# Skyrme functional from a three-body pseudopotential of second order in gradients: Formalism for central terms

J. Sadoudi,[1,2,3] T. Duguet,[1,4] J. Meyer,[5] and M. Bender[2,3]

[1]*CEA-Saclay DSM/Irfu/SPhN, F-91191 Gif sur Yvette Cedex, France*

[2]*Université Bordeaux, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

[3]*CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

[4]*National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA*

[5]*Université de Lyon, F-69003 Lyon, France; Université Lyon 1, 43 Boulevard du 11 Novembre 1918, F-69622 Villeurbanne cedex, France; and CNRS-IN2P3, UMR 5822, Institute de Physique Nucléaire de Lyon*

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**Background:** In one way or another, all modern parametrizations of the nuclear energy density functional (EDF) do not respect the exchange symmetry associated with Pauli's principle. It has been recently shown that this practice jeopardizes multireference (MR) EDF calculations by contaminating the energy with spurious self-interactions that, for example, lead to finite steps or even divergences when plotting it as a function of collective coordinates [J. Dobaczewski *et al.*, Phys. Rev. C **76**, 054315 (2007); D. Lacroix *et al.*, Phys. Rev. C **79**, 044318 (2009)]. As of today, the only viable option to bypass these pathologies is to rely on EDF kernels that enforce Pauli's principle from the outset by strictly and exactly deriving from a *genuine*, i.e., density-independent, Hamilton operator.

**Purpose:** The objective is to build cutting-edge parametrizations of the EDF kernel deriving from a pseudopotential that can be safely employed in symmetry restoration and configuration mixing calculations.

**Methods:** We wish to develop the most general Skyrme-like EDF parametrization containing linear, bilinear, and trilinear terms in the density matrices with up to two gradients, under the key constraint that it derives strictly from an effective Hamilton operator. While linear and bilinear terms are obtained from a standard one-body kinetic energy operator and a (density-independent) two-body Skyrme pseudopotential, the most general three-body Skyrme-like pseudopotential containing up to two gradient operators is constructed to generate the trilinear part. The present study is limited to central terms. Spin orbit and tensor will be addressed in a forthcoming paper.

**Results:** The most general central Skyrme-type zero-range three-body interaction is built up to second order in derivatives. The complete trilinear EDF, including time-odd and $T = 1$ pairing parts, is derived along with the corresponding normal and anomalous fields entering the Hartree-Fock-Bogoliubov equations of motion. Its building blocks are the same local densities that the standard Skyrme functional is constructed from. The central three-body pseudopotential is defined out of six independent parameters. Expressions for bulk properties of symmetric, isospin-asymmetric, and spin-polarized homogeneous nuclear matter, as well as associated Landau parameters, are given.

**Conclusions:** This study establishes a first step towards a new generation of nuclear EDFs that respect Pauli's principle and that can be safely used in predictive and spuriosity-free SR and MR EDF calculations.

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## I. INTRODUCTION

Methods based on an energy density functional (EDF) are at present the only available microscopic tools to address all medium- and heavy-mass nuclei within one consistent framework. They allow for a unified description of many phenomena in nuclear structure and dynamics over the entire chart of nuclei [1–4]. The EDF method coexists on two levels: One level is usually characterized as "mean-field" and frequently identified with Hartree-Fock (HF), HF + BCS, and Hartree-Fock-Bogoliubov (HFB) methods. The second level is often qualified as "beyond mean-field," a notion used for both the random phase approximation (RPA) and its extensions on the one hand and symmetry restorations and the generator coordinate method (GCM) on the other hand. Throughout this article we refer to mean-field methods as *single-reference* (SR) EDF methods, as all densities entering the kernel are constructed from a single product state. Symmetry restoration and GCM are denoted as *multireference* (MR) EDF methods, as the densities entering the kernel are constructed from pairs of product states belonging to a large set of reference states. An overview over the SR- and MR-EDF formalisms can be found in Ref. [5].

In the literature, one finds nuclear EDF kernels of many different forms, being either local or nonlocal and being either relativistic or nonrelativistic. For the purpose of the present study, there is a third categorization of energy functionals that has to be made that concerns the handling of Pauli's exclusion principle. Its most obvious consequence, namely that all single-particle levels are occupied by at most one nucleon, is always satisfied at the level of individual densities used to build the EDF given that one-body density matrices are explicitly computed from antisymmetric product states of either Slater or Bogoliubov type. However, a violation of Pauli's principle may arise when multiplying two or even more such densities

 

to build bilinear, trilinear, etc., terms in the EDF kernel. Terms of a given power in the density matrices have to combine in a very specific way to cancel out the unphysical interaction of a particle with itself or that of a pair of particles with itself [6–11] and to provide an antisymmetric residual interaction [8].

As of today, the only practical way to enforce all aspects of exchange symmetry is to set up the off-diagonal EDF kernel as the matrix elements of a *genuine*, i.e., density-independent, operator between two product states of Bogoliubov type, taking all exchange and pairing terms into account without any approximation or simplification. Such an effective Hamilton operator is typically meant to be the sum of the kinetic energy operator and a pseudopotential. By virtue of the generalized Wick theorem [12–14], the resulting kernel takes the form of a specific functional of one-body transition density matrices built from the two product states. In what follows, such EDF kernels are said to be *pseudopotential based*.

None of the modern, e.g., Skyrme, Gogny, or relativistic, parametrizations belong to this category of pseudopotential-based kernels. The most remote are kernels directly built on the level of combinations of one-body densities or density matrices without making reference to any underlying operator. In what follows, such EDF kernels are said to belong to the category of *general functionals*. In that case, the form of the EDF kernel is typically constrained by all symmetries of the nuclear Hamiltonian [15] but the exchange symmetry. Frequently used examples are the EDF kernels constructed by Fayans and collaborators [16] and the Barcelona-Catania-Paris parametrization [17].

The large majority of existing parametrizations, however, falls between the pseudopotential-based kernels and the general functionals. We denote those as *hybrid* parametrizations. The paradigm here consists of relating the interaction part of the EDF kernel to the expectation value of a *density-dependent*, and therefore state-dependent, effective interaction, keeping all exchange and pairing terms. Prominent examples are the Gogny family of parametrizations [18–21] and those derived from the density-dependent M3Y interaction by Nakada [22]. Also, very few Skyrme parametrizations were constructed along this line; examples are SkP [23], SkS1-SkS4 [24], SkE2, and SkE4 [25]. For most of the other Skyrme parametrizations, the link to the density-dependent effective interactions is only kept for some terms, but not for all.[1] First of all, the particle-hole (i.e., normal) and particle-particle (i.e., pairing or anomalous) parts of almost all Skyrme parametrizations are entirely unrelated. As a matter of fact, only the particle-hole part of the kernel is usually referred to as the *Skyrme EDF*, which is then combined with the pairing EDF of the respective author's preference. Second, specific exchange terms in the energy functional are often modified or simply set to zero for reasons of phenomenology. The latter practice mainly concerns spin-orbit and spin-tensor terms [3,4,27–30] and the so-called time-odd terms entering the particle-hole part of the EDF [3,4,26,31–34]. Such modifications bring the functionals close to the spirit of the general functionals.

Among the existing functionals, Gogny or M3Y-based parametrizations are the closest to the concept of a pseudopotential-based EDF kernel. Still, from the point of view of Pauli's exclusion principle, they are fundamentally different given that the exchange symmetry is not respected by the density-dependent term. In that respect, general and hybrid functionals all belong to the same category. Indeed, it makes no difference that the exchange symmetry is broken by just one term in the functional or by many of them.

In spite of the many successes of general and hybrid functionals, there are good reasons to revisit pseudopotential-based EDF kernels. Indeed, it was recently demonstrated [6,7] that any breaking of Pauli's principle contaminates the EDF kernel with spurious contributions that can jeopardize MR-EDF calculations [35–40]. The problem manifests itself through finite steps and/or even divergences when plotting the symmetry-restored energy as a function of a collective coordinate [7,35,39–41]. Even more striking, contaminated kernels can lead to *nonzero* (non-normalized) energies when restoring good *negative* particle number [7], which is impossible for projected operator matrix elements. Generally speaking, the results of MR-EDF calculations based on hybrid or general functionals depend on how the sums and/or integrals over the collective coordinates are discretized. Decreasing the step sizes often amplifies the contamination with spurious contributions as they become better resolved [7]. In addition, using nonanalytical functions for the density dependence, such as the popular $\rho^{\alpha}(\vec{r})$ dependence, introduces a further problem into the MR EDF frame by making the EDF kernel a multivalued function of the collective coordinates [41].

In the use of the Gogny functional, whose only breaking of Pauli's principle relates to its density-dependent term, a special treatment of the latter has been used in some MR calculations to bypass the problem invoked above [38,42]. Besides not being consistent with the definition of the rest of the EDF kernel, this recipe cannot be expected to work for all configuration mixings of interest [43].

Isospin and angular-momentum projected MR EDF calculations of Refs. [44,45] employ a kernel that derives strictly from a simple two-body Skyrme pseudopotential without density dependence. In doing so, the pathologies alluded to above are fully avoided by construction. As these calculations neglect pairing correlations altogether, it is of no concern that the two-body Skyrme pseudopotentials employed fail to provide reasonable pairing correlations. To the best of our knowledge, there has been only one recent attempt by us to construct a Skyrme pseudopotential *without any density dependence* that is meant to be used in both the particle-hole and the particle-particle parts of the EDF [46]. This was achieved by adding gradientless three- and four-body contact terms to a standard velocity-dependent two-body Skyrme pseudopotential. However, the best parameter fit generated

[1] As a relic of the historical origin of the Skyrme effective interaction as a pseudopotential, general or hybrid Skyrme parametrizations are frequently defined in terms of the parameters of a density-dependent effective interaction, to which is added a list modifications of the EDF generated by an actual density-dependent two-body effective interaction [3,4]. This ambivalence of the Skyrme EDF and the representation of its parameters is a source of confusion and frequently provokes its inconsistent use in RPA and in the calculation of infinite nuclear-matter properties [3,10,26].

in this way did, by far, not match the performance of modern hybrids or general Skyrme parametrizations. As a matter of fact, it turned out to be impossible to have simultaneously appropriate empirical nuclear-matter properties, attractive pairing and stability against infinite- and finite-size instabilities [46]. This limitation points to the necessity of introducing additional higher-order terms.

Aiming at a strict pseudopotential-based approach, there are two possible directions of enriching a Skyrme-like parametrization. One is to include terms containing a higher number of gradient operators in the two-body pseudopotential. Terms of this kind have already been suggested in the seminal papers by Skyrme [47–49]. Their most general form has recently been worked out systematically up to sixth order [50]. The associated EDF kernel remains strictly bilinear, but is expressed in terms of a larger set of local densities invoking more derivatives than is the case for the standard Skyrme functional. An alternative is to stick to the second order in gradients, but to consider many-body operators, e.g., velocity-dependent three-body interactions. The associated EDF kernel can still be expressed in terms of the same set of local densities as the bilinear one deriving from the standard Skyrme two-body pseudopotential, but contains higher-order polynomials.

The number of contributions to infinite nuclear-matter properties that originate from fourth-order gradient operators in the two-body pseudopotential is much smaller than the number of those originating from second-order terms [51]. In the end, one mainly obtains a multitude of contributions that influence surface properties of finite nuclei. Consequently, many-body terms might offer an easier access to a decoupling of nuclear-matter properties from pairing and instabilities. This is thus the route we wish to pursue in the present work. Ultimately, one may, of course, combine both types of extensions. However, and although those two extensions are systematic, one should note that no strong formal argument exists at this point to declare one to be superior to the other. Even though "naturalness" can be invoked [52] in the context of Skyrme EDF parametrizations, this concept has not yet been proven to provide a truly meaningful and systematic power counting at finite density.[2] A formal framework that establishes a hierarchy of terms in the EDF is currently missing and clearly deserves attention in the future.

Skyrme-type contact three-body pseudopotentials containing up to two gradient operators have been already used in the past [25,54–63]. None of these developments has been systematic and aimed at the complete set of possible terms. Also, not all of these studies have combined their three-body pseudopotential with a Skyrme-type two-body interaction. Additionally, all these studies limited themselves to central interactions, and none of them aimed at the most general structure. Only time-even contributions to the normal part of the resulting EDF were discussed, if at all, and spherical symmetry was assumed and exploited in all cases to simplify the resulting energy functional and one-body fields.

The aim of the present study is to supersede the existing body of work in several respects.

(1) Constructing the most general contact three-body pseudopotential containing up to two gradient operators. In the present study, we focus on its *central* part, i.e., on terms that do not couple the orientation of spins and momenta. Central terms are the most important ones for our goal of replacing the traditional density-dependence of the standard Skyrme EDF. At the SR-EDF level, only central terms contribute to properties of nonpolarized infinite nuclear matter and therefore to bulk properties of even-even nuclei. By contrast, three-body spin-orbit and tensor interactions produce terms that allow for the fine-tuning of the nucleon-number dependence of shell structure. These will be discussed elsewhere [64].
(2) Deriving the complete trilinear EDF kernel from the three-body pseudopotential, i.e., providing time-even and time-odd contributions to the normal part of the EDF along with the complete pairing part, in a form that is suited for symmetry-unrestricted SR and MR calculations. We limit ourselves to the case where single-particle states, and consequently the one-body density matrices, retain a good neutron or proton character.
(3) Deriving the expressions of the corresponding one-body fields entering the HFB Hamiltonian matrix.
(4) Computing infinite nuclear-matter properties and associated Landau parameters.

As will become clear below, there exists a large number of possible central three-body contact operators that respect symmetries of the exact nuclear Hamiltonian. Only a small subset of these, however, provide linearly independent contributions to the EDF kernel. To find a complete irreducible set of such operators, we proceed in the following way.

(1) Write all possible operator structures consistent with symmetries of the underlying nuclear Hamiltonian.
(2) Derive the corresponding EDF kernel.
(3) Perform the singular-value decomposition (SVD) of the matrix expressing the coupling constants multiplying each contribution to the EDF kernel in terms of the parameters entering the underlying pseudopotential and determine the number of independent parameters defining the latter.

Owing to the large number of possible three-body terms, the above tasks cannot be accomplished safely on the basis of pen and paper. Consequently, a formal algebra code has been developed to carry them out [65]. The code also derives contributions to normal and anomalous one-body potentials, bulk properties of infinite nuclear matter, and associated Landau parameters.

The paper is organized as follows. Section II introduces the building blocks needed to construct the pseudopotential in a pedestrian, though necessary for the following discussion, fashion. Section III outlines the use of pseudopotentials with gradients within the context of the nuclear EDF method. The central three-body Skyrme-like pseudopotential is then built in Sec. IV. The construction of the standard two-body

[2]We note that Weinberg's power counting based on naive dimensional analysis already does not provide an appropriate power counting for in-vacuum nuclear interactions based on chiral effective field theory [53].

Skyrme pseudopotential is provided as a reference throughout. Section V details bilinear and trilinear contributions to the EDF kernel derived from two- and three-body central pseudopotentials. Expressions are given there in the so-called isoscalar-isovector representation. Section VI concludes the discussion and gives perspectives for future work, some already under way. Appendixes provide further details on (i) the derivation of infinite nuclear-matter properties at zero and nonzero spin and isospin asymmetry, as well as associated Landau parameters, (ii) the formulation of the EDF kernel in the so-called neutron-proton representation, (iii) the explicit expressions of normal and anomalous one-body fields entering the HFB Hamilton matrix, (iv) the algebraic steps needed to derive the EDF kernel from the pseudopotential, and (v) a verification of the local gauge invariance of the functional.

## II. BASIC INGREDIENTS

This section introduces the necessary ingredients to set up the three-body pseudopotential and to compute the EDF kernel that derives from it.

### A. Introductory remarks

In addition to invariances of the pseudopotential under time-reversal, parity, rotational, translational, and Galilean transformations, we also assume it to be isospin invariant. Translational and Galilean transformations are special cases of local gauge transformations [50]. The invariance of the EDF under the latter has been invoked as a possible guiding principle for the construction of pseudopotentials and general EDF kernels [50,66–68]. We check the local gauge invariance for the pseudopotential-based EDF constructed here in Appendix E.

The EDF is derived assuming pure proton and neutron one-body density matrices, which excludes at this stage the possibility of having $T = 0$ or $T = 1$ proton-neutron pairing [69,70]. Such correlations, however, have never been addressed so far in a systematic and complete fashion in nuclear EDF calculations anyway. When needed, extensions of the present work to this case are straightforward.

The formulation of the three-body contact potentials, however, is not a straightforward generalization of the formalism usually used to set up the standard Skyrme two-body interaction. To illustrate these differences and to validate our procedure, we describe two- and three-body terms side by side.

The Coulomb energy is omitted from the present discussion because its evaluation is standard. In a strict pseudopotential-based framework, its exchange and pairing contributions have to be calculated exactly [38,42]. By contrast, the kinetic energy is kept at various places throughout the paper as it contributes to nuclear-matter properties discussed in Appendix B.

### B. Coordinate basis

The coordinate representation $\{|\vec{r}\sigma q\rangle\} \equiv \{|\vec{r}\rangle \otimes |\sigma\rangle \otimes |q\rangle\}$ labels nucleon states with the position vector $\vec{r} \in \mathbb{R}^3$, the spin projection $\sigma = \pm 1/2$, and the isospin component[3] $q = \pm 1/2$ such that

$$\hat{\vec{r}}\,|\vec{r}\sigma q\rangle = \vec{r}\,|\vec{r}\sigma q\rangle, \tag{1a}$$

$$\hat{\vec{s}}^{\,2}\,|\vec{r}\sigma q\rangle = \frac{3\hbar^2}{4}|\vec{r}\sigma q\rangle, \tag{1b}$$

$$\hat{s}_z|\vec{r}\sigma q\rangle = \hbar\sigma|\vec{r}\sigma q\rangle, \tag{1c}$$

$$\hat{\tau}^2|\vec{r}\sigma q\rangle = \frac{3\hbar^2}{4}|\vec{r}\sigma q\rangle, \tag{1d}$$

$$\hat{\tau}_z|\vec{r}\sigma q\rangle = \hbar q|\vec{r}\sigma q\rangle. \tag{1e}$$

This constitutes a continuous orthonormal direct-product basis of the one-body Hilbert space $\mathcal{H}_1 = \mathcal{H}_{1,\vec{r}} \otimes \mathcal{H}_{1,\sigma} \otimes \mathcal{H}_{1,q}$. Associated orthogonality and completeness relations are given by

$$\langle\vec{r}\sigma q|\vec{r}\,'\sigma' q'\rangle = \delta(\vec{r} - \vec{r}\,')\delta_{\sigma\sigma'}\delta_{qq'}, \tag{2a}$$

$$\int d^3r \sum_{\sigma}\sum_{q} |\vec{r}\sigma q\rangle\langle\vec{r}\sigma q| = \hat{\mathbb{1}}_1, \tag{2b}$$

where $\mathbb{1}_1 = \mathbb{1}_{1,\vec{r}} \otimes \mathbb{1}_{1\sigma} \otimes \mathbb{1}_{1,q}$ is the unity operator on $\mathcal{H}_1$. Introducing a complete set of orthogonal single-particle wave functions,

$$\langle\vec{r}\sigma q|i\rangle \equiv \varphi_i(\vec{r}\sigma q), \tag{3}$$

creation and annihilation operators of a nucleon at coordinates $\{\vec{r}\sigma q\}$ are given by

$$a_{\vec{r}\sigma q} \equiv \sum_i \varphi_i(\vec{r}\sigma q)\, a_i, \tag{4a}$$

$$a^\dagger_{\vec{r}\sigma q} \equiv \sum_i \varphi^*_i(\vec{r}\sigma q)\, a^\dagger_i. \tag{4b}$$

The pseudopotentials constructed below act on two-body ($\mathcal{H}_2$) and three-body ($\mathcal{H}_3$) Hilbert spaces. We thus introduce bases of $\mathcal{H}_2$ and $\mathcal{H}_3$ through tensor products of the one-body basis $\{|\vec{r}\sigma q\rangle\} \equiv \{|\xi\rangle\}$. This provides non-antisymmetrized basis states,

$$|\xi_3\xi_4\rangle \equiv |1 : \vec{r}_3\sigma_3 q_3, 2 : \vec{r}_4\sigma_4 q_4\rangle \tag{5a}$$

$$\equiv |\vec{r}_3\sigma_3 q_3, \vec{r}_4\sigma_4 q_4\rangle, \tag{5b}$$

$$|\xi_4\xi_5\xi_6\rangle \equiv |1 : \vec{r}_4\sigma_4 q_4, 2 : \vec{r}_5\sigma_5 q_5, 3 : \vec{r}_6\sigma_6 q_6\rangle \tag{5c}$$

$$\equiv |\vec{r}_4\sigma_4 q_4, \vec{r}_5\sigma_5 q_5, \vec{r}_6\sigma_6 q_6\rangle, \tag{5d}$$

where the shorthand notation is used whenever possible. In such non-antisymmetrized states, each individual nucleon occupies a well-defined single-particle state. This is made very explicit in Eqs. (5a) and (5c), but only implicit in Eqs. (5b) and (5d) for brevity. It is clear from the former equations that the particle index (i.e., being the first, second, or third particle in a two- or three-body state) should not be confused with the indices labeling different states in the single-particle basis. For example, in Eq. (5a) nucleon 1 occupies single-particle

[3]The quantum number $q$ is sometimes labeled by a letter, i.e., $n$ for neutrons and $p$ for protons, instead of $+1/2$ for neutrons and $-1/2$ for protons.

state $|\vec{r}_3\sigma_3 q_3\rangle$, whereas nucleon 2 occupies the state $|\vec{r}_4\sigma_4 q_4\rangle$. Associated orthogonality,

$$\langle\xi_1\xi_2|\xi_3\xi_4\rangle = \delta_{\xi_1\xi_3}\delta_{\xi_2\xi_4}, \tag{6a}$$

$$\langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle = \delta_{\xi_1\xi_4}\delta_{\xi_2\xi_5}\delta_{\xi_3\xi_6}, \tag{6b}$$

and completeness relations,

$$\iint \mathrm{d}\xi_1\mathrm{d}\xi_2\ |\xi_1\xi_2\rangle\langle\xi_1\xi_2| = \hat{\mathbb{1}}_2, \tag{7a}$$

$$\iiint \mathrm{d}\xi_1\mathrm{d}\xi_2\mathrm{d}\xi_3\ |\xi_1\xi_2\xi_3\rangle\langle\xi_1\xi_2\xi_3| = \hat{\mathbb{1}}_3, \tag{7b}$$

can be derived from Eq. (2), where

$$\delta_{\xi_1\xi_2} \equiv \delta(\vec{r}_1 - \vec{r}_2)\delta_{\sigma_1\sigma_2}\delta_{q_1q_2}, \tag{8a}$$

$$\int \mathrm{d}\xi \equiv \int \mathrm{d}^3r \sum_{\sigma=\pm1/2}\sum_{q=\pm1/2}. \tag{8b}$$

### C. $\delta$ and gradient operators

#### 1. $\delta$ operators

The $\delta$ operator $\hat{\delta}^r_{ij}$ describes an interaction between nucleons $i$ and $j$ located at the same position. Its two-body and three-body matrix elements in coordinate representation are given by

$$\langle\xi_1\xi_2|\hat{\delta}^r_{12}|\xi_3\xi_4\rangle = \langle\xi_1\xi_2|\xi_3\xi_4\rangle\delta(\vec{r}_3 - \vec{r}_4), \tag{9a}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\delta}^r_{12}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\delta(\vec{r}_4 - \vec{r}_5), \tag{9b}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\delta}^r_{13}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\delta(\vec{r}_4 - \vec{r}_6), \tag{9c}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\delta}^r_{23}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\delta(\vec{r}_5 - \vec{r}_6). \tag{9d}$$

#### 2. Gradient operators

The one-body gradient operator is introduced through matrix elements connecting coordinate and configuration basis states,

$$\vec{\nabla}_{\vec{r}}\ \varphi_i(\xi) \equiv \langle\xi|\hat{\vec{\nabla}}|i\rangle = \int \mathrm{d}\xi'\langle\xi|\hat{\vec{\nabla}}|\xi'\rangle\varphi_i(\xi'). \tag{10}$$

From the definition of its Hermitian conjugate $\langle i|\hat{\vec{\nabla}}^\dagger|\xi\rangle = [\langle\xi|\hat{\vec{\nabla}}|i\rangle]^*$ it follows that

$$\vec{\nabla}_{\vec{r}}\ \varphi_i^*(\xi) = \langle i|\hat{\vec{\nabla}}^\dagger|\xi\rangle = \int \mathrm{d}\xi'\varphi_i^*(\xi')\langle\xi'|\hat{\vec{\nabla}}^\dagger|\xi\rangle. \tag{11}$$

Matrix elements of the gradient operator and of its Hermitian conjugate in coordinate basis can deduce directly from Eqs. (10) and (11)

$$\langle\xi_1|\hat{\vec{\nabla}}|\xi_2\rangle = \langle\xi_1|\xi_2\rangle\vec{\nabla}_{\vec{r}_2}, \tag{12a}$$

$$\langle\xi_1|\hat{\vec{\nabla}}^\dagger|\xi_2\rangle = \vec{\nabla}_{\vec{r}_1}\langle\xi_1|\xi_2\rangle, \tag{12b}$$

where the convention used states that $\vec{\nabla}_{\vec{r}}$ acts on functions depending on $\vec{r}$ located to its right, whereas $\vec{\nabla}_{\vec{r}}$ acts on functions depending on $\vec{r}$ located to its left. The momentum operator $\hat{\vec{p}} \equiv -\mathrm{i}\hbar\hat{\vec{\nabla}}$ being Hermitian, it follows trivially that $\langle i|\hat{\vec{\nabla}}|j\rangle = -\langle i|\hat{\vec{\nabla}}^\dagger|j\rangle$ is anti-Hermitian, such that

$$\langle\xi_1|\hat{\vec{\nabla}}|\xi_2\rangle = \langle\xi_1|\xi_2\rangle\vec{\nabla}_{\vec{r}_2} = -\vec{\nabla}_{\vec{r}_1}\langle\xi_1|\xi_2\rangle, \tag{13a}$$

$$\langle\xi_1|\hat{\vec{\nabla}}^\dagger|\xi_2\rangle = \vec{\nabla}_{\vec{r}_1}\langle\xi_1|\xi_2\rangle = -\langle\xi_1|\xi_2\rangle\vec{\nabla}_{\vec{r}_2}. \tag{13b}$$

#### 3. Relative momentum operators

The gradient structure of the pseudopotential involves relative momentum operators associated with particles $i$ and $j$,

$$\hat{\vec{k}}_{ij} \equiv \frac{1}{2\hbar}(\hat{\vec{p}}_i - \hat{\vec{p}}_j) = -\frac{\mathrm{i}}{2}(\hat{\vec{\nabla}}_i - \hat{\vec{\nabla}}_j), \tag{14}$$

where $\hat{\vec{\nabla}}_i$ acts on particle $i$. Using that $\hat{\vec{k}}_{ij}$ is Hermitian $\hat{\vec{k}}_{12} = \hat{\vec{k}}_{12}^\dagger$, we first provide two- and three-body matrix elements connecting coordinate and configuration basis states,

$$\langle\xi_1\xi_2|\hat{\vec{k}}_{12}|ij\rangle = \big[\vec{k}_{\vec{r}_1\vec{r}_2}\ \varphi_i(\xi_1)\varphi_j(\xi_2)\big], \tag{15a}$$

$$\langle ij|\hat{\vec{k}}_{12}|\xi_1\xi_2\rangle = \big[\vec{k}^*_{\vec{r}_1\vec{r}_2}\ \varphi_i^*(\xi_1)\varphi_j^*(\xi_2)\big], \tag{15b}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{12}|ijk\rangle = \big[\vec{k}_{\vec{r}_1\vec{r}_2}\ \varphi_i(\xi_1)\varphi_j(\xi_2)\varphi_k(\xi_3)\big], \tag{15c}$$

$$\langle ijk|\hat{\vec{k}}_{12}|\xi_1\xi_2\xi_3\rangle = \big[\vec{k}^*_{\vec{r}_1\vec{r}_2}\ \varphi_i^*(\xi_1)\varphi_j^*(\xi_2)\varphi_k^*(\xi_3)\big], \tag{15d}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{13}|ijk\rangle = \big[\vec{k}_{\vec{r}_1\vec{r}_3}\ \varphi_i(\xi_1)\varphi_j(\xi_2)\varphi_k(\xi_3)\big], \tag{15e}$$

$$\langle ijk|\hat{\vec{k}}_{13}|\xi_1\xi_2\xi_3\rangle = \big[\vec{k}^*_{\vec{r}_1\vec{r}_3}\ \varphi_i^*(\xi_1)\varphi_j^*(\xi_2)\varphi_k^*(\xi_3)\big], \tag{15f}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{23}|ijk\rangle = \big[\vec{k}_{\vec{r}_2\vec{r}_3}\ \varphi_i(\xi_1)\varphi_j(\xi_2)\varphi_k(\xi_3)\big], \tag{15g}$$

$$\langle ijk|\hat{\vec{k}}_{23}|\xi_1\xi_2\xi_3\rangle = \big[\vec{k}^*_{\vec{r}_2\vec{r}_3}\ \varphi_i^*(\xi_1)\varphi_j^*(\xi_2)\varphi_k^*(\xi_3)\big], \tag{15h}$$

where

$$\vec{k}_{\vec{r}_i\vec{r}_j} \equiv -\frac{\mathrm{i}}{2}\big(\vec{\nabla}_{\vec{r}_i} - \vec{\nabla}_{\vec{r}_j}\big), \tag{16}$$

while $\vec{k}^*_{\vec{r}_i\vec{r}_j}$ denotes its complex conjugate. The brackets in Eq. (15) indicate that $\vec{k}_{\vec{r}_i\vec{r}_j}$ acts only on the wave functions located inside. Matrix elements in the coordinate basis can be deduced to take the form

$$\langle\xi_1\xi_2|\hat{\vec{k}}_{12}|\xi_3\xi_4\rangle = \langle\xi_1\xi_2|\xi_3\xi_4\rangle\ \vec{k}_{\vec{r}_3\vec{r}_4} \tag{17a}$$

$$= \vec{k}^*_{\vec{r}_1\vec{r}_2}\ \langle\xi_1\xi_2|\xi_3\xi_4\rangle, \tag{17b}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{12}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\ \vec{k}_{\vec{r}_4\vec{r}_5} \tag{17c}$$

$$= \vec{k}^*_{\vec{r}_1\vec{r}_2}\ \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle, \tag{17d}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{13}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\ \vec{k}_{\vec{r}_4\vec{r}_6} \tag{17e}$$

$$= \vec{k}^*_{\vec{r}_1\vec{r}_3}\ \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle, \tag{17f}$$

$$\langle\xi_1\xi_2\xi_3|\hat{\vec{k}}_{23}|\xi_4\xi_5\xi_6\rangle = \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle\ \vec{k}_{\vec{r}_5\vec{r}_6} \tag{17g}$$

$$= \vec{k}^*_{\vec{r}_2\vec{r}_3}\ \langle\xi_1\xi_2\xi_3|\xi_4\xi_5\xi_6\rangle, \tag{17h}$$

where $\vec{k}_{\vec{r}_i\vec{r}_j}$ acts on functions located to its right, while $\vec{k}^*_{\vec{r}_i\vec{r}_j}$ acts on functions located to its left. The quantum mechanical

operator $\hat{\vec{k}}_{ij}$ has to be distinguished from its position-space matrix element $\vec{k}_{\vec{r}_3\vec{r}_4}$ that is a differential operator on $\mathbb{R}^3 \otimes \mathbb{R}^3$.

Thorough definitions of the matrix elements of elementary operators have been given above. Matrix elements of a *product* of such elementary operators can be computed in a pedestrian way by inserting as many completeness relations as necessary to invoke matrix elements of the elementary operators.[4] Let us consider as an example two types of matrix elements that will have to be considered for the two-body Skyrme pseudopotential. By virtue of Eqs. (17b) and (17a), and by inserting enough completeness relations on $\mathcal{H}_2$, one obtains

$$\begin{aligned}\langle\xi_1\xi_2|\hat{\delta}^r_{12}\hat{\vec{k}}^2_{12}|\xi_3\xi_4\rangle &= \langle\xi_1\xi_2|\xi_3\xi_4\rangle\delta(\vec{r}_3-\vec{r}_4)\,\vec{k}^2_{\vec{r}_3\vec{r}_4}\\ &= \delta(\vec{r}_1-\vec{r}_2)\,\vec{k}^{*2}_{\vec{r}_1\vec{r}_2}\,\langle\xi_1\xi_2|\xi_3\xi_4\rangle, \quad (18a)\\ \langle\xi_1\xi_2|\hat{\vec{k}}_{12}\cdot\hat{\delta}^r_{12}\hat{\vec{k}}_{12}|\xi_3\xi_4\rangle &= \vec{k}^*_{\vec{r}_1\vec{r}_2}\langle\xi_1\xi_2|\xi_3\xi_4\rangle\delta(\vec{r}_3-\vec{r}_4)\,\vec{k}_{\vec{r}_3\vec{r}_4}\\ &= \langle\xi_1\xi_2|\xi_3\xi_4\rangle\vec{k}_{\vec{r}_3\vec{r}_4}\delta(\vec{r}_3-\vec{r}_4)\,\vec{k}_{\vec{r}_3\vec{r}_4}\\ &= \vec{k}^*_{\vec{r}_1\vec{r}_2}\cdot\delta(\vec{r}_1-\vec{r}_2)\,\vec{k}^*_{\vec{r}_1\vec{r}_2}\langle\xi_1\xi_2|\xi_3\xi_4\rangle. \quad (18b)\end{aligned}$$

Any of the alternative formulas can be used when evaluating matrix elements of the interaction given that the resulting expressions can be related by one or several integrations by parts. Proceeding as above, one can easily show that gradient and $\delta$ operators do not commute,

$$\hat{\vec{k}}_{ij}\hat{\delta}^r_{ij} \neq \hat{\delta}^r_{ij}\hat{\vec{k}}_{ij} = \big(\hat{\vec{k}}_{ij}\hat{\delta}^r_{ij}\big)^\dagger. \quad (19)$$

### D. Position-, spin-, and isospin-exchange operators

Two-body coordinate-exchange operators will be used to formulate the pseudopotential. Additionally, such operators are elementary building blocks of the antisymmetrizers that will enter the calculation of the EDF kernel; see Eq. (38). Applying the exchange operator $\hat{P}_{ij} = \hat{P}_{ji}$, which acts on the coordinates of particles $i$ and $j$, with $i \neq j$, two- and three-body basis states are transformed according to

$$\begin{aligned}\hat{P}_{12}|\xi_3\xi_4\rangle &\equiv |\xi_4\xi_3\rangle, \quad (20a)\\ \hat{P}_{12}|\xi_4\xi_5\xi_6\rangle &\equiv |\xi_5\xi_4\xi_6\rangle, \quad (20b)\\ \hat{P}_{13}|\xi_4\xi_5\xi_6\rangle &\equiv |\xi_6\xi_5\xi_4\rangle, \quad (20c)\\ \hat{P}_{23}|\xi_4\xi_5\xi_6\rangle &\equiv |\xi_4\xi_6\xi_5\rangle, \quad (20d)\end{aligned}$$

and similarly in any other basis representation. Of course, applying the same exchange operator twice gives back the original state. Furthermore, different exchange operators acting on the same space do, in general, not commute with one another, i.e.,

$$\begin{aligned}\hat{P}_{12}\hat{P}_{13} &= \hat{P}_{13}\hat{P}_{23} = \hat{P}_{23}\hat{P}_{12}, \quad (21a)\\ \hat{P}_{12}\hat{P}_{23} &= \hat{P}_{23}\hat{P}_{13} = \hat{P}_{13}\hat{P}_{12}. \quad (21b)\end{aligned}$$

[4]Taking shortcuts by "applying" operators sequentially on bras or kets rather than resorting to *matrix elements* of elementary operators might sometimes lead to ambiguous computational steps.

In coordinate representation, exchange operators factorize into position-, spin-, and isospin-exchange operators $\hat{P}_{ij} \equiv \hat{P}^r_{ij}\hat{P}^\sigma_{ij}\hat{P}^q_{ij}$ that only exchange the corresponding coordinates, e.g.,

$$\begin{aligned}\hat{P}^r_{12}|\xi_4\xi_5\xi_6\rangle &\equiv |\vec{r}_5\sigma_4q_4,\vec{r}_4\sigma_5q_5,\vec{r}_6\sigma_6q_6\rangle, \quad (22a)\\ \hat{P}^\sigma_{12}|\xi_4\xi_5\xi_6\rangle &\equiv |\vec{r}_4\sigma_5q_4,\vec{r}_5\sigma_4q_5,\vec{r}_6\sigma_6q_6\rangle, \quad (22b)\\ \hat{P}^q_{12}|\xi_4\xi_5\xi_6\rangle &\equiv |\vec{r}_4\sigma_4q_5,\vec{r}_5\sigma_5q_4,\vec{r}_6\sigma_6q_6\rangle. \quad (22c)\end{aligned}$$

Coordinate-exchange operators do not commute with relative momentum operators. One finds that

$$\begin{aligned}\hat{\vec{k}}_{ij}\,\hat{P}^r_{ij} &= \hat{P}^r_{ij}\,\hat{\vec{k}}_{ji} = -\hat{P}^r_{ij}\,\hat{\vec{k}}_{ij}, \quad (23a)\\ \hat{\vec{k}}_{ij}\,\hat{P}^r_{kj} &= \hat{P}^r_{kj}\,\hat{\vec{k}}_{ik}, \quad (23b)\\ \hat{\vec{k}}_{ij}\,\hat{P}^r_{ik} &= \hat{P}^r_{ik}\,\hat{\vec{k}}_{kj}, \quad (23c)\end{aligned}$$

i.e., in general, the commutation with a position-exchange operator changes the particle indices involved in the gradient operator. In the particular case where particle indices are the same in both operators, they anticommute; see Eq. (23a). These features can be established in a pedestrian way, e.g.,

$$\begin{aligned}\langle\vec{r}_1\vec{r}_2\vec{r}_3|\hat{\vec{k}}_{12}\hat{P}^r_{12}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle &= \langle\vec{r}_1\vec{r}_2\vec{r}_3|\vec{r}_5\vec{r}_4\vec{r}_6\rangle\vec{k}_{\vec{r}_5\vec{r}_4} \quad (24a)\\ &= -\langle\vec{r}_1\vec{r}_2\vec{r}_3|\,\hat{P}^r_{12}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle\vec{k}_{\vec{r}_4\vec{r}_5}\\ &= -\langle\vec{r}_1\vec{r}_2\vec{r}_3|\,\hat{P}^r_{12}\hat{\vec{k}}_{12}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle,\\ \langle\vec{r}_1\vec{r}_2\vec{r}_3|\hat{\vec{k}}_{12}\hat{P}^r_{13}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle &= \langle\vec{r}_1\vec{r}_2\vec{r}_3|\vec{r}_6\vec{r}_5\vec{r}_4\rangle\vec{k}_{\vec{r}_6\vec{r}_5}\\ &= \langle\vec{r}_1\vec{r}_2\vec{r}_3|\,\hat{P}^r_{13}\hat{\vec{k}}_{32}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle. \quad (24b)\end{aligned}$$

This indicates that it may not be equivalent to have position-exchange operators located to the right or to the left of gradient operators in three-body potentials. Also, while it is always possible to replace $\hat{P}^r_{ij}$ directly with $\pm1$ in the matrix elements of the two-body potential by virtue of Eq. (23a), where the sign ultimately depends on the parity associated with the combination of gradient operators at play, this is in most cases not possible in matrix elements of three-body operators.

To evaluate matrix elements of the pseudopotential, it turns out to be useful to write spin-exchange operators in terms of spin Pauli matrices [71],

$$\hat{P}^\sigma_{ij} = \tfrac{1}{2}(1 + \hat{\vec{\sigma}}_i\cdot\hat{\vec{\sigma}}_j). \quad (25)$$

Recalling that

$$\hat{\sigma}_{i,\mu}\hat{\sigma}_{i,\nu} = \delta_{\mu\nu}1 + \mathrm{i}\sum_\kappa \epsilon_{\mu\nu\kappa}\hat{\sigma}_{i,\kappa}, \quad (26)$$

when both Pauli matrices act on the same particle $i$, with $\mu,\nu,\kappa \in \{x,y,z\}$ and $\epsilon_{\mu\nu\kappa}$ denoting the Levi-Civita symbol, the product of two spin-exchange operators can be expressed as

$$\hat{P}^\sigma_{12}\hat{P}^\sigma_{13} = \frac{1}{4}\Bigg(1 + \hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_2 + \hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_3 + \hat{\vec{\sigma}}_2\cdot\hat{\vec{\sigma}}_3 + \mathrm{i}\sum_{\mu\nu\kappa}\epsilon_{\mu\nu\kappa}\hat{\sigma}_{1,\kappa}\hat{\sigma}_{2,\mu}\hat{\sigma}_{3,\nu}\Bigg), \quad (27a)$$

$$\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23} = \frac{1}{4}\left(1 + \hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_2 + \hat{\vec{\sigma}}_2\cdot\hat{\vec{\sigma}}_3 + \hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_3 + \mathrm{i}\sum_{\mu\nu\kappa}\epsilon_{\mu\nu\kappa}\hat{\sigma}_{1,\mu}\hat{\sigma}_{2,\kappa}\hat{\sigma}_{3,\nu}\right). \quad (27b)$$

### E. Antisymmetrization operators

Let us introduce $\hat{\mathcal{A}}_{12}$ and $\hat{\mathcal{A}}_{123}$ as the two- and three-body antisymmetrizers, respectively, under the form

$$\hat{\mathcal{A}}_{12} \equiv (1 - \hat{P}_{12}), \quad (28a)$$

$$\hat{\mathcal{A}}_{123} \equiv \hat{\mathcal{A}}_{12}(1 - \hat{P}_{13} - \hat{P}_{23}) = (1 - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{12}\hat{P}_{13} + \hat{P}_{12}\hat{P}_{23}). \quad (28b)$$

We introduce $\hat{\mathcal{A}}^{12}_{123}$ as another useful combination of exchange operators,

$$\hat{\mathcal{A}}^{12}_{123} \equiv (1 - \hat{P}_{13} - \hat{P}_{23}). \quad (28c)$$

Basic properties of two-body exchange operators lead to

$$\hat{P}_{12}\hat{\mathcal{A}}_{12}|ij\rangle = -\hat{\mathcal{A}}_{12}|ij\rangle, \quad (29a)$$

$$\hat{P}_{12}\hat{\mathcal{A}}_{123}|ijk\rangle = -\hat{\mathcal{A}}_{123}|ijk\rangle, \quad (29b)$$

$$\hat{P}_{13}\hat{\mathcal{A}}_{123}|ijk\rangle = -\hat{\mathcal{A}}_{123}|ijk\rangle, \quad (29c)$$

$$\hat{P}_{23}\hat{\mathcal{A}}_{123}|ijk\rangle = -\hat{\mathcal{A}}_{123}|ijk\rangle, \quad (29d)$$

from which trivially follows that

$$\hat{P}^{r}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle = -\hat{P}^{\sigma}_{ij}\hat{P}^{q}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle, \quad (30a)$$

$$\hat{P}^{\sigma}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle = -\hat{P}^{r}_{ij}\hat{P}^{q}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle, \quad (30b)$$

$$\hat{P}^{q}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle = -\hat{P}^{r}_{ij}\hat{P}^{\sigma}_{ij}\mathcal{A}_{123}|\xi_4\xi_5\xi_6\rangle. \quad (30c)$$

## III. THE ENERGY DENSITY FUNCTIONAL

Before coming to the construction of the pseudopotential itself, let us explain its use within the context of EDF calculations.

### A. Reference states

The EDF method originates from the picture of a nucleus as an ensemble of quasiparticles moving independently in their self-created average field. It relies on the use of product states of Bogoliubov quasiparticles,

$$|\Phi\rangle = \mathcal{N}_\Phi \prod_\mu \beta_\mu|0\rangle, \quad (31)$$

where $\{\beta^\dagger_\mu\}$ and $\{\beta_\mu\}$ denote quasiparticle creation and annihilation operators relating to an arbitrary one-body basis $\{a^\dagger_\alpha, a_\alpha\}$ through a unitary canonical transformation of Bogoliubov type [13,14],

$$\beta_\mu = \sum_i (U^\dagger_{\mu i}a_i + V^\dagger_{\mu i}a^\dagger_i), \quad (32a)$$

$$\beta^\dagger_\mu = \sum_i (V_{i\mu}a_i + U_{i\mu}a^\dagger_i). \quad (32b)$$

The factor $\mathcal{N}_\Phi$ in Eq. (31) ensures the normalization $\langle\Phi|\Phi\rangle = 1$ of the quasiparticle vacuum.

### B. Pseudopotential-based EDF kernel

Within the pseudopotential-based formulation of the EDF method, the energy kernel is derived from a pseudo-Hamiltonian that reads, in an arbitrary basis, as

$$\hat{H}_{\mathrm{pseudo}} = \sum_{ij} a^\dagger_i t^{(1)}_{ij} a_j \quad (33a)$$

$$+ \frac{1}{2!}\sum_{ijkl} a^\dagger_i a^\dagger_j v^{(2)}_{ijkl} a_l a_k \quad (33b)$$

$$+ \frac{1}{3!}\sum_{ijklmn} a^\dagger_i a^\dagger_j a^\dagger_k v^{(3)}_{ijklmn} a_n a_m a_l + \cdots, \quad (33c)$$

where

$$t^{(1)}_{ij} \equiv \langle i|\hat{t}|j\rangle, \quad (34a)$$

$$v^{(2)}_{ijkl} \equiv \langle ij|\hat{v}_{12}|kl\rangle, \quad (34b)$$

$$v^{(3)}_{ijklmn} \equiv \langle ijk|\hat{v}_{123}|lmn\rangle, \quad (34c)$$

denote matrix elements of the effective one-body kinetic energy operator and non-antisymmetrized matrix elements of two-body, three-body . . . (density-independent) pseudopotentials. In the present work, we do limit ourselves to two- and three-body pseudopotentials, but the further extension of the formalism to four-body and higher operators is straightforward, though cumbersome.

The corresponding SR, i.e., diagonal, EDF kernel is computed as

$$E \equiv \langle\Phi|\hat{H}_{\mathrm{pseudo}}|\Phi\rangle \quad (35a)$$

$$= E[\rho, \kappa, \kappa^*] \quad (35b)$$

and takes the form of a functional of one-body density matrices

$$\rho_{ij} \equiv \langle\Phi|a^\dagger_j a_i|\Phi\rangle, \quad (36a)$$

$$\kappa_{ij} \equiv \langle\Phi|a_j a_i|\Phi\rangle, \quad (36b)$$

$$\kappa^*_{ij} \equiv \langle\Phi|a^\dagger_i a^\dagger_j|\Phi\rangle, \quad (36c)$$

by virtue of Wick's theorem [72]. The normal density matrix is Hermitian $\rho_{ij} = \rho^*_{ji}$, whereas the anomalous density matrix is skew symmetric $\kappa_{ij} = -\kappa_{ji}$.

Multireference calculations invoke an extension of the SR EDF kernel to define the *off-diagonal* kernel involving two different Bogoliubov states. As opposed to hybrid and general functionals [73], such an extension is formally straightforward and unambiguous for a pseudopotential-based parametrization. By virtue of the generalized (i.e., off-diagonal) Wick theorem [12–14], the off-diagonal energy is obtained from

$E[\rho,\kappa,\kappa^*]$ by replacing the density matrices of Eq. (36) with *transition* (i.e., off-diagonal) density matrices [5], and multiplying the entire EDF kernel with a norm kernel.

### C. EDF kernel in a configuration basis

When evaluating Eq. (35a), the resulting terms can be grouped according to their content in normal and anomalous density matrices

$$E[\rho,\kappa,\kappa^*] \equiv E^{\rho} + E^{\rho\rho} + E^{\kappa\kappa} + E^{\rho\rho\rho} + E^{\kappa\kappa\rho}. \quad (37)$$

There are several equivalent possibilities of how these can be expressed. We choose a form where each given product of density matrices appears only once and where the antisymmetrization is done explicitly in the matrix elements by virtue of the antisymmetrization operators $\hat{\mathcal{A}}_{12}$, $\hat{\mathcal{A}}_{123}$, and $\hat{\mathcal{A}}^{12}_{123}$ of Eq. (28)

$$E^{\rho} = \sum_{ij}\langle i|\hat{t}|j\rangle\rho_{ji}, \quad (38a)$$

$$E^{\rho\rho} = \frac{1}{2}\sum_{ijkl}\langle ij|\hat{v}_{12}\hat{\mathcal{A}}_{12}|kl\rangle\rho_{ki}\rho_{lj}, \quad (38b)$$

$$E^{\kappa\kappa} = \frac{1}{2}\sum_{ijkl}\langle ij|\hat{v}_{12}|kl\rangle\kappa^*_{ij}\kappa_{kl} \quad (38c)$$

$$= \frac{1}{4}\sum_{ijkl}\langle ij|\hat{v}_{12}\hat{\mathcal{A}}_{12}|kl\rangle\kappa^*_{ij}\kappa_{kl}, \quad (38d)$$

$$E^{\rho\rho\rho} = \frac{1}{6}\sum_{ijklmn}\langle ijk|\hat{v}_{123}\hat{\mathcal{A}}_{123}|lmn\rangle\rho_{li}\rho_{mj}\rho_{nk}, \quad (38e)$$

$$E^{\kappa\kappa\rho} = \frac{1}{6}\sum_{ijklmn}\langle ijk|\hat{\mathcal{A}}^{12}_{123}\hat{v}_{123}\hat{\mathcal{A}}^{12}_{123}|lmn\rangle\kappa^*_{ij}\kappa_{lm}\rho_{nk} \quad (38f)$$

$$= \frac{1}{2}\sum_{ijklmn}\langle ijk|\hat{v}_{123}\hat{\mathcal{A}}^{12}_{123}|lmn\rangle\kappa^*_{ij}\kappa_{lm}\rho_{nk} \quad (38g)$$

$$= \frac{1}{4}\sum_{ijklmn}\langle ijk|\hat{v}_{123}\hat{\mathcal{A}}_{123}|lmn\rangle\kappa^*_{ij}\kappa_{lm}\rho_{nk}. \quad (38h)$$

Exploiting relations (21) and the cyclic nature of the particle trace in expressions containing normal density matrices only, e.g.,

$$\sum_{ijkl}\langle ij|\hat{P}_{12}\hat{v}_{12}|kl\rangle\rho_{ki}\rho_{lj} = \sum_{ijkl}\langle ij|\hat{v}_{12}\hat{P}_{12}|kl\rangle\rho_{ki}\rho_{lj}, \quad (39)$$

as well as the skew symmetry of the pairing tensor, antisymmetrizers and exchange operators can be placed either to the left or to the right of the pseudopotential according to what is shown in Eqs. (38).

### D. Symmetry under particle exchange

Because we are dealing with identical particles, pseudopotential operators must be symmetric under the exchange of any pair of nucleons, i.e.,

$$\hat{v}_{\overline{12}} = \hat{v}_{\overline{21}}, \quad (40a)$$

$$\hat{v}_{\overline{123}} = \hat{v}_{\overline{213}} = \hat{v}_{\overline{132}} = \hat{v}_{\overline{321}} = \hat{v}_{\overline{231}} = \hat{v}_{\overline{312}}, \quad (40b)$$

where the bar over a certain set of particle indices indicates from here on the symmetry of the operator under any permutation within that set. In matrix elements, exchanging particles corresponds to exchanging the complete set of associated single-particle quantum numbers in *both* the bra and the ket. This leads to symmetry properties of the kind

$$\langle ij|\hat{v}_{\overline{12}}|kl\rangle = \langle ji|\hat{v}_{\overline{12}}|lk\rangle, \quad (41a)$$

$$\langle ijk|\hat{v}_{\overline{123}}|lmn\rangle = \langle kij|\hat{v}_{\overline{123}}|nlm\rangle. \quad (41b)$$

When constructing a two-body Hermitian operator out of $\delta$ and relative momentum operators, along with exchange operators, the symmetry of the potential under particle exchange is automatically fulfilled. When the three-body potential is constructed from the same two-body building blocks, its symmetry under permutation of the particle indices is not as automatically fulfilled. This property, however, can always be enforced by constructing the pseudopotential as the sum of six permutations over the particle indices of a nonsymmetric potential $\hat{v}'_{123}$. More convenient for our purpose is to take advantage of the fact that any fully symmetric operator $\hat{v}_{\overline{123}}$ can be decomposed into the sum of three parts that are symmetric under the exchange of two particles,

$$\hat{v}_{\overline{123}} \equiv \hat{v}_{\overline{123}} + \hat{v}_{\overline{132}} + \hat{v}_{\overline{231}}. \quad (42)$$

We use this property to build explicitly $\hat{v}_{\overline{123}}$, with the other two parts being obtained through the application of two-body exchange operators

$$\hat{v}_{\overline{123}} = \hat{v}_{\overline{123}} + \hat{P}_{23}\hat{v}_{\overline{123}}\hat{P}_{23} + \hat{P}_{13}\hat{v}_{\overline{123}}\hat{P}_{13}. \quad (43)$$

Invoking the skew symmetry of $\kappa$ [Eq. (43)] allows one to rewrite trilinear contributions to the EDF kernel in terms of $\hat{v}_{\overline{123}}$ only, i.e.,

$$E^{\rho\rho\rho} = \frac{1}{2}\sum_{ijklmn}\langle ijk|\hat{v}_{\overline{123}}\hat{\mathcal{A}}_{123}|lmn\rangle\rho_{li}\rho_{mj}\rho_{nk}, \quad (44a)$$

$$E^{\kappa\kappa\rho} = \frac{1}{2}\sum_{ijklmn}\langle ijk|\hat{\mathcal{A}}^{12}_{123}\hat{v}_{\overline{123}}\hat{\mathcal{A}}^{12}_{123}|lmn\rangle\kappa^*_{ij}\kappa_{lm}\rho_{nk}. \quad (44b)$$

## IV. BUILDING THE PSEUDOPOTENTIAL

In this section, we describe the setup of two- and three-body Skyrme-type pseudopotentials containing up to two gradient operators.

### A. Generic structure

We build Hermitian two- and three-body operators out of two-body $\delta$, relative momentum, and exchange operators such that symmetries listed in Sec. II A are fulfilled. To the best of our knowledge, all earlier attempts to construct Skyrme-type three-body contact interactions were limited to operator structures where $\hat{v}_{\overline{123}}$ is set up by inserting an additional $\delta$ function into a subset of the standard two-body

Skyrme interaction [25,54–63]. As seen below, this does not generate the most general set of three-body terms.

We separate two- and three-body pseudopotentials into a sum of terms that all are functions of the elementary two-body operators, i.e.,

$$\hat{v}_{\overline{12}} \equiv \sum_i \hat{v}^i_{\overline{12}}\big[\hat{P}^{\{t_i,x_i\}}_{12}, \hat{k}^{(\dagger)}_{12}, \hat{\delta}^r_{12}\big], \tag{45a}$$

$$\hat{v}_{\overline{123}} \equiv \sum_i \hat{v}^i_{\overline{123}}\big[\hat{P}^{\{u_i,y_i\}}_{123}, \hat{k}^{(\dagger)}_{12}, \hat{k}^{(\dagger)}_{23}, \hat{k}^{(\dagger)}_{13}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big]. \tag{45b}$$

The index $i$ labels the possible coordinate-space structures, i.e., terms with a different content in gradient operators. The number of such terms is limited by the number of interacting nucleons (i.e., two and three in the present case) and the number of gradient operators allowed (i.e., up to two in the present case). Each of these can be combined with a large number of distinct combinations of two-body exchange operators, represented by $\hat{P}^{\{t_i,x_i\}}_{12}$ and $\hat{P}^{\{u_i,y_i\}}_{123}$.

### B. Structure in coordinate space

Each function $\hat{v}^i_{\overline{12}}$ contains a set of parameters denoted as $t_i$ and $x_{ij}$, and each function $\hat{v}^i_{\overline{123}}$ contains a set of parameters denoted as $u_i$ and $y_{ij}$. Parameters $t_i$ and $u_i$ represent the overall coupling strength of a given coordinate space operator, whereas $x_{ij}$ and $y_{ij}$ weigh the possible combinations of spin- and isospin-exchange operators, labeled by $j$.

We first specify the dependence of functions $\hat{v}^i_{\overline{12}}$ and $\hat{v}^i_{\overline{123}}$ on gradient operators and $\delta$ functions by forming all possible Hermitian scalars. Using for now the most simple spin and isospin dependence under the form of unit operators in spin and isospin space, one obtains

$$\hat{v}^0_{\overline{12}}\big(\hat{\mathbb{1}}_{2,\sigma q}, \hat{\delta}^r_{12}\big) \equiv \hat{\mathbb{1}}_{2,\sigma q}\hat{\delta}^r_{12}, \tag{46a}$$

$$\hat{v}^1_{\overline{12}}\big(\hat{\mathbb{1}}_{2,\sigma q}, \hat{k}^{(\dagger)}_{12}, \hat{\delta}^r_{12}\big) \equiv \hat{\mathbb{1}}_{2,\sigma q}\tfrac{1}{2}\big(\hat{k}^\dagger_{12}\cdot\hat{k}^\dagger_{12}\hat{\delta}^r_{12} + \hat{\delta}^r_{12}\hat{k}_{12}\cdot\hat{k}_{12}\big), \tag{46b}$$

$$\hat{v}^2_{\overline{12}}\big(\hat{\mathbb{1}}_{2,\sigma q}, \hat{k}^{(\dagger)}_{12}, \hat{\delta}^r_{12}\big) \equiv \hat{\mathbb{1}}_{2,\sigma q}\hat{k}^\dagger_{12}\hat{\delta}^r_{12}\cdot\hat{k}_{12}, \tag{46c}$$

for two-body terms and

$$\hat{v}^0_{\overline{123}}\big(\hat{\mathbb{1}}_{3,\sigma q}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big) \equiv \hat{\mathbb{1}}_{3,\sigma q}\hat{\delta}^r_{13}\hat{\delta}^r_{23}, \tag{46d}$$

$$\hat{v}^1_{\overline{123}}\big(\hat{\mathbb{1}}_{3,\sigma q}, \hat{k}^{(\dagger)}_{12}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big) \equiv \hat{\mathbb{1}}_{3,\sigma q}\tfrac{1}{2}\big(\hat{k}^\dagger_{12}\cdot\hat{k}^\dagger_{12}\hat{\delta}^r_{13}\hat{\delta}^r_{23} + \hat{\delta}^r_{13}\hat{\delta}^r_{23}\hat{k}_{12}\cdot\hat{k}_{12}\big), \tag{46e}$$

$$\hat{v}^2_{\overline{123}}\big(\hat{\mathbb{1}}_{3,\sigma q}, \hat{k}^{(\dagger)}_{12}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big) \equiv \hat{\mathbb{1}}_{3,\sigma q}\hat{k}^\dagger_{12}\hat{\delta}^r_{13}\hat{\delta}^r_{23}\cdot\hat{k}_{12}, \tag{46f}$$

$$\hat{v}^3_{\overline{123}}\big(\hat{\mathbb{1}}_{3,\sigma q}, \hat{k}^{(\dagger)}_{23}, \hat{k}^{(\dagger)}_{13}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big) \equiv \hat{\mathbb{1}}_{3,\sigma q}\tfrac{1}{2}\big(\hat{k}^\dagger_{23}\cdot\hat{k}^\dagger_{13}\hat{\delta}^r_{13}\hat{\delta}^r_{23} + \hat{\delta}^r_{13}\hat{\delta}^r_{23}\hat{k}_{13}\cdot\hat{k}_{23}\big), \tag{46g}$$

$$\hat{v}^4_{\overline{123}}\big(\hat{\mathbb{1}}_{3,\sigma q}, \hat{k}^{(\dagger)}_{23}, \hat{k}^{(\dagger)}_{13}, \hat{\delta}^r_{13}\hat{\delta}^r_{23}\big) \equiv \hat{\mathbb{1}}_{3,\sigma q}\tfrac{1}{2}\big(\hat{k}^\dagger_{13}\hat{\delta}^r_{13}\hat{\delta}^r_{23}\cdot\hat{k}_{23} + \hat{k}^\dagger_{23}\hat{\delta}^r_{13}\hat{\delta}^r_{23}\cdot\hat{k}_{13}\big), \tag{46h}$$

for three-body terms. The list of arguments has been reduced to those that each function actually depends on.

### C. Structure in spin and isospin spaces

As the next step, we deduce the most general operators $\hat{P}^{\{t_i,x_i\}}_{12}$ and $\hat{P}^{\{u_i,y_i\}}_{123}$ that accompany each term in Eq. (46). For terms involving two Hermitian conjugate contributions, one has to employ $\hat{P}^{\{t_i,x_i\}}_{12}$ or $\hat{P}^{\{u_i,y_i\}}_{123}$ for one and $\hat{P}^{\{t_i,x_i\}\dagger}_{12}$ and $\hat{P}^{\{u_i,y_i\}\dagger}_{123}$ for the other, such that the overall operator remains indeed Hermitian.

*A priori*, the most general form is given by the sum of two- and three-body terms obtained by multiplying position-, spin-, and isospin-exchange operators in all possible ways. In the end, $\hat{P}^{\{t_i,x_i\}}_{12}$ and $\hat{P}^{\{u_i,y_i\}}_{123}$ can be expressed solely in terms of spin- and isospin-exchange operators by virtue of Eq. (30). While $\hat{P}^{\{t_i,x_i\}}_{12} = \hat{P}^{\{t_i,x_i\}\,\dagger}_{12}$ derives from the Hermiticity of exchange operators defined in Eq. (22), the same does not hold in general for $\hat{P}^{\{u_i,y_i\}}_{123}$, because products of exchange operators of the same type (i.e., space, spin or isospin) associated with different pairs of particles do not commute.

All terms in Eq. (46) but those entering $\hat{v}^4_{\overline{123}}$ are individually symmetric under the exchange of particles 1 and 2 such that they have to be joined by a spin-isospin operator that itself is symmetric under such an exchange. These considerations lead to the following general spin-isospin operators acting on $\mathcal{H}_2$ and $\mathcal{H}_3$ that are symmetric under the exchange of particles 1 and 2,

$$\hat{P}^{\{t_i,x_i\}}_{\overline{12}} \equiv t_i\big(\hat{\mathbb{1}}_2 + x_{i1}\hat{P}^\sigma_{12} + x_{i2}\hat{P}^q_{12} + x_{i3}\hat{P}^\sigma_{12}\hat{P}^q_{12}\big), \tag{47a}$$

$$\begin{aligned}\hat{P}^{\{u_i,y_i\}}_{\overline{123}} \equiv\ & u_i\big[\hat{\mathbb{1}}_3 + y_{i1}\hat{P}^\sigma_{12} + y_{i2}\big(\hat{P}^\sigma_{13} + \hat{P}^\sigma_{23}\big) + y_{i3}\big(\hat{P}^\sigma_{12}\hat{P}^\sigma_{13} + \hat{P}^\sigma_{12}\hat{P}^\sigma_{23}\big) + y_{i10}\hat{P}^q_{12}\\ & + y_{i11}\hat{P}^\sigma_{12}\hat{P}^q_{12} + y_{i12}\big(\hat{P}^\sigma_{13}\hat{P}^q_{12} + \hat{P}^\sigma_{23}\hat{P}^q_{12}\big) + y_{i13}\big(\hat{P}^\sigma_{12}\hat{P}^\sigma_{13}\hat{P}^q_{12} + \hat{P}^\sigma_{12}\hat{P}^\sigma_{23}\hat{P}^q_{12}\big) + y_{i20}\big(\hat{P}^q_{13} + \hat{P}^q_{23}\big)\\ & + y_{i21}\big(\hat{P}^\sigma_{12}\hat{P}^q_{13} + \hat{P}^\sigma_{12}\hat{P}^q_{23}\big) + y_{i22}\big(\hat{P}^\sigma_{13}\hat{P}^q_{13} + \hat{P}^\sigma_{23}\hat{P}^q_{23}\big) + y_{i23}\big(\hat{P}^\sigma_{13}\hat{P}^q_{23} + \hat{P}^\sigma_{23}\hat{P}^q_{13}\big)\end{aligned}$$

$$+ y_{i24}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}\big) + y_{i25}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{23}\big) + y_{i30}\big(\hat{P}^{q}_{12}\hat{P}^{q}_{13} + \hat{P}^{q}_{12}\hat{P}^{q}_{23}\big)$$
$$+ y_{i31}\big(\hat{P}^{\sigma}_{12}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{q}_{12}\hat{P}^{q}_{23}\big) + y_{i32}\big(\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{23}\hat{P}^{q}_{12}\hat{P}^{q}_{23}\big) + y_{i33}\big(\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{23} + \hat{P}^{\sigma}_{23}\hat{P}^{q}_{12}\hat{P}^{q}_{13}\big)$$
$$+ y_{i34}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{12}\hat{P}^{q}_{23} + y_{i35}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{23} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{12}\hat{P}^{q}_{13}\big)\big]. \tag{47b}$$

As for terms entering $\hat{v}^{4}_{\overline{123}}$, we have to introduce two other functions of spin- and isospin-exchange operators, the first of which only depends on particles 1 and 2, whereas the second one depends on all particles and is not symmetric under the exchange of particles 1 and 2,

$$\hat{P}^{\{u_i,y_i\}}_{123,a} \equiv u_i\big(\hat{\mathbb{1}}_3 + y_{i1}\hat{P}^{\sigma}_{12} + y_{i2}\hat{P}^{q}_{12} + y_{i3}\hat{P}^{\sigma}_{12}\hat{P}^{q}_{12}\big), \tag{48a}$$
$$\begin{aligned}\hat{P}^{\{u_i,y_i\}}_{123,b} \equiv u_i\big(&y_{i2}\hat{P}^{\sigma}_{13} + y_{i3}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13} + y_{i12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12} + y_{i13}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12} + y_{i20}\hat{P}^{q}_{13} + y_{i21}\hat{P}^{\sigma}_{12}\hat{P}^{q}_{13} + y_{i22}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13}\\ &+ y_{i23}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{23} + y_{i24}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13} + y_{i25}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{13} + y_{i30}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + y_{i31}\hat{P}^{\sigma}_{12}\hat{P}^{q}_{12}\hat{P}^{q}_{13}\\ &+ y_{i32}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + y_{i33}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{23} + y_{i34}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{13} + y_{i35}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{23}\big).\end{aligned} \tag{48b}$$

It has to be noted that

$$\hat{P}^{\{u_i,y_i\}}_{\overline{123}} = \hat{P}^{\{u_i,y_i\}}_{123,a} + \hat{P}^{\{u_i,y_i\}}_{123,b} + \hat{P}^{\{u_i,y_i\}}_{213,b}; \tag{49}$$

i.e., operators $\hat{P}^{\{u_i,y_i\}}_{123,a}$ and $\hat{P}^{\{u_i,y_i\}}_{123,b}$ are nothing but subparts of $\hat{P}^{\{u_i,y_i\}}_{\overline{123}}$. Also, one has that $\hat{P}^{\{u_i,y_i\}}_{123,a} = \hat{P}^{\{u_i,y_i\}\dagger}_{123,a}$.

Whenever a given term displays good parity under the exchange of the spatial coordinates of particles $i$ and $j$, one can replace $\hat{P}^{r}_{ij}$ by $\pm 1$ in its matrix elements *a priori*. For instance, it can be easily seen that $\hat{v}^{2}_{\overline{12}}$ changes its sign under particle exchange; hence, it has negative parity. As a consequence, one can make the replacement $\hat{v}^{2}_{\overline{12}}\hat{P}^{r}_{12} = \hat{v}^{2}_{\overline{12}}$ in its matrix elements. Whenever such property can be exploited, one can use Eq. (30) to re-express $\hat{P}^{q}_{ij}$ in terms of $\hat{P}^{\sigma}_{ij}$. This can be done in Eqs. (46a), (46b), (46c), (46e), and (46f) for $\hat{P}^{q}_{12}$, as well as in Eq. (46d) for $\hat{P}^{q}_{12}$, $\hat{P}^{q}_{13}$, and $\hat{P}^{q}_{23}$. In the end, these considerations bring $\hat{P}^{\{t_i,x_i\}}_{\overline{12}}$ and $\hat{P}^{\{u_i,y_i\}}_{\overline{123}}$ into the simpler form,

$$\hat{P}^{\{t_i,x_i\}}_{\overline{12},\alpha} = t_i\big(\hat{\mathbb{1}}_2 + x_i\hat{P}^{\sigma}_{12}\big), \tag{50a}$$
$$\hat{P}^{\{u_i,y_i\}}_{\overline{123},\alpha} = u_i\big[\hat{\mathbb{1}}_3 + y_{i1}\hat{P}^{\sigma}_{12} + y_{i2}\big(\hat{P}^{\sigma}_{13} + \hat{P}^{\sigma}_{23}\big) + y_{i3}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\big)\big], \tag{50b}$$
$$\begin{aligned}\hat{P}^{\{u_i,y_i\}}_{\overline{123},\beta} = u_i\big[&\hat{\mathbb{1}}_3 + y_{i1}\hat{P}^{\sigma}_{12} + y_{i2}\big(\hat{P}^{\sigma}_{13} + \hat{P}^{\sigma}_{23}\big) + y_{i3}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\big) + y_{i20}\big(\hat{P}^{q}_{13} + \hat{P}^{q}_{23}\big)\\ &+ y_{i21}\big(\hat{P}^{\sigma}_{12}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{q}_{23}\big) + y_{i22}\big(\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}\big) + y_{i23}\big(\hat{P}^{\sigma}_{13}\hat{P}^{q}_{23} + \hat{P}^{\sigma}_{23}\hat{P}^{q}_{13}\big)\\ &+ y_{i24}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}\big) + y_{i25}\big(\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{13} + \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{23}\big)\big].\end{aligned} \tag{50c}$$

No such reductions, however, are possible in Eqs. (46g) and (46h). In the end, the complete exploitation of the symmetry relations listed above leads to the following set of the most general possible structures,

$$\hat{v}^{0}_{\overline{12}} \equiv \hat{P}^{\{t_0,x_0\}}_{\overline{12},\alpha}\hat{\delta}^{r}_{12}, \tag{51a}$$
$$\hat{v}^{1}_{\overline{12}} \equiv \tfrac{1}{2}\hat{P}^{\{t_1,x_1\}}_{\overline{12},\alpha}\big[\hat{\vec{k}}^{\dagger}_{12}\cdot\hat{\vec{k}}^{\dagger}_{12}\hat{\delta}^{r}_{12} + \hat{\delta}^{r}_{12}\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}_{12}\big], \tag{51b}$$
$$\hat{v}^{2}_{\overline{12}} \equiv \hat{P}^{\{t_2,x_2\}}_{\overline{12},\alpha}\hat{\vec{k}}^{\dagger}_{12}\hat{\delta}^{r}_{12}\cdot\hat{\vec{k}}_{12}, \tag{51c}$$

for two-body terms and

$$\hat{v}^{0}_{\overline{123}} \equiv \tfrac{1}{2}\big[\hat{P}^{\{u_0,y_0\},\dagger}_{\overline{123},\alpha} + \hat{P}^{\{u_0,y_0\}}_{\overline{123},\alpha}\big]\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}, \tag{51d}$$
$$\hat{v}^{1}_{\overline{123}} \equiv \tfrac{1}{2}\big[\hat{P}^{\{u_1,y_1\},\dagger}_{\overline{123},\beta}\hat{\vec{k}}^{\dagger}_{12}\cdot\hat{\vec{k}}^{\dagger}_{12}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23} + \hat{P}^{\{u_1,y_1\}}_{\overline{123},\beta}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\hat{\vec{k}}_{12}\cdot\hat{\vec{k}}_{12}\big], \tag{51e}$$
$$\hat{v}^{2}_{\overline{123}} \equiv \tfrac{1}{2}\big[\hat{P}^{\{u_2,y_2\},\dagger}_{\overline{123},\beta} + \hat{P}^{\{u_2,y_2\}}_{\overline{123},\beta}\big]\hat{\vec{k}}^{\dagger}_{12}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{12}, \tag{51f}$$
$$\hat{v}^{3}_{\overline{123}} \equiv \tfrac{1}{2}\big[\hat{P}^{\{u_3,y_3\},\dagger}_{\overline{123}}\hat{\vec{k}}^{\dagger}_{23}\cdot\hat{\vec{k}}^{\dagger}_{13}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23} + \hat{P}^{\{u_3,y_3\}}_{\overline{123}}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\hat{\vec{k}}_{13}\cdot\hat{\vec{k}}_{23}\big], \tag{51g}$$
$$\begin{aligned}\hat{v}^{4}_{\overline{123}} \equiv\ &\tfrac{1}{2}\hat{P}^{\{u_4,y_4\}}_{123,a}\big[\hat{\vec{k}}^{\dagger}_{13}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{23} + \hat{\vec{k}}^{\dagger}_{23}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{13}\big]\\ &+ \tfrac{1}{2}\big[\hat{P}^{\{u_4,y_{41}\},\dagger}_{123,b} + \hat{P}^{\{u_4,y_{41}\}}_{213,b}\big]\hat{\vec{k}}^{\dagger}_{23}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{13} + \tfrac{1}{2}\big[\hat{P}^{\{u_4,y_{41}\},\dagger}_{213,b} + \hat{P}^{\{u_4,y_{41}\}}_{123,b}\big]\hat{\vec{k}}^{\dagger}_{13}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{23}\\ &+ \tfrac{1}{2}\big[\hat{P}^{\{u_4,y_{42}\},\dagger}_{213,b} + \hat{P}^{\{u_4,y_{42}\}}_{123,b}\big]\hat{\vec{k}}^{\dagger}_{23}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{13} + \tfrac{1}{2}\big[\hat{P}^{\{u_4,y_{42}\},\dagger}_{123,b} + \hat{P}^{\{u_4,y_{42}\}}_{213,b}\big]\hat{\vec{k}}^{\dagger}_{13}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{23},\end{aligned} \tag{51h}$$

for three-body terms. At this stage, $\hat{v}_{\overline{12}}$ is defined out of six coupling constants, whereas $\hat{v}_{\overline{123}}$ includes altogether about 70 parameters. The two-body terms correspond already to the final form of Skyrme's standard central two-body vertex. For the three-body pseudopotential, however, it can be expected that many terms are, in fact, linearly dependent. Further redundancies among these terms, however, become increasingly difficult to detect, and we do not attempt to find them by hand. Instead, the task is carried out by a formal algebra code that constructs first the complete energy functional deriving from Eq. (51) and then analyzes the correlations between the original terms in the pseudopotential.

## V. DERIVING THE EDF KERNEL

We now provide the full expression of the EDF kernel obtained from the two- and three-body pseudopotentials given in Eq. (51). The mathematical steps actually taken by the numerical code to derive the results are sketched in Appendix C. Correlations among the terms in the original pseudopotentials are then identified using a SVD. This allows us to deduce a set of linearly independent central three-body Skyrme-like pseudopotentials.

### A. Ingredients of the EDF kernel

#### 1. Density matrices

In coordinate representation, the normal and anomalous one-body density matrices read

$$\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q') \equiv \langle\Phi|a^{\dagger}_{\vec{r}\,'\sigma' q'}a_{\vec{r}\sigma q}|\Phi\rangle = \sum_{ij}\varphi^{*}_{j}(\vec{r}\,'\sigma' q')\varphi_{i}(\vec{r}\sigma q)\rho_{ij}, \tag{52a}$$

$$\kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q') \equiv \langle\Phi|a_{\vec{r}\,'\sigma' q'}a_{\vec{r}\sigma q}|\Phi\rangle = \sum_{ij}\varphi_{j}(\vec{r}\,'\sigma' q')\varphi_{i}(\vec{r}\sigma q)\kappa_{ij}. \tag{52b}$$

We assume pure proton and neutron density matrices, such that $\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = \kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = 0$ when $q \neq q'$. As already noted, the normal density matrix is Hermitian, i.e., $\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = \rho^{*}(\vec{r}\,'\sigma' q',\vec{r}\sigma q)$, whereas the pair tensor is skew symmetric, i.e., $\kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = -\kappa(\vec{r}\,'\sigma' q',\vec{r}\sigma q)$.

### B. Nonlocal densities

When assuming pure proton and neutron single-particle states, the most straightforward representation of the densities is obtained in terms of proton and neutron densities. In this case, nonlocal normal and anomalous densities take the form

$$\rho_{q}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma q), \tag{53a}$$

$$s_{q,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma'\sigma}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q)\langle\sigma'|\hat{\sigma}_{\nu}|\sigma\rangle, \tag{53b}$$

$$\tilde{\rho}_{q}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma}2\bar{\sigma}\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma} q), \tag{53c}$$

$$\tilde{s}_{q,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma'\sigma}2\bar{\sigma}'\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}' q)\langle\sigma'|\hat{\sigma}_{\nu}|\sigma\rangle. \tag{53d}$$

One further introduces kinetic densities

$$\tau_{q}(\vec{r},\vec{r}\,') \equiv \sum_{\mu}\nabla_{\vec{r},\mu}\nabla_{\vec{r}\,',\mu}\rho_{q}(\vec{r},\vec{r}\,'), \tag{53e}$$

$$T_{q,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\mu}\nabla_{\vec{r},\mu}\nabla_{\vec{r}\,',\mu}s_{q,\nu}(\vec{r},\vec{r}\,'), \tag{53f}$$

$$\tilde{\tau}_{q}(\vec{r},\vec{r}\,') \equiv \sum_{\mu}\nabla_{\vec{r},\mu}\nabla_{\vec{r}\,',\mu}\tilde{\rho}_{q}(\vec{r},\vec{r}\,'), \tag{53g}$$

$$\tilde{T}_{q,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\mu}\nabla_{\vec{r},\mu}\nabla_{\vec{r}\,',\mu}\tilde{s}_{q,\nu}(\vec{r},\vec{r}\,'), \tag{53h}$$

and currents

$$j_{q,\mu}(\vec{r},\vec{r}\,') \equiv -\frac{\mathrm{i}}{2}(\nabla_{\vec{r},\mu}-\nabla_{\vec{r}\,',\mu})\rho_{q}(\vec{r},\vec{r}\,'), \tag{53i}$$

$$J_{q,\mu\nu}(\vec{r},\vec{r}\,'), \equiv -\frac{\mathrm{i}}{2}(\nabla_{\vec{r},\mu}-\nabla_{\vec{r}\,',\mu})s_{q,\nu}(\vec{r},\vec{r}\,'), \tag{53j}$$

$$\tilde{j}_{q,\mu}(\vec{r},\vec{r}\,') \equiv -\frac{\mathrm{i}}{2}(\nabla_{\vec{r},\mu}-\nabla_{\vec{r}\,',\mu})\tilde{\rho}_{q}(\vec{r},\vec{r}\,'), \tag{53k}$$

$$\tilde{J}_{q,\mu\nu}(\vec{r},\vec{r}\,') \equiv -\frac{\mathrm{i}}{2}(\nabla_{\vec{r},\mu}-\nabla_{\vec{r}\,',\mu})\tilde{s}_{q,\nu}(\vec{r},\vec{r}\,'), \tag{53l}$$

where $\bar{\sigma} = -\sigma$. Greek indices taking values $x$, $y$, or $z$ refer to Cartesian components of spatial vectors and tensors. Densities without Greek index such as $\rho$ and $\tilde{\rho}$ are scalars. Densities in Eq. (53) denote nonlocal matter, spin, pair, pair-spin, kinetic, spin-kinetic, pair-kinetic, pair-spin-kinetic, current, spin-current, pair-current, and pair-spin-current densities for a given nucleon species $q$, respectively.

The particular definition of the pairing densities $\tilde{\rho}_{q}(\vec{r},\vec{r}\,')$ and $\tilde{s}_{q,\nu}(\vec{r},\vec{r}\,')$ involves the time reversal of coordinates $\vec{r}\,'\sigma' q'$, which is done to provide a compact representation of the EDF kernel derived from contact interactions in terms of a local densities, which cannot be achieved in terms of $\kappa$ owing to its being skew symmetric [23,66].

The nonlocal pair density is symmetric under coordinate exchange, whereas the pair-spin density is skew symmetric

$$\tilde{\rho}_{q}(\vec{r}\,',\vec{r}) = +\tilde{\rho}_{q}(\vec{r},\vec{r}\,'), \tag{54a}$$

$$\tilde{s}_{q,\nu}(\vec{r}\,',\vec{r}) = -\tilde{s}_{q,\nu}(\vec{r},\vec{r}\,'). \tag{54b}$$

Instead of constructing them from the pair tensor (52b), the pair densities could alternatively also be derived from a pair density matrix defined as [23,66]

$$\tilde{\rho}(\vec{r}\sigma q,\vec{r}\,'\sigma' q') \equiv 2\sigma'\kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q'). \tag{55}$$

The full normal and pair density matrices can be expressed in terms of the nonlocal densities, which is equivalent to expanding a complex $2\times 2$ matrix in spin space over the unit matrix and Pauli matrices, which together form a complete basis of that space,

$$\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = \tfrac{1}{2}\big[\rho_{q}(\vec{r},\vec{r}\,')\delta_{\sigma\sigma'} + \vec{s}_{q}(\vec{r},\vec{r}\,')\cdot\langle\sigma|\hat{\vec{\sigma}}|\sigma'\rangle\big]\delta_{qq'}, \tag{56a}$$

$$\tilde{\rho}(\vec{r}\sigma q,\vec{r}\,'\sigma' q') = \tfrac{1}{2}\big[\tilde{\rho}_{q}(\vec{r},\vec{r}\,')\delta_{\sigma\sigma'} + \tilde{\vec{s}}_{q}(\vec{r},\vec{r}\,')\cdot\langle\sigma|\hat{\vec{\sigma}}|\sigma'\rangle\big]\delta_{qq'}. \tag{56b}$$

### C. Local densities

Ultimately, the expression of the EDF kernel invokes local densities obtained from the nonlocalones

through

$$\mathcal{P}_q(\vec{r}) \equiv \mathcal{P}_q(\vec{r},\vec{r}), \tag{57}$$

$$\tilde{\mathcal{P}}_q(\vec{r}) \equiv \tilde{\mathcal{P}}_q(\vec{r},\vec{r}), \tag{58}$$

where $\mathcal{P}_q$ and $\tilde{\mathcal{P}}_q$ represent any of the normal or anomalous densities in Eq. (53). The local pair densities $\tilde{s}_{q,\nu}(\vec{r})$, $\tilde{T}_{q,\nu}(\vec{r})$, and $\tilde{j}_{q,\mu}(\vec{r})$ turn out to be zero,

$$\tilde{s}_{q,\nu}(\vec{r}) = \tilde{T}_{q,\nu}(\vec{r}) = \tilde{j}_{q,\mu}(\vec{r}) = 0, \tag{59}$$

because the corresponding nonlocal densities (53) are skew symmetric under the exchange of $\vec{r}$ and $\vec{r}\,'$ [Eq. (54)].

Single-reference EDF calculations based on time-reversal-breaking quasiparticle vacua [Eq. (31)] involve pair densities that are, in general, complex. The energy being real, the EDF kernel necessarily contains also their complex conjugate deriving from $\tilde{\rho}^*_q(\vec{r},\vec{r}\,') = \sum_\sigma 2\bar{\sigma}\kappa^*(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}q) = \sum_\sigma 2\bar{\sigma}\langle\Phi|a^\dagger_{\vec{r}\sigma q}a^\dagger_{\vec{r}\,'\bar{\sigma}q}|\Phi\rangle$, etc.

### D. Isoscalar and isovector densities

We now recouple the density matrices to isoscalars and isovectors, which allow for a more transparent representation of the physics contained in an energy functional,

$$\rho_0(\vec{r},\vec{r}\,') \equiv \sum_{\sigma q}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma q), \tag{60a}$$

$$\rho_{1,\mathfrak{a}}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma q' q}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma q')\tau_{\mathfrak{a},q'q}, \tag{60b}$$

$$s_{0,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma' \sigma q}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q)\sigma_{\nu,\sigma'\sigma}, \tag{60c}$$

$$s_{1,\mathfrak{a},\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma'\sigma q' q}\rho(\vec{r}\sigma q,\vec{r}\,'\sigma' q')\sigma_{\nu,\sigma'\sigma}\tau_{\mathfrak{a},q'q}, \tag{60d}$$

$$\breve{\rho}_0(\vec{r},\vec{r}\,') \equiv \sum_{\sigma q} 4\bar{\sigma}\bar{q}\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}\bar{q}), \tag{60e}$$

$$\breve{\rho}_{1,\mathfrak{a}}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma q' q} 4\bar{\sigma}\bar{q}'\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}\bar{q}')\tau_{\mathfrak{a},q'q}, \tag{60f}$$

$$\breve{s}_{0,\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma' \sigma q} 4\bar{\sigma}'\bar{q}\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}'\bar{q})\sigma_{\nu,\sigma'\sigma}, \tag{60g}$$

$$\breve{s}_{1,\mathfrak{a},\nu}(\vec{r},\vec{r}\,') \equiv \sum_{\sigma'\sigma q' q} 4\bar{\sigma}'\bar{q}'\kappa(\vec{r}\sigma q,\vec{r}\,'\bar{\sigma}'\bar{q}')\sigma_{\nu,\sigma'\sigma}\tau_{\mathfrak{a},q'q}, \tag{60h}$$

where $\sigma_{\nu,\sigma'\sigma} \equiv \langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle$ and $\tau_{\mathfrak{a},q'q} \equiv \langle q'|\hat{\tau}_\mathfrak{a}|q\rangle$ are matrix elements of spin and isospin Pauli matrices, respectively, whereas $\bar{q} \equiv -q$. Densities with index 0 are isoscalar, whereas densities with index $(1,\mathfrak{a})$ are Cartesian components of isovector densities, with the index in fractur labeling its components $\mathfrak{a} \in \{1,2,3\}$.

In this representation, local densities are obtained in the same manner as above in Eq. (57).

When limiting oneself to pure proton and neutron density matrices as done here, it follows that [69,70]

(i) the first ($\mathfrak{a} = 1$) and second ($\mathfrak{a} = 2$) isovector components of all normal densities are zero,
(ii) all isoscalar pairing densities are zero,
(iii) the third component ($\mathfrak{a} = 3$) of all isovector pairing densities is zero.

For the sake of compact notation, normal isovector densities are written without reference to the isospin component

$$\rho_1 \equiv \rho_{1,3} \tag{61}$$

in what follows. For pair densities, however, the index for the third isospin component has to be kept.

### E. Link between the two representations

The definition of the pair densities in isoscalar/isovector representation labeled with a "breve," such as $\breve{\rho}_t(\vec{r})$, differs from the ones labeled with a "tilde," such as $\tilde{\rho}_q(\vec{r})$, by a transformation in isospin that is the homolog of the transformation in spin space that leads from $\kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q')$ to $\tilde{\rho}(\vec{r}\sigma q,\vec{r}\,'\sigma' q')$ [69,70]. Both transformations are performed to obtain local pair densities from the skew-symmetric $\kappa(\vec{r}\sigma q,\vec{r}\,'\sigma' q')$. As long as densities are represented in proton-neutron representation, only the transformation in spin space is needed, whereas the recoupling of the local densities in isospin space requires also the transformation in isospin space. For any normal density $\mathcal{P}$, the transformation between the two representations is given by

$$\mathcal{P}_n \equiv \tfrac{1}{2}(\mathcal{P}_0 + \mathcal{P}_1), \tag{62a}$$

$$\mathcal{P}_p \equiv \tfrac{1}{2}(\mathcal{P}_0 - \mathcal{P}_1). \tag{62b}$$

The first ($\breve{\mathcal{P}}_{1,1}$) and second ($\breve{\mathcal{P}}_{1,2}$) isovector components of the pairing densities are related to neutron and proton pairing densities $\tilde{\mathcal{P}}_q$, $q \in \{n,p\}$, according to [69]

$$\tilde{\mathcal{P}}_n \equiv \tfrac{1}{2}(\breve{\mathcal{P}}_{1,1} + \mathrm{i}\breve{\mathcal{P}}_{1,2}), \tag{63a}$$

$$\tilde{\mathcal{P}}_p \equiv \tfrac{1}{2}(\breve{\mathcal{P}}_{1,1} - \mathrm{i}\breve{\mathcal{P}}_{1,2}). \tag{63b}$$

### F. Deriving the energy functional

The analytical derivation of the EDF kernel from the three-body pseudopotential considered here is more cumbersome than for the usual two-body Skyrme pseudopotential. The main reason relates to the large number of terms obtained by multiplying the antisymmetrizer $\mathcal{A}_{123}$ with the exchange operators of Eqs. (48), (48a), and (50). Still, the intrinsic difficulty of calculating each individual term is the same and, for most of them, the evaluation can be done in the same manner as for the two-body Skyrme interaction. A slight complication arises in a small number of terms where position-exchange operators cannot be directly replaced with $\pm 1$ in the matrix elements. For those terms, one has to pay additional attention to which nonlocal density the gradient operators do act.

In the end, the main challenge is to handle the sheer number of terms to be evaluated. The numerical code that performs the necessary algebraic manipulations is based on shape recognition and has been written as a Unix shell script [65]. To present how the calculation proceeds in the code, Appendix C lists the steps to be taken to reduce the matrix elements of the pseudopotential to an EDF kernel that depends on local densities only for a few typical terms arising from the three-body pseudopotential.

### G. Redundant terms in the pseudopotential

Having derived the energy functional from the two- and three-body pseudopotentials, we are now looking for strict correlations between its terms. The analysis is performed at the level of the EDF kernel, i.e., examining whether the energy functional deriving from different potential terms are linearly dependent. To do so, we apply the SVD to the matrix relating the coupling constants multiplying each term in the EDF kernel to the set of parameters entering the pseudopotential. Whenever such a correlation is identified, the number of independent terms in the original pseudopotential is reduced.

Two-body terms in Eq. (51) serve as a consistency check for the procedure. In this case, the formal algebra code gives the well-known energy functional of Refs. [23,69,70], and the correlation analysis confirms that all terms are linearly independent, as expected.

Most of the redundancies in the three-body pseudopotential are easily identified given that the functional obtained from one term is often directly proportional to the functional derived from another term; see Table I for the identification of such strict proportionality. For a smaller number of terms, however, only the SVD can reveal their more intricate interdependency; see Table II. For example, the energy functional obtained from the term with parameter $u_2 y_{221}$ in Eq. (51) equals the sum of the energy functionals obtained from the terms with parameters $u_2$, $u_2 y_{21}$, and $u_2 y_{22}$ with relative weights $-1$, $+2$, and $-1$, respectively. The two terms containing a single spin or isospin-exchange operator in $\hat{P}^{\{u_0,y_0\}}_{\overline{123},\alpha}$ [Eq. (51d)] give an energy functional that is zero. The term with simultaneous spin and isospin exchange (or, equivalently, a position exchange) in Eq. (51d) provides the same energy functional as the term without an exchange operator, such that the three-body term without gradient is in the end defined by a single free parameter, as expected from earlier studies [8,59]. Last, but not least, it turns out that all gradient terms of Eqs. (51g) and (51h) are fully correlated to those in Eqs. (51e) and (51f), respectively.

TABLE I. Equivalent terms in the three-body pseudopotential of Eq. (51).

| Term | | Correlated terms |
|---|---|---|
| $u_0$ | $\leftarrow$ | $u_0 y_{03}$ |
| $u_0 y_{01}$ | $\leftarrow$ | $u_0 y_{02}$ |
| $u_1$ | $\leftarrow$ | $u_1 y_{13}, u_3 y_{30}, u_3 y_{33}, u_1 y_{121}, u_1 y_{122}, u_3 y_{321}, u_3 y_{322}, u_1 y_{123}, u_3 y_{323}$ |
| $u_1 y_{11}$ | $\leftarrow$ | $u_1 y_{12}, u_3 y_{31}, u_3 y_{32}, u_1 y_{120}, u_1 y_{125}, u_3 y_{320}, u_3 y_{325}, u_1 y_{124}, u_3 y_{324}$ |
| $u_2$ | $\leftarrow$ | $u_4, u_4 y_{43}, u_5 y_{522}, u_6 y_{622}, u_2 y_{222}, u_5 y_{534}, u_6 y_{634}$ |
| $u_2 y_{21}$ | $\leftarrow$ | $u_5 y_{52}, u_5 y_{513}, u_6 y_{62}, u_5 y_{520}, u_6 y_{620}, u_2 y_{225}, u_5 y_{525}, u_5 y_{531}, u_6 y_{624}, u_2 y_{224}, u_6 y_{632}, u_6 y_{633}$ |
| $u_2 y_{22}$ | $\leftarrow$ | $u_4 y_{42}, u_6 y_{613}, u_5 y_{532}, u_5 y_{533}$ |
| $u_2 y_{23}$ | $\leftarrow$ | $u_5 y_{512}, u_6 y_{612}, u_5 y_{530}, u_5 y_{535}$ |
| $u_2 y_{220}$ | $\leftarrow$ | $u_4 y_{41}, u_5 y_{524}, u_6 y_{625}, u_6 y_{631}$ |
| $u_2 y_{221}$ | $\leftarrow$ | $u_5 y_{53}, u_5 y_{521}, u_6 y_{621}, u_6 y_{635}$ |
| $u_2 y_{223}$ | $\leftarrow$ | $y_{63}, u_5 y_{523}, u_6 y_{623}, u_6 y_{630}$ |

TABLE II. Correlations between terms of the pseudopotential Eq. (51). See text.

| Term | $u_2$ | $u_2 y_{21}$ | $u_2 y_{22}$ |
|---|---|---|---|
| $u_2 y_{23} =$ | $-1$ | $+1$ | $+1$ |
| $u_2 y_{220} =$ | | $+1$ | $-1$ |
| $u_2 y_{221} =$ | $-1$ | $+2$ | $-1$ |
| $u_2 y_{223} =$ | $+2$ | $-3$ | |

### H. Final form of the pseudopotential

The irreducible set of central three-body operators containing two gradients is not unique as there are many equivalent possibilities to select independent terms. For consistency with the standard representation of the central part of the two-body Skyrme interaction,

$$\hat{v}_{\overline{12}} = t_0\big(\hat{\mathbb{1}}_2 + x_0\hat{P}^\sigma_{12}\big)\hat{\delta}^r_{12} \tag{64a}$$

$$+\frac{t_1}{2}\big(\hat{\mathbb{1}}_2 + x_1\hat{P}^\sigma_{12}\big)\big(\hat{\vec{k}}^{\dagger 2}_{12}\,\hat{\delta}^r_{12} + \hat{\delta}^r_{12}\,\hat{\vec{k}}^{2}_{12}\big) \tag{64b}$$

$$+t_2\big(\hat{\mathbb{1}}_2 + x_2\hat{P}^\sigma_{12}\big)\hat{\vec{k}}^{\dagger}_{12}\,\hat{\delta}^r_{12}\cdot\hat{\vec{k}}_{12}, \tag{64c}$$

we choose a form that contains only spin-exchange operators. This leads to

$$\hat{v}_{\overline{123}} = u_0\,\hat{\delta}^r_{13}\hat{\delta}^r_{23} \tag{64d}$$

$$+\frac{u_1}{2}\big(\hat{\mathbb{1}}_3 + y_1\hat{P}^\sigma_{12}\big)\big(\hat{\vec{k}}^{\dagger 2}_{12}\hat{\delta}^r_{13}\hat{\delta}^r_{23} + \hat{\delta}^r_{13}\hat{\delta}^r_{23}\hat{\vec{k}}^{2}_{12}\big) \tag{64e}$$

$$+u_2\big(\hat{\mathbb{1}}_3 + y_{21}\hat{P}^\sigma_{12}\big)\hat{\vec{k}}^{\dagger}_{12}\,\hat{\delta}^r_{13}\hat{\delta}^r_{23}\cdot\hat{\vec{k}}_{12} \tag{64f}$$

$$+u_2 y_{22}\big(\hat{P}^\sigma_{13} + \hat{P}^\sigma_{23}\big)\hat{\vec{k}}^{\dagger}_{12}\,\hat{\delta}^r_{13}\hat{\delta}^r_{23}\cdot\hat{\vec{k}}_{12}, \tag{64g}$$

where $u_0$, $u_1$, $y_1$, $u_2$, $y_{21}$, and $y_{22}$ denote the final set of free parameters complementing $t_0$, $x_0$, $t_1$, $x_1$, $t_2$, and $x_2$. There are altogether 12 parameters for the central terms.

The complexity of the final three-body pseudopotential is tremendously reduced compared to the original expression [Eq. (51)]. As a matter of fact, its spatial content can be obtained by inserting a mere $\delta$ operator $\hat{\delta}^r_{23}$ into the central two-body terms. Still, the spin-isospin structure in Eq. (64g) is richer than that of the corresponding two-body operator of Eq. (64c), such that the form of the three-body pseudopotential could not have been completely guessed by analogy with the two-body terms.

Compared to three-body contact potentials with two gradients studied in the past, our final form contains one term, Eq. (64g), that, to the best of our knowledge, has never been considered before; see Table III. As a matter of fact, most published work considered an even smaller subset. Most importantly, these earlier works [54–58,60,62] discussed only nuclear matter and/or spherical nuclei and ignored the possibility of pairing correlations, such that they present only incomplete expressions for the energy functional and the corresponding one-body fields.

### I. Energy functional

Starting from a Skyrme-like pseudopotential, each term of the resulting energy functional can be expressed as the integral

TABLE III. Three-body terms in Eq. (64) labeled by their parameters that have been considered in earlier work as indicated by +.

| Reference | $u_0$ | $u_1$ | $u_1y_1$ | $u_2$ | $u_2y_{21}$ | $u_2y_{22}$ |
|---|---|---|---|---|---|---|
| [54] | + | + | − | − | − | − |
| [55] | + | + | − | − | − | − |
| [56] | + | − | − | + | + | − |
| [60] | + | + | − | − | − | − |
| [57] | + | + | − | + | + | − |
| [58] | + | + | − | − | − | − |
| [62] | + | + | + | + | + | − |

over a local energy density, i.e.,

$$E^{\rho} \equiv \int d^3r\ \mathcal{E}^{\rho}(\vec{r}), \tag{65a}$$

$$E^{\rho\rho} \equiv \int d^3r\ \mathcal{E}^{\rho\rho}(\vec{r}), \tag{65b}$$

$$E^{\kappa\kappa} \equiv \int d^3r\ \mathcal{E}^{\kappa\kappa}(\vec{r}), \tag{65c}$$

$$E^{\rho\rho\rho} \equiv \int d^3r\ \mathcal{E}^{\rho\rho\rho}(\vec{r}), \tag{65d}$$

$$E^{\kappa\kappa\rho} \equiv \int d^3r\ \mathcal{E}^{\kappa\kappa\rho}(\vec{r}). \tag{65e}$$

We give now the energy functional in a representation using isoscalar and isovector densities. Its representation in terms of proton and neutron densities can be found in Appendix A.

#### 1. Linear part

Omitting the argument $\vec{r}$ of the local densities for brevity, the linear energy density associated with the effective one-body kinetic energy operator is given by

$$\mathcal{E}^{\rho} = \frac{\hbar^2}{2m}\tau_0. \tag{66}$$

#### 2. Bilinear part

The normal part of the bilinear energy density is well known and reads

$$\begin{aligned}\mathcal{E}^{\rho\rho} = \sum_{t=0,1}\Bigg[ & A_t^{\rho}\rho_t\rho_t + A_t^{\tau}\rho_t\tau_t + A_t^{\nabla\rho}(\vec{\nabla}\rho_t)\cdot(\vec{\nabla}\rho_t) \\ & + \sum_{\mu\nu} A_t^{J} J_{t,\mu\nu}J_{t,\mu\nu} + A_t^{s}\vec{s}_t\cdot\vec{s}_t + A_t^{T}\vec{s}_t\cdot\vec{T}_t \\ & + A_t^{j}\vec{j}_t\cdot\vec{j}_t + \sum_{\mu\nu} A_t^{\nabla s}(\nabla_\mu s_{t,\nu})(\nabla_\mu s_{t,\nu})\Bigg],\end{aligned} \tag{67}$$

whereas its anomalous part is given by

$$\begin{aligned}\mathcal{E}^{\kappa\kappa} = \sum_{\mathfrak{a}=1,2}\Bigg[ & A^{\check{\rho}}\check{\rho}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{a}} + A^{\check{\tau}^*}\check{\tau}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{a}} + A^{\check{\tau}}\check{\tau}_{1,\mathfrak{a}}\check{\rho}^*_{1,\mathfrak{a}} \\ & + A^{\nabla\check{\rho}}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\cdot(\vec{\nabla}\check{\rho}_{1,\mathfrak{a}}) + \sum_{\mu\nu} A^{\check{J}}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{J}_{1,\mathfrak{a},\mu\nu}\Bigg].\end{aligned} \tag{68}$$

The relations between the coupling constants of the energy functional and the pseudopotential parameters are listed in Tables IV and V.

#### 3. Trilinear part

The normal part of the trilinear energy density reads

$$\begin{aligned}\mathcal{E}^{\rho\rho\rho} = \sum_{t=0,1}\Bigg\{ & B_t^{\rho}\rho_t\rho_t\rho_0 + B_t^{s}\vec{s}_t\cdot\vec{s}_t\rho_0 + B_t^{\tau}\rho_t\tau_t\rho_0 + B_t^{\tau s}\tau_t\vec{s}_t\cdot\vec{s}_0 + B_t^{T}\vec{s}_t\cdot\vec{T}_t\rho_0 + B_{t\bar{t}}^{T}\vec{s}_t\cdot\vec{T}_{\bar{t}}\rho_1 \\ & + B_t^{\nabla\rho}(\vec{\nabla}\rho_t)\cdot(\vec{\nabla}\rho_t)\rho_0 + B_t^{j}\vec{j}_t\cdot\vec{j}_t\rho_0 + \sum_{\mu\nu}\Big[B_t^{\nabla s}(\nabla_\mu s_{t,\nu})(\nabla_\mu s_{t,\nu})\rho_0 + B_t^{\nabla\rho s}(\nabla_\mu\rho_t)(\nabla_\mu s_{t,\nu})s_{0,\nu} \\ & + B_{t\bar{t}}^{\nabla\rho s}(\nabla_\mu\rho_t)(\nabla_\mu s_{\bar{t},\nu})s_{1,\nu} + B_t^{J}J_{t,\mu\nu}J_{t,\mu\nu}\rho_0 + B_t^{Js}j_{t,\mu}J_{t,\mu\nu}s_{0,\nu} + B_{t\bar{t}}^{Js}j_{t,\mu}J_{\bar{t},\mu\nu}s_{1,\nu}\Big] \\ & + \sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\Big[B_t^{\nabla sJ}(\nabla_\mu s_{t,\nu})J_{t,\mu\lambda}s_{0,\kappa} + B_{t\bar{t}}^{\nabla sJ}(\nabla_\mu s_{t,\nu})J_{\bar{t},\mu\lambda}s_{1,\kappa}\Big]\Bigg\} + B_{10}^{s}\vec{s}_1\cdot\vec{s}_0\rho_1 + B_{10}^{\tau}\rho_1\tau_0\rho_1 + B_{10}^{\tau s}\tau_0\vec{s}_1\cdot\vec{s}_1 \\ & + B_{10}^{\nabla\rho}(\vec{\nabla}\rho_1)\cdot(\vec{\nabla}\rho_0)\rho_1 + \sum_{\mu\nu}B_{10}^{\nabla s}(\nabla_\mu s_{1,\nu})(\nabla_\mu s_{0,\nu})\rho_1 + B_{10}^{j}\vec{j}_1\cdot\vec{j}_0\rho_1 + \sum_{\mu\nu}B_{10}^{J}J_{1,\mu\nu}J_{0,\mu\nu}\rho_1,\end{aligned} \tag{69}$$

whereas its anomalous part is given by

$$\begin{aligned}\mathcal{E}^{\kappa\kappa\rho} = \sum_{\mathfrak{a}=1,2}\Bigg\{ & B_0^{\check{\rho}}\check{\rho}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{a}}\rho_0 + B_0^{\check{\tau}^*}\check{\tau}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{a}}\rho_0 + B_0^{\check{\tau}}\check{\rho}^*_{1,\mathfrak{a}}\check{\tau}_{1,\mathfrak{a}}\rho_0 + B_0^{\check{\rho}\tau}\check{\rho}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{a}}\tau_0 + B_0^{\nabla\check{\rho}}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\cdot(\vec{\nabla}\check{\rho}_{1,\mathfrak{a}})\rho_0 \\ & + B_0^{\nabla\check{\rho}^*\check{\rho}}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\check{\rho}_{1,\mathfrak{a}}\cdot(\vec{\nabla}\rho_0) + B_0^{\check{\rho}^*\nabla\check{\rho}}\check{\rho}^*_{1,\mathfrak{a}}(\vec{\nabla}\check{\rho}_{1,\mathfrak{a}})\cdot(\vec{\nabla}\rho_0) + \mathrm{i}B_0^{\nabla\check{\rho}^*j}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\check{\rho}_{1,\mathfrak{a}}\cdot\vec{j}_0 + \mathrm{i}B_0^{\nabla\check{\rho}j}\check{\rho}^*_{1,\mathfrak{a}}(\vec{\nabla}\check{\rho}_{1,\mathfrak{a}})\cdot\vec{j}_0 \\ & + \sum_{\mu\nu}\Big[B_0^{\check{J}}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{J}_{1,\mathfrak{a},\mu\nu}\rho_0 + B_0^{\check{J}^*\check{\rho}}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{\rho}_{1,\mathfrak{a}}J_{0,\mu\nu} + B_0^{\check{\rho}^*\check{J}}\check{\rho}^*_{1,\mathfrak{a}}\check{J}_{1,\mathfrak{a},\mu\nu}J_{0,\mu\nu} + \mathrm{i}B_0^{\nabla\check{\rho}^*\check{J}}(\nabla_\mu\check{\rho}^*_{1,\mathfrak{a}})\check{J}_{1,\mathfrak{a},\mu\nu}s_{0,\nu} \\ & + \mathrm{i}B_0^{\check{J}^*\nabla\check{\rho}}\check{J}^*_{1,\mathfrak{a},\mu\nu}(\nabla_\mu\check{\rho}_{1,\mathfrak{a}})s_{0,\nu} + \mathrm{i}B_0^{\check{J}^*\nabla s}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{\rho}_{1,\mathfrak{a}}(\nabla_\mu s_{0,\nu}) + \mathrm{i}B_0^{\check{J}\nabla s}\check{\rho}^*_{1,\mathfrak{a}}\check{J}_{1,\mathfrak{a},\mu\nu}(\nabla_\mu s_{0,\nu})\Big]\Bigg\}\end{aligned}$$

$$+\sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\left[\mathrm{i}B_0^{\check{J}^2 s}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{J}_{1,\mathfrak{a},\mu\lambda}s_{0,\kappa}\right]\Big\}+\sum_{\mathfrak{a},\mathfrak{b}=1,2}\sum_{\mathfrak{c}=3}\epsilon_{\mathfrak{a}\mathfrak{b}\mathfrak{c}}\Big\{\mathrm{i}B_1^{\check{\rho}}\check{\rho}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{b}}\rho_{1,\mathfrak{c}}+\mathrm{i}B_1^{\check{\tau}^*}\check{\tau}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{b}}\rho_{1,\mathfrak{c}}+\mathrm{i}B_1^{\check{\tau}}\check{\rho}^*_{1,\mathfrak{a}}\check{\tau}_{1,\mathfrak{b}}\rho_{1,\mathfrak{c}}$$
$$+\mathrm{i}B_1^{\check{\rho}\tau}\check{\rho}^*_{1,\mathfrak{a}}\check{\rho}_{1,\mathfrak{b}}\tau_{1,\mathfrak{c}}+\mathrm{i}B_1^{\nabla\check{\rho}}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\cdot(\vec{\nabla}\check{\rho}_{1,\mathfrak{b}})\rho_{1,\mathfrak{c}}+\mathrm{i}B_1^{\nabla\check{\rho}^*\check{\rho}}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\check{\rho}_{1,\mathfrak{b}}\cdot(\vec{\nabla}\rho_{1,\mathfrak{c}})+\mathrm{i}B_1^{\check{\rho}^*\nabla\check{\rho}}\check{\rho}^*_{1,\mathfrak{a}}(\vec{\nabla}\check{\rho}_{1,\mathfrak{b}})\cdot(\vec{\nabla}\rho_{1,\mathfrak{c}})$$
$$+B_1^{\nabla\check{\rho}^* j}(\vec{\nabla}\check{\rho}^*_{1,\mathfrak{a}})\check{\rho}_{1,\mathfrak{b}}\cdot\vec{j}_{1,\mathfrak{c}}+B_1^{\nabla\check{\rho}j}\check{\rho}^*_{1,\mathfrak{a}}(\vec{\nabla}\check{\rho}_{1,\mathfrak{b}})\cdot\vec{j}_{1,\mathfrak{c}}+\sum_{\mu\nu}\Big[\mathrm{i}B_1^{\check{J}}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{J}_{1,\mathfrak{b},\mu\nu}\rho_{1,\mathfrak{c}}+\mathrm{i}B_1^{\check{J}^*\check{\rho}}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{\rho}_{1,\mathfrak{b}}J_{1,\mathfrak{c},\mu\nu}$$
$$+\mathrm{i}B_1^{\check{\rho}^*\check{J}}\check{\rho}^*_{1,\mathfrak{a}}\check{J}_{1,\mathfrak{b},\mu\nu}J_{1,\mathfrak{c},\mu\nu}+B_1^{\nabla\check{\rho}^*\check{J}}(\nabla_\mu\check{\rho}^*_{1,\mathfrak{a}})\check{J}_{1,\mathfrak{b},\mu\nu}s_{1,\mathfrak{c},\nu}+B_1^{\check{J}^*\nabla\check{\rho}}\check{J}^*_{1,\mathfrak{a},\mu\nu}(\nabla_\mu\check{\rho}_{1,\mathfrak{b}})s_{1,\mathfrak{c},\nu}$$
$$+B_1^{\check{J}^*\nabla s}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{\rho}_{1,\mathfrak{b}}(\nabla_\mu s_{1,\mathfrak{c},\nu})+B_1^{\check{J}\nabla s}\check{\rho}^*_{1,\mathfrak{a}}\check{J}_{1,\mathfrak{b},\mu\nu}(\nabla_\mu s_{1,\mathfrak{c},\nu})\Big]+\sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\left[B_1^{\check{J}^2 s}\check{J}^*_{1,\mathfrak{a},\mu\nu}\check{J}_{1,\mathfrak{b},\mu\lambda}s_{1,\mathfrak{c},\kappa}\right]\Big\}. \tag{70}$$

Sums over Greek indices run over $x$, $y$, and $z$ components of spatial vectors, whereas sums over indices in fractur are over isovector components. In the normal part of the trilinear EDF, the notation $\bar{t}$ is such that $\bar{t}=1$ (0) whenever $t=0$ (1). Coupling constants are related to pseudopotential parameters according to Tables VI and VII.

#### 4. Discussion

A few further comments on the structure of bilinear and trilinear contributions to the EDF kernel are in order.

In the case of pure proton and neutron density matrices, as considered here, only a pairing functional of isovector character remains [69,70], as all isoscalar pair densities are zero; see Sec. V D. The generic isospin structure of the terms containing isovector densities is

$$\sum_{\mathfrak{a}}\mathcal{P}_{1,\mathfrak{a}}\mathcal{P}'_{1,\mathfrak{a}}=\mathcal{P}_{1,3}\,\mathcal{P}'_{1,3}, \tag{71a}$$

$$\sum_{\mathfrak{a}}\check{\mathcal{P}}^*_{1,\mathfrak{a}}\check{\mathcal{P}}'_{1,\mathfrak{a}}=\check{\mathcal{P}}^*_{1,1}\check{\mathcal{P}}'_{1,1}+\check{\mathcal{P}}^*_{1,2}\check{\mathcal{P}}'_{1,2}, \tag{71b}$$

$$\sum_{\mathfrak{a}}\mathcal{P}_{1,\mathfrak{a}}\mathcal{P}'_{1,\mathfrak{a}}\mathcal{P}''_0=\mathcal{P}_{1,3}\,\mathcal{P}'_{1,3}\mathcal{P}''_0, \tag{71c}$$

$$\sum_{\mathfrak{a}}\check{\mathcal{P}}^*_{1,\mathfrak{a}}\check{\mathcal{P}}'_{1,\mathfrak{a}}\mathcal{P}''_0=(\check{\mathcal{P}}^*_{1,1}\check{\mathcal{P}}'_{1,1}+\check{\mathcal{P}}^*_{1,2}\check{\mathcal{P}}'_{1,2})\mathcal{P}''_0, \tag{71d}$$

$$\sum_{\mathfrak{a}\mathfrak{b}\mathfrak{c}}\epsilon_{\mathfrak{a}\mathfrak{b}\mathfrak{c}}\check{\mathcal{P}}^*_{1,\mathfrak{a}}\check{\mathcal{P}}'_{1,\mathfrak{b}}\mathcal{P}''_{1,\mathfrak{c}}=(\check{\mathcal{P}}^*_{1,1}\check{\mathcal{P}}'_{1,2}-\check{\mathcal{P}}^*_{1,2}\check{\mathcal{P}}'_{1,1})\mathcal{P}''_{1,3}. \tag{71e}$$

Equations (71a) to (71d) correspond to scalar products of two isovectors coupled to isospin zero (and which might be multiplied by a normal isoscalar density), whereas Eq. (71e) displays a triple product of three isovectors that are thereby also coupled to an isoscalar.

As all pair densities are, in general, complex, all terms containing two different pair densities $\check{\mathcal{P}}^*$ and $\check{\mathcal{P}}'$ taking the form $\check{\mathcal{P}}^*\check{\mathcal{P}}'+\check{\mathcal{P}}\check{\mathcal{P}}'^*$ for the functional kernel to be real.

The bilinear part of the functional does not contain all possible combinations of local densities compatible with spatial symmetries [15,69]. Indeed, some of those combinations only emerge in the functional derived from spin-orbit and -tensor forces [28,34]. The same applies to the trilinear part of the functional. We postpone the discussion of spin-orbit and -tensor terms to a future publication [64].

There are two equivalent ways of writing the terms with derivatives of local densities in the bilinear part of the EDF, i.e., the third and last term in Eq. (67) and the last term in Eq. (68), which differ from each other by an integration by parts [15]. Usually, these terms are expressed in terms of Laplacians [3,15,28,30,34]. Trilinear terms, however, do not offer such a freedom. For internal consistency, we thus define associated terms in the bilinear part of the EDF in terms of first derivatives of local densities, at variance with most of the literature.

Trilinear terms $\mathcal{E}^{\rho\rho\rho}$ and $\mathcal{E}^{\kappa\kappa\rho}$ display a much more complex structure than would be obtained by adding a mere density

TABLE IV. Coefficients of the normal part of the bilinear EDF kernel [Eq. (67)] as a function of the parameters of the pseudopotential of Eqs. (64a)–(64c). Missing entries are zero.

| | $t_0$ | $t_0x_0$ | $t_1$ | $t_1x_1$ | $t_2$ | $t_2x_2$ |
|---|---|---|---|---|---|---|
| $A_0^\rho$ = | $+\frac{3}{8}$ | | | | | |
| $A_1^\rho$ = | $-\frac{1}{8}$ | $-\frac{1}{4}$ | | | | |
| $A_0^s$ = | $-\frac{1}{8}$ | $+\frac{1}{4}$ | | | | |
| $A_1^s$ = | $-\frac{1}{8}$ | | | | | |
| $A_0^\tau$ = | | | $+\frac{3}{16}$ | | $+\frac{5}{16}$ | $+\frac{1}{4}$ |
| $A_1^\tau$ = | | | $-\frac{1}{16}$ | $-\frac{1}{8}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ |
| $A_0^T$ = | | | $-\frac{1}{16}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ |
| $A_1^T$ = | | | $-\frac{1}{16}$ | | $+\frac{1}{16}$ | |
| $A_0^{\nabla\rho}$ = | | | $+\frac{9}{64}$ | | $-\frac{5}{64}$ | $-\frac{1}{16}$ |
| $A_1^{\nabla\rho}$ = | | | $-\frac{3}{64}$ | $-\frac{3}{32}$ | $-\frac{1}{64}$ | $-\frac{1}{32}$ |
| $A_0^{\nabla s}$ = | | | $-\frac{3}{64}$ | $+\frac{3}{32}$ | $-\frac{1}{64}$ | $-\frac{1}{32}$ |
| $A_1^{\nabla s}$ = | | | $-\frac{3}{64}$ | | $-\frac{1}{64}$ | |
| $A_0^j$ = | | | $-\frac{3}{16}$ | | $-\frac{5}{16}$ | $-\frac{1}{4}$ |
| $A_1^j$ = | | | $+\frac{1}{16}$ | $+\frac{1}{8}$ | $-\frac{1}{16}$ | $-\frac{1}{8}$ |
| $A_0^J$ = | | | $+\frac{1}{16}$ | $-\frac{1}{8}$ | $-\frac{1}{16}$ | $-\frac{1}{8}$ |
| $A_1^J$ = | | | $+\frac{1}{16}$ | | $-\frac{1}{16}$ | |

TABLE V. Same as Table IV, but for the anomalous part of the bilinear EDF kernel [Eq. (68)].

| | $t_0$ | $t_0x_0$ | $t_1$ | $t_1x_1$ | $t_2$ | $t_2x_2$ |
|---|---|---|---|---|---|---|
| $A^{\check{\rho}}$ = | $+\frac{1}{8}$ | $-\frac{1}{8}$ | | | | |
| $A^{\check{\tau}^*}$ = | | | $+\frac{1}{16}$ | $-\frac{1}{16}$ | | |
| $A^{\check{\tau}}$ = | | | $+\frac{1}{16}$ | $-\frac{1}{16}$ | | |
| $A^{\nabla\check{\rho}}$ = | | | $+\frac{1}{32}$ | $-\frac{1}{32}$ | | |
| $A^{\check{J}}$ = | | | | | $+\frac{1}{8}$ | $+\frac{1}{8}$ |

TABLE VI. Same as Table IV for the normal part of the trilinear EDF [Eq. (69)].

| | $u_0$ | $u_1$ | $u_1 y_1$ | $u_2$ | $u_2 y_{21}$ | $u_2 y_{22}$ |
|---|---|---|---|---|---|---|
| $B_0^{\rho} =$ | $+\frac{3}{16}$ | | | | | |
| $B_1^{\rho} =$ | $-\frac{3}{16}$ | | | | | |
| $B_0^{\tau} =$ | | $+\frac{3}{32}$ | | $+\frac{15}{64}$ | $+\frac{3}{16}$ | $+\frac{3}{32}$ |
| $B_{10}^{\tau} =$ | | $-\frac{1}{32}$ | $+\frac{1}{32}$ | $-\frac{5}{64}$ | $-\frac{1}{16}$ | $-\frac{7}{32}$ |
| $B_1^{\tau} =$ | | $-\frac{1}{16}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ |
| $B_0^{\nabla\rho} =$ | | $+\frac{15}{128}$ | | $-\frac{15}{256}$ | $-\frac{3}{64}$ | $-\frac{3}{128}$ |
| $B_{10}^{\nabla\rho} =$ | | $-\frac{5}{64}$ | $+\frac{1}{32}$ | $+\frac{5}{128}$ | $+\frac{1}{32}$ | $+\frac{7}{64}$ |
| $B_1^{\nabla\rho} =$ | | $-\frac{5}{128}$ | $-\frac{1}{32}$ | $-\frac{7}{256}$ | $-\frac{1}{32}$ | $-\frac{5}{128}$ |
| $B_0^{J} =$ | | $+\frac{1}{32}$ | $-\frac{1}{16}$ | $-\frac{7}{64}$ | $-\frac{1}{8}$ | $+\frac{1}{32}$ |
| $B_{10}^{J} =$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ | $+\frac{1}{32}$ | | $+\frac{3}{16}$ |
| $B_1^{J} =$ | | $+\frac{1}{32}$ | | $-\frac{7}{64}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ |
| $B_0^{s} =$ | $-\frac{3}{16}$ | | | | | |
| $B_{10}^{s} =$ | $+\frac{3}{8}$ | | | | | |
| $B_1^{s} =$ | $-\frac{3}{16}$ | | | | | |
| $B_0^{T} =$ | | $-\frac{1}{16}$ | $+\frac{1}{32}$ | $+\frac{1}{32}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ |
| $B_{10}^{T} =$ | | $+\frac{1}{16}$ | $-\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{16}$ | $-\frac{1}{8}$ |
| $B_{01}^{T} =$ | | $+\frac{1}{16}$ | | $-\frac{1}{32}$ | | |
| $B_1^{T} =$ | | $-\frac{1}{16}$ | | $+\frac{1}{32}$ | | |
| $B_0^{\tau s} =$ | | $-\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{5}{64}$ | $-\frac{1}{16}$ | $+\frac{5}{32}$ |
| $B_{10}^{\tau s} =$ | | $-\frac{1}{32}$ | | $-\frac{5}{64}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ |
| $B_1^{\tau s} =$ | | $+\frac{1}{16}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B_0^{\nabla s} =$ | | $-\frac{5}{128}$ | $+\frac{1}{32}$ | $-\frac{7}{256}$ | $-\frac{1}{32}$ | $+\frac{1}{128}$ |
| $B_{10}^{\nabla s} =$ | | $+\frac{5}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{128}$ | | $+\frac{3}{64}$ |
| $B_1^{\nabla s} =$ | | $-\frac{5}{128}$ | | $-\frac{7}{256}$ | $-\frac{1}{64}$ | $-\frac{1}{128}$ |
| $B_0^{\nabla\rho s} =$ | | $-\frac{5}{64}$ | $-\frac{1}{32}$ | $+\frac{5}{128}$ | $+\frac{1}{32}$ | $-\frac{5}{64}$ |
| $B_{01}^{\nabla\rho s} =$ | | $-\frac{5}{64}$ | | $+\frac{5}{128}$ | $+\frac{1}{32}$ | $+\frac{1}{64}$ |
| $B_{10}^{\nabla\rho s} =$ | | $+\frac{5}{64}$ | | $+\frac{1}{128}$ | $+\frac{1}{32}$ | $+\frac{1}{64}$ |
| $B_1^{\nabla\rho s} =$ | | $+\frac{5}{64}$ | $+\frac{1}{32}$ | $+\frac{1}{128}$ | | $-\frac{3}{64}$ |
| $B_0^{Js} =$ | | $+\frac{1}{16}$ | $+\frac{1}{16}$ | $+\frac{5}{32}$ | $+\frac{1}{8}$ | $-\frac{5}{16}$ |
| $B_{01}^{Js} =$ | | $+\frac{1}{16}$ | | $+\frac{5}{32}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ |
| $B_{10}^{Js} =$ | | $-\frac{1}{16}$ | | $+\frac{1}{32}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ |
| $B_1^{Js} =$ | | $-\frac{1}{16}$ | $-\frac{1}{16}$ | $+\frac{1}{32}$ | | $-\frac{3}{16}$ |
| $B_0^{\nabla s J} =$ | | | | $-\frac{3}{64}$ | $-\frac{3}{32}$ | $+\frac{3}{32}$ |
| $B_{01}^{\nabla s J} =$ | | | $+\frac{1}{16}$ | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_{10}^{\nabla s J} =$ | | | $-\frac{1}{32}$ | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_1^{\nabla s J} =$ | | | $-\frac{1}{32}$ | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_0^{j} =$ | | $-\frac{3}{32}$ | | $-\frac{15}{64}$ | $-\frac{3}{16}$ | $-\frac{3}{32}$ |
| $B_{10}^{j} =$ | | $+\frac{1}{16}$ | $-\frac{1}{16}$ | $+\frac{5}{32}$ | $+\frac{1}{8}$ | $+\frac{7}{16}$ |
| $B_1^{j} =$ | | $+\frac{1}{32}$ | $+\frac{1}{16}$ | $-\frac{7}{64}$ | $-\frac{1}{8}$ | $-\frac{5}{32}$ |

dependence to the coupling constants entering $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$. Although one can find trilinear terms that do have the structure of terms appearing in the bilinear part of the functional times $\rho_0(\vec{r})$, relative weights between isoscalar and isovector terms, or between time-even, time-odd, and pairing terms, are not the same as in their bilinear counterparts. This is a consequence of Pauli's exclusion principle that is fully preserved for energy functionals deriving from a three-body pseudopotential, but violated for functionals deriving from density-dependent two-body interactions; see the discussion in Refs. [8,60] regarding terms without gradients.

TABLE VII. Same as Table IV, but for the anomalous part of the trilinear EDF kernel [Eq. (70)].

| | $u_0$ | $u_1$ | $u_1 y_1$ | $u_2$ | $u_2 y_{21}$ | $u_2 y_{22}$ |
|---|---|---|---|---|---|---|
| $B_0^{\check\rho} =$ | $+\frac{3}{16}$ | | | | | |
| $B_0^{\check\tau^*} =$ | | $+\frac{3}{64}$ | $-\frac{3}{128}$ | | | |
| $B_0^{\check\tau} =$ | | $+\frac{3}{64}$ | $-\frac{3}{128}$ | | | |
| $B_0^{\check\rho\tau} =$ | | $+\frac{1}{32}$ | $+\frac{1}{64}$ | $+\frac{5}{64}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ |
| $B_0^{\nabla\check\rho} =$ | | $+\frac{1}{32}$ | $-\frac{1}{128}$ | $+\frac{5}{256}$ | $+\frac{1}{64}$ | $-\frac{1}{64}$ |
| $B_0^{\nabla\check\rho^*\check\rho} =$ | | $+\frac{5}{128}$ | $+\frac{1}{128}$ | $-\frac{5}{256}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B_0^{\check\rho^*\nabla\check\rho} =$ | | $+\frac{5}{128}$ | $+\frac{1}{128}$ | $-\frac{5}{256}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B_0^{\nabla\check\rho^* j} =$ | | $-\frac{1}{64}$ | $-\frac{1}{128}$ | $-\frac{5}{128}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_0^{\nabla\check\rho j} =$ | | $+\frac{1}{64}$ | $+\frac{1}{128}$ | $+\frac{5}{128}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B_0^{\check J} =$ | | | | $+\frac{9}{64}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ |
| $B_0^{J^*\check\rho} =$ | | | $-\frac{1}{64}$ | $-\frac{3}{64}$ | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B_0^{\check\rho^* J} =$ | | | $-\frac{1}{64}$ | $-\frac{3}{64}$ | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B_0^{\nabla\check\rho^*\check J} =$ | | | $+\frac{1}{128}$ | $+\frac{3}{128}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B_0^{\check J^*\nabla\check\rho} =$ | | | $-\frac{1}{128}$ | $-\frac{3}{128}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_0^{J^*\nabla s} =$ | | | $-\frac{1}{64}$ | $+\frac{3}{128}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B_0^{\check J\nabla s} =$ | | | $+\frac{1}{64}$ | $-\frac{3}{128}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_0^{\check J^2 s} =$ | | | | $+\frac{3}{64}$ | $+\frac{1}{32}$ | $-\frac{1}{8}$ |
| $B_1^{\check\rho} =$ | $-\frac{3}{16}$ | | | | | |
| $B_1^{\check\tau^*} =$ | | $-\frac{3}{64}$ | $+\frac{3}{128}$ | | | |
| $B_1^{\check\tau} =$ | | $-\frac{3}{64}$ | $+\frac{3}{128}$ | | | |
| $B_1^{\check\rho\tau} =$ | | $-\frac{1}{32}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B_1^{\nabla\check\rho} =$ | | $-\frac{1}{32}$ | $+\frac{1}{128}$ | $+\frac{1}{256}$ | $+\frac{1}{128}$ | $-\frac{1}{128}$ |
| $B_1^{\nabla\check\rho^*\check\rho} =$ | | $-\frac{5}{128}$ | $-\frac{1}{128}$ | $-\frac{1}{256}$ | $-\frac{1}{128}$ | $+\frac{1}{128}$ |
| $B_1^{\check\rho^*\nabla\check\rho} =$ | | $-\frac{5}{128}$ | $-\frac{1}{128}$ | $-\frac{1}{256}$ | $-\frac{1}{128}$ | $+\frac{1}{128}$ |
| $B_1^{\nabla\check\rho^* j} =$ | | $-\frac{1}{64}$ | $-\frac{1}{128}$ | $+\frac{1}{128}$ | $+\frac{1}{64}$ | $-\frac{1}{64}$ |
| $B_1^{\nabla\check\rho j} =$ | | $+\frac{1}{64}$ | $+\frac{1}{128}$ | $-\frac{1}{128}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B_1^{\check J} =$ | | | | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $-\frac{5}{32}$ |
| $B_1^{\check J^*\check\rho} =$ | | | $+\frac{1}{64}$ | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_1^{\check\rho^* J} =$ | | | $+\frac{1}{64}$ | $-\frac{3}{64}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B_1^{\nabla\check\rho^*\check J} =$ | | | $+\frac{1}{128}$ | $-\frac{3}{128}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B_1^{\check J^*\nabla\check\rho} =$ | | | $-\frac{1}{128}$ | $+\frac{3}{128}$ | $+\frac{1}{64}$ | $-\frac{1}{64}$ |
| $B_1^{J^*\nabla s} =$ | | | $-\frac{1}{64}$ | $-\frac{3}{128}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B_1^{\check J\nabla s} =$ | | | $+\frac{1}{64}$ | $+\frac{3}{128}$ | $+\frac{1}{64}$ | $-\frac{1}{64}$ |
| $B_1^{\check J^2 s} =$ | | | | $-\frac{3}{64}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ |

Keeping the coupling constants consistent with Tables IV, V, VI, and VII, the energy functional (66)–(70) is invariant under arbitrary local gauge transformations; see Appendix E. This property indicates the local character of the underlying pseudopotential [14]. Galilean invariance, which is a necessary requirement for interactions to be meaningfully used in dynamical calculations such as time-dependent HF, is one special case of the more general invariance under arbitrary gauge transformations and therefore automatically fulfilled.

The first critical check that the formal algebra code is proceeding correctly is provided by the fact that well-known results (EDF, one-body fields, infinite matter properties) associated with the central part of the (density-independent) two-body Skyrme interaction are recovered. For the trilinear

part, two nontrivial, though indirect, tests give us further confidence; i.e., (i) the local gauge invariance of the EDF kernel is exactly fulfilled as mentioned above and (ii) the numerical code that tracks both the real and the imaginary parts of the EDF kernel computes the latter to be strictly zero for each Hermitian piece of the pseudopotential.

Properties of homogeneous nuclear matter, both symmetric and asymmetric in isospin and/or spin, along with Landau parameters, are discussed in in Appendix B. Additionally, the energy functional in the often-used proton-neutron representation is provided in Appendix B, whereas the expressions for the associated one-body fields entering the HFB equations of motion are listed in Appendix D.

## VI. CONCLUSIONS AND OUTLOOK

We have constructed the most general central Skyrme-type three-body pseudopotential containing up to two derivatives, derived the corresponding EDF (i.e., time-even and time-odd contributions to the normal part of the EDF along with the complete anomalous part) and one-body fields as well as computed an extensive set of infinite nuclear-matter properties. Our objective is to build EDF parametrizations that derive strictly from (density-independent) two- and three-body Skyrme-like pseudopotentials as required for spuriosity-free MR calculations.

The main observations and conclusions of the present work are as follows.

(i) The central three-body pseudopotential is defined out of six independent parameters in total. Combined with the central part of the two-body Skyrme pseudopotential, this leads to a total of 12 parameters prior to considering spin-orbit and -tensor terms.
(ii) The structure of some of the three-body terms containing gradients cannot be conjectured by just inserting an additional $\delta$ function into a two-body Skyrme interaction of standard form.
(iii) The EDF trilinear kernel possesses a much more complex structure than the functional resulting from a density-dependent two-body vertex, in particular as far as time-odd and pairing parts are concerned.

The main points for future studies are as follows.

(i) The structure of the *effective* three-body interaction to be used in nuclear EDF calculations has been investigated in Ref. [74] on the basis of a general analysis of low-density finite fermion systems. The starting point of the inquiry is the Lee and Yang expansion of the ground-state energy of an homogeneous low-density fermionic gas governed by a short-range two-body interaction [75]. Combining this expansion with *ab initio* Green's function Monte Carlo calculations of dilute fermions in a harmonic trap, it is concluded that the finite range and nonlocality of the effective three-body interaction, resulting in a nonlocal trilinear energy kernel, may play an important role in inhomogeneous systems. Whether our much more computationally friendly Skyrme-like parametrization of the trilinear energy kernel based on a momentum expansion to second order can fully account for these nonlocality effects remains to be demonstrated. The toy system studied in Ref. [74] could constitute a useful test case to address this question in the near future, at the price of extending the analysis to the part of the effective three-body interaction induced by genuine three-body forces.
(ii) The discussion regarding three-body spin-orbit and -tensor pseudopotentials constructed along the same lines as here will be given elsewhere [64]. These do not contribute to bulk properties of nonpolarized nuclear matter, but can be used to fine tune the nucleon-number dependence of the shell structure with more freedom than when using two-body spin-orbit and -tensor interactions only [28,30].
(iii) A first tentative adjustment of the parameters of the newly derived EDF kernel, complemented by the Coulomb interaction, is currently under way [76]. The most important question to answer before proceeding further regards the capacity of the presently developed pseudopotential-based EDF to give a satisfying description of bulk properties of nuclei, including pairing correlations.
(iv) To avoid ultraviolet divergences, a contact interaction such as ours has to be accompanied by a cutoff when used in HFB [77] or beyond-mean-field calculations, such as RPA, Quasiparticle RPA or many-body perturbation theory [78,79]. The preservation of the Pauli principle, which is the prime motivation of our work, demands that one and the same cutoff is consistently used everywhere. An important question to be answered will concern how to formulate such a cutoff that can be efficiently used in all many-body methods of interest in a representation-independent manner.
(v) When combined with a Coulomb energy functional that contains exact exchange and pairing contributions, the pseudopotential-based EDF constructed here can be safely used in MR EDF calculations performing symmetry restoration and/or configuration mixing based on the GCM.

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## APPENDIX A: NEUTRON-PROTON REPRESENTATION OF THE EDF

A widely used alternative to the representation of the EDF kernel in terms of isoscalar and isovector densities presented in Sec. V I is a representation in terms of proton and neutron densities.

### 1. Energy density

#### *a. Linear part*

The kinetic energy density is given by

$$\mathcal{E}^{\rho} = \frac{\hbar^2}{2m} \sum_q \tau_q. \tag{A1}$$

### *b. Bilinear part*

The normal part of the bilinear energy density reads

$$\begin{aligned}\mathcal{E}^{\rho\rho} = \sum_q \Big\{ & A^{\rho_1\rho_1}\rho_q\rho_q + A^{\rho_1\rho_2}\rho_q\rho_{\bar{q}} + A^{s_1s_1}\vec{s}_q\cdot\vec{s}_q + A^{s_1s_2}\vec{s}_q\cdot\vec{s}_{\bar{q}} + A^{\tau_1\rho_1}\tau_q\rho_q + A^{\tau_1\rho_2}\tau_q\rho_{\bar{q}} + A^{T_1s_1}\vec{T}_q\cdot\vec{s}_q + A^{T_1s_2}\vec{T}_q\cdot\vec{s}_{\bar{q}} \\ & + A^{\nabla\rho_1\nabla\rho_1}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_q) + A^{\nabla\rho_1\nabla\rho_2}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_{\bar{q}}) + \sum_{\mu\nu}\big[A^{\nabla s_1\nabla s_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{q,\nu}) + A^{\nabla s_1\nabla s_2}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{\bar{q},\nu}) \\ & + A^{J_1J_1}J_{q,\mu\nu}J_{q,\mu\nu} + A^{J_1J_2}J_{q,\mu\nu}J_{\bar{q},\mu\nu}\big] + A^{j_1j_1}\vec{j}_q\cdot\vec{j}_q + A^{j_1j_2}\vec{j}_q\cdot\vec{j}_{\bar{q}}\Big\}, \end{aligned} \tag{A2}$$

whereas its anomalous part takes the form

$$\mathcal{E}^{\kappa\kappa} = \sum_q \left[ A^{\tilde{\rho}_1^*\tilde{\rho}_1}\tilde{\rho}_q^*\tilde{\rho}_q + A^{\tilde{\tau}_1^*\tilde{\rho}_1}\tilde{\tau}_q^*\tilde{\rho}_q + A^{\tilde{\tau}_1\tilde{\rho}_1^*}\tilde{\tau}_q\tilde{\rho}_q^* + A^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot(\vec{\nabla}\tilde{\rho}_q) + \sum_{\mu\nu} A_1^{\tilde{J}_1^*\tilde{J}_1}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\nu}\right]. \tag{A3}$$

Index $\bar{q}$ appearing in the sums over nucleon species $q$ denotes nucleons of the other kind, $\bar{q}\neq q$. The relation between the parameters of the pseudopotential and the coefficients of the energy functional are given in Tables VIII and IX.

### *c. Trilinear part*

The normal part of the trilinear energy density reads

$$\begin{aligned}\mathcal{E}^{\rho\rho\rho} = \sum_q \Big\{ & B^{\rho_1\rho_1\rho_2}\rho_q\rho_q\rho_{\bar{q}} + B^{s_1s_1\rho_2}\vec{s}_q\cdot\vec{s}_q\rho_{\bar{q}} + B^{\tau_1\rho_1\rho_2}\tau_q\rho_q\rho_{\bar{q}} + B^{\tau_1\rho_1\rho_1}\tau_q\rho_q\rho_q + B^{\tau_1\rho_2\rho_2}\tau_q\rho_{\bar{q}}\rho_{\bar{q}} + B^{T_1s_1\rho_2}\vec{T}_q\cdot\vec{s}_q\rho_{\bar{q}} \\ & + B^{T_1s_2\rho_1}\vec{T}_q\cdot\vec{s}_{\bar{q}}\rho_q + B^{\tau_1s_1s_1}\tau_q\vec{s}_q\cdot\vec{s}_q + B^{\tau_1s_1s_2}\tau_q\vec{s}_q\cdot\vec{s}_{\bar{q}} + B^{\tau_1s_2s_2}\tau_q\vec{s}_{\bar{q}}\cdot\vec{s}_{\bar{q}} + B^{\nabla\rho_1\nabla\rho_1\rho_1}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_q)\rho_q \\ & + B^{\nabla\rho_1\nabla\rho_1\rho_2}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_q)\rho_{\bar{q}} + B^{\nabla\rho_1\nabla\rho_2\rho_1}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_{\bar{q}})\rho_q + B^{j_1j_1\rho_1}\vec{j}_q\cdot\vec{j}_q\rho_q + B^{j_1j_1\rho_2}\vec{j}_q\cdot\vec{j}_q\rho_{\bar{q}} + B^{j_1j_2\rho_1}\vec{j}_q\cdot\vec{j}_{\bar{q}}\rho_q \\ & + \sum_{\mu\nu}\big[B^{\nabla s_1\nabla s_1\rho_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{q,\nu})\rho_q + B^{\nabla s_1\nabla s_1\rho_2}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{q,\nu})\rho_{\bar{q}} + B^{\nabla s_1\nabla s_2\rho_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{\bar{q},\nu})\rho_q \\ & + B^{\nabla\rho_1\nabla s_1s_1}(\nabla_\mu\rho_q)(\nabla_\mu s_{q,\nu})s_{q,\nu} + B^{\nabla\rho_1\nabla s_1s_2}(\nabla_\mu\rho_q)(\nabla_\mu s_{q,\nu})s_{\bar{q},\nu} + B^{\nabla\rho_1\nabla s_2s_1}(\nabla_\mu\rho_q)(\nabla_\mu s_{\bar{q},\nu})s_{q,\nu} \\ & + B^{\nabla\rho_1\nabla s_2s_2}(\nabla_\mu\rho_q)(\nabla_\mu s_{\bar{q},\nu})s_{\bar{q},\nu} + B^{J_1J_1\rho_1}J_{q,\mu\nu}J_{q,\mu\nu}\rho_q + B^{J_1J_1\rho_2}J_{q,\mu\nu}J_{q,\mu\nu}\rho_{\bar{q}} + B^{J_1J_2\rho_1}J_{q,\mu\nu}J_{\bar{q},\mu\nu}\rho_q \\ & + B^{j_1J_1s_1}j_{q,\mu}J_{q,\mu\nu}s_{q,\nu} + B^{j_1J_1s_2}j_{q,\mu}J_{q,\mu\nu}s_{\bar{q},\nu} + B^{j_1J_2s_1}j_{q,\mu}J_{\bar{q},\mu\nu}s_{q,\nu} + B^{j_1J_2s_2}j_{q,\mu}J_{\bar{q},\mu\nu}s_{\bar{q},\nu}\big] \\ & + \sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\big[B^{\nabla s_1J_1s_1}(\nabla_\mu s_{q,\nu})J_{q,\mu\lambda}s_{q,\kappa} + B^{\nabla s_1J_1s_2}(\nabla_\mu s_{q,\nu})J_{q,\mu\lambda}s_{\bar{q},\kappa} + B^{\nabla s_1J_2s_1}(\nabla_\mu s_{q,\nu})J_{\bar{q},\mu\lambda}s_{q,\kappa} \\ & + B^{\nabla s_1J_2s_2}(\nabla_\mu s_{q,\nu})J_{\bar{q},\mu\lambda}s_{\bar{q},\kappa}\big]\Big\}, \end{aligned} \tag{A4}$$

whereas its anomalous part is given by

$$\begin{aligned}\mathcal{E}^{\kappa\kappa\rho} = \sum_q \Big\{ & B^{\tilde{\rho}_1^*\tilde{\rho}_1\rho_2}\tilde{\rho}_q^*\tilde{\rho}_q\rho_{\bar{q}} + B^{\tau_1\tilde{\rho}_1^*\tilde{\rho}_1}\tau_q\tilde{\rho}_q^*\tilde{\rho}_q + B^{\tau_2\tilde{\rho}_1^*\tilde{\rho}_1}\tau_{\bar{q}}\tilde{\rho}_q^*\tilde{\rho}_q + B^{\tilde{\tau}_1^*\tilde{\rho}_1\rho_2}\tilde{\tau}_q^*\tilde{\rho}_q\rho_{\bar{q}} + B^{\tilde{\tau}_1\tilde{\rho}_1^*\rho_2}\tilde{\tau}_q\tilde{\rho}_q^*\rho_{\bar{q}} \\ & + B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot(\vec{\nabla}\tilde{\rho}_q)\rho_q + B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_2}(\vec{\nabla}\tilde{\rho}_q^*)\cdot(\vec{\nabla}\tilde{\rho}_q)\rho_{\bar{q}} + B^{\nabla\tilde{\rho}_1^*\nabla\rho_1\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot(\vec{\nabla}\rho_q)\tilde{\rho}_q \\ & + B^{\nabla\tilde{\rho}_1\nabla\rho_1\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_q)\cdot(\vec{\nabla}\rho_q)\tilde{\rho}_q^* + B^{\nabla\tilde{\rho}_1^*\nabla\rho_2\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot(\vec{\nabla}\rho_{\bar{q}})\tilde{\rho}_q + B^{\nabla\tilde{\rho}_1\nabla\rho_2\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_q)\cdot(\vec{\nabla}\rho_{\bar{q}})\tilde{\rho}_q^* \\ & + \mathrm{i}B^{\nabla\tilde{\rho}_1^*j_1\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot\vec{j}_{q,\mu}\tilde{\rho}_q + \mathrm{i}B^{\nabla\tilde{\rho}_1^*j_2\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}_q^*)\cdot\vec{j}_{\bar{q}}\tilde{\rho}_q + \mathrm{i}B^{\nabla\tilde{\rho}_1j_1\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_q)\cdot\vec{j}_q\tilde{\rho}_q^* + \mathrm{i}B^{\nabla\tilde{\rho}_1j_2\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_q)\cdot\vec{j}_{\bar{q}}\tilde{\rho}_q^* \\ & + \sum_{\mu\nu}\big[B^{\tilde{J}_1^*\tilde{J}_1\rho_1}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\nu}\rho_q + B^{\tilde{J}_1^*\tilde{J}_1\rho_2}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\nu}\rho_{\bar{q}} + B^{\tilde{J}_1^*J_1\tilde{\rho}_1}\tilde{J}^*_{q,\mu\nu}J_{q,\mu\nu}\tilde{\rho}_q + B^{\tilde{J}_1^*J_2\tilde{\rho}_1}\tilde{J}^*_{q,\mu\nu}J_{\bar{q},\mu\nu}\tilde{\rho}_q \\ & + B^{\tilde{J}_1J_1\tilde{\rho}_1^*}\tilde{J}_{q,\mu\nu}J_{q,\mu\nu}\tilde{\rho}_q^* + B^{\tilde{J}_1J_2\tilde{\rho}_1^*}\tilde{J}_{q,\mu\nu}J_{\bar{q},\mu\nu}\tilde{\rho}_q^* + \mathrm{i}B^{\nabla\tilde{\rho}_1^*\tilde{J}_1s_1}(\nabla_\mu\tilde{\rho}_q^*)\tilde{J}_{q,\mu\nu}s_{q,\nu} + \mathrm{i}B^{\nabla\tilde{\rho}_1^*\tilde{J}_1s_2}(\nabla_\mu\tilde{\rho}_q^*)\tilde{J}_{q,\mu\nu}s_{\bar{q},\nu} \\ & + \mathrm{i}B^{\nabla\tilde{\rho}_1\tilde{J}_1^*s_1}(\nabla_\mu\tilde{\rho}_q)\tilde{J}^*_{q,\mu\nu}s_{q,\nu} + \mathrm{i}B^{\nabla\tilde{\rho}_1\tilde{J}_1^*s_2}(\nabla_\mu\tilde{\rho}_q)\tilde{J}^*_{q,\mu\nu}s_{\bar{q},\nu} + \mathrm{i}B^{\nabla s_1\tilde{J}_1^*\tilde{\rho}_1}(\nabla_\mu s_{q,\nu})\tilde{J}^*_{q,\mu\nu}\tilde{\rho}_q \\ & + \mathrm{i}B^{\nabla s_2\tilde{J}_1^*\tilde{\rho}_1}(\nabla_\mu s_{\bar{q},\nu})\tilde{J}^*_{q,\mu\nu}\tilde{\rho}_q + \mathrm{i}B^{\nabla s_1\tilde{J}_1\tilde{\rho}_1^*}(\nabla_\mu s_{q,\nu})\tilde{J}_{q,\mu\nu}\tilde{\rho}_q^* + \mathrm{i}B^{\nabla s_2\tilde{J}_1\tilde{\rho}_1^*}(\nabla_\mu s_{\bar{q},\nu})\tilde{J}_{q,\mu\nu}\tilde{\rho}_q^*\big] \\ & + \sum_{\mu\nu\lambda\kappa}\epsilon_{\nu\lambda\kappa}\big[\mathrm{i}B^{\tilde{J}_1^*\tilde{J}_1s_1}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\lambda}s_{q,\kappa} + \mathrm{i}B^{\tilde{J}_1^*\tilde{J}_1s_2}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\lambda}s_{\bar{q},\kappa}\big]\Big\}. \end{aligned} \tag{A5}$$

The relations between the parameters of the pseudopotential and the coefficients of the energy functional are listed in Tables X and XI.

TABLE VIII. Coupling constants of the normal bilinear part of the EDF in neutron-proton representation [Eq. (A2)] as a function of the pseudopotential parameters of Eqs. (64a) to (64c). Missing entries are zero.

| | $t_0$ | $t_0x_0$ | $t_1$ | $t_1x_1$ | $t_2$ | $t_2x_2$ |
|---|---|---|---|---|---|---|
| $A^{\rho_1\rho_1} =$ | $+\frac{1}{4}$ | $-\frac{1}{4}$ | | | | |
| $A^{\rho_1\rho_2} =$ | $+\frac{1}{2}$ | $+\frac{1}{4}$ | | | | |
| $A^{s_1s_1} =$ | $-\frac{1}{4}$ | $+\frac{1}{4}$ | | | | |
| $A^{s_1s_2} =$ | | $+\frac{1}{4}$ | | | | |
| $A^{\tau_1\rho_1} =$ | | | $+\frac{1}{8}$ | $-\frac{1}{8}$ | $+\frac{3}{8}$ | $+\frac{3}{8}$ |
| $A^{\tau_1\rho_2} =$ | | | $+\frac{1}{4}$ | $+\frac{1}{8}$ | $+\frac{1}{4}$ | $+\frac{1}{8}$ |
| $A^{T_1s_1} =$ | | | $-\frac{1}{8}$ | $+\frac{1}{8}$ | $+\frac{1}{8}$ | $+\frac{1}{8}$ |
| $A^{T_1s_2} =$ | | | | $+\frac{1}{8}$ | | $+\frac{1}{8}$ |
| $A^{\nabla\rho_1\nabla\rho_1} =$ | | | $+\frac{3}{32}$ | $-\frac{3}{32}$ | $-\frac{3}{32}$ | $-\frac{3}{32}$ |
| $A^{\nabla\rho_1\nabla\rho_2} =$ | | | $+\frac{3}{16}$ | $+\frac{3}{32}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ |
| $A^{\nabla s_1\nabla s_1} =$ | | | $-\frac{3}{32}$ | $+\frac{3}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{32}$ |
| $A^{\nabla s_1\nabla s_2} =$ | | | | $+\frac{3}{32}$ | | $-\frac{1}{32}$ |
| $A^{j_1j_1} =$ | | | $-\frac{1}{8}$ | $+\frac{1}{8}$ | $-\frac{3}{8}$ | $-\frac{3}{8}$ |
| $A^{j_1j_2} =$ | | | $-\frac{1}{4}$ | $-\frac{1}{8}$ | $-\frac{1}{4}$ | $-\frac{1}{8}$ |
| $A^{J_1J_1} =$ | | | $+\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ |
| $A^{J_1J_2} =$ | | | | $-\frac{1}{8}$ | | $-\frac{1}{8}$ |

## APPENDIX B: INFINITE NUCLEAR MATTER

### 1. General definitions

A first insight into the physics described by a given energy functional is provided by the analysis of the model system of homogeneous infinite nuclear matter (INM), where the Coulomb interaction is neglected. Although it is an idealized system, INM has relevance to the study of several real systems, e.g., the physics of neutron stars or the dynamics of supernovae explosions. In this context, one is first and foremost interested in computing the equation of state (EOS) of such a system, i.e., its energy per nucleon as a function of its density. Below, pairing correlations are omitted as they little impact bulk properties such as the EOS. However, one should note that pairing properties, such as pairing gaps, of INM are of importance to the physics of neutron stars; see, e.g., Ref. [80].

Infinite nuclear matter being translationally invariant, it is convenient to use a plane-wave basis,

$$\langle \vec{r}\sigma q|\vec{k}\sigma' q'\rangle = \varphi_{\vec{k}\sigma' q'}(\vec{r}\sigma q) = (2\pi)^{-\frac{3}{2}}\exp(\mathrm{i}\vec{k}\cdot\vec{r})\delta_{\sigma\sigma'}\delta_{qq'}, \tag{B1}$$

TABLE IX. Same as Table VIII, but for the anomalous bilinear part of the EDF [Eq. (A3)].

| | $t_0$ | $t_0x_0$ | $t_1$ | $t_1x_1$ | $t_2$ | $t_2x_2$ |
|---|---|---|---|---|---|---|
| $A^{\tilde{\rho}_1^*\tilde{\rho}_1} =$ | $+\frac{1}{4}$ | $-\frac{1}{4}$ | | | | |
| $A^{\tilde{\tau}_1^*\tilde{\rho}_1} =$ | | | $+\frac{1}{8}$ | $-\frac{1}{8}$ | | |
| $A^{\tilde{\tau}_1\tilde{\rho}_1^*} =$ | | | $+\frac{1}{8}$ | $-\frac{1}{8}$ | | |
| $A^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1} =$ | | | $+\frac{1}{16}$ | $-\frac{1}{16}$ | | |
| $A_1^{\tilde{J}_1^*\tilde{J}_1} =$ | | | | | $+\frac{1}{4}$ | $+\frac{1}{4}$ |

TABLE X. Same as Table VIII for the normal part of the trilinear EDF kernel [Eq. (A4)].

| | $u_0$ | $u_1$ | $u_1y_1$ | $u_2$ | $u_2y_{21}$ | $u_2y_{22}$ |
|---|---|---|---|---|---|---|
| $B^{\rho_1\rho_1\rho_2} =$ | $+\frac{3}{4}$ | | | | | |
| $B^{s_1s_1\rho_2} =$ | $-\frac{3}{4}$ | | | | | |
| $B^{\tau_1\rho_1\rho_1} =$ | | | | $+\frac{3}{16}$ | $+\frac{3}{16}$ | $-\frac{3}{16}$ |
| $B^{\tau_1\rho_1\rho_2} =$ | | $+\frac{1}{4}$ | $-\frac{1}{16}$ | $+\frac{5}{8}$ | $+\frac{1}{2}$ | $+\frac{5}{8}$ |
| $B^{\tau_1\rho_2\rho_2} =$ | | $+\frac{1}{8}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ |
| $B^{T_1s_1\rho_2} =$ | | $-\frac{1}{4}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ | $+\frac{1}{8}$ | $+\frac{1}{4}$ |
| $B^{T_1s_2\rho_1} =$ | | | $+\frac{1}{16}$ | | $+\frac{1}{8}$ | $+\frac{1}{4}$ |
| $B^{\tau_1s_1s_1} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{\tau_1s_1s_2} =$ | | | $-\frac{1}{16}$ | | | $+\frac{3}{8}$ |
| $B^{\tau_1s_2s_2} =$ | | $-\frac{1}{8}$ | $-\frac{1}{16}$ | $-\frac{1}{8}$ | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B^{\nabla\rho_1\nabla\rho_1\rho_1} =$ | | | | $-\frac{3}{64}$ | $-\frac{3}{64}$ | $+\frac{3}{64}$ |
| $B^{\nabla\rho_1\nabla\rho_1\rho_2} =$ | | $+\frac{5}{32}$ | $-\frac{1}{16}$ | $-\frac{1}{8}$ | $-\frac{7}{64}$ | $-\frac{11}{64}$ |
| $B^{\nabla\rho_1\nabla\rho_2\rho_1} =$ | | $+\frac{5}{16}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B^{\nabla s_1\nabla s_1\rho_1} =$ | | | | $-\frac{3}{64}$ | $-\frac{3}{64}$ | $+\frac{3}{64}$ |
| $B^{\nabla s_1\nabla s_1\rho_2} =$ | | $-\frac{5}{32}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ | $-\frac{3}{64}$ | $-\frac{3}{64}$ |
| $B^{\nabla s_1\nabla s_2\rho_1} =$ | | | $+\frac{1}{16}$ | | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B^{\nabla\rho_1\nabla s_1s_1} =$ | | | | $+\frac{3}{32}$ | $+\frac{3}{32}$ | $-\frac{3}{32}$ |
| $B^{\nabla\rho_1\nabla s_1s_2} =$ | | | | | $-\frac{1}{32}$ | $-\frac{5}{32}$ |
| $B^{\nabla\rho_1\nabla s_2s_1} =$ | | | $-\frac{1}{16}$ | | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B^{\nabla\rho_1\nabla s_2s_2} =$ | | $-\frac{5}{16}$ | $-\frac{1}{16}$ | $+\frac{1}{16}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B^{j_1j_1\rho_1} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{j_1j_1\rho_2} =$ | | $-\frac{1}{8}$ | $+\frac{1}{8}$ | $-\frac{1}{2}$ | $-\frac{7}{16}$ | $-\frac{11}{16}$ |
| $B^{j_1j_2\rho_1} =$ | | $-\frac{1}{4}$ | $-\frac{1}{8}$ | $-\frac{1}{4}$ | $-\frac{1}{8}$ | $+\frac{1}{8}$ |
| $B^{J_1J_1\rho_1} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{J_1J_1\rho_2} =$ | | $+\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{4}$ | $-\frac{3}{16}$ | $-\frac{3}{16}$ |
| $B^{J_1J_2\rho_1} =$ | | | $-\frac{1}{8}$ | | $-\frac{1}{8}$ | $+\frac{1}{8}$ |
| $B^{j_1J_1s_1} =$ | | | | $+\frac{3}{8}$ | $+\frac{3}{8}$ | $-\frac{3}{8}$ |
| $B^{j_1J_1s_2} =$ | | | | | $-\frac{1}{8}$ | $-\frac{5}{8}$ |
| $B^{j_1J_2s_1} =$ | | | $+\frac{1}{8}$ | | $+\frac{1}{8}$ | $-\frac{1}{8}$ |
| $B^{j_1J_2s_2} =$ | | $+\frac{1}{4}$ | $+\frac{1}{8}$ | $+\frac{1}{4}$ | $+\frac{1}{8}$ | $-\frac{1}{8}$ |
| $B^{\nabla s_1J_1s_1} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{\nabla s_1J_1s_2} =$ | | | $-\frac{1}{16}$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B^{\nabla s_1J_2s_1} =$ | | | $-\frac{1}{16}$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B^{\nabla s_1J_2s_2} =$ | | | $+\frac{1}{8}$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ |

where $q\sigma = \{n\uparrow, n\downarrow, p\uparrow, p\downarrow\}$ labels proton/neutron states with spin up/down. Neglecting pairing, the SR state reduces to a Slater determinant obtained by filling individual orbitals $\varphi_{\vec{k}\sigma' q'}(\vec{r}\sigma q)$ up to the Fermi momentum; i.e., the normal density matrix is diagonal in the plane-wave basis and equal to 1 for states characterized by $|\vec{k}| \leqslant k_{F,q\sigma}$ and 0 otherwise, where $k_{F,q\sigma}$ denotes the spin- and isospin-dependent Fermi momentum. In doing so, we make the usual assumption that the respective Fermi surface is spherical for each particle species and spin direction.

When calculating densities for each of the combinations $q\sigma$, the sum over basis states $(i, j)$ in Eq. (57) becomes an integral over the Fermi spheres of radius $k_{F,q\sigma}$, leading to

TABLE XI. Same as Table VIII, but for the anomalous part of the trilinear EDF kernel [Eq. (A5)].

| | $u_0$ | $u_1$ | $u_1y_1$ | $u_2$ | $u_2y_{21}$ | $u_2y_{22}$ |
|---|---|---|---|---|---|---|
| $B^{\tilde{\rho}_1^*\tilde{\rho}_1\rho_2} =$ | $+\frac{3}{4}$ | | | | | |
| $B^{\tilde{\tau}_1^*\tilde{\rho}_1\rho_2} =$ | | $+\frac{3}{16}$ | $-\frac{3}{32}$ | | | |
| $B^{\tilde{\tau}_1\tilde{\rho}_1^*\rho_2} =$ | | $+\frac{3}{16}$ | $-\frac{3}{32}$ | | | |
| $B^{\tau_1\tilde{\rho}_1^*\tilde{\rho}_1} =$ | | | | $+\frac{3}{16}$ | $+\frac{3}{16}$ | $-\frac{3}{16}$ |
| $B^{\tau_2\tilde{\rho}_1^*\tilde{\rho}_1} =$ | | $+\frac{1}{8}$ | $+\frac{1}{16}$ | $+\frac{1}{8}$ | $+\frac{1}{16}$ | $-\frac{1}{16}$ |
| $B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_1} =$ | | | | $+\frac{3}{64}$ | $+\frac{3}{64}$ | $-\frac{3}{64}$ |
| $B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_2} =$ | | $+\frac{1}{8}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ | $+\frac{1}{64}$ | $-\frac{1}{64}$ |
| $B^{\nabla\tilde{\rho}_1^*\nabla\rho_1\tilde{\rho}_1} =$ | | | | $-\frac{3}{64}$ | $-\frac{3}{64}$ | $+\frac{3}{64}$ |
| $B^{\nabla\tilde{\rho}_1^*\nabla\rho_2\tilde{\rho}_1} =$ | | $+\frac{5}{32}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B^{\nabla\tilde{\rho}_1\nabla\rho_1\tilde{\rho}_1^*} =$ | | | | $-\frac{3}{64}$ | $-\frac{3}{64}$ | $+\frac{3}{64}$ |
| $B^{\nabla\tilde{\rho}_1\nabla\rho_2\tilde{\rho}_1^*} =$ | | $+\frac{5}{32}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{64}$ | $+\frac{1}{64}$ |
| $B^{\tilde{J}_1^*\tilde{J}_1\rho_1} =$ | | | | $+\frac{3}{16}$ | $+\frac{3}{16}$ | $-\frac{3}{16}$ |
| $B^{\tilde{J}_1^*\tilde{J}_1\rho_2} =$ | | | | $+\frac{3}{8}$ | $+\frac{5}{16}$ | $+\frac{7}{16}$ |
| $B^{\tilde{J}_1^*J_1\tilde{\rho}_1} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{\tilde{J}_1^*J_2\tilde{\rho}_1} =$ | | | $-\frac{1}{16}$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B^{\tilde{J}_1J_1\tilde{\rho}_1^*} =$ | | | | $-\frac{3}{16}$ | $-\frac{3}{16}$ | $+\frac{3}{16}$ |
| $B^{\tilde{J}_1J_2\tilde{\rho}_1^*} =$ | | | $-\frac{1}{16}$ | | $-\frac{1}{16}$ | $+\frac{1}{16}$ |
| $B^{\tilde{J}_1^*\tilde{J}_1s_1} =$ | | | | $+\frac{3}{16}$ | $+\frac{3}{16}$ | $-\frac{3}{16}$ |
| $B^{\tilde{J}_1^*\tilde{J}_1s_2} =$ | | | | | $-\frac{1}{16}$ | $-\frac{5}{16}$ |
| $B^{\nabla\tilde{\rho}_1^*\tilde{J}_1s_1} =$ | | | | $+\frac{3}{32}$ | $+\frac{3}{32}$ | $-\frac{3}{32}$ |
| $B^{\nabla\tilde{\rho}_1^*\tilde{J}_1s_2} =$ | | | $+\frac{1}{32}$ | | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B^{\nabla\tilde{\rho}_1^*j_1\tilde{\rho}_1} =$ | | | | $-\frac{3}{32}$ | $-\frac{3}{32}$ | $+\frac{3}{32}$ |
| $B^{\nabla\tilde{\rho}_1^*j_2\tilde{\rho}_1} =$ | | $-\frac{1}{16}$ | $-\frac{1}{32}$ | $-\frac{1}{16}$ | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B^{\nabla\tilde{\rho}_1\tilde{J}_1^*s_1} =$ | | | | $-\frac{3}{32}$ | $-\frac{3}{32}$ | $+\frac{3}{32}$ |
| $B^{\nabla\tilde{\rho}_1\tilde{J}_1^*s_2} =$ | | | $-\frac{1}{32}$ | | $-\frac{1}{32}$ | $+\frac{1}{32}$ |
| $B^{\nabla s_1\tilde{J}_1^*\tilde{\rho}_1} =$ | | | | $+\frac{3}{32}$ | $+\frac{3}{32}$ | $-\frac{3}{32}$ |
| $B^{\nabla s_2\tilde{J}_1^*\tilde{\rho}_1} =$ | | | $-\frac{1}{16}$ | | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B^{\nabla\tilde{\rho}_1j_1\tilde{\rho}_1^*} =$ | | | | $+\frac{3}{32}$ | $+\frac{3}{32}$ | $-\frac{3}{32}$ |
| $B^{\nabla\tilde{\rho}_1j_2\tilde{\rho}_1^*} =$ | | $+\frac{1}{16}$ | $+\frac{1}{32}$ | $+\frac{1}{16}$ | $+\frac{1}{32}$ | $-\frac{1}{32}$ |
| $B^{\nabla s_1\tilde{J}_1\tilde{\rho}_1^*} =$ | | | | $-\frac{3}{32}$ | $-\frac{3}{32}$ | $+\frac{3}{32}$ |
| $B^{\nabla s_2\tilde{J}_1\tilde{\rho}_1^*} =$ | | | $+\frac{1}{16}$ | | $-\frac{1}{32}$ | $+\frac{1}{32}$ |

expressions for the matter and kinetic densities of the form

$$\rho_{q\sigma} = \frac{1}{6\pi^2}k_{F,q\sigma}^3, \tag{B2a}$$

$$\tau_{q\sigma} = \frac{3}{20}\,\frac{2}{3\pi^2}\,k_{F,q\sigma}^5. \tag{B2b}$$

With the choice of a Fermi surface centered at $\vec{k}=0$, current densities vanish $\vec{j}_{q\sigma}=0$. Also, all gradients of local densities are zero $\nabla_\nu\rho_{q\sigma}=0$ by construction, as are the pair densities.

The densities (B2a) for the four different combinations of spin and particle species can be recoupled to scalar-isoscalar $\rho_0$, scalar-isovector $\rho_1$, vector-isoscalar $s_0$, and vector-isovector $s_1$ densities [26],

$$\rho_0 = \rho_{n\uparrow}+\rho_{n\downarrow}+\rho_{p\uparrow}+\rho_{p\downarrow}, \tag{B3a}$$

$$\rho_1 = \rho_{n\uparrow}+\rho_{n\downarrow}-\rho_{p\uparrow}-\rho_{p\downarrow}, \tag{B3b}$$

$$s_0 = \rho_{n\uparrow}-\rho_{n\downarrow}+\rho_{p\uparrow}-\rho_{p\downarrow}, \tag{B3c}$$

$$s_1 = \rho_{n\uparrow}-\rho_{n\downarrow}-\rho_{p\uparrow}+\rho_{p\downarrow}. \tag{B3d}$$

The inverse relationships read

$$\rho_{n\uparrow} = \tfrac{1}{4}(1+I_\tau+I_\sigma+I_{\sigma\tau})\rho_0, \tag{B4a}$$

$$\rho_{n\downarrow} = \tfrac{1}{4}(1+I_\tau-I_\sigma-I_{\sigma\tau})\rho_0, \tag{B4b}$$

$$\rho_{p\uparrow} = \tfrac{1}{4}(1-I_\tau+I_\sigma-I_{\sigma\tau})\rho_0, \tag{B4c}$$

$$\rho_{p\downarrow} = \tfrac{1}{4}(1-I_\tau-I_\sigma+I_{\sigma\tau})\rho_0, \tag{B4d}$$

where the relative isospin $I_\tau \equiv \rho_1/\rho_0$, spin $I_\sigma \equiv s_0/\rho_0$, and spin-isospin $I_{\sigma\tau} \equiv s_1/\rho_0$ excesses, taking values $-1 \leqslant I_i \leqslant 1$, have been introduced. Typical cases of interest are (i) symmetric nuclear matter ($I_\tau = I_\sigma = I_{\sigma\tau} = 0$), (ii) isospin-asymmetric nuclear matter ($I_\tau \neq 0$), (iii) spin-polarized nuclear matter ($I_\sigma \neq 0$), and (iv) isospin-asymmetric spin-polarized nuclear matter ($I_\tau \neq 0$, $I_\sigma \neq 0$ and $I_{\sigma\tau} \neq 0$), but the definitions given above allow also for the coverage of all intermediate cases.

In analogy to Eq. (B3) one can also define isoscalar and isovector kinetic densities using Eqs. (B2a) and (B2b),

$$\tau_0 = \tau_{n\uparrow}+\tau_{n\downarrow}+\tau_{p\uparrow}+\tau_{p\downarrow} = \tfrac{3}{5}c_s\rho_0^{\frac{5}{3}}F_{5/3}^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau}), \tag{B5a}$$

$$\tau_1 = \tau_{n\uparrow}+\tau_{n\downarrow}-\tau_{p\uparrow}-\tau_{p\downarrow} = \tfrac{3}{5}c_s\rho_0^{\frac{5}{3}}F_{5/3}^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}), \tag{B5b}$$

$$T_0 = \tau_{n\uparrow}-\tau_{n\downarrow}+\tau_{p\uparrow}-\tau_{p\downarrow} = \tfrac{3}{5}c_s\rho_0^{\frac{5}{3}}F_{5/3}^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau}), \tag{B5c}$$

$$T_1 = \tau_{n\uparrow}-\tau_{n\downarrow}-\tau_{p\uparrow}+\tau_{p\downarrow} = \tfrac{3}{5}c_s\rho_0^{\frac{5}{3}}F_{5/3}^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau}), \tag{B5d}$$

where $c_s \equiv (3\pi^2/2)^{\frac{2}{3}}$ and $c_n \equiv (3\pi^2)^{\frac{2}{3}}$ and where functions $F$ of the relative isospin, spin, and spin-isospin excesses introduced in Ref. [26] have been used. Their definitions are listed in Appendix B 2 along with useful properties.

As mentioned above, the main quantity of interest is the EOS that can be easily calculated from Eqs. (66), (67), and (69). The fact that most of the local densities are zero in INM implies that quantities of interest will be expressed in terms of a limited number of couplings.

### 2. *F* functions

The kinetic densities in INM can be expressed in a very compact manner in terms of functions $F_m^{(0)}(I_\tau, I_\sigma, I_{\sigma\tau})$, $F_m^{(\tau)}(I_\tau, I_\sigma, I_{\sigma\tau})$, $F_m^{(\sigma)}(I_\tau, I_\sigma, I_{\sigma\tau})$, and $F_m^{(\sigma\tau)}(I_\tau, I_\sigma, I_{\sigma\tau})$ that have been introduced in Ref. [26]:

$$F_m^{(0)} \equiv \tfrac{1}{4}\big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m+(1+I_\tau-I_\sigma-I_{\sigma\tau})^m +(1-I_\tau+I_\sigma-I_{\sigma\tau})^m+(1-I_\tau-I_\sigma+I_{\sigma\tau})^m\big], \tag{B6a}$$

$$F_m^{(\tau)} \equiv \tfrac{1}{4}\big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m+(1+I_\tau-I_\sigma-I_{\sigma\tau})^m -(1-I_\tau+I_\sigma-I_{\sigma\tau})^m-(1-I_\tau-I_\sigma+I_{\sigma\tau})^m\big], \tag{B6b}$$

$$F_m^{(\sigma)} \equiv \tfrac{1}{4}\big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m-(1+I_\tau-I_\sigma-I_{\sigma\tau})^m +(1-I_\tau+I_\sigma-I_{\sigma\tau})^m-(1-I_\tau-I_\sigma+I_{\sigma\tau})^m\big], \tag{B6c}$$

$$F_m^{(\sigma\tau)} \equiv \tfrac{1}{4}\big[(1+I_\tau+I_\sigma+I_{\sigma\tau})^m-(1+I_\tau-I_\sigma-I_{\sigma\tau})^m -(1-I_\tau+I_\sigma-I_{\sigma\tau})^m+(1-I_\tau-I_\sigma+I_{\sigma\tau})^m\big]. \tag{B6d}$$

Their first derivatives with respect to spin, isospin, and spin-isospin excesses that are needed for the derivation of some nuclear-matter properties are

$$\frac{\partial F_m^{(\tau)}}{\partial I_\tau}=\frac{\partial F_m^{(\sigma)}}{\partial I_\sigma}=\frac{\partial F_m^{(\sigma\tau)}}{\partial I_{\sigma\tau}}=mF_{m-1}^{(0)}, \tag{B7a}$$

$$\frac{\partial F_m^{(0)}}{\partial I_\tau}=\frac{\partial F_m^{(\sigma)}}{\partial I_{\sigma\tau}}=\frac{\partial F_m^{(\sigma\tau)}}{\partial I_\sigma}=mF_{m-1}^{(\tau)}, \tag{B7b}$$

$$\frac{\partial F_m^{(0)}}{\partial I_\sigma}=\frac{\partial F_m^{(\tau)}}{\partial I_{\sigma\tau}}=\frac{\partial F_m^{(\sigma\tau)}}{\partial I_\tau}=mF_{m-1}^{(\sigma)}, \tag{B7c}$$

$$\frac{\partial F_m^{(0)}}{\partial I_{\sigma\tau}}=\frac{\partial F_m^{(\tau)}}{\partial I_\sigma}=\frac{\partial F_m^{(\sigma)}}{\partial I_\tau}=mF_{m-1}^{(\sigma\tau)}, \tag{B7d}$$

whereas their second derivatives are given by

$$\frac{\partial^2 F_m^{(j)}}{\partial I_i^2}=m(m-1)F_{m-2}^{(j)}, \tag{B8}$$

for any $i,\ j\in\{0,\tau,\sigma,\sigma\tau\}$. Special values that are appear in the nuclear-matter properties discussed below are

$$F_0^{(0)}(I_\tau,I_\sigma,I_{\sigma\tau})=1,\quad F_0^{(i)}(I_\tau,I_\sigma,I_{\sigma\tau})=0, \tag{B9a}$$

$$F_1^{(0)}(I_\tau,I_\sigma,I_{\sigma\tau})=1,\quad F_1^{(i)}(I_\tau,I_\sigma,I_{\sigma\tau})=I_i, \tag{B9b}$$

and

$$F_m^{(0)}(0,0,0)=1, \tag{B10a}$$

$$F_m^{(i)}(0,0,0)=0, \tag{B10b}$$

$$F_m^{(\tau)}(0,1,0)=F_m^{(\tau)}(0,0,1)=0, \tag{B10c}$$

$$F_m^{(\sigma)}(1,0,0)=F_m^{(\sigma)}(0,0,1)=0, \tag{B10d}$$

$$F_m^{(\sigma\tau)}(1,0,0)=F_m^{(\sigma\tau)}(0,1,0)=0, \tag{B10e}$$

$$F_m^{(0)}(1,0,0)=F_m^{(0)}(0,1,0)=F_m^{(0)}(0,0,1)=2^{m-1}, \tag{B10f}$$

$$F_m^{(\tau)}(1,0,0)=F_m^{(\sigma)}(0,1,0)=F_m^{(\sigma\tau)}(0,0,1)=2^{m-1}, \tag{B10g}$$

$$F_m^{(0)}(1,1,1)=F_m^{(i)}(1,1,1)=4^{m-1}, \tag{B10h}$$

where $i\in\{\tau,\sigma,\sigma\tau\}$.

### 3. Symmetric nuclear matter

Symmetric nuclear matter (SNM) is characterized by an equal number of protons and neutrons as well as of spin-up and spin-down particles in both nucleons species, $\rho_1=I_\tau=0$ and $I_\sigma=I_{\sigma\tau}=0$. Only $\rho_0$ and $\tau_0$ are nonzero, i.e., $\rho_n=\rho_p=\frac{1}{2}\rho_0$ and $\tau_n=\tau_p=\frac{1}{2}\tau_0$. The resulting energy per particle reads

$$\frac{E_H}{A}\equiv\frac{\mathcal{E}_H}{\rho_0}=\frac{3}{5}\frac{\hbar^2}{2m}c_s\,\rho_0^{\frac{2}{3}}+\big(A_0^\rho+B_0^\rho\,\rho_0\big)\rho_0 +\frac{3}{5}c_s\big(A_0^\tau+B_0^\tau\rho_0\big)\rho_0^{\frac{5}{3}}. \tag{B11}$$

Symmetric nuclear matter presents a stable state such that a minimum energy is obtained for some finite value of the density $\rho_{\rm sat}$. The pressure of the fluid relates to the first derivative of the EOS with respect to the isoscalar density, which in SNM reads

$$P\equiv\rho_0^2\frac{\partial E_H/A}{\partial\rho_0}\bigg|_A =\frac{2}{5}\frac{\hbar^2}{2m}c_s\,\rho_0^{\frac{5}{3}}+\big(A_0^\rho\ +2B_0^\rho\ \rho_0\big)\rho_0^2 +c_s\bigg(A_0^\tau\ +\frac{8}{5}B_0^\tau\ \rho_0\bigg)\rho_0^{\frac{8}{3}}. \tag{B12}$$

The saturation density $\rho_{\rm sat}$ is naturally obtained as the solution of $P(\rho_{\rm sat})=0$.

The incompressibility of the nuclear fluid relates to the second derivative of the EOS with respect to the isoscalar density and expresses the energy cost to compress the nuclear fluid. It is defined as

$$K\equiv\frac{18P}{\rho_0}+9\rho_0^2\frac{\partial^2 E_H/A}{\partial\rho_0^2}, \tag{B13}$$

such that at equilibrium

$$K_\infty\equiv 9\rho_0^2\frac{\partial^2 E_H/A}{\partial\rho_0^2}\bigg|_{\rho_0=\rho_{\rm sat}} =-\frac{6}{5}\frac{\hbar^2}{2m}c_s\,\rho_{\rm sat}^{\frac{2}{3}}+18B_0^\rho\ \rho_{\rm sat}^2+\ 6c_s\big(A_0^\tau\ +4B_0^\tau\ \rho_0\big)\rho_{\rm sat}^{\frac{5}{3}}, \tag{B14}$$

which needs to be positive for the system to be stable against density fluctuations.

### 4. Asymmetric nuclear matter

More general cases of homogeneous nuclear matter are characterized by (i) unequal proton- and neutron-matter densities, i.e., $I_\tau\neq 0$, (ii) a global spin polarization, i.e., $I_\sigma\neq 0$ and (iii) a spin polarization that differs for neutron and proton species, i.e., $I_{\sigma\tau}\neq 0$. Based on Eqs. (66), (67), and (69), the EOS of such a nuclear fluid is given by

$$\begin{aligned}\frac{E_H}{A}=&\frac{3}{5}\frac{\hbar^2}{2m}c_sF_{5/3}^{(0)}(I_\tau,I_\sigma,I_{\sigma\tau})\rho_0^{\frac{2}{3}}+\big(A_0^\rho+B_0^\rho\ \rho_0\big)\rho_0+\big(A_1^\rho+B_1^\rho\ \rho_0\big)\rho_0I_\tau^2+\big(A_0^s+B_0^s\ \rho_0\big)\rho_0I_\sigma^2+B_{10}^s\,\rho_0^2I_\sigma I_\tau I_{\sigma\tau}\\ &+\big(A_1^s+B_1^s\ \rho_0\big)\rho_0I_{\sigma\tau}^2+\frac{3}{5}\big[\big(A_0^\tau+B_0^\tau\ \rho_0+B_{10}^\tau\,\rho_0I_\tau^2+B_0^{\tau s}\ \rho_0I_\sigma^2+B_{10}^{\tau s}\,\rho_0I_{\sigma\tau}^2\big)F_{5/3}^{(0)}(I_\tau,I_\sigma,I_{\sigma\tau})\\ &+\big(A_1^\tau\ I_\tau+B_1^\tau\ \rho_0I_\tau+B_1^{\tau s}\ \rho_0I_\sigma I_{\sigma\tau}\big)F_{5/3}^{(\tau)}\big(I_\tau,I_\sigma,I_{\sigma\tau}\big)+\big(A_0^T\ I_\sigma+B_0^T\ \rho_0I_\sigma+B_{10}^T\,\rho_0I_\tau I_{\sigma\tau}\big)F_{5/3}^{(\sigma)}(I_\tau,I_\sigma,I_{\sigma\tau})\\ &+\big(A_1^T\ I_{\sigma\tau}+B_1^T\ \rho_0I_{\sigma\tau}+B_{01}^T\,\rho_0I_\sigma I_\tau\big)F_{5/3}^{(\sigma\tau)}(I_\tau,I_\sigma,I_{\sigma\tau})\big]c_s\rho_0^{\frac{5}{3}}.\end{aligned} \tag{B15}$$

Spin, isospin, and spin-isospin symmetry energies are analogs of $K_\infty$ with respect to spin, isospin, and spin-isospin excesses, respectively, i.e., they characterize the stiffness of the EOS with respect to generating such nonzero excesses. At saturation of SNM, i.e., when $I_\sigma = I_\tau = I_{\sigma\tau} = 0$ and $\rho_0 = \rho_{\rm sat}$, the three symmetry energies are given by

$$a_\tau \equiv \frac{1}{2}\frac{\partial^2 E_H/A}{\partial I_\tau^2}\bigg|_{I_\sigma=I_\tau=I_{\sigma\tau}=0} = \frac{1}{3}\frac{\hbar^2}{2m}c_s\rho_0^{\frac{2}{3}} + \big(A_1^\rho + B_1^\rho\,\rho_0\big)\,\rho_0 + \bigg[\frac{1}{3}\big(A_0^\tau + B_0^\tau\,\rho_0\big) + A_1^\tau + B_1^\tau\,\rho_0 + \frac{3}{5}B_{10}^\tau\,\rho_0\bigg]c_s\rho_0^{\frac{5}{3}}, \tag{B16a}$$

$$a_\sigma \equiv \frac{1}{2}\frac{\partial^2 E_H/A}{\partial I_\sigma^2}\bigg|_{I_\sigma=I_\tau=I_{\sigma\tau}=0} = \frac{1}{3}\frac{\hbar^2}{2m}c_s\rho_0^{\frac{2}{3}} + \big(A_0^s + B_0^s\,\rho_0\big)\,\rho_0 + \bigg[\frac{1}{3}\big(A_0^\tau + B_0^\tau\,\rho_0\big) + A_0^T + B_0^T\,\rho_0 + \frac{3}{5}B_0^{\tau s}\,\rho_0\bigg]c_s\rho_0^{\frac{5}{3}}, \tag{B16b}$$

$$a_{\sigma\tau} \equiv \frac{1}{2}\frac{\partial^2 E_H/A}{\partial I_{\sigma\tau}^2}\bigg|_{I_\sigma=I_\tau=I_{\sigma\tau}=0} = \frac{1}{3}\frac{\hbar^2}{2m}c_s\rho_0^{\frac{2}{3}} + \big(A_1^s + B_1^s\,\rho_0\big)\,\rho_0 + \bigg[\frac{1}{3}\big(A_0^\tau + B_0^\tau\,\rho_0\big) + A_1^T + B_1^T\,\rho_0 + \frac{3}{5}B_{10}^{\tau s}\,\rho_0\bigg]c_s\rho_0^{\frac{5}{3}}, \tag{B16c}$$

and must be positive for the minimum of the EOS to be stable.

Two other quantities of interest are intimately connected to the skin thickness of heavy isospin-asymmetric nuclei, i.e., to the difference between their neutron and proton radii. These quantities are the density-symmetry coefficient $L$,

$$\begin{aligned} L &\equiv 3\rho\frac{\partial}{\partial\rho}\left(\frac{1}{2}\frac{\partial^2 E_H/A}{\partial I_\tau^2}\right)\bigg|_{I_\sigma=I_\tau=I_{\sigma\tau}=0} \\ &= \frac{2}{3}\frac{\hbar^2}{2m}c_s\rho_0^{\frac{2}{3}} + 3\big(A_1^\rho + 2B_1^\rho\,\rho_0\big)\rho_0 \\ &\quad + \left(\frac{5}{3}A_0^\tau + \frac{8}{3}B_0^\tau\,\rho_0 + 5A_1^\tau + 8B_1^\tau\,\rho_0 + \frac{24}{5}B_{10}^\tau\,\rho_0\right)c_s\rho_0^{\frac{5}{3}}, \end{aligned} \tag{B17}$$

and the symmetry incompressibility coefficient,

$$\begin{aligned} K_{\rm sym} &\equiv 9\rho^2\frac{\partial^2}{\partial\rho^2}\left(\frac{1}{2}\frac{\partial^2 E_H/A}{\partial I_\tau^2}\right)\bigg|_{I_\sigma=I_\tau=I_{\sigma\tau}=0} \\ &= -\frac{2}{3}\frac{\hbar^2}{2m}c_s\rho_0^{\frac{2}{3}} + \frac{10}{3}\big(A_0^\tau + 4B_0^\tau\,\rho_0\big)c_s\rho_0^{\frac{5}{3}} \\ &\quad + 18B_1^\rho\,\rho_0^2 + \big[10\big(A_1^\tau + 4B_1^\tau\rho_0\big) + 24B_{10}^\tau\rho_0\big]c_s\rho_0^{\frac{5}{3}}. \end{aligned} \tag{B18}$$

### 5. Pure neutron matter

A particular case of isospin-asymmetric nuclear matter is (spin-saturated) pure neutron matter (PNM) obtained for $I_\tau = 1$, $I_\sigma = I_{\sigma\tau} = 0$. The EOS of PNM reads

$$\begin{aligned} \frac{E_H}{A} &= \frac{3}{5}\frac{\hbar^2}{2m}c_n\rho_0^{\frac{2}{3}} + \big(A_0^\rho\ + B_0^\rho\,\rho_0\big)\rho_0 \\ &\quad + \big(A_1^\rho\ + B_1^\rho\,\rho_0\big)\rho_0 + \frac{3}{5}c_n\big(A_0^\tau\ + B_0^\tau\,\rho_0\big)\rho_0^{\frac{5}{3}} \\ &\quad + \frac{3}{5}c_n\big(A_1^\tau\ + B_1^\tau\,\rho_0 + B_{10}^\tau\,\rho_0\big)\rho_0^{\frac{5}{3}}. \end{aligned} \tag{B19}$$

### 6. Effective masses

The average energy of a nucleon inside the nuclear medium is the sum of a kinetic term plus a momentum-dependent self-energy term[5] coming from its interaction with all the other nucleons. This energy can be rewritten as a kinetic energy term involving an effective mass. One can thus define four different effective masses for neutron or proton with spin-up or -down, i.e., $m^*_{n\uparrow}$, $m^*_{n\downarrow}$, $m^*_{p\uparrow}$, and $m^*_{p\downarrow}$. The expressions for such effective masses at arbitrary values of the spin, isospin, and spin-isospin excesses read as

$$\begin{aligned} \frac{m}{m^*_{q\sigma}} &\equiv \frac{2m}{\hbar^2}\frac{\partial\mathcal{E}_H}{\partial\tau_{q\sigma}} \\ &= 1 + \frac{2m}{\hbar^2}\big[\big(A_0^\tau + B_0^\tau\rho_0\big)\rho_0 \\ &\quad + \big(A_1^\tau + B_1^\tau\rho_0\big)\eta_q I_\tau\rho_0 + \big(A_0^T + B_0^T\rho_0\big)\eta_\sigma I_\sigma\rho_0 \\ &\quad + \big(A_1^T + B_1^T\rho_0\big)\eta_\sigma\eta_q I_{\sigma\tau}\rho_0 \\ &\quad + \big(B_{10}^\tau I_\tau^2 + B_0^{\tau s}I_\sigma^2 + B_{10}^{\tau s}I_{\sigma\tau}^2 + B_1^{\tau s}\eta_q I_\sigma I_{\sigma\tau} \\ &\quad + B_{10}^T\eta_\sigma I_\tau I_{\sigma\tau} + B_{01}^T\eta_\sigma\eta_q I_\tau I_\sigma\big)\rho_0^2\big], \end{aligned} \tag{B20}$$

where

$$\eta_q = \begin{cases} +1 & \text{for } q = n, \\ -1 & \text{for } q = p, \end{cases} \tag{B21}$$

$$\eta_\sigma = \begin{cases} +1 & \text{for } \sigma = \uparrow, \\ -1 & \text{for } \sigma = \downarrow. \end{cases} \tag{B22}$$

One can further define effective masses of the particle species $q$

$$\begin{aligned} \frac{m}{m^*_q} &\equiv \frac{1}{2}\left(\frac{m}{m^*_{q\uparrow}} + \frac{m}{m^*_{q\downarrow}}\right) \\ &= 1 + \frac{2m}{\hbar^2}\big[\big(A_0^\tau + B_0^\tau\rho_0\big)\rho_0 + \big(A_1^\tau + B_1^\tau\rho_0\big)\eta_q I_\tau\rho_0 \\ &\quad + \big(B_{10}^\tau I_\tau^2 + B_0^{\tau s}I_\sigma^2 + B_{10}^{\tau s}I_{\sigma\tau}^2 + B_1^{\tau s}\eta_q I_\sigma I_{\sigma\tau}\big)\rho_0^2\big], \end{aligned} \tag{B23a}$$

[5]The standard notion of (physical) self-energy that appears in many-body theories is not to be confused with the notion of spurious self-interaction in energy functionals as invoked in the Introduction.

and of particles with spin orientation $\sigma$

$$\frac{m}{m^*_\sigma} \equiv \frac{1}{2}\left(\frac{m}{m^*_{n\sigma}} + \frac{m}{m^*_{p\sigma}}\right) = 1 + \frac{2m}{\hbar^2}\big[\big(A^\tau_0 + B^\tau_0\rho_0\big)\rho_0 + \big(A^T_0 + B^T_0\rho_0\big)\eta_\sigma I_\sigma \rho_0 + \big(B^\tau_{10} I^2_\tau + B^{\tau s}_0 I^2_\sigma + B^{\tau s}_{10} I^2_{\sigma\tau} + B^T_{10}\eta_\sigma I_\tau I_{\sigma\tau}\big)\rho_0^2\big]. \tag{B23b}$$

Equivalently, one can define scalar-isoscalar, scalar-isovector, vector-isoscalar, and vector-isovector effective masses $m^*_{st}$,

$$\frac{m}{m^*_{00}} \equiv \frac{1}{4}\left(\frac{m}{m^*_{n\uparrow}} + \frac{m}{m^*_{n\downarrow}} + \frac{m}{m^*_{p\uparrow}} + \frac{m}{m^*_{p\downarrow}}\right) = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}_H}{\partial \tau_0}, \tag{B24a}$$

$$\frac{m}{m^*_{01}} \equiv \frac{1}{4}\left(\frac{m}{m^*_{n\uparrow}} + \frac{m}{m^*_{n\downarrow}} - \frac{m}{m^*_{p\uparrow}} - \frac{m}{m^*_{p\downarrow}}\right) = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}_H}{\partial \tau_1}, \tag{B24b}$$

$$\frac{m}{m^*_{10}} \equiv \frac{1}{4}\left(\frac{m}{m^*_{n\uparrow}} - \frac{m}{m^*_{n\downarrow}} + \frac{m}{m^*_{p\uparrow}} - \frac{m}{m^*_{p\downarrow}}\right) = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}_H}{\partial T_0}, \tag{B24c}$$

$$\frac{m}{m^*_{11}} \equiv \frac{1}{4}\left(\frac{m}{m^*_{n\uparrow}} - \frac{m}{m^*_{n\downarrow}} - \frac{m}{m^*_{p\uparrow}} + \frac{m}{m^*_{p\downarrow}}\right) = \frac{2m}{\hbar^2}\frac{\partial \mathcal{E}_H}{\partial T_1}, \tag{B24d}$$

which for our functional gives

$$\frac{m}{m^*_{00}} = 1 + \frac{2m}{\hbar^2}\big[\big(A^\tau_0 + B^\tau_0\rho_0\big)\rho_0 + \big(B^\tau_{10} I^2_\tau + B^{\tau s}_0 I^2_\sigma + B^{\tau s}_{10} I^2_{\sigma\tau}\big)\rho_0^2\big], \tag{B25a}$$

$$\frac{m}{m^*_{01}} = \frac{2m}{\hbar^2}\big[\big(A^\tau_1 + B^\tau_1\rho_0\big) I_\tau \rho_0 + B^{\tau s}_1 I_\sigma I_{\sigma\tau}\rho_0^2\big], \tag{B25b}$$

$$\frac{m}{m^*_{10}} = \frac{2m}{\hbar^2}\big[\big(A^T_0 + B^T_0\rho_0\big) I_\sigma \rho_0 + B^T_{10} I_\tau I_{\sigma\tau}\rho_0^2\big], \tag{B25c}$$

$$\frac{m}{m^*_{11}} = \frac{2m}{\hbar^2}\big[\big(A^T_1 + B^T_1\rho_0\big) I_{\sigma\tau}\rho_0 + B^T_{01} I_\tau I_\sigma \rho_0^2\big]. \tag{B25d}$$

The implication of these nonstandard definitions of the effective masses will be expanded on in a forthcoming publication [81]. Note that $m^*_{01}$ is different than the usual definition of the isovector effective mass. The various effective masses at the saturation point of SNM can be trivially obtained from the expressions given above by setting $I_\tau = I_\sigma = I_{\sigma\tau} = 0$.

### 7. Landau parameters

#### *a. Introduction*

Landau parameters are interesting quantities [82–84] to compute for several reasons. Two sum rules must be fulfilled by Landau parameters for the Pauli principle to be respected [85]. In the present case where the EDF kernel does derive from a pseudopotential, the two sum rules are fulfilled analytically by construction.

There are also two other sum rules that derive from the antisymmetry of the scattering amplitude, which is determined by the residual interaction. The antisymmetry of the residual interaction itself, to which Landau parameters are related, however, does not ensure the antisymmetry of the observable scattering amplitude [86].

Landau parameters can also be used to detect and control infinite-wavelength instabilities. Such instabilities appear when Landau parameters do not respect the stability conditions [85,87],

$$1 + \frac{X_l}{2l+1} > 0, \tag{B26}$$

where $X_l = \{F_l, F'_l, G_l, G'_l\}$ with $l = 0, 1$ denotes the Landau parameters. In particular, four of the Landau parameters, $F_0$, $F'_0$, $G_0$, and $G'_0$ are also related to the stiffness of the EOS, i.e., its second derivatives with respect to density, isospin, spin, and spin-isospin fluctuations. This leads to the following relationships at saturation:

$$K_\infty = 6\frac{\hbar^2 k_F^2}{2m^*_0}(1 + F_0), \tag{B27a}$$

$$a_\tau = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m^*_0}(1 + F'_0), \tag{B27b}$$

$$a_\sigma = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m^*_0}(1 + G_0), \tag{B27c}$$

$$a_{\sigma\tau} = \frac{1}{3}\frac{\hbar^2 k_F^2}{2m^*_0}(1 + G'_0). \tag{B27d}$$

For the EOS of SNM to have a stable minimum, all these second derivatives have to be larger than zero, such that $F_0$, $F'_0$, $G_0$, and $G'_0$ are greater than $-1$, which is equivalent to the stability conditions (B26).

It has to be noted that parametrizations must not only be stable against infinite wavelength instabilities signaled by Landau parameters, but also against finite-size instabilities that probe gradient terms in the EDF [32–34,88,89]. The control of finite-size instabilities for the newly proposed Skyrme-like parametrizations will be discussed in a forthcoming publication.

#### *b. Definition*

Landau parameters are calculated via the residual particle-hole interaction in INM, which, in general, is defined through

$$v^{\rm res}_{12} \equiv \langle \vec{r}'_1\sigma'_1 q_1, \vec{r}'_2\sigma'_2 q_2 | \hat{v}^{\rm res}_{12} | \vec{r}_1\sigma_1 q_1, \vec{r}_2\sigma_2 q_2\rangle = \frac{\partial^2 \mathcal{E}}{\partial\rho(\vec{r}'_2\sigma'_2 q_2, \vec{r}_2\sigma_2 q_2)\partial\rho(\vec{r}'_1\sigma'_1 q_1, \vec{r}_1\sigma_1 q_1)} \tag{B28}$$

and can be written in INM, for momenta lying on the Fermi surface, as

$$v^{\rm res}_{12} = N_0^{-1}\sum_l [F_l + F'_l\ \tau_1\circ\tau_2 + G_l\ \vec{\sigma}_1\cdot\vec{\sigma}_2 + G'_l\ \vec{\sigma}_1\cdot\vec{\sigma}_2\ \tau_1\circ\tau_2] P_l(\cos\theta), \tag{B29}$$

TABLE XII. Landau parameters expressed in terms of the pseudopotential parameters. Missing entries are zero.

| | $f_0$ | $f_0'$ | $g_0$ | $g_0'$ | $f_1$ | $f_1'$ | $g_1$ | $g_1'$ |
|---|---|---|---|---|---|---|---|---|
| $t_0$ | $\frac{3}{4}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | | | | |
| $t_0x_0$ | | $-\frac{1}{2}$ | $\frac{1}{2}$ | | | | | |
| $t_1k_F^2$ | $\frac{3}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{3}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ |
| $t_1x_1k_F^2$ | | $-\frac{1}{4}$ | $\frac{1}{4}$ | | | $\frac{1}{4}$ | $-\frac{1}{4}$ | |
| $t_2k_F^2$ | $\frac{5}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | $-\frac{5}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ | $-\frac{1}{8}$ |
| $t_2x_2k_F^2$ | $\frac{1}{2}$ | $\frac{1}{4}$ | $\frac{1}{4}$ | | $-\frac{1}{2}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | |
| $u_0\rho_0$ | $\frac{9}{8}$ | $-\frac{3}{8}$ | $-\frac{3}{8}$ | $-\frac{3}{8}$ | | | | |
| $u_1\rho_0k_F^2$ | $\frac{39}{80}$ | $-\frac{13}{80}$ | $-\frac{13}{80}$ | $-\frac{13}{80}$ | $-\frac{3}{16}$ | $\frac{1}{16}$ | $\frac{1}{16}$ | $\frac{1}{16}$ |
| $u_1y_1\rho_0k_F^2$ | | $-\frac{1}{40}$ | $\frac{1}{40}$ | | | $\frac{1}{8}$ | $-\frac{1}{8}$ | |
| $u_2\rho_0k_F^2$ | $\frac{39}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{1}{32}$ | $-\frac{15}{32}$ | $-\frac{7}{32}$ | $-\frac{7}{32}$ | $-\frac{7}{32}$ |
| $u_2y_{21}\rho_0k_F^2$ | $\frac{39}{40}$ | $\frac{1}{20}$ | $\frac{1}{20}$ | $-\frac{3}{40}$ | $-\frac{3}{8}$ | $-\frac{1}{4}$ | $-\frac{1}{4}$ | $-\frac{1}{8}$ |
| $u_2y_{22}\rho_0k_F^2$ | $\frac{39}{80}$ | $-\frac{31}{80}$ | $\frac{35}{80}$ | $-\frac{3}{80}$ | $-\frac{3}{16}$ | $-\frac{5}{16}$ | $\frac{1}{16}$ | $-\frac{1}{16}$ |

where coefficients $F_l$, $F_l'$, $G_l$, and $G_l'$ are Landau parameters, $N_0 \equiv 2m_0^* k_F/\pi^2\hbar^2$ is a normalization factor, $P_l(x)$ are Legendre polynomials, and $\theta$ is the angle between the incoming momentum of nucleon 1 and the outgoing momentum of nucleon 2. In the present case, Landau parameters read explicitly as

$$f_0 = 2A_0^\rho + 2A_0^\tau\, k_F^2 + 6B_0^\rho\, \rho_0 + 2B_0^\tau\, \tau_0 + 4B_0^\tau\, k_F^2\rho_0, \tag{B30a}$$

$$f_0' = 2A_1^\rho + 2A_1^\tau\, k_F^2 + 2B_1^\rho\, \rho_0 + 2B_{10}^\tau\, \tau_0 + 2B_1^\tau\, k_F^2\rho_0, \tag{B30b}$$

$$g_0 = 2A_0^s + 2A_0^T\, k_F^2 + 2B_0^s\, \rho_0 + 2B_0^{\tau s}\, \tau_0 + 2B_0^T\, k_F^2\rho_0, \tag{B30c}$$

$$g_0' = 2A_1^s + 2A_1^T\, k_F^2 + 2B_1^s\, \rho_0 + 2B_{10}^{\tau s}\, \tau_0 + 2B_1^T\, k_F^2\rho_0, \tag{B30d}$$

$$f_1 = 2A_0^j\, k_F^2 + 2B_0^j\, k_F^2\rho_0, \tag{B30e}$$

$$f_1' = 2A_1^j\, k_F^2 + 2B_1^j\, k_F^2\rho_0, \tag{B30f}$$

$$g_1 = 2A_0^J\, k_F^2 + 2B_0^J\, k_F^2\rho_0, \tag{B30g}$$

$$g_1' = 2A_1^J\, k_F^2 + 2B_1^J\, k_F^2\rho_0, \tag{B30h}$$

where $f_l \equiv F_l/N_0$, $f_l' \equiv F_l'/N_0$, $g_l \equiv G_l/N_0$, and $g_l' \equiv G_l'/N_0$ and where we have used Eq. (B5) to express $\tau_0$ in terms of $k_F^2$ and $\rho_0$. The Landau parameters with $l \geqslant 2$ are zero for a Skyrme-type interaction with only up to two gradients. The expressions for the Landau parameters in terms of the pseudopotential parameters are given in Table XII.

#### c. Sum rules from the residual interaction

The EDF from which the residual interaction derives has been constructed from an antisymmetrized vertex such that the Pauli principle is respected throughout. When the antisymmetrized vertex is a two-body pseudopotential multiplied by a two-body antisymmetrizer, taking two derivatives of the EDF with respect to nonlocal densities gives back the original antisymmetrized vertex. When the antisymmetrized vertex is made of two- plus three-body pseudopotentials multiplied by appropriate antisymmetrizers, the residual particle-hole interaction remains an antisymmetrized two-body vertex. Consequently, the exclusion principle demands that the residual interaction Eq. (B29) is antisymmetric under the exchange of incoming or outgoing particles. This is equivalent to requiring that incoming and outgoing two-body states carry odd values of $L + S + T$, where $L$ denotes the two-body orbital angular momentum of the relative motion, whereas $S$ and $T$ characterize the two-body spin and isospin, respectively. Starting from Eq. (B29) with $\vec{p}_1 = \vec{p}_2'$, i.e., $\theta = 0$, and requiring that the antisymmetry holds for each spin-isospin channel separately, provides two sum rules,

$$\sum_l (F_l + F_l' + G_l + G_l') = 0, \tag{B31a}$$

$$\sum_l (F_l - 3F_l' - 3G_l + 9G_l') = 0, \tag{B31b}$$

where we have used that $P_l(1) = 1$ for all $l$. Equation (B31a) holds for spin and isospin triplet ($S = T = 1$) two-body states, for which $\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \tau_1 \circ \tau_2 = 1$. Equation (B31b) holds for spin and isospin singlet ($S = T = 0$) two-body states for which $\vec{\sigma}_1 \cdot \vec{\sigma}_2 = \tau_1 \circ \tau_2 = -3$. In both cases the relative orbital angular momentum of the two-body state is odd.

Sum rules (B31) are fulfilled for Landau parameters derived from the presently developed two- plus three-body pseudopotential; see Table XII. This property provides a stringent test that the derivation of the EDF and of the residual interaction are correct.

Note that in the presence of tensor-type pseudopotentials there are additional contributions to the sum rules [84,89,90].

#### d. Sum rules from the scattering amplitude

The residual particle-hole interaction is not a physically observable quantity in contrast to the scattering amplitude $\Gamma_{12}$ associated with the motion of a particle-hole pair [86]. The latter is related to the former through an integral equation, such that the particle-hole interaction can be seen as the irreducible vertex and the scattering amplitude as the total vertex. Analogs to Eq. (B31) can be derived from the antisymmetry of the scattering amplitude. Plugging the expansion of the scattering amplitude on Legendre polynomials,

$$\Gamma_{12} \equiv N_0^{-1} \sum_l [B_l + C_l\, \tau_1 \circ \tau_2 + D_l\, \vec{\sigma}_1 \cdot \vec{\sigma}_2 + E_l\, \vec{\sigma}_1 \cdot \vec{\sigma}_2\, \tau_1 \circ \tau_2] P_l(\cos\theta), \tag{B32}$$

into the integral equation that relates it to the residual interaction (B29), one obtains, in the absence of tensor terms, the relationships [82,86,91]

$$B_l = \frac{F_l}{1 + F_l/(2l+1)}, \tag{B33a}$$

$$C_l = \frac{F_l'}{1 + F_l'/(2l+1)}, \tag{B33b}$$

$$D_l = \frac{G_l}{1 + G_l/(2l+1)}, \tag{B33c}$$

$$E_l = \frac{G_l'}{1 + G_l'/(2l+1)}. \tag{B33d}$$

The reasoning used in Appendix B 7 c now provides sum rules for the expansion coefficients of $\Gamma_{12}$,

$$\sum_l (B_l + C_l + D_l + E_l) = 0, \tag{B34a}$$

$$\sum_l (B_l - 3C_l - 3D_l + 9E_l) = 0, \tag{B34b}$$

which can be rearranged as [91]

$$\sum_l (B_l + 3E_l) = 0, \tag{B35a}$$

$$\sum_l \left(\frac{2}{3}B_l + C_l + D_l\right) = 0. \tag{B35b}$$

In Born approximation, i.e., when the magnitude of Landau parameters entering Eq. (B33) are negligible compared to $2l+1$, Eq. (B34) reduces to Eq. (B31). However, Landau parameters are not small in nuclear matter, such that, physically speaking, sum rule (B31) cannot be justified starting from the scattering amplitude.

Interestingly, the antisymmetric character of the residual particle-hole interaction does not guarantee the antisymmetry of the scattering amplitude, which is frequently broken in practice. Through the iteration process of the integral equation, reducible diagrams might appear without their Pauli principle counterparts [86,92], which is a fingerprint of the lack of complexity of the irreducible residual interaction. Inserting density dependencies into the pseudopotential has allowed in some cases to effectively compensate for such missing diagrams [86] at the price of compromising the antisymmetry of the residual interaction itself and thus of violating Eq. (B31). In the end, fulfilling both the antisymmetry of the irreducible vertex and of the scattering amplitude is a difficult task. In the present case, the former is ensured analytically, whereas the latter is not. The extent to which it is violated will depend on the values of the parameters that result from a given fit.

## APPENDIX C: STEPS TO DERIVE THE EDF KERNEL

This section lists the steps to derive the energy functional in proton-neutron representation from the pseudopotentials defined in Eq. (51). We limit the illustration to a few normal and anomalous terms resulting from the operator $\hat{v}^{\rm ex} = u_2 y_{21}\, \hat{P}^{\sigma}_{12}\, \hat{\vec{k}}^{\dagger}_{12} \hat{\delta}^{r}_{13} \hat{\delta}^{r}_{23} \cdot \hat{\vec{k}}_{12}$, one of the terms contained in $\hat{v}^{2}_{\overline{123}}$ [Eq. (46f)]. Such an operator is used in Eqs. (44a) and (44b) where one has to multiply it to the antisymmetrizers. For the normal part one must thus evaluate $\hat{P}^{\sigma}_{12}\hat{\mathcal{A}}_{123}$, which leads to

$$\hat{P}^{\sigma}_{12}\hat{\mathcal{A}}_{123} = \hat{P}^{\sigma}_{12} - \hat{P}^{r}_{12}\hat{P}^{q}_{12} - \hat{P}^{r}_{23}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23} - \hat{P}^{r}_{13}\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{13} + \hat{P}^{r}_{12}\hat{P}^{r}_{23}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{12}\hat{P}^{q}_{23} + \hat{P}^{r}_{12}\hat{P}^{r}_{13}\hat{P}^{\sigma}_{13}\hat{P}^{q}_{12}\hat{P}^{q}_{13}. \tag{C1}$$

Selecting only the third term as an example, i.e., $-\hat{v}^{ex}P_{23}$, which is also obtained in the pairing part when evaluating $\hat{\mathcal{A}}^{12}_{123}\hat{P}^{\sigma}_{12}\hat{\mathcal{A}}^{12}_{123}$, one computes its matrix elements by inserting closure relations on $\mathcal{H}_3$ in the coordinate basis according to

$$-\langle ijk|\hat{v}^{ex}P_{23}|lmn\rangle = -\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6\; \varphi^{\dagger}_i(\xi_1)\varphi^{\dagger}_j(\xi_2)\varphi^{\dagger}_k(\xi_3)\langle \xi_1\xi_2\xi_3|\hat{v}^{ex}P_{23}|\xi_4\xi_5\xi_6\rangle \varphi_l(\xi_4)\varphi_m(\xi_5)\varphi_n(\xi_6). \tag{C2}$$

### 1. Spatial part of the matrix element

Using Eqs. (17) and (22), one obtains

$$\langle \vec{r}_1\vec{r}_2\vec{r}_3|\hat{\vec{k}}^{\dagger}_{12}\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}\cdot\hat{\vec{k}}_{12}\hat{P}^{r}_{23}|\vec{r}_4\vec{r}_5\vec{r}_6\rangle = \vec{k}^{*}_{\vec{r}_1\vec{r}_2}\,\langle \vec{r}_1\vec{r}_2\vec{r}_3|\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}|\vec{r}_4\vec{r}_6\vec{r}_5\rangle\,\vec{k}_{\vec{r}_4\vec{r}_6}. \tag{C3}$$

Applying the gradients on the wave functions to the right and to the left, one can write

$$\begin{aligned}
-\langle ijk|\hat{v}^{ex}P_{23}|lmn\rangle &= -\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6\; \langle \sigma_1 q_1 \sigma_2 q_2 \sigma_3 q_3|\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}|\sigma_4 q_4 \sigma_5 q_5 \sigma_6 q_6\rangle\; \langle \vec{r}_1\vec{r}_2\vec{r}_3|\hat{\delta}^{r}_{13}\hat{\delta}^{r}_{23}|\vec{r}_4\vec{r}_6\vec{r}_5\rangle \\
&\quad\times \vec{k}^{*}_{\vec{r}_1\vec{r}_2}\vec{k}_{\vec{r}_4\vec{r}_6}\;\varphi^{\dagger}_i(\xi_1)\varphi^{\dagger}_j(\xi_2)\varphi^{\dagger}_k(\xi_3)\varphi_l(\xi_4)\varphi_m(\xi_5)\varphi_n(\xi_6) \qquad \text{(C4a)} \\
&= -\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6\; \langle \sigma_1 q_1 \sigma_2 q_2 \sigma_3 q_3|\hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}|\sigma_4 q_4 \sigma_5 q_5 \sigma_6 q_6\rangle\; \delta(\vec{r}_1-\vec{r}_4)\delta(\vec{r}_2-\vec{r}_6) \\
&\quad\times \delta(\vec{r}_3-\vec{r}_5)\delta(\vec{r}_4-\vec{r}_5)\delta(\vec{r}_6-\vec{r}_5)\;\vec{k}^{*}_{\vec{r}_1\vec{r}_2}\vec{k}_{\vec{r}_4\vec{r}_6}\;\varphi^{\dagger}_i(\xi_1)\varphi^{\dagger}_j(\xi_2)\varphi^{\dagger}_k(\xi_3)\varphi_l(\xi_4)\varphi_m(\xi_5)\varphi_n(\xi_6). \qquad \text{(C4b)}
\end{aligned}$$

With that at hand, Eqs. (44a) and (44b) become

$$E^{\rho\rho\rho}_{ex} = -\frac{1}{2}\sum_{ijklmn}\langle ijk|\hat{v}^{ex}P_{23}|lmn\rangle\,\rho_{li}\,\rho_{mj}\,\rho_{nk} \tag{C5a}$$

$$= -\frac{1}{2}\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6 \left\langle \hat{P}^{\sigma}_{12}\hat{P}^{\sigma}_{23}\hat{P}^{q}_{23}\right\rangle \delta(\{\vec{r}\}=\vec{r})\;\vec{k}^{*}_{\vec{r}_1\vec{r}_2}\vec{k}_{\vec{r}_4\vec{r}_6}\;\rho(\xi_4,\xi_1)\rho(\xi_5,\xi_2)\rho(\xi_6,\xi_3), \tag{C5b}$$

$$E_{ex}^{\kappa\kappa\rho} = -\frac{1}{2}\sum_{ijklmn}\langle ijk|\hat{v}^{ex}P_{23}|lmn\rangle\kappa_{ij}^{*}\kappa_{lm}\rho_{nk} \tag{C5c}$$

$$= -\frac{1}{2}\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6 \left\langle \hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\hat{P}_{23}^{q}\right\rangle \delta(\{\vec{r}\}=\vec{r})\,\vec{k}^{*}_{\vec{r}_1\vec{r}_2}\cdot\vec{k}_{\vec{r}_4\vec{r}_6}\,\kappa^{*}(\xi_1,\xi_2)\kappa(\xi_4,\xi_5)\rho(\xi_6,\xi_3), \tag{C5d}$$

where we have introduced the shorthands

$$\left\langle \hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\hat{P}_{23}^{q}\right\rangle \equiv \langle\sigma_1 q_1\sigma_2 q_2\sigma_3 q_3|\hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\hat{P}_{23}^{q}|\sigma_4 q_4\sigma_5 q_5\sigma_6 q_6\rangle, \tag{C6a}$$

$$\delta(\{\vec{r}\}=\vec{r}) \equiv \delta(\vec{r}_1-\vec{r}_4)\delta(\vec{r}_2-\vec{r}_6)\delta(\vec{r}_3-\vec{r}_5)\delta(\vec{r}_4-\vec{r}_5)\delta(\vec{r}_6-\vec{r}_5). \tag{C6b}$$

### 2. Isospin part of the matrix element

The matrix element of the isospin-exchange operator is trivially evaluated using Eq. (22),

$$\langle q_1 q_2 q_3|\hat{P}_{23}^{q}|q_4 q_5 q_6\rangle = \langle q_1 q_2 q_3|q_4 q_6 q_5\rangle = \delta_{q_1 q_4}\delta_{q_2 q_6}\delta_{q_3 q_5}. \tag{C7}$$

Recalling that local densities are diagonal in isospin, the integrand is null if $q_4 \neq q_1$, $q_5 \neq q_2$, $q_6 \neq q_3$ for the normal part and if $q_1 \neq q_2$, $q_4 \neq q_5$, $q_6 \neq q_3$ for the anomalous part. One thus obtains

$$E_{ex}^{\rho\rho\rho} = -\frac{1}{2}\int d\zeta_1 d\zeta_2 d\zeta_3 d\zeta_4 d\zeta_5 d\zeta_6 \sum_{q_1,q_2}\left\langle \hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\right\rangle \delta(\{\vec{r}\}=\vec{r})\vec{k}^{*}_{\vec{r}_1\vec{r}_2}\cdot\vec{k}_{\vec{r}_4\vec{r}_6}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_2}(\zeta_5,\zeta_2)\rho_{q_2}(\zeta_6,\zeta_3), \tag{C8a}$$

$$E_{ex}^{\kappa\kappa\rho} = -\frac{1}{2}\int d\zeta_1 d\zeta_2 d\zeta_3 d\zeta_4 d\zeta_5 d\zeta_6 \sum_{q_1}\left\langle \hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\right\rangle \delta(\{\vec{r}\}=\vec{r})\,\vec{k}^{*}_{\vec{r}_1\vec{r}_2}\cdot\vec{k}_{\vec{r}_4\vec{r}_6}\,\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C8b}$$

where $\zeta \equiv \vec{r},\sigma$ and $\langle\hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}\rangle \equiv \langle\sigma_1\sigma_2\sigma_3|\hat{P}_{12}^{\sigma}\hat{P}_{23}^{\sigma}|\sigma_4\sigma_5\sigma_6\rangle$. More generally, matrix elements at play in the normal part of the EDF are

$$\langle q_1 q_2 q_3|1|q_4 q_5 q_6\rangle \to \sum_{q_1,q_2,q_3}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_2}(\zeta_5,\zeta_2)\rho_{q_3}(\zeta_6,\zeta_3), \tag{C9a}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1,q_3}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_1}(\zeta_5,\zeta_2)\rho_{q_3}(\zeta_6,\zeta_3), \tag{C9b}$$

$$\langle q_1 q_2 q_3|\hat{P}_{23}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1,q_2}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_2}(\zeta_5,\zeta_2)\rho_{q_2}(\zeta_6,\zeta_3), \tag{C9c}$$

$$\langle q_1 q_2 q_3|\hat{P}_{13}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1,q_2}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_2}(\zeta_5,\zeta_2)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C9d}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}\hat{P}_{23}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_1}(\zeta_5,\zeta_2)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C9e}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}\hat{P}_{13}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\rho_{q_1}(\zeta_4,\zeta_1)\rho_{q_1}(\zeta_5,\zeta_2)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C9f}$$

whereas those at play for the pairing part are

$$\langle q_1 q_2 q_3|1|q_4 q_5 q_6\rangle \to \sum_{q_1,q_2}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_2}(\zeta_6,\zeta_3), \tag{C10a}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1,q_2}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_2}(\zeta_6,\zeta_3), \tag{C10b}$$

$$\langle q_1 q_2 q_3|\hat{P}_{23}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C10c}$$

$$\langle q_1 q_2 q_3|\hat{P}_{13}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C10d}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}\hat{P}_{23}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3), \tag{C10e}$$

$$\langle q_1 q_2 q_3|\hat{P}_{12}^{q}\hat{P}_{13}^{q}|q_4 q_5 q_6\rangle \to \sum_{q_1}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3). \tag{C10f}$$

### 3. Spin part of the matrix element for the normal energy

Using Eqs. (27), one arrives straightforwardly after one step of algebraic computation at

$$E_{ex}^{\rho\rho\rho} = -\frac{1}{8}\int d^3r_1 d^3r_2 d^3r_3 d^3r_4 d^3r_5 d^3r_6 \sum_{q_1,q_2} \delta(\{\vec{r}\}=\vec{r})\, \vec{k}^{*}_{\vec{r}_1\vec{r}_2}\cdot\vec{k}_{\vec{r}_4\vec{r}_6}\Big[\rho_{q_1}(\vec{r}_4,\vec{r}_1)\rho_{q_2}(\vec{r}_5,\vec{r}_2)\rho_{q_2}(\vec{r}_6,\vec{r}_3)$$
$$+\vec{s}_{q_1}(\vec{r}_4,\vec{r}_1)\cdot\vec{s}_{q_2}(\vec{r}_5,\vec{r}_2)\rho_{q_2}(\vec{r}_6,\vec{r}_3)+\rho_{q_1}(\vec{r}_4,\vec{r}_1)\vec{s}_{q_2}(\vec{r}_5,\vec{r}_2)\cdot\vec{s}_{q_2}(\vec{r}_6,\vec{r}_3)+\vec{s}_{q_1}(\vec{r}_4,\vec{r}_1)\rho_{q_2}(\vec{r}_5,\vec{r}_2)\cdot\vec{s}_{q_2}(\vec{r}_6,\vec{r}_3)$$
$$+\mathrm{i}\sum_{\nu\kappa\lambda}\epsilon_{\nu\kappa\lambda}s_{q_1,\nu}(\vec{r}_4,\vec{r}_1)s_{q_2,\lambda}(\vec{r}_5,\vec{r}_2)s_{q_2,\kappa}(\vec{r}_6,\vec{r}_3)\Big], \tag{C11}$$

where Eqs. (53a) and (53b) have been utilized under the form

$$\sum_{\sigma_1\sigma_4}\langle\sigma_1|1|\sigma_4\rangle\rho_{q_1}(\zeta_4,\zeta_1)=\rho_{q_1}(\vec{r}_4,\vec{r}_1), \tag{C12a}$$
$$\sum_{\sigma_1\sigma_4}\langle\sigma_1|\hat{\sigma}_\nu|\sigma_4\rangle\rho_{q_1}(\zeta_4,\zeta_1)=s_{q_1,\nu}(\vec{r}_4,\vec{r}_1). \tag{C12b}$$

### 4. Spin part of the matrix element for the pairing energy

Expressing the pairing part of the EDF kernel in terms of nonlocal pair-spin densities is trickier. Using Eq. (27) to express spin-exchange operators in terms of spin Pauli matrices, let us take one resulting term, i.e., the one proportional to $\hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_2$, to illustrate the procedure. One needs to compute

$$\sum_{\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6}\langle\hat{\vec{\sigma}}_1\cdot\hat{\vec{\sigma}}_2\rangle\,\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3)=\sum_{\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\sigma_2|\hat{\vec{\sigma}}|\sigma_5\rangle\,\delta_{\sigma_3\sigma_6}\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\zeta_6,\zeta_3)$$
$$=\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\sigma_2|\hat{\vec{\sigma}}|\sigma_5\rangle\,\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)\rho_{q_1}(\vec{r}_6,\vec{r}_3). \tag{C13}$$

To do so, one exploits the relations

$$\kappa_q(\vec{r}\sigma,\vec{r}\,'\sigma')=2\bar{\sigma}'\tilde{\rho}_q(\vec{r}\sigma,\vec{r}\,'\bar{\sigma}'), \tag{C14a}$$
$$\kappa^{*}_q(\vec{r}\sigma,\vec{r}\,'\sigma')=2\bar{\sigma}'\tilde{\rho}^{*}_q(\vec{r}\sigma,\vec{r}\,'\bar{\sigma}') \tag{C14b}$$

[Eqs. (56) and (54)], as well as the following set of relations involving matrix elements of spin Pauli matrices,

$$\langle\sigma_1|\hat{\sigma}_\mu|\sigma_2\rangle=-4\sigma_1\sigma_2\langle\bar{\sigma}_2|\hat{\sigma}_\mu|\bar{\sigma}_1\rangle, \tag{C15a}$$
$$\hat{\sigma}_\nu\hat{\sigma}_\nu=\delta_{\nu\nu}, \tag{C15b}$$
$$\sum_\sigma\langle\sigma|\hat{\sigma}_\nu|\sigma\rangle=0, \tag{C15c}$$
$$\sum_\sigma\langle\sigma|\sigma\rangle=2, \tag{C15d}$$
$$\sum_\sigma\langle\sigma|\hat{\sigma}_\mu\hat{\sigma}_\nu\hat{\sigma}_\lambda\hat{\sigma}_\kappa|\sigma\rangle=\delta_{\mu\nu}\delta_{\lambda\kappa}-\delta_{\mu\lambda}\delta_{\nu\kappa}+\delta_{\mu\kappa}\delta_{\nu\lambda}, \tag{C15e}$$

to perform the following algebraic manipulations:

$$\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\sigma_2|\hat{\vec{\sigma}}|\sigma_5\rangle\,\kappa^{*}_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)$$
$$=\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\sigma_2|\hat{\vec{\sigma}}|\sigma_5\rangle\,4\sigma_2\sigma_5\tilde{\rho}^{*}_{q_1}(\vec{r}_1\sigma_1,\vec{r}_2\bar{\sigma}_2)\tilde{\rho}_{q_1}(\vec{r}_4\sigma_4,\vec{r}_5\bar{\sigma}_5)$$
$$=-\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\bar{\sigma}_5|\hat{\vec{\sigma}}|\bar{\sigma}_2\rangle\,\tilde{\rho}^{*}_{q_1}(\vec{r}_1\sigma_1,\vec{r}_2\bar{\sigma}_2)\tilde{\rho}_{q_1}(\vec{r}_4\sigma_4,\vec{r}_5\bar{\sigma}_5)$$
$$=-\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1|\hat{\vec{\sigma}}|\sigma_4\rangle\cdot\langle\sigma_5|\hat{\vec{\sigma}}|\sigma_2\rangle\,\tilde{\rho}^{*}_{q_1}(\vec{r}_1\sigma_1,\vec{r}_2\sigma_2)\tilde{\rho}_{q_1}(\vec{r}_4\sigma_4,\vec{r}_5\sigma_5)$$

$$
\begin{aligned}
&= -\frac{1}{4}\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\sum_{\nu}\langle\sigma_1|\hat{\sigma}_\nu|\sigma_4\rangle\ \langle\sigma_5|\hat{\sigma}_\nu|\sigma_2\rangle\left[\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\delta_{\sigma_1\sigma_2}+\sum_{\kappa}\tilde{s}^*_{q_1,\kappa}(\vec{r}_1,\vec{r}_2)\ \langle\sigma_2|\sigma_\kappa|\sigma_1\rangle\right]\\
&\quad\times\left[\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)\delta_{\sigma_4\sigma_5}+\sum_{\lambda}\tilde{s}_{q_1,\lambda}(\vec{r}_4,\vec{r}_5)\ \langle\sigma_4|\sigma_\lambda|\sigma_5\rangle\right]\\
&= -\frac{1}{4}\left[\sum_{\sigma}\sum_{\nu}\langle\sigma|\hat{\sigma}_\nu\hat{\sigma}_\nu|\sigma\rangle\ \tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)+\sum_{\sigma}\sum_{\nu\lambda}\langle\sigma|\hat{\sigma}_\nu\hat{\sigma}_\nu\hat{\sigma}_\lambda|\sigma\rangle\ \tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\lambda}(\vec{r}_4,\vec{r}_5)\right.\\
&\quad\left.+\sum_{\sigma}\sum_{\nu\kappa}\langle\sigma|\hat{\sigma}_\nu\hat{\sigma}_\nu\hat{\sigma}_\kappa|\sigma\rangle\ \tilde{s}^*_{q_1,\kappa}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)+\sum_{\sigma}\sum_{\nu\lambda\kappa}\langle\sigma|\hat{\sigma}_\nu\hat{\sigma}_\lambda\hat{\sigma}_\nu\hat{\sigma}_\kappa|\sigma\rangle\ \tilde{s}^*_{q_1,\kappa}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\lambda}(\vec{r}_4,\vec{r}_5)\right]\\
&= -\frac{1}{2}\left[3\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)-\sum_{\lambda}\tilde{s}^*_{q_1,\lambda}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\lambda}(\vec{r}_4,\vec{r}_5)\right].
\end{aligned}
\tag{C16}
$$

The normal density matrix $\rho_{q_1}(\vec{r}_6,\vec{r}_3)$ in Eq. (C13) is not involved in these manipulations and has been omitted for brevity. Altogether, the evaluation of Eq. (C5d) requires the identities

$$
\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1\sigma_2|1|\sigma_4\sigma_5\rangle\ \kappa^*_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)=\frac{1}{2}\left[\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)+\sum_{\nu}\tilde{s}^*_{q_1,\nu}(\vec{r}_1,\vec{r}_2)\ \tilde{s}_{q_1,\nu}(\vec{r}_4,\vec{r}_5)\right],
\tag{C17a}
$$

$$
\begin{aligned}
\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1\sigma_2|\hat{\sigma}_{1,\nu}|\sigma_4\sigma_5\rangle\ \kappa^*_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)&=\frac{1}{2}\left[\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\nu}(\vec{r}_4,\vec{r}_5)+\tilde{s}^*_{q_1,\nu}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)\right.\\
&\quad\left.-\mathrm{i}\sum_{\lambda\kappa}\epsilon_{\nu\lambda\kappa}\tilde{s}^*_{q_1,\lambda}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\kappa}(\vec{r}_4,\vec{r}_5)\right],
\end{aligned}
\tag{C17b}
$$

$$
\begin{aligned}
\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1\sigma_2|\hat{\sigma}_{2,\nu}|\sigma_4\sigma_5\rangle\ \kappa^*_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)&=-\frac{1}{2}\left[\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\nu}(\vec{r}_4,\vec{r}_5)+\tilde{s}^*_{q_1,\nu}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)\right.\\
&\quad\left.+\mathrm{i}\sum_{\lambda\kappa}\epsilon_{\nu\lambda\kappa}\tilde{s}^*_{q_1,\lambda}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\kappa}(\vec{r}_4,\vec{r}_5)\right],
\end{aligned}
\tag{C17c}
$$

$$
\sum_{\sigma_1\sigma_2\sigma_4\sigma_5}\langle\sigma_1\sigma_2|\hat{\sigma}_{1,\nu}\hat{\sigma}_{2,\nu}|\sigma_4\sigma_5\rangle\ \kappa^*_{q_1}(\zeta_1,\zeta_2)\kappa_{q_1}(\zeta_4,\zeta_5)=-\frac{1}{2}\left[3\tilde{\rho}^*_{q_1}(\vec{r}_1,\vec{r}_2)\tilde{\rho}_{q_1}(\vec{r}_4,\vec{r}_5)-\tilde{s}^*_{q_1,\nu}(\vec{r}_1,\vec{r}_2)\tilde{s}_{q_1,\nu}(\vec{r}_4,\vec{r}_5)\right].
\tag{C17d}
$$

#### 5. Applying gradient operators

Now that the matrix element has been evaluated, the integrand contains $\delta$ functions and differential operators acting on nonlocal densities. The latter must be evaluated prior to utilizing the former. Simple rules can be obtained that express the action of specific combinations of gradient operators on nonlocal densities in terms of local densities [93,94]. Those rules work identically for $\rho_q(\vec{r},\vec{r}\,')$, $s_{q,\mu}(\vec{r},\vec{r}\,')$, $\tilde{\rho}_q(\vec{r}\,',\vec{r})$, or $\tilde{s}_{q,\nu}(\vec{r}\,',\vec{r})$. Defining $\mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}$, $\mathcal{P}^{\vec{r}}_{q,(\nu)}$, $\mathcal{T}^{\vec{r}}_{q,(\nu)}$, and $\mathcal{J}^{\vec{r}}_{q,\mu(\nu)}$ as generic notation for the densities, for each column on the right-hand side of the table,

$$
\begin{aligned}
\mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}&\equiv\{\rho_q(\vec{r}\,',\vec{r})\,;\ s_{q,\nu}(\vec{r}\,',\vec{r})\,;\ \tilde{\rho}_q(\vec{r}\,',\vec{r})\,;\ \tilde{s}_{q,\nu}(\vec{r}\,',\vec{r})\},\\
\mathcal{P}^{\vec{r}}_{q,(\nu)}&\equiv\{\rho_q(\vec{r})\,;\ s_{q,\nu}(\vec{r})\,;\ \tilde{\rho}_q(\vec{r})\,;\ \tilde{s}_{q,\nu}(\vec{r})\},\\
\mathcal{T}^{\vec{r}}_{q,(\nu)}&\equiv\{\tau_q(\vec{r})\,;\ T_{q,\nu}(\vec{r})\,;\ \tilde{\tau}_q(\vec{r})\,;\ \tilde{T}_{q,\nu}(\vec{r})\},\\
\mathcal{J}^{\vec{r}}_{q,\mu(\nu)}&\equiv\{j_{q,\mu}(\vec{r})\,;\ J_{q,\mu\nu}(\vec{r})\,;\ \tilde{j}_{q,\mu}(\vec{r})\,;\ \tilde{J}_{q,\mu\nu}(\vec{r})\},
\end{aligned}
$$

there is a set of four relations

$$
\nabla_{\vec{r},\mu}\ \mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}\big|_{\vec{r}=\vec{r}\,'}=\tfrac{1}{2}\nabla_\mu\mathcal{P}^{\vec{r}}_{q,(\nu)}+\mathrm{i}\mathcal{J}^{\vec{r}}_{q,\mu(\nu)},
\tag{C18a}
$$

$$
\nabla_{\vec{r}\,',\mu}\ \mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}\big|_{\vec{r}=\vec{r}\,'}=\tfrac{1}{2}\nabla_\mu\mathcal{P}^{\vec{r}}_{q,(\nu)}-\mathrm{i}\mathcal{J}^{\vec{r}}_{q,\mu(\nu)},
\tag{C18b}
$$

$$
\Delta_{\vec{r}}\ \mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}\big|_{\vec{r}=\vec{r}\,'}=\tfrac{1}{2}\Delta\mathcal{P}^{\vec{r}}_{q,(\nu)}-\mathcal{T}^{\vec{r}}_{q,(\nu)}+\mathrm{i}\vec{\nabla}\cdot\vec{\mathcal{J}}^{\vec{r}}_{q,(\nu)},
\tag{C18c}
$$

$$
\Delta_{\vec{r}\,'}\ \mathcal{P}^{\vec{r}\vec{r}\,'}_{q,(\nu)}\big|_{\vec{r}=\vec{r}\,'}=\tfrac{1}{2}\Delta\mathcal{P}^{\vec{r}}_{q,(\nu)}-\mathcal{T}^{\vec{r}}_{q,(\nu)}-\mathrm{i}\vec{\nabla}\cdot\vec{\mathcal{J}}^{\vec{r}}_{q,(\nu)}.
\tag{C18d}
$$

Applying those rules and exploiting the $\delta$ functions, one ends up with a local energy density expressed in terms of the local densities of interest.

## APPENDIX D: ONE-BODY FIELDS

Having the explicit expression of the EDF kernel at hand, its contributions to the one-body fields entering the HFB equations can be derived. Normal and anomalous fields are gathered into the HFB Hamiltonian matrix [13,14],

$$
\mathcal{H}\equiv\begin{pmatrix}h^q & \Delta^q\\ -\Delta^{q*} & -h^{q*}\end{pmatrix},
\tag{D1}
$$

and are respectively defined as

$$h^q_{\beta\alpha} \equiv \frac{\delta E}{\delta \rho^q_{\alpha\beta}}, \quad \Delta^q_{\alpha\beta} \equiv \frac{\delta E}{\delta \kappa^{q*}_{\alpha\beta}}, \tag{D2}$$

for $\beta \leqslant \alpha$. Field $h$ is Hermitian, $h^q_{\beta\alpha} = h^{q*}_{\alpha\beta}$, whereas $\Delta^q$ is skew symmetric $\Delta^q_{\beta\alpha} = -\Delta^q_{\alpha\beta}$. These fields can be specified either in a configuration basis $\{\alpha, \beta\} \in \{i, j\}$ or in coordinate representation $\{\alpha, \beta\} \in \{\xi, \xi'\}$.

Below, we explicitly provide contributions to the HFB Hamiltonian that derive from the energy functional defined by Eqs. (A2), (A3), (A4), and (A5), which constitutes just a part of the complete EDF kernel. In a realistic calculation, additional terms contribute to the one-body fields in the HFB equation, such as the center-of-mass correction, the Coulomb interaction, as well as constraints, in particular the obligatory one on neutron and proton numbers. None of these are specified here.

The EDF being a functional of local densities, it is of advantage to calculate contributions to the matrix elements of the one-body fields in a configuration basis through the chain rule

$$\begin{aligned} h^q_{ji} = \int d^3r \Bigg[ & \frac{\delta \mathcal{E}}{\delta \rho_q(\vec{r})} \frac{\delta \rho_q(\vec{r})}{\delta \rho^q_{ij}} + \frac{\delta \mathcal{E}}{\delta \tau_q(\vec{r})} \frac{\delta \tau_q(\vec{r})}{\delta \rho^q_{ij}} \\ & + \sum_{\mu\nu} \frac{\delta \mathcal{E}}{\delta J_{q,\mu\nu}(\vec{r})} \frac{\delta J_{q,\mu\nu}(\vec{r})}{\delta \rho^q_{ij}} + \sum_{\mu} \frac{\delta \mathcal{E}}{\delta s_{q,\mu}(\vec{r})} \frac{\delta s_{q,\mu}(\vec{r})}{\delta \rho^q_{ij}} \\ & + \sum_{\mu} \frac{\delta \mathcal{E}}{\delta T_{q,\mu}(\vec{r})} \frac{\delta T_{q,\mu}(\vec{r})}{\delta \rho^q_{ij}} + \sum_{\mu} \frac{\delta \mathcal{E}}{\delta j_{q,\mu}(\vec{r})} \frac{\delta j_{q,\mu}(\vec{r})}{\delta \rho^q_{ij}} \Bigg], \end{aligned} \tag{D3a}$$

$$\begin{aligned} \Delta^q_{ij} = \int d^3r \Bigg[ & \frac{\delta \mathcal{E}}{\delta \tilde{\rho}^*_q(\vec{r})} \frac{\delta \tilde{\rho}^*_q(\vec{r})}{\delta \kappa^{q*}_{ij}} + \frac{\delta \mathcal{E}}{\delta \tilde{\tau}^*_q(\vec{r})} \frac{\delta \tilde{\tau}^*_q(\vec{r})}{\delta \kappa^{q*}_{ij}} \\ & + \sum_{\mu\nu} \frac{\delta \mathcal{E}}{\delta \tilde{J}^*_{q,\mu\nu}(\vec{r})} \frac{\delta \tilde{J}^*_{q,\mu\nu}(\vec{r})}{\delta \kappa^{q*}_{ij}} \Bigg]. \end{aligned} \tag{D3b}$$

The functional derivatives of the local densities can be obtained for $j \leqslant i$ as

$$\frac{\delta \rho_q(\vec{r})}{\delta \rho^q_{ij}} = \sum_{\sigma} \varphi^*_j(\vec{r}\sigma q)\varphi_i(\vec{r}\sigma q), \tag{D4a}$$

$$\frac{\delta \tau_q(\vec{r})}{\delta \rho^q_{ij}} = \sum_{\sigma} [\vec{\nabla}\varphi^*_j(\vec{r}\sigma q)] \cdot [\vec{\nabla}\varphi_i(\vec{r}\sigma q)], \tag{D4b}$$

$$\begin{aligned} \frac{\delta J_{q,\mu\nu}(\vec{r})}{\delta \rho^q_{ij}} = & -\sum_{\sigma\sigma'} \frac{\mathrm{i}}{2} \{\varphi^*_j(\vec{r}\sigma' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \nabla_\mu \varphi_i(\vec{r}\sigma q) \\ & - \nabla_\mu \varphi^*_j(\vec{r}\sigma' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \varphi_i(\vec{r}\sigma q)\}, \end{aligned} \tag{D4c}$$

$$\frac{\delta s_{q,\nu}(\vec{r})}{\delta \rho^q_{ij}} = \sum_{\sigma\sigma'} \varphi^*_j(\vec{r}\sigma' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \varphi_i(\vec{r}\sigma q), \tag{D4d}$$

$$\frac{\delta T_{q,\nu}(\vec{r})}{\delta \rho^q_{ij}} = \sum_{\sigma\sigma'} \vec{\nabla}\varphi^*_j(\vec{r}\sigma' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \cdot \vec{\nabla}\varphi_i(\vec{r}\sigma q), \tag{D4e}$$

$$\begin{aligned} \frac{\delta j_{q,\mu}(\vec{r})}{\delta \rho^q_{ij}} = & -\sum_{\sigma} \frac{\mathrm{i}}{2} \{\varphi^*_j(\vec{r}\sigma q)[\nabla_\mu \varphi_i(\vec{r}\sigma q)] \\ & - [\nabla_\mu \varphi^*_j(\vec{r}\sigma q)]\varphi_i(\vec{r}\sigma q)\}, \end{aligned} \tag{D4f}$$

$$\frac{\delta \tilde{\rho}^*_q(\vec{r})}{\delta \kappa^{q*}_{ij}} = \sum_{\sigma} 4\bar{\sigma}\varphi^*_i(\vec{r}\bar{\sigma} q)\varphi^*_j(\vec{r}\sigma q), \tag{D4g}$$

$$\frac{\delta \tilde{\tau}^*_q(\vec{r})}{\delta \kappa^{q*}_{ij}} = \sum_{\sigma} 4\bar{\sigma}[\vec{\nabla}\varphi^*_i(\vec{r}\bar{\sigma} q)] \cdot [\vec{\nabla}\varphi^*_j(\vec{r}\sigma q)], \tag{D4h}$$

$$\begin{aligned} \frac{\delta \tilde{J}^*_{q,\mu\nu}(\vec{r})}{\delta \kappa^{q*}_{ij}} = & -\sum_{\sigma\sigma'} 4\bar{\sigma}' \frac{\mathrm{i}}{2} \{\varphi^*_i(\vec{r}\bar{\sigma}' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \nabla_\mu \varphi^*_j(\vec{r}\sigma q) \\ & - \nabla_\mu \varphi^*_i(\vec{r}\bar{\sigma}' q)\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle \varphi^*_j(\vec{r}\sigma q)\}. \end{aligned} \tag{D4i}$$

The functional derivatives of the local energy density $\mathcal{E}$ define the local potentials,

$$U_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \rho_q(\vec{r})}, \tag{D5a}$$

$$B_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tau_q(\vec{r})}, \tag{D5b}$$

$$W_{q,\mu\nu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta J_{q,\mu\nu}(\vec{r})}, \tag{D5c}$$

$$S_{q,\mu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta s_{q,\mu}(\vec{r})}, \tag{D5d}$$

$$C_{q,\mu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta T_{q,\mu}(\vec{r})}, \tag{D5e}$$

$$A_{q,\mu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta j_{q,\mu}(\vec{r})}, \tag{D5f}$$

$$\tilde{U}_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tilde{\rho}^*_q(\vec{r})}, \tag{D5g}$$

$$\tilde{B}_q(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tilde{\tau}^*_q(\vec{r})}, \tag{D5h}$$

$$\tilde{W}_{q,\mu\nu}(\vec{r}) \equiv \frac{\delta \mathcal{E}}{\delta \tilde{J}^*_{q,\mu\nu}(\vec{r})}. \tag{D5i}$$

Matrix elements in the configuration basis can be related to those in the coordinate basis through

$$h^q_{ji} \equiv \iint d^3r d^3r' \sum_{\sigma\sigma'} \varphi^*_j(\vec{r}\,'\sigma' q) h^q(\vec{r}\sigma, \vec{r}\,'\sigma')\varphi_i(\vec{r}\sigma q), \tag{D6a}$$

$$\Delta^q_{ij} \equiv \iint d^3r d^3r' \sum_{\sigma\sigma'} 4\bar{\sigma}'\varphi^*_j(\vec{r}\,'\bar{\sigma}' q)\tilde{h}^q(\vec{r}\sigma, \vec{r}\,'\sigma')\varphi^*_i(\vec{r}\sigma q). \tag{D6b}$$

In the present case, fields are local in coordinate space representation, i.e.,

$$h^q(\vec{r}\sigma, \vec{r}\,'\sigma') \equiv \delta(\vec{r} - \vec{r}\,')h^q_{\sigma\sigma'}(\vec{r}), \tag{D7a}$$

$$\tilde{h}^q(\vec{r}\sigma, \vec{r}\,'\sigma') \equiv \delta(\vec{r} - \vec{r}\,')\tilde{h}^q_{\sigma\sigma'}(\vec{r}), \tag{D7b}$$

with the generic structure

$$h^q_{\sigma\sigma'}(\vec{r}) = U_q(\vec{r})\delta_{\sigma\sigma'} - \sum_\mu \nabla_\mu B_q(\vec{r})\nabla_\mu \delta_{\sigma\sigma'} - \frac{\mathrm{i}}{2}\sum_{\mu\nu}[W_{q,\mu\nu}(\vec{r})\nabla_\mu\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle + \nabla_\mu\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle W_{q,\mu\nu}(\vec{r})]$$
$$+\sum_\nu S_{q,\nu}(\vec{r})\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle - \sum_{\mu\nu}\nabla_\mu C_{q,\nu}(\vec{r})\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle\nabla_\mu - \sum_\mu \frac{\mathrm{i}}{2}[A_{q,\mu}(\vec{r})\nabla_\mu + \nabla_\mu A_{q,\mu}(\vec{r})]\delta_{\sigma\sigma'}, \tag{D8a}$$

$$\tilde{h}^q_{\sigma\sigma'}(\vec{r}) = \tilde{U}_q(\vec{r})\delta_{\sigma\sigma'} - \sum_\mu \nabla_\mu \tilde{B}_q(\vec{r})\nabla_\mu \delta_{\sigma\sigma'} - \frac{\mathrm{i}}{2}\sum_{\mu\nu}[\tilde{W}_{q,\mu\nu}(\vec{r})\nabla_\mu\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle + \nabla_\mu\langle\sigma'|\hat{\sigma}_\nu|\sigma\rangle\tilde{W}_{q,\mu\nu}(\vec{r})]. \tag{D8b}$$

In Eq. (D8a), gradient operators act to their right on both the local potentials and on the wave function the fields $h^q_{\sigma\sigma'}(\vec{r})$ and $\tilde{h}^q_{\sigma\sigma'}(\vec{r})$ are applied to. For the functional constructed here, the overall structure of the two fields is the same as for traditional Skyrme EDF parametrizations, the only difference being additional terms the local potentials.

### 1. Local potentials

Explicit expressions of the local potentials deriving from the EDF kernel defined through Eqs. (A2), (A3), (A4), and (A5) are given by

$$\begin{aligned}
U_q &= 2A^{\rho_1\rho_1}\rho_q + 2A^{\rho_1\rho_2}\rho_{\bar{q}} + A^{\tau_1\rho_1}\tau_q + A^{\tau_1\rho_2}\tau_{\bar{q}} - 2A^{\nabla\rho_1\nabla\rho_1}\Delta\rho_q - 2A^{\nabla\rho_1\nabla\rho_2}\Delta\rho_{\bar{q}} \\
&+2B^{\rho_1\rho_1\rho_2}\rho_q\rho_{\bar{q}} + B^{\rho_1\rho_1\rho_2}\rho_{\bar{q}}\rho_{\bar{q}} + B^{s_1s_1\rho_2}\vec{s}_{\bar{q}}\cdot\vec{s}_{\bar{q}} + B^{\tilde{\rho}_1^*\tilde{\rho}_1\rho_2}\tilde{\rho}^*_{\bar{q}}\tilde{\rho}_{\bar{q}} + 2B^{\tau_1\rho_1\rho_1}\tau_q\rho_q \\
&+B^{\tau_1\rho_1\rho_2}\tau_q\rho_{\bar{q}} + B^{\tau_1\rho_1\rho_2}\tau_{\bar{q}}\rho_{\bar{q}} + 2B^{\tau_1\rho_2\rho_2}\tau_{\bar{q}}\rho_q + B^{T_1s_1\rho_2}\vec{T}_{\bar{q}}\cdot\vec{s}_{\bar{q}} + B^{T_1s_2\rho_1}\vec{T}_q\cdot\vec{s}_{\bar{q}} + B^{\tilde{\tau}_1^*\tilde{\rho}_1\rho_2}\tilde{\tau}^*_{\bar{q}}\tilde{\rho}_{\bar{q}} + B^{\tilde{\tau}_1\tilde{\rho}_1^*\rho_2}\tilde{\tau}_{\bar{q}}\tilde{\rho}^*_{\bar{q}} \\
&-2B^{\nabla\rho_1\nabla\rho_1\rho_1}(\Delta\rho_q)\rho_q - B^{\nabla\rho_1\nabla\rho_1\rho_1}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_q) - 2B^{\nabla\rho_1\nabla\rho_1\rho_2}(\Delta\rho_q)\rho_{\bar{q}} - 2B^{\nabla\rho_1\nabla\rho_1\rho_2}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}\rho_{\bar{q}}) \\
&+B^{\nabla\rho_1\nabla\rho_1\rho_2}(\vec{\nabla}\rho_{\bar{q}})\cdot(\vec{\nabla}\rho_{\bar{q}}) - B^{\nabla\rho_1\nabla\rho_2\rho_1}(\Delta\rho_{\bar{q}})\rho_q - B^{\nabla\rho_1\nabla\rho_2\rho_1}(\Delta\rho_{\bar{q}})\rho_{\bar{q}} - B^{\nabla\rho_1\nabla\rho_2\rho_1}(\vec{\nabla}\rho_{\bar{q}})\cdot(\vec{\nabla}\rho_{\bar{q}}) \\
&+\sum_{\mu\nu}[B^{\nabla s_1\nabla s_1\rho_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{q,\nu}) + B^{\nabla s_1\nabla s_1\rho_2}(\nabla_\mu s_{\bar{q},\nu})(\nabla_\mu s_{\bar{q},\nu}) + B^{\nabla s_1\nabla s_2\rho_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{\bar{q},\nu})] \\
&- B^{\nabla\rho_1\nabla s_1 s_1}(\Delta\vec{s}_q)\cdot\vec{s}_q - B^{\nabla\rho_1\nabla s_1 s_2}(\Delta\vec{s}_q)\cdot\vec{s}_{\bar{q}} - B^{\nabla\rho_1\nabla s_2 s_1}(\Delta\vec{s}_{\bar{q}})\cdot\vec{s}_q - B^{\nabla\rho_1\nabla s_2 s_2}(\Delta\vec{s}_{\bar{q}})\cdot\vec{s}_{\bar{q}} \\
&+\sum_{\mu\nu}[-B^{\nabla\rho_1\nabla s_1 s_1}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{q,\nu}) - B^{\nabla\rho_1\nabla s_1 s_2}(\nabla_\mu s_{q,\nu})(\nabla_\mu s_{\bar{q},\nu}) - B^{\nabla\rho_1\nabla s_2 s_1}(\nabla_\mu s_{\bar{q},\nu})(\nabla_\mu s_{q,\nu}) \\
&- B^{\nabla\rho_1\nabla s_2 s_2}(\nabla_\mu s_{\bar{q},\nu})(\nabla_\mu s_{\bar{q},\nu})] + B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_1}(\vec{\nabla}\tilde{\rho}^*_q)\cdot(\vec{\nabla}\tilde{\rho}_q) + B^{\nabla\tilde{\rho}_1^*\nabla\tilde{\rho}_1\rho_2}(\vec{\nabla}\tilde{\rho}^*_{\bar{q}})\cdot(\vec{\nabla}\tilde{\rho}_{\bar{q}}) \\
&- B^{\nabla\tilde{\rho}_1^*\nabla\rho_1\tilde{\rho}_1}(\Delta\tilde{\rho}^*_q)\tilde{\rho}_q - B^{\nabla\tilde{\rho}_1^*\nabla\rho_1\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}^*_q)\cdot(\vec{\nabla}\tilde{\rho}_q) - B^{\nabla\tilde{\rho}_1^*\nabla\rho_2\tilde{\rho}_1}(\Delta\tilde{\rho}^*_{\bar{q}})\tilde{\rho}_{\bar{q}} - B^{\nabla\tilde{\rho}_1^*\nabla\rho_2\tilde{\rho}_1}(\vec{\nabla}\tilde{\rho}^*_{\bar{q}})\cdot(\vec{\nabla}\tilde{\rho}_{\bar{q}}) \\
&- B^{\nabla\tilde{\rho}_1\nabla\rho_1\tilde{\rho}_1^*}(\Delta\tilde{\rho}_q)\tilde{\rho}^*_q - B^{\nabla\tilde{\rho}_1\nabla\rho_1\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_q)\cdot(\vec{\nabla}\tilde{\rho}^*_q) - B^{\nabla\tilde{\rho}_1\nabla\rho_2\tilde{\rho}_1^*}(\Delta\tilde{\rho}_{\bar{q}})\tilde{\rho}^*_{\bar{q}} - B^{\nabla\tilde{\rho}_1\nabla\rho_2\tilde{\rho}_1^*}(\vec{\nabla}\tilde{\rho}_{\bar{q}})\cdot(\vec{\nabla}\tilde{\rho}^*_{\bar{q}}) \\
&+ B^{j_1j_1\rho_1}\vec{j}_q\cdot\vec{j}_q + B^{j_1j_1\rho_2}\vec{j}_{\bar{q}}\cdot\vec{j}_{\bar{q}} + B^{j_1j_2\rho_1}\vec{j}_q\cdot\vec{j}_{\bar{q}} + \sum_{\mu\nu}[B^{J_1J_1\rho_1}J_{q,\mu\nu}J_{q,\mu\nu} + B^{J_1J_1\rho_2}J_{\bar{q},\mu\nu}J_{\bar{q},\mu\nu} \\
&+ B^{J_1J_2\rho_1}J_{q,\mu\nu}J_{\bar{q},\mu\nu} + B^{\tilde{J}_1^*\tilde{J}_1\rho_1}\tilde{J}^*_{q,\mu\nu}\tilde{J}_{q,\mu\nu} + B^{\tilde{J}_1^*\tilde{J}_1\rho_2}\tilde{J}^*_{\bar{q},\mu\nu}\tilde{J}_{\bar{q},\mu\nu}],
\end{aligned} \tag{D9a}$$

$$\begin{aligned}
S_{q,\nu} &= 2A^{s_1s_1}s_{q,\nu} + 2A^{s_1s_2}s_{\bar{q},\nu} + A^{T_1s_1}T_{q,\nu} + A^{T_1s_2}T_{\bar{q},\nu} - 2A^{\nabla s_1\nabla s_1}\Delta s_{q,\nu} - 2A^{\nabla s_1\nabla s_2}\Delta s_{\bar{q},\nu} \\
&+2B^{s_1s_1\rho_2}s_{q,\nu}\rho_{\bar{q}} + B^{T_1s_1\rho_2}T_{q,\nu}\rho_{\bar{q}} + B^{T_1s_2\rho_1}T_{\bar{q},\nu}\rho_{\bar{q}} \\
&+2B^{\tau_1s_1s_1}\tau_q s_{q,\nu} + B^{\tau_1s_1s_2}\tau_q s_{\bar{q},\nu} + B^{\tau_1s_1s_2}\tau_{\bar{q}}s_{\bar{q},\nu} + 2B^{\tau_1s_2s_2}\tau_{\bar{q}}s_{q,\nu} - 2B^{\nabla s_1\nabla s_1\rho_1}(\Delta s_{q,\nu})\rho_q \\
&- 2B^{\nabla s_1\nabla s_1\rho_1}(\vec{\nabla}s_{q,\nu})\cdot(\vec{\nabla}\rho_q) - 2B^{\nabla s_1\nabla s_1\rho_2}(\Delta s_{q,\nu})\rho_{\bar{q}} - 2B^{\nabla s_1\nabla s_1\rho_2}(\vec{\nabla}s_{q,\nu})\cdot(\vec{\nabla}\rho_{\bar{q}}) \\
&- B^{\nabla s_1\nabla s_2\rho_1}(\Delta s_{\bar{q},\nu})\rho_q - B^{\nabla s_1\nabla s_2\rho_1}(\Delta s_{\bar{q},\nu})\rho_{\bar{q}} - B^{\nabla s_1\nabla s_2\rho_1}(\vec{\nabla}s_{\bar{q},\nu})\cdot(\vec{\nabla}\rho_q) - B^{\nabla s_1\nabla s_2\rho_1}(\vec{\nabla}s_{\bar{q},\nu})\cdot(\vec{\nabla}\rho_{\bar{q}}) \\
&- B^{\nabla\rho_1\nabla s_1 s_1}(\Delta\rho_q)s_{q,\nu} - B^{\nabla\rho_1\nabla s_1 s_2}(\Delta\rho_q)s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_1 s_2}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}s_{\bar{q},\nu}) + B^{\nabla\rho_1\nabla s_1 s_2}(\vec{\nabla}\rho_{\bar{q}})\cdot(\vec{\nabla}s_{\bar{q},\nu}) \\
&- B^{\nabla\rho_1\nabla s_2 s_1}(\Delta\rho_{\bar{q}})s_{\bar{q},\nu} - B^{\nabla\rho_1\nabla s_2 s_1}(\vec{\nabla}\rho_{\bar{q}})\cdot(\vec{\nabla}s_{\bar{q},\nu}) + B^{\nabla\rho_1\nabla s_2 s_1}(\vec{\nabla}\rho_q)\cdot(\vec{\nabla}s_{\bar{q},\nu}) - B^{\nabla\rho_1\nabla s_2 s_2}(\Delta\rho_{\bar{q}})s_{q,\nu} \\
&+ \sum_\mu[B^{j_1J_1s_1}j_{q,\mu}J_{q,\mu\nu} + B^{j_1J_1s_2}j_{\bar{q},\mu}J_{\bar{q},\mu\nu} + B^{j_1J_2s_1}j_{q,\mu}J_{\bar{q},\mu\nu} + B^{j_1J_2s_2}j_{\bar{q},\mu}J_{q,\mu\nu}]
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{\mu\lambda\kappa}\epsilon_{\nu\lambda\kappa}[-B^{\nabla s_1 J_1 s_1}(\nabla_\mu J_{q,\mu\lambda})s_{q,\kappa}-B^{\nabla s_1 J_1 s_1}J_{q,\mu\lambda}(\nabla_\mu s_{q,\kappa})+B^{\nabla s_1 J_1 s_1}(\nabla_\mu s_{q,\lambda})J_{q,\mu\kappa}\\
&-B^{\nabla s_1 J_1 s_2}(\nabla_\mu J_{q,\mu\lambda})s_{\bar q,\kappa}-B^{\nabla s_1 J_1 s_2}J_{q,\mu\lambda}(\nabla_\mu s_{\bar q,\kappa})+B^{\nabla s_1 J_1 s_2}(\nabla_\mu s_{\bar q,\lambda})J_{\bar q,\mu\kappa}-B^{\nabla s_1 J_2 s_1}(\nabla_\mu J_{\bar q,\mu\lambda})s_{q,\kappa}\\
&+2B^{\nabla s_1 J_2 s_1}(\nabla_\mu s_{q,\lambda})J_{\bar q,\mu\kappa}-B^{\nabla s_1 J_2 s_2}(\nabla_\mu J_{\bar q,\mu\lambda})s_{\bar q,\kappa}-B^{\nabla s_1 J_2 s_2}J_{\bar q,\mu\lambda}(\nabla_\mu s_{\bar q,\kappa})+B^{\nabla s_1 J_2 s_2}(\nabla_\mu s_{\bar q,\lambda})J_{q,\mu\kappa}\\
&+\mathrm{i}B^{\tilde J_1^* \tilde J_1 s_1}\tilde J^*_{q,\mu\lambda}\tilde J_{q,\mu\kappa}+\mathrm{i}B^{\tilde J_1^* \tilde J_1 s_2}\tilde J^*_{\bar q,\mu\lambda}\tilde J_{\bar q,\mu\kappa}]+\sum_\mu[\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_1}(\nabla_\mu\tilde\rho_q^*)\tilde J_{q,\mu\nu}+\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_2}(\nabla_\mu\tilde\rho_{\bar q}^*)\tilde J_{\bar q,\mu\nu}\\
&+\mathrm{i}B^{\nabla\tilde\rho_1\tilde J_1^* s_1}(\nabla_\mu\tilde\rho_q)\tilde J^*_{q,\mu\nu}+\mathrm{i}B^{\nabla\tilde\rho_1\tilde J_1^* s_2}(\nabla_\mu\tilde\rho_{\bar q})\tilde J^*_{\bar q,\mu\nu}-\mathrm{i}B^{\nabla s_1\tilde J_1^*\tilde\rho_1}(\nabla_\mu\tilde J^*_{q,\mu\nu})\tilde\rho_q-\mathrm{i}B^{\nabla s_1\tilde J_1^*\tilde\rho_1}\tilde J^*_{q,\mu\nu}(\nabla_\mu\tilde\rho_q)\\
&-\mathrm{i}B^{\nabla s_2\tilde J_1^*\tilde\rho_1}(\nabla_\mu\tilde J^*_{\bar q,\mu\nu})\tilde\rho_{\bar q}-\mathrm{i}B^{\nabla s_2\tilde J_1^*\tilde\rho_1}\tilde J^*_{\bar q,\mu\nu}(\nabla_\mu\tilde\rho_{\bar q})-\mathrm{i}B^{\nabla s_1\tilde J_1\tilde\rho_1^*}(\nabla_\mu\tilde J_{q,\mu\nu})\tilde\rho_q^*-\mathrm{i}B^{\nabla s_1\tilde J_1\tilde\rho_1^*}\tilde J_{q,\mu\nu}(\nabla_\mu\tilde\rho_q^*)\\
&-\mathrm{i}B^{\nabla s_2\tilde J_1\tilde\rho_1^*}(\nabla_\mu\tilde J_{\bar q,\mu\nu})\tilde\rho_{\bar q}^*-\mathrm{i}B^{\nabla s_2\tilde J_1\tilde\rho_1^*}\tilde J_{\bar q,\mu\nu}(\nabla_\mu\tilde\rho_{\bar q}^*)],
\end{aligned}
\tag{D9b}
$$

$$
\begin{aligned}
B_q=&\frac{\hbar^2}{2m}+A^{\tau_1\rho_1}\rho_q+A^{\tau_1\rho_2}\rho_{\bar q}+B^{\tau_1\rho_1\rho_1}\rho_q\rho_q+B^{\tau_1\rho_1\rho_2}\rho_q\rho_{\bar q}+B^{\tau_1\rho_2\rho_2}\rho_{\bar q}\rho_{\bar q}+B^{\tau_1 s_1 s_1}\vec s_q\cdot\vec s_q\\
&+B^{\tau_1 s_1 s_2}\vec s_q\cdot\vec s_{\bar q}+B^{\tau_1 s_2 s_2}\vec s_{\bar q}\cdot\vec s_{\bar q}+B^{\tau_1\tilde\rho_1^*\tilde\rho_1}\tilde\rho_q^*\tilde\rho_q+B^{\tau_2\tilde\rho_1^*\tilde\rho_1}\tilde\rho_{\bar q}^*\tilde\rho_{\bar q},
\end{aligned}
\tag{D9c}
$$

$$
C_{q,\nu}=A^{T_1 s_1}s_{q,\nu}+A^{T_1 s_2}s_{\bar q,\nu}+B^{T_1 s_1\rho_2}s_{q,\nu}\rho_{\bar q}+B^{T_1 s_2\rho_1}s_{\bar q,\nu}\rho_q,
\tag{D9d}
$$

$$
\begin{aligned}
A_{q,\mu}=&2A^{j_1 j_1}j_{q,\mu}+2A^{j_1 j_2}j_{\bar q,\mu}+2B^{j_1 j_1\rho_1}j_{q,\mu}\rho_q+2B^{j_1 j_1\rho_2}j_{q,\mu}\rho_{\bar q}+B^{j_1 j_2\rho_1}j_{\bar q,\mu}\rho_q+B^{j_1 j_2\rho_1}j_{\bar q,\mu}\rho_{\bar q}\\
&+\sum_\nu(B^{j_1 J_1 s_1}J_{q,\mu\nu}s_{q,\nu}+B^{j_1 J_1 s_2}J_{q,\mu\nu}s_{\bar q,\nu}+B^{j_1 J_2 s_1}J_{\bar q,\mu\nu}s_{q,\nu}+B^{j_1 J_2 s_2}J_{\bar q,\mu\nu}s_{\bar q,\nu})\\
&+\mathrm{i}B^{\nabla\tilde\rho_1^* j_1\tilde\rho_1}(\nabla_\mu\tilde\rho_q^*)\tilde\rho_q+\mathrm{i}B^{\nabla\tilde\rho_1^* j_2\tilde\rho_1}(\nabla_\mu\tilde\rho_{\bar q}^*)\tilde\rho_{\bar q}+\mathrm{i}B^{\nabla\tilde\rho_1 j_1\tilde\rho_1^*}(\nabla_\mu\tilde\rho_q)\tilde\rho_q^*+\mathrm{i}B^{\nabla\tilde\rho_1 j_2\tilde\rho_1^*}(\nabla_\mu\tilde\rho_{\bar q})\tilde\rho_{\bar q}^*,
\end{aligned}
\tag{D9e}
$$

$$
\begin{aligned}
W_{q,\mu\nu}=&2A^{J_1 J_1}J_{q,\mu\nu}+2A^{J_1 J_2}J_{\bar q,\mu\nu}+2B^{J_1 J_1\rho_1}J_{q,\mu\nu}\rho_q+2B^{J_1 J_1\rho_2}J_{q,\mu\nu}\rho_{\bar q}\\
&+B^{J_1 J_2\rho_1}J_{\bar q,\mu\nu}\rho_q+B^{J_1 J_2\rho_1}J_{\bar q,\mu\nu}\rho_{\bar q}+B^{j_1 J_1 s_1}j_{q,\mu}s_{q,\nu}+B^{j_1 J_1 s_2}j_{q,\mu}s_{\bar q,\nu}+B^{j_1 J_2 s_1}j_{\bar q,\mu}s_{\bar q,\nu}\\
&+B^{j_1 J_2 s_2}j_{\bar q,\mu}s_{q,\nu}+B^{\tilde J_1^* J_1\tilde\rho_1}\tilde J^*_{q,\mu\nu}\tilde\rho_q+B^{\tilde J_1^* J_2\tilde\rho_1}\tilde J^*_{\bar q,\mu\nu}\tilde\rho_{\bar q}+B^{\tilde J_1 J_1\tilde\rho_1^*}\tilde J_{q,\mu\nu}\tilde\rho_q^*+B^{\tilde J_1 J_2\tilde\rho_1^*}\tilde J_{\bar q,\mu\nu}\tilde\rho_{\bar q}^*\\
&+\sum_{\lambda\kappa}\epsilon_{\nu\lambda\kappa}[-B^{\nabla s_1 J_1 s_1}(\nabla_\mu s_{q,\lambda})s_{q,\kappa}-B^{\nabla s_1 J_1 s_2}(\nabla_\mu s_{q,\lambda})s_{\bar q,\kappa}-B^{\nabla s_1 J_2 s_1}(\nabla_\mu s_{\bar q,\lambda})s_{\bar q,\kappa}\\
&-B^{\nabla s_1 J_2 s_2}(\nabla_\mu s_{\bar q,\lambda})s_{q,\kappa}],
\end{aligned}
\tag{D9f}
$$

$$
\begin{aligned}
\tilde U_q=&A^{\tilde\rho_1^*\tilde\rho_1}\tilde\rho_q+A^{\tilde\tau_1\tilde\rho_1^*}\tilde\tau_q-A^{\nabla\tilde\rho_1^*\nabla\tilde\rho_1}\Delta\tilde\rho_q+B^{\tilde\rho_1^*\tilde\rho_1\rho_2}\tilde\rho_q\rho_{\bar q}+B^{\tilde\tau_1\tilde\rho_1^*\rho_2}\tilde\tau_q\rho_{\bar q}+B^{\tau_1\tilde\rho_1^*\tilde\rho_1}\tau_q\tilde\rho_q+B^{\tau_2\tilde\rho_1^*\tilde\rho_1}\tau_{\bar q}\tilde\rho_q\\
&-B^{\nabla\tilde\rho_1^*\nabla\tilde\rho_1\rho_1}(\Delta\tilde\rho_q)\rho_q-B^{\nabla\tilde\rho_1^*\nabla\tilde\rho_1\rho_1}(\vec\nabla\tilde\rho_q)\cdot(\vec\nabla\rho_q)-B^{\nabla\tilde\rho_1^*\nabla\tilde\rho_1\rho_2}(\Delta\tilde\rho_q)\rho_{\bar q}-B^{\nabla\tilde\rho_1^*\nabla\tilde\rho_1\rho_2}(\vec\nabla\tilde\rho_q)\cdot(\vec\nabla\rho_{\bar q})\\
&-B^{\nabla\tilde\rho_1^*\nabla\rho_1\tilde\rho_1}(\Delta\rho_q)\tilde\rho_q-B^{\nabla\tilde\rho_1^*\nabla\rho_1\tilde\rho_1}(\vec\nabla\rho_q)\cdot(\vec\nabla\tilde\rho_q)-B^{\nabla\tilde\rho_1^*\nabla\rho_2\tilde\rho_1}(\Delta\rho_{\bar q})\tilde\rho_q-B^{\nabla\tilde\rho_1^*\nabla\rho_2\tilde\rho_1}(\vec\nabla\rho_{\bar q})\cdot(\vec\nabla\tilde\rho_q)\\
&+B^{\nabla\tilde\rho_1\nabla\rho_1\tilde\rho_1^*}(\vec\nabla\tilde\rho_q)\cdot(\vec\nabla\rho_q)+B^{\nabla\tilde\rho_1\nabla\rho_2\tilde\rho_1^*}(\vec\nabla\tilde\rho_q)\cdot(\vec\nabla\rho_{\bar q})+\sum_{\mu\nu}[B^{\tilde J_1 J_1\tilde\rho_1^*}\tilde J_{q,\mu\nu}J_{q,\mu\nu}+B^{\tilde J_1 J_2\tilde\rho_1^*}\tilde J_{q,\mu\nu}J_{\bar q,\mu\nu}\\
&-\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_1}\nabla_\mu\tilde J_{q,\mu\nu}s_{q,\nu}-\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_1}\tilde J_{q,\mu\nu}\nabla_\mu s_{q,\nu}-\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_2}\nabla_\mu\tilde J_{q,\mu\nu}s_{\bar q,\nu}-\mathrm{i}B^{\nabla\tilde\rho_1^*\tilde J_1 s_2}\tilde J_{q,\mu\nu}\nabla_\mu s_{\bar q,\nu}]\\
&-\mathrm{i}B^{\nabla\tilde\rho_1^* j_1\tilde\rho_1}(\vec\nabla\cdot\vec j_q)\tilde\rho_q-\mathrm{i}B^{\nabla\tilde\rho_1^* j_1\tilde\rho_1}\vec j_q\cdot(\vec\nabla\tilde\rho_q)-\mathrm{i}B^{\nabla\tilde\rho_1^* j_2\tilde\rho_1}(\vec\nabla\cdot\vec j_{\bar q})\tilde\rho_q-\mathrm{i}B^{\nabla\tilde\rho_1^* j_2\tilde\rho_1}\vec j_{\bar q}\cdot(\vec\nabla\tilde\rho_q)\\
&+\mathrm{i}B^{\nabla\tilde\rho_1 j_1\tilde\rho_1^*}(\vec\nabla\tilde\rho_q)\cdot\vec j_q+\mathrm{i}B^{\nabla\tilde\rho_1 j_2\tilde\rho_1^*}(\vec\nabla\tilde\rho_q)\cdot\vec j_{\bar q}+\sum_{\mu\nu}[\mathrm{i}B^{\nabla s_1\tilde J_1\tilde\rho_1^*}(\nabla_\mu s_{q,\nu})\tilde J_{q,\mu\nu}+\mathrm{i}B^{\nabla s_2\tilde J_1\tilde\rho_1^*}(\nabla_\mu s_{\bar q,\nu})\tilde J_{q,\mu\nu}],
\end{aligned}
\tag{D9g}
$$

$$
\tilde B_q=A^{\tilde\tau_1^*\tilde\rho_1}\tilde\rho_q+B^{\tilde\tau_1^*\tilde\rho_1\rho_2}\tilde\rho_q\rho_{\bar q},
\tag{D9h}
$$

$$
\begin{aligned}
\tilde W_{q,\mu\nu}=&A_1^{\tilde J_1^*\tilde J_1}\tilde J_{q,\mu\nu}+B^{\tilde J_1^*\tilde J_1\rho_1}\tilde J_{q,\mu\nu}\rho_q+B^{\tilde J_1^*\tilde J_1\rho_2}\tilde J_{q,\mu\nu}\rho_{\bar q}+B^{\tilde J_1^* J_1\tilde\rho_1}J_{q,\mu\nu}\tilde\rho_q\\
&+B^{\tilde J_1^* J_2\tilde\rho_1}J_{\bar q,\mu\nu}\tilde\rho_q+\mathrm{i}B^{\nabla\tilde\rho_1\tilde J_1^* s_1}(\nabla_\mu\tilde\rho_q)s_{q,\nu}+\mathrm{i}B^{\nabla\tilde\rho_1\tilde J_1^* s_2}(\nabla_\mu\tilde\rho_q)s_{\bar q,\nu}+\mathrm{i}B^{\nabla s_1\tilde J_1^*\tilde\rho_1}(\nabla_\mu s_{q,\nu})\tilde\rho_q\\
&+\mathrm{i}B^{\nabla s_2\tilde J_1^*\tilde\rho_1}(\nabla_\mu s_{\bar q,\nu})\tilde\rho_q+\sum_{\lambda\kappa}\epsilon_{\nu\lambda\kappa}[\mathrm{i}B^{\tilde J_1^*\tilde J_1 s_1}\tilde J_{q,\mu\lambda}s_{q,\kappa}+\mathrm{i}B^{\tilde J_1^*\tilde J_1 s_2}\tilde J_{q,\mu\lambda}s_{\bar q,\kappa}].
\end{aligned}
\tag{D9i}
$$

## APPENDIX E: LOCAL GAUGE INVARIANCE

### 1. Gauge transformations

The invariance of the energy under local gauge transformation traces back to the locality of the underlying interaction [14]. Given that realistic nuclear interactions have no reason to be local, invariance of the diagonal EDF kernel under general local gauge transformations does not have to be required. However, invariance under Galilean transformations is mandatory. Given that Galilean transformations are nothing but a particular case of local gauge transformations, we now test the invariance of the nuclear EDF under the latter as a way to verify its invariance under the former. That the the newly developed EDF kernel happens to be invariant under general local gauge transformations indicates that the dependence of the pseudopotential up to second order in gradients represents an internally consistent approximation to a local finite-range three-body potential.

Let us now characterize the behavior of the EDF kernel under general gauge transformations [66]. To do so, we first define the transformation law of the one-body density matrices, i.e.,

$$\rho'(\vec{r}\,\sigma q, \vec{r}\,'\sigma' q') = e^{\mathrm{i}(\phi(\vec{r})-\phi(\vec{r}\,'))}\rho(\vec{r}\sigma q, \vec{r}\,'\sigma' q'), \tag{E1a}$$

$$\kappa'(\vec{r}\,\sigma q, \vec{r}\,'\sigma' q') = e^{\mathrm{i}(\phi(\vec{r})+\phi(\vec{r}\,'))}\kappa(\vec{r}\sigma q, \vec{r}\,'\sigma' q'). \tag{E1b}$$

Galilean transformations are nothing but the particular gauge transformations obtained for $\phi(\vec{r}) = \vec{p}\cdot\vec{r}/\hbar$, where $\vec{p}$ characterizes the Galilean boost. Based on Eq. (E1), the transformation law of the local densities from which the EDF kernel is built is obtained as

$$\rho'_q = \rho_q, \tag{E2a}$$

$$\tau'_q = \tau_q + 2\vec{j}_q\cdot(\vec{\nabla}\phi) + \rho_q(\vec{\nabla}\phi)^2, \tag{E2b}$$

$$\vec{j}'_q = \vec{j}_q + \rho_q(\vec{\nabla}\phi), \tag{E2c}$$

$$s'_{q,\nu} = s_{q,\nu}, \tag{E2d}$$

$$T'_{q,\nu} = T_{q,\nu} + \sum_\mu [2J_{q,\mu\nu}(\nabla_\mu\phi) + s_{q,\nu}(\nabla_\mu\phi)^2], \tag{E2e}$$

$$J'_{q,\mu\nu} = J_{q,\mu\nu} + s_{q,\nu}(\nabla_\mu\phi), \tag{E2f}$$

$$\tilde{\rho}'_q = e^{2\mathrm{i}\phi}\tilde{\rho}_q, \tag{E2g}$$

$$\tilde{\tau}'_q = e^{2\mathrm{i}\phi}[\tilde{\tau}_q + \mathrm{i}(\vec{\nabla}\tilde{\rho}_q)\cdot(\vec{\nabla}\phi) - \tilde{\rho}_q(\vec{r})(\vec{\nabla}\phi)^2], \tag{E2h}$$

$$\tilde{J}'_{q,\mu\nu} = e^{2\mathrm{i}\phi}\tilde{J}_{q,\mu\nu}. \tag{E2i}$$

Although Eq. (E2) makes use of neutron and proton densities, the same transformation laws hold for isoscalar and isovector densities. The latter are used in the following to characterize the gauge invariance of the EDF kernel.

### 2. Normal part of the EDF kernel

The gauge invariance of the normal part of the EDF kernel requires that

$$\mathcal{E}^{\rho\rho'} - \mathcal{E}^{\rho\rho} \equiv [\mathcal{E}^{\rho\rho}]_{\mathcal{G}} = 0, \tag{E3a}$$

$$\mathcal{E}^{\rho\rho\rho'} - \mathcal{E}^{\rho\rho\rho} \equiv [\mathcal{E}^{\rho\rho\rho}]_{\mathcal{G}} = 0, \tag{E3b}$$

where $\mathcal{E}^{\rho\rho'}$ and $\mathcal{E}^{\rho\rho\rho'}$ denote energy densities computed from the gauge-transformed densities defined in Eq. (E2). In Eq. (E3), square brackets with index $\mathcal{G}$ have to be zero for the EDF kernel to be gauge invariant. Such conditions can be fulfilled only if specific correlations between coupling constants are at play. Gauge transformation only affects normal densities $\tau_t$, $T_{t,\nu}$, $j_{t,\mu}$, and $J_{t,\mu\nu}$, following Eq. (E2). The fact that $\tau'_t - \tau_t$, $T'_{t,\nu} - T_{t,\nu}$, $j'_{t,\mu} - j_{t,\mu}$, and $J'_{t,\mu\nu} - J_{t,\mu\nu}$ depend on densities $j_{t,\mu}$, $J_{t,\mu\nu}$, $\rho_t$, and $s_{t,\nu}$ in addition to the gauge function $\phi(\vec{r})$, implies that correlations only involve coefficients multiplying densities $\tau_t$, $T_{t,\nu}$, $j_{t,\mu}$, and $J_{t,\mu\nu}$ having the same spin and isospin character.

For the bilinear functional, the two densities involved in a given term are either both isoscalar or isovector and both scalar or vector, such that each gauge invariant combination involves only two terms of the functional. As a result, condition Eq. (E3a) is equivalent to requiring that

$$\left[A_t^\tau\ \tau_t\rho_t + A_t^j\ \vec{j}_t\cdot\vec{j}_t\right]_{\mathcal{G}} = 0, \tag{E4a}$$

$$\left[A_t^T\ \vec{s}_t\cdot\vec{T}_t + \sum_{\mu\nu} A_t^J\ J_{t,\mu\nu}J_{t,\mu\nu}\right]_{\mathcal{G}} = 0, \tag{E4b}$$

for $t \in \{0, 1\}$ and is fulfilled whenever [66]

$$A_t^\tau = -A_t^j, \quad A_t^T = -A_t^J. \tag{E5}$$

For the trilinear functional, such combinations can involve many more terms as two isovector or vector densities are always multiplied by an isoscalar or scalar density. Condition (E3b) gives rise to seven independent relations that read

$$0 = \left[B_0^\tau\rho_0\tau_0\rho_0 + B_0^j\rho_0\vec{j}_0\cdot\vec{j}_0\right]_{\mathcal{G}}, \tag{E6a}$$

$$0 = \left[B_0^T\rho_0\vec{T}_0\cdot\vec{s}_0 + B_0^{\tau s}\vec{s}_0\tau_0\cdot\vec{s}_0 + \sum_{\mu\nu} B_0^J\rho_0 J_{0,\mu\nu}J_{0,\mu\nu} + \sum_{\mu\nu} B_0^{Js}s_{0,\nu}j_{0,\mu}J_{0,\mu\nu}\right]_{\mathcal{G}}, \tag{E6b}$$

$$0 = \left[B_1^\tau\rho_0\tau_1\rho_1 + B_{10}^\tau\rho_1\tau_0\rho_1 + B_1^j\rho_0\vec{j}_1\cdot\vec{j}_1 + B_{10}^j\rho_1\vec{j}_1\cdot\vec{j}_0\right]_{\mathcal{G}}, \tag{E6c}$$

$$0 = \left[B_1^T\rho_0\vec{T}_1\cdot\vec{s}_1 + B_{10}^{\tau s}\vec{s}_1\tau_0\cdot\vec{s}_1 + \sum_{\mu\nu} B_1^J\rho_0 J_{1,\mu\nu}J_{1,\mu\nu} + \sum_{\mu\nu} B_{01}^{Js}s_{1,\nu}j_{0,\mu}J_{1,\mu\nu}\right]_{\mathcal{G}}, \tag{E6d}$$

$$0 = \left[B_{10}^T\rho_1\vec{T}_0\cdot\vec{s}_1 + B_{01}^T\rho_1\vec{T}_1\cdot\vec{s}_0 + B_1^{\tau s}\vec{s}_0\tau_1\cdot\vec{s}_1 + \sum_{\mu\nu} B_{10}^J\rho_1 J_{1,\mu\nu}J_{0,\mu\nu} + \sum_{\mu\nu} B_1^{Js}s_{0,\nu}j_{1,\mu}J_{1,\mu\nu} + \sum_{\mu\nu} B_{10}^{Js}s_{1,\nu}j_{1,\mu}J_{0,\mu\nu}\right]_{\mathcal{G}}, \tag{E6e}$$

$$0 = \left[\sum_{\mu\nu\lambda k} \epsilon_{\nu\lambda k}B_0^{\nabla sJ}s_{0,k}(\nabla_\mu s_{0,\nu})J_{0,\mu\lambda}\right]_{\mathcal{G}}, \tag{E6f}$$

$$0 = \Bigg\{ \sum_{\mu\nu\lambda k} \epsilon_{\nu\lambda k} \Big[ B_1^{\nabla s J} s_{0,k} (\nabla_\mu s_{1,\nu}) J_{1,\mu\lambda} + B_{10}^{\nabla s J} s_{1,k} (\nabla_\mu s_{1,\nu}) J_{0,\mu\lambda} + B_{01}^{\nabla s J} s_{1,k} (\nabla_\mu s_{0,\nu}) J_{1,\mu\lambda} \Big] \Bigg\}_{\mathcal{G}}. \tag{E6g}$$

Condition (E6a) involves functional terms containing scalar-isoscalar densities. Condition (E6b) involves functional terms containing isoscalar densities among which two are vector densities. Condition (E6c) involves functional terms containing two isovector densities and no vector densities. Conditions (E6d) and (E6e) involve functional terms containing two isovector densities and two vector densities. Condition (E6f) involves functional terms containing three vector-isoscalar densities. Finally, condition (E6g) involves all the functional terms with three spin densities, among which two are isovector. Correlations between coupling constants resulting from conditions Eq. (E6) read

$$\text{Eq. (E6a)} \Rightarrow B_0^\tau + B_0^j = 0, \tag{E7a}$$

$$\text{Eq. (E6b)} \Rightarrow \begin{cases} 2B_0^{\tau s} + B_0^{Js} = 0, \\ 2B_0^T + 2B_0^J + B_0^{Js} = 0, \end{cases} \tag{E7b}$$

$$\text{Eq. (E6c)} \Rightarrow \begin{cases} 2B_{10}^\tau + B_{10}^j = 0, \\ 2B_1^\tau + 2B_1^j + B_{10}^j = 0, \end{cases} \tag{E7c}$$

$$\text{Eq. (E6d)} \Rightarrow \begin{cases} 2B_{10}^{\tau s} + B_{01}^{Js} = 0, \\ 2B_1^T + 2B_1^J + B_{01}^{Js} = 0, \end{cases} \tag{E7d}$$

$$\text{Eq. (E6e)} \Rightarrow \begin{cases} 2B_1^{\tau s} + B_1^{Js} + B_{10}^{Js} = 0, \\ 2B_{10}^T + B_{10}^J + B_{10}^{Js} = 0, \\ 2B_{01}^T + B_{10}^J + B_1^{Js} = 0, \end{cases} \tag{E7e}$$

$$\text{Eq. (E6g)} \Rightarrow B_1^{\nabla s J} - B_{10}^{\nabla s J} = 0, \tag{E7f}$$

while Eq. (E6f) is respected for all $B_0^{\nabla s J}$. Conditions (E7) are fulfilled by our functional coefficients; see Tables IV and VI.

### 3. Anomalous part of the EDF kernel

The same strategy is followed for the anomalous part of the EDF kernel. The analog of condition (E3) is

$$\mathcal{E}^{\kappa\kappa\prime} - \mathcal{E}^{\kappa\kappa} \equiv [\mathcal{E}^{\kappa\kappa}]_{\mathcal{G}} = 0, \tag{E8a}$$

$$\mathcal{E}^{\kappa\kappa\kappa\prime} - \mathcal{E}^{\kappa\kappa\kappa} \equiv [\mathcal{E}^{\kappa\kappa\kappa}]_{\mathcal{G}} = 0. \tag{E8b}$$

As seen from Eq. (E2), all anomalous local densities are affected by gauge transformations. However, each pairing density enters the energy density with the complex conjugate of another pairing density, such that bilinear products of the form $\breve{\rho}^*\breve{\rho}$, $\breve{J}^*\breve{J}$, $\breve{\rho}^*\breve{J}$, or $\breve{J}^*\breve{\rho}$ are effectively gauge invariant. As a result, only $\breve{\tau}$ or derivatives of $\breve{\rho}$ and $\breve{J}$ have to be explicitly dealt with. For trilinear terms a gauge dependence might also arise from the third, then normal, local density. Again, correlations will only involve coefficients multiplying densities of same spin and isospin character.

For the bilinear functional, condition (E8a) is equivalent to requiring

$$\Big[ A^{\breve{\tau}^*} \sum_{\mathfrak{a}=1,2} \breve{\tau}_{1,\mathfrak{a}}^* \breve{\rho}_{1,\mathfrak{a}} + A^{\breve{\tau}} \sum_{\mathfrak{a}=1,2} \breve{\tau}_{1,\mathfrak{a}} \breve{\rho}_{1,\mathfrak{a}}^* + A^{\nabla\breve{\rho}} \sum_{\mathfrak{a}=1,2} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \cdot (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}) \Big]_{\mathcal{G}} = 0, \tag{E9}$$

which is fulfilled for

$$A^{\nabla\breve{\rho}} = \tfrac{1}{2} A^{\breve{\tau}^*} = \tfrac{1}{2} A^{\breve{\tau}}. \tag{E10}$$

For the trilinear functional, condition (E8b) gives rise to eight independent gauge-invariant conditions that read

$$0 = \Big[ \sum_{\mathfrak{a}=1,2} \Big\{ B_0^{\breve{\tau}^*} \breve{\tau}_{1,\mathfrak{a}}^* \breve{\rho}_{1,\mathfrak{a}} \rho_0 + B_0^{\breve{\tau}} \breve{\rho}_{1,\mathfrak{a}}^* \breve{\tau}_{1,\mathfrak{a}} \rho_0 + B_0^{\breve{\rho}\tau} \breve{\rho}_{1,\mathfrak{a}}^* \breve{\rho}_{1,\mathfrak{a}} \tau_0 + B_0^{\nabla\breve{\rho}} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \cdot (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}) \rho_0 + \mathrm{i} B_0^{\nabla\breve{\rho}^* j} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \breve{\rho}_{1,\mathfrak{a}} \cdot \vec{j}_0 + \mathrm{i} B_0^{\nabla\breve{\rho} j} \breve{\rho}_{1,\mathfrak{a}}^* (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}) \cdot \vec{j}_0 \Big\} \Big]_{\mathcal{G}}, \tag{E11a}$$

$$0 = \Big[ \sum_{\mathfrak{a}=1,2} \Big\{ B_0^{\nabla\breve{\rho}^*\breve{\rho}} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \breve{\rho}_{1,\mathfrak{a}} \cdot (\vec{\nabla}\rho_0) + B_0^{\breve{\rho}^*\nabla\breve{\rho}} \breve{\rho}_{1,\mathfrak{a}}^* (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}) \cdot (\vec{\nabla}\rho_0) \Big\} \Big]_{\mathcal{G}}, \tag{E11b}$$

$$0 = \Big[ \sum_{\mathfrak{a}=1,2} \sum_{\mu\nu} \Big\{ B_0^{\breve{\rho}^*\breve{J}} \breve{\rho}_{1,\mathfrak{a}}^* \breve{J}_{1,\mathfrak{a},\mu\nu} J_{0,\mu\nu} + \mathrm{i} B_0^{\nabla\breve{\rho}^*\breve{J}} (\nabla_\mu \breve{\rho}_{1,\mathfrak{a}}^*) \breve{J}_{1,\mathfrak{a},\mu\nu} s_{0,\nu} \Big\} \Big]_{\mathcal{G}}, \tag{E11c}$$

$$0 = \Big[ \sum_{\mathfrak{a}=1,2} \sum_{\mu\nu} \Big\{ B_0^{\breve{J}^*\breve{\rho}} \breve{J}_{1,\mathfrak{a},\mu\nu}^* \breve{\rho}_{1,\mathfrak{a}} J_{0,\mu\nu} + \mathrm{i} B_0^{\breve{J}^*\nabla\breve{\rho}} \breve{J}_{1,\mathfrak{a},\mu\nu}^* (\nabla_\mu \breve{\rho}_{1,\mathfrak{a}}) s_{0,\nu} \Big\} \Big]_{\mathcal{G}}, \tag{E11d}$$

$$0 = \Big[ \sum_{\mathfrak{a},\mathfrak{b}=1,2} \sum_{\mathfrak{c}=3} \epsilon_{\mathfrak{a}\mathfrak{b}\mathfrak{c}} \Big\{ \mathrm{i} B_1^{\breve{\tau}^*} \breve{\tau}_{1,\mathfrak{a}}^* \breve{\rho}_{1,\mathfrak{b}} \rho_{1,\mathfrak{c}} + \mathrm{i} B_1^{\breve{\tau}} \breve{\rho}_{1,\mathfrak{a}}^* \breve{\tau}_{1,\mathfrak{b}} \rho_{1,\mathfrak{c}} + \mathrm{i} B_1^{\breve{\rho}\tau} \breve{\rho}_{1,\mathfrak{a}}^* \breve{\rho}_{1,\mathfrak{b}} \tau_{1,\mathfrak{c}} + \mathrm{i} B_1^{\nabla\breve{\rho}} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \cdot (\vec{\nabla}\breve{\rho}_{1,\mathfrak{b}}) \rho_{1,\mathfrak{c}} + B_1^{\nabla\breve{\rho}^* j} (\vec{\nabla}\breve{\rho}_{1,\mathfrak{a}}^*) \breve{\rho}_{1,\mathfrak{b}} \cdot \vec{j}_{1,\mathfrak{c}} + B_1^{\nabla\breve{\rho} j} \breve{\rho}_{1,\mathfrak{a}}^* (\vec{\nabla}\breve{\rho}_{1,\mathfrak{b}}) \cdot \vec{j}_{1,\mathfrak{c}} \Big\} \Big], \tag{E11e}$$

$$0 = \left[ \sum_{a,b=1,2} \sum_{c=3} \epsilon_{abc} \left\{ \mathrm{i} B_1^{\nabla \check{\rho}^* \check{\rho}} (\vec{\nabla} \check{\rho}^*_{1,a}) \check{\rho}_{1,b} \cdot (\vec{\nabla} \rho_{1,c}) + \mathrm{i} B_1^{\check{\rho}^* \nabla \check{\rho}} \check{\rho}^*_{1,a} (\vec{\nabla} \check{\rho}_{1,b}) \cdot (\vec{\nabla} \rho_{1,c}) \right\} \right]_{\mathcal{G}}, \tag{E11f}$$

$$0 = \left[ \sum_{a,b=1,2} \sum_{c=3} \epsilon_{abc} \sum_{\mu\nu} \left\{ \mathrm{i} B_1^{\check{\rho}^* \check{J}} \check{\rho}^*_{1,a} \check{J}_{1,b,\mu\nu} J_{1,c,\mu\nu} + B_1^{\nabla \check{\rho}^* \check{J}} (\nabla_\mu \check{\rho}^*_{1,a}) \check{J}_{1,b,\mu\nu} s_{1,c,\nu} \right\} \right]_{\mathcal{G}}, \tag{E11g}$$

$$0 = \left[ \sum_{a,b=1,2} \sum_{c=3} \epsilon_{abc} \sum_{\mu\nu} \left\{ \mathrm{i} B_1^{\check{J}^* \check{\rho}} \check{J}^*_{1,a,\mu\nu} \check{\rho}_{1,b} J_{1,c,\mu\nu} + B_1^{\check{J}^* \nabla \check{\rho}} \check{J}^*_{1,a,\mu\nu} (\nabla_\mu \check{\rho}_{1,b}) s_{1,c,\nu} \right\} \right]_{\mathcal{G}}. \tag{E11h}$$

These relations must be independently fulfilled, which requires that the coupling constants satisfy

$$\text{Eq. (E11a)} \Rightarrow \begin{cases} -B_0^{\check{\tau}^*} + 2B_0^{\nabla \check{\rho}} + B_0^{\nabla \check{\rho}^* j} = 0, \\ B_0^{\check{\tau}} - 2B_0^{\nabla \check{\rho}} + B_0^{\nabla \check{\rho} j} = 0, \\ B_0^{\check{\rho}\tau} + B_0^{\nabla \check{\rho}^* j} - B_0^{\nabla \check{\rho} j} = 0, \end{cases} \tag{E12a}$$

$$\text{Eq. (E11b)} \Rightarrow B_0^{\nabla \check{\rho}^* \check{\rho}} = B_0^{\check{\rho}^* \nabla \check{\rho}}, \tag{E12b}$$

$$\text{Eq. (E11c)} \Rightarrow B_0^{\check{\rho}^* \check{J}} = -2B_0^{\nabla \check{\rho}^* \check{J}}, \tag{E12c}$$

$$\text{Eq. (E11d)} \Rightarrow B_0^{\check{J}^* \check{\rho}} = 2B_0^{\check{J}^* \nabla \check{\rho}}, \tag{E12d}$$

$$\text{Eq. (E11e)} \Rightarrow \begin{cases} -B_1^{\check{\tau}^*} + 2B_1^{\nabla \check{\rho}} - B_1^{\nabla \check{\rho}^* j} = 0, \\ B_1^{\check{\tau}} - 2B_1^{\nabla \check{\rho}} - B_1^{\nabla \check{\rho} j} = 0, \\ B_1^{\check{\rho}\tau} - B_1^{\nabla \check{\rho}^* j} + B_1^{\nabla \check{\rho} j} = 0, \end{cases} \tag{E12e}$$

$$\text{Eq. (E11f)} \Rightarrow B_1^{\nabla \check{\rho}^* \check{\rho}} = B_1^{\check{\rho}^* \nabla \check{\rho}}, \tag{E12f}$$

$$\text{Eq. (E11g)} \Rightarrow B_1^{\check{\rho}^* \check{J}} = 2B_1^{\nabla \check{\rho}^* \check{J}}, \tag{E12g}$$

$$\text{Eq. (E11h)} \Rightarrow B_1^{\check{J}^* \check{\rho}} = -2B_1^{\check{J}^* \nabla \check{\rho}}, \tag{E12h}$$

which is indeed the case our EDF kernel; see Tables V and VII.


[1] Ph. Quentin and H. Flocard, Annu. Rev. Nucl. Part. Sci. **28**, 523 (1978).
[2] K. Bennaceur, P. Bonche, and J. Meyer, C. R. Phys. **4**, 555 (2003).
[3] M. Bender, P.-H. Heenen, and P.-G. Reinhard, Rev. Mod. Phys. **75**, 121 (2003).
[4] J. Erler, P. Klüpfel, and P.-G. Reinhard, J. Phys. G **38**, 033101 (2011).
[5] T. Duguet, arXiv:1309.0440 [*The Euroschool Lectures on Physics with Exotic Beams*, edited by C. Scheidenberger and M. Pfützner, Lecture Notes in Physics Vol. IV (Springer Verlag, Berlin, Heidelberg) (to be published)].
[6] D. Lacroix, T. Duguet, and M. Bender, Phys. Rev. C **79**, 044318 (2009).
[7] M. Bender, T. Duguet, and D. Lacroix, Phys. Rev. C **79**, 044319 (2009).
[8] S. Stringari and D. M. Brink, Nucl. Phys. A **304**, 307 (1978).
[9] M. Bender, P.-G. Reinhard, J. Dobaczewski, and W. Nazarewicz (unpublished).
[10] N. Chamel, Phys. Rev. C **82**, 061307(R) (2010).
[11] J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[12] R. Balian and E. Brézin, Nuovo Cimento **64**, 37 (1969).
[13] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer-Verlag, New York, 1980).
[14] J. P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems* (MIT Press, Cambridge, MA, 1986).
[15] J. Dobaczewski and J. Dudek, Acta Phys. Pol. B **27**, 45 (1996).
[16] S. A. Fayans, S. V. Tolokonnikov, E. L. Trykov, and D. Zawischa, Nucl. Phys. A **676**, 49 (2000).
[17] M. Baldo, P. Schuck, and X. Viñas, Phys. Lett. B **663**, 390 (2008); M. Baldo, L. M. Robledo, P. Schuck, and X. Viñas, Phys. Rev. C **87**, 064305 (2013).
[18] D. Gogny, in *Proceedings of the International Conference on Nuclear Self-Consistent Fields*, edited by G. Ripka and M. Porneuf, International Centre for Theoretical Physics, Trieste (North-Holland, Amsterdam, 1975), p. 333.
[19] J. Dechargé and D. Gogny, Phys. Rev. C **21**, 1568 (1980).
[20] F. Chappert, M. Girod, and S. Hilaire, Phys. Lett. B **668**, 420 (2008).
[21] S. Goriely, S. Hilaire, M. Girod, and S. Péru, Phys. Rev. Lett. **102**, 242501 (2009).
[22] H. Nakada, Phys. Rev. C **68**, 014316 (2003); **81**, 027301 (2010); **87**, 014336 (2013).
[23] J. Dobaczewski, H. Flocard, and J. Treiner, Nucl. Phys. A **422**, 103 (1984).
[24] J. M. G. Gómez, C. Prieto, and J. Navarro, Nucl. Phys. A **549**, 125 (1992).
[25] M. Waroquier, J. Sau, K. Heyde, P. Van Isacker, and H. Vincx, Phys. Rev. C **19**, 1983 (1979).
[26] M. Bender, J. Dobaczewski, J. Engel, and W. Nazarewicz, Phys. Rev. C **65**, 054322 (2002).

[27] P.-G. Reinhard and H. Flocard, Nucl. Phys. A **584**, 467 (1995).
[28] T. Lesinski, M. Bender, K. Bennaceur, T. Duguet, and J. Meyer, Phys. Rev. C **76**, 014312 (2007).
[29] M. Zalewski, J. Dobaczewski, W. Satuła, and T. R. Werner, Phys. Rev. C **77**, 024316 (2008).
[30] M. Bender, K. Bennaceur, T. Duguet, P.-H. Heenen, T. Lesinski, and J. Meyer, Phys. Rev. C **80**, 064302 (2009).
[31] T. Duguet, P. Bonche, P.-H. Heenen, and J. Meyer, Phys. Rev. C **65**, 014310 (2001).
[32] K. J. Pototzky, J. Erler, P.-G. Reinhard, and V. O. Nesterenko, Eur. Phys. J. A **46**, 299 (2010).
[33] N. Schunck, J. Dobaczewski, J. McDonnell, J. Moré, W. Nazarewicz, J. Sarich, and M. V. Stoitsov, Phys. Rev. C **81**, 024316 (2010).
[34] V. Hellemans, P.-H. Heenen, and M. Bender, Phys. Rev. C **85**, 014326 (2012).
[35] N. Tajima, H. Flocard, P. Bonche, J. Dobaczewski, and P.-H. Heenen, Nucl. Phys. A **542**, 355 (1992).
[36] F. Dönau, Phys. Rev. C **58**, 872 (1998).
[37] D. Almehed, S. Frauendorf, and F. Dönau, Phys. Rev. C **63**, 044311 (2001).
[38] M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A **696**, 467 (2001).
[39] J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, and P.-G. Reinhard, Phys. Rev. C **76**, 054315 (2007).
[40] H. Zduńczuk, J. Dobaczewski, and W. Satuła, Int. J. Mod. Phys. E **16**, 377 (2007).
[41] T. Duguet, M. Bender, K. Bennaceur, D. Lacroix, and T. Lesinski, Phys. Rev. C **79**, 044320 (2009).
[42] T. R. Rodriguez, J. L. Egido, and L. M. Robledo, Phys. Rev. C **72**, 064303 (2005).
[43] L. M. Robledo, Int. J. Mod. Phys. E **16**, 337 (2007); J. Phys. G **37**, 064020 (2010).
[44] W. Satuła, J. Dobaczewski, W. Nazarewicz, and M. Rafalski, Phys. Rev. C **81**, 054310 (2010).
[45] W. Satuła, J. Dobaczewski, W. Nazarewicz, and T. R. Werner, Phys. Rev. C **86**, 054316 (2012).
[46] J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Phys. Scr. T **154**, 014013 (2013).
[47] T. H. R. Skyrme, Philos. Mag. **1**, 1043 (1956).
[48] J. S. Bell and T. H. R. Skyrme, Philos. Mag. **1**, 1055 (1956).
[49] T. H. R. Skyrme, Nucl. Phys. **9**, 615 (1959).
[50] F. Raimondi, B. G. Carlsson, J. Dobaczewski, and J. Toivanen, Phys. Rev. C **84**, 064303 (2011).
[51] D. Davesne, A. Pastore, and J. Navarro, J. Phys. G **40**, 095104 (2013).
[52] M. Kortelainen, R. J. Furnstahl, W. Nazarewicz, and M. V. Stoitsov, Phys. Rev. C **82**, 011304 (2010).
[53] B. Long, talk given at The 7th International Workshop on Chiral Dynamics, August 2012, Newport News, Virginia, arXiv:1307.0582.
[54] J. P. Blaizot, B. Grammaticos, and K. F. Liu, in *Proceedings of the International Conference on Nuclear Self-Consistent Fields*, edited by G. Ripka and M. Porneuf, International Center for Theoretical Physics, Trieste (North-Holland, Amsterdam, 1975), p. 259.
[55] K. F. Liu, Phys. Lett. B **60**, 9 (1975).
[56] N. Onishi and J. W. Negele, Nucl. Phys. A **301**, 336 (1978).
[57] A. Arima, N. Onishi, T. Inoue, Y. Akiyama, and T. Suzuki, Nucl. Phys. A **459**, 286 (1986).
[58] D. C. Zheng, L. Zamick, and S. Moszkowski, Ann. Phys. (NY) **201**, 342 (1990).
[59] M. Waroquier, K. Heyde, and H. Vincx, Phys. Rev. C **13**, 1664 (1976).
[60] M. Waroquier, K. Heyde, and G. Wenes, Nucl. Phys. A **404**, 269 (1983).
[61] M. Waroquier, G. Wenes, and K. Heyde, Nucl. Phys. A **404**, 298 (1983).
[62] K.-F. Liu, H. Luo, Z. Ma, Q. Shen, and S. A. Moszkowski, Nucl. Phys. A **534**, 1 (1991).
[63] K.-F. Liu, Z. Ma, and H.-D. Luo, Nucl. Phys. A **534**, 58 (1991).
[64] J. Sadoudi *et al*. (unpublished).
[65] J. Sadoudi, Thèse, Université Paris-Sud XI, 2011.
[66] J. Dobaczewski and J. Dudek, Phys. Rev. C **52**, 1827 (1995); **55**, 3177(E) (1997).
[67] B. G. Carlsson, J. Dobaczewski, and M. Kortelainen, Phys. Rev. C **78**, 044326 (2008); **81**, 029904(E) (2010).
[68] F. Raimondi, B. G. Carlsson, and J. Dobaczewski, Phys. Rev. C **83**, 054311 (2011).
[69] E. Perlinska, S. G. Rohoziński, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. C **69**, 014316 (2004).
[70] S. G. Rohoziński, J. Dobaczewski, and W. Nazarewicz, Phys. Rev. C **81**, 014313 (2010).
[71] S. G. Nilsson and I. Ragnarsson, *Shapes and Shells in Nuclear Structure* (Cambridge University Press, Cambridge, U.K., 1995).
[72] G. C. Wick, Phys. Rev. **80**, 268 (1950).
[73] T. Duguet and J. Sadoudi, J. Phys. G **37**, 064009 (2010).
[74] A. Gezerlis and G. F. Bertsch, Phys. Rev. Lett. **105**, 212501 (2010).
[75] T. D. Lee and C. N. Yang, Phys. Rev. **105**, 1119 (1957).
[76] K. Bennaceur *et al*. (unpublished).
[77] A. Bulgac and Y. Yu, Phys. Rev. Lett. **88**, 042504 (2002).
[78] K. Moghrabi, M. Grasso, X. Roca-Maza, and G. Colò, Phys. Rev. C **85**, 044323 (2012).
[79] B. G. Carlsson, J. Toivanen, and U. von Barth, Phys. Rev. C **87**, 054303 (2013).
[80] N. Chamel, S. Goriely, and J. M. Pearson, in *Fifty Years of Nuclear BCS: Pairing in Finite Systems*, edited by R. Broglia and W. Zelevinsky (World Scientific, Singapore, 2013), p. 284.
[81] J. Meyer *et al*. (unpublished).
[82] S.-O. Bäckman, Nucl. Phys. A **130**, 427 (1969).
[83] B. D. Chang, Phys. Lett. B **56**, 205 (1975).
[84] L.-G. Cao, G. Colò, and H. Sagawa, Phys. Rev. C **81**, 044302 (2010).
[85] A. B. Midgal, *Theory of Finite Fermi Systems and Applications to Atomic Nuclei* (Wiley, New York, 1967).
[86] D. Gogny and R. Padjen, Nucl. Phys. A **293**, 365 (1977).
[87] I. Y. Pomeranchuk, Sov. Phys. JETP **8**, 361 (1959).
[88] T. Lesinski, K. Bennaceur, T. Duguet, and J. Meyer, Phys. Rev. C **74**, 044315 (2006).
[89] A. Pastore, D. Davesne, Y. Lallouet, M. Martini, K. Bennaceur, and J. Meyer, Phys. Rev. C **85**, 054317 (2012).
[90] G. E. Brown, S.-O. Bäckman, E. Oset, and W. Weise, Nucl. Phys. A **286**, 191 (1977).
[91] B. L. Friman and A. K. Dhar, Phys. Lett. B **85**, 1 (1979).
[92] S. Babu and G. E. Brown, Ann. Phys. (NY) **78**, 1 (1973).
[93] D. Vautherin and D. M. Brink, Phys. Rev. C **5**, 626 (1972).
[94] Y. M. Engel, D. M. Brink, K. Goeke, S. J. Krieger, and D. Vautherin, Nucl. Phys. A **249**, 215 (1975).