. (33) coincides with the KS equation. In this case the residual correlation energy functional $E_{RC}[\tilde{n}]$ corresponds to the sum of the direct (Hartree) term and the exchange and correlation energy in the KS method.

Here we consider a more general case, setting $\tilde{H}$ to be the $N$-particle Hamiltonian with an effective NN interaction:

$$\tilde{H} = T + \sum_{i \neq j} \tilde{v}^{NN}_{ij} + \sum_{i \neq j} v^{\text{Coul}}_{ij}.$$  

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We will use the effective NN force of the form

$$\tilde{v}_{ij}^{NN} = \tilde{v}_{ij}^e + \tilde{v}_{ij}^{so},$$

where the central part of the effective force is given by

$$\tilde{v}_{ij}^e = \sum_n [w_n + b_n P_{ij}^c - h_n P_{ij}^r - m_n P_{ij}^c P_{ij}^r] v_n(s),$$

where $w_n, b_n, h_n, m_n$ are the parameters of the force ($n = 1, 2, \ldots$), $P_{ij}^c$ and $P_{ij}^r$ are the spin and isospin exchange operators and $v_n(s)$ ($s = r_i - r_j$) are the radial formfactors of the central part of the effective force. For the sake of simplicity we will consider only one term in the sum (40) i.e. we will drop index $n$ in the following. The spin-orbit part of the force is chosen as follows

$$\tilde{v}_{ij}^{so} = iW_0(\sigma_i + \sigma_j) \cdot [k' \times \delta(r_i - r_j)k],$$

where $k = \frac{1}{2i}(\nabla_i - \nabla_j)$ denotes the operator acting on the right and $k' = -\frac{1}{2i}(\nabla_i - \nabla_j)$ is the operator acting on the left.

It was mentioned that the choice of the effective Hamiltonian $\tilde{H}$ and the effective interactions is rather arbitrary. Practically the operator $\tilde{H}$ is confined only by the above formal mathematical conditions. The situation is quite different in the usual HF method where there are no other ingredients apart from the effective forces which are taken to be density dependent in order to ensure the nuclear saturation. In our approach the particular choice of $\tilde{H}$ is compensated by the addition of the residual correlation energy $E_{RC}[\tilde{n}]$, which contains all necessary density dependence of the total energy functional. In the applications of the method the functional $E_{RC}[\tilde{n}]$ is parametrized phenomenologically, the parameters are adjusted to describe nuclear ground-state properties. Following this ideology the effective interactions entering operator $\tilde{H}$ are taken to be density independent. Thus, we would like to stress that the effective interactions in our DFT approach are not exactly the same as in HF theory.

Let us define the density $\mathcal{H}_0$ of the quasi-local HF energy functional $\mathcal{E}_0^{QL}[\rho_{QL}]$ as follows

$$\mathcal{E}_0^{QL} = \int d\mathbf{r} \mathcal{H}_0(\mathbf{r}).$$

According to (38)-(41) the energy density $\mathcal{H}_0$ is described by six terms:

$$\mathcal{H}_0 = \frac{\hbar^2}{2m} (\tau_n + \tau_p) + \mathcal{H}_{\text{Dir}}^{\text{Nucl}} + \mathcal{H}_{\text{Exch}}^{\text{Nucl}} + \mathcal{H}_{\text{Dir}}^{\text{Coul}} + \mathcal{H}_{\text{Exch}}^{\text{Coul}} + \mathcal{H}_{\text{so}}.$$  

The direct nuclear energy density $\mathcal{H}_{\text{Dir}}^{\text{Nucl}}$ comes from the central part of the NN force and is given by

$$\mathcal{H}_{\text{Dir}}^{\text{Nucl}}(\mathbf{r}) = \frac{1}{2} \int d\mathbf{r}' \{(w + \frac{b}{2})n(\mathbf{r})n(\mathbf{r}') - (h + \frac{m}{2})[n_p(\mathbf{r})n_p(\mathbf{r}') + n_n(\mathbf{r})n_n(\mathbf{r})]\} v(|\mathbf{r} - \mathbf{r}'|).$$

The density of the Coulomb direct energy is

$$\mathcal{H}_{\text{Dir}}^{\text{Coul}}(\mathbf{r}) = \frac{e^2}{2} \int d\mathbf{r}' \frac{n_p(\mathbf{r})n_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$ 

These direct energies give the contribution to the so-called Hartree functional. To calculate the exchange terms that come from the central part of the NN force we use the recently proposed ETF approximation for the DM up to $\hbar^2$ order [8]. Notice that there are other possible options to obtain the quasi-local energy functional based on the Negele-Vautherin and Campi-Bouyssy DM expansions [4, 5, 6]. In our approach for spin-saturated nuclei the nuclear exchange energy density is given by two terms

$$\mathcal{H}_{\text{Exch}}^{\text{Nucl}} = \mathcal{H}_{\text{Exch,0}}^{\text{Nucl}} + \mathcal{H}_{\text{Exch},2}^{\text{Nucl}}.$$
The first term is calculated to $\hbar^0$ order (which corresponds to the Slater approximation for the DM):
\[ H_{\text{Nuc}}^\text{Exch,0}(r) = \int ds v(s) \left( \frac{1}{2} X_{\epsilon_1} \sum_{q} \left( n_q(r) \hat{j}_1(k_q s) \right)^2 + X_{\epsilon_2} n_n(r) \hat{j}_1(k_n s) n_p(r) \hat{j}_1(k_p s) \right), \]  
(47)
where $k_q(r) = (3\pi^2 n_q(r))^{1/3}$ is the Fermi momentum, $\hat{j}_1(x) = 3j_1(x)/x$, $j_1(x)$ is the spherical Bessel function and $X_{\epsilon_1} = m + h/2 - b - w/2$, $X_{\epsilon_2} = m + h/2$. The second term corresponds to the $\hbar^2$ correction:
\[ H_{\text{Nuc}}^\text{Exch,2}(r) = \sum_q \frac{\hbar^2}{2m} \left[ [(f_q - 1) (\tau_q - \frac{3}{5} k_q^2 n_q - \frac{1}{4} \Delta n_q) + k_q f_q \hat{f}_q \left( \frac{\nabla n_q}{n_q}^2 - \frac{1}{36} \Delta n_q \right)] \right]. \]  
(48)
In this equation $f_q = f_q(r, k_q)$, $f_q' = (\partial f_q(r, k)/\partial k)_{k=k_q}$. The function $f_q(r, k)$ is the inverse of the position- and momentum-dependent effective mass and is defined in the ETF approximation by
\[ f_q(r, k) = 1 + m \frac{\partial V^\text{Nuc}_{\text{Exch},q}(r, k)}{\hbar^2 k}, \]  
(49)
where $V^\text{Nuc}_{\text{Exch},q}$ is the Wigner transform of the exchange potential in the Thomas-Fermi approximation:
\[ V^\text{Nuc}_{\text{Exch},p}(r, k) = \int dse^{-i k s} v(s) \left[ X_{\epsilon_1} n_p(r) \hat{j}_1(k_p s) + X_{\epsilon_2} n_n(r) \hat{j}_1(k_n s) \right] \]  
(50)
and analogously for $V^\text{Nuc}_{\text{Exch},n}$ with the permutation of indices $p$ and $n$ (see [8] for details). It is worthwhile noting that within the semiclassical ETF approximation the kinetic-energy density is a functional of the local density. Then the energy functional obtained would only depend on the local particle density and spin density. However, it was found in [8] that the use of the quantal kinetic energy in Eq.(48), which yields the radial-dependent effective mass, improves agreement with results of the full HF calculation significantly. It motivates us to use the anzatz (31) for $\tau_q$ in the present paper.

The Coulomb exchange energy consists of the Slater term and the second-order correction that in the ETF approximation is written as [17, 8]:
\[ H_{\text{Exch}}^\text{Coul}(r) = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} \frac{7}{432\pi (3\pi^2)^{1/3}} \frac{(\nabla n_p)^2}{n_p^{4/3}}. \]  
(51)
Finally, the spin-orbit energy density is given by
\[ H^{so}(r) = -\frac{1}{2} W_0 [n(r) \nabla J + n_n(r) \nabla J_n + n_p(r) \nabla J_p], \]  
(52)
where $J = J_p + J_n$.

It is worthwhile noting that in this section we replace the exact quasi-local functional $\mathcal{E}_0^{QL}$ by the approximate functional calculated within the ETF approximation. The difference between them gives a very small contribution (see the following sections), but it cannot be totally included within the residual correlation term because it depends on the $\rho_{QL}$ while the latter only depends on the $\hat{n}$. The determination of the residual correlation energy $E_{RC}[\hat{n}]$ will be specified in the next section.

5 THE ENERGY FUNCTIONAL AND SINGLE-PARTICLE EQUATIONS FOR THE GOGNY FORCE

The formulae (44), (46)-(50) are valid for any radial formfactor $v(s)$ of the central part of the effective forces. Here we give the explicit expressions for the above-defined quantities in the case
of a Gaussian formfactor \( v(s) = \exp(-s^2/a^2) \) entering in the Gogny-type effective forces which are used in the numerical applications of our method. Assuming spherical symmetry of the particle densities we get from Eqs. (44) and (47)

\[
H_{\text{Dir}}(r) = \frac{\pi a^2}{2r} \int_0^\infty dr' r' \left\{ \exp\left( -\frac{(r - r')^2}{a^2} \right) - \exp\left( -\frac{(r + r')^2}{a^2} \right) \right\} \\
\times \left\{ (w + \frac{b}{2})n(r)n(r') - (h + \frac{m}{2})[n_p(r)n_p(r') + n_n(r)n_n(r')] \right\},
\]

(53)

\[
H_{\text{Nucl}}^{\text{Dir},0}(r) = \frac{2}{3\pi^{5/2} a^3} \\
\times \left\{ Xe_1 \sum_q \left( \frac{\sqrt{\pi}}{2} a^3 k_q^3 \text{erf}(ak_q) + \frac{a^2 k_q^2}{2} - 1 \right) \exp(-a^2 k_q^2) - \frac{3a^2 k_q^2}{2} + 1 \right\} \\
+ Xe_2 \sum_{\eta = \pm 1} \eta \left[ \frac{\sqrt{\pi}}{2} a^3 (k_n + \eta k_p)(k_n^2 + k_p^2 - \eta k_n k_p) \text{erf}\left( \frac{a}{2}(k_n + \eta k_p) \right) \right] \\
+ \left( a^2 (k_n^2 + k_p^2 - \eta k_n k_p) - 2 \right) \exp\left( -\frac{a^2}{4}(k_n + \eta k_p)^2 \right) \}.
\]

(54)

The second-order correction to the exchange nuclear energy density (48) can be rewritten in the following way:

\[
H_{\text{Exch},2}(r) = \sum_q \left( F_q(\tau_q - \frac{3}{5} k_n^2 n_q - \frac{1}{4} \Delta n_q) + G_q\left( \frac{1}{27} \left( \nabla n_q \right)^2 - \frac{1}{36} \Delta n_q \right) \right),
\]

(55)

where the explicit value of the functions \( F_q \) and \( G_q \) calculated with a Gaussian formfactor are given in Appendix 1.

The SPP is defined following Eq.(36). According to (28), (42) and (43) we split it into five pieces:

\[
U_q = U_{\text{Dir},q}^{\text{Nucl}} + U_{\text{Exch},q}^{\text{Nucl}} + U_{\text{Dir},q}^{\text{Coul}} + U_{\text{Exch},q}^{\text{Coul}} + U_q^{RC},
\]

(56)

where the direct nuclear SPP is given by

\[
U_{\text{Dir},q}^{\text{Nucl}}(r) = \frac{\pi a^2}{r} \int_0^\infty dr' r' \left\{ \exp\left( -\frac{(r - r')^2}{a^2} \right) - \exp\left( -\frac{(r + r')^2}{a^2} \right) \right\} \\
\times \left\{ (w + \frac{b}{2})n(r') - (h + \frac{m}{2})n_q(r') \right\}.
\]

(57)

The exchange nuclear potential consists of two parts following (46):

\[
U_{\text{Exch},q}^{\text{Nucl}} = U_{\text{Exch},q,0}^{\text{Nucl}} + U_{\text{Exch},q,2}^{\text{Nucl}},
\]

(58)

where, for example, the Slater part of the exchange SPP acting on the protons is given by

\[
U_{\text{Exch},p,0}^{\text{Nucl}} = \frac{2}{\sqrt{\pi} a^3 k_p^3} Xe_1 \left[ \frac{\sqrt{\pi}}{2} a^3 k_p^3 \text{erf}(ak_p) + a^2 k_p^2 \exp(-a^2 k_p^2) - a^2 k_p^2 \right] \\
+ 2Xe_2 \sum_{\eta = \pm 1} \eta \left[ \frac{\sqrt{\pi}}{4} a^3 k_p^3 \text{erf}\left( \frac{a}{2}(k_p + \eta k_n) \right) + \frac{1}{2} a^2 k_p^2 \exp(-\frac{a^2}{4}(k_p + \eta k_n)^2) \right].
\]

(59)
For the second-order contribution to the exchange SPP, we have

\[ U^{\text{Nucl Exch,}p,2} = \pi^2 \left\{ \frac{1}{k_p} \left[ F^p_{n} (\tau_p - \frac{3}{5} k_p^2 n_p) + \frac{1}{27} \left( \frac{3G_p}{k_p^2} - G_p^p \right) \frac{(\nabla n_p)^2}{n_p} \right] \\
- \frac{1}{36} \left( 8G_p^p + G_p^p + 9F^p_p \right) \Delta n_p + F^p_n (\tau_n - \frac{3}{5} k_n^2 n_n) + \frac{1}{27} G_n^p (\nabla n_n)^2/n_n \right\} \]

\[ - \frac{1}{36} (G_n^p + 9F^p_n) \Delta n_n - \frac{2}{27k_n} G_n^p (\nabla n_n)^2/n_n \]

\[ - F_p k_n^2 - \Delta F_p - \frac{1}{36} \Delta G_p, \]

where the functions \( F_q^p, G_q^p, \Delta F_q \) and \( \Delta G_q \) used in Eq. (60) are also given in Appendix 1. The formulae for the Slater and \( \bar{h}^2 \) contributions to the nuclear exchange potential acting on neutrons are obtained by replacing \( n \) by \( p \) and \( p \) by \( n \) in Eqs.(59) and (60).

The Coulomb direct and exchange potentials, entering Eq. (56), are not equal to zero only for protons. In the explicit form we have

\[ U^{\text{Coul Dir,}p}(r) = e^2 \int \frac{d r' n_p(r')}{|r - r'|}, \]

\[ U^{\text{Coul Exch,}p}(r) = - \left( \frac{3}{\pi} n_p(r) \right)^{1/3}. \]

The inclusion of the \( \bar{h}^2 \)-correction to the Coulomb exchange energy (second term in Eq. (51)) in the SPP leads to the unphysical behaviour of the potential at \( r \to \infty \). We thus only calculate its contribution to the binding energy as a perturbation.

The radial dependent effective mass \( m^*_q(r) \) and the form factor \( W_q(r) \) of the spin-orbit potential are defined according to Eqs. (35), (37), (42), (43), (52) and (55) by the relations

\[ \frac{\bar{h}^2}{2m^*_q(r)} = \frac{\bar{h}^2}{2m} + F_q, \]

\[ W_q(r) = \frac{1}{2} W_0 (\nabla n + \nabla n_q). \]

Now we shall turn to the determination of the residual correlation energy. We take it in the form of the phenomenological ansatz

\[ E_{RC}[\hat{n}] = \frac{t_3}{4} \int d r n^\alpha(r) \left[ (2 + x_3)n^2(r) - (2x_3 + 1) \left( n_p^2(r) + n_n^2(r) \right) \right]. \]

The parameters \( t_3, x_3 \) and \( \alpha \) together with the parameters of the Hamiltonian \( \hat{H} \) have to be chosen from the condition of the best description of the nuclear ground-state properties. In the calculations, which are presented in the next section, we use the well-known parameter set of the D1S Gogny force. Let us note that the formula (65) is the standard ansatz which enters not only a density-dependent part of the Gogny forces but, for example, a density-dependent part of the Skyrme forces. Eq. (65) leads to the following contribution into the SPP in accordance with the definition (56):

\[ U^{RC}_q = \frac{t_3}{4} n^{\alpha-1} \left[ (2 + \alpha)(2 + x_3)n^2 - (2x_3 + 1) \left( \alpha(n_p^2 + n_n^2) + 2n_q n \right) \right]. \]
6 NUMERICAL RESULTS

In this section we want to check our local approximation to the HF method using finite-range Gogny forces. First of all, we compare the exact HF ground-state binding energies as well as the rms radii of the neutron and proton densities of some magic nuclei computed with the Gogny D1S force [18] with our DFT results. In this comparison we use two different quasi-local functionals : DFT-$h^0$, where the exchange energy coming from the finite-range part of the interaction is taken at pure Thomas-Fermi level (Slater approach) and DFT-$h^2$ where the ETF-$h^2$ contributions have been added to the Slater part. Notice that in this DFT-$h^2$ approach the semiclassical kinetic-energy density entering Eq. (48) has been replaced by the corresponding quantal density for the reasons pointed out above. In both DFT calculations we solve the local Schrödinger equation (33) for neutrons and protons with the potentials and effective masses reported in the previous section. Table 1 collects all these binding energies and radii which have been computed taking into account the two-body centre-of-mass correction. In our calculation we take into account this correction as explained in Appendix 2. We would like to say in passing that the numerical value of this two-body centre-of-mass correction along the whole periodic table is very well reproduced by using the pocket formula based on the harmonic oscillator and derived in [19].

From Table 1 we can see that the DFT-$h^2$ binding energies reproduce the HF values fairly well. The differences between HF and DFT-$h^2$ are smaller than 1% for all the considered nuclei from $^{40}$Ca to $^{208}$Pb and in the case of $^{16}$O the relative difference is only 1.8%. The DFT-$h^0$ binding energies show larger discrepancies with the full HF results. The relative differences range from 7% in $^{16}$O to 1% in the heaviest nucleus considered $^{208}$Pb. As regards the rms radii of the neutron and proton densities, the full HF values are again better reproduced by the DFT-$h^2$ approximation than by the DFT-$h^0$ approach. These results show the importance of the $h^2$ corrections in the local approximation to the HF exchange energy. It should be pointed out that the eigenvalues $\epsilon_i$ in Eq. (33) have no rigorous physical sense in the DFT except for the energy of the last filled level, which corresponds to the neutron or proton separation energy (chemical potential). Table 1 also displays the neutron and proton chemical potentials obtained using the DFT-$h^0$, DFT-$h^2$ and HF approximations. The DFT-$h^2$ chemical potentials differ from the HF chemical potentials by less than 1 MeV while the shift of the DFT-$h^0$ separation energies with respect to the the full HF values is larger and can be around 3 MeV for light nuclei.

It is important to note that the agreement of the proposed DFT approximations with the full HF results is determined by the treatment of the non-local effects. The contribution of the pointed effects can be quantified in terms of the effective mass in nuclear matter. The results of Table 1 show that for effective forces with an effective mass over the bare mass of around 0.7, as in the case of the Gogny forces [20], the non-local effects can be very well accounted for the DFT-$h^2$ functional proposed in this paper. However, for forces where the non-local effects are larger, the result of our DFT-$h^2$ approximation is worse when compared with the HF results, but is still better than other suitable choices of the exchange-energy localization such as the Negele-Vautherin or Campi-Bouyssy approaches (see Ref.[8] for more details about this point).

Figures 1 and 2 displays the neutron and proton densities for $^{40}$Ca and $^{208}$Pb obtained using the D1S force in the full HF (solid line) as well as in the DFT-$h^2$ (dashed line) and DFT-$h^0$ (short-dashed line) calculations. The DFT proton and neutron densities nicely reproduce the surface and the tail of the full HF densities. In the region near the centre of the nuclei, the DFT density follows the full HF density profile very well although a small shift between the full HF and DFT proton and neutron densities appears in this central region. These differences can be attributed to the fact that our DFT description of the s-orbitals, whose wave functions mainly provide the proton and neutron densities at the centre of the nuclei, show some small differences with the corresponding HF s-orbitals. Comparing the DFT-$h^0$ and DFT-$h^2$ densities, it can be seen that including the $h^2$ contributions in our local approximation, one obtains a better agreement with the full HF densities.

Figures 3 and 4 display the radial dependence of the neutron and proton effective masses over the bare nucleon mass calculated with the DFT-$h^2$ approach (see Eq. (63)) for $^{40}$Ca and $^{208}$Pb nuclei (solid lines). Because there is no explicit radial-dependent effective mass in the full
Figure 1: Neutron and proton densities of the nucleus $^{40}$Ca calculated with the D1S Gogny force using the DFT-$h^0$ (short-dashed line) and DFT-$h^2$ (dashed line) approaches compared with the full HF densities (solid line).
Figure 2: Same as Figure 1 for the nucleus $^{208}\text{Pb}$. 
Figure 3: Neutron and proton radial dependence of the effective mass of the nucleus $^{40}\text{Ca}$ calculated with the D1S Gogny force using the DFT-$\hbar^2$ approach (solid line) compared with the corresponding HF effective masses obtained with the Skyrme SIII force (dashed line).
Figure 4: Same as Figure 3 for the nucleus $^{208}\text{Pb}$.
Table 1: Total binding energies $B$ (in MeV), neutron $r_n$ and proton $r_p$ rms radii (in fm) and separation energies of neutrons $S_n$ and protons $S_p$ (in MeV) of some magic nuclei computed with the D1S Gogny force using the DFT-$h^0$ and DFT-$h^2$ approaches compared with the full HF results.

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HF calculation of finite nuclei using the Gogny forces, we compare the DFT-$h^2$ results with the neutron and proton effective mass over the bare nucleon mass obtained using the Skyrme III force [21] (dashed lines). We find that the DFT-$h^2$ results exhibit similar trends to those of the Skyrme effective masses. The differences between the two calculations are basically due to the different values of the nucleon effective mass in nuclear matter which are $m^*/m = 0.70$ for the Gogny D1S force and $m^*/m = 0.76$ for the Skyrme III interaction.

7 SUMMARY

In the present paper we propose a non-local extension of the DFT and its quasi-local reduction. To this aim we define an energy functional which depends on the Slater-determinant DM with the occupation numbers being either 1 or 0. This enables us to avoid the difficulties of the non-local DFT reported in [13]. Defining the uncorrelated kinetic-energy densities and spin densities we construct the quasi-local energy functional and rigorously derive the single particle equations with the radial-dependent effective mass and the spin-orbit potential.

In order to define the energy functional of the Slater-determinant DM one has to introduce an effective Hamiltonian which ensures its existence. This feature of nucleon systems arises from the specific properties of the bare NN force in contrast to the Coulomb force in electron systems. In our approach the total energy functional consists of HF part and residual correlation energy. The HF energy functional can be calculated directly, while the residual correlation energy is considered phenomenologically. Using the recently proposed semiclassical ETF approximation for the DM [8] we obtain a quasi-local energy density functional only depending on the local particle, kinetic-energy and spin densities. The resulting single-particle equations of motion contain the local mean-field potential, the uncorrelated effective mass and spin-orbit potential. Using the finite range density-dependent Gogny force they are calculated analytically. The use of a different effective force such as M3Y will be reported in a forthcoming publication.
We apply our method to the calculations of the nuclear ground-state properties and compare it with the exact HF solutions using the Gogny D1S force. We obtain a very good agreement in the description of the binding energies and root mean square radii. The single-particle energies of the highest occupied neutron and proton levels in the full HF calculation are well reproduced by our local approximation. The particle densities are also in good agreement with the exact HF densities. We analyze the radial dependent effective mass within our approach. Comparing it with the result obtained with the Skyrme III interaction, it also exhibits a very reasonable behavior.

In conclusion, our approach has the following advantages: it handles local differential equations in contrast to the integro-differential equations in the HF approach, at the same time the quality of the obtained results is sufficiently high; our method enables one to construct a quasi-local energy density functional on the base of the effective forces with arbitrary radial formfactors; the method can be straightforwardly generalized to the non-spherical case.

Acknowledgments

The authors are grateful to the Gogny group for providing us the HF results with the Gogny force and to M. Centelles for a careful reading of the manuscript. One of us also acknowledges financial support from DGCYT (Spain) under grant PB98-1247 and from DGR (Catalonia) under grant 2000SGR-00024.
In this appendix we present the explicit expressions for the functions $F_q$, $G_q$, $F_{q'}$, $G_{q'}$, $\Delta F_q$ and $\Delta G_q$ calculated with a Gaussian formfactor. These functions are used to obtain the second-order contributions to the exchange nuclear energy density (55) and the corresponding SPP (60). In the following, excepting Eqs. (70) and (71), we assume that $q' \neq q$.

\begin{align}
F_q &= -\frac{a^2}{2\sqrt{\pi}} \left\{ X e_1 z_q^3 \exp\left(-\frac{z_q^2}{2}\right) Q_1 \left(\frac{z_q^2}{2}\right) + X e_2 z_q^3 \exp\left(-\frac{z_q^2}{2} + \frac{z_{q'}^2}{4}\right) Q_1 \left(\frac{z_q^2 + z_{q'}^2}{2}\right) \right\}, \\
G_q &= \frac{a^2}{4\sqrt{\pi}} z_q^2 \left\{ X e_1 z_q^3 \exp\left(-\frac{z_q^2}{2}\right) \left[ Q_1 \left(\frac{z_q^2}{2}\right) - z_q^2 Q_2 \left(\frac{z_q^2}{2}\right) \right] \right. \\
&\quad+ \left. X e_2 z_q^3 \exp\left(-\frac{z_q^2 + z_{q'}^2}{4}\right) \left[ Q_1 \left(\frac{z_q^2 + z_{q'}^2}{2}\right) - z_q^2 Q_2 \left(\frac{z_q^2 + z_{q'}^2}{2}\right) \right] \right\},
\end{align}

where $z_q = ak_q$ and the functions $Q_m(x)$ are defined by

\begin{align}
Q_0(x) &= \frac{\sinh(x)}{x}, \quad Q_{m+1} = \frac{1}{2x} \frac{dQ_m(x)}{dx}.
\end{align}

The functions $F_{q'}$, $G_{q'}$, $F_{q''}$, $F''_{q''}$ and $G_{q''}$ (the two last functions needed to obtain $\Delta F_q$ and $\Delta G_q$, see below) are defined as:

\begin{align}
F_{q'} &= \frac{1}{k_{q'}} \frac{\partial F_q}{\partial k_{q'}}, \quad F_{q''} = \frac{\partial^2 F_q}{\partial k_{q'}^2}, \\
G_{q'} &= \frac{1}{k_{q'}} \frac{\partial G_q}{\partial k_{q'}}, \quad G_{q''} = \frac{\partial^2 G_q}{\partial k_{q'}^2},
\end{align}

and their explicit form is:

\begin{align}
F_q &= -\frac{a^4}{4\sqrt{\pi}} \left\{ 2X e_1 e_0 z_q \left[ (3 - z_q^2) Q_1(x_q) + z_q^2 Q_2(x_q) \right] + X e_2 e_0 z_q^3 \left[ z_q^2 Q_2(x_0) - Q_1(x_0) \right] \right\}, \\
F_{q'} &= -\frac{a^4}{4\sqrt{\pi}} X e_2 e_0 z_{q'} \left[ (6 - z_{q'}^2) Q_1(x_0) + z_{q'}^2 z_q^2 Q_2(x_0) \right], \\
F_{qq} &= -\frac{a^4}{8\sqrt{\pi}} \left\{ 4X e_1 e_q z_q \left[ (2 - z_q^2) (3 - 2z_q^2) Q_1(x_q) - z_q^4 (1 + 2z_q^2) Q_2(x_q) \right] - X e_2 e_0 z_q^3 \left[ (2 - z_q^2 - z_q^2) Q_1(x_0) + 2z_q^2 (4 + z_q^2) Q_2(x_0) \right] \right\}, \\
F_{q'q'} &= -\frac{a^4}{8\sqrt{\pi}} X e_2 e_0 z_{q'} \left[ (24 - 14z_{q'}^2 + z_{q'}^2 z_{q'}^2) Q_1(x_0) + 2z_{q'}^2 z_q^2 (2 - z_{q'}^2) Q_2(x_0) \right], \\
F_{qq'} &= \frac{a^4}{8\sqrt{\pi}} X e_2 e_0 z_q z_{q'}^2 \left[ (6 - 2z_{q'}^2) Q_1(x_0) + z_{q'}^2 (z_q^2 + z_{q'}^2) Q_2(x_0) \right], \\
G_{q'} &= \frac{a^4}{8\sqrt{\pi}} \left\{ 2X e_1 e_q z_q^3 \left[ (5 - 2z_q^2) Q_1(x_q) + z_q^2 (3 + 2z_q^2) Q_2(x_q) \right] + X e_2 e_0 z_{q'}^3 \left[ (4 - z_{q'}^2 - z_{q'}^2) Q_1(x_0) + 2z_{q'}^2 (3 + z_{q'}^2) Q_2(x_0) \right] \right\}, \\
G_q &= \frac{a^4}{8\sqrt{\pi}} X e_2 e_0 z_q^2 z_{q'} \left[ (6 - 2z_{q'}^2) Q_1(x_0) + z_{q'}^2 (z_q^2 + z_{q'}^2) Q_2(x_0) \right],
\end{align}
\[ G_{qq} = \frac{a^4}{16\pi} [8X_e e_0 z_q^3 [(10 - 7z_q^2 + 2z_q^4)Q_1(x_q) - z_q^2(6 + z_q^2 + 2z_q^4)Q_2(x_q)] \\
+ X_e e_0 z_q^3 [(8 - 10z_q^2 + 4z_q^2 + 3z_q^2 z_q^2 + z_q^4)Q_1(x_0) \\
- z_q^2(48 + 10z_q^2 + z_q^2 + 3z_q^4)Q_2(x_0)]], \quad \text{(79)} \]

\[ G_{qq'} = \frac{a^4}{16\pi} X_e e_0 z_q z_{q'} [(24 - 22z_q^2 + 3z_{q'}^2 + z_q^2 z_{q'})Q_1(x_0) \\
+ z_{q'}^2(4z_q^2 + 2z_q^2 - 3z_q^2 z_{q'}^2 - z_{q'}^4)Q_2(x_0)], \quad \text{(80)} \]

\[ G_{qq''} = \frac{a^4}{16\pi} X_e e_0 z_q z_{q''} [(24 - 6z_q^2 - 8z_q^2 z_{q''} + 3z_{q''}^2 + z_q^2)Q_1(x_0) \\
+ z_{q''}^2(4z_q^2 - 6z_q^2 - 3z_q^2 z_{q''}^2 - z_{q''}^4)Q_2(x_0)], \quad \text{(81)} \]

where \( z_q = a k_q, x_q = \frac{z_q^2}{2}, x_0 = z_p z_n/2, e_q = \exp(-x_q), e_0 = \exp(-(x_p + x_n)/2) \). Finally \( \Delta F_q \) and \( \Delta G_q \) are given by:

\[ \Delta F_q = \frac{\pi^2}{3} \left( \frac{1}{k_q} [(F_{qq} - 2F_q)(\nabla n_q)^2_{n_q} + 3F_q^2 \Delta n_q] \\
+ \frac{1}{k_{q'}} [(F_{qq'} - 2F_{q'}) (\nabla n_{q'})^2_{n_q'} + 3F_{q'}^2 \Delta n_{q'}] + \frac{6\pi^2}{k_q k_{q'}} F_{qq'} (\nabla n_q)(\nabla n_{q'}) \right), \quad \text{(82)} \]

\[ \Delta G_q = \frac{\pi^2}{3} \left( \frac{1}{k_q} [(G_{qq} - 2G_q)(\nabla n_q)^2_{n_q} + 3G_q^2 \Delta n_q] \\
+ \frac{1}{k_{q'}} [(G_{qq'} - 2G_{q'}) (\nabla n_{q'})^2_{n_q'} + 3G_{q'}^2 \Delta n_{q'}] + \frac{6\pi^2}{k_q k_{q'}} G_{qq'} (\nabla n_q)(\nabla n_{q'}) \right). \quad \text{(83)} \]
Appendix 2

In this Appendix we describe briefly the method to calculate the centre-of-mass correction to the ground-state energy. As is well known, the general idea consists of subtracting the quantity

\[ E^{CM} = \langle \Psi_{GS} | \frac{P^2}{2M} | \Psi_{GS} \rangle \]  

from \( E_{GS} \). Here \( P \) is the total momentum operator, \( M \) is the total mass of a nucleus. Usually the quantity \( E^{CM} \) is represented as a sum of two terms:

\[ E^{CM} = E_1^{CM} + E_2^{CM}, \]  

where \( E_1^{CM} \) is the one-body, \( E_2^{CM} \) is the two-body centre-of-mass kinetic energy. The quantity \( E_1^{CM} \) is defined by formulae:

\[ E_1^{CM} = \sum_q E_{1,q}^{CM}, \quad E_{1,q}^{CM} = \frac{1}{2M} \text{Sp} \left( p^2 \rho_q \right), \]  

where in accordance with the definition (6) the following notation is introduced

\[ \rho_q = \rho_q(r, r') = \sum_{\sigma} \rho(r, \sigma, q, r', \sigma, q). \]  

Hereinafter the symbol \( \text{Sp} \) denotes the trace over the space variables. The subtraction of \( E_1^{CM} \) leads to the simple renormalization of the nucleon mass in the single-particle Hamiltonian \( h_q \):

\[ m_q \rightarrow \bar{m}_{1,q}, \quad \bar{m}_{1,q} = M/(M - m_q). \]  

The reasonable method for the evaluation of the quantity \( E_2^{CM} \) is the Hartree-Fock approximation for the ground-state wave function \( \Psi_{GS} \) in Eq. (84). In addition we adopt the following approximation for the single-particle DM:

\[ \rho(r, \sigma, q, r', \sigma', q) = \frac{1}{2} \delta_{\sigma, \sigma'} \rho_q(r, r'). \]  

With these assumptions we have

\[ E_2^{CM} = \sum_q E_{2,q}^{CM}, \quad E_{2,q}^{CM} = -\frac{1}{2} \text{Sp} \left( K_{2,q}^{CM} \rho_q \right), \]  

where the single-particle operator \( K_{2,q}^{CM} \) is defined as

\[ K_{2,q}^{CM} = \frac{1}{2M} p \rho_q p. \]  

In contrast to the one-body contribution, the subtraction of \( E_2^{CM} \) leads to the additional non-locality in the \( h_q \) because in the self-consistent approach we have to add the non-local operator \( K_{2,q}^{CM} \) to the single-particle kinetic-energy operator. So the total correction to the \( h_q \) is:

\[ \frac{p^2}{2m_q} \rightarrow \frac{p^2}{2\bar{m}_{1,q}} + K_{2,q}^{CM}. \]  

In the local or quasi-local DFT and in similar approaches the non-locality of \( K_{2,q}^{CM} \) in Eq. (92) leads to unpleasant difficulties. So we use the simplified method, proposed in Ref. [16], to take into account the contribution of the operator \( K_{2,q}^{CM} \) in the single-particle equations.
Let us write the density matrix $\rho_q$ in the form:

$$\rho_q(r, r') = 2 \int \frac{dk}{(2\pi)^3} \bar{n}_q(R, k) e^{iks},$$

(93)

where $R = (r + r')/2$, $s = r' - r$, $\bar{n}_q(R, k)$ is the momentum distribution function. The approximation consists of replacing function $\bar{n}_q(R, k)$ in Eq. (93) by some effective constant value $\bar{n}^{CM}_q$. Substituting Eq. (93) with $\bar{n}_q(R, k) = \bar{n}^{CM}_q$ into Eq. (91) we get

$$\tilde{K}^{CM}_{2,q} = \bar{n}^{CM}_q \frac{p^2}{M}.$$  

(94)

The value of $\bar{n}^{CM}_q$ is defined by the substitution of $\tilde{K}^{CM}_{2,q}$ into Eq. (90) instead of $K^{CM}_{2,q}$. Taking into account Eqs. (86) and (94) we obtain:

$$\bar{n}^{CM}_q = -E^{CM}_{2,q} / E^{CM}_{1,q}.$$  

(95)

The quantities $E^{CM}_{1,q}$ and $E^{CM}_{2,q}$ are defined everywhere by Eqs. (86), (90) which can be rewritten in the following forms making use of Eq. (21) for the Slater-determinant density matrix

$$E^{CM}_{1,q} = \frac{\hbar^2}{2M} \sum_{i=1}^{N} \sum_{\sigma} \int dr |\nabla \varphi_i(r, \sigma, q)|^2,$$

(96)

$$E^{CM}_{2,q} = -\frac{\hbar^2}{2M} \sum_{i=1}^{N} \sum_{\sigma} \int dr \varphi_i^*(r, \sigma, q) \nabla \varphi_i(r, \sigma, q)^2.$$  

(97)

It is easy to prove, using Eqs. (96), (97) and the completeness of the set of functions $\varphi_i$, that $|E^{CM}_{2,q}| < |E^{CM}_{1,q}|$ and consequently:

$$0 < \bar{n}^{CM}_q < 1.$$  

(98)

One can also prove that in the limit cases ($\bar{n}^{CM}_q \to 0$ and $\bar{n}^{CM}_q \to 1$) the action of the approximate operator $\tilde{K}^{CM}_{2,q}$ upon the wave functions of the occupied orbitals $\varphi_i$ coincides with the action of the initial operator $K^{CM}_{2,q}$ as defined by Eq. (91). So Eq. (94) can be considered as the interpolation formula.

The total centre-of-mass correction to the $h_q$ in this method is reduced to the renormalization of the nucleon mass as in the one-body case:

$$\frac{p^2}{2m_q} - \frac{p^2}{2\bar{m}_q}, \quad \frac{m_q}{\bar{m}_q} = \frac{M}{M + (2\bar{n}^{CM}_q - 1)m_q}.$$  

(99)
References