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Quasilocal density functional theory and its application within the extended Thomas-Fermi approximation

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In this paper we propose a generalization of the density functional theory. The theory leads to single-particle equations of motion with a quasilocal mean-field operator, which contains a quasiparticle position-dependent effective mass and a spin-orbit potential. The energy density functional is constructed using the extended Thomas-Fermi approximation and the ground-state properties of doubly magic nuclei are considered within the framework of this approach. Calculations were performed using the finite-range Gogny D1S forces and the results are compared with the exact Hartree-Fock calculations.

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I. INTRODUCTION

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 a mean field produced by effective nucleon-nucleon forces which are generally nonlocal and density dependent. In this case, one can refer to the density-dependent Hartree-Fock method (DDHF) if necessary to distinguish it from the HF method *ab initio* used in atomic physics and quantum chemistry. The resulting equations of motion contain a nonlocal single-particle potential (SPP) which is determined self-consistently. Comprehensive studies of nuclear ground-state properties within the DDHF method have been carried out with zero-range Skyrme-like forces (see, for example, Refs. [1–3], and references therein). The status of this problem is not 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 nonlocality of the SPP. For example, the complete solution of the HF equations was carried out in Ref. [4] for finite-range effective forces with a Gaussian form factor using a harmonic oscillator basis. Furthermore, the M3Y effective forces with a Yukawa form factor were employed in Ref. [5] within the Campi and Bouyssy [6] local approximation for the single-particle density matrix.

Thus, the problem of localization of the nonlocal SPP becomes extremely important. As is well known, the nonlocal exchange Fock part of the SPP is determined using the nonlocal 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 these equations do not contain any integral operators which lead to difficulties in the general nonlocal case. For instance, the Negele and Vautherin expansion of the DM [7] and its modification by Campi and Bouyssy [6] enable the HF energy to be expressed in the pointed functional form. Recently, another approach based on the extended Thomas-Fermi (ETF, see, for instance, Ref. [8]) method has been proposed in Ref. [9].

An alternative approach to the mean-field theory, which is widely used in applications to electron systems, is based on the Kohn-Sham (KS) [10] method within the framework of density functional theory (DFT). The original version of this theory (which we shall call the local DFT) was developed in the pioneering paper of Hohenberg and Kohn (HK) [11], where an energy functional that only depends on the local particle density was considered. Later on other versions of the DFT were proposed (see, for example, Refs. [12,13]). In particular, the nonlocal extension of this theory was discussed by Gilbert in Ref. [14] where the functional dependence on the DM was included.

The main merit of the KS scheme is the following: it provides a means of obtaining single-particle equations of motion for the local DFT. These equations contain the local mean-field potential, which must 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. As regards 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 which 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. Furthermore, the spin-orbit potential at least 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 assumes that any kinetic-energy density and spin density can be produced by the many-particle wave function describing the noninteracting system in some external potential with a spin-orbit component. However, in contrast to the case of the local particle density (see Ref. [15]), this statement *has not been proved*.

To include the radial-dependent effective mass and the spin-orbit potential in a rigorous way, one would have to use the nonlocal extension of the DFT and 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 nonlocal energy functional leads to serious difficulties in view of the specific properties of the pseudo-Hamiltonian obtained (see Ref. [14] for details).

The main goal of the present paper is to develop the modification of the nonlocal generalization of the DFT which would be free from the above-mentioned shortcomings of the nonlocal theory. To this end we define an energy functional that depends on the DM produced by a determinant wave function (in what follows we shall refer to it as a Slater-determinant DM). Although this DM generally does not correspond to any interacting fermion system, we will nevertheless 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 nonlocal SPP. This approach is described in Sec. II of the paper.

In Sec. III the quasilocal reduction of the DFT is developed. Within the quasilocal 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 Sec. IV we derive a semiclassical HF energy functional within the quasilocal scheme starting from the recently proposed expansion of the DM in the extended Thomas-Fermi method [9]. In the fifth section we apply our method to the description of the ground-state properties of some doubly magic spherical nuclei. To illustrate our approach, we use the effective two-body finite-range forces with Gaussian form factors. The residual correlation term is taken phenomenologically. The main results are given in the summary. In Appendices A and B some auxiliary formulas for the SPP with a Gaussian form factor are given. In Appendix C we describe a simple method to take into account the two-body correction of the center-of-mass motion to the binding energy.

II. THE NONLOCAL 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 nonrelativistic many-particle Hamiltonian. The explicit form of this operator is not important here. One can associate it with the usual formula:

$$H=T+\sum_{i\neq j} v_{ij}^{NN}+\sum_{i\neq j} v_{ij}^{Coul}+\cdots, \tag{1}$$

where

$$T=-\sum_i \frac{\hbar^2}{2m}\Delta_i \tag{2}$$

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 ellipses denotes the many-particle interactions if needed.

The HK energy functional [11], 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, Refs. [12,13]):

$$E_{HK}[n]=\inf_{\Psi\to n}\langle\Psi|H|\Psi\rangle, \tag{3}$$

where $|\Psi\rangle$ is an arbitrary normalized N-particle state. The short notation $\Psi\to n$ hereafter means the many-to-one mapping of the wave function $\Psi(x_1,\ldots,x_N)$ to the local density $n(\boldsymbol{r})$, i.e., it means that the following equalities are fulfilled:

$$n(\boldsymbol{r})=n_p(\boldsymbol{r})+n_n(\boldsymbol{r}), \tag{4}$$

$$n_q(\boldsymbol{r})=\sum_\sigma \rho(x,x), \tag{5}$$

$$\rho(x,x')=N\int \Psi(x,x_2,\ldots,x_N)\times\Psi^*(x',x_2,\ldots,x_N)dx_2\cdots dx_N, \tag{6}$$

where $\rho(x,x')$ is the single-particle DM, $x=\{\boldsymbol{r},\sigma,q\}$ includes the spatial $\boldsymbol{r}$ and spin σ variables, and the index of nucleon type $q=n,p$. The integration over x includes the summation over σ and q.

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

In the local DFT the minimum of the functional $E_{HK}[n]$ is proved to be 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 [15]:

If $n(\boldsymbol{r})\geqslant 0$, $\int n(\boldsymbol{r})d\boldsymbol{r}=N$, $\int(\boldsymbol{\nabla}\sqrt{n(\boldsymbol{r})})^2 d\boldsymbol{r}<\infty$, *then there exists an N-particle Slater-determinant wave function* Ψ_0 *built up from an orthonormal set of N single-particle wave functions* φ_i:

$$\Psi_0(x_1,\ldots,x_N)=(N!)^{-1/2}\det\{\varphi_i(x_j)\}, \tag{7}$$

such that $\Psi_0 \to n(\boldsymbol{r})$. In other words there is a many-to-one mapping of N-particle Slater-determinant wave functions onto the local particle density $n(\boldsymbol{r})$.

It is worth noting that it is not necessary for the Slater-determinant wave function Ψ_0 to be the ground-state wave function of some noninteracting system. In principle, it can correspond to some excited state of this system.

This theorem enables one to define the kinetic-energy functional $T_0[n]$ for a system of noninteracting particles:

$$T_0[n] = \inf_{\Psi_0 \to n} \langle \Psi_0 | T | \Psi_0 \rangle, \tag{8}$$

and to divide the HK functional $E_{HK}[n]$ into two parts:

$$E_{HK}[n] = T_0[n] + W[n], \tag{9}$$

where the energy functional $W[n]$ contains the potential energy as well as the correlation part of the kinetic energy.

Since the density n is produced by some Slater-determinant wave function, we have from Eqs. (5)–(7)

$$n_q(\boldsymbol{r}) = \sum_{i=1}^{N} \sum_{\sigma} |\varphi_i(\boldsymbol{r},\sigma,q)|^2. \tag{10}$$

By the same reasoning the kinetic-energy functional of the noninteracting system (8) can be written as

$$T_0[n] = \sum_{i=1}^{N} \frac{\hbar^2}{2m} \sum_{\sigma,q} \int |\boldsymbol{\nabla} \varphi_i(\boldsymbol{r},\sigma,q)|^2 d\boldsymbol{r}. \tag{11}$$

Notice that one could define the kinetic-energy functional on the basis of a more general set of N-particle wave functions:

$$T[n] = \inf_{\Psi \to n} \langle \Psi | T | \Psi \rangle. \tag{12}$$

However, this functional cannot be written in the form (11) and it is thus useless in deriving KS equations.

Applying the variational principle to the functional $E_{HK}[n]$ with functions φ_i, φ_i^* as functional variables, one obtains in accordance with Eqs. (4) and (9)–(11) the following KS equations:

$$h_{HK}\varphi_i = \varepsilon_i \varphi_i, \tag{13}$$

with

$$h_{HK} = -\frac{\hbar^2}{2m}\Delta + U(\boldsymbol{r}), \tag{14}$$

where $U(\boldsymbol{r}) = \delta W/\delta n$ is the local mean-field potential and ε_i are the Lagrange multipliers to ensure the normalization condition of the single-particle wave functions φ_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 shall not do this in the present paper.

Equation (14) does not contain either 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 nonlocal extension of the DFT. Let us define the energy functional

$$\mathcal{E}_0[\rho_0] = \inf_{\Psi_0 \to \rho_0} \langle \Psi_0 | \tilde{H} | \Psi_0 \rangle, \tag{15}$$

where Ψ_0 is any Slater-determinant wave function of the form (7), ρ_0 is the single-particle DM produced by Ψ_0 according to Eq. (6) (i.e., the 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 Eq. (15) exists.

The functional $\mathcal{E}_0[\rho_0]$ has the form of the HF energy functional built up on the basis of the effective Hamiltonian $\tilde{H}$. Thus in what follows we shall also refer to it as the HF energy functional. Let us define the residual correlation energy E_{RC} as follows:

$$E_{RC}[\hat{n}] = E[\hat{n}] - E_0[\hat{n}], \tag{16}$$

where $\hat{n} = \{n_p, n_n\}$ and

$$E[\hat{n}] = \inf_{\Psi \to \hat{n}} \langle \Psi | H | \Psi \rangle, \tag{17}$$

$$\begin{aligned} E_0[\hat{n}] &= \inf_{\Psi_0 \to \hat{n}} \langle \Psi_0 | \tilde{H} | \Psi_0 \rangle = \inf_{\rho_0 \to \hat{n}} \inf_{\Psi_0 \to \rho_0} \langle \Psi_0 | \tilde{H} | \Psi_0 \rangle \\ &= \inf_{\rho_0 \to \hat{n}} \mathcal{E}_0[\rho_0]. \end{aligned} \tag{18}$$

Because functionals $E[\hat{n}]$ and $E_0[\hat{n}]$ only depend on the local density $\hat{n}$, by definition the same is true for the functional $E_{RC}[\hat{n}]$. 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 Ψ. The auxiliary functional $E_0[\hat{n}]$ (as well as the kinetic-energy functional $T_0[n]$ in 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 nonlocal DFT is defined as

$$\mathcal{E}[\rho_0] = \mathcal{E}_0[\rho_0] + E_{RC}[\hat{n}], \tag{19}$$

where ρ_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 speculate as to whether these functionals are known or not. The most important thing is that they are rigorously defined.

The main property of the functional $\mathcal{E}[\rho_0]$ is expressed by the following equalities:

$$\inf_{\rho_0} \mathcal{E}[\rho_0] = \inf_{\hat{n}} \inf_{\rho_0 \to \hat{n}} \mathcal{E}[\rho_0] = \inf_{\hat{n}} E[\hat{n}] = E_{GS}, \tag{20}$$

where E_{GS} is the *true* ground-state energy of the interacting system as in the case of HK theory. It is important to note that our energy functional $\mathcal{E}$ is not uniquely defined by Eq. (19) and depends on $\tilde{H}$ explicitly.

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 Eq. (20) is a minimum. In addition, we use the general formula for the Slater-determinant DM ρ_0 which follows from Eqs. (6) and (7). Namely,

$$\rho_0(x,x') = \sum_{i=1}^{N} \varphi_i(x)\varphi_i^*(x'), \tag{21}$$

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 φ_i, φ_i^* as functional variables according to Eq. (21) we obtain the following set of single-particle equations:

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

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

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

$$U_{RC}(x) = U_{RC}(\boldsymbol{r},q) = \frac{\delta E_{RC}}{\delta n_q(\boldsymbol{r})}. \tag{24}$$

It is worth noting that the occupation numbers of the Slater-determinant DM are fixed to either 1 or 0. Thus, we avoid difficulties arising from the uncertainty of the occupation numbers in the theory developed in Ref. [14].

It should also be stressed that our approach is not aimed at the complete description of nuclear dynamics. It only provides an exact description of a few ground-state characteristics: the ground-state energy, and the local particle density together with the referred quantities. For a review of nuclear many-body theories giving more comprehensive treatment of the nuclear dynamics, see, for example, Refs. [8,16]. However, a discussion on the relationship between our approach and the DDHF method seems to be more relevant. As has been mentioned above, the DFT is the exact theory. It means that the minimum of the energy functional $\mathcal{E}[\rho_0]$ (if it is attained) yields the *exact* ground-state energy and the *exact* local particle density. Generally this is not fulfilled for the DDHF energy functional. In a sense, the DDHF method can be considered as a phenomenological realization of our nonlocal generalization of the DFT. In this case the contribution of the density-dependent part of the effective forces to the DDHF energy functional plays the role of residual correlation energy E_{RC}. In most of the DDHF schemes (see, for example, Refs. [2,4]) this contribution (which is E_{RC} in our notation) has the form

$$E_{RC}[\hat{n}] = \int d\boldsymbol{r}\varepsilon_{RC}(\boldsymbol{r}), \tag{25}$$

where the energy density $\varepsilon_{RC}(\boldsymbol{r})$ is just an algebraic function of the local densities. In the general case this formula is not true for the *exact* E_{RC}, and must be considered only as an approximation. However, if we assume that it is possible to represent the functional E_{RC} in such a form, then one could choose the parameters and the density dependence of the effective forces in the DDHF method in such a way that the DDHF energy functional would be equal to the exact DFT energy functional $\mathcal{E}$. As a corollary under these assumptions the DDHF method is able to reproduce the *exact* ground-state energy and *exact* local particle densities.

III. REDUCTION TO THE QUASILOCAL 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 τ_q, and spin $\boldsymbol{J}_q$ densities for neutrons and protons:

$$n_q(\boldsymbol{r}) = \sum_{\sigma} \int dx'\,\delta(x-x')\rho_0(x,x'), \tag{26}$$

$$\tau_q(\boldsymbol{r}) = \sum_{\sigma} \int dx'\,\delta(x-x')(\boldsymbol{\nabla}_r\boldsymbol{\nabla}_{r'})\rho_0(x,x'), \tag{27}$$

$$\boldsymbol{J}_q(\boldsymbol{r}) = i\sum_{\sigma} \int dx'\,\delta(\boldsymbol{r}-\boldsymbol{r}')\,\delta_{q,q'}[(\boldsymbol{\sigma})_{\sigma',\sigma}\times\boldsymbol{\nabla}_r]\rho_0(x,x'), \tag{28}$$

where $\delta(x-x') = \delta(\boldsymbol{r}-\boldsymbol{r}')\,\delta_{\sigma,\sigma'}\delta_{q,q'}$, and the quantities τ_q and $\boldsymbol{J}_q$ are the *uncorrelated* neutron and proton kinetic-energy and spin densities, respectively. Introducing the short notation $\rho_{QL} \equiv \{n_p, n_n, \tau_p, \tau_n, \boldsymbol{J}_p, \boldsymbol{J}_n\}$, let us define the quasilocal energy functional as follows:

$$\mathcal{E}^{QL}[\rho_{QL}] = \mathcal{E}_0^{QL}[\rho_{QL}] + E_{RC}[\hat{n}], \tag{29}$$

where

$$\mathcal{E}_0^{QL}[\rho_{QL}] = \inf_{\rho_0 \to \rho_{QL}} \mathcal{E}_0[\rho_0]. \tag{30}$$

Notice that the many-to-one mapping $\rho_0 \to \rho_{QL}$ is established according to Eqs. (26)–(28), and that the set $\hat{n} = \{n_p, n_n\}$ enters ρ_{QL}: $\hat{n} \in \rho_{QL}$.

From Eqs. (19), (20), (29), and (30) we have

$$\inf_{\rho_{QL}} \mathcal{E}^{QL}[\rho_{QL}] = E_{GS}. \tag{31}$$

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

$$\tau_q(\boldsymbol{r}) = \sum_{i=1}^{N} \sum_{\sigma} |\boldsymbol{\nabla}\varphi_i(\boldsymbol{r},\sigma,q)|^2, \tag{32}$$

$$\boldsymbol{J}_q(\boldsymbol{r}) = i\sum_{i=1}^{N} \sum_{\sigma,\sigma'} \varphi_i^*(\boldsymbol{r},\sigma',q)[(\boldsymbol{\sigma})_{\sigma',\sigma}\times\boldsymbol{\nabla}]\varphi_i(\boldsymbol{r},\sigma,q), \tag{33}$$

one can apply the variational principle to the energy functional $\mathcal{E}^{QL}[\rho_{QL}]$ with φ_i, φ_i^* as functional variables. The resulting single-particle equations are

$$h_q\varphi_i=\varepsilon_i\varphi_i, \tag{34}$$

where

$$h_q=-\boldsymbol{\nabla}\frac{\hbar^2}{2m_q^*(\boldsymbol{r})}\boldsymbol{\nabla}+U_q(\boldsymbol{r})-i\boldsymbol{W}_q(\boldsymbol{r})\cdot[\boldsymbol{\nabla}\times\boldsymbol{\sigma}], \tag{35}$$

$$\frac{\hbar^2}{2m_q^*(\boldsymbol{r})}=\frac{\delta\mathcal{E}^{QL}}{\delta\tau_q(\boldsymbol{r})}, \tag{36}$$

$$U_q(\boldsymbol{r})=\frac{\delta\mathcal{E}^{QL}}{\delta n_q(\boldsymbol{r})}, \tag{37}$$

$$\boldsymbol{W}_q(\boldsymbol{r})=\frac{\delta\mathcal{E}^{QL}}{\delta\boldsymbol{J}_q(\boldsymbol{r})}. \tag{38}$$

These expressions are general to the exact quasilocal DFT. If the DDHF energy functional were equal to the exact quasilocal expression (see above) these expressions would correspond to those reported in Refs. [5,7]. If the functional $\mathcal{E}^{QL}$ is known, we 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 τ_q and spin density $\boldsymbol{J}_q$ 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 out in the Introduction, the energy functional dependence on the exact kinetic-energy and spin densities could be introduced, for example, by the application of the above quasilocal reduction procedure to the energy functional of the nonlocal theory developed in Ref. [14]. However, the mapping of the Slater-determinant wave functions Ψ_0 onto the *exact* kinetic-energy and spin densities is not defined, in contrast to the mapping onto the *exact* local density, i.e., Eqs. (32) and (33) are incorrect for the exact kinetic-energy and spin densities. As a consequence, it is impossible to derive the single-particle equations such as Eqs. (34)–(38).

IV. THE EXTENDED THOMAS-FERMI APPROXIMATION IN THE QUASILOCAL DFT

We would now like to turn our attention to the effective Hamiltonian $\tilde{H}$. It has been mentioned that its choice is rather arbitrary. The operator $\tilde{H}$ is confined only by the following formal mathematical conditions. First, the energy functional $\mathcal{E}_0$ has to be well defined. While the functional $E[\hat{n}]$ is always defined, this is not the case for the functionals $\mathcal{E}_0[\rho_0]$ and $E_0[\hat{n}]$. Indeed, the matrix element of the true microscopic Hamiltonian with the bare *NN* interaction H over the Slater-determinant wave functions can diverge due to the short-range singularity of the forces, as it happens in standard many-body theory. Thus, we will use a Hamiltonian $\tilde{H}$ with an *effective* two-body *NN* interaction whose matrix elements are well defined. Secondly, the local energy functional $E[\hat{n}]$ obviously has the minimal property that is necessary to apply the variational principle. However, this may not be true for the nonlocal energy functional $\mathcal{E}[\rho_0]$ [in spite of the fact that the equality (20) is always true]. Because the functional $\mathcal{E}[\rho_0]$ depends on $\tilde{H}$ explicitly [see Eqs. (19) and (15)] one has to choose $\tilde{H}$ to ensure the minimal property of the energy functional $\mathcal{E}[\rho_0]$. 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 $m_q^*=m$, $\boldsymbol{W}_q=0$, and Eq. (34) coincides with the KS equation. In this case the residual correlation energy functional $E_{RC}[\hat{n}]$ corresponds to the sum of the direct (Hartree) term and the exchange and correlation energies 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:

$$\tilde{H}=T+\sum_{i\neq j}\tilde{v}_{ij}^{NN}+\sum_{i\neq j}v_{ij}^{Coul}. \tag{39}$$

We will use the effective *NN* forces entering $\tilde{H}$ in the form

$$\tilde{v}_{ij}^{NN}=\hat{v}_{ij}^{c}+\hat{v}_{ij}^{so}, \tag{40}$$

where the central part of the effective forces is given by

$$\hat{v}_{ij}^{c}=\sum_n[w_n+b_nP_{ij}^{\sigma}-h_nP_{ij}^{\tau}-m_nP_{ij}^{\sigma}P_{ij}^{\tau}]v_n(s), \tag{41}$$

w_n, b_n, h_n, and m_n are the parameters of the forces ($n=1,2,\ldots$), P_{ij}^{σ} and P_{ij}^{τ} are the spin and isospin exchange operators, and $v_n(s)$ ($\boldsymbol{s}=\boldsymbol{r}_i-\boldsymbol{r}_j$) are the radial form factors of the central part of the effective forces. The spin-orbit part of the forces is chosen in the form used in the Skyrme and Gogny interactions [2,4] as follows:

$$\hat{v}_{ij}^{so}=iW_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j)\cdot[\boldsymbol{k}'\times\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)\boldsymbol{k}], \tag{42}$$

where $\boldsymbol{k}=1/2i(\boldsymbol{\nabla}_i-\boldsymbol{\nabla}_j)$ denotes the operator acting on the right and $\boldsymbol{k}'=-1/2i(\overleftarrow{\boldsymbol{\nabla}}_i-\overleftarrow{\boldsymbol{\nabla}}_j)$ is the operator acting on the left.

In our approach this natural, but particular, choice of $\tilde{H}$ is compensated for by the addition of the formally defined, but, strictly speaking, unknown residual correlation energy $E_{RC}[\hat{n}]$, which contains all necessary density dependence of the total energy functional. In the applications of the method the functional $E_{RC}[\hat{n}]$ is parametrized phenomenologically and the parameters are adjusted to describe nuclear ground-state properties. Following this ideology the effective interactions entering the operator $\tilde{H}$ are taken to be density independent. The situation is quite different in the usual DDHF method, where there are no other ingredients apart from the effective forces which are taken to be density dependent in order to ensure nuclear saturation. Thus, we would like to stress that the effective interactions in our DFT approach are not exactly the same as in the DDHF theory. Therefore, the effective *NN* forces (40) entering $\widetilde{H}$ could, for example, be chosen as the finite-range part of the Gogny forces or the density-independent part of the M3Y [17] interaction.

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

$$\mathcal{E}_0^{QL}=\int d\boldsymbol{r}\mathcal{H}_0(\boldsymbol{r}). \tag{43}$$

According to Eqs. (39)–(42) the energy density $\mathcal{H}_0$ is described by six terms,

$$\mathcal{H}_0=\frac{\hbar^2}{2m}(\tau_n+\tau_p)+\mathcal{H}_{Dir}^{Nucl}+\mathcal{H}_{Exch}^{Nucl}+\mathcal{H}_{Dir}^{Coul}+\mathcal{H}_{Exch}^{Coul}+\mathcal{H}^{so}. \tag{44}$$

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

$$\mathcal{H}_{Dir}^{Nucl}(\boldsymbol{r})=\frac{1}{2}\int d\boldsymbol{r}'\left\{\left(w+\frac{b}{2}\right)n(\boldsymbol{r})n(\boldsymbol{r}')-\left(h+\frac{m}{2}\right)\right.$$
$$\left.\times[n_p(\boldsymbol{r})n_p(\boldsymbol{r}')+n_n(\boldsymbol{r})n_n(\boldsymbol{r}')]\right\}v(|\boldsymbol{r}-\boldsymbol{r}'|). \tag{45}$$

The density of the Coulomb direct energy is

$$\mathcal{H}_{Dir}^{Coul}(\boldsymbol{r})=\frac{e^2}{2}\int d\boldsymbol{r}'\frac{n_p(\boldsymbol{r})n_p(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}. \tag{46}$$

These direct energies give the contribution to the so-called Hartree functional. Up to now we have developed the *exact* theory. In the following step we will make some approximations that are similar to those used in Refs. [5,7]. To calculate the exchange terms that come from the central part of the *NN* forces we use the recently proposed ETF approximation for the DM up to $\hbar^2$ order [9]. Notice that there are other possible options to obtain the quasilocal energy functional based on the Negele-Vautherin and Campi-Bouyssy DM expansions [5–7]. In our approach for spin-saturated nuclei the nuclear exchange energy density is given by two terms,

$$\mathcal{H}_{Exch}^{Nucl}=\mathcal{H}_{Exch,0}^{Nucl}+\mathcal{H}_{Exch,2}^{Nucl}. \tag{47}$$

The first term is calculated to $\hbar^0$ order (which corresponds to the Slater approximation for the DM):

$$\mathcal{H}_{Exch,0}^{Nucl}(\boldsymbol{r})=\int d\boldsymbol{s}v(s)\left\{\frac{1}{2}X_{e1}\sum_q[n_q(\boldsymbol{r})\hat{j}_1(k_qs)]^2\right.$$
$$\left.+X_{e2}n_n(\boldsymbol{r})\hat{j}_1(k_ns)n_p(\boldsymbol{r})\hat{j}_1(k_ps)\right\}, \tag{48}$$

where $k_q(\boldsymbol{r})=[3\pi^2n_q(\boldsymbol{r})]^{1/3}$ is the Fermi momentum, $\hat{j}_1(x)=3j_1(x)/x$, $j_1(x)$ is the spherical Bessel function, and $X_{e1}=m+h/2-b-w/2$, $X_{e2}=m+h/2$. The second term corresponds to the $\hbar^2$ correction:

$$\mathcal{H}_{Exch,2}^{Nucl}(\boldsymbol{r})=\sum_q\frac{\hbar^2}{2m}\left\{(f_q-1)\left(\tau_q-\frac{3}{5}k_q^2n_q-\frac{1}{4}\Delta n_q\right)\right.$$
$$\left.+k_qf_q'\left[\frac{1}{27}\frac{(\boldsymbol{\nabla}n_q)^2}{n_q}-\frac{1}{36}\Delta n_q\right]\right\}. \tag{49}$$

In this equation $f_q=f_q(\boldsymbol{r},k_q)$, $f_q'=(\partial f_q(\boldsymbol{r},k)/\partial k)_{k=k_q}$. The function $f_q(\boldsymbol{r},k)$ is the inverse of the position- and momentum-dependent effective mass and is defined in the ETF approximation by

$$f_q(\boldsymbol{r},k)=1+\frac{m}{\hbar^2k}\frac{\partial V_{Exch,q}^{Nucl}(\boldsymbol{r},k)}{\partial k}, \tag{50}$$

where $V_{Exch,q}^{Nucl}$ is the Wigner transform of the exchange potential in the Thomas-Fermi approximation

$$V_{Exch,p}^{Nucl}(\boldsymbol{r},k)=\int d\boldsymbol{s}e^{-i\boldsymbol{k}\boldsymbol{s}}v(s)[X_{e1}n_p(\boldsymbol{r})\hat{j}_1(k_ps)$$
$$+X_{e2}n_n(\boldsymbol{r})\hat{j}_1(k_ns)] \tag{51}$$

and analogously for $V_{Exch,n}^{Nucl}$ with the permutation of indices p and n (see Ref. [9] for details). It is worth noting that within the semiclassical ETF approximation the kinetic-energy density is a functional of the local density. Thus, the energy functional obtained would only depend on the local particle density and spin density. However, it was found in Ref. [9] that the use of the quantal kinetic energy in Eq. (49), which yields the radial-dependent effective mass, significantly improves agreement with results of the full HF calculation. This has led us to use the ansatz (32) for τ_q in the present paper.

The Coulomb exchange energy consists of the Slater term and the second-order correction, which in the ETF approximation, is written as [9,18]

$$\mathcal{H}_{Exch}^{Coul}(\boldsymbol{r})=-\frac{3}{4}\left(\frac{3}{\pi}\right)^{1/3}n_p^{4/3}-\frac{7}{432\pi(3\pi^2)^{1/3}}\frac{(\boldsymbol{\nabla}n_p)^2}{n_p^{4/3}}. \tag{52}$$

Finally, the spin-orbit energy density is given by

$$\mathcal{H}^{so}(\boldsymbol{r})=-\frac{1}{2}W_0[n(\boldsymbol{r})\boldsymbol{\nabla}\boldsymbol{J}+n_n(\boldsymbol{r})\boldsymbol{\nabla}\boldsymbol{J}_n+n_p(\boldsymbol{r})\boldsymbol{\nabla}\boldsymbol{J}_p], \tag{53}$$

where $\boldsymbol{J}=\boldsymbol{J}_p+\boldsymbol{J}_n$.

It is important to point out that in this section we replace the exact quasilocal 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 this difference depends on the ρ_{QL} (due to the τ_n, τ_p, $\boldsymbol{J}_n$, and $\boldsymbol{J}_p$ dependencies), while the latter only depends on the $\hat{n}$.

The formulas (45) and (47)–(51) are valid for any radial form factor $v(s)$ of the central part of the effective forces. In this paper we use the effective interaction with a Gaussian form factor. The reason for this is the following. It was pointed out that under some assumptions the DDHF energy functional may coincide with the exact DFT functional. Thus, if the effective forces, which provide a sufficiently good description of the nuclear ground-state properties within the framework of the DDHF approach, are known (as in the case of the Gogny forces), it is reasonable to use them to construct the energy functional $\mathcal{E}$ in our theory. The DDHF effective forces can be split into two parts: the density-independent and the density-dependent expressions. The first part can be used to construct the HF energy functional $\mathcal{E}_0$ of our theory. The functional E_{RC} is then simply the DDHF energy functional calculated with the density-dependent part of the forces. In the applications of the method, which are presented in the next section, we employ the well-known parameter set of the D1S Gogny forces [19] which is successfully used in the DDHF calculations of the nuclear properties. The radial dependence of the Gogny forces is determined by the Gaussian form factor, which explains our choice. These considerations enable the use of the density-dependent part of the Gogny forces in order to approximate the residual correlation energy entering our energy functional. We therefore take E_{RC} in the form of the phenomenological ansatz

$$E_{RC}[\hat{n}]=\frac{t_3}{4}\int d\boldsymbol{r}n^{\alpha}(\boldsymbol{r})\{(2+x_3)n^2(\boldsymbol{r}) -(2x_3+1)[n_p^2(\boldsymbol{r})+n_n^2(\boldsymbol{r})]\}. \tag{54}$$

Although this form is probably too simplistic, it enables the saturation mechanism to be reproduced. We also would like to point out that the formula (54) is a standard ansatz which does not only enter the density-dependent part of the Gogny forces, but is also used in, for example, the density-dependent part of the Skyrme forces. The explicit expressions for the above-defined energy densities and for the SPP in the case of a Gaussian form factor $v(s)=\exp(-s^2/a^2)$ are given in Appendix A.

The parameters entering E_{RC} and $\widetilde{H}$ should be chosen in such a way that our quasilocal ETF approach would reproduce finite nuclei experimental data. However, in the numerical applications of our model presented in this paper, the parameters t_3, x_3, and α in Eq. (54) together with the parameters of the effective two-body Hamiltonian $\widetilde{H}$, are chosen to be equal to the corresponding parameters of the set D1S. In this way, rather than reproducing the experimental data in the best way possible, we are examining whether our quasilocal ETF approach is able to reproduce the full DDHF results obtained with the D1S forces.

The Gogny forces are purely phenomenological in the sense that these interactions have a predetermined form whose parameters are fitted to reproduce global properties of nuclei and nuclear matter. The Gaussian form factor is chosen due to its computational advantages in the full DDHF calculations of deformed nuclei. However, these forces simultaneously provide a good description of the mean-field and the pairing properties. From a more fundamental point of view, an effective interaction could be derived from a G matrix calculation, as in the case of the density-dependent M3Y forces used in Ref. [5]. However, the contributions of the different spin-isospin channels to the binding energy of nuclear matter calculated with the Gogny D1 forces compared with the same values obtained with the Brueckner-Hartree-Fock theory with a realistic two-body interaction show reasonable agreement in the even parts ($S=0$, $T=1$ and $S=1$, $T=0$) at least for momenta from zero to 1.5 fm^{-1} (see Fig. 1 of Ref. [4]). Although these forces are phenomenological, they can be considered to be a reasonable parametrization of the G matrix which provides the correct saturation properties [4]. On the other hand, a study of the equation of state for cold asymmetric nuclear matter [20] shows that at low densities and moderate asymmetries, which are relevant for the description of terrestrial finite nuclei, the Gogny D1 forces agree reasonably well with the results obtained with the realistic UV14+TNI interaction [21], although agreement fails at high densities and asymmetries.

V. NUMERICAL RESULTS

In this section we check our quasilocal DFT approximation as compared with the full DDHF 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 forces [19] with our DFT results. In this comparison we use two different quasilocal functionals: DFT-$\hbar^0$, where the exchange energy coming from the finite-range part of the interaction is taken at a pure Thomas-Fermi level (Slater approach), and DFT-$\hbar^2$, where the ETF-$\hbar^2$ contributions have been added to the Slater part. Notice that in this DFT-$\hbar^2$ approach the semiclassical kinetic-energy density entering Eq. (49) has been replaced by the corresponding quantal density for reasons pointed out above. In both DFT calculations we solve the local Schrödinger Eq. (34) for neutrons and protons with the potentials and effective masses reported in Appendix A. Table I collects all these binding energies and radii which have been computed taking into account the two-body center-of-mass correction. In our calculation we take into account this correction as explained in Appendix C. We would like to say in passing that the numerical value of this two-body center-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 Ref. [22].

From Table I we can see that the DFT-$\hbar^2$ binding energies reproduce the HF values fairly well. The differences between HF and DFT-$\hbar^2$ 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-$\hbar^0$ 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-$\hbar^2$ approximation than by the DFT-$\hbar^0$ approach. These results show the importance of the $\hbar^2$ corrections in the local approximation to the HF exchange

TABLE I. 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 forces using the DFT-$\hbar^0$ and DFT-$\hbar^2$ approaches compared with the full HF results.

		^{16}O	^{40}Ca	^{48}Ca	^{90}Zr	^{132}Sn	^{208}Pb
B	DFT-$\hbar^0$	120.2	329.6	407.5	772.1	1092.9	1623.3
	DFT-$\hbar^2$	127.3	341.9	415.0	783.9	1101.2	1636.6
	HF	129.6	344.6	416.7	785.6	1103.0	1638.9
	experiment	127.6	342.1	416.0	783.9	1102.9	1636.4
r_n	DFT-$\hbar^0$	2.72	3.41	3.62	4.29	4.87	5.59
	DFT-$\hbar^2$	2.69	3.39	3.61	4.28	4.86	5.58
	HF	2.65	3.37	3.58	4.27	4.84	5.57
r_p	DFT-$\hbar^0$	2.75	3.46	3.47	4.24	4.66	5.44
	DFT-$\hbar^2$	2.71	3.44	3.46	4.23	4.66	5.44
	HF	2.67	3.41	3.44	4.21	4.65	5.44
S_n	DFT-$\hbar^0$	12.20	13.21	9.31	11.87	7.49	7.45
	DFT-$\hbar^2$	14.55	15.36	9.52	12.02	7.59	8.03
	HF	15.08	16.04	9.66	11.88	7.68	7.80
	experiment	15.66	15.64	9.95	11.97	7.31	7.37
S_p	DFT-$\hbar^0$	8.98	6.43	14.07	7.43	15.52	8.17
	DFT-$\hbar^2$	11.24	8.45	16.51	8.25	15.94	9.29
	HF	12.53	9.27	17.09	8.36	16.23	9.51
	experiment	12.13	8.33	15.81	8.36	15.34	8.01

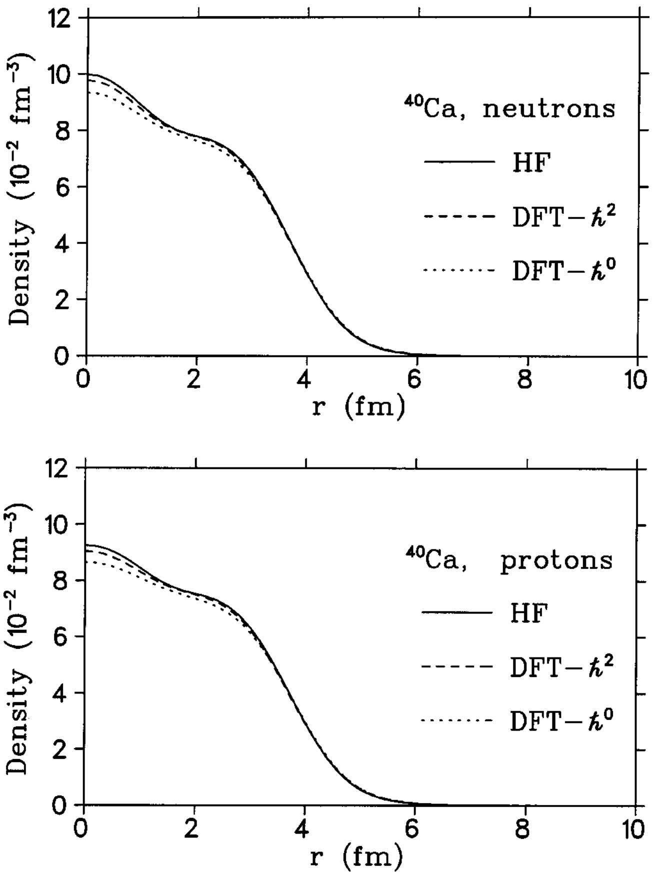

FIG. 1. Neutron and proton densities of the nucleus ^{40}Ca calculated with the D1S Gogny forces using the DFT-$\hbar^0$ (dotted lines) and DFT-$\hbar^2$ (dashed lines) approaches compared with the full HF densities (solid lines).

energy. It should be pointed out that the eigenvalues ε_i in Eq. (34) 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 I also displays the neutron and proton chemical potentials obtained using the DFT-$\hbar^0$, DFT-$\hbar^2$, and HF approximations. The DFT-$\hbar^2$ chemical potentials differ from the HF chemical potentials by less than 1 MeV, while the shift of the DFT-$\hbar^0$ separation energies with respect to the full HF values is larger and can be approximately 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 nonlocal effects. The contribution of the pointed effects can be quantified in terms of the effective mass in nuclear matter. The results of Table I show that for effective forces with an effective mass of approximately 0.7, as in the case of the Gogny forces [23], the nonlocal effects can be very well accounted for by the DFT-$\hbar^2$ functional proposed in this paper. However, for forces where the nonlocal effects are larger, the result of our DFT-$\hbar^2$ 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. [9] for more details on this point).

Figures 1 and 2 display the neutron and proton densities for ^{40}Ca and ^{208}Pb obtained using the D1S forces in the full HF (solid lines) as well as in the DFT-$\hbar^2$ (dashed lines) and DFT-$\hbar^0$ (dotted lines) calculations. The DFT proton and neutron densities nicely reproduce the surface and the tail of the full HF densities. In the region near the center 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 center of the nuclei, show some small differences with the corresponding HF s orbitals. Comparing the DFT-$\hbar^0$ and DFT-$\hbar^2$ densities, it can be seen that by including the $\hbar^2$ contributions in our local approximation, we obtain better agreement with the full HF densities.

Figure 3 displays the radial dependence of the neutron and proton effective masses calculated with the DFT-$\hbar^2$ approach [see Eq. (A13)] for the ^{208}Pb nucleus (solid lines). Because there is no explicit radial-dependent effective mass in the full HF calculation of finite nuclei using the Gogny forces, we compare the DFT-$\hbar^2$ results with the neutron and proton effective masses obtained using the Skyrme SIII forces [24] (dashed lines). We find that the DFT-$\hbar^2$ 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 forces and $m^*/m = 0.76$ for the Skyrme SIII interaction.

The neutron and proton SPP of the nucleus ^{208}Pb calcu-

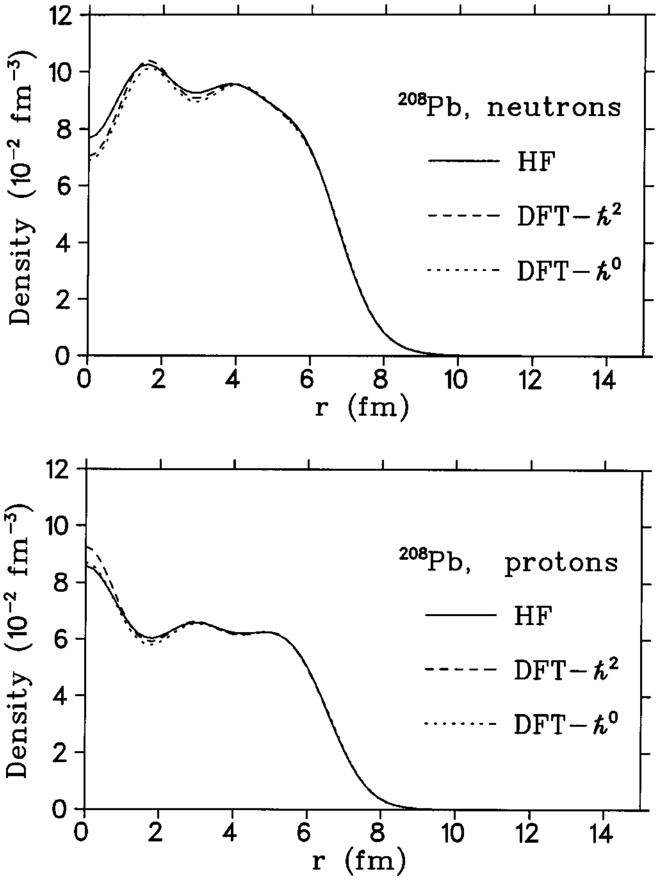

FIG. 2. Same as in Fig. 1 for the nucleus ^{208}Pb.

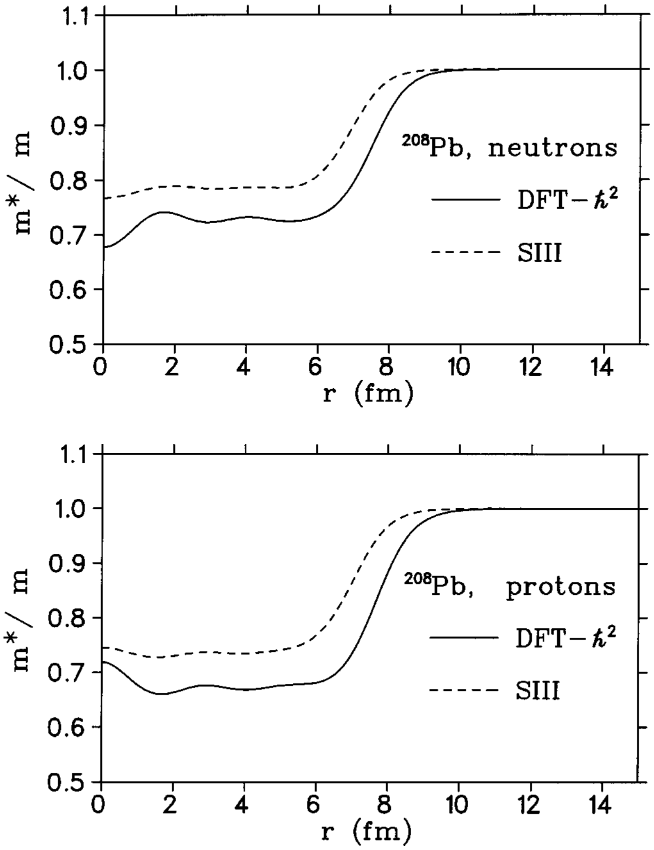

FIG. 3. Radial dependence of the neutron and proton effective masses of the nucleus ^{208}Pb calculated with the D1S Gogny forces using the DFT-$\hbar^2$ approach (solid lines) compared with the corresponding HF effective masses obtained with the Skyrme SIII forces (dashed lines).

lated within the framework of the DFT-$\hbar^2$ approximation are presented in Fig. 4. The contributions of the direct ($U_{Dir,q}^{Nucl}$) and exchange ($U_{Exch,q}^{Nucl}$) nuclear potentials are displayed. Note that the total SPP U_q also includes the contribution of the residual correlation potential U_q^{RC} according to Eq. (A4). The results show that contributions from the direct nuclear and residual correlation potentials are large, whereas there is only a small contribution from exchange nuclear potential. This is due to the particular structure of the Gogny forces. Modern effective interactions derived from a Brueckner calculation [5] give a strong exchange contribution when compared with the direct part.

VI. SUMMARY

In the present paper we propose a nonlocal extension of the DFT and its quasilocal reduction. To this end we define an energy functional which depends on the Slater-determinant DM where the occupation numbers are either 1 or 0. This enables us to avoid the difficulties of the nonlocal DFT reported in Ref. [14]. Defining the uncorrelated kinetic-energy densities and spin densities, we construct the quasilocal 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* forces in contrast to the Coulomb force in electron systems. In our approach the total energy functional consists of the HF part and the 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 [9], we obtain a quasilocal energy density functional which only depends 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 the spin-orbit potential. Using the finite-range density-dependent Gogny forces they are calculated analytically. The use of the different effective forces such as M3Y will be reported in the future.

Our method has been used to calculate some nuclear ground-state properties using the Gogny D1S forces and our results are compared with those of the exact HF calculations. Very good agreement is obtained 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. The radial-dependent

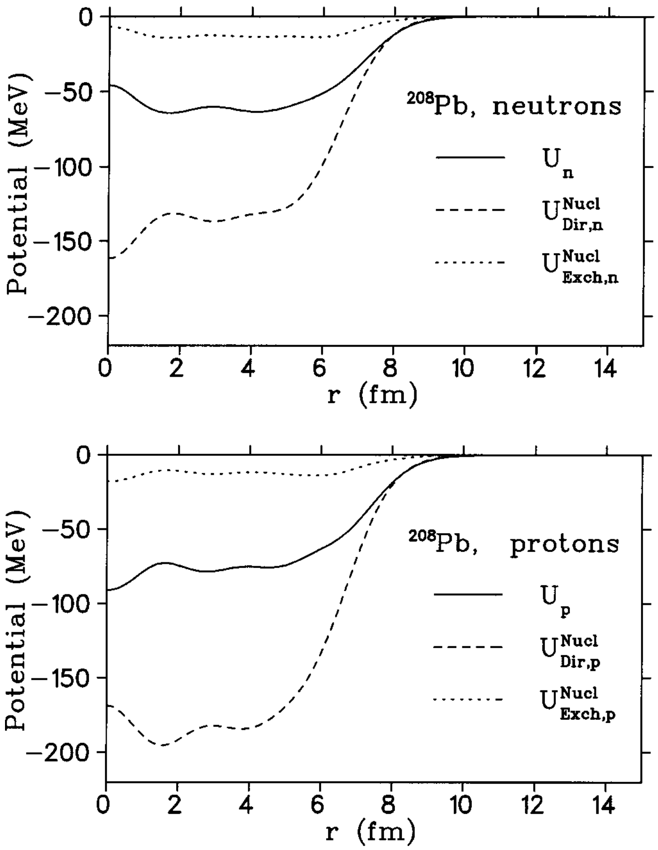

FIG. 4. Neutron and proton single-particle potentials of the nucleus ^{208}Pb calculated with the D1S Gogny forces within the framework of the DFT-$\hbar^2$ approximation: the total SPP U_q without the Coulomb contribution for protons (solid lines), the direct nuclear SPP $U^{Nucl}_{Dir,q}$ (dashed lines), and the exchange nuclear SPP $U^{Nucl}_{Exch,q}$ (dotted lines). See Eqs. (A4)–(A8) for details.

effective mass and SPP have also been analyzed within our approach.

In conclusion, our approach has the following advantages: it handles local differential equations in contrast to the integrodifferential equations in the HF approach and the quality of the obtained results is sufficiently high; our method enables one to construct a quasilocal energy density functional on the basis of effective forces with arbitrary radial form factors; and the method can be straightforwardly generalized to the nonspherical case.

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APPENDIX A

In this appendix we present the formulas for the energy densities and for the SPP in the case of the single Gaussian form factor $v(s)=\exp(-s^2/a^2)$. Assuming spherical symmetry of the particle densities, we obtain from Eqs. (45) and (48)

$$\mathcal{H}^{Nucl}_{Dir}(\mathbf{r})=\frac{\pi a^2}{2r}\int_0^\infty dr'r'\left\{\exp\left[-\frac{(r-r')^2}{a^2}\right]-\exp\left[-\frac{(r+r')^2}{a^2}\right]\right\}\left\{\left(w+\frac{b}{2}\right)n(r)n(r')-\left(h+\frac{m}{2}\right)[n_p(r)n_p(r')+n_n(r)n_n(r')]\right\}, \tag{A1}$$

$$\begin{aligned}\mathcal{H}^{Nucl}_{Exch,0}(\mathbf{r})=\frac{2}{3\pi^{5/2}a^3}\Bigg\{&X_{e1}\sum_q\left[\frac{\sqrt{\pi}}{2}a^3k_q^3\mathrm{erf}(ak_q)+\left(\frac{a^2k_q^2}{2}-1\right)\exp(-a^2k_q^2)-\frac{3a^2k_q^2}{2}+1\right]\\&+X_{e2}\sum_{\eta=\pm1}\eta\Bigg[\frac{\sqrt{\pi}}{2}a^3(k_n+\eta k_p)\\&\times(k_n^2+k_p^2-\eta k_nk_p)\mathrm{erf}\left(\frac{a}{2}(k_n+\eta k_p)\right)\\&+(a^2(k_n^2+k_p^2-\eta k_nk_p)-2)\\&\times\exp\left(-\frac{a^2}{4}(k_n+\eta k_p)^2\right)\Bigg]\Bigg\}.\end{aligned} \tag{A2}$$

The second-order correction to the exchange nuclear energy density (49) can be rewritten in the following way:

$$\mathcal{H}^{Nucl}_{Exch,2}(\mathbf{r})=\sum_q\left[F_q\left(\tau_q-\frac{3}{5}k_q^2n_q-\frac{1}{4}\Delta n_q\right)+G_q\left(\frac{1}{27}\frac{(\boldsymbol{\nabla}n_q)^2}{n_q}-\frac{1}{36}\Delta n_q\right)\right], \tag{A3}$$

where the explicit formulas for the functions F_q and G_q in the case of a Gaussian form factor are given below in Appendix B.

The SPP is defined following Eq. (37). According to Eqs. (29), (43), and (44) it is split into six parts:

$$U_q=U^{Nucl}_{Dir,q}+U^{Nucl}_{Exch,q}+U^{Coul}_{Dir,q}+U^{Coul}_{Exch,q}+U^{so}_q+U^{RC}_q, \tag{A4}$$

where the direct nuclear SPP is given by

$$U^{Nucl}_{Dir,q}(\boldsymbol{r}) = \frac{\pi a^2}{r}\int_0^\infty dr' r' \left\{ \exp\left[-\frac{(r-r')^2}{a^2} \right] - \exp\left[-\frac{(r+r')^2}{a^2} \right] \right\} \left[\left(w + \frac{b}{2} \right) n(r') - \left(h + \frac{m}{2} \right) n_q(r') \right]. \tag{A5}$$

The exchange nuclear potential consists of two parts following Eq. (47):

$$U^{Nucl}_{Exch,q} = U^{Nucl}_{Exch,q,0} + U^{Nucl}_{Exch,q,2}, \tag{A6}$$

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

$$U^{Nucl}_{Exch,p,0} = \frac{2}{\sqrt{\pi} a^3 k_p^3} \left\{ X_{e1} \left[\frac{\sqrt{\pi}}{2} a^3 k_p^3 \mathrm{erf}(a k_p) + a^2 k_p^2 \exp(-a^2 k_p^2) - a^2 k_p^2 \right] + 2 X_{e2} \sum_{\eta=\pm 1} \eta \left[\frac{\sqrt{\pi}}{4} a^3 k_p^3 \mathrm{erf}\left(\frac{a}{2}(k_p + \eta k_n) \right) + \frac{1}{2} a^2 k_p^2 \exp\left(-\frac{a^2}{4}(k_p + \eta k_n)^2 \right) \right] \right\}. \tag{A7}$$

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

$$U^{Nucl}_{Exch,p,2} = \pi^2 \left\{ \frac{1}{k_p} \left[F^p_p \left(\tau_p - \frac{3}{5} k_p^2 n_p \right) + \frac{1}{27} \left(\frac{3 G_p}{k_p^2} - G^p_p \right) \times \frac{(\boldsymbol{\nabla} n_p)^2}{n_p} - \frac{1}{36} \left(\frac{8 G_p}{k_p^2} + G^p_p + 9 F^p_p \right) \Delta n_p + F^p_n \left(\tau_n - \frac{3}{5} k_n^2 n_n \right) + \frac{1}{27} G^p_n \frac{(\boldsymbol{\nabla} n_n)^2}{n_n} - \frac{1}{36} (G^p_n + 9 F^p_n) \Delta n_n \right] - \frac{2}{27 k_n} G^n_p \frac{(\boldsymbol{\nabla} n_p)(\boldsymbol{\nabla} n_n)}{n_p} \right\} - F_p k_p^2 - \frac{1}{4} \Delta F_p - \frac{1}{36} \Delta G_p, \tag{A8}$$

where the functions $F^{q'}_q$, $G^{q'}_q$, ΔF_q, and ΔG_q used in Eq. (A8) are given in Appendix B. The formulas for the Slater and $\hbar^2$ contributions to the nuclear exchange potential acting on neutrons are obtained by replacing n by p and p by n in Eqs. (A7) and (A8).

The Coulomb direct and exchange potentials, entering Eq. (A4), are only not equal to zero for protons. In the explicit form we have

$$U^{Coul}_{Dir,p}(\boldsymbol{r}) = e^2 \int d\boldsymbol{r}' \frac{n_p(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|}, \tag{A9}$$

$$U^{Coul}_{Exch,p}(\boldsymbol{r}) = -\left[\frac{3}{\pi} n_p(\boldsymbol{r}) \right]^{1/3}. \tag{A10}$$

Including the $\hbar^2$ correction to the Coulomb exchange energy [second term in Eq. (52)] in the SPP leads to the unphysical behavior of the potential at $r \to \infty$. Its contribution to the binding energy is thus calculated as a perturbation.

The contribution of the spin-orbit energy to the SPP is given by

$$U^{so}_q = -\frac{1}{2} W_0 (\boldsymbol{\nabla} \boldsymbol{J} + \boldsymbol{\nabla} \boldsymbol{J}_q). \tag{A11}$$

Finally, the contribution of the residual correlation energy into the SPP is defined by Eqs. (37) and (54). Thus according to the notation (A4) we have

$$U^{RC}_q = \frac{t_3}{4} n^{\alpha-1} \{ (2+\alpha)(2+x_3) n^2 - (2x_3+1)[\alpha(n_p^2 + n_n^2) + 2 n_q n] \}. \tag{A12}$$

The radial-dependent effective mass $m^*_q(\boldsymbol{r})$ and the form factor $\boldsymbol{W}_q(\boldsymbol{r})$ of the spin-orbit potential are defined according to Eqs. (36), (38), (43), (44), (53), and (A3) by the relations

$$\frac{\hbar^2}{2 m^*_q(\boldsymbol{r})} = \frac{\hbar^2}{2m} + F_q, \tag{A13}$$

$$\boldsymbol{W}_q(\boldsymbol{r}) = \frac{1}{2} W_0 (\boldsymbol{\nabla} n + \boldsymbol{\nabla} n_q). \tag{A14}$$

A similar expression for the radial-dependent effective mass (A13) also appears in the independent particle Hamiltonian obtained in Refs. [5,7].

APPENDIX B

In this appendix we present the explicit expressions for the functions F_q, G_q, $F^{q'}_q$, $G^{q'}_q$, ΔF_q, and ΔG_q calculated with a Gaussian form factor. These functions are used to obtain the second-order contributions to the exchange nuclear energy density (A3) and the corresponding SPP (A8). In the following, with the exception of Eqs. (B4) and (B5), we assume that $q' \neq q$:

$$F_q = -\frac{a^2}{2\sqrt{\pi}} \left\{ X_{e1} z_q^3 \exp\left(-\frac{z_q^2}{2} \right) Q_1\left(\frac{z_q^2}{2} \right) + X_{e2} z_{q'}^3, \exp\left(-\frac{z_q^2 + z_{q'}^2}{4} \right) Q_1\left(\frac{z_q z_{q'}}{2} \right) \right\}, \tag{B1}$$

$$G_q=\frac{a^2}{4\sqrt{\pi}}z_q^2\left\{X_{e1}z_q^3\exp\left(-\frac{z_q^2}{2}\right)\left[Q_1\left(\frac{z_q^2}{2}\right)-z_q^2Q_2\left(\frac{z_q^2}{2}\right)\right]\right.$$
$$+X_{e2}z_{q'}^3\exp\left(-\frac{z_q^2+z_{q'}^2}{4}\right)\left[Q_1\left(\frac{z_qz_{q'}}{2}\right)\right.$$
$$\left.\left.-z_{q'}^2Q_2\left(\frac{z_qz_{q'}}{2}\right)\right]\right\}, \tag{B2}$$

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

$$Q_0(x)=\frac{\sinh(x)}{x},\quad Q_{m+1}=\frac{1}{2x}\frac{dQ_m(x)}{dx}. \tag{B3}$$

The functions $F_q^{q'}$, $G_q^{q'}$, $F_q^{q'q''}$, and $G_q^{q'q''}$ (the last two functions needed to obtain ΔF_q and ΔG_q, see below) are defined as

$$F_q^{q'}=\frac{1}{k_{q'}}\frac{\partial F_q}{\partial k_{q'}},\quad F_q^{q'q''}=\frac{\partial^2 F_q}{\partial k_{q'}\partial k_{q''}}, \tag{B4}$$

$$G_q^{q'}=\frac{1}{k_{q'}}\frac{\partial G_q}{\partial k_{q'}},\quad G_q^{q'q''}=\frac{\partial^2 G_q}{\partial k_{q'}\partial k_{q''}}, \tag{B5}$$

and their explicit form is

$$F_q^q=-\frac{a^4}{4\sqrt{\pi}}\{2X_{e1}e_qz_q[(3-z_q^2)Q_1(x_q)+z_q^4Q_2(x_q)]$$
$$+X_{e2}e_0z_{q'}^3[z_{q'}^2Q_2(x_0)-Q_1(x_0)]\}, \tag{B6}$$

$$F_q^{q'}=-\frac{a^4}{4\sqrt{\pi}}X_{e2}e_0z_{q'}[(6-z_{q'}^2)Q_1(x_0)+z_q^2z_{q'}^2Q_2(x_0)], \tag{B7}$$

$$F_q^{qq}=-\frac{a^4}{8\sqrt{\pi}}\{4X_{e1}e_qz_q[(2-z_q^2)(3-2z_q^2)Q_1(x_q)$$
$$-z_q^4(1+2z_q^2)Q_2(x_q)]-X_{e2}e_0z_{q'}^3[(2-z_q^2-z_{q'}^2)$$
$$\times Q_1(x_0)+2z_{q'}^2(4+z_q^2)Q_2(x_0)]\}, \tag{B8}$$

$$F_q^{q'q'}=-\frac{a^4}{8\sqrt{\pi}}X_{e2}e_0z_{q'}[(24-14z_{q'}^2+z_q^2z_{q'}^2+z_{q'}^4)Q_1(x_0)$$
$$+2z_q^2z_{q'}^2(2-z_{q'}^2)Q_2(x_0)], \tag{B9}$$

$$F_q^{qq'}=\frac{a^4}{8\sqrt{\pi}}X_{e2}e_0z_qz_{q'}^2[(6-2z_{q'}^2)Q_1(x_0)$$
$$+z_{q'}^2(z_q^2+z_{q'}^2)Q_2(x_0)], \tag{B10}$$

$$G_q^q=\frac{a^4}{8\sqrt{\pi}}\{2X_{e1}e_qz_q^3[(5-2z_q^2)Q_1(x_q)+z_q^2(3$$
$$+2z_q^2)Q_2(x_q)]+X_{e2}e_0z_{q'}^3[(4-z_q^2-z_{q'}^2)Q_1(x_0)$$
$$+2z_{q'}^2(3+z_q^2)Q_2(x_0)]\}, \tag{B11}$$

$$G_q^{q'}=\frac{a^4}{8\sqrt{\pi}}X_{e2}e_0z_q^2z_{q'}[(6-2z_{q'}^2)Q_1(x_0)$$
$$+z_{q'}^2(z_q^2+z_{q'}^2)Q_2(x_0)], \tag{B12}$$

$$G_q^{qq}=\frac{a^4}{16\sqrt{\pi}}\{8X_{e1}e_qz_q^3[(10-7z_q^2+2z_q^4)Q_1(x_q)$$
$$-z_q^2(6+z_q^2+2z_q^4)Q_2(x_q)]$$
$$+X_{e2}e_0z_{q'}^3[(8-10z_q^2+4z_{q'}^2$$
$$+3z_q^2z_{q'}^2+z_q^4)Q_1(x_0)$$
$$-z_{q'}^2(48+10z_q^2+z_q^2z_{q'}^2+3z_q^4)Q_2(x_0)]\}, \tag{B13}$$

$$G_q^{q'q'}=\frac{a^4}{16\sqrt{\pi}}X_{e2}e_0z_q^2z_{q'}[(24-22z_{q'}^2+3z_{q'}^4+z_q^2z_{q'}^2)Q_1(x_0)$$
$$+z_{q'}^2(4z_q^2+2z_{q'}^2-3z_q^2z_{q'}^2-z_{q'}^4)Q_2(x_0)], \tag{B14}$$

$$G_q^{qq'}=\frac{a^4}{16\sqrt{\pi}}X_{e2}e_0z_qz_{q'}^2[(24-6z_q^2-8z_{q'}^2+3z_q^2z_{q'}^2+z_{q'}^4)$$
$$\times Q_1(x_0)+z_{q'}^2(4z_q^2-6z_{q'}^2-3z_q^2z_{q'}^2-z_q^4)Q_2(x_0)], \tag{B15}$$

where $z_q=ak_q$, $x_q=z_q^2/2$, $x_0=z_pz_n/2$, $e_q=\exp(-x_q)$, and $e_0=\exp(-(x_p+x_n)/2)$. Finally, ΔF_q and ΔG_q are given by

$$\Delta F_q=\frac{\pi^2}{3}\left\{\frac{1}{k_q}\left[(F_q^{qq}-2F_q^q)\frac{(\boldsymbol{\nabla}n_q)^2}{n_q}+3F_q^q\Delta n_q\right]\right.$$
$$+\frac{1}{k_{q'}}\left[(F_q^{q'q'}-2F_q^{q'})\frac{(\boldsymbol{\nabla}n_{q'})^2}{n_{q'}}+3F_q^{q'}\Delta n_{q'}\right]$$
$$\left.+\frac{6\pi^2}{k_q^2k_{q'}^2}F_q^{qq'}(\boldsymbol{\nabla}n_q)(\boldsymbol{\nabla}n_{q'})\right\}, \tag{B16}$$

$$\Delta G_q=\frac{\pi^2}{3}\left\{\frac{1}{k_q}\left[(G_q^{qq}-2G_q^q)\frac{(\boldsymbol{\nabla}n_q)^2}{n_q}+3G_q^q\Delta n_q\right]\right.$$
$$+\frac{1}{k_{q'}}\left[(G_q^{q'q'}-2G_q^{q'})\frac{(\boldsymbol{\nabla}n_{q'})^2}{n_{q'}}+3G_q^{q'}\Delta n_{q'}\right]$$
$$\left.+\frac{6\pi^2}{k_q^2k_{q'}^2}G_q^{qq'}(\boldsymbol{\nabla}n_q)(\boldsymbol{\nabla}n_{q'})\right\}. \tag{B17}$$

APPENDIX C

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

$$E^{\text{c.m.}}=\left\langle \Psi_{\text{g.s.}}\left|\frac{\mathbf{P}^2}{2M}\right|\Psi_{\text{g.s.}}\right\rangle \tag{C1}$$

from $E_{\text{g.s.}}$. Here $\mathbf{P}$ is the total momentum operator, and M is the total mass of a nucleus. Usually the quantity $E^{\text{c.m.}}$ is represented as a sum of two terms:

$$E^{\text{c.m.}}=E_1^{\text{c.m.}}+E_2^{\text{c.m.}}, \tag{C2}$$

where $E_1^{\text{c.m.}}$ is the one-body and $E_2^{\text{c.m.}}$ is the two-body center-of-mass kinetic energy. The quantity $E_1^{\text{c.m.}}$ is defined by the following formulas:

$$E_1^{\text{c.m.}}=\sum_q E_{1,q}^{\text{c.m.}}, \quad E_{1,q}^{\text{c.m.}}=\frac{1}{2M}\text{Sp}(\mathbf{p}^2\rho_q), \tag{C3}$$

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

$$\rho_q=\rho_q(\mathbf{r},\mathbf{r}')=\sum_\sigma \rho(\mathbf{r},\sigma,q,\ \mathbf{r}',\sigma,q). \tag{C4}$$

Hereinafter the symbol Sp denotes the trace over the space variables. The subtraction of $E_1^{\text{c.m.}}$ leads to the simple renormalization of the nucleon mass in the single-particle Hamiltonian h_q: $m_q\to\overline{m}_{1,q}$,

$$\overline{m}_{1,q}/m_q=M/(M-m_q). \tag{C5}$$

The most reasonable method for the evaluation of the quantity $E_2^{\text{c.m.}}$ is the Hartree-Fock approximation for the ground-state wave function $\Psi_{\text{g.s.}}$ in Eq. (C1). In addition, we adopt the following approximation for the single-particle DM:

$$\rho(\mathbf{r},\sigma,q,\ \mathbf{r}',\sigma',q)=\frac{1}{2}\delta_{\sigma,\sigma'}\rho_q(\mathbf{r},\mathbf{r}'). \tag{C6}$$

With these assumptions we have

$$E_2^{\text{c.m.}}=\sum_q E_{2,q}^{\text{c.m.}}, \quad E_{2,q}^{\text{c.m.}}=-\frac{1}{2}\text{Sp}(K_{2,q}^{\text{c.m.}}\rho_q), \tag{C7}$$

where the single-particle operator $K_{2,q}^{\text{c.m.}}$ is defined as

$$K_{2,q}^{\text{c.m.}}=\frac{1}{2M}\mathbf{p}\rho_q\mathbf{p}. \tag{C8}$$

In contrast to the one-body contribution, the subtraction of $E_2^{\text{c.m.}}$ leads to additional nonlocality in the h_q, since in the self-consistent approach we have to add the nonlocal operator $K_{2,q}^{\text{c.m.}}$ to the single-particle kinetic-energy operator. Thus the total correction to h_q is

$$\frac{\mathbf{p}^2}{2m_q}\to\frac{\mathbf{p}^2}{2\overline{m}_{1,q}}+K_{2,q}^{\text{c.m.}}. \tag{C9}$$

In the local or quasilocal DFT and in similar approaches nonlocality of $K_{2,q}^{\text{c.m.}}$ in Eq. (C9) leads to unpleasant difficulties. We therefore use the simplified method, proposed in Ref. [25], in which we take the contribution of the operator $K_{2,q}^{\text{c.m.}}$ in the single-particle equations into account.

Let us write the density matrix ρ_q in the form

$$\rho_q(\mathbf{r},\ \mathbf{r}')=2\int \frac{d\mathbf{k}}{(2\pi)^3}\overline{n}_q(\mathbf{R},\ \mathbf{k})e^{i\mathbf{ks}}, \tag{C10}$$

where $\mathbf{R}=(\mathbf{r}+\mathbf{r}')/2$, $\mathbf{s}=\mathbf{r}'-\mathbf{r}$, and $\overline{n}_q(\mathbf{R},\ \mathbf{k})$ is the momentum distribution function. The approximation consists of replacing the function $\overline{n}_q(\mathbf{R},\ \mathbf{k})$ in Eq. (C10) by some effective constant value $\overline{n}_q^{\text{c.m.}}$. Substituting Eq. (C10) with $\overline{n}_q(\mathbf{R},\ \mathbf{k})=\overline{n}_q^{\text{c.m.}}$ into Eq. (C8) we get

$$\tilde{K}_{2,q}^{\text{c.m.}}=\overline{n}_q^{\text{c.m.}}\frac{\mathbf{p}^2}{M}. \tag{C11}$$

The value of $\overline{n}_q^{\text{c.m.}}$ is defined by the substitution of $\tilde{K}_{2,q}^{\text{c.m.}}$ into Eq. (C7) instead of $K_{2,q}^{\text{c.m.}}$. Taking into account Eqs. (C3) and (C11) we obtain

$$\overline{n}_q^{\text{c.m.}}=-E_{2,q}^{\text{c.m.}}/E_{1,q}^{\text{c.m.}}. \tag{C12}$$

The quantities $E_{1,q}^{\text{c.m.}}$ and $E_{2,q}^{\text{c.m.}}$ are defined everywhere by Eqs. (C3) and (C7) which can be rewritten in the following forms making use of Eq. (21) for the Slater-determinant density matrix:

$$E_{1,q}^{\text{c.m.}}=\frac{\hbar^2}{2M}\sum_{i=1}^{N}\sum_\sigma\int d\mathbf{r}|\boldsymbol{\nabla}\varphi_i(\mathbf{r},\ \sigma,\ q)|^2, \tag{C13}$$

$$E_{2,q}^{\text{c.m.}}=-\frac{\hbar^2}{2M}\sum_{i=1}^{N}\sum_{i'=1}^{N}\left|\sum_\sigma\int d\mathbf{r}\varphi_i^*(\mathbf{r},\ \sigma,\ q)\times\boldsymbol{\nabla}\varphi_{i'}(\mathbf{r},\ \sigma,\ q)\right|^2. \tag{C14}$$

It is easy to prove, using Eqs. (C13) and (C14) and the completeness of the set of functions φ_i, that $|E_{2,q}^{\text{c.m.}}|<|E_{1,q}^{\text{c.m.}}|$ and consequently

$$0<\overline{n}_q^{\text{c.m.}}<1. \tag{C15}$$

One can also prove that in the limiting cases ($\overline{n}_q^{\text{c.m.}} \to 0$ and $\overline{n}_q^{\text{c.m.}} \to 1$) the action of the approximate operator $\widetilde{K}_{2,q}^{\text{c.m.}}$ upon the wave functions of the occupied orbitals φ_i coincides with the action of the initial operator $K_{2,q}^{\text{c.m.}}$ as defined by Eq. (C8). Thus Eq. (C11) can be considered as the interpolation formula.

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

$$\frac{\mathbf{p}^2}{2m_q} \to \frac{\mathbf{p}^2}{2\overline{m}_q}, \quad \frac{\overline{m}_q}{m_q} = \frac{M}{M + (2\overline{n}_q^{\text{c.m.}} - 1)m_q}. \tag{C16}$$

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