The Negele-Vautherin density matrix expansion applied to the Gogny force

J. Dobaczewski

Institute of Theoretical Physics, University of Warsaw, Hoża 69, PL-00681 Warsaw, Poland

Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland

B.G. Carlsson

Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland

M. Kortelainen

Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA

Abstract.

We use the Negele-Vautherin density matrix expansion to derive a quasi-local density functional for the description of systems of fermions interacting with short-ranged interactions composed of arbitrary finite-range central, spin-orbit, and tensor components. Terms that are absent in the original Negele-Vautherin approach owing to the angle averaging of the density matrix are fixed by employing a gauge invariance condition. We obtain the Kohn-Sham interaction energies in all spin-isospin channels, including the exchange terms, expressed as functions of the local densities and their derivatives up to second (next to leading) order. We illustrate the method by determining the coupling constants of the Skyrme functional or Skyrme force that correspond to the finite-range Gogny central force. The resulting self-consistent solutions reproduce the Gogny-force binding energies and radii within the precision of 1-2%.

PACS numbers: 21.60.Jz, 21.10.Dr, 21.30.-x

1. Introduction

The search for a universal energy density functional (EDF) [1], that would be able to provide a spectroscopic-quality [2] description of atomic nuclei, is at the focus of the present-day studies in nuclear structure. Recently, several advanced phenomenological analyses were aimed at improving the standard relativistic [3] or nonrelativistic local [4, 2, 5, 6, 7] or nonlocal functionals [8]. A significant ongoing effort is also devoted to microscopic derivations of the functionals (see, for example, Refs. [9, 10, 11].) One of the central points of the current EDF studies is the question: to what extent can the finite-range effective interactions be approximated as quasi-local density functionals?

The framework to build the quasi-local theory was set up in the seminal paper by Negele and Vautherin (NV) [12], which introduced the so-called density matrix expansion (DME) method. Later, other methods to achieve the same goal, like the semiclassical expansion [13, 14] were also proposed and studied. The original NV expansion, for the scalar density, allowed for treating only the even-order terms in relative coordinates, and thus was applicable only to even-power gradient densities. In the present study, we revisit the NV expansion by adding the odd-power gradient densities through the local gauge-invariance condition. There are two other important differences of the present approach with respect to the NV original, namely, (i) we treat the spin (vector) densities analogously to the scalar densities and (ii) we apply a different DME for the direct terms. These differences are motivated by the effective-theory [15] interpretation of the DME advocated in the present study. The ultimate test of these ideas can only be obtained by analysing microscopic properties of nuclear densities [11].

We present a complete set of expressions in all spin-isospin channels, applicable to arbitrary finite-range central, spin-orbit, and tensor interactions. Our study is focused on applying the NV expansion to the Gogny interaction [16, 17]. This allows us to look at the correct scale of the interaction range that properly characterizes nuclear lowenergy phenomena. By performing expansion up to second order (or next-to-leading order, NLO), one obtains the local Skyrme functional [18, 19]. In this way, we establish a firm link between two different, local and nonlocal, very successful functionals.

The paper is organized as follows. In Section 2, we introduce reformulation of the NV expansion in terms of particles without spin. Discussion of this example allows us to present details of the approach without complications that otherwise could have obscured the main ideas. In Sections 3 and 4, we present results with spin and isospin degrees of freedom reintroduced, with Section 4 containing applications of the formalism to the Gogny force. Conclusions are given in Section 5, and Appendix A contains the discussion of spin and isospin polarized nuclear matter. Preliminary results of the present study were published in Ref. [20].

2. Local energy density for spinless particles of one kind

In this section, we consider the simplest (and academic) case of fermions with no spin and no isospin. First we recall that for an arbitrary non-local finite-range interaction $V(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2)$, the Kohn-Sham interaction energy [21] has the form

$$\mathcal{E}^{\text{int}} = \frac{1}{2} \int d^3 \mathbf{r}'_1 d^3 \mathbf{r}'_2 d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 V(\mathbf{r}'_1, \mathbf{r}'_2; \mathbf{r}_1, \mathbf{r}_2) \times (\rho(\mathbf{r}_1, \mathbf{r}'_1) \rho(\mathbf{r}_2, \mathbf{r}'_2) - \rho(\mathbf{r}_2, \mathbf{r}'_1) \rho(\mathbf{r}_1, \mathbf{r}'_2)), \qquad (1)$$

The Negele-Vautherin density matrix expansion applied to the Gogny force

whereas for a local interaction,

$$V(\mathbf{r}_{1}',\mathbf{r}_{2}';\mathbf{r}_{1},\mathbf{r}_{2}) = \delta(\mathbf{r}_{1}'-\mathbf{r}_{1})\delta(\mathbf{r}_{2}'-\mathbf{r}_{2})V(\mathbf{r}_{1},\mathbf{r}_{2}),$$
(2)

the interaction energy reduces to:

$$\mathcal{E}^{\text{int}} = \frac{1}{2} \int d^3 \boldsymbol{r}_1 d^3 \boldsymbol{r}_2 V(\boldsymbol{r}_1, \boldsymbol{r}_2) \Big(\rho(\boldsymbol{r}_1) \rho(\boldsymbol{r}_2) - \rho(\boldsymbol{r}_2, \boldsymbol{r}_1) \rho(\boldsymbol{r}_1, \boldsymbol{r}_2) \Big),$$
(3)

where $\rho(\mathbf{r}_1) \equiv \rho(\mathbf{r}_1, \mathbf{r}_1)$ and $\rho(\mathbf{r}_2) \equiv \rho(\mathbf{r}_2, \mathbf{r}_2)$ are local densities. As is well known, the first term in Eq. (3) (the direct term) depends only on local densities, whereas the second one (the exchange term) depends on the modulus squared of the non-local density. This markedly different structure of the two terms requires separate treatment, as discussed in the following two subsections.

2.1. Direct interaction energy

In nuclei, the range of interaction is significantly smaller than the typical scale of the distance at which the local density varies. Therefore, we may expand the local densities $\rho(\mathbf{r}_1)$ and $\rho(\mathbf{r}_2)$ around their average position, and use this expansion to calculate the direct term in Eq. (3).

Denoting the standard total (\mathbf{R}) and relative (\mathbf{r}) coordinates and derivatives as

$$R = \frac{1}{2}(r_1 + r_2), \qquad r = r_1 - r_2,$$
 (4)

$$\boldsymbol{\nabla} = \frac{\partial}{\partial \boldsymbol{R}} = \frac{\partial}{\partial \boldsymbol{r}_1} + \frac{\partial}{\partial \boldsymbol{r}_2}, \qquad \boldsymbol{\partial} = \frac{\partial}{\partial \boldsymbol{r}} = \frac{1}{2} \left(\frac{\partial}{\partial \boldsymbol{r}_1} - \frac{\partial}{\partial \boldsymbol{r}_2} \right), \tag{5}$$

we have the expansion of local densities to second order,

$$\rho(\boldsymbol{r}_1) = \rho(\boldsymbol{R} + \frac{1}{2}\boldsymbol{r}) = \rho(\boldsymbol{R}) + \frac{1}{2}r_a\nabla_a\rho(\boldsymbol{R}) + \frac{1}{8}r_ar_b\nabla_a\nabla_b\rho(\boldsymbol{R}) + \dots, \quad (6)$$

$$\rho(\boldsymbol{r}_2) = \rho(\boldsymbol{R} - \frac{1}{2}\boldsymbol{r}) = \rho(\boldsymbol{R}) - \frac{1}{2}r_a\nabla_a\rho(\boldsymbol{R}) + \frac{1}{8}r_ar_b\nabla_a\nabla_b\rho(\boldsymbol{R}) + \dots, \quad (7)$$

and hence

$$\rho(\boldsymbol{r}_1)\rho(\boldsymbol{r}_2) = \rho^2(\boldsymbol{R}) + \frac{1}{4}r_a r_b \Big(\rho(\boldsymbol{R})\nabla_a \nabla_b \rho(\boldsymbol{R}) - [\nabla_a \rho(\boldsymbol{R})][\nabla_b \rho(\boldsymbol{R})]\Big) + \dots, (8)$$

where we implicitly assumed the summation over the repeated Cartesian indices a and b.

Assuming that the local potential $V(\mathbf{r}_1, \mathbf{r}_2)$ depends only on the distance between the interacting particles, $V(\mathbf{r}_1, \mathbf{r}_2) = V(|\mathbf{r}_1 - \mathbf{r}_2|) = V(r)$, the direct interaction energy is given by the integral of a local energy density $\mathcal{H}_{dir}^{int}(\mathbf{R})$,

$$\mathcal{E}_{\rm dir}^{\rm int} = \int d^3 \boldsymbol{R} \, \mathcal{H}_{\rm dir}^{\rm int}(\boldsymbol{R}), \tag{9}$$

where up to second order,

$$\mathcal{H}_{\rm dir}^{\rm int}(\boldsymbol{R}) = \frac{1}{2} \Big[V_0 \rho^2 + \frac{1}{12} V_2 \Big(\rho \Delta \rho - (\boldsymbol{\nabla} \rho)^2 \Big) \Big] + \dots,$$
(10)

where the coupling constants, V_0 and V_2 , are given by the lowest two moments of the interaction,

$$V_n = \int d^3 \mathbf{r} \, r^n V(r) = 4\pi \int dr \, r^{n+2} V(r).$$
(11)

After integrating by parts, the two second-order terms in Eq. (10) are identical, so we can equally well use:

$$\mathcal{H}_{\rm dir}^{\rm int}(\boldsymbol{R}) = \frac{1}{2} \Big[V_0 \rho^2 + \frac{1}{6} V_2 \rho \Delta \rho \Big] + \dots, \qquad (12)$$

We see that the separation of scales between the range of interaction and the rate of change of the local density leads to a dramatic collapse of information that is transferred from the interaction potential to the interaction energy. Namely, the two constants, V_0 and V_2 , completely characterize the interaction in the direct term, and the detailed form of the potential V(r) becomes irrelevant. Moreover, it can be easily checked that in this approximation, the direct energy density is exactly equal to that corresponding to the contact force corrected by the second-order gradient pseudopotential,

$$\tilde{V}(\boldsymbol{r}) = V_0 \delta(\boldsymbol{r}) - \frac{2}{3} V_2 \boldsymbol{\partial} \cdot \delta(\boldsymbol{r}) \boldsymbol{\partial}.$$
(13)

2.2. Exchange interaction energy

In the exchange term of Eq. (3), the non-zero range of the interaction probes the nonlocal space dependence of the density matrix. For short-range interactions, one can expand $\rho(\mathbf{R}, \mathbf{r})$ to second order with respect to the variable \mathbf{r} , which gives

$$\rho(\boldsymbol{r}_1, \boldsymbol{r}_2) = \rho(\boldsymbol{R}, \boldsymbol{r}) = \rho(\boldsymbol{R}) + r_a \partial_a \rho(\boldsymbol{R}, \boldsymbol{r}) + \frac{1}{2} r_a r_b \partial_a \partial_b \rho(\boldsymbol{R}, \boldsymbol{r}) + \dots$$
$$= \rho(\boldsymbol{R}) + i r_a j_a(\boldsymbol{R}) + \frac{1}{2} r_a r_b \left[\frac{1}{4} \nabla_a \nabla_b \rho(\boldsymbol{R}) - \tau_{ab}(\boldsymbol{R}) \right] + \dots (14)$$

where derivatives ∂_i are always calculated at $r_a=0$, and therefore, the result can be expressed in terms of the standard current and kinetic densities [22]:

$$j_a(\boldsymbol{R}) = \frac{1}{i} \partial_a \rho(\boldsymbol{R}, \boldsymbol{r})_{\boldsymbol{r}=0}, \qquad \tau_{ab}(\boldsymbol{R}) = \nabla_a^{(1)} \nabla_b^{(2)} \rho(\boldsymbol{r}_1, \boldsymbol{r}_2)_{\boldsymbol{r}_1=\boldsymbol{r}_2}.$$
 (15)

This parabolic approximation does not ensure that $\rho(\mathbf{r}_1, \mathbf{r}_2) \longrightarrow 0$ for large $r = |\mathbf{r}| = |\mathbf{r}_1 - \mathbf{r}_2|$. In the spirit of the DME [12], one can improve it by introducing three functions of r, $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$ [20] that vanish at large r, i.e., we define the quasi-local approximation of the density matrix by:

$$\rho(\boldsymbol{r}_1, \boldsymbol{r}_2) = \pi_0(r)\rho(\boldsymbol{R}) + \pi_1(r)r_a\partial_a\rho(\boldsymbol{R}, \boldsymbol{r}) + \frac{1}{2}\pi_2(r)r_ar_b\partial_a\partial_b\rho(\boldsymbol{R}, \boldsymbol{r}) + \dots$$
$$= \pi_0(r)\rho(\boldsymbol{R}) + i\pi_1(r)r_aj_a\rho(\boldsymbol{R}) + \frac{1}{2}\pi_2(r)r_ar_b\left[\frac{1}{4}\nabla_a\nabla_b\rho(\boldsymbol{R}) - \tau_{ab}(\boldsymbol{R})\right] + \dots(16)$$

Such a postulate has to be compatible with the Taylor expansion of Eq. (14), which requires that

$$\pi_0(0) = \pi_1(0) = \pi_2(0) = 1$$
 and $\pi'_0(0) = \pi'_1(0) = \pi''_0(0) = 0.$ (17)

Of course, for $\pi_0(r) = \pi_1(r) = \pi_2(r) = 1$, one reverts to the parabolic approximation (14).

The product of nonlocal densities in the exchange integral of Eq. (3) to second order reads

$$\rho(\boldsymbol{r}_{1},\boldsymbol{r}_{2})\rho(\boldsymbol{r}_{2},\boldsymbol{r}_{1}) = \pi_{0}^{2}(r)\rho^{2}(\boldsymbol{R}) + \pi_{0}(r)\pi_{2}(r)r_{a}r_{b}\left\{\rho(\boldsymbol{R})\partial_{a}\partial_{b}\rho(\boldsymbol{R},\boldsymbol{r}) - [\partial_{a}\rho(\boldsymbol{R},\boldsymbol{r})][\partial_{b}\rho(\boldsymbol{R},\boldsymbol{r})]\right\} + \dots = \pi_{0}^{2}(r)\rho^{2}(\boldsymbol{R}) + \pi_{0}(r)\pi_{2}(r)r_{a}r_{b}\left\{\frac{1}{4}\rho(\boldsymbol{R})\nabla_{a}\nabla_{b}\rho(\boldsymbol{R}) - \rho(\boldsymbol{R})\tau_{ab}(\boldsymbol{R}) + j_{a}(\boldsymbol{R})j_{b}(\boldsymbol{R})\right\} + \dots , \quad (18)$$

The Negele-Vautherin density matrix expansion applied to the Gogny force

where we have introduced the supplementary condition:

$$\pi_1^2(r) = \pi_0(r)\pi_2(r). \tag{19}$$

This condition ensures that the quasi-local approximation of Eq. (16) is compatible with the local gauge invariance [23]. Indeed, the left-hand side of Eq. (18) is manifestly invariant with respect to the local gauge transformation,

$$\rho'(\mathbf{r}_1, \mathbf{r}_2) = e^{i\phi(\mathbf{r}_1) - i\phi(\mathbf{r}_2)}\rho(\mathbf{r}_1, \mathbf{r}_2),$$
(20)

and only the difference of terms in the curly brackets in Eq. (18) is invariant with respect to the same transformation [22, 19].

Functions $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$ also depend on the parameters defining the approximation (16). In particular, when the infinite matter is used to define functions $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$, like in the DME, they parametrically depend on the Fermi momentum k_F . By associating the local density $\rho(\mathbf{R})$ with k_F , functions $\pi_0(r)$, $\pi_1(r)$, and $\pi_2(r)$ become dependent on $\rho(\mathbf{R})$, and hence the damping of the density matrix in the non-local direction \mathbf{r} can be different in different local points \mathbf{R} . However, in order to keep the notation simple, we do not explicitly indicate this possible dependence on density.

Within the quasi-local approximation, one obtains the exchange interaction energy,

$$\mathcal{E}_{\text{exc}}^{\text{int}} = \int d^3 \boldsymbol{R} \, \mathcal{H}_{\text{exc}}^{\text{int}}(\boldsymbol{R}), \tag{21}$$

where up to second order,

$$\mathcal{H}_{\rm exc}^{\rm int}(\boldsymbol{R}) = -\frac{1}{2} \Big[V_{\pi 0}^{00} \rho^2 + \frac{1}{3} V_{\pi 2}^{02} \Big(\frac{1}{4} \rho \Delta \rho - (\rho \tau - \boldsymbol{j}^2) \Big) \Big] + \dots, \qquad (22)$$

and where $\tau = \tau_{aa}$. The coupling constants, $V_{\pi 0}^{00}$ and $V_{\pi 2}^{02}$, are given by the following moments of the interaction,

$$V_{\pi n}^{ij} = \int d^3 \boldsymbol{r} \, r^n \pi_i(r) \pi_j(r) V(r) = 4\pi \int dr \, r^{n+2} \pi_i(r) \pi_j(r) V(r).$$
(23)

Unlike the coupling constants defining the direct term (11), these in Eq. (23) have to be understood as the running coupling constants, which in the DME depend on the scale of the Fermi momentum k_F or density $\rho(\mathbf{R})$.

Again, the separation of scales between the range of interaction and the rate of change of the density matrix in the non-local direction results in the dependence of the local energy density on two coupling constants only, and not on the details of the interaction. For the parabolic approximation of Eq. (14), the coupling constants that define the direct and exchange energies are identical, i.e., $V_{\pi 0}^{00} = V_0$ and $V_{\pi 2}^{02} = V_2$; however, for the quasi-local approximation of Eq. (16) they are different. This important observation is discussed in Sec. 3.2 in more detail.

In nuclei, the separation of scales discussed above is not very well pronounced. The characteristic parameter, which defines these relative scales, is equal to $k_F a$, where a stands for the range of the interaction. For example, within the Gogny interaction, which we analyze in detail in Sec. 4, there are two components with the ranges of a = 0.7 and 1.2 fm, whereas $k_F = 1.35 \text{ fm}^{-1}$, which gives values of $k_F a = 0.95$ and 1.62 that are dangerously close to 1. Therefore, in the expansion of the local energy density (22), one cannot really count on the moments $V_{\pi n}^{ij}$ decreasing with the increasing order n.

Instead, as demonstrated by Negele and Vautherin [12], one can hope for tremendously improving the convergence by using at each order the proper counterterms, which make each order vanish in the infinite matter. Without repeating the original NV construction, here we only note that the net result consists of adding and subtracting in Eq. (16) the infinite-matter term, that is,

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \nu_0(r)\rho(\mathbf{R}) + i\nu_1(r)r_a j_a \rho(\mathbf{R}) + \frac{1}{2}\nu_2(r)r_a r_b \left[\frac{1}{4}\nabla_a \nabla_b \rho(\mathbf{R}) - \tau_{ab}(\mathbf{R}) + \frac{1}{5}\delta_{ab}k_F^2 \rho(\mathbf{R})\right] + \dots , \quad (24)$$

where we have defined functions $\nu_i(r)$ such that:

$$\nu_0(r) = \pi_0(r) - \frac{1}{10}(k_F r)^2 \pi_2, \qquad \nu_1(r) = \pi_1(r), \qquad \nu_2(r) = \pi_2(r).$$
(25)

By neglecting the term quadratic in ν_2 , we can now use the approximation (24) to calculate the product of densities in Eq. (18), which gives

$$\rho(\boldsymbol{r}_1, \boldsymbol{r}_2)\rho(\boldsymbol{r}_2, \boldsymbol{r}_1) = \nu_0^2(r)\rho^2(\boldsymbol{R}) + \nu_0(r)\nu_2(r)r_ar_b\left\{\frac{1}{4}\rho(\boldsymbol{R})\nabla_a\nabla_b\rho(\boldsymbol{R}) - \rho(\boldsymbol{R})\tau_{ab}(\boldsymbol{R}) + \frac{1}{5}\delta_{ab}k_F^2\rho^2(\boldsymbol{R}) + j_a(\boldsymbol{R})j_b(\boldsymbol{R})\right\} + \dots , \qquad (26)$$

where again the gauge invariance requires that

$$\nu_1^2(r) = \nu_0(r)\nu_2(r). \tag{27}$$

We note that the gauge-invariance conditions for the functions $\pi_i(r)$ and $\nu_i(r)$, Eqs. (19) and (27), are compatible with one another only up to the term $\pi_2^2(r)$, which was shifted to higher orders. Finally, approximation (26) gives the energy density analogous to (22),

$$\mathcal{H}_{\text{exc}}^{\text{int}}(\boldsymbol{R}) = -\frac{1}{2} \Big[V_{\nu 0}^{00} \rho^2 + \frac{1}{3} V_{\nu 2}^{02} \Big(\frac{1}{4} \rho \Delta \rho - (\rho \tau - \boldsymbol{j}^2) + \frac{3}{5} k_F^2 \rho^2 \Big) \Big] + \dots, \quad (28)$$

where the coupling constants, $V_{\nu 0}^{00}$ and $V_{\nu 2}^{02}$, are given by the moments of the interaction calculated for functions $\nu_i(r)$, namely,

$$V_{\nu n}^{ij} = \int d^3 \boldsymbol{r} \, r^n \nu_i(r) \nu_j(r) V(r) = 4\pi \int dr \, r^{n+2} \nu_i(r) \nu_j(r) V(r).$$
(29)

We see that the two sets of auxiliary functions, $\pi_i(r)$ and $\nu_i(r)$, are suitable for discussing the approximate forms of the nonlocal density $\rho(\mathbf{r}_1, \mathbf{r}_2)$ and exchange energy density $\mathcal{H}_{\text{exc}}^{\text{int}}(\mathbf{R})$, respectively. Although for the nonlocal density they correspond to a simple reshuffling of terms, which gives relations (25) between $\pi_i(r)$ and $\nu_i(r)$, for the exchange energy density they constitute entirely different approximations, given in Eqs. (22) and (28), with expansion (28) having a larger potential for faster convergence. Only this latter expansion is further discussed.

2.3. Determination of functions $\pi_i(r)$

For a given nonlocal density $\rho(\mathbf{r}_1, \mathbf{r}_2)$, the auxiliary functions $\pi_i(r)$ or $\nu_i(r)$, which define its quasi-local approximation, can be calculated as their best possible approximations in terms of local densities. However, the usefulness of the expansion relies on the assumption that generic forms of these functions can be estimated and then applied to all many-body systems of a given kind.

The standard Slater approximation [24, 25], which is routinely used to evaluate the Coulomb exchange energy (cf. Refs. [26, 27]), corresponds to

$$\pi_0(r) = \nu_0(r) = \frac{3j_1(k_F r)}{k_F r} \quad \text{and} \quad \pi_2(r) = 0.$$
(30)

The NV expansion [12] gives a second-order estimate by making the momentum expansion around the Fermi momentum k_F of an infinite system. This gives:

$$\pi_0(r) = \frac{6j_1(k_F r) + 21j_3(k_F r)}{2k_F r} \simeq 1 - \frac{(k_F r)^4}{504},\tag{31}$$

$$\pi_2(r) = \frac{105j_3(k_F r)}{(k_F r)^3} \simeq 1 - \frac{(k_F r)^2}{18} + \frac{(k_F r)^4}{792},\tag{32}$$

$$\nu_0(r) = \frac{3j_1(k_F r)}{k_F r} \simeq 1 - \frac{(k_F r)^2}{10} + \frac{(k_F r)^4}{280},\tag{33}$$

where $j_n(k_F r)$ are the spherical Bessel functions.

The NV functions $\pi_0(r)$, $\pi_2(r)$, and $\nu_0(r)$ are plotted in Fig. 1 with solid, dashed, and dotted lines, respectively. One can see that for large $k_F r$, functions $\pi_0(r)$ and $\pi_2(r)$ have zeros close to one another and the same signs. Indeed, asymptotically both behave like $\cos(k_F r)/k_F r$. Therefore, the gauge-invariance condition (19) can be satisfied almost everywhere. On the other hand, functions $\nu_0(r)$ and $\nu_2(r) = \pi_2(r)$, have asymptotically opposite signs, and the corresponding gauge-invariance condition (27) can be almost nowhere satisfied. Nevertheless, as discussed in Sec. 2.2, what really matters are the moments of interaction (23) and (29), where functions $\pi_i(r)$ and $\nu_i(r)$ are probed only within the range of the interaction, that is, up to $k_F r \simeq 1$ -2. Therefore, for the NV expansion, one can safely use approximations:

$$\pi_1(r) = +\sqrt{|\pi_0(r)\pi_2(r)|},\tag{34}$$

$$\nu_1(r) = +\sqrt{|\nu_0(r)\nu_2(r)|},\tag{35}$$

which are valid up to the first zero of j_3 or j_1 , respectively, that is, up to $k_F r \simeq 7.0$ and 4.5.

By the same token, we can replace in Eqs. (31)–(33) the Bessel functions by Gaussians having the same leading-order dependence on $k_F r$, namely,

$$\pi_0(r) = \exp\left(-\frac{(k_F r)^4}{504}\right),$$
(36)

$$\pi_2(r) = \exp\left(-\frac{(k_F r)^2}{18} - \frac{(k_F r)^4}{1100}\right),\tag{37}$$

$$\nu_0(r) = \exp\left(-\frac{(k_F r)^4}{504}\right) - \frac{(k_F r)^2}{10} \exp\left(-\frac{(k_F r)^2}{18} - \frac{(k_F r)^4}{1100}\right).$$
 (38)

As seen in the bottom panel of Fig. 1, in this way, in the region of small $k_F r$, one obtains a very good reproduction of the NV functions $\pi_i(r)$ and $\nu_i(r)$.

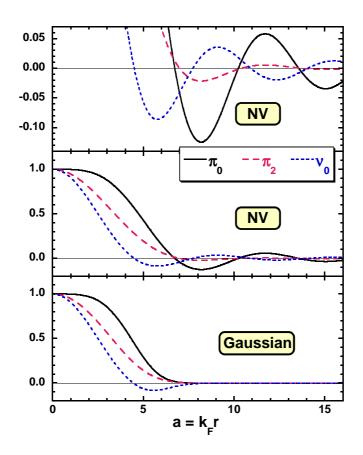


Figure 1. Dependence of the functions $\pi_0(r)$ (solid lines), $\pi_2(r)$ (dashed lines), and $\nu_0(r)$ (dotted lines) on $k_F r$. The top and middle panels show the NV functions of Eqs. (31)–(33), with the top panel plotted in expanded scale to better show the details at large $k_F r$. The bottom panel shows the functions $\pi_0(r)$, $\pi_2(r)$, and $\nu_0(r)$ approximated by Gaussians as in Eqs. (36)–(38).

3. Local energy density for particles with spin and isospin

3.1. Density matrix expansion with spin and isospin

For nucleons, the density matrix $\rho(\mathbf{r}_1\sigma_1\tau_1, \mathbf{r}_2\sigma_2\tau_2)$ depends not only on positions \mathbf{r}_1 and \mathbf{r}_2 but also on spin $\sigma_1, \sigma_2 = \pm 1$ and isospin $\tau_1, \tau_2 = \pm 1$ coordinates. Since the strong two-body interaction is assumed to be isospin and rotationally invariant, it is convenient to represent the standard density matrix $\rho(\mathbf{r}_1\sigma_1\tau_1, \mathbf{r}_2\sigma_2\tau_2)$ through nonlocal densities $\rho_{\mu k}(\mathbf{r}_1, \mathbf{r}_2)$ as:

$$\rho(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}_2\sigma_2\tau_2) = \frac{1}{4} \sum_{\mu=0, x, y, z} \sum_{k=0}^3 \rho_{\mu k}(\boldsymbol{r}_1, \boldsymbol{r}_2) \langle \sigma_1 | \sigma_\mu | \sigma_2 \rangle \langle \tau_1 | \tau_k | \tau_2 \rangle,$$
(39)

where σ_0 ($\sigma_{x,y,z}$) and τ_0 ($\tau_{1,2,3}$) are the unity (Pauli) matrices in the spin and isospin coordinates, respectively. For $\mu = 0$ and $\mu = x, y, z$, the densities are scalars and vectors, respectively, and for k = 0 and k = 1, 2, 3, they are isoscalars and isovectors, so altogether the density matrix is split into the four standard spin-isospin channels.

For the direct term, we can proceed as in Sec. 2.1, by making the Taylor expansions of local densities (at $\mathbf{r}_1 = \mathbf{r}_2$) in each spin-isospin channel; that is, similarly as in Eqs. (6) and (7), we have

$$\rho_{\mu k}(\boldsymbol{R} \pm \frac{1}{2}\boldsymbol{r}) = \rho_{\mu k}(\boldsymbol{R}) \pm \frac{1}{2}r_a \nabla_a \rho_{\mu k}(\boldsymbol{R}) + \frac{1}{8}r_a r_b \nabla_a \nabla_b \rho_{\mu k}(\boldsymbol{R}) + \dots \qquad (40)$$

For the exchange term, Sec. 2.2, the analogous Taylor expansions of nonlocal densities, similarly as in Eq. (14), read

$$\rho_{\mu k}(\boldsymbol{R}, \pm \boldsymbol{r}) = \rho_{\mu k}(\boldsymbol{R}) \pm i r_a j_{\mu a k}(\boldsymbol{R}) + \frac{1}{2} r_a r_b \left[\frac{1}{4} \nabla_a \nabla_b \rho_{\mu k}(\boldsymbol{R}) - \tau_{\mu a b k}(\boldsymbol{R}) \right] + \dots, \quad (41)$$

where the current $(j_{\mu ak}(\mathbf{R}))$ and kinetic $(\tau_{\mu abk}(\mathbf{R}))$ densities are defined in each channel as in Eqs. (15), namely,

$$j_{\mu ak}(\mathbf{R}) = \frac{1}{i} \partial_a \rho_{\mu k}(\mathbf{R}, \mathbf{r})_{\mathbf{r}=0}, \qquad \tau_{\mu abk}(\mathbf{R}) = \nabla_a^{(1)} \nabla_b^{(2)} \rho_{\mu k}(\mathbf{r}_1, \mathbf{r}_2)_{\mathbf{r}_1 = \mathbf{r}_2}.$$
(42)

The local density approximation of densities in all channels, analogous to Eqs. (16) and (24), is now postulated as

$$\rho_{\mu k}(\boldsymbol{R}, \pm \boldsymbol{r}) = \pi_0(r)\rho_{\mu k}(\boldsymbol{R}) \pm i\pi_1(r)r_a j_{\mu ak}(\boldsymbol{R}) + \frac{1}{2}\pi_2(r)r_a r_b \left[\frac{1}{4}\nabla_a \nabla_b \rho_{\mu k}(\boldsymbol{R}) - \tau_{\mu abk}(\boldsymbol{R})\right] + \dots , \qquad (43)$$

and

$$\rho_{\mu k}(\boldsymbol{R}, \pm \boldsymbol{r}) = \nu_0(r)\rho_{\mu k}(\boldsymbol{R}) \pm i\nu_1(r)r_a j_{\mu ak}\rho(\boldsymbol{R}) + \frac{1}{2}\nu_2(r)r_a r_b \left[\frac{1}{4}\nabla_a\nabla_b\rho_{\mu k}(\boldsymbol{R}) - \tau_{\mu abk}(\boldsymbol{R}) + \frac{1}{5}\delta_{ab}k_F^2\rho_{\mu k}(\boldsymbol{R})\right] + \dots \quad (44)$$

At this point, we have assumed that functions $\pi_i(r)$ and $\nu_i(r)$ are channelindependent, that is, that they are scalar-isoscalar functions. In Appendix A we discuss this point in more detail, and we show that the postulate of simply channel-dependent functions $\pi_i(r)$ and $\nu_i(r)$ is incompatible with properties of infinite matter, whereas the proper treatment of the problem leads immediately to the channel mixing and the energy density, which is not invariant with respect to rotational and isospin symmetries. This question certainly requires further study, whereas at the moment, a consistent approach can only be obtained by assuming the scalar-isoscalar functions $\pi_i(r)$ and $\nu_i(r)$.

We can now apply derivations presented in Secs. 2.1 and 2.2 to the general case of an arbitrary finite-range local nuclear interaction composed of the standard central, spin-orbit, and tensor terms:

$$\hat{V}(\boldsymbol{r}_{1},\boldsymbol{r}_{2}) = W(r) + B(r)P_{\sigma} - H(r)P_{\tau} - M(r)P_{\sigma}P_{\tau} + \left[P(r) + Q(r)P_{\tau}\right]\boldsymbol{L} \cdot \boldsymbol{S} + \left[R(r) + S(r)P_{\tau}\right]S_{12},$$
(45)

where $r = |\boldsymbol{r}| = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$, and

$$P_{\sigma} = \frac{1}{2}(1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2), \qquad P_{\tau} = \frac{1}{2}(1 + \vec{\tau}_1 \circ \vec{\tau}_2), \tag{46}$$

$$\boldsymbol{L} = -i\hbar\boldsymbol{r}\times\boldsymbol{\partial}, \qquad \boldsymbol{S} = \frac{\hbar}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2), \qquad S_{12} = \frac{3}{r^2}(\boldsymbol{\sigma}_1 \cdot \boldsymbol{r})(\boldsymbol{\sigma}_2 \cdot \boldsymbol{r}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2.$$
(47)

After straightforward but lengthy calculations, one obtains the interaction energy in the form of a local integral, analogous to that for the Skyrme interaction [28, 22, 19],

$$\mathcal{E}^{\text{int}} = \int d^{3}\boldsymbol{R} \sum_{k=0}^{3} \left[C_{t}^{\rho} \rho_{k}^{2} + C_{t}^{\Delta\rho} \rho_{k} \Delta\rho_{k} + C_{t}^{\tau} \left(\rho_{k} \tau_{k} - \boldsymbol{j}_{k}^{2} \right) + C_{t}^{s} \boldsymbol{s}_{k}^{2} + C_{t}^{\Delta s} \boldsymbol{s}_{k} \cdot \Delta \boldsymbol{s}_{k} + C_{t}^{T} \left(\boldsymbol{s}_{k} \cdot \boldsymbol{T}_{k} - \boldsymbol{J}_{abk} \boldsymbol{J}_{abk} \right) + C_{t}^{F} \left(\boldsymbol{s}_{k} \cdot \boldsymbol{F}_{k} - \frac{1}{2} \boldsymbol{J}_{aak} \boldsymbol{J}_{bbk} - \frac{1}{2} \boldsymbol{J}_{abk} \boldsymbol{J}_{bak} \right) + C_{t}^{\nabla s} \left(\boldsymbol{\nabla} \cdot \boldsymbol{s}_{k} \right)^{2} + C_{t}^{\nabla J} \left(\rho_{k} \boldsymbol{\nabla} \cdot \boldsymbol{J}_{k} + \boldsymbol{s}_{k} \cdot \left(\boldsymbol{\nabla} \times \boldsymbol{j}_{k} \right) \right) \right],$$
(48)

where $\rho_k \equiv \rho_{0k}$, $\tau_k \equiv \tau_{0bbk}$, $\mathbf{j}_{ak} \equiv j_{0ak}$, $\mathbf{s}_{ak} \equiv \rho_{ak}$, $\mathbf{T}_{ak} \equiv \tau_{abbk}$, $\mathbf{F}_{ak} \equiv \frac{1}{2}(\tau_{babk} + \tau_{bbak})$, $J_{abk} \equiv j_{abk}$, and $\mathbf{J}_{ak} \equiv \epsilon_{abc} j_{cbk}$ are the standard local densities. The isoscalar (t = 0) and isovector (t = 1) coupling constants C_t correspond to k = 0 and k = 1, 2, 3, respectively.

The coupling constants of the local energy density (48) are related to moments of the interaction in the following way:

$$8 \begin{pmatrix} C_0^{\rho} \\ C_1^{\rho} \\ C_0^{s} \\ C_1^{s} \\ C_1^{s} \end{pmatrix} = \begin{pmatrix} 4 & 2-2-1 \\ 0 & 0-2-1 \\ 0 & 2 & 0-1 \\ 0 & 0 & 0-1 \end{pmatrix} \begin{pmatrix} W_0 + M_{\nu 0}^{00} + \frac{1}{5} M_{\nu 2}^{02} k_F^2 \\ B_0 + H_{\nu 0}^{00} + \frac{1}{5} H_{\nu 2}^{02} k_F^2 \\ H_0 + B_{\nu 0}^{00} + \frac{1}{5} B_{\nu 2}^{02} k_F^2 \\ M_0 + W_{\nu 0}^{00} + \frac{1}{5} W_{\nu 2}^{02} k_F^2 \end{pmatrix},$$
(49)

$$96 \begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^{\pi} \\ C_0^{\pi} \\ C_1^{\pi} \\ C_0^{\pi} \\ C_1^{\pi} \\ C_0^{\Lambda s} \\ C_1^{\Lambda s} \\ C_1^{T} \\ C_0^{T} \\ C_1^{T} \\ C_0^{T} \\ C_1^{T} \\ C_0^{T} \\ C_1^{T} \\ C_1^{T} \\ C_1^{T} \\ C_1^{T} \\ C_1^{F} \\ C_1^{\Gamma} \\ C_1^{\Gamma} \\ C_1^{\Gamma} \\ C_1^{F} \\ C_1^{\nabla s} \\ C_1^{$$

$$24 \begin{pmatrix} C_0^{\nabla J} \\ C_1^{\nabla J} \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} P_2 + Q_{\nu 2}^{01} \\ Q_2 + P_{\nu 2}^{01} \end{pmatrix}.$$
(51)

All the coupling constants of the local energy density (48) depend linearly on the following moments of potentials:

$$X_{n} = \int d^{3} \boldsymbol{r} \, r^{n} X(r) = 4\pi \int d\, r \, r^{n+2} X(r), \qquad (52)$$

$$X_{\nu n}^{ij} = \int d^3 \boldsymbol{r} \, r^n \nu_i(r) \nu_j(r) X(r), = 4\pi \int d\, r \, r^{n+2} \nu_i(r) \nu_j(r) X(r), \tag{53}$$

where X stands for W, B, H, M, P, Q, R, or S.

Again we see that whenever expansions of density matrices, Eqs. (40) and (44), are sufficiently accurate within the ranges of interactions, information about these interactions collapses to a few lowest moments. Short-range details of these interactions are, therefore, entirely irrelevant for low-energy characteristics of nuclear states. This is typical of all physical situations, where scales of interaction and observation are well separated, as specified in the effective field theories. The energy density characterizing the low-energy effects is local and depends on local densities and their derivatives up to second order, whereas the dynamic information is contained in a few coupling constants.

Moreover, the detailed large-r dependence of auxiliary functions $\nu_i(r)$ on position r is also irrelevant, because all that matters are moments (53) which define the coupling constants (49)–(51) describing the exchange energy, and these are influenced only by the small-r properties of functions $\nu_i(r)$. Finally, the most important feature is the k_F or density dependence of $\nu_i(r)$, which determines the density dependence of the coupling constants.

3.2. Local energy density corresponding to the Skyrme force

In general, the number of moments entering Eqs. (49)–(51) is higher than the number of coupling constants, and all the coupling constants are independent. However, it is extremely instructive to check what happens in the vacuum limit of $k_F = 0$. This situation is obtained by setting $\nu_i(r) = 1$, which gives the direct and exchange moments equal to one another, namely, $X_{\nu n}^{ij} = X_n$, and the coupling constants of Eqs. (49)–(51) collapse to:

$$8 \begin{pmatrix} C_0^{\rho} \\ C_1^{\rho} \\ C_0^s \\ C_1^s \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ -1 & -2 \\ -1 & 2 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} W_0 + M_0 \\ B_0 + H_0 \end{pmatrix},$$
(54)

$$96 \begin{pmatrix} C_0^{\Delta\rho} \\ C_1^{\Delta\rho} \\ C_0^{\sigma} \\ C_0^{\sigma} \\ C_1^{\sigma} \\ C_0^{\sigma} \\ C_1^{\sigma} \\ C_0^{\Delta s} \\ C_1^{\sigma} \\ C_1^{\sigma} \\ C_1^{\sigma} \\ C_1^{T} \\ C_0^{T} \\ C_0^{T} \\ C_1^{T} \\ C_0^{F} \\ C_1^{\Gamma} \\ C_0^{\Gamma} \\ C_1^{\nabla s} \\ C_1^{\nabla s} \\ C_1^{\nabla s} \end{pmatrix} = \begin{pmatrix} 7 & 2-2 & 2 & 0 & 0 \\ -1 & -2 & -4 & -2 & 0 & 0 \\ 4 & 8 & -8 & -16 & 0 & 0 \\ -1 & 4 & 2 & -2 & -3 & 0 \\ -1 & 0 & 0 & -2 & 1 & -2 \\ 4 & 0 & -8 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & -4 & -8 \\ 4 & 0 & 0 & 0 & 0 & 12 & 24 \\ 0 & 0 & 0 & 0 & 0 & 12 & 20 \\ 0 & 0 & 0 & 0 & 0 & -9 & 0 \\ 0 & 0 & 0 & 0 & 0 & -9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & -6 \end{pmatrix}$$
(55)

The Negele-Vautherin density matrix expansion applied to the Gogny force

$$24 \begin{pmatrix} C_0^{\nabla J} \\ C_1^{\nabla J} \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \end{pmatrix} \begin{pmatrix} P_2 + Q_2 \end{pmatrix}.$$
(56)

These coupling constants correspond exactly to those obtained for the Skyrme force (see Ref. [19] for the notations and conventions used), namely,

$$t_0 = W_0 + M_0$$
, $t_0 x_0 = B_0 + H_0$, (57)

$$t_1 = -\frac{1}{3}(W_2 + M_2)$$
, $t_1 x_1 = -\frac{1}{3}(B_2 + H_2),$ (58)

$$t_2 = \frac{1}{3}(W_2 - M_2)$$
, $t_2 x_2 = \frac{1}{3}(B_2 - H_2)$, (59)

$$t_e = \frac{1}{15}(S_2 - R_2)$$
, $t_o = \frac{1}{15}(S_2 + R_2)$, (60)

$$W = -\frac{1}{6}(P_2 + Q_2) \qquad . \tag{61}$$

The same relations are also obtained by using in the exchange term the pure Taylor expansions (41); that is, by setting $\pi(r) = 1$, which gives $X_{\pi n}^{ij} = X_n$, and by using the classification of terms as in Eqs. (21)–(23). This second way of obtaining the approximate coupling constants leads to results independent of k_F , which are, of course, identical to those obtained at $k_F = 0$ above.

Relations (54)–(56) imply that the coupling constants of the energy functional (48) are dependent of one another, and in fact, half of them determines the other half. This is exactly the situation encountered when the energy density is calculated for the Skyrme interaction. Then one obtains (cf. Ref. [23]):

$$3\begin{pmatrix} C_0^s\\ C_1^s \end{pmatrix} = \begin{pmatrix} -2 & -3\\ -1 & 0 \end{pmatrix} \begin{pmatrix} C_0^\rho\\ C_1^\rho \end{pmatrix},$$
(62)

$$24 \begin{pmatrix} C_0^{\Delta s} \\ C_1^{\Delta s} \\ C_0^T \\ C_1^T \\ C_0^{\nabla s} \\ C_1^T \\ C_0^{\nabla s} \\ C_1^{\nabla s} \end{pmatrix} = \begin{pmatrix} -12 & -12 & 3 & 9 & 0 & -6 \\ -4 & -4 & 3 & -3 & -2 & 4 \\ 16 & 48 & -4 & 12 & -8 & 0 \\ 16 & -16 & 4 & -12 & 0 & -8 \\ 0 & 0 & 0 & 0 & 0 & -18 \\ 0 & 0 & 0 & 0 & -6 & 12 \end{pmatrix} \begin{pmatrix} C_0^{\Delta \rho} \\ C_1^{\Delta \rho} \\ C_0^T \\ C_0^T \\ C_1^T \\ C_0^F \\ C_1^F \end{pmatrix}, \quad (63)$$
$$C_0^{\nabla J} = 3C_1^{\nabla J}.$$

It is obvious that the above relations among the coupling constants result from an oversimplified approximation to the exchange energy of the finite-range interaction.

We recall here [23, 29] that without the tensor terms, relations (62) and (63) allow us to determine the time-odd coupling constants C_t^s , $C_t^{\Delta s}$, and C_t^T as functions of the time-even coupling constants C_t^{ρ} , $C_t^{\Delta \rho}$, and C_t^{τ} . Since the time-even coupling constants are usually adjusted solely to the time-even observables, the resulting values of the time-odd coupling constants are simply "fictitious" or "illusory", as noted already in Ref. [30]. In a more realistic case of relations (49) and (50), these constraints are no longer valid, and the time-odd properties of the functional are independent of the timeeven properties. This independence requires breaking the link between the Skyrme force

12

Table 1. The NV coupling constants (49)–(50) calculated for the Gogny interaction D1S [17] for the Fermi momenta of $k_F = 0$ and $1.35 \,\mathrm{fm}^{-1}$. First-order coupling constants, C_t^{ρ} and $C_t^{\Delta s}$, are in units of MeV fm³ and the second-order coupling constants, $C_t^{\Delta \rho}$, C_t^{τ} , $C_t^{\Delta s}$, and C_t^{T} , are in units of MeV fm⁵.

	<i>t</i> =	= 0	t = 1		
	$k_F = 0$	$k_{F} = 1.35$	$k_F = 0$	$k_F = 1.35$	
C_t^{ρ}	-665.1658	-600.6156	468.5360	428.3580	
C_t^s	-25.09219	-57.13246	221.7219	230.3318	
$C_t^{\Delta \rho}$	-125.3365	-84.66327	56.65570	31.22042	
C_t^{τ}	236.9227	74.22964	-141.9368	-40.19573	
$C_t^{\Delta s}$	10.72944	-10.25276	58.80425	65.14281	
C_t^T	-80.70182	3.226982	-10.87263	-36.22687	

Table 2. The standard Skyrme-force parameters (57)–(59) calculated for the Gogny interaction D1S [17] for the Fermi momenta of $k_F = 0$ and 1.35 fm^{-1} . These parameters correspond to the time-even sector of the Skyrme functional. Parameter t_0 is in units of MeV fm³; parameters t_1 and t_2 are in units of MeV fm⁵, and parameters x_0, x_1 , and x_2 are dimensionless.

	$k_F = 0$	$k_F = 1.35$
t_0	-1773.775	-1601.642
t_1	984.3584	550.5103
t_2	810.3964	-166.0710
x_0	0.5565848	0.5697973
x_1	0.2488322	0.09972511
x_2	-0.9915809	-0.5517191

and the density functional.

4. Application to the Gogny interaction

In this section, we apply the results of Sec. 3 to the finite-range part of the Gogny interaction D1S [17]. This amounts to calculating moments (52) and (53) of the Gaussian functions with the two ranges of 0.7 and 1.2 fm, which constitute the central part of the Gogny interaction. Because this interaction does not contain any finite-range spin-orbit or tensor force in Eqs. (50) and (51), the moments P, Q, R, and S are set to zero. On the other hand, the zero-range spin-orbit and density-dependent terms of the Gogny interaction are left unchanged.

In Table 1 we show values of coupling constants (49)–(51) calculated in the vacuum $(k_F = 0)$ and at the saturation density $(k_F = 1.35 \,\mathrm{fm}^{-1})$. Similarly, Table 2 shows

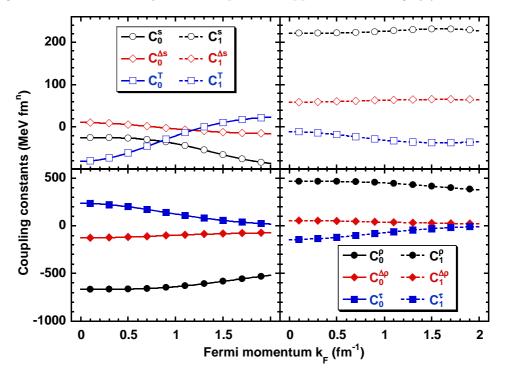


Figure 2. Dependence of the NV coupling constants (49)–(50), calculated for the Gogny interaction D1S [17], on the Fermi momentum k_F . Full and open symbols (lower and upper panels) show values of the time-even and time-odd coupling constants, respectively. Solid and dashed lines (left and right panels) show values of the isoscalar and isovector coupling constants, respectively. Units are specified in the caption to Table 1.

values of the Skyrme-force parameters (57)–(59) corresponding to the time-even coupling constants. In Figs. 2 and 3 we plot the coupling constants and Skyrme-force parameters, respectively, as functions of the Fermi momentum.

The most important observation resulting from values shown in Tables 1 and 2 and Figs. 2 and 3 pertains to a significant density (or k_F) dependence of the coupling constants and Skyrme-force parameters. The strongest dependence is obtained for the isoscalar tensor coupling constant C_0^T . (Note that the central finite-range Gogny interaction induces significant values of the tensor coupling constants C_t^T , even if this force does not contain any explicit tensor term.) Also the kinetic coupling constants C_t^{τ} exhibit a strong density dependence, going almost to zero at $k_F \sim 2 \text{ fm}^{-1}$. We note that the obtained density dependencies do not, in general, follow any power laws. Significantly stronger density dependencies are obtained for the Skyrme-force parameters (Fig. 3). The pole appearing in the parameter x_2 is a consequence of the fact that parameters t_2 and t_2x_2 , derived in Eq. (59), change signs at slightly different values of the Fermi momentum.

Let us now consider the question of whether parameters calculated at any fixed value of the Fermi momentum can provide a reasonable alternative. To analyze this point, we first note that the zero-order coupling constants given in Eq. (49) depend on

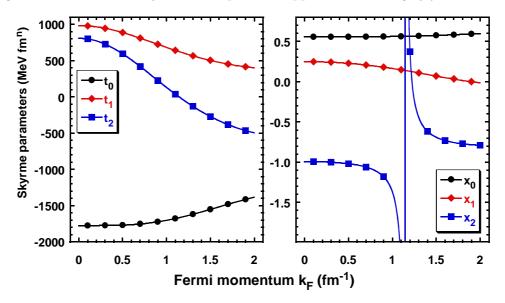


Figure 3. Dependence of the standard Skyrme-force parameters (57)–(59), calculated for the Gogny interaction D1S [17], on the Fermi momentum k_F . These parameters correspond to the time-even sector of the Skyrme functional. Units are specified in the caption of Table 2.

 k_F (i) implicitly through the moments of Eq. (53) and (ii) explicitly through the k_F^2 term, that is,

$$C_t^{\rho}(k_F) = C_{t,0}^{\rho}(k_F) + C_{t,2/3}^{\rho}(k_F)\rho^{2/3},$$
(65)

$$C_t^s(k_F) = C_{t,0}^s(k_F) + C_{t,2/3}^s(k_F)\rho^{2/3},$$
(66)

where we employed the standard association of the Fermi energy with density, namely, $\rho = 2k_F^3/3\pi^2$. Therefore, we can consider fixed values of the coupling constants calculated at a given Fermi momentum k_F^0 as

$$C_t^{\rho}(k_F^0)$$
 and $C_t^s(k_F^0)$, or (67)

$$C_{t,0}^{\rho}(k_F^0), C_{t,2/3}^{\rho}(k_F^0), C_{t,0}^s(k_F^0), \text{ and } C_{t,2/3}^s(k_F^0).$$
 (68)

The second option gives the coupling constants that still depend on the density as $\rho^{2/3}$, in analogy with the standard density-dependent term, which for the Gogny force depends on the density as $\rho^{1/3}$, and which in the present study is alway kept untouched.

In the upper and lower panels of Fig. 4, thin lines show the nuclear matter equations of state (energy per particle in function of density or Fermi momentum) obtained for the coupling constants fixed according to prescriptions (67) and (68), respectively. For comparison, thick lines show the NV results obtained for density-dependent coupling constants. Since in the nuclear matter, the factor multiplying the term $\nu_0(r)\nu_2(r)$ in Eq. (18) vanishes exactly (by construction), the thick lines correspond to the exact Gogny force results.

Equations of state calculated with prescription (68) for fixed values of k_F^0 from 1.35 to 1.98 fm⁻¹ with the step of 0.07 fm⁻¹ completely miss the saturation point. This means

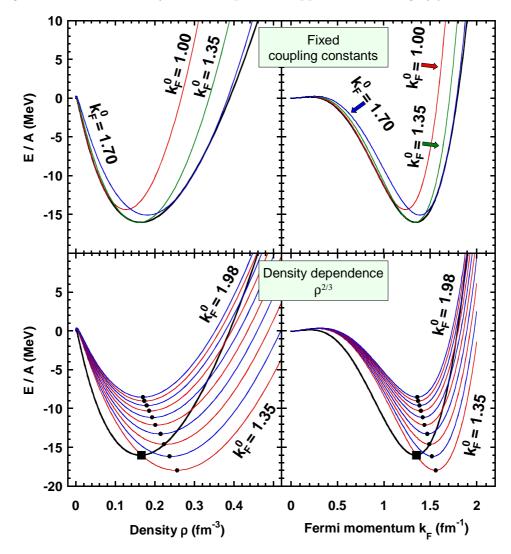


Figure 4. Dependence of the infinite-matter energy per particle on the density (left panels) or Fermi momentum (right panels). Thick lines show the NV results for density-dependent coupling constants. Thin lines show the NV results for fixed coupling constants calculated at the given values of k_F^0 . Upper and lower panels show results for fixed coupling constants (67) and for coupling constants (68) that depend on density as $\rho^{2/3}$. The full square and circles mark the minima of curves.

that Skyrme forces with constant parameters (68) derived by the NV expansion cannot be equivalent to the finite-range Gogny interaction. On the other hand, prescription (67), for fixed value of $k_F^0 = 1.35 \,\mathrm{fm}^{-1}$, reproduces the equation of state fairly well, with some deviations seen only at densities beyond the saturation point. For comparison, we also show results obtained with $k_F^0 = 1$ and $1.7 \,\mathrm{fm}^{-1}$, which fit the equation of state at low and high densities, respectively. These results show that the explicit dependence on the Fermi momentum, which appears in the NV expansion, cannot be used to define the density dependence of the coupling constants.

The full density dependence of all Skyrme-force parameters was recently

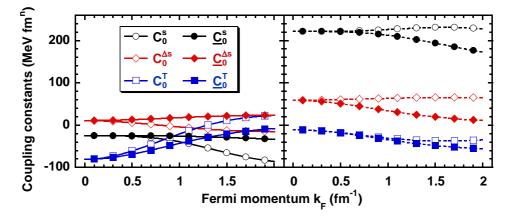


Figure 5. Similar to Fig. 2 except for the time-odd NV coupling constants only. The open symbols show exact results (49)–(50) as plotted in Fig. 2, whereas the full symbols show results inferred from the time-even sector by using Eqs. (62) and (63). Solid and dashed lines (left and right panels) show values of the isoscalar and isovector coupling constants, respectively.

Table 3. Similar to Table 1 except for the time-odd NV coupling constants inferred from the time-even sector by using Eqs. (62) and (63) for a Fermi momentum of $1.35 \,\mathrm{fm}^{-1}$.

	t = 0	t = 1
C_t^s	-27.94756	200.2052
$C_t^{\Delta s}$	20.92673	23.21032
C_t^T	-26.47083	-44.78631

implemented in a spherical self-consistent code [31]. Here we use this implementation to test the results of the NV expansion against the full-fledged solutions known for the Gogny D1S force [32, 33]. In Table 4, we show results obtained for three sets of Skyrme-force parameters:

- S1Sa: fixed parameters given in Table 2 for $k_F^0 = 1.35 \,\mathrm{fm}^{-1}$, used together with the standard D1S parameters [17] of the zero-range spin-orbit ($W = 130 \,\mathrm{MeV} \,\mathrm{fm}^5$) and density-dependent ($t_3 = 1390.60 \,\mathrm{MeV} \,\mathrm{fm}^4$) terms.
- S1Sb: density-dependent parameters shown in Fig. 3, implemented for $\rho = 2k_F^3/3\pi^2$ and used with the standard values of W and t_3 .
- S1Sc: fixed parameters identical to those of S1Sa, but with the value of $t_3 = 1385.35 \text{ MeV fm}^4$ slightly changed, so as to bring the ground-state energy of ²⁰⁸Pb exactly to the true D1S value [33].

Table 4 shows the ground-state energies E of seven doubly magic spherical nuclei, calculated by using the Skyrme-force parameters S1Sa, S1Sb, and S1Sc, and compared with the Gogny-force energies E_G . To facilitate the comparison, we also show relative

differences $\Delta E = (E - E_G)/|E_G|$ in percent along with the corresponding RMS deviations (the last row in Table 4).

On can see that for the Skyrme-force parameters S1Sa and S1Sb, which are directly derived from the Gogny force by using the NV expansion, one obtains the nuclear binding energies smaller by 1–2% as compared to those given by the original Gogny force. This should be considered a very good result, although it cannot compete in precision of describing experimental data with the original Gogny or Skyrme forces, which have parameters directly fitted to experimental binding energies. A simple rescaling of the parameter t_3 brings the RMS deviation to below 0.4%, and makes the Skyrme force S1Sc competitive with most other standard Skyrme parameterizations. At the same time, the analogous RMS deviations obtained for the neutron and proton radii are 0.20 and 0.30% (S1Sa), 1.01 and 0.94% (S1Sb), and 0.26 and 0.44% (S1Sc), respectively.

We note here in passing that in this study we defined the S1Sb parameter set by considering the density-dependent coupling constants $C_t^{\Delta\rho}$ (Fig. 3) that multiply densities $\rho_t \Delta \rho_t$. An attempt of using the same coupling constants along with densities $-(\nabla \rho_t)^2$ gives, in fact, the RMS deviations of binding energies (5.34%), neutron radii (2.44%), and proton radii (2.27%), which are significantly worse than those of S1Sb (Table 4). This shows that the prescription to replace in EDFs integrated by parts (see Refs. [29, 31]) the Fermi momentum by $\rho = 2k_F^3/3\pi^2$ may lead to significantly different results. Another recipy is to associate k_F with density before taking products of the two density matrices which means both of the above terms will be active. However in order to have a better correspondence with the traditional Skyrme functionals we have made this association after taking the product.

It is not our purpose here to propose that any of the Skyrme-force parameterizations introduced in the present work are better solutions to the problem of finding the best agreement with data. It is already known that within the standard second-order Skyrme-force parameterizations, a spectroscopic-quality [2] force cannot be found [34]. Nevertheless, it is gratifying to see that the NV expansion allows us to bridge the gap between the non-local and quasi-local EDFs, or between the finite-range and zero-range effective forces. A more quantitative discussion of the accuracy of the NV expansion will be possible by considering higher-order NV expansions [35].

Finally, in Fig. 5 we compare the time-odd coupling constants calculated by using Eqs. (49) and (50) with those corresponding to the Skyrme-force parameters; that is, calculated by using Eqs. (62) and (63). Similarly, Table 3 lists the numerical values of the Skyrme-force time-odd coupling constants. As one can see, differences between both sets of the time-odd coupling constants, shown in Fig. 5 with open and full symbols, are quite substantial. These results illustrate the fact that the NV expansion of the Gogny force leads to the Skyrme functional and not to the Skyrme force.

We conclude this section by noting that functions $\pi_i(r)$ approximated by Gaussians (see Eqs. (36)–(38) and Fig. 1) lead to the coupling constants and Skyrme-force parameters, which, when plotted in the scales of Figs. 2, 3, and 5, are indistinguishable from those presented in these figures.

force energies E_G . All energies are in MeV.							
	D1S [33]	S1Sa		S1Sb		S1Sc	
	E_G	E	ΔE	E	ΔE	E	ΔE
^{40}Ca	-342.689	-335.312	2.15%	-340.642	0.60%	-339.369	0.97%
$^{48}\mathrm{Ca}$	-414.330	-409.118	1.26%	-410.698	0.88%	-414.213	0.03%
56 Ni	-481.111	-473.497	1.58%	-471.970	1.90%	-479.843	0.26%
⁷⁸ Ni	-637.845	-630.447	1.16%	-629.066	1.38%	-638.837	-0.16%
$^{100}\mathrm{Sn}$	-828.024	-814.568	1.63%	-814.896	1.59%	-826.453	0.19%
$^{132}\mathrm{Sn}$	-1101.670	-1086.272	1.40%	-1086.867	1.34%	-1101.445	0.02%
$^{208}\mathrm{Pb}$	-1637.291	-1612.634	1.51%	-1617.419	1.21%	-1637.291	0.00%
RMS	n.a.	n.a.	1.56%	n.a.	1.33%	n.a.	0.39%

Table 4. Binding energies E of seven doubly magic nuclei calculated by using the Skyrme-force parameters S1Sa, S1Sb, and S1Sc (see text) compared with the Gogny-force energies E_G . All energies are in MeV.

5. Conclusions

In the present study, we derived a set of compact expressions giving the local energy density corresponding to the Kohn-Sham potential energy for an arbitrary local finiterange central, spin-orbit, and tensor interactions. The method is based on the Negele-Vautherin density matrix expansion augmented by the odd-power gradient terms fulfilling the gauge-invariance condition. The coupling constants of the local energy density depend on a set of moments of the interaction conforming to the ideas of the effective theory. The expansion is based on the separation of scales between the range of the force and space characteristics of the one-body density matrix. It leads to a representation of dynamical properties of the system in terms of a set of numbers, whereby complicated short-range characteristics of effective interactions remain unresolved.

We pointed out the fact that to correctly describe the exchange properties of the functional, proper treatment of the density matrix in the nonlocal direction is essential. This immediately leads to the local energy density that does not correspond to an averaged zero-range pseudopotential. Therefore, the Negele-Vautherin expansion performed up to NLO leads to the Skyrme functional and not to the Skyrme force. Within this formalism, the only way to define the Skyrme force is to match it to the time-even properties of the non-local functional, disregarding those pertaining to the time-odd channel.

We applied the general NLO expressions to the case of the central finite-range part of the Gogny interaction. It turns out that the obtained coupling constants of the local Skyrme functional quite strongly depend on the Fermi momentum or on the density. Nevertheless, the equation of state obtained for fixed coupling constants, calculated at the saturation point of $k_F = 1.35 \,\mathrm{fm}^{-1}$, fairly well reproduces the exact Gognyforce result. On the other hand, partial density dependence, inferred from the explicit dependence of the coupling constants on k_F , gives very unsatisfactory results.

By solving the self-consistent equations with the Skyrme-force parameters derived from the Gogny force, one obtains an excellent agreement (up to 1-2%) of binding energies and radii with those corresponding to the true Gogny force. This shows that the ideas of the effective theory, whereby the finite-range nuclear forces are sufficiently short-range to be replaced by contact quasi-potentials, are applicable to low-energy nuclear observables.

We also discussed properties of the one-body density matrix for the spin and isospin polarized infinite nuclear matter. In this case, one obtains the nonlocal densities with mixed spin-isospin channels. As a result, the local energy density is not invariant but covariant with respect to rotational and isospin symmetries; that is, it does not have the form of the standard Skyrme functional. It means that the standard Negele-Vautherin expansion can only be performed for unpolarized densities.

Interesting comments by Thomas Duguet are gratefully acknowledged. This work was supported by the Polish Ministry of Science and Higher Education under Contract No. N N 202 328234, by the Academy of Finland and University of Jyväskylä within the FIDIPRO program, and by the U.S. Department of Energy under Contract Nos. DE-FC02-09ER41583 (UNEDF SciDAC Collaboration) and DE-FG02-96ER40963 (University of Tennessee).

Appendix A. Spin and isospin polarized infinite nuclear matter

Let us consider the infinite nuclear matter with spin and isospin polarizations, which is described by the one-body Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta - \boldsymbol{H} \cdot \boldsymbol{\sigma} - \vec{\lambda} \circ \vec{\tau}, \qquad (A.1)$$

where $\boldsymbol{\sigma}$ and \boldsymbol{H} are the space vectors of spin Pauli matrices and spin-polarization Lagrange multipliers, respectively, and $\vec{\tau}$ and $\vec{\lambda}$ are the isovectors of the analogous isospin Pauli matrices and isospin-polarization Lagrange multipliers, whereas the dot "·" (circle "o") denotes the scalar (isoscalar) product. Each eigenstate of Hamiltonian (A.1) is a Slater determinant that depends on the orientations of the Lagrange multipliers \boldsymbol{H} and $\vec{\lambda}$ in the space and isospace, respectively. However, since the kinetic energy is scalar and isoscalar, we can arbitrarily fix these orientations to \boldsymbol{H}_z and $\vec{\lambda}_3$, which gives the nonlocal densities for spin-up and spin-down ($\boldsymbol{\sigma} = \pm 1$) neutrons and protons ($\boldsymbol{\tau} = \pm 1$) in the form,

$$\bar{\rho}_{\sigma\tau}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \int_{|\boldsymbol{k}| < k_{F, \sigma\tau}} \mathrm{d}^3 \boldsymbol{k} \, e^{i \boldsymbol{k} \cdot (\boldsymbol{r}_1 - \boldsymbol{r}_2)} = \bar{\rho}_{\sigma\tau} \bar{\pi}_{\sigma\tau}(\boldsymbol{r}). \tag{A.2}$$

The system simply separates into four independent Fermi spheres for spin-up and spindown neutrons and protons, with four constant densities $\bar{\rho}_{\sigma\tau}$, whereas the dependence on The Negele-Vautherin density matrix expansion applied to the Gogny force

the relative position vector \mathbf{r} is given by four scalar functions $\bar{\pi}_{\sigma\tau}(r)$ [compare Eq. (30)],

$$\bar{\pi}_{\sigma\tau}(r) = \frac{3j_1(k_{F,\sigma\tau}r)}{k_{F,\sigma\tau}r}.$$
(A.3)

We note that the spin-isospin indices $\sigma\tau$ pertain here to the preselected quantization axis defined by the chosen directions of \boldsymbol{H} and $\vec{\lambda}$, which define an "intrinsic" reference frame. In this reference frame, densities are marked with a bar symbol.

The ground state of the system is obtained by filling the four Fermi spheres up to the common Fermi energy ϵ_F ,

$$\epsilon_F = \epsilon_{F,\sigma\tau} = \frac{\hbar^2 k_{F,\sigma\tau}^2}{2m} - \boldsymbol{H}_z \sigma - \vec{\lambda}_3 \tau, \qquad (A.4)$$

which defines the four Fermi momenta $k_{F,\sigma\tau}$. Finally, by varying ϵ_F , one obtains systems with different total densities $\rho = \sum_{\sigma\tau} \bar{\rho}_{\sigma\tau}$.

It is, of course, clear that for the asymmetric and polarized infinite nuclear matter, the density matrix of Eq. (39) is diagonal in spin and isospin,

$$\bar{\rho}(\boldsymbol{r}_1\sigma_1\tau_1, \boldsymbol{r}_2\sigma_2\tau_2) = \bar{\rho}_{\sigma_1\tau_1}(\boldsymbol{r}_1, \boldsymbol{r}_2)\delta_{\sigma_1\sigma_2}\delta_{\tau_1\tau_2}$$
(A.5)

and thus the nonlocal densities $\bar{\rho}_{\mu k}(\mathbf{r}_1, \mathbf{r}_2)$ have non-zero components only for $\mu = 0$ or z and k = 0 or 3, that is,

where we have abbreviated the indices of $\sigma\tau$ just to their signs. After expressing the right-hand side of this equation in terms nonlocal densities (A.2), one obtains:

$$\begin{pmatrix} \bar{\rho}_{00}(\boldsymbol{r}_{1},\boldsymbol{r}_{2})\\ \bar{\rho}_{03}(\boldsymbol{r}_{1},\boldsymbol{r}_{2})\\ \bar{\rho}_{z0}(\boldsymbol{r}_{1},\boldsymbol{r}_{2})\\ \bar{\rho}_{z3}(\boldsymbol{r}_{1},\boldsymbol{r}_{2}) \end{pmatrix} = \begin{pmatrix} \bar{\pi}_{00}(r) & \bar{\pi}_{03}(r) & \bar{\pi}_{z0}(r) & \bar{\pi}_{z3}(r) \\ \bar{\pi}_{00}(r) & \bar{\pi}_{z3}(r) & \bar{\pi}_{z0}(r) & \bar{\pi}_{z0}(r) \\ \bar{\pi}_{z0}(r) & \bar{\pi}_{z3}(r) & \bar{\pi}_{00}(r) & \bar{\pi}_{03}(r) \\ \bar{\pi}_{z3}(r) & \bar{\pi}_{z0}(r) & \bar{\pi}_{03}(r) & \bar{\pi}_{00}(r) \end{pmatrix} \begin{pmatrix} \bar{\rho}_{00} \\ \bar{\rho}_{03} \\ \bar{\rho}_{z0} \\ \bar{\rho}_{z0} \\ \bar{\rho}_{z3} \end{pmatrix}, \quad (A.7)$$

where functions $\bar{\pi}_{\mu k}(r)$ are defined similarly as in Eq. (A.6), namely,

Already here we see the main problem: for the spin and isospin polarized systems, the spin-isospin channels of nonlocal densities $\bar{\rho}_{\mu k}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ in Eq. (A.7) are linear combinations of the spin-isospin channels of local densities $\bar{\rho}_{\mu k}$; that is, the spin-isospin channels become mixed.

To make the preceding result even more clear, we note that the spin-isospin directions of the Lagrange multipliers \boldsymbol{H} and $\vec{\lambda}$ can be arbitrarily varied and the spin-isospin directions of the nonlocal densities $\rho_{\mu k}(\boldsymbol{r}_1, \boldsymbol{r}_2)$, local densities $\rho_{\mu k}$, and functions

 $\pi_{\mu k}(r)$ are always aligned with those of the Lagrange multipliers. Therefore, we can use the directions of the local densities instead of those pertaining to the Lagrange multipliers. By using the standard densities [19] in the (i) scalar-isoscalar channel $(\rho = \rho_{00})$, (ii) vector-isoscalar channel ($\mathbf{s}_{\mu} = \rho_{\mu 0}$, for $\mu = x, y, z$), (iii) scalar-isovector channel ($\vec{\rho}_k = \rho_{0k}$, for k = 1, 2, 3), and (iv) vector-isovector channel ($\vec{s}_{\mu k} = \rho_{\mu k}$, for $\mu = x, y, z$ and k = 1, 2, 3), we then define functions $\pi(r)$ in the four channels as,

$$\begin{aligned}
\pi(r) &= \bar{\pi}_{00}(r), \\
\pi(r) &= \frac{s}{|s|} \bar{\pi}_{03}(r), \\
\vec{\pi}(r) &= \frac{\vec{\rho}}{|\vec{\rho}|} \bar{\pi}_{z0}(r), \\
\vec{\pi}(r) &= \frac{\vec{s}}{|\vec{s}|} \bar{\pi}_{z3}(r).
\end{aligned} \tag{A.9}$$

Here, the "intrinsic" functions $\bar{\pi}_{\mu k}(r)$ do not depend on the spin-isospin directions; that is, they are defined by the following Fermi energies,

$$\epsilon_F = \epsilon_{F,\sigma\tau} = \frac{\hbar^2 k_{F,\sigma\tau}^2}{2m} - |\boldsymbol{H}|\sigma - |\vec{\lambda}|\tau.$$
(A.10)

Finally, definitions (A.9) allow us to present densities in the "laboratory" reference frame as [compare Eq. (A.7)],

$$\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho \,\pi(r) + \vec{\rho} \circ \vec{\pi}(r) + \mathbf{s} \cdot \mathbf{\pi}(r) + \vec{\mathbf{s}} \cdot \circ \vec{\mathbf{\pi}}(r), \tag{A.11}$$

$$\vec{\rho}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \vec{\rho} \,\pi(r) + \rho \,\vec{\pi}(r) + \vec{\boldsymbol{s}} \cdot \boldsymbol{\pi}(r) + \boldsymbol{\boldsymbol{s}} \cdot \vec{\boldsymbol{\pi}}(r), \tag{A.12}$$

$$\boldsymbol{s}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \boldsymbol{s}\,\pi(r) + \boldsymbol{\vec{s}}\circ\,\boldsymbol{\vec{\pi}}(r) + \rho\,\boldsymbol{\pi}(r) + \boldsymbol{\vec{\rho}}\circ\boldsymbol{\vec{\pi}}(r), \tag{A.13}$$

$$\vec{\boldsymbol{s}}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \vec{\boldsymbol{s}} \,\pi(r) + \boldsymbol{s} \,\vec{\pi}(r) + \vec{\rho} \,\boldsymbol{\pi}(r) + \rho \,\vec{\boldsymbol{\pi}}(r). \tag{A.14}$$

Note that the same scalar-isoscalar function $\pi(r)$ multiplies all local densities in the first terms of Eqs. (A.11)–(A.14). Therefore, the postulate of using different functions in different channels [11] is not compatible with the results obtained for the polarized nuclear matter.

Again we see that the spin-isospin channels of nonlocal densities are mixed, namely, local densities in all channels contribute to every channel in the nonlocal density. As a consequence, the energy density is not invariant but only covariant with respect to the spin-isospin rotations (see the discussion in the Appendix A of Ref. [5]). Therefore, the NV expansion performed in the polarized nuclear matter does not lead to the standard local functional of Eq. (48). On the other hand, derivation in the unpolarized nuclear matter corresponds to all functions $\bar{\rho}_{\sigma\tau}(r)$ equal to one another, which leads to vanishing functions $\vec{\pi}(r)$, $\pi(r)$, and $\vec{\pi}(r)$. Then, in Eqs. (A.11)–(A.14), only the first terms survive and the spin-isospin channels are not mixed. Such a situation corresponds to postulating a channel-independent function $\pi(r)$, which we employed in Sec. 3.

- [1] G.F. Bertsch, D.J. Dean, and W. Nazarewicz, SciDAC Review 6, Winter 2007, p. 42.
- [2] M. Zalewski, J. Dobaczewski, W. Satuła, and T.R. Werner, Phys. Rev. C 77, 024316 (2008).
- [3] W.H. Long, P. Ring, Nguyen Van Giai, and J. Meng, arXiv:0812.1103.
- [4] T. Lesinski, M. Bender, K. Bennaceur, T. Duguet, and J. Meyer, Phys. Rev. C 76, 014312 (2007).
- [5] B.G. Carlsson, J. Dobaczewski, and M. Kortelainen, Phys. Rev. C 78, 044326 (2008).

- [6] M. Bender, K. Bennaceur, T. Duguet, P.-H. Heenen, T. Lesinski, and J. Meyer, Phys. Rev. C 80, 064302 (2009).
- [7] M. Zalewski, P. Olbratowski, and W. Satuła, arXiv:1002.2051.
- [8] N. Chamel, S. Goriely, and J.M. Pearson, Nucl. Phys. A 812, 72 (2008).
- [9] P. Finelli, N. Kaiser, D. Vretenar, and W. Weise, Nucl. Phys. A770, 1 (2006).
- [10] S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. A 39, 219 (2009).
- [11] B. Gebremariam, T. Duguet, and S.K. Bogner, arXiv:0910.4979.
- [12] J.W. Negele and D. Vautherin, Phys. Rev. C 5, 1472 (1972).
- [13] V.B. Soubbotin and X. Viñas, Nuc. Phys A665, 291 (2000).
- [14] V.B. Soubbotin, V.I. Tselyaev, and X. Viñas, Phys. Rev. C 67, 014324 (2003).
- [15] G.P. Lepage, Lectures given at the VIII Jorge Andre Swieca Summer School (Brazil, 1997), nuclth/9706029.
- [16] J. Dechargé and D. Gogny, Phys. Rev. C21, 1568 (1980).
- [17] J.-F. Berger, M. Girod, and D. Gogny, Comput. Phys. Comm. 63, 365 (1991).
- [18] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. 75, 121 (2003).
- [19] E. Perlińska, S.G. Rohoziński, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. C 69, 014316 (2004).
- [20] J. Dobaczewski, in *Trends in Field Theory Research*, ed. O. Kovras (Nova Science Publishers, New York, 2005) p. 157, nucl-th/0301069.
- [21] W. Kohn and L.J. Sham, Phys. Rev. 140, A1133 (1965).
- [22] Y.M. Engel, D.M. Brink, K. Goeke, S.J. Krieger, and D. Vautherin, Nucl. Phys. A249, 215 (1975).
- [23] J. Dobaczewski and J. Dudek, Phys. Rev. C52, 1827 (1995); C55, 3177(E) (1997).
- [24] J.C. Slater, Phys. Rev. 81, 385 (1951).
- [25] O. Bokanowski and N.J. Mauser, Math. Models Methods Appl. Sci. 9, 941 (1999).
- [26] C. Titin-Schnaider and P. Quentin, Phys. Lett. 49B, 397 (1974).
- [27] J. Skalski, Phys. Rev. C63, 024312 (2001).
- [28] H. Flocard, Thesis 1975, Orsay, Série A, N^o 1543.
- [29] J. Dobaczewski and J. Dudek, Acta Phys. Pol. B27, 45 (1996).
- [30] J.W. Negele, in Effective Interactions and Operators in Nuclei, Lecture Notes in Physics 40 (Springer, Berlin, 1975), p. 270.
- [31] M. Kortelainen *et al.*, to be published.
- [32] J.-P. Delaroche, M. Girod, J. Libert, H. Goutte, S. Hilaire, S. Péru, N. Pillet, and G.F. Bertsch, Phys. Rev. C 81, 014303 (2010).
- [33] http://www-phynu.cea.fr/HFB-5DCH-table.htm.
- [34] M. Kortelainen, J. Dobaczewski, K. Mizuyama, and J. Toivanen, Phys. Rev. C 77, 064307 (2008).
- [35] B.G. Carlsson *et al.*, to be published.