

Local density approximation for proton-neutron pairing correlations: FormalismE. Perlińska,^{1,2,*} S. G. Rohoziński,^{1,†} J. Dobaczewski,^{1,‡} and W. Nazarewicz^{1,3,4,§}¹*Institute of Theoretical Physics, Warsaw University, Hoża 69, PL-00681 Warsaw, Poland*²*Institute of Physical Chemistry of the Polish Academy of Sciences, Kasprzaka 44/52, PL-01224 Warsaw, Poland*³*Department of Physics and Astronomy, The University of Tennessee, Knoxville, Tennessee 37996, USA*⁴*Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA*

(Received 1 October 2003; published 30 January 2004)

In the present study we generalize the self-consistent Hartree-Fock-Bogoliubov (HFB) theory formulated in the coordinate space to the case which incorporates an arbitrary mixing between protons and neutrons in the particle-hole (p - h) and particle-particle (p - p or pairing) channels. We define the HFB density matrices, discuss their spin-isospin structure, and construct the most general energy-density functional that is quadratic in local densities. The consequences of the local gauge invariance are discussed and the particular case of the Skyrme energy-density functional is studied. By varying the total energy with respect to the density matrices the self-consistent one-body HFB Hamiltonian is obtained and the structure of the resulting mean fields is shown. The consequences of the time-reversal symmetry, charge invariance, and proton-neutron symmetry are summarized. The complete list of expressions required to calculate total energy is presented.

DOI: 10.1103/PhysRevC.69.014316

PACS number(s): 21.60.Jz, 21.30.Fe, 71.15.Mb

I. INTRODUCTION

One of the main goals of nuclear theory is to build the unified microscopic framework for heavy nuclei in which the bulk nuclear properties, nuclear excitations, and nuclear reactions can be described on the same footing. Microscopic theory also provides the solid foundation for phenomenological models and coupling schemes which have been applied so successfully to explain specific nuclear properties. Exotic short-lived nuclei are very important in this quest. The abnormal neutron-to-proton ratios of these nuclei isolate and amplify important features, which are not clearly visible in stable systems.

For medium-mass and heavy nuclei, a critical challenge is the quest for the universal energy-density functional, which will be able to describe properties of finite nuclei as well as extended asymmetric nucleonic matter (e.g., as found in neutron stars). Self-consistent methods based on the density functional theory have already achieved a level of sophistication and precision which allows analyses of experimental data for a wide range of properties and for arbitrarily heavy nuclei. For instance, self-consistent Hartree-Fock and Hartree-Fock-Bogoliubov (HFB) models are now able to reproduce measured nuclear binding energies with an impressive rms error of ~ 700 keV [1,2]. However, much work remains to be done. Developing a universal nuclear density functional will require a better understanding of the density dependence, isospin effects, pairing, as well as an improved treatment of many-body correlations. All those aspects are essential for the structure of proton-rich nuclei with $N \approx Z$, which are expected to exhibit proton-neutron (pn) pairing

[3]; it is precisely in those nuclei that the state-of-the-art microscopic mass formula needs to be supplemented by a phenomenological Wigner term [1,2].

In spite of an impressive experimental progress in the heavy $N \approx Z$ region, it is still unclear (i) what the specific fingerprints of the pn pairing are and (ii) what is the interplay between the like-particle and pn ($T=0, 1$) p - h , and p - p channels. Before attempting to answer these questions, established theoretical models of nuclear pairing need to be generalized to properly account for pn correlations. The present work is a step in this direction. We propose the general HFB formalism which fully incorporates the pn mixing on the mean-field level. The resulting density matrices have a very rich spin-isospin structure, which, in the presence of static pn pairing, can produce novel mean fields and deformations.

The paper is organized as follows. Section II contains a brief review of the pn pairing. Section III discusses the density matrices (scalar, vector, and tensor), both in the p - n and p - p channel. The discussion is based on the coordinate-space HFB formalism [4–6], which was introduced earlier to describe pairing correlations between like nucleons. This method is the tool of choice when dealing with weakly bound heavy nuclei [7]. The energy functional is constructed in Sec. IV, the associated mean fields are derived in Sec. V, and Sec. VI deals with the resulting coordinate-space HFB equations. In the discussion of pn pairing, the notion of self-consistent symmetries, especially those associated with charge invariance and time reversal, is crucial, and we devote Sec. VII to this topic. Finally, conclusions are contained in Sec. VIII.

II. PROTON-NEUTRON PAIRING, A CONCISE OVERVIEW

A unique aspect of proton-rich nuclei with $N \approx Z$ is that neutrons and protons occupy the same single-particle orbitals. Consequently, due to the large spatial overlaps between

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neutron and proton single-particle wave functions, pn pairing is expected to be present in those systems.

So far, the strongest evidence for enhanced pn correlations around the $N=Z$ line comes from the measured binding energies [8–16] and the isospin structure of the low-lying states in odd-odd nuclei [16–28]. The pn correlations are also expected to play some role in single- β decay [29–31], double- β decay [32–38], transfer reactions [39–45] (see, however, Ref. [16]), structure of low-lying collective states [46], α decay and α correlations [45,47–52], structure of high spin states [14,20,53–79], and in properties of low-density nuclear matter [80–90].

Actually, the pn pairing is not “the new kid on the block” but it has a long history and is ultimately connected to the charge invariance of the strong Hamiltonian. (For reference, in 1932 Heisenberg introduced isotopic spin [91] and in 1936 Wigner introduced the nuclear $SU(4)$ supermultiplets [92].) An important step was the adaptation of Racah’s concept of seniority by Racah and Talmi [93], and Flowers [94] in 1952. In the independent quasiparticle (BCS) picture [95], pairing condensate appears as a result of an attractive interaction between quasiparticles near the Fermi surface. The term “nuclear superconductivity” was first used by Pines at the 1957 Rehovot conference to point out that the new BCS theory might also apply to nuclei [96]. This was formally accomplished in the late 1950s [97,98] and shortly afterwards the importance of pn pairing was emphasized [47,99,100] and a number of theoretical papers dealing with the generalization of the BCS theory to the pn pairing case appeared [101–103].

Independently, group-theoretical methods based on the quasispin formalism were developed. Many insights were gained by simple solvable models employing symmetry-dictated interactions [104–111]. Two families of models were used, one based on the j - j coupling with the symmetry $SO(5)$ (appropriate for the $T=1$ pairing) and the other based on the L - S coupling with the symmetry $SO(8)$ (appropriate for the $T=0$ and $T=1$ pairing). These models have been consecutively developed and applied to various physically interesting cases [36,42,44,45,112–114]. Among many techniques used to solve the problem of pn pairing with schematic interactions, worth mentioning are the exact methods [43,115,116] used to describe isovector states of a charge-independent pairing Hamiltonian.

Properties of pn pairing (at low and high spins, in cold and hot nuclei) have been studied within the large-scale shell model (diagonalization shell-model, variational shell model, and Monte Carlo shell model) [20,21,64,69,70,90,117–123]. It was concluded that the isovector pairing in the dominating $J=0$ channel mainly acts between time-reversed states within the same shell. On the other hand, isoscalar pairing can also involve coupling (mainly $J=1$) between spin-orbit partners. Consequently, spin-orbit splitting plays a crucial role in understanding the $T=0$ pairing [20].

It is to be noted that it is by no means obvious how to extract “pairing correlations” from the realistic shell-model calculations. The “pairing Hamiltonian” is an integral part of the residual shell-model interaction. The shell-model Hamiltonian is usually written in the p - p representation, but it also can be transformed to the p - h representation by means of the

Pandya transformation [124]. This means that the high- J interaction between pairs can translate into the low- J interaction in the p - h channel. It is only in the mean-field theory that the division into “particle-hole” and “particle-particle” channels appears naturally. One way of translating the shell-model results into mean-field language is by means of correlators, such as the number of $T=0$ and $T=1$ pairs in the shell-model wave function [69,112,120,125].

The extension of the interacting boson models (IBM) to the case of pn bosons had to wait until 1980, when IBM-3 (only $T=1$ pairs [126]) and IBM-4 (both ($T=1, S=0$) and ($T=0, S=1$) bosons [127]) were proposed. For recent applications of various algebraic models, see Refs. [26,128–138].

An alternative strategy to the pn pairing problem is via the mean-field approach. Here, the major conceptual step was the proposition that quasiparticles are mixtures not only particles and holes but also protons and neutrons. The resulting HFB quasiparticle vacuum is a superposition of wave functions corresponding to even-even and odd-odd nuclei with different particle numbers. Unlike in the standard nn and pp pairing cases, the coefficients of the Bogoliubov transformation are, in general, complex. Generalized Bogoliubov transformation, generalized gap equations, and pn pairing fields are discussed in Refs. [3,53,55,57,62,65,67,68,101,139–161].

The problem of the spontaneous isospin breaking in the mean-field theory was realized soon after the development of the generalized quasiparticle approach [48,144,148]. The symmetry is broken by the independent (separate) treatment of $T=1$ proton and neutron pairing correlations and by the BCS quasiparticle mean field (the generalized product wave function is not an eigenstate of isospin). Several techniques have been developed to restore isospin. They include the generator coordinate method, random phase approximation, Kamlah expansion, isocranking, and exact projection [15,16,27,37,48,67,144,148,162–166]. It is fair to say, however, that in spite of many attempts to extend the quasiparticle approach to incorporate the effect of pn correlations, no symmetry-unrestricted mean-field calculations of pn pairing, based on realistic effective interaction and the isospin-conserving formalism have been carried out.

III. DENSITY MATRICES IN THE ISOSPIN SPACE

We begin with the discussion of the building blocks of the HFB theory: one-body density matrices. In the HFB theory, expectation values of all observables and, in particular, of the nuclear Hamiltonian can be expressed as functionals of the density matrix $\hat{\rho}$ and the pairing tensor $\hat{\kappa}$ defined as [167]

$$\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = \langle \Psi | a_{\mathbf{r}'s't'}^\dagger a_{\mathbf{r}st} | \Psi \rangle, \quad (1a)$$

$$\hat{\kappa}(\mathbf{r}st, \mathbf{r}'s't') = \langle \Psi | a_{\mathbf{r}'s't'} a_{\mathbf{r}st} | \Psi \rangle, \quad (1b)$$

where $a_{\mathbf{r}st}^\dagger$ and $a_{\mathbf{r}st}$ create and annihilate, respectively, nucleons at point \mathbf{r} , spin $s = \pm \frac{1}{2}$ and isospin $t = \pm \frac{1}{2}$, while $|\Psi\rangle$ is the HFB independent-quasiparticle state. Instead of using the antisymmetric pairing tensor it is more convenient to introduce the p - p density matrices that can be defined in two forms, $\hat{\hat{\rho}}$

or $\hat{\rho}$, denoted by “tilde” and “breve,” respectively,

$$\hat{\tilde{\rho}}(\mathbf{r}st, \mathbf{r}'s't') = -2s't' \langle \Psi | a_{r'-s't'} a_{rst} | \Psi \rangle, \quad (2a)$$

$$\hat{\breve{\rho}}(\mathbf{r}st, \mathbf{r}'s't') = 4s't' \langle \Psi | a_{r'-s't'} a_{rst} | \Psi \rangle. \quad (2b)$$

In Ref. [5], p - p density matrix $\hat{\rho}$ was used to treat the n - n and p - p pairing correlations without the proton-neutron mixing. It was then shown that for conserved time-reversal symmetry $\hat{\rho}$ is Hermitian, and leads to p - p local densities that have the structure which is analogous to that of the p - h local densities. However, in the case of the proton-neutron mixing studied here, we decided to use the p - p density matrix $\hat{\breve{\rho}}$, because it allows a more transparent treatment of the isoscalar and isovector pairing channels. Detailed discussion of this point will be presented in Sec. III C below.

With each of density matrices of Eqs. (1a) and (2b) three other matrices are associated: the Hermitian conjugate matrices defined as

$$\hat{\rho}^+(\mathbf{r}st, \mathbf{r}'s't') = \hat{\rho}^*(\mathbf{r}'s't', \mathbf{r}st), \quad (3a)$$

$$\hat{\breve{\rho}}^+(\mathbf{r}st, \mathbf{r}'s't') = \hat{\breve{\rho}}^*(\mathbf{r}'s't', \mathbf{r}st), \quad (3b)$$

the time-reversed matrices defined as

$$\hat{\rho}^T(\mathbf{r}st, \mathbf{r}'s't') = 4ss' \hat{\rho}^*(\mathbf{r}-st, \mathbf{r}'-s't'), \quad (4a)$$

$$\hat{\breve{\rho}}^T(\mathbf{r}st, \mathbf{r}'s't') = 4ss' \hat{\breve{\rho}}^*(\mathbf{r}-st, \mathbf{r}'-s't'), \quad (4b)$$

the charge-reversed matrices defined as

$$\hat{\rho}^C(\mathbf{r}st, \mathbf{r}'s't') = 4tt' \hat{\rho}(\mathbf{r}s-t, \mathbf{r}'s'-t'), \quad (5a)$$

$$\hat{\breve{\rho}}^C(\mathbf{r}st, \mathbf{r}'s't') = 4tt' \hat{\breve{\rho}}(\mathbf{r}s-t, \mathbf{r}'s'-t'), \quad (5b)$$

where the asterisk stands for the complex conjugation.

Here and below we present full sets of expressions even in those cases when they could, in principle, be replaced by verbal descriptions. We do so in order to avoid possible confusion at the expense of a slight increase in the length of the paper. We think that such an approach is highly beneficial to the reader, because in many cases small but significant differences appear in expressions that otherwise could have seemed analogous to one another.

The charge-reversal operation C defined in Eq. (5) exchanges the neutron and proton charges, or equivalently, flips their isospin projections. Note that the time reversal is anti-linear while the charge reversal is a linear operation, and that they commute with one another. Symmetries of the density matrices can be conveniently expressed in terms of just the Hermitian conjugation, and time and charge reversals, namely, it follows from definitions (1a) and (2b) that

$$\hat{\rho}^+ = \hat{\rho}, \quad (6a)$$

$$\hat{\rho}^+ = -\hat{\rho}^{TC}, \quad (6b)$$

where the superscript TC denotes superposition of the time (4) and charge (5) reversals.

For $|\Psi\rangle$ being an independent-quasiparticle state the density matrices fulfill the following kinematical conditions:

$$\hat{\rho} \bullet \hat{\rho} = \hat{\rho} \bullet \hat{\rho}^{TC}, \quad (7a)$$

$$\hat{\rho} = \hat{\rho} \bullet \hat{\rho} + \hat{\rho} \bullet \hat{\rho}^+, \quad (7b)$$

where \bullet stands for integration over spatial coordinates and summation over spin and isospin indices, denoted by $\int dx$, e.g.,

$$\begin{aligned} (\hat{\rho} \bullet \hat{\rho})(\mathbf{r}_1s_1t_1, \mathbf{r}_2s_2t_2) &= (\hat{\rho} \bullet \hat{\rho})(x_1, x_2) = \int dx \hat{\rho}(x_1, x) \hat{\rho}(x, x_2) \\ &= \int d^3\mathbf{r} \sum_{st} \hat{\rho}(\mathbf{r}_1s_1t_1, \mathbf{r}st) \hat{\rho}(\mathbf{r}st, \mathbf{r}_2s_2t_2), \end{aligned} \quad (8)$$

where we also abbreviated the space-spin-isospin variables by $x \equiv \{\mathbf{r}st\}$. Equations (7) secure the projectivity of the generalized density matrix

$$\hat{\mathcal{R}} = \hat{\mathcal{W}} \hat{\mathcal{R}} \hat{\mathcal{W}}^+ = \begin{pmatrix} \hat{\rho} & \hat{\rho} \\ \hat{\rho}^+ & \hat{1} - \hat{\rho}^{TC} \end{pmatrix}, \quad (9)$$

where $\hat{1} := \delta(x-x') := \delta(\mathbf{r}-\mathbf{r}') \delta_{ss'} \delta_{tt'}$ and the unitary matrix $\hat{\mathcal{W}}$,

$$\hat{\mathcal{W}} = \begin{pmatrix} \hat{1} & 0 \\ 0 & -\hat{\sigma}_y \hat{\tau}_2 \end{pmatrix}, \quad (10)$$

transforms the standard generalized density matrix $\hat{\mathcal{R}}$ (cf. Ref. [167]) to the breve representation.

When the pairing correlations of only like nucleons are taken into account, none but the diagonal (off-diagonal) matrix elements of density matrix $\hat{\rho}(\hat{\rho})$ in isospin indices are considered. However, in a general case of pairing correlations between both, like and unlike nucleons, the remaining matrix elements become relevant as well. Therefore, in the following sections we specify the spin-isospin structure of the p - h and p - p density matrices explicitly.

A. Nonlocal densities

The density matrices in the spin and isospin spaces can be expressed as linear combinations of the unity and Pauli matrices. To write the corresponding formulas the following notation is assumed. Vectors and vector operators in the physical three-dimensional space are denoted with boldface symbols, e.g., \mathbf{r} or ∇ , and the second rank tensors with sans serif symbols, e.g., \mathbf{J} . Scalar products of three-dimensional space vectors are, as usual, denoted with the central dot, $\mathbf{r} \cdot \nabla$. The components of vectors and tensors are labeled with indices a, b, c and the names of axes are x, y , and z , e.g., $\mathbf{r} = (\mathbf{r}_x, \mathbf{r}_y, \mathbf{r}_z)$. In order to make a clear distinction, vectors in isospace are denoted with arrows and scalar products of them with the circle: $\vec{v} \circ \vec{w}$. The components of isovectors are labeled with indices i, k , and the names of isoaxes are 1, 2, and 3, e.g., $\vec{v} = (v_1, v_2, v_3)$. Finally, isoscalars are marked with

subscript “0,” and we often combine formulas for isoscalars and isovectors by letting the indices run through all the four values, e.g., $k=0, 1, 2, 3$.

With this convention the density matrices have the following form:

$$\begin{aligned} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') &= \frac{1}{4}\rho_0(\mathbf{r}, \mathbf{r}')\delta_{ss'}\delta_{tt'} + \frac{1}{4}\delta_{ss'}\tilde{\rho}(\mathbf{r}, \mathbf{r}') \circ \hat{\tau}_{tt'} \\ &+ \frac{1}{4}\mathbf{s}_0(\mathbf{r}, \mathbf{r}') \cdot \hat{\boldsymbol{\sigma}}_{ss'}\delta_{tt'} + \frac{1}{4}\tilde{\mathbf{s}}(\mathbf{r}, \mathbf{r}') \cdot \hat{\boldsymbol{\sigma}}_{ss'} \circ \hat{\tau}_{tt'}, \end{aligned} \quad (11a)$$

$$\begin{aligned} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') &= \frac{1}{4}\check{\rho}_0(\mathbf{r}, \mathbf{r}')\delta_{ss'}\delta_{tt'} + \frac{1}{4}\delta_{ss'}\check{\tilde{\rho}}(\mathbf{r}, \mathbf{r}') \circ \hat{\tau}_{tt'} \\ &+ \frac{1}{4}\check{\mathbf{s}}_0(\mathbf{r}, \mathbf{r}') \cdot \hat{\boldsymbol{\sigma}}_{ss'}\delta_{tt'} + \frac{1}{4}\check{\tilde{\mathbf{s}}}(\mathbf{r}, \mathbf{r}') \cdot \hat{\boldsymbol{\sigma}}_{ss'} \circ \hat{\tau}_{tt'}, \end{aligned} \quad (11b)$$

where $\hat{\tau}_{tt'} = (\hat{\tau}_{tt'}^1, \hat{\tau}_{tt'}^2, \hat{\tau}_{tt'}^3)$ and $\hat{\boldsymbol{\sigma}}_{ss'} = (\hat{\boldsymbol{\sigma}}_{ss'}^x, \hat{\boldsymbol{\sigma}}_{ss'}^y, \hat{\boldsymbol{\sigma}}_{ss'}^z)$ are the isospin and spin Pauli matrices, respectively, which are accompanied by the corresponding unity matrices, $\hat{\tau}_{tt'}^0 = \delta_{tt'}$ and $\hat{\boldsymbol{\sigma}}_{ss'}^u = \delta_{ss'}$. The density matrices defined in Eqs. (1a) and (2b) are now expressed by several functions of the pair of position vectors \mathbf{r} and \mathbf{r}' . To avoid confusion, the functions appearing on the right-hand sides of Eqs. (11) will be called the (non-local) density functions or, simply, densities, unlike the density matrices of Eqs. (1a) and (2b) appearing on the left-hand sides.

The densities are traces in spin and isospin indices of the following combinations of the density and the Pauli matrices.

(1) Scalar densities are the following.

(a) p - h isoscalar and isovector densities

$$\rho_0(\mathbf{r}, \mathbf{r}') = \sum_{st} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st), \quad (12a)$$

$$\tilde{\rho}(\mathbf{r}, \mathbf{r}') = \sum_{stt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st') \hat{\tau}_{t't}. \quad (12b)$$

(b) p - p isoscalar and isovector densities

$$\check{\rho}_0(\mathbf{r}, \mathbf{r}') = \sum_{st} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st), \quad (13a)$$

$$\check{\tilde{\rho}}(\mathbf{r}, \mathbf{r}') = \sum_{stt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'st') \hat{\tau}_{t't}. \quad (13b)$$

(2) Vector densities are the following.

(a) p - h spin isoscalar and isovector densities

$$\mathbf{s}_0(\mathbf{r}, \mathbf{r}') = \sum_{ss't} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't) \hat{\boldsymbol{\sigma}}_{s's}, \quad (14a)$$

$$\tilde{\mathbf{s}}(\mathbf{r}, \mathbf{r}') = \sum_{ss'tt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') \hat{\boldsymbol{\sigma}}_{s's} \hat{\tau}_{t't}. \quad (14b)$$

(b) p - p spin isoscalar and isovector densities

$$\check{\mathbf{s}}_0(\mathbf{r}, \mathbf{r}') = \sum_{ss't} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't) \hat{\boldsymbol{\sigma}}_{s's}, \quad (15a)$$

$$\check{\tilde{\mathbf{s}}}(\mathbf{r}, \mathbf{r}') = \sum_{ss'tt'} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') \hat{\boldsymbol{\sigma}}_{s's} \hat{\tau}_{t't}. \quad (15b)$$

Since the p - h density matrix and the Pauli matrices are both Hermitian, all the p - h densities are Hermitian too,

$$\rho_0(\mathbf{r}, \mathbf{r}') = \rho_0^*(\mathbf{r}', \mathbf{r}), \quad (16a)$$

$$\tilde{\rho}(\mathbf{r}, \mathbf{r}') = \tilde{\rho}^*(\mathbf{r}', \mathbf{r}), \quad (16b)$$

$$\mathbf{s}_0(\mathbf{r}, \mathbf{r}') = \mathbf{s}_0^*(\mathbf{r}', \mathbf{r}), \quad (16c)$$

$$\tilde{\mathbf{s}}(\mathbf{r}, \mathbf{r}') = \tilde{\mathbf{s}}^*(\mathbf{r}', \mathbf{r}), \quad (16d)$$

and hence, their real parts are symmetric, while the imaginary parts are antisymmetric, with respect to transposition of spatial arguments \mathbf{r} and \mathbf{r}' .

On the other hand, the unity matrices $\hat{\boldsymbol{\sigma}}_{ss'}^u = \delta_{ss'}$ and $\hat{\tau}_{tt'}^0 = \delta_{tt'}$ (scalar and isoscalar) are TC symmetric, while the vector and isovector Pauli matrices are TC antisymmetric, i.e.,

$$\hat{\boldsymbol{\sigma}}_{ss'} = -4ss' \hat{\boldsymbol{\sigma}}_{-s-s'}^*, \quad (17a)$$

$$\hat{\tau}_{tt'} = -4tt' \hat{\tau}_{-t-t'}^*. \quad (17b)$$

We should stress here again that operation TC is antilinear, and therefore, complex conjugation appears in all right-hand sides of Eqs. (17), although only the Pauli matrices σ_y and τ_2 are imaginary.

Since the p - p density matrix transforms under TC as in Eq. (6b), the p - p densities are either symmetric (scalar-isovector and vector-isoscalar) or antisymmetric (scalar-isoscalar and vector-isovector) under the transposition of their arguments, namely,

$$\check{\rho}_0(\mathbf{r}, \mathbf{r}') = -\check{\rho}_0(\mathbf{r}', \mathbf{r}), \quad (18a)$$

$$\check{\tilde{\rho}}(\mathbf{r}, \mathbf{r}') = \check{\tilde{\rho}}(\mathbf{r}', \mathbf{r}), \quad (18b)$$

$$\check{\mathbf{s}}_0(\mathbf{r}, \mathbf{r}') = \check{\mathbf{s}}_0(\mathbf{r}', \mathbf{r}), \quad (18c)$$

$$\check{\tilde{\mathbf{s}}}(\mathbf{r}, \mathbf{r}') = -\check{\tilde{\mathbf{s}}}(\mathbf{r}', \mathbf{r}). \quad (18d)$$

Equations (16) and (18) are fulfilled independently of any other symmetries conserved by the system; they result from general properties (6) of density matrices $\hat{\rho}$ and $\hat{\tilde{\rho}}$.

B. Local densities

In the HFB theory with the zero-range Skyrme interaction [168,169] or in the local density approximation (LDA) (cf. Refs. [167,170]), the energy functional depends only on local densities and on local densities built from derivatives up to the second order. These local densities are obtained by setting $\mathbf{r}' = \mathbf{r}$ in Eqs. (12)–(15) after the derivatives are performed. They will be denoted by having one spatial argu-

ment to distinguish them from the nonlocal densities that have two. Moreover, for local densities the spatial argument will often be omitted in order to lighten the notation.

Following the standard definitions [171,172], a number of local densities are introduced.

(1) Scalar densities are the following.

(a) Particle and pairing densities

$$\rho_k(\mathbf{r}) = \rho_k(\mathbf{r}, \mathbf{r}')_{\mathbf{r}=\mathbf{r}'}, \quad (19a)$$

$$\check{\rho}(\mathbf{r}) = \check{\rho}(\mathbf{r}, \mathbf{r}')_{\mathbf{r}=\mathbf{r}'}. \quad (19b)$$

(b) p - h and p - p kinetic densities

$$\tau_k(\mathbf{r}) = [(\nabla \cdot \nabla')\rho_k(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (20a)$$

$$\check{\tau}(\mathbf{r}) = [(\nabla \cdot \nabla')\check{\rho}(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}. \quad (20b)$$

(2) Vector densities are the following.

(a) p - h and p - p spin (pseudovector) densities

$$s_k(\mathbf{r}) = s_k(\mathbf{r}, \mathbf{r}')_{\mathbf{r}=\mathbf{r}'}, \quad (21a)$$

$$\check{s}_0(\mathbf{r}) = \check{s}_0(\mathbf{r}, \mathbf{r}')_{\mathbf{r}=\mathbf{r}'}. \quad (21b)$$

(b) p - h and p - p spin-kinetic (pseudovector) densities

$$\mathbf{T}_k(\mathbf{r}) = [(\nabla \cdot \nabla')s_k(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (22a)$$

$$\check{\mathbf{T}}_0(\mathbf{r}) = [(\nabla \cdot \nabla')\check{s}_0(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}. \quad (22b)$$

(c) p - h and p - p current (vector) densities

$$\mathbf{j}_k(\mathbf{r}) = \frac{1}{2i}[(\nabla - \nabla')\rho_k(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (23a)$$

$$\check{\mathbf{j}}_0(\mathbf{r}) = \frac{1}{2i}[(\nabla - \nabla')\check{\rho}_0(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}. \quad (23b)$$

(d) p - h and p - p tensor-kinetic (pseudovector) densities

$$\mathbf{F}_k(\mathbf{r}) = \frac{1}{2}[(\nabla \otimes \nabla' + \nabla' \otimes \nabla) \cdot s_k(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (24a)$$

$$\check{\mathbf{F}}_0(\mathbf{r}) = \frac{1}{2}[(\nabla \otimes \nabla' + \nabla' \otimes \nabla) \cdot \check{s}_0(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}. \quad (24b)$$

(3) Tensor densities are the following.

p - h and p - p spin-current (pseudotensor) densities

$$\mathbf{J}_k(\mathbf{r}) = \frac{1}{2i}[(\nabla - \nabla') \otimes s_k(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (25a)$$

$$\check{\mathbf{J}}(\mathbf{r}) = \frac{1}{2i}[(\nabla - \nabla') \otimes \check{s}(\mathbf{r}, \mathbf{r}')]_{\mathbf{r}=\mathbf{r}'}, \quad (25b)$$

where $k=0, 1, 2, 3$, and \otimes stands for the tensor product of vectors in the physical space, e.g., $(\mathbf{v} \otimes \mathbf{w})_{ab} \equiv v_a w_b$ and $[(\mathbf{v} \otimes \mathbf{w}) \cdot \mathbf{z}]_a \equiv v_a (\mathbf{w} \cdot \mathbf{z})$. Note that for particle, pairing, kinetic, spin, spin-kinetic, and tensor-kinetic densities only the sym-

metric nonlocal densities contribute, while for the current and spin-current densities only antisymmetric ones contribute. It is then clear that for each p - h density there exist both isoscalar and isovector component, while for the p - p densities, the isovector component exists only for the pairing, kinetic, and spin-current densities, while the isoscalar one exists only for spin, spin-kinetic, tensor-kinetic, and current densities.

We note here in passing that the complete list of all local densities (up to the derivatives of the second order) also includes the kinetic and spin-kinetic densities in which the two derivatives are coupled to a tensor, i.e., $\nabla \otimes \nabla'$. The resulting local densities are usually disregarded, because they do not have counterparts to form useful terms in the local energy density. There is one set of exceptions, which has been overlooked in the systematic construction presented in Ref. [173], and appears in the averaging of a zero-range tensor force [171], namely, the set of the tensor-kinetic local densities (24). In Sec. IV we define terms in the energy density that depend on the tensor-kinetic densities.

All tensor densities (25) can be decomposed into trace, antisymmetric, and symmetric parts, giving the standard pseudoscalar, vector, and pseudotensor components that we show here to fix the notation

$$J_k(\mathbf{r}) = \sum_{a=x,y,z} J_{kaa}(\mathbf{r}), \quad (26a)$$

$$\check{\mathbf{J}}(\mathbf{r}) = \sum_{a=x,y,z} \check{\mathbf{J}}_{aa}(\mathbf{r}), \quad (26b)$$

$$\mathbf{J}_{ka}(\mathbf{r}) = \sum_{b,c=x,y,z} \epsilon_{abc} J_{kbc}(\mathbf{r}), \quad (27a)$$

$$\check{\mathbf{J}}_a(\mathbf{r}) = \sum_{b,c=x,y,z} \epsilon_{abc} \check{\mathbf{J}}_{bc}(\mathbf{r}), \quad (27b)$$

$$\underline{\mathbf{J}}_{kab}(\mathbf{r}) = \frac{1}{2}J_{kab}(\mathbf{r}) + \frac{1}{2}J_{kba}(\mathbf{r}) - \frac{1}{3}J_k(\mathbf{r})\delta_{ab}, \quad (28a)$$

$$\check{\underline{\mathbf{J}}}_{ab}(\mathbf{r}) = \frac{1}{2}\check{\mathbf{J}}_{ab}(\mathbf{r}) + \frac{1}{2}\check{\mathbf{J}}_{ba}(\mathbf{r}) - \frac{1}{3}\check{\mathbf{J}}(\mathbf{r})\delta_{ab}, \quad (28b)$$

where $k=0, 1, 2, 3$.

It follows from Eqs. (16) and (18) that the p - h densities are all real whereas the p - p densities are in general complex and thus the complex-conjugate densities are relevant. The p - p densities become real or imaginary only when the time-reversal symmetry is conserved, see Sec. VII.

Instead of the isoscalar and the third component of isovector p - h density one can always use the neutron and the proton one, e.g.,

$$\rho_n(\mathbf{r}) = \frac{1}{2}[\rho_0(\mathbf{r}) + \rho_3(\mathbf{r})], \quad (29a)$$

$$\rho_p(\mathbf{r}) = \frac{1}{2}[\rho_0(\mathbf{r}) - \rho_3(\mathbf{r})], \quad (29b)$$

and just the same for all other p - h densities. Similarly, instead of the $k=1, 2$ isovector p - p densities one can use the neutron and proton pairing density, i.e.,

$$\check{\rho}_n(\mathbf{r}) = \frac{1}{2}[\check{\rho}_1(\mathbf{r}) + i\check{\rho}_2(\mathbf{r})], \quad (30a)$$

$$\check{\rho}_p(\mathbf{r}) = \frac{1}{2}[\check{\rho}_1(\mathbf{r}) - i\check{\rho}_2(\mathbf{r})], \quad (30b)$$

and just the same for all other p - p densities.

C. The TC symmetry

When constructing the energy-density functional (Sec. IV) from the local densities (19)–(25) one should ensure that it is invariant with respect to the following: 1° spatial rotations, 2° isospin rotations, 3° space inversion, and 4° time reversal. All the local densities of Sec. III B have definite transformation properties with respect to the first three of those, 1°–3°, so one can easily construct the corresponding invariants by multiplying densities of the same type by one another. For example, a product of any pseudovector-isoscalar density with itself, or with any other pseudovector-isoscalar density, is an invariant.

The time-reversal symmetry cannot be immediately treated on the same footing, because the time-reversal and the isospin rotations do not commute. However, as noted in Ref. [174], for problems involving the isospin symmetry it is more convenient to use the TC symmetry instead of the time reversal. Indeed, since the charge reversal C is equivalent to a rotation by the angle π about the isoaxis $k=2$, for conserved isospin the conservation of TC is equivalent to conservation of T alone. Therefore, in order to construct the energy density which is also time-reversal invariant, we should classify the local densities according to the TC symmetry and then multiply by one another only densities with the same TC transformation properties.

To this end, we split the p - h and p - p density matrices into parts that are symmetric and antisymmetric with respect to the TC reversal, i.e., explicitly,

$$\hat{\rho}_\pm(x, x') = \frac{1}{2}[\hat{\rho}(x, x') \pm 16ss'tt'\hat{\rho}^*(\bar{x}, \bar{x}')], \quad (31a)$$

$$\hat{\rho}_\pm(x, x') = \frac{1}{2}[\hat{\rho}(x, x') \pm 16ss'tt'\hat{\rho}^*(\bar{x}, \bar{x}')], \quad (31b)$$

where we used a short-hand notation of $\bar{x} \equiv \{\mathbf{r}, -s, -t\}$. In conjunction with the TC transformation properties of the Pauli matrices (17), one then immediately obtains that the corresponding nonlocal densities of Sec. III A are either real or imaginary, i.e.,

$$\rho_{0\pm}(\mathbf{r}, \mathbf{r}') = \pm \rho_{0\pm}^*(\mathbf{r}, \mathbf{r}'), \quad (32a)$$

$$\tilde{\rho}_\pm(\mathbf{r}, \mathbf{r}') = \mp \tilde{\rho}_\pm^*(\mathbf{r}, \mathbf{r}'), \quad (32b)$$

$$s_{0\pm}(\mathbf{r}, \mathbf{r}') = \mp s_{0\pm}^*(\mathbf{r}, \mathbf{r}'), \quad (32c)$$

$$\vec{s}_\pm(\mathbf{r}, \mathbf{r}') = \pm \vec{s}_\pm^*(\mathbf{r}, \mathbf{r}') \quad (32d)$$

and

$$\check{\rho}_{0\pm}(\mathbf{r}, \mathbf{r}') = \pm \check{\rho}_{0\pm}^*(\mathbf{r}, \mathbf{r}'), \quad (33a)$$

$$\check{\tilde{\rho}}_\pm(\mathbf{r}, \mathbf{r}') = \mp \check{\tilde{\rho}}_\pm^*(\mathbf{r}, \mathbf{r}'), \quad (33b)$$

$$\check{s}_{0\pm}(\mathbf{r}, \mathbf{r}') = \mp \check{s}_{0\pm}^*(\mathbf{r}, \mathbf{r}'), \quad (33c)$$

$$\check{\vec{s}}_\pm(\mathbf{r}, \mathbf{r}') = \pm \check{\vec{s}}_\pm^*(\mathbf{r}, \mathbf{r}'). \quad (33d)$$

This result shows that real and imaginary parts of nonlocal densities (12)–(15) have opposite TC transformation properties. From Eqs. (32) one then obtains classification of local p - h densities, namely, the isoscalar densities $\rho_0(\mathbf{r})$, $\tau_0(\mathbf{r})$, and $J_0(\mathbf{r})$ are TC symmetric and $s_0(\mathbf{r})$, $\mathbf{T}_0(\mathbf{r})$, $\mathbf{F}_0(\mathbf{r})$, and $\mathbf{j}_0(\mathbf{r})$ are TC antisymmetric, while the isovector densities $\vec{\rho}(\mathbf{r})$, $\vec{\tau}(\mathbf{r})$, and $\vec{J}(\mathbf{r})$ are TC antisymmetric and $\vec{s}(\mathbf{r})$, $\vec{T}(\mathbf{r})$, $\vec{F}(\mathbf{r})$, and $\vec{j}(\mathbf{r})$ are TC symmetric.

The rules of constructing the p - h energy density are thus identical to those valid in the case of no proton-neutron mixing [172]. On the other hand, from Eqs. (33) one obtains classification of local p - p densities, namely, real parts of all p - p densities are TC antisymmetric and imaginary parts are TC symmetric. The p - p energy density must therefore be built by multiplying real parts of different densities with one another, and separately imaginary parts also with one another. These rules are at the base of the energy-density functional constructed in Sec. IV.

IV. THE ENERGY-DENSITY FUNCTIONAL

In the HFB theory the expectation value of Hamiltonian in state $|\Psi\rangle$ is a functional of the density matrices, and reads

$$\begin{aligned} E_{\text{HFB}} &= \langle \Psi | H | \Psi \rangle = \bar{H}[\hat{\rho}, \hat{\rho}, \hat{\rho}^\pm] \\ &= \text{Tr}(\hat{T} \cdot \hat{\rho}) + \frac{1}{2} \text{Tr}(\hat{\Gamma} \cdot \hat{\rho} + \hat{\Gamma}^\dagger \cdot \hat{\rho}^\dagger), \end{aligned} \quad (34)$$

where Tr denotes integration over spatial coordinates and summation over spin and isospin indices. Nuclear many-body Hamiltonian H ,

$$\begin{aligned} H &= \int dx' dx \hat{T}(x', x) a_x^\dagger a_x \\ &+ \frac{1}{4} \int dx'_1 dx'_2 dx_1 dx_2 \hat{V}(x'_1 x'_2, x_1 x_2) a_{x'_1}^\dagger a_{x'_2}^\dagger a_{x_2} a_{x_1} \end{aligned} \quad (35)$$

is composed of one-body kinetic energy T and two-body interaction V , being expressed in Eq. (35) by matrix $\hat{T}(x', x)$ and the antisymmetrized matrix elements $\hat{V}(x'_1 x'_2, x_1 x_2)$, respectively. Matrices $\hat{\Gamma}$ and $\hat{\Gamma}^\dagger$ are the single-particle (p - h) and pairing (p - p) self-consistent potentials, respectively,

$$\hat{\Gamma}(x'_1, x_1) = \int dx'_2 dx_2 \hat{V}_{p-h}(x'_1 x'_2, x_1 x_2) \hat{\rho}(x_2, x'_2), \quad (36)$$

$$\hat{\Gamma}(x'_1, x'_2) = \int dx_1 dx_2 F_2 \hat{V}_{p-p}(x'_1 \bar{x}'_2, x_1 \bar{x}_2) \hat{\rho}(x_1, x_2), \quad (37)$$

where $F_2 = 8s'_2 t'_2 t_2$ and $\bar{x} \equiv \{\mathbf{r}, -s, -t\}$. In Eqs. (36) and (37) we have indicated that the p - h and p - p potentials can be determined by *different* two-body interactions, V_{p-h} and V_{p-p} , called effective interactions in the p - h and the p - p channel, respectively. This places further derivations in the framework of the energy-density formalism that is not based on a definite Hamiltonian (35). Moreover, effective interactions, V_{p-h} and V_{p-p} , are supposed to be, in general, density dependent.

In the case of the Skyrme effective interaction as well as in the framework of the LDA, the energy functional of Eq. (34) is a three-dimensional spatial integral,

$$\bar{H} = \int d^3r \mathcal{H}(\mathbf{r}), \quad (38)$$

of local energy density $\mathcal{H}(\mathbf{r})$ that is a real, scalar, time-even, and isoscalar function of local densities and their first and second derivatives. (Isospin-breaking terms, such as those resulting from different neutron and proton masses and from the Coulomb interaction, can be easily added and, for simplicity, are not considered in the present study.) In the case of no proton-neutron mixing, the construction of the most general energy density that is quadratic in one-body local densities was presented in detail in Ref. [173]. With the proton-neutron mixing included, the construction can be performed analogically by including the additional nonzero local densities derived in Sec. III. Then the energy density can be written in the following form:

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m} \tau_0(\mathbf{r}) + \sum_{t=0,1} [\chi_t(\mathbf{r}) + \check{\chi}_t(\mathbf{r})], \quad (39)$$

where we assumed that the neutron and proton masses are equal.

The p - h and p - p interaction energy densities, $\chi_t(\mathbf{r})$ and $\check{\chi}_t$, for $t=0$ depend quadratically on the isoscalar densities, and for $t=1$ on the isovector ones. Based on general rules of constructing the energy density, Sec. III C, one obtains

$$\begin{aligned} \chi_0(\mathbf{r}) = & C_0^p \rho_0^2 + C_0^{\Delta p} \rho_0 \Delta \rho_0 + C_0^{\tau} \rho_0 \tau_0 + C_0^{J_0} J_0^2 + C_0^{J_1} J_0^2 + C_0^{J_2} J_0^2 \\ & + C_0^{\nabla J} \rho_0 \nabla \cdot \mathbf{J}_0 + C_0^s s_0^2 + C_0^{\Delta s} s_0 \cdot \Delta s_0 + C_0^{\mathbf{T}} s_0 \cdot \mathbf{T}_0 \\ & + C_0^j J_0^2 + C_0^{\nabla j} s_0 \cdot (\nabla \times \mathbf{j}_0) + C_0^{\nabla s} (\nabla \cdot s_0)^2 + C_0^F s_0 \cdot \mathbf{F}_0, \end{aligned} \quad (40a)$$

$$\begin{aligned} \chi_1(\mathbf{r}) = & C_1^p \bar{\rho}^2 + C_1^{\Delta p} \bar{\rho} \circ \Delta \bar{\rho} + C_1^{\tau} \bar{\rho} \circ \bar{\tau} + C_1^{J_0} \bar{J}^2 + C_1^{J_1} \bar{J}^2 + C_1^{J_2} \bar{J}^2 \\ & + C_1^{\nabla J} \bar{\rho} \circ \nabla \cdot \bar{\mathbf{J}} + C_1^s \bar{s}^2 + C_1^{\Delta s} \bar{s} \circ \Delta \bar{s} + C_1^{\mathbf{T}} \bar{s} \circ \bar{\mathbf{T}} + C_1^j \bar{J}^2 \\ & + C_1^{\nabla j} \bar{s} \circ (\nabla \times \bar{\mathbf{j}}) + C_1^{\nabla s} (\nabla \cdot \bar{s})^2 + C_1^F \bar{s} \circ \bar{\mathbf{F}}, \end{aligned} \quad (40b)$$

where \times stands for the vector product, and

$$\begin{aligned} \check{\chi}_0(\mathbf{r}) = & \check{C}_0^s |\check{s}_0|^2 + \check{C}_0^{\Delta s} \text{Re}(\check{s}_0^* \circ \Delta \check{s}_0) + \check{C}_0^{\mathbf{T}} \text{Re}(\check{s}_0^* \circ \check{\mathbf{T}}_0) + \check{C}_0^j |\check{J}_0|^2 \\ & + \check{C}_0^{\nabla j} \text{Re}[\check{s}_0^* \cdot (\nabla \times \check{\mathbf{j}}_0)] + \check{C}_0^{\nabla s} |\nabla \cdot \check{s}_0|^2 \\ & + \check{C}_0^F \text{Re}(\check{s}_0^* \cdot \check{\mathbf{F}}_0), \end{aligned} \quad (41a)$$

$$\begin{aligned} \check{\chi}_1(\mathbf{r}) = & \check{C}_1^p |\check{\rho}|^2 + \check{C}_1^{\Delta p} \text{Re}(\check{\rho}^* \circ \Delta \check{\rho}) + \check{C}_1^{\tau} \text{Re}(\check{\rho}^* \circ \check{\tau}) + \check{C}_1^{J_0} |\check{J}|^2 \\ & + \check{C}_1^{J_1} |\check{J}|^2 + \check{C}_1^{J_2} |\check{J}|^2 + \check{C}_1^{\nabla J} \text{Re}(\check{\rho}^* \circ \nabla \cdot \check{\mathbf{J}}). \end{aligned} \quad (41b)$$

In Eqs. (40) and (41) squares always denote total lengths in space and/or isospace, for complex densities taken in the complex sense, e.g., $|\check{\mathbf{J}}(\mathbf{r})|^2 = \sum_{ak} \check{J}_{ak}^* \check{J}_{ak}$. In the p - p energy density (41) we show only terms in which the products of real parts are added to products of imaginary parts. According to the rules based on the TC symmetry, Sec. III C, similar terms with both products subtracted from one another are also allowed. We do not show them explicitly, because they have exactly the form of Eq. (41), but without complex conjugations and with absolute values replaced by real parts of products.

When the effective interaction is density dependent all coupling constants, C 's and \check{C} 's, may also depend on density. If this is the case, however, terms that can be transformed into one another by integration by parts are not anymore equivalent. Then, five more types of terms may appear in the energy density, see Ref. [173]; we do not consider such a possibility in the present study. Note that in the p - h channel all coupling constants appear in two flavors, for $t=0$ and 1, while in the p - p channel each one appears exclusively either for $t=0$ or for $t=1$.

The expression (39) is fairly general. In particular, *it is not based on any particular two-body interaction*. However, if one assumes that the underlying two-body potential is local and momentum independent, the form of Eq. (39) can be simplified and the number of coupling constants can be reduced. Two particular cases of practical interest are discussed in the following.

A. Local gauge invariance

Under a local gauge transformation [175], many-body wave function is multiplied by position-dependent phase factor

$$|\Psi'\rangle = \exp \left\{ i \sum_{j=1}^A \phi(\mathbf{r}_j) \right\} |\Psi\rangle, \quad (42)$$

which induces the following gauge transformations of density matrices (1a) and (2b):

$$\hat{\rho}'(\mathbf{r}st, \mathbf{r}'s't') = e^{i\phi(\mathbf{r}) - i\phi(\mathbf{r}')} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't'), \quad (43a)$$

$$\hat{\rho}'(\mathbf{r}st, \mathbf{r}'s't') = e^{i\phi(\mathbf{r}) + i\phi(\mathbf{r}')} \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't'). \quad (43b)$$

The Galilean transformation is a local gauge transformation for $\phi(\mathbf{r}) = \mathbf{p} \cdot \mathbf{r}$, where \mathbf{p} is a constant boost momentum. In analogy to that one can introduce the local momentum field defined by

$$\mathbf{p}(\mathbf{r}) = \nabla \phi(\mathbf{r}). \quad (44)$$

Local and momentum-independent interaction is invariant with respect to local gauge transformation, and hence energy densities (40) and (41) must then also be independent of the local gauge. The question whether it is possible to model nuclear effective interactions in the p - h and p - p channels by a local and momentum-independent interaction is open. Therefore, gauge transformation of the energy density can, in principle, be respected or not, depending on a choice of dynamics one makes.

It is easy to tell when the local energy densities (40) and (41) are local gauge invariant, because properties of local densities (19)–(25) under gauge transformation read explicitly

$$\rho'_k = \rho_k, \quad (45a)$$

$$\tau'_k = \tau_k + 2\mathbf{p} \cdot \mathbf{j}_k + \mathbf{p}^2 \rho_k, \quad (45b)$$

$$\mathbf{s}'_k = \mathbf{s}_k, \quad (45c)$$

$$\mathbf{T}'_k = \mathbf{T}_k + 2\mathbf{p} \cdot \mathbf{J}_k + \mathbf{p}^2 \mathbf{s}_k, \quad (45d)$$

$$\mathbf{j}'_k = \mathbf{j}_k + \mathbf{p} \rho_k, \quad (45e)$$

$$\mathbf{F}'_k = \mathbf{F}_k + \mathbf{p} \mathbf{J}_k + \mathbf{J}_k \cdot \mathbf{p} + \mathbf{p}(\mathbf{p} \cdot \mathbf{s}_k), \quad (45f)$$

$$\mathbf{J}'_k = \mathbf{J}_k + \mathbf{p} \otimes \mathbf{s}_k, \quad (45g)$$

where $k=0, 1, 2, 3$, and

$$\vec{\rho}' = e^{2i\phi} \vec{\rho}, \quad (46a)$$

$$\vec{\tau}' = e^{2i\phi} (\vec{\tau} + i\mathbf{p} \cdot \nabla \vec{\rho} - \mathbf{p}^2 \vec{\rho}), \quad (46b)$$

$$\check{s}'_0 = e^{2i\phi} \check{s}_0, \quad (46c)$$

$$\check{\mathbf{T}}'_0 = e^{2i\phi} [\check{\mathbf{T}}_0 + i(\mathbf{p} \cdot \nabla) \check{s}_0 - \mathbf{p}^2 \check{s}_0], \quad (46d)$$

$$\check{\mathbf{J}}'_0 = e^{2i\phi} \check{\mathbf{J}}_0, \quad (46e)$$

$$\check{\mathbf{F}}'_0 = e^{2i\phi} \left(\check{\mathbf{F}}_0 + \frac{i}{2} (\nabla \cdot \check{s}_0) \mathbf{p} + \frac{i}{2} (\nabla \otimes \check{s}_0) \cdot \mathbf{p} - (\mathbf{p} \cdot \check{s}_0) \mathbf{p} \right), \quad (46f)$$

$$\check{\mathbf{J}}'_0 = e^{2i\phi} \check{\mathbf{J}}_0. \quad (46g)$$

Since all local p - p densities (46) are multiplied under the gauge transformation by phase factors $e^{2i\phi(\mathbf{r})}$, products of local p - p densities are not gauge invariant. Therefore, all terms not shown explicitly in the p - p energy density [see discussion below Eq. (41)] violate the gauge invariance. On the other hand, products of complex-conjugate p - p densities and p - p densities may be gauge invariant. This obviously is the case for the pairing, spin, current, and spin-current p - p den-

sities, while only specific combinations of kinetic, spin-kinetic, and tensor-kinetic densities are gauge invariant.

Complete list of all p - h and p - p gauge-invariant combinations of local densities reads

$$G_k^\tau(\mathbf{r}) = \rho_k \tau_k - \mathbf{J}_k^2, \quad (47a)$$

$$G_k^T(\mathbf{r}) = \mathbf{s}_k \cdot \mathbf{T}_k - \mathbf{J}_k^2 = \mathbf{s}_k \cdot \mathbf{T}_k - \frac{1}{3} \mathbf{J}_k^2 - \frac{1}{2} \mathbf{J}_k^2 - \mathbf{J}_k^2, \quad (47b)$$

$$G_k^{\nabla J}(\mathbf{r}) = \rho_k \nabla \cdot \mathbf{J}_k + \mathbf{s}_k \cdot (\nabla \times \mathbf{j}_k), \quad (47c)$$

$$\begin{aligned} G_k^F(\mathbf{r}) &= \mathbf{s}_k \cdot \mathbf{F}_k - \frac{1}{2} \left(\sum_a \mathbf{J}_{kaa} \right)^2 - \frac{1}{2} \sum_{ab} \mathbf{J}_{kab} \mathbf{J}_{kba} \\ &= \mathbf{s}_k \cdot \mathbf{F}_k - \frac{2}{3} \mathbf{J}_k^2 + \frac{1}{4} \mathbf{J}_k^2 - \frac{1}{2} \mathbf{J}_k^2, \end{aligned} \quad (47d)$$

where $k=0, 1, 2, 3$, and

$$\check{G}_0^T(\mathbf{r}) = \text{Re}(\check{s}_0^* \cdot \check{\mathbf{T}}_0) - \frac{1}{4} \text{Re}(\check{s}_0^* \cdot \Delta \check{s}_0), \quad (48a)$$

$$\check{G}_F^0(\mathbf{r}) = \text{Re}(\check{s}_0^* \cdot \check{\mathbf{F}}_0) + \frac{1}{4} |\nabla \cdot \check{s}_0|^2, \quad (48b)$$

$$\check{G}_k^\tau(\mathbf{r}) = \text{Re}(\check{\rho}_k^* \check{\tau}_k) - \frac{1}{4} \text{Re}(\check{\rho}_k^* \Delta \check{\rho}_k), \quad (48c)$$

where $k=1, 2, 3$. Note that terms of the p - p energy density that depend on $\nabla \times \check{\mathbf{J}}_0$ and $\nabla \cdot \check{\mathbf{J}}_0$ are not gauge invariant.

Finally, energy density given by Eqs. (40) and (41) is gauge invariant provided the coupling constants fulfill the following constraints:

$$C_t^j = -C_t^\tau, \quad (49a)$$

$$C_t^{J0} = -\frac{1}{3} C_t^T - \frac{2}{3} C_t^F, \quad (49b)$$

$$C_t^{J1} = -\frac{1}{2} C_t^T + \frac{1}{4} C_t^F, \quad (49c)$$

$$C_t^{J2} = -C_t^T - \frac{1}{2} C_t^F, \quad (49d)$$

$$C_t^{\nabla j} = +C_t^{\nabla J}, \quad (49e)$$

for $t=0, 1$, and

$$\check{C}_0^{\Delta s} = -\frac{1}{4} \check{C}_0^T, \quad (50a)$$

$$\check{C}_0^{\nabla s} = +\frac{1}{4} \check{C}_0^F, \quad (50b)$$

$$\check{C}_0^{\nabla j} = 0, \quad (50c)$$

$$\check{C}_1^{\Delta\rho} = -\frac{1}{4}\check{C}_1^{\tau}, \quad (50d)$$

$$\check{C}_1^{\nabla J} = 0. \quad (50e)$$

B. Skyrme interaction energy functional

The Skyrme interaction [168,169] is a zero-range local force that depends on relative momenta up to the second order. The complete list of terms giving its matrix element in the position-spin-isospin representation, including the tensor components [171,176], reads

$$\begin{aligned} & \hat{V}(\mathbf{r}'_1 s'_1 t'_1 \mathbf{r}'_2 s'_2 t'_2, \mathbf{r}_1 s_1 t_1 \mathbf{r}_2 s_2 t_2) \\ &= \left\{ t_0 (\hat{\delta}^\sigma + x_0 \hat{P}^\sigma) + \frac{1}{6} t_3 (\hat{\delta}^\sigma + x_3 \hat{P}^\sigma) \rho_0^\alpha \left[\frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2) \right] \right. \\ &+ \frac{1}{2} t_1 (\hat{\delta}^\sigma + x_1 \hat{P}^\sigma) [\hat{\mathbf{k}}'^2 + \hat{\mathbf{k}}^2] \\ &+ \frac{1}{2} t_e [\hat{\mathbf{k}}'^* \cdot \hat{\mathbf{S}} \cdot \hat{\mathbf{k}}'^* + \hat{\mathbf{k}} \cdot \hat{\mathbf{S}} \cdot \hat{\mathbf{k}}] \\ &+ t_2 (\hat{\delta}^\sigma + x_2 \hat{P}^\sigma) \hat{\mathbf{k}}'^* \cdot \hat{\mathbf{k}} + t_0 \hat{\mathbf{k}}'^* \cdot \hat{\mathbf{S}} \cdot \hat{\mathbf{k}} \\ &\left. + i W_0 \hat{\mathbf{S}} \cdot [\hat{\mathbf{k}}'^* \times \hat{\mathbf{k}}] \right\} (\hat{\delta}^\sigma \hat{\delta}^\tau - \hat{P}^\sigma \hat{P}^\tau P^M) \hat{\delta}_{12}, \quad (51) \end{aligned}$$

where

$$\hat{\delta}_{s'_1 s'_2 s_1 s_2}^\sigma = \delta_{s'_1 s_1} \delta_{s'_2 s_2}, \quad (52a)$$

$$\hat{\delta}_{t'_1 t'_2 t_1 t_2}^\tau = \delta_{t'_1 t_1} \delta_{t'_2 t_2} \quad (52b)$$

and

$$\hat{P}_{s'_1 s'_2 s_1 s_2}^\sigma = \frac{1}{2} (\hat{\delta}_{s'_1 s'_2 s_1 s_2}^\sigma + \hat{\boldsymbol{\sigma}}_{s'_1 s_1} \cdot \hat{\boldsymbol{\sigma}}_{s'_2 s_2}) = \delta_{s'_1 s_2} \delta_{s'_2 s_1}, \quad (53a)$$

$$\hat{P}_{t'_1 t'_2 t_1 t_2}^\tau = \frac{1}{2} (\hat{\delta}_{t'_1 t'_2 t_1 t_2}^\tau + \hat{\boldsymbol{\tau}}_{t'_1 t_1} \circ \hat{\boldsymbol{\tau}}_{t'_2 t_2}) = \delta_{t'_1 t_2} \delta_{t'_2 t_1} \quad (53b)$$

are the spin and isospin unity and exchange operators, respectively, and

$$\hat{\mathbf{S}}_{s'_1 s'_2 s_1 s_2} = \hat{\boldsymbol{\sigma}}_{s'_1 s_1} \delta_{s'_2 s_2} + \hat{\boldsymbol{\sigma}}_{s'_2 s_2} \delta_{s'_1 s_1}, \quad (54a)$$

$$\hat{\mathbf{S}}_{s'_1 s'_2 s_1 s_2}^{ab} = \frac{3}{2} (\hat{\boldsymbol{\sigma}}_{s'_1 s_1}^a \hat{\boldsymbol{\sigma}}_{s'_2 s_2}^b + \hat{\boldsymbol{\sigma}}_{s'_1 s_1}^b \hat{\boldsymbol{\sigma}}_{s'_2 s_2}^a) - \delta_{ab} \hat{\boldsymbol{\sigma}}_{s'_1 s_1} \cdot \hat{\boldsymbol{\sigma}}_{s'_2 s_2} \quad (54b)$$

are two-body vector and tensor spin operators, respectively. The relative momentum operators

$$\hat{\mathbf{k}} = \frac{1}{2i} (\nabla_1 - \nabla_2), \quad (55a)$$

$$\hat{\mathbf{k}}' = \frac{1}{2i} (\nabla'_1 - \nabla'_2), \quad (55b)$$

act on the δ functions in $\hat{\delta}_{12}$,

$$\begin{aligned} \hat{\delta}_{12}(\mathbf{r}'_1 \mathbf{r}'_2, \mathbf{r}_1 \mathbf{r}_2) &= \delta(\mathbf{r}'_1 - \mathbf{r}_1) \delta(\mathbf{r}'_2 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ &= \delta(\mathbf{r}'_1 - \mathbf{r}_2) \delta(\mathbf{r}'_2 - \mathbf{r}_1) \delta(\mathbf{r}_2 - \mathbf{r}_1). \quad (56) \end{aligned}$$

This action has to be understood in the standard sense of derivatives of distributions.

Whenever the Skyrme interaction (51) is inserted into integrals, such as in Eqs. (35)–(37), the integration by parts transfers the derivatives onto appropriate variables in the remaining parts of integrands.

Numbers P^M are equal to +1 or –1 depending on whether in a given term the power of momentum $\hat{\mathbf{k}}$ is even or odd, respectively. Skyrme interaction written in the form of the integral kernel (51) is explicitly antisymmetric with respect to exchanging left or right pairs of variables pertaining to particles 1 and 2.

The Skyrme HFB energy density can be calculated by inserting the Skyrme interaction (51) directly into expressions (36), (37), and (34). Results for the p - h channel were published by many authors, see, e.g., Refs. [169,172,175,177], although often some terms of interaction (51) were neglected and/or restricted symmetries were used. Results for the p - p channel were previously published with tensor terms and the proton-neutron mixing neglected [5]. Here we aim at presenting the complete set of results.

Calculations leading to expressions for the Skyrme energy density are tedious, but can be efficiently performed by noting two simplifying facts. First, the two-body spin operators obey conditions

$$\hat{S} \hat{P}^\sigma = \hat{S}, \quad (57)$$

$$\hat{S} \hat{P}^\sigma = \hat{S}, \quad (58)$$

and hence only terms up to linear in spin and isospin Pauli matrices appear in the antisymmetrized interaction. Second, the Pauli matrices in Eq. (51) pertain to the p - h coupling channel, while the momenta to the p - p coupling channel. Hence, calculations may become very easy once a common, p - h or p - p , coupling channel is used for all the elements of interaction. This requires either recoupling momenta to the p - h channel or recoupling the Pauli matrices to the p - p channel. To this end, we separately consider the p - h and p - p energy densities.

1. The p - h channel

In the p - h energy density, indices of the Pauli matrices are contracted directly with density matrices of particles 1 and 2, and immediately give nonlocal densities through appropriate traces in Eqs. (12)–(15). However, the relative momentum

operators (55) affect both particles at the same time, and hence have to be first recoupled to forms where the two particles are acted upon independently, i.e.,

$$\frac{1}{2}(\hat{\mathbf{k}}'^2 + \hat{\mathbf{k}}^2) = \frac{1}{8}(\hat{\mathbf{K}}_1^2 + \hat{\mathbf{K}}_2^2 - \hat{\mathbf{K}}_1 \cdot \hat{\mathbf{K}}_2 - 4\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2) + \frac{1}{4}(\nabla_1 \cdot \nabla'_1 + \nabla_2 \cdot \nabla'_2), \quad (59a)$$

$$\hat{\mathbf{k}}'^* \cdot \hat{\mathbf{k}} = \frac{1}{8}(\hat{\mathbf{K}}_1 \cdot \hat{\mathbf{K}}_2 - 4\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2) + \frac{1}{4}(\nabla_1 \cdot \nabla'_1 + \nabla_2 \cdot \nabla'_2), \quad (59b)$$

$$\hat{\mathbf{k}}'^* \times \hat{\mathbf{k}} = \frac{1}{4}(\hat{\mathbf{K}}_1 - \hat{\mathbf{K}}_2) \times (\hat{\mathbf{k}}_2 - \hat{\mathbf{k}}_1), \quad (59c)$$

$$\begin{aligned} \hat{\mathbf{k}}'^* \otimes \hat{\mathbf{k}}'^* + \hat{\mathbf{k}} \otimes \hat{\mathbf{k}} &= \frac{1}{4}(\hat{\mathbf{K}}_1 \otimes \hat{\mathbf{K}}_1 + \hat{\mathbf{K}}_2 \otimes \hat{\mathbf{K}}_2) - \frac{1}{8}(\hat{\mathbf{K}}_1 \otimes \hat{\mathbf{K}}_2 + \hat{\mathbf{K}}_2 \otimes \hat{\mathbf{K}}_1) \\ &\quad - \frac{1}{2}(\hat{\mathbf{k}}_1 \otimes \hat{\mathbf{k}}_2 + \hat{\mathbf{k}}_2 \otimes \hat{\mathbf{k}}_1) \\ &\quad + \frac{1}{4}(\nabla_1 \otimes \nabla'_1 + \nabla_2 \otimes \nabla'_2) + \frac{1}{4}(\nabla'_1 \otimes \nabla_1 \\ &\quad + \nabla'_2 \otimes \nabla_2), \end{aligned} \quad (59d)$$

$$\begin{aligned} \hat{\mathbf{k}}'^* \otimes \hat{\mathbf{k}} + \hat{\mathbf{k}} \otimes \hat{\mathbf{k}}'^* &= \frac{1}{8}(\hat{\mathbf{K}}_1 \otimes \hat{\mathbf{K}}_2 + \hat{\mathbf{K}}_2 \otimes \hat{\mathbf{K}}_1) - \frac{1}{2}(\hat{\mathbf{k}}_1 \otimes \hat{\mathbf{k}}_2 + \hat{\mathbf{k}}_2 \otimes \hat{\mathbf{k}}_1) \\ &\quad + \frac{1}{4}(\nabla_1 \otimes \nabla'_1 + \nabla_2 \otimes \nabla'_2) \\ &\quad + \frac{1}{4}(\nabla'_1 \otimes \nabla_1 + \nabla'_2 \otimes \nabla_2), \end{aligned} \quad (59e)$$

where

$$\hat{\mathbf{k}}_1 = \frac{1}{2i}(\nabla_1 - \nabla'_1), \quad (60a)$$

$$\hat{\mathbf{k}}_2 = \frac{1}{2i}(\nabla_2 - \nabla'_2) \quad (60b)$$

and

$$\hat{\mathbf{K}}_1 = -i(\nabla_1 + \nabla'_1), \quad (61a)$$

$$\hat{\mathbf{K}}_2 = -i(\nabla_2 + \nabla'_2). \quad (61b)$$

Final results can now be easily obtained by noting that relative momenta (60) lead to the current densities (23a) and (25a), total momenta (61) lead to derivatives of local densities, and the scalar and tensor products of individual momenta lead to kinetic densities (20a), (22a), and (24a).

The zero-order (density-dependent) p - h coupling constants of the energy density (40) are expressed by the Skyrme force parameters as

TABLE I. Second-order coupling constants of the p - h energy density (40) as functions of parameters of the Skyrme interaction (51), expressed by the formula $C=(A/192)(at_1+bt_1x_1+ct_2+dt_2x_2+et_e+ft_o+gW_0)$.

	A	a	b	c	d	e	f	g
$C_0^{\Delta\rho}$	3	-9	0	5	4	0	0	0
C_0^τ	12	3	0	5	4	0	0	0
$C_0^{J_0}$	-4	-1	2	1	2	10	30	0
$C_0^{J_1}$	-6	-1	2	1	2	-5	-15	0
$C_0^{J_2}$	-12	-1	2	1	2	1	3	0
$C_0^{\nabla J}$	48	0	0	0	0	0	0	-3
$C_0^{\Delta s}$	3	3	-6	1	2	6	-6	0
C_0^τ	12	-1	2	1	2	-2	-6	0
C_0^j	-12	3	0	5	4	0	0	0
$C_0^{\nabla s}$	18	0	0	0	0	3	-3	0
C_0^F	72	0	0	0	0	1	3	0
$C_0^{\nabla j}$	48	0	0	0	0	0	0	-3
$C_1^{\Delta\rho}$	3	3	6	1	2	0	0	0
C_1^τ	12	-1	-2	1	2	0	0	0
$C_1^{J_0}$	-4	-1	0	1	0	-10	10	0
$C_1^{J_1}$	-6	-1	0	1	0	5	-5	0
$C_1^{J_2}$	-12	-1	0	1	0	-1	1	0
$C_1^{\nabla J}$	48	0	0	0	0	0	0	-1
$C_1^{\Delta s}$	3	3	0	1	0	-6	-2	0
C_1^τ	12	-1	0	1	0	2	-2	0
C_1^j	-12	-1	-2	1	2	0	0	0
$C_1^{\nabla s}$	18	0	0	0	0	-3	-1	0
C_1^F	72	0	0	0	0	-1	1	0
$C_1^{\nabla j}$	48	0	0	0	0	0	0	-1

$$C_0^\rho = \frac{3}{8}t_0 + \frac{3}{48}t_3\rho_0^\alpha(\mathbf{r}), \quad (62a)$$

$$C_0^s = \frac{1}{8}t_0(2x_0 - 1) + \frac{1}{48}t_3(2x_3 - 1)\rho_0^\alpha(\mathbf{r}), \quad (62b)$$

$$C_1^\rho = -\frac{1}{8}t_0(2x_0 + 1) - \frac{1}{48}t_3(2x_3 + 1)\rho_0^\alpha(\mathbf{r}), \quad (62c)$$

$$C_1^s = -\frac{1}{8}t_0 - \frac{1}{48}t_3\rho_0^\alpha(\mathbf{r}), \quad (62d)$$

and the second-order coupling constants are given in Table I. One can immediately see that the gauge-invariance conditions (49) are fulfilled. This is so because the momentum-dependent terms of the Skyrme interaction obey the Galilean invariance [172,175]

Since seven Skyrme force parameters define 24 second-order p - h coupling constants, in the resulting Skyrme energy density there is a high degree of dependency. First, as is well

known [178], a single spin-orbit parameter W_0 determines all four spin-orbit coupling constants $C_t^{\nabla J}$ and $C_t^{\nabla j}$, for $t=0$ and 1. Second, four Skyrme parameters, t_1 , x_1 , t_2 , and x_2 , uniquely determine four coupling constants $C_t^{\Delta\rho}$ and C_t^{τ} , for $t=0$ and 1. Third, two tensor Skyrme parameters, t_e and t_o , uniquely determine either isoscalar or isovector coupling constants, $C_t^{\nabla s}$ and C_t^F . Once such a role of the seven Skyrme parameters is fixed, values of the remaining coupling constants are also uniquely fixed.

2. The p - p channel

In the p - p energy density, each operator of the relative momentum, $\hat{\mathbf{k}}'$ and $\hat{\mathbf{k}}$, acts on variables of the same density matrix, and thus no recoupling is necessary. Terms of the interaction that are linear in momenta then lead to current densities (23b) and (25b), while terms that are quadratic in momenta lead to derivatives of local densities and to kinetic densities (20b), (22b), and (24b), because

$$\hat{\mathbf{k}}^2 = -\frac{1}{4}(\nabla_1 + \nabla_2)^2 + \nabla_1 \cdot \nabla_2, \quad (63a)$$

$$\hat{\mathbf{k}} \otimes \hat{\mathbf{k}} = -\frac{1}{4}(\nabla_1 + \nabla_2) \otimes (\nabla_1 + \nabla_2) + \frac{1}{2}(\nabla_1 \otimes \nabla_2 + \nabla_2 \otimes \nabla_1). \quad (63b)$$

However, in the p - p energy density, indices of Pauli matrices couple together the two density matrices, and hence do require recoupling to the p - p channel. These recoupling formulas can be obtained by means of the standard algebra of angular momentum. A sum of the three Clebsch-Gordan coefficients appropriate to the present case reads [179]

$$\begin{aligned} & 4s_2' s_2 \sum_{\mu_1 \mu_2} \langle \frac{1}{2} s_1 \lambda_1 \mu_1 | \frac{1}{2} s_1' | \frac{1}{2} - s_2 \lambda_2 \mu_2 | \frac{1}{2} - s_2' \rangle \\ & \quad \times \langle \lambda_1 - \mu_1 \lambda_2 - \mu_2 | \lambda \mu \rangle \\ & = \sum_{l' m', lm} (-1)^{\lambda_1 - \lambda_2 + l'} (2l' + 1) \\ & \quad \times (2l + 1) \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \lambda_1 \\ \frac{1}{2} & \frac{1}{2} & \lambda_2 \\ l' & l & \lambda \end{Bmatrix} \times \langle \frac{1}{2} s_2' l' m' | \frac{1}{2} s_1' \rangle \langle \frac{1}{2} s_1 l m | \frac{1}{2} s_2 \rangle \\ & \quad \times \langle l' - m' l - m | \lambda \mu \rangle. \end{aligned} \quad (64)$$

Taking relevant combinations of $\lambda_1, \lambda_2=0, 1$ and $\lambda=0, 1, 2$, one obtains

$$4s_2' s_2 \hat{\delta}_{s_1', -s_2', -s_1, -s_2}^{\sigma} = \frac{1}{2} \delta_{s_2' s_1'}^{\sigma} \delta_{s_2 s_1} + \frac{1}{2} \boldsymbol{\sigma}_{s_2' s_1'}^* \cdot \boldsymbol{\sigma}_{s_2 s_1}, \quad (65a)$$

$$4s_2' s_2 \hat{P}_{s_1', -s_2', -s_1, -s_2}^{\sigma} = -\frac{1}{2} \delta_{s_2' s_1'}^{\sigma} \delta_{s_2 s_1} + \frac{1}{2} \boldsymbol{\sigma}_{s_2' s_1'}^* \cdot \boldsymbol{\sigma}_{s_2 s_1}, \quad (65b)$$

$$4s_2' s_2 \hat{S}_{s_1', -s_2', -s_1, -s_2} = -i \boldsymbol{\sigma}_{s_2' s_1'}^* \times \boldsymbol{\sigma}_{s_2 s_1}, \quad (65c)$$

TABLE II. Second-order coupling constants of the p - p energy density (41) as functions of parameters of the Skyrme interaction (51), expressed by the formula $\check{C} = (A/96)(at_1 + bt_1 x_1 + ct_2 + dt_2 x_2 + et_e + ft_o + gW_0)$.

	A	a	b	c	d	e	f	g
$\check{C}_0^{\Delta s}$	-3	1	1	0	0	2	0	0
\check{C}_0^{τ}	12	1	1	0	0	2	0	0
\check{C}_0^j	12	0	0	1	-1	0	0	0
$\check{C}_0^{\nabla s}$	-18	0	0	0	0	1	0	0
\check{C}_0^F	-72	0	0	0	0	1	0	0
$\check{C}_0^{\nabla j}$	0	0	0	0	0	0	0	0
$\check{C}_1^{\Delta\rho}$	-3	1	-1	0	0	0	0	0
\check{C}_1^{τ}	12	1	-1	0	0	0	0	0
\check{C}_1^{j0}	4	0	0	1	1	0	-10	4
\check{C}_1^{j1}	6	0	0	1	1	0	5	2
\check{C}_1^{j2}	12	0	0	1	1	0	-1	-2
$\check{C}_1^{\nabla j}$	0	0	0	0	0	0	0	0

$$\begin{aligned} 4s_2' s_2 \hat{S}_{s_1', -s_2', -s_1, -s_2}^{ab} &= -\frac{3}{2} (\boldsymbol{\sigma}_{s_2' s_1'}^{a*} \boldsymbol{\sigma}_{s_2 s_1}^b + \boldsymbol{\sigma}_{s_2' s_1'}^{b*} \boldsymbol{\sigma}_{s_2 s_1}^a) \\ & \quad + \delta_{ab} \boldsymbol{\sigma}_{s_2' s_1'}^* \cdot \boldsymbol{\sigma}_{s_2 s_1}, \end{aligned} \quad (65d)$$

and the formulas similar to Eqs. (65a) and (65b) are obtained for $\hat{\delta}^{\sigma}$ and \hat{P}^{τ} , respectively.

The two zero-order (density-dependent) p - p coupling constants of the energy density (41) are related to the Skyrme parameters in the following way:

$$\check{C}_0^s = \frac{1}{8} t_0 (1 + x_0) + \frac{1}{48} t_3 (1 + x_3) \rho_0^\alpha(\mathbf{r}), \quad (66a)$$

$$\check{C}_1^p = \frac{1}{8} t_0 (1 - x_0) + \frac{1}{48} t_3 (1 - x_3) \rho_0^\alpha(\mathbf{r}), \quad (66b)$$

and the second-order p - p coupling constants are given in Table II. Similar to the p - h case, the gauge-invariance conditions (50) are met.

Equivalently, the density-dependent zero-range pairing force V_{pair} can be used in the p - p channel [180–183],

$$V_{\text{pair}}(\mathbf{r}, \mathbf{r}') = f_{\text{pair}}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'), \quad (67)$$

for

$$f_{\text{pair}}(\mathbf{r}) = V_0 \left\{ 1 + x_0 \hat{P}^{\sigma} - \left[\frac{\rho_0(\mathbf{r})}{\rho_c} \right]^\alpha (1 + x_3 \hat{P}^{\sigma}) \right\}, \quad (68)$$

where \hat{P}^{σ} is the spin-exchange operator (53a). In such a case, coupling constants (66) read

$$\check{C}_0^s = \frac{1}{8} V_0 (1 + x_0) - \frac{1}{8} V_0 (1 + x_3) \left[\frac{\rho_0(\mathbf{r})}{\rho_c} \right]^\alpha, \quad (69a)$$

$$\check{C}_1^p = \frac{1}{8}V_0(1-x_0) - \frac{1}{8}V_0(1-x_3) \left[\frac{\rho_0(\mathbf{r})}{\rho_c} \right]^\alpha. \quad (69b)$$

Note that when only the isovector pairing is used, as in most LDA applications to date, the exchange parameters x_0 and x_3 are redundant in the definition of the isovector coupling constant \check{C}_1^p , and hence are usually set to 0. However, if one wants to independently model the isoscalar and isovector pairing intensity, one has to use nonzero values of x_0 and x_3 .

For the Gogny interaction [167], the zero-range density-dependent term t_3 with $\alpha=1/3$ was used in order to enforce proper saturation properties. The corresponding exchange parameter $x_3=1$ was used to prevent this zero-range force from contributing to the isovector pairing channel. However, such a choice, when applied literally to the proton-neutron mixing case, might lead to a very strong repulsive isoscalar pairing interaction.

The term of $\check{\chi}$ coming from the spin-orbit interaction contains the combination of components of the p - p spin-current density $\check{\mathbf{J}}$,

$$\sum_{ab} (\check{\mathbf{J}}_{aa}^* \circ \check{\mathbf{J}}_{bb} - \check{\mathbf{J}}_{ab}^* \circ \check{\mathbf{J}}_{ba}) = \frac{2}{3}|\check{\mathbf{J}}|^2 + \frac{1}{2}|\check{\mathbf{J}}|^2 - |\check{\mathbf{J}}|^2, \quad (70)$$

that is different from that coming from the tensor t_0 term,

$$\begin{aligned} \sum_{ab} \left(\check{\mathbf{J}}_{ab}^* \circ \check{\mathbf{J}}_{ab} - \frac{3}{2}\check{\mathbf{J}}_{aa}^* \circ \check{\mathbf{J}}_{bb} - \frac{3}{2}\check{\mathbf{J}}_{ab}^* \circ \check{\mathbf{J}}_{ba} \right) \\ = -\frac{5}{3}|\check{\mathbf{J}}|^2 + \frac{5}{4}|\check{\mathbf{J}}|^2 - \frac{1}{2}|\check{\mathbf{J}}|^2, \end{aligned} \quad (71)$$

and from that coming from the central t_2 term,

$$|\check{\mathbf{J}}|^2 = \sum_{ab} (\check{\mathbf{J}}_{ab}^* \circ \check{\mathbf{J}}_{ab}) = \frac{1}{3}|\check{\mathbf{J}}|^2 + \frac{1}{2}|\check{\mathbf{J}}|^2 + |\check{\mathbf{J}}|^2. \quad (72)$$

Therefore, by setting appropriate values of the $t_2(1+x_2)$, W_0 , and t_0 parameters, one can obtain arbitrary values of the spin-current coupling constants \check{C}_1^{j0} , \check{C}_1^{j1} , and \check{C}_1^{j2} . Similarly, parameter $t_2(1-x_2)$ allows for fixing an arbitrary value of the current coupling constant \check{C}_0^j . On the other hand, parameter $t_1(1+x_1)$ defines two isoscalar coupling constants, $\check{C}_0^{\Delta s}$ and \check{C}_0^T , parameter t_e defines another two isoscalar coupling constants, $\check{C}_0^{\nabla s}$ and \check{C}_0^F , and parameter $t_1(1-x_1)$ defines two isovector coupling constants, $\check{C}_1^{\Delta\rho}$ and \check{C}_1^{τ} ; hence, these pairs of coupling constants are not independent from one another. These three pairs of dependencies reflect, in fact, the three gauge invariance conditions (48). In this way, seven Skyrme force parameters determine ten coupling constants in the p - p channel. Finally, the Skyrme interaction does not give any nonzero values for the spin-orbit coupling constants $\check{C}_0^{\nabla j}$ and \check{C}_1^{jI} . Therefore, up to the gauge invariance conditions, the Skyrme interaction fully determines the energy density in the p - p channel.

V. THE P - H AND P - P MEAN FIELDS

By varying the energy functional (34) with respect to the density matrices one obtains the p - h and p - p mean-field Hamiltonians,

$$\begin{aligned} \hat{h}(\mathbf{r}'s't', \mathbf{r}st) &= \frac{\overline{\delta H[\hat{\rho}, \hat{\rho}, \hat{\rho}^+]}}{\delta \hat{\rho}(\mathbf{r}st, \mathbf{r}'s't')} \\ &= -\frac{\hbar^2}{2m} \delta(\mathbf{r}-\mathbf{r}') \nabla \cdot \nabla \delta_{s't} \delta_{t't} + \hat{\Gamma}(\mathbf{r}'s't', \mathbf{r}st) \\ &\quad + \hat{\Gamma}_r(\mathbf{r}'s't', \mathbf{r}st), \end{aligned} \quad (73a)$$

$$\begin{aligned} \hat{h}(\mathbf{r}'s't', \mathbf{r}st) &= \frac{\overline{\delta H[\hat{\rho}, \hat{\rho}, \hat{\rho}^+]}}{\delta \hat{\rho}^+(\mathbf{r}st, \mathbf{r}'s't')} \\ &= \hat{\Gamma}(\mathbf{r}'s't', \mathbf{r}st) + \hat{\Gamma}_r(\mathbf{r}'s't', \mathbf{r}st). \end{aligned} \quad (73b)$$

The rearrangement potentials $\hat{\Gamma}_r$ and $\hat{\Gamma}_r$ result from the density dependence of effective interactions on the p - h and p - p densities, respectively. Usually effective interactions are assumed to depend only on the p - h density matrix (most often, only on the isoscalar particle density ρ_0). In that case the p - p rearrangement potential vanishes. However, one cannot forget that the dependence of the p - p interaction on the particle density results in a corresponding contribution to the p - h rearrangement potential. In what follows, to simplify the presentation we do not show the rearrangement terms explicitly.

Within the LDA, the mean-field Hamiltonians being originally, such as the Skyrme interaction of Eq. (51), either distributions or derivatives of distributions can, when acting as the integral kernels, be expressed as local, momentum-dependent operators, i.e.,

$$\hat{h}(\mathbf{r}'s't', \mathbf{r}st) = \delta(\mathbf{r}-\mathbf{r}') \hat{h}(\mathbf{r}; s't', st), \quad (74a)$$

$$\hat{h}(\mathbf{r}'s't', \mathbf{r}st) = \delta(\mathbf{r}-\mathbf{r}') \hat{h}(\mathbf{r}; s't', st). \quad (74b)$$

The kinetic energy term in Eq. (73a) is already expressed in such a form. The mean-fields Hamiltonians are the second-order operators in momentum and matrices in the spin and isospin spaces. The isospin structure of the local p - h and p - p mean-field Hamiltonians reads

$$\hat{h}(\mathbf{r}; s't', st) = h_0(\mathbf{r}; s', s) \delta_{t't} + \vec{h}(\mathbf{r}; s', s) \circ \hat{\tau}_{t't}, \quad (75a)$$

$$\hat{h}(\mathbf{r}; s't', st) = \check{h}_0(\mathbf{r}; s', s) \delta_{t't} + \vec{\check{h}}(\mathbf{r}; s', s) \circ \hat{\tau}_{t't}, \quad (75b)$$

respectively. The isoscalar and isovector parts of the p - h mean-field Hamiltonian can be presented in the compact form

$$\begin{aligned}
h_k(\mathbf{r}; s', s) = & -\frac{\hbar^2}{2m} \nabla^2 \delta_{s's} \delta_{k0} + U_k \delta_{s's} + \boldsymbol{\Sigma}_k \cdot \hat{\boldsymbol{\sigma}}_{s's} + \frac{1}{2i} [\mathbf{I}_k \delta_{s's} \\
& + (\mathbf{B}_k \cdot \hat{\boldsymbol{\sigma}}_{s's}) \cdot \nabla + \frac{1}{2i} \nabla \cdot [\mathbf{I}_k \delta_{s's} + (\mathbf{B}_k \cdot \hat{\boldsymbol{\sigma}}_{s's})] \\
& - \nabla \cdot [M_k \delta_{s's} + \mathbf{C}_k \cdot \hat{\boldsymbol{\sigma}}_{s's}] \nabla - \nabla \cdot \mathbf{D}_k \hat{\boldsymbol{\sigma}}_{s's} \cdot \nabla
\end{aligned} \quad (76)$$

for $k=0, 1, 2, 3$, and where

$$(\mathbf{B} \cdot \hat{\boldsymbol{\sigma}})_a = \sum_b \mathbf{B}_{ab} \hat{\boldsymbol{\sigma}}^b \quad (77)$$

for $a=x, y, z$ is the a th component of a space vector. The names of symbols are inspired by those introduced in Ref. [172]. Since the p - h density matrix is Hermitian, the p - h mean-field Hamiltonian is also Hermitian and, thus, all the potentials, M_k , U_k , \mathbf{B}_k , \mathbf{C}_k , \mathbf{D}_k , \mathbf{I}_k , and $\boldsymbol{\Sigma}_k$ are real.

The general form of the mean-field Hamiltonian (76) can be constructed from the momentum $-i\nabla$ and spin $\hat{\boldsymbol{\sigma}}$ operators, based only on the symmetry properties. Apart from the one-body kinetic energy [the first term in Eq. (76)], the expansion in momentum gives (i) zero-order terms with scalar (U_k) and pseudovector ($\boldsymbol{\Sigma}_k$) potentials, (ii) first-order terms with vector (\mathbf{I}_k) and pseudotensor (\mathbf{B}_k) potentials, (iii) second-order-scalar terms with scalar (M_k) and pseudoscalar (\mathbf{C}_k) effective masses, and (iv) second-order-tensor terms. In principle, the most general form of the last category should involve tensor and third-order-pseudotensor potentials. However, in Eq. (76) we show only the particular form of it that corresponds to the energy density (40).

According to Eqs. (73) the p - h mean-field Hamiltonian is the functional derivative of the energy functional over the Hermitian p - h density matrix. Functional derivatives of integrals of type

$$\overline{\langle f\rho \rangle} = \int \delta(\mathbf{r}_1 - \mathbf{r}_2) f(\mathbf{r}_1) \rho(\mathbf{r}_1, \mathbf{r}_2) d^3\mathbf{r}_1 d^3\mathbf{r}_2, \quad (78)$$

where function f is treated as independent of densities and ρ represents a p - h nonlocal density, can easily be calculated using Eqs. (12) and (14). Bearing in mind that

$$\frac{\delta \hat{\rho}(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2)}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = \delta(\mathbf{r}_1 - \mathbf{r}) \delta(\mathbf{r}_2 - \mathbf{r}') \delta_{s_1 s} \delta_{s_2 s'} \delta_{t_1 t} \delta_{t_2 t'}, \quad (79)$$

one has

$$\frac{\overline{\delta \langle f \rho_k \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = \delta(\mathbf{r}' - \mathbf{r}) f(\mathbf{r}) \delta_{s's} \hat{\tau}_{t't}^k, \quad (80a)$$

$$\frac{\overline{\delta \langle f s_k \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = \delta(\mathbf{r}' - \mathbf{r}) f(\mathbf{r}) \hat{\boldsymbol{\sigma}}_{s's} \hat{\tau}_{t't}^k \quad (80b)$$

for $k=0, 1, 2, 3$. The functional derivatives of integrals of local differential densities are obtained from Eqs. (80) through integration by parts. Then, the functional derivatives become dependent on derivatives of the Dirac δ function and

thus, in accordance with Eqs. (74), again act as local differential operators. They read

$$\frac{\overline{\delta \langle f \mathbf{j}_k \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = \frac{1}{2i} \delta(\mathbf{r}' - \mathbf{r}) [\nabla f(\mathbf{r}) + f(\mathbf{r}) \nabla] \delta_{s's} \hat{\tau}_{t't}^k, \quad (81a)$$

$$\frac{\overline{\delta \langle f \mathbf{j}_{kab} \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = \frac{1}{2i} \delta(\mathbf{r}' - \mathbf{r}) [\nabla_a f(\mathbf{r}) + f(\mathbf{r}) \nabla_a] \hat{\boldsymbol{\sigma}}_{s's}^b \hat{\tau}_{t't}^k, \quad (81b)$$

$$\frac{\overline{\delta \langle f \nabla_a \nabla'_b \rho_k \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = -\delta(\mathbf{r}' - \mathbf{r}) \nabla_a f(\mathbf{r}) \nabla_b \delta_{s's} \hat{\tau}_{t't}^k, \quad (82a)$$

$$\frac{\overline{\delta \langle f \nabla_a \nabla'_b s_{kc} \rangle}}{\delta \hat{\rho}(\mathbf{r} s t, \mathbf{r}' s' t')} = -\delta(\mathbf{r}' - \mathbf{r}) \nabla_a f(\mathbf{r}) \nabla_b \hat{\boldsymbol{\sigma}}_{s's}^c \hat{\tau}_{t't}^k \quad (82b)$$

for $k=0, 1, 2, 3$ and $a, b, c=x, y, z$. Calculations of the functional derivatives over the density matrix are equivalent to the rules for variations over single-particle wave functions given by Engel *et al.* [172]. Using formulas given above, Eqs. (80)–(82), one obtains the following relations between the potentials defining the p - h mean field (76) and the local p - h densities defining the energy density (40),

$$U_k(\mathbf{r}) = 2C_t^p \rho_k + 2C_t^{\Delta p} \Delta \rho_k + C_t^\tau \tau_k + C_t^{\nabla j} \nabla \cdot \mathbf{J}_k, \quad (83a)$$

$$\begin{aligned}
\boldsymbol{\Sigma}_k(\mathbf{r}) = & 2C_t^s s_k + 2(C_t^{\Delta s} - C_t^{\nabla s}) \Delta s_k - 2C_t^{\nabla s} \nabla \times (\nabla \times s_k) \\
& + C_t^T \mathbf{T}_k + C_t^F \mathbf{F}_k + C_t^{\nabla j} \nabla \times \mathbf{j}_k,
\end{aligned} \quad (83b)$$

$$\mathbf{I}_k(\mathbf{r}) = 2C_t^j \mathbf{j}_k + C_t^{\nabla j} \nabla \times s_k, \quad (83c)$$

$$\mathbf{B}_k(\mathbf{r}) = 2C_t^{j0} \mathbf{j}_k \delta - 2C_t^{j1} \boldsymbol{\epsilon} \cdot \mathbf{J}_k + 2C_t^{j2} \underline{\mathbf{j}}_k + C_t^{\nabla j} \boldsymbol{\epsilon} \cdot \nabla \rho_k, \quad (83d)$$

$$M_k(\mathbf{r}) = C_t^\tau \rho_k, \quad (83e)$$

$$C_k(\mathbf{r}) = C_t^T s_k, \quad (83f)$$

$$D_k(\mathbf{r}) = C_t^F s_k, \quad (83g)$$

for $k=0, 1, 2, 3$. All coupling constants C_t in Eqs. (83) are taken with $t=0$ for $k=0$ (isoscalsars) and with $t=1$ for $k=1, 2, 3$ (isovectors). Symbol δ is the unit space tensor, and $\boldsymbol{\epsilon} \cdot \mathbf{J}$ stands for the antisymmetric space tensor with components $(\boldsymbol{\epsilon} \cdot \mathbf{J})_{ab} = \sum_c \epsilon_{acb} \mathbf{J}_c$, so that, according to Eq. (77), its action on a vector is obviously the vector product $(\boldsymbol{\epsilon} \cdot \mathbf{J}) \cdot \hat{\boldsymbol{\sigma}} = \mathbf{J} \times \hat{\boldsymbol{\sigma}}$.

The p - p mean-field Hamiltonian has the following isoscalar and isovector components:

$$\begin{aligned} \check{h}_0(\mathbf{r}; s', s) &= \check{\Sigma}_0 \cdot \check{\sigma}_{s't'} + \frac{1}{2i} \{ \check{\nabla} \cdot \check{I}_0 \delta_{s't'} + \check{I}_0 \delta_{s't'} \cdot \check{\nabla} \} \\ &\quad - \check{\nabla} \cdot [\check{C}_0 \cdot \check{\sigma}_{s't'}] \check{\nabla} - \check{\nabla} \cdot \check{D}_0 \check{\sigma}_{s't'} \cdot \check{\nabla}, \end{aligned} \quad (84a)$$

$$\begin{aligned} \check{h}(\mathbf{r}; s', s) &= \check{U}(\mathbf{r}) \delta_{s't'} + \frac{1}{2i} \{ \check{\nabla} \cdot [\check{B}(\mathbf{r}) \cdot \check{\sigma}_{s't'}] + [\check{B}(\mathbf{r}) \cdot \check{\sigma}_{s't'}] \cdot \check{\nabla} \} \\ &\quad - \check{\nabla} \cdot \check{M} \delta_{s't'} \check{\nabla}. \end{aligned} \quad (84b)$$

Contrary to the p - h Hamiltonian (76), the p - p Hamiltonian (84) can be non-Hermitian, because potentials \check{C}_0 , \check{D}_0 , \check{I}_0 , $\check{\Sigma}_0$, \check{M} , \check{U} , and \check{B} are, in general, complex quantities. This is so, because the p - p density matrix is, in general, not Hermitian. Therefore, the energy functional should be treated as a functional of both $\hat{\rho}$ and $\hat{\rho}^\dagger$.

The p - p mean-field Hamiltonian is the functional derivative of the energy functional over $\hat{\rho}^\dagger$, whereas the Hermitian conjugate Hamiltonian is the functional derivative over $\hat{\rho}$. The p - p densities are, according to Eqs. (13) and (15), functions of $\hat{\rho}$, while the complex-conjugate densities are functions of $\hat{\rho}^\dagger$.

When calculating the p - p functional derivatives, one cannot forget that the p - p density matrix fulfills symmetry condition (6b), implying that the p - p densities are either symmetric or antisymmetric functions, Eqs. (18). Therefore, the calculation of functional derivatives over either $\hat{\rho}$ or $\hat{\rho}^\dagger$ is similar to that leading to Eqs. (80)–(82), however, instead of Eq. (79) one has

$$\begin{aligned} \frac{\delta \hat{\rho}^\dagger(\mathbf{r}_1 s_1 t_1, \mathbf{r}_2 s_2 t_2)}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} &= \delta(\mathbf{r}_1 - \mathbf{r}) \delta(\mathbf{r}_2 - \mathbf{r}') \delta_{s_1 s} \delta_{s_2 s'} \delta_{t_1 t} \delta_{t_2 t'} \\ &\quad - 16 s s' t t' \delta(\mathbf{r}_1 - \mathbf{r}') \\ &\quad \times \delta(\mathbf{r}_2 - \mathbf{r}) \delta_{s_1 - s'} \delta_{s_2 - s} \delta_{t_1 - t'} \delta_{t_2 - t}. \end{aligned} \quad (85)$$

In the expressions for functional derivatives, this gives either cancellation or addition of terms coming from the two components of the right-hand side of Eq. (85). Finally, the non-vanishing derivatives are

$$\frac{\delta \langle f \check{\rho}^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = 2 \delta(\mathbf{r}' - \mathbf{r}) f(\mathbf{r}) \delta_{s't'} \hat{\tau}_{t't}, \quad (86a)$$

$$\frac{\delta \langle f \check{s}_0^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = 2 \delta(\mathbf{r}' - \mathbf{r}) f(\mathbf{r}) \hat{\sigma}_{s't'} \hat{\tau}_{t't}^0, \quad (86b)$$

$$\frac{\delta \langle f \check{J}_0^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = -i \delta(\mathbf{r}' - \mathbf{r}) [\check{\nabla} f(\mathbf{r}) + f(\mathbf{r}) \check{\nabla}] \delta_{s't'} \hat{\tau}_{t't}^0, \quad (87a)$$

$$\frac{\delta \langle f \check{J}_{ab}^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = -i \delta(\mathbf{r}' - \mathbf{r}) [\check{\nabla}_a f(\mathbf{r}) + f(\mathbf{r}) \check{\nabla}_a] \hat{\sigma}_{s't'} \hat{\tau}_{t't}, \quad (87b)$$

$$\frac{\delta \langle f \check{\nabla}_a \check{\nabla}_b \check{s}_0^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = -2 \delta(\mathbf{r}' - \mathbf{r}) \check{\nabla}_a f(\mathbf{r}) \check{\nabla}_b \delta_{s't'} \hat{\tau}_{t't}, \quad (88a)$$

$$\frac{\delta \langle f \check{\nabla}_a \check{\nabla}_b \check{s}_{0c}^\dagger \rangle}{\delta \hat{\rho}^\dagger(\mathbf{r} s t, \mathbf{r}' s' t')} = -2 \delta(\mathbf{r}' - \mathbf{r}) \check{\nabla}_a f(\mathbf{r}) \check{\nabla}_b \hat{\sigma}_{s't'} \hat{\tau}_{t't}^0 \quad (88b)$$

for $a, b, c = x, y, z$.

Using Eqs. (86) and (87) one obtains the following relations between the potentials defining the p - p mean-field Hamiltonian (84) and the local p - p densities defining the energy density (41):

$$\begin{aligned} \check{\Sigma}_0(\mathbf{r}) &= 2 \check{C}_0^s \check{s}_0 + 2(\check{C}_0^{\Delta s} - \check{C}_0^{\nabla s}) \Delta \check{s}_0 - 2 \check{C}_0^{\nabla s} \check{\nabla} \times (\check{\nabla} \times \check{s}_0) \\ &\quad + \check{C}_0^T \check{T}_0 + \check{C}_0^F \check{F}_0 + \check{C}_0^J \check{\nabla} \times \check{J}_0, \end{aligned} \quad (89a)$$

$$\check{I}_0(\mathbf{r}) = 2 \check{C}_0^j \check{J}_0 + \check{C}_0^{\nabla j} \check{\nabla} \times \check{s}_0, \quad (89b)$$

$$\check{C}_0(\mathbf{r}) = \check{C}_0^T \check{s}_0, \quad (89c)$$

$$\check{D}_0(\mathbf{r}) = \check{C}_0^F \check{s}_0, \quad (89d)$$

$$\check{U}(\mathbf{r}) = 2 \check{C}_1^p \check{\rho} + 2 \check{C}_1^{\Delta p} \Delta \check{\rho} + \check{C}_1^{\nabla p} \check{\nabla} \cdot \check{J}_k, \quad (89e)$$

$$\check{B}(\mathbf{r}) = 2 \check{C}_1^{J0} \check{J} \delta - 2 \check{C}_1^{J1} \epsilon \cdot \check{J} + 2 \check{C}_1^{J2} \check{J} \cdot \check{\nabla} + \check{C}_1^{\nabla J} \epsilon \cdot \check{\nabla} \check{\rho}, \quad (89f)$$

$$\check{M}(\mathbf{r}) = \check{C}_1^{\tau} \check{\rho}. \quad (89g)$$

In the case of the zero-range pairing force (67), the isovector p - p potential is proportional to the p - p isovector density while the isoscalar field has a very different structure, i.e., it is proportional to the scalar product of spin $\hat{\sigma}$ and the p - p spin density \check{s}_0 . This immediately suggests that there exists a connection between the isoscalar pairing and the p - p spin saturation, which is influenced by the spin-orbit splitting. In this context, let us remind the shell-model study [20] which discusses the relation between the magnitude of the $T=0$ pairing and the spin-orbit splitting.

VI. THE HFB EQUATIONS

Minimization of the energy functional of Eq. (34) with respect to the p - h and p - p density matrices, which fulfill Eqs. (7) under auxiliary conditions

$$\int d^3r \rho_n(\mathbf{r}) = N, \quad (90a)$$

$$\int d^3r \rho_p(\mathbf{r}) = Z, \quad (90b)$$

leads to the HFB equation of the form

$$[\hat{\mathcal{H}}, \hat{\mathcal{R}}] = 0. \quad (91)$$

The generalized density matrix $\hat{\mathcal{R}}$ is given by Eq. (9) and the generalized mean-field Hamiltonian is defined as

$$\hat{\mathcal{H}} = \hat{\mathcal{W}} \hat{\mathcal{H}} \hat{\mathcal{W}}^\dagger = \begin{pmatrix} \hat{h} - \hat{\lambda} & \hat{h} \\ \hat{h}^\dagger & -\hat{h}^{TC} + \hat{\lambda} \end{pmatrix}, \quad (92)$$

with the Lagrange multiplier given by

$$\hat{\lambda} = \frac{1}{2}(\lambda_n + \lambda_p) + \frac{1}{2}(\lambda_n - \lambda_p) \hat{\tau}^3, \quad (93)$$

where λ_n and λ_p are the neutron and proton Fermi levels, respectively.

The usual method of solving the HFB equation (91) is to solve in a self-consistent way the eigenvalue problem,

$$\hat{\mathcal{H}}(x', x) \cdot \Phi(x; E) = E \Phi(x'; E), \quad (94)$$

for the generalized mean-field Hamiltonian, and then to construct the generalized density matrix,

$$\hat{\mathcal{R}}(x, x') = \sum_{E \in \mathcal{E}} \Phi(x; E) \Phi^\dagger(x'; E), \quad (95)$$

as a projection operator onto the set of the quasihole (occupied) states Φ belonging to a subset of energy spectrum, \mathcal{E} . For a local mean-field Hamiltonian, Eq. (94) is a system of eight second-order differential equations, in general with complex coefficients. Usual four dimensions corresponding to upper and lower HFB components and to two spin projections are here multiplied by another factor of 2 due to the isospin projections. Altogether, Eq. (94) corresponds to a system of 16 equations within the domain of real numbers. When specific symmetry conditions are imposed on solutions, this number can be reduced in a standard way, see Ref. [184] for the analysis pertaining to spherical symmetry.

The energy spectrum of generalized mean-field Hamiltonian has been discussed in Ref. [5]. The only difference with the present case is that here the eigenvalue problems for neutrons and protons in Eq. (94) cannot be separated. It is well known that the eigenvalues of $\hat{\mathcal{H}}$ appear in pairs of opposite signs. For each quasihole state of energy E ,

$$\Phi(\mathbf{r}st; E) = \begin{pmatrix} \varphi(\mathbf{r}st; E) \\ \psi(\mathbf{r}st; E) \end{pmatrix}, \quad (96)$$

there exists a quasiparticle state

$$\Phi(\mathbf{r}st; -E) = 4st \begin{pmatrix} \psi^*(\mathbf{r} - s - t; E) \\ \varphi^*(\mathbf{r} - s - t; E) \end{pmatrix} \quad (97)$$

belonging to energy $-E$. In the case of the absence of external fields, bound states (when φ and ψ are both localized) exist only when both Fermi levels, λ_n and λ_p , are negative. Discrete quasihole energy levels lie within the range $\mathcal{L} < E < -\mathcal{L}$, where $\mathcal{L} = \max(\lambda_n, \lambda_p) < 0$. The ground-state solution corresponds to occupying states having negative energies; then the set \mathcal{E} consists of a number of discrete levels lying inside segment $(\mathcal{L}, 0)$ and the continuous spectrum with $-\infty < E < \mathcal{L}$.

Traditionally, one solves Eq. (94) for the quasiparticle states of positive energies rather than for the negative ones. Then, the discrete spectrum is within the segment $0 < E < -\mathcal{L}$ and energies $E > -\mathcal{L}$ belong to the continuum. Having found the wave functions $\Phi(\mathbf{r}st; E)$ for $E > 0$ one uses Eq. (97) to construct the density matrix, i.e.,

$$\hat{\mathcal{R}}(x, x') = \sum_{E > 0} \Phi(x; -E) \Phi^\dagger(x'; -E). \quad (98)$$

The p - h and p - p density matrices are then expressed as

$$\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = 16ss'tt' \sum_{E > 0} \psi^*(\mathbf{r} - s - t; E) \psi(\mathbf{r}' - s' - t'; E), \quad (99a)$$

$$\hat{\rho}(\mathbf{r}st, \mathbf{r}'s't') = 16ss'tt' \sum_{E > 0} \psi^*(\mathbf{r} - s - t; E) \varphi(\mathbf{r}' - s - t'; E). \quad (99b)$$

VII. CONSERVED SYMMETRIES

Conserved and broken symmetries are one of the most important elements of description of many-body systems. Within the mean-field approach, the theorem about self-consistent symmetries [167] tells us that mean-field states may or may not have all the symmetries of the Hamiltonian, depending on interactions and the system studied. Within the HFB approach, the symmetry is conserved when the generalized density matrix $\hat{\mathcal{R}}$ and the generalized Hamiltonian $\hat{\mathcal{H}}$ both commute with the symmetry operator \hat{U} , i.e., $[\hat{\mathcal{R}}, \hat{U}] = 0$ and $[\hat{\mathcal{H}}, \hat{U}] = 0$ or

$$\hat{U} \hat{\mathcal{R}} \hat{U}^\dagger = \hat{\mathcal{R}}, \quad (100a)$$

$$\hat{U} \hat{\mathcal{H}} \hat{U}^\dagger = \hat{\mathcal{H}}, \quad (100b)$$

where

$$\hat{U} = \begin{pmatrix} \hat{U} & 0 \\ 0 & \hat{U}^* \end{pmatrix}, \quad (101)$$

and \hat{U} is a unitary matrix of the single-particle symmetry operator. For the breve representation used in the present

study, the symmetry operator is given) by [cf. Eq. (9)]

$$\hat{\mathcal{U}} = \hat{\mathcal{N}}\hat{\mathcal{L}}\hat{\mathcal{N}}^\dagger = \begin{pmatrix} \hat{U} & 0 \\ 0 & \hat{U}^{TC} \end{pmatrix}, \quad (102)$$

and then

$$\hat{\mathcal{U}}\hat{\mathcal{R}}\hat{\mathcal{U}}^\dagger = \hat{\mathcal{R}}, \quad (103a)$$

$$\hat{\mathcal{U}}\hat{\mathcal{H}}\hat{\mathcal{U}}^\dagger = \hat{\mathcal{H}}. \quad (103b)$$

In the previous sections we have presented the most general set of expressions pertaining to the situation when no symmetries were *a priori* conserved. Below we discuss consequences of conserved symmetries.

A. Proton-neutron symmetry

The standard case of no proton-neutron mixing can be described by the conserved proton-neutron symmetry given by

$$\hat{U}_{pn} = i \exp(-i\pi\hat{T}_3) = i \exp\left(-\frac{i}{2}\pi\hat{\tau}_3\right) = \hat{\tau}_3. \quad (104)$$

In other words, the iso-3 signature (multiplied by i) is then the conserved symmetry. Note that conservation of projection of the isospin on the third axis (the charge conservation) would require that the iso-3 rotation about an arbitrary angle be conserved, while the iso-3 signature corresponds only to rotation about π . Within the HFB approach, the charge symmetry is broken in the same way as is the particle number symmetry.

Since the TC -transformed symmetry operator reads $\hat{U}_{pn}^{TC} = -\hat{\tau}_3$, we obtain from Eq. (103a) that

$$\hat{\tau}_3\hat{\rho}\hat{\tau}_3 = \hat{\rho}, \quad (105a)$$

$$\hat{\tau}_3\hat{\rho}\hat{\tau}_3 = -\hat{\rho}, \quad (105b)$$

and analogous properties hold for the mean-field Hamiltonians, \hat{h} and \hat{h} , respectively. It is then clear that without the proton-neutron mixing the p - h density matrices and Hamiltonians have only the $k=0$ and 3 isospin components, while the p - p ones have (in the breve representation) only the $k=1$ and 2 isospin components, cf. Eqs. (29) and (30).

B. Time-reversal symmetry

In the case of time-reversal invariance, $\hat{\rho}^T = \hat{\rho}$ and $\hat{\rho}^T = \hat{\rho}$, see Eqs. (4), the p - h and p - p densities fulfill additional conditions

$$\rho_0(\mathbf{r}, \mathbf{r}') = \rho_0^*(\mathbf{r}, \mathbf{r}'), \quad (106a)$$

$$\rho_k(\mathbf{r}, \mathbf{r}') = -(-1)^k \rho_k^*(\mathbf{r}, \mathbf{r}'), \quad (106b)$$

$$s_0(\mathbf{r}, \mathbf{r}') = -s_0^*(\mathbf{r}, \mathbf{r}'), \quad (106c)$$

$$s_k(\mathbf{r}, \mathbf{r}') = (-1)^k s_k^*(\mathbf{r}, \mathbf{r}') \quad (106d)$$

and

$$\check{\rho}_0(\mathbf{r}, \mathbf{r}') = \check{\rho}_0^*(\mathbf{r}, \mathbf{r}'), \quad (107a)$$

$$\check{\rho}_k(\mathbf{r}, \mathbf{r}') = -(-1)^k \check{\rho}_k^*(\mathbf{r}, \mathbf{r}'), \quad (107b)$$

$$\check{s}_0(\mathbf{r}, \mathbf{r}') = -\check{s}_0^*(\mathbf{r}, \mathbf{r}'), \quad (107c)$$

$$\check{s}_k(\mathbf{r}, \mathbf{r}') = (-1)^k \check{s}_k^*(\mathbf{r}, \mathbf{r}'), \quad (107d)$$

where $k=1, 2, 3$. Due to the fact that the $k=2$ Pauli matrix $\hat{\tau}^2$ is imaginary, the time reversal acts differently on the $k=2$ isovector components than on the $k=1, 3$ components of all isovector densities. At the first sight, this seems to be a bizarre property. Indeed, the isospin quantum number is introduced to take into account the fact that there are two kinds of nucleons in nature, and each kind has its own, apparently unrelated to one another, time-reversal operation.

However, the use of the standard isospin formalism implies something more, namely, the neutron wave function (isospin up) can be obtained from the proton wave function (isospin down) by an action of the (real) $\hat{\tau}^1$ Pauli matrix. Therefore, the relative phases of the neutron and proton wave functions are fixed by the phase convention that has been used to choose the isospin Pauli matrices. As a consequence, the time-reversal properties of neutrons and protons are not any more independent from one another. Of course, this is not a spurious quirk of the mathematics we use, but a reflection of a deeper fact that by mixing the neutron and proton wave functions we introduce complex mixing coefficients that do affect the time-reversal properties of the mixed wave function. Conservation of the time reversal means that these mixing coefficients must follow rules dictated by the time reversal, which implies differences between the $k=2$ and $k=1, 3$ isodirections. Therefore, we see here that from basic arguments it follows that conservation of the time reversal *must imply the isospin symmetry breaking*. The only isorotations that are compatible with the time reversal are those about the $k=2$ isoaxis. (The influence of the time-odd fields on the magnitude of the Wigner energy was pointed out in Ref. [12].)

TABLE III. Symmetries of the p - h (left) and p - p (right) densities in general case (no conserved symmetries imposed), and in case of the time-reversal symmetry conserved. Real (Re) and imaginary (Im) parts are symmetric (S) or antisymmetric (A) under exchange of their spatial arguments, as indicated in the table.

Density	General		Time reversal		Density	General		Time reversal	
	Re	Im	Re	Im		Re	Im	Re	Im
$\rho_0(\mathbf{r}, \mathbf{r}')$	S	A	S	0	$\check{\rho}_0(\mathbf{r}, \mathbf{r}')$	A	A	A	0
$\rho_2(\mathbf{r}, \mathbf{r}')$	S	A	0	A	$\check{\rho}_2(\mathbf{r}, \mathbf{r}')$	S	S	0	S
$\rho_{1,3}(\mathbf{r}, \mathbf{r}')$	S	A	S	0	$\check{\rho}_{1,3}(\mathbf{r}, \mathbf{r}')$	S	S	S	0
$s_0(\mathbf{r}, \mathbf{r}')$	S	A	0	A	$\check{s}_0(\mathbf{r}, \mathbf{r}')$	S	S	0	S
$s_2(\mathbf{r}, \mathbf{r}')$	S	A	S	0	$\check{s}_2(\mathbf{r}, \mathbf{r}')$	A	A	A	0
$s_{1,3}(\mathbf{r}, \mathbf{r}')$	S	A	0	A	$\check{s}_{1,3}(\mathbf{r}, \mathbf{r}')$	A	A	0	A

Table III summarizes properties of p - h and p - p densities under the exchange of their spatial arguments. When no conserved symmetry is imposed, all densities are complex, and their real and imaginary parts are either symmetric or antisymmetric. For conserved time reversal, all densities become either real or imaginary and are either symmetric or antisymmetric. Recall that symmetric parts contribute only to particle, kinetic, spin, spin-kinetic, and tensor-kinetic local densities, while the antisymmetric parts contribute only to the current and spin-current local densities. Therefore, local densities are complex, real, imaginary, or vanishing, depending on whether time-reversal, proton-neutron, or both symmetries are conserved. Table IV presents these properties for all local p - h and p - p densities.

In previous studies, e.g., in Refs. [3,62,65,152,153], the $T=1$ pairing fields were associated with the real part of the pairing tensor, while the $T=0$ pairing was represented by the imaginary part of the pairing tensor. Such a structure was

obtained for specific phase conventions and symmetries. On the other hand, as shown in Table IV, the general case corresponding to no conserved symmetries (e.g., for rotating states) requires that all the pn densities be complex.

To summarize this section, we now enumerate all nonzero densities when the time reversal is conserved or not, and/or the proton-neutron mixing is present or not. By counting as one density each component of a vector, tensor, or isovector, we obtain the following four options.

- (i) 1° time-reversal broken plus proton-neutron mixing.
 - (a) 23 real p - h isoscalar densities: $\rho_0(\mathbf{r})$, $\tau_0(\mathbf{r})$, $\mathbf{J}_0(\mathbf{r})$, $s_0(\mathbf{r})$, $\mathbf{T}_0(\mathbf{r})$, $\mathbf{j}_0(\mathbf{r})$, and $\mathbf{F}_0(\mathbf{r})$.
 - (b) 69 real p - h isovector densities: $\vec{\rho}(\mathbf{r})$, $\vec{\tau}(\mathbf{r})$, $\vec{\mathbf{J}}(\mathbf{r})$, $\vec{s}(\mathbf{r})$, $\vec{\mathbf{T}}(\mathbf{r})$, $\vec{\mathbf{j}}(\mathbf{r})$, and $\vec{\mathbf{F}}(\mathbf{r})$.
 - (c) 12 complex p - p isoscalar densities: $\check{s}_0(\mathbf{r})$, $\check{\mathbf{T}}_0(\mathbf{r})$, $\check{\mathbf{j}}_0(\mathbf{r})$, and $\check{\mathbf{F}}_0(\mathbf{r})$.

TABLE IV. Properties of the local p - h and p - p densities in general case (no conserved symmetries imposed), and in case of the time-reversal, proton-neutron, or both symmetries conserved. The $k=0, 1, 2$, or 3 isospin components of densities are complex (C), real (R), imaginary (I), or zero (0), as indicated in the table.

k	0	General			Time reversal			Proton neutron			Both					
		1	2	3	0	1	2	3	0	1	2	3	0	1	2	3
ρ_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
τ_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
\mathbf{J}_k	R	R	R	R	R	R	0	R	R	0	0	R	R	0	0	R
s_k	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
\mathbf{T}_k	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
\mathbf{j}_k	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
\mathbf{F}_k	R	R	R	R	0	0	R	0	R	0	0	R	0	0	0	0
$\check{\rho}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
$\check{\tau}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
$\check{\mathbf{J}}_k$	0	C	C	C	0	R	I	R	0	C	C	0	0	R	I	0
\check{s}_k	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\check{\mathbf{T}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\check{\mathbf{j}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0
$\check{\mathbf{F}}_k$	C	0	0	0	I	0	0	0	0	0	0	0	0	0	0	0

(d) 33 complex p - p isovector densities: $\check{\rho}(\mathbf{r})$, $\check{\tau}(\mathbf{r})$, and $\check{\mathbf{J}}(\mathbf{r})$.

(ii) 2° time-reversal conserved plus proton-neutron mixing.

(a) 11 real p - h isoscalar densities: $\rho_0(\mathbf{r})$, $\tau_0(\mathbf{r})$, and $\mathbf{J}_0(\mathbf{r})$.

(b) 30 real p - h isovector densities: $\rho_{1,3}(\mathbf{r})$, $\tau_{1,3}(\mathbf{r})$, $\mathbf{J}_{1,3}(\mathbf{r})$, $s_2(\mathbf{r})$, $\mathbf{T}_2(\mathbf{r})$, $\mathbf{j}_2(\mathbf{r})$, and $\mathbf{J}_2(\mathbf{r})$.

(c) 12 imaginary p - p isoscalar densities: $\check{s}_0(\mathbf{r})$, $\check{\mathbf{T}}_0(\mathbf{r})$, $\check{\mathbf{j}}_0(\mathbf{r})$, and $\check{\mathbf{F}}_0(\mathbf{r})$.

(d) 33 p - p isovector densities, 22 real $\check{\rho}_{1,3}(\mathbf{r})$, $\check{\tau}_{1,3}(\mathbf{r})$, $\check{\mathbf{J}}_{1,3}(\mathbf{r})$ and 11 imaginary $\check{\rho}_2(\mathbf{r})$, $\check{\tau}_2(\mathbf{r})$, $\check{\mathbf{J}}_2(\mathbf{r})$.

(iii) 3° time-reversal broken, no proton-neutron mixing.

(a) 23 real p - h isoscalar densities: $\rho_0(\mathbf{r})$, $\tau_0(\mathbf{r})$, $\mathbf{J}_0(\mathbf{r})$, $s_0(\mathbf{r})$, $\mathbf{T}_0(\mathbf{r})$, $\mathbf{j}_0(\mathbf{r})$, and $\mathbf{F}_0(\mathbf{r})$.

(b) 23 real p - h isovector densities: $\rho_3(\mathbf{r})$, $\tau_3(\mathbf{r})$, $\mathbf{J}_3(\mathbf{r})$, $s_3(\mathbf{r})$, $\mathbf{T}_3(\mathbf{r})$, $\mathbf{j}_3(\mathbf{r})$, and $\mathbf{F}_3(\mathbf{r})$.

(c) 22 complex p - p isovector densities: $\check{\rho}_{1,2}(\mathbf{r})$, $\check{\tau}_{1,2}(\mathbf{r})$, and $\check{\mathbf{J}}_{1,2}(\mathbf{r})$.

(iv) 4° time-reversal conserved, no proton-neutron mixing.

(a) 11 real p - h isoscalar densities: $\rho_0(\mathbf{r})$, $\tau_0(\mathbf{r})$, and $\mathbf{J}_0(\mathbf{r})$.

(b) 11 real p - h isovector densities: $\rho_3(\mathbf{r})$, $\tau_3(\mathbf{r})$, and $\mathbf{J}_3(\mathbf{r})$.

(c) 22 p - p isovector densities, 11 real $\check{\rho}_1(\mathbf{r})$, $\check{\tau}_1(\mathbf{r})$, $\check{\mathbf{J}}_1(\mathbf{r})$ and 11 imaginary $\check{\rho}_2(\mathbf{r})$, $\check{\tau}_2(\mathbf{r})$, $\check{\mathbf{J}}_2(\mathbf{r})$.

VIII. CONCLUSIONS

Experimental studies of the heavy $N \sim Z$ nuclei have sparked renewed interest in physics of pn correlations, especially pn pairing. While the appearance of the $T=1$ pn pairing is a simple consequence of the charge invariance, in spite of vigorous research, no hard evidence for the elusive $T=0$ pairing phase has yet been found. There are conflicting messages coming from calculations based on the quasiparticle

approach. In some models, the $T=0$ and $T=1$ pairing modes are mutually exclusive, while in others they are not. What is clear, however, that predictions of calculations that impose some symmetry constraints (which can rule out the presence of some pairing fields) should be taken with the grain of salt.

In this work, we propose the most general nuclear energy-density functional which is quadratic in isoscalar and isovector densities. To this end, we discuss the isospin structure of the density matrices and self-consistent mean fields that appear in the coordinate-space HFB theory allowing for a microscopic description of pairing correlations in all isospin channels. The resulting expressions incorporate an arbitrary mixing between protons and neutrons. No particular self-consistent symmetries of the energy-density functional have been imposed, however, the consequences of the time-reversal and proton-neutron symmetry are discussed. The obtained nuclear energy-density functional (39)–(41) does not have to be related to any given local potential. However, if the underlying potential is local and velocity independent, the potential energy density is invariant with respect to a local gauge transformation. The resulting densities appear in certain gauge-invariant combinations (47) and (48) which lead to a significant simplification of the functional.

The self-consistent wave functions obtained by solving the generalized HFB equations are not eigenstates of isospin. This is a serious drawback of the quasiparticle approach. To cure this problem, isospin should be restored by means of, e.g., projection techniques. While this can be carried out in a straightforward manner for energy functionals that are related to a two-body potential, the restoration of spontaneously broken symmetries of a general density functional poses a conceptual dilemma [185–188] and a serious challenge that is left for the future work.

ACKNOWLEDGMENTS

This work was supported in part by the Polish Committee for Scientific Research (KBN) under Contract No. 5 P03B 014 21, by the Foundation for Polish Science (FNP), and by the U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963 (University of Tennessee) and DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory).

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