Self-consistent symmetries in the proton-neutron Hartree-Fock-Bogoliubov approach

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Symmetry properties of densities and mean fields appearing in the nuclear Density Functional Theory with pairing are studied. We consider energy functionals that depend only on local densities and their derivatives. The most important self-consistent symmetries are discussed: spherical, axial, space-inversion, and mirror symmetries. In each case, the consequences of breaking or conserving the time-reversal and/or proton-neutron symmetries are discussed and summarized in a tabulated form, useful in practical applications.

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I. INTRODUCTION

The nuclear Density Functional Theory (DFT) is a theoretical tool of choice for describing complex, open-shell nuclei, for which the dimension of the configuration space becomes intractable for other methods of theoretical nuclear structure, such as ab initio and configuration interaction (shell model) techniques. The main building blocks of nuclear DFT are the effective fields, often represented by local proton and neutron densities and their derivatives. When compared to the electronic DFT, the unique features of the nuclear variant are: (i) the presence of two kinds of fermions, protons and neutrons; (ii) the essential role of nucleonic pairing; and (iii) the absence of external potential and the need for symmetry restoration in a self-bound system.

At the heart of the DFT lies the energy density functional that is built from the nucleonic intrinsic density matrices. The requirement that the total energy be minimal under a variation of the densities leads to the Hartree-Fock-Bogoliubov (HFB; or Bogoliubov-de Gennes) equations. They form a set of non-linear integro-differential equations which has to be solved iteratively for the self-consistent densities.

The quasi-particle vacuum associated with the DFT solution is a highly correlated state. This is partly because the DFT description is performed in a frame of reference attached to the nucleus, the intrinsic frame, in which the nuclear mean field may spontaneously break the symmetry of the original Hamiltonian, or energy density. While the resulting deformed solutions do not obey symmetries present in the laboratory system, they acquire lower binding through long-range polarization effects. Additional correlations may be gained by means of symmetry restoration. Such a strategy, rooted in the nuclear Jahn-Teller effect, has proven to be very effective in nuclear mean-field calculations.

Since the symmetry breaking is essential for determining the optimal mean field of the nucleus, the self-consistent symmetries present in the model may often determine physics. A self-consistent symmetry (SCS) is a unitary or antiunitary transformation \( S \), which commutes with the HFB Hamiltonian. Due to self-consistency, \( S \) also commutes with DFT densities. The associated DFT energy density \( \mathcal{H} \) is referred to as symmetry invariant:

\[
\mathcal{H}^S(r) = \mathcal{H}(r).
\]

The above definition of SCS that can often be found in the literature is too limiting when it comes to the DFT. Indeed, invariance of the energy density itself is not a prerequisite for the invariance of the energy density functional (EDF). Actually, the EDF is invariant with respect to \( S \) also when the energy density is covariant with \( S \), i.e.,

\[
\mathcal{H}^S(r) = \mathcal{H}(S^+ r S).
\]

The energy density that meets is referred to as symmetry covariant, see discussion in Appendix A of Ref. The existence of SCS has a profound impact on self-consistent solutions. If the initial density matrix employed at the first iteration of HFB equations contains a SCS, then that symmetry will propagate through to the final DFT solution. Therefore, the introduction of SCS restricts the generality of the self-consistent density matrix and may lead to an erroneous estimate of the DFT energy and deformation of the system.

A considerable literature exists on nuclear collective modes associated with spontaneously broken symmetries. Ground-state deformations of nuclei, including those in the pairing channel, have been reviewed in Refs. In the presence of angular momentum, new deformations of magnetic character may appear in the rotating nuclear mean field. High-spin particle-hole (p-h) and particle-particle (p-p or pairing) deformations, both isoscalar and isovector, have been discussed in detail in Refs., which also contain a general discussion of spontaneous symmetry-breaking phenomena in rotating nuclei (see also for a recent update).
Symmetry properties of Hartree-Fock (HF) densities were studied in Ref. [22] in the context of a double point group D_{2h}^P that contains three mutually perpendicular symmetry axes of the second order, space inversion, and time reversal. The associated symmetry-breaking schemes have been outlined in the following Ref. [24].

In this paper, we extend the discussion of Refs. [22,23] to the pairing channel and transition densities using the coordinate-space HF theory which incorporates an arbitrary mixing between protons and neutrons in the p-h and p-p channels [24]. The constraints imposed on DFT densities by the time-reversal and proton-neutron (p-n) symmetries are studied for various spatial geometries (spherical, axial, space-inversion, mirror, and D_{2h}). The details pertaining to the p-n HF theory in the Local Density Approximation (LDA) can be found in Ref. [24]. Throughout our work, we refer to this previous paper as I.

Our interest in a general HFB formalism that incorporates an arbitrary mixing between proton and neutron quasiparticles is motivated by numerous phenomena that are present in medium-mass and heavy nuclei with \(N\approx Z\). These include: p-n pairing correlations; alpha decay and alpha clustering; local increase in binding energy that contains three mutually perpendicular symmetry axes of the second order, space inversion, and time reversal. The associated symmetry-breaking schemes have been outlined in the following Ref. [24].

The paper is organized as follows. Section II introduces the local DFT densities and defines transformation rules for density matrices. The symmetries of interest, both in the position-spin space and in the isotopic space are discussed in Sec III. Symmetry properties of densities are studied in Sec. IV for (i) spherical symmetry (with and without space inversion); (ii) axial symmetry (with and without space inversion); and (iii) D_{2h} symmetry. When going beyond the mean-field approximation, e.g., by using the Generator Coordinate Method or projection techniques, multi-reference transition densities appear. The associated symmetry properties are summarized in Sec. V. Previous self-consistent calculations of p-n pairing are commented upon in Sec. VI in the context of our findings. Section VII summarizes the main results of our study. Finally, Appendix A is devoted to the generalized Cayley-Hamilton theorem for irreducible spherical tensors and tensor fields.

II. DENSITIES AND FIELDS

A. Density matrices and mean fields in the p-h and p-p channels

To fix the notation, we begin with a brief recapitulation of definitions and basic properties of the one-body HFB density matrices in p-h and p-p channels, see I for details. The p-h and p-p density matrices are defined, respectively, as

\[
\hat{\rho}(r, s) = \langle \Psi | a_{r,s}^+ a_{r,s} | \Psi \rangle, \quad \hat{\rho}(r, s) = 4s^2 \langle \Psi | a_{r,s}^+ a_{r,s} | \Psi \rangle,
\]

where \(a_{r,s}^+\) and \(a_{r,s}\) create and annihilate, respectively, nucleons at point \(r\), spin \(s=\pm \frac{1}{2}\), and isospin \(t=\pm \frac{1}{2}\), while \(|\Psi\rangle\) is the HFB independent-quasiparticle state.

The p-h and p-p density matrices form together the projective generalized “breve” density matrix,

\[
\hat{\tilde{R}}(x, x') = \begin{pmatrix} \hat{\tilde{\rho}}(x, x') & \hat{\tilde{\sigma}}(x, x') \\ \hat{\tilde{\sigma}}^+(x, x') & 1 - \hat{\tilde{\rho}}(x, x') \end{pmatrix},
\]

where we abbreviated the position-spin-isospin variables by \(x=rst\) and \(1 := \delta(x-x') := \delta(r-r')\delta(s,s')\delta(t,t')\).

In I, we found that instead of using the usual antisymmetric pairing tensor \(\tilde{\rho}\), it is more convenient to introduce the above p-p (or anomalous) density matrix, \(\hat{\tilde{\rho}}\). The relation between the standard density matrix \(\hat{\tilde{R}}(x, x')\) and \(\hat{\tilde{R}}(x, x')\) is given by a unitary transformation \(\hat{W}\)

\[
\hat{W} = \begin{pmatrix} 1 & 0 \\ 0 & \hat{\tilde{\sigma}}^+(2) \end{pmatrix}.
\]

The quantities expressed in the representation \(\hat{W}\) are indicated by a “breve” symbol in the following.

Throughout our paper we apply the following naming convention. The matrices are denoted by “hat”; the quantities expressed in the representation \(\hat{W}\) are marked by “breve”; the matrices in a double HFB space are denoted by the calligraphic capital letters. As in I, we label space vectors by boldface symbols and their scalar products by the central dot, e.g., \(r \cdot \nabla\); 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., \(r = (r_x, r_y, r_z)\). Here we note that similarly as in I, the individual vector components are also shown in boldface.

Vectors in isospace (isovectors) are labeled by arrows with their scalar products in the isospace denoted by the circle, e.g., \(\vec{v} \cdot \vec{w}\). The components of isovectors are labeled with indices \(i, k\), and the names of iso-axes are 1, 2, and 3. Isoscalars are marked with subscript “0”, and we often combine formulæ for isoscalars and isovectors by letting the indices run through all the four values, e.g., \(k=0,1,2,3\).

The symbol \(\int dx\) represents integration over spatial coordinates and summation over spin and isospin indices, and \(\bullet\) denotes the matrix multiplication and integration/summation \(\int dx\). The asterisk stands for the
complex conjugation. The spin and isospin Pauli matrices are, respectively, \( \hat{\sigma}_{ss'} = (\hat{\sigma}_s^x, \hat{\sigma}_s^y, \hat{\sigma}_s^z) \) and \( \hat{\tau}_{tt'} = (\hat{\tau}_t^{(1)}, \hat{\tau}_t^{(2)}, \hat{\tau}_t^{(3)}) \), and the corresponding unity matrices are \( \hat{1}_{tt'} = \delta_{tt'} \) and \( \hat{1}_{ss'} = \delta_{ss'} \).

Under TC, the product of time reversal \( T \) and charge reversal \( C \) (a rotation by \( \pi \) in isospin space around the second axis), the density matrices (3) and (4) become:

\[
\hat{\rho}^{TC}(r st, r's't') = 16 s's't' \hat{\rho}^r (r - s - t, r' - s' - t') \quad (7a)
\]

\[
\hat{\tau}^{TC}(r st, r's't') = 16 s's't' \hat{\tau}^r (r - s - t, r' - s' - t') \quad (7b)
\]

The symmetries of \( \hat{\rho} \) and \( \hat{\tau} \) can be conveniently expressed in terms of just the Hermitian conjugation and TC:

\[
\hat{\rho}^+ = \hat{\rho}, \quad (8a)
\]

\[
\hat{\tau}^+ = -\hat{\tau}^{TC}. \quad (8b)
\]

Expressed in terms of spin-isospin components, the density matrices can be written as:

\[
\hat{\rho}(r st, r's't') = \frac{1}{4} \rho_0(r, r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(r, r') \circ \hat{\tau}_{tt'} + \frac{1}{4} \hat{s}_0(r, r') \cdot \sigma_{ss'} \circ \hat{\tau}_{tt'}, \quad (9a)
\]

\[
\hat{\tau}(r st, r's't') = \frac{1}{4} \rho_0(r, r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\tau}(r, r') \circ \hat{\tau}_{tt'} + \frac{1}{4} \hat{s}_0(r, r') \cdot \sigma_{ss'} \circ \hat{\tau}_{tt'}. \quad (9b)
\]

To avoid confusion, the functions of two position vectors \( r \) and \( r' \) appearing on the right-hand sides of Eqs. (12) will be called the *nonlocal* density functions or, simply, densities, unlike the density matrices (3) and (4) appearing on the left-hand sides.

Since the p-h density matrix and the Pauli matrices are both Hermitian, according to (I-16) all p-h densities are Hermitian as well; hence, their real parts are symmetric, while the imaginary parts are antisymmetric with respect to exchanging \( r \) and \( r' \). Similarly, transformation properties of Pauli matrices under time-reversal and charge conjugation (I-17) make the p-p densities either symmetric (scalar-isovector and vector-isoscalar) or antisymmetric (scalar-isoscalar and vector-iso-vector) with respect to exchanging \( r \) and \( r' \), see Eq. (I-18). These properties are fulfilled independently of any other symmetries conserved by the system; they are consequences of definitions of density matrices \( \hat{\rho} \) and \( \hat{\tau} \).

In the HFB theory with the zero-range Skyrme interaction [25, 26], or in the local density approximation (LDA; cf. Refs. [17, 18]), the energy functional depends only on *local* densities, and on local densities built from derivatives up to a given order, see Refs. [11, 12] for systematic constructions. The local densities are denoted by having only one spatial argument to distinguish them from the nonlocal densities. Following the standard definitions [29, 31] in the present study we employ definitions of local p-h and p-p densities according to Ref. 1. For the sake of completeness, we repeat them here:

- **scalar densities**:

  - particle and pairing densities:

    \[
    \rho_k(r) = \rho_k(r, r')_{r=r'}, \quad (10a)
    \]

    \[
    \bar{\rho}(r) = \bar{\rho}(r, r')_{r=r'}, \quad (10b)
    \]

- **vector densities**:

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

    \[
    s_k(r) = s_k(r, r')_{r=r'}, \quad (12a)
    \]

    \[
    s_0(r) = s_0(r, r')_{r=r'}, \quad (12b)
    \]

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

    \[
    T_k(r) = [(\nabla \cdot \nabla') s_k(r, r')]_{r=r'}, \quad (13a)
    \]

    \[
    T_0(r) = [(\nabla \cdot \nabla') s_0(r, r')]_{r=r'}, \quad (13b)
    \]

- **current densities**:

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

    \[
    j_k(r) = \frac{1}{2} [(\nabla - \nabla') j_k(r, r')]_{r=r'}, \quad (14a)
    \]

    \[
    j_0(r) = \frac{1}{2} [(\nabla - \nabla') j_0(r, r')]_{r=r'}, \quad (14b)
    \]

  - p-h and p-p tensor-kinetic (pseudotensor) densities:

    \[
    F_k(r) = \frac{1}{2} [(\nabla \otimes \nabla' + \nabla' \otimes \nabla) \cdot s_k(r, r')]_{r=r'}, \quad (15a)
    \]

    \[
    F_0(r) = \frac{1}{2} [(\nabla \otimes \nabla' + \nabla' \otimes \nabla) \cdot s_0(r, r')]_{r=r'}, \quad (15b)
    \]

- **tensor densities**:

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

    \[
    J_k(r) = \frac{1}{2} [(\nabla - \nabla') \otimes s_k(r, r')]_{r=r'}, \quad (16a)
    \]

    \[
    J_0(r) = \frac{1}{2} [(\nabla - \nabla') \otimes s_0(r, r')]_{r=r'}, \quad (16b)
    \]
where \(k=0,1,2,3\), and \(\otimes\) stands for the tensor product of vectors in the physical space, e.g., \((\mathbf{v} \otimes \mathbf{w})_a = v_a w_b \) and \(((\mathbf{v} \otimes \mathbf{w}) \cdot \mathbf{z})_a = v_a (w \cdot z)\).

The kinetic, spin-kinetic, and tensor-kinetic densities are, in fact, equal to contractions of the following 2nd-order and 3rd-order tensor densities:

\[
\tau_{kbc}(r) = \left[ \nabla_b \nabla_c \rho_k(r) (r') \right]_{r=r'}, \quad (17a)
\]

\[
\bar{\tau}_b(r) = \sum_{b=x,y,z} \tau_{bb}(r), \quad (18a)
\]

\[
T_{kbc}(r) = \left[ \nabla_b \nabla_c s_{kbc}(r) (r') \right]_{r=r'}, \quad (17c)
\]

\[
\bar{T}_{bdc}(r) = \left[ \nabla_b \nabla_c s_{bdc}(r) (r') \right]_{r=r'}, \quad (17d)
\]

namely,

\[
\tau_k(r) = \sum_{b=x,y,z} \tau_{bb}(r), \quad (18b)
\]

\[
\bar{T}_{kd}(r) = \sum_{b=x,y,z} T_{kbdb}(r), \quad (18c)
\]

\[
T_{bd}(r) = \sum_{b=x,y,z} \bar{T}_{bd}(r), \quad (18d)
\]

\[
\bar{T}_{bd}(r) = \sum_{b=x,y,z} \bar{T}_{bdc}(r), \quad (18e)
\]

\[
\bar{T}_{bb}(r) = \sum_{c=x,y,z} \bar{T}_{bdc}(r), \quad (18f)
\]

All pseudotensor densities can be decomposed into trace, antisymmetric, and symmetric components \((I-26)-(I-28)\), that is, into pseudoscalar \(J_k(r)\) and \(\bar{J}(r)\); vector \(J_k(r)\) and \(\bar{J}(r)\); and pseudotensor \(\underline{J}(r)\) and \(\bar{\underline{J}}(r)\) densities.

In the case of the Skyrme effective interaction, as well as in the framework of the energy density functional approach, the energy functional is a three-dimensional spatial integral,

\[
\mathcal{H} = \int d^3r \mathcal{H}(r), \quad (19)
\]

of the local energy density \(\mathcal{H}(r)\) that is supposed to be a real, scalar, time-even, and isoscalar function of local densities and their derivatives.

Minimization of the energy functional with respect to the p-h and p-p density matrices under auxiliary conditions

\[
\int d^3r \rho_0(r) = A \quad (20)
\]

and

\[
\int d^3r \rho_3(r) = N - Z = 2T_3, \quad (21)
\]

leads to the common eigenvalue problem for the generalized density matrix \(\bar{\mathcal{R}}\) and the generalized mean-field Hamiltonian matrix defined as

\[
\bar{\mathcal{H}} = \left( \begin{array}{cc} \hat{h} - \bar{\lambda} & \hat{\lambda} \\ \bar{\lambda} & -\hat{h}^{TC} + \bar{\lambda} \end{array} \right), \quad (22)
\]

with the Lagrange multiplier matrix given by

\[
\bar{\lambda} = \frac{1}{2}(\lambda_n + \lambda_p) \mathbf{I} + \frac{1}{2}(\lambda_n - \lambda_p) \hat{r}^{(3)} = \lambda_0 \mathbf{I} + \lambda_3 \hat{r}^{(3)}, \quad (23)
\]

where \(\lambda_n\) and \(\lambda_p\) are the neutron and proton Fermi levels, respectively.

B. Transformation rules for the density matrices

A general Hermitian one-body operator in the Fock space can be written as

\[
G = \int d^3r' \sum_{s't'} \int d^3r \sum_{st} \tilde{g}(r's't', rst) a^+_s r'_t a_{rst}, \quad (24)
\]

where

\[
\tilde{g}(r's't', rst) = \langle r's't'|g|rst \rangle \quad (25)
\]

is the matrix element of the single-particle operator \(g\) acting in the space of one-body wave functions. Let us now consider a unitary transformation \(U\) in the Fock space generated by \(G\):

\[
U = e^{i\alpha G}, \quad (26)
\]

where \(\alpha\) is a real parameter. By making use of the Baker-Campbell-Hausdorff relations, the annihilation and creation operators transform under \(U\) as:

\[
U^+_a r_{st} U = \int d^3r' \sum_{s't'} \hat{u}(r_{st}, r's't') a^+_{r's't'}, \quad (27a)
\]

\[
U^+_a r_{st} U = \int d^3r' \sum_{s't'} \hat{\tilde{u}}(r's't', r_{st}) a^+_s r'_t, \quad (27b)
\]

where

\[
\hat{u}(r's't', r_{st}) = \langle r's't'|e^{i\alpha g}|rst \rangle. \quad (28)
\]

From Eqs. 27 it follows that the density matrices calculated for the transformed state \(U|\Psi\rangle\), i.e., the transformed density matrices, are:
The generalized density matrix (5) transformed under 
where \( \hat{K} \) is a linear unitary operator and 
\( \hat{K} \) is the matrix complex conjugation operator associated with the position-spin-isospin representation. One has to remember that the decomposition (30) and definition of \( \hat{K} \) (37) does not depend on any specific choice of the single-particle basis \( \phi_i(rst) \). The advantage of such a choice is that properties of antilinear symmetries (like the time reversal) directly translate into the complex-conjugation properties of densities. However, other choices of \( K \) can be useful when the complex-conjugation properties of matrix elements of operators in the given basis \( \phi_i(rst) \) are considered.

**III. SYMMETRIES**

Let us suppose that \( U \) (or \( U_K \)) is a symmetry transformation of the nuclear many-body Hamiltonian, \( H \), i.e.,

\[
UHU^+ = H.
\]

The generalized density matrix \( \hat{\rho} \) and mean-field Hamiltonian \( \hat{H} \), obtained through the minimization procedure, may, but need not, obey the symmetry \( U \). It can be only proved [7] that if \( U \) is a symmetry of \( H \) then the transformed generalized mean-field Hamiltonian depends functionally on the transformed generalized density matrix in the same way as the original Hamiltonian on the original density:

\[
\hat{H}^U \{ \hat{\rho} \} = \hat{U} \hat{H} \{ \hat{\rho} \} \hat{U}^+ = \hat{H} \{ \hat{U}^U \}.
\]

This means that in order to understand the symmetries of the mean field, it suffices to analyze the symmetries of the underlying density matrix. The nuclear Hamiltonian is supposed to conserve numbers of protons and neutrons, and to be invariant under space rotations.
\(D(\alpha, \beta, \gamma)\), space inversion \(P\), time reversal \(T\), and rotations in the isotopic space (isorotations) \(D_\tau(\alpha_\tau, \beta_\tau, \gamma_\tau)\).

(Throughout the present paper, to denote rotations we use symbols \(D\), \(d\), and \(D\) instead of the usual letter \(R\). The symbol \(R\) is reserved for the generalized density matrix.) In the space-spin-isospin basis, the single-particle matrix elements of corresponding operators \(d\), \(p\), \(t\), and \(d_t\) are:

\[
\hat{d}^{\alpha\beta\gamma}(r's't', r, st) = \delta(r' - r)\delta_{l't'} e^{i\alpha_{l'}(r_l) e^{i\beta_{l'}(r_l) e^{i\gamma_{l'}(r_l)}} \times \hat{a}_{s'\sigma}(\sigma, \alpha\beta\gamma),
\]

\[
\hat{p}(r's't', r, st) = \delta(r' + r)\delta_{s's'} \hat{\sigma}_{l't'},
\]

\[
\hat{t}(r's't', r, st) = \delta(r' - r)(-i\hat{a}^\dagger_{s's'})\delta_{l't'} \hat{\kappa},
\]

\[
\hat{a}^{\alpha\beta\gamma\tau}_r(r's't', r, st) = \delta(r' - r)\delta_{s's'} \hat{\tau}_{l't'}(\tau, \alpha\beta\gamma\tau),
\]

respectively, where \(\hat{u}(r)\) is the single-particle orbital-angular-momentum operator, \(\hat{L}(r) = L(r) + \frac{\hbar}{2}\sigma\) is the total single-particle orbital-angular-momentum operator, \(\alpha\), \(\beta\), and \(\gamma\) (\(\alpha_r, \beta_r\), and \(\gamma_r\)) are the Euler angles of rotations in space (isospace). The spin rotation matrix \(\hat{a}_{s's'}\), being the function of the Pauli matrices and Euler angles, reads

\[
\hat{a}_{s's'}(\sigma, \alpha\beta\gamma) = (e^{i\frac{\beta}{2}\sigma_z} e^{i\frac{\alpha}{2}\sigma_y} e^{i\frac{\gamma}{2}\sigma_x})_{s's'}
\]

\[
= \cos\frac{\beta}{2} \left(\cos\frac{\gamma + \alpha}{2}\sigma_{z's'} + i \sin\frac{\gamma + \alpha}{2}\sigma_{y's'}\right) + i \sin\frac{\beta}{2} \left(\cos\frac{\alpha - \gamma}{2}\sigma_{y's'} + i \sin\frac{\gamma - \alpha}{2}\sigma_{x's'}\right),
\]

and the isospin rotation matrix \(\hat{a}_{l't'}(\tau, \alpha\beta\gamma\tau)\) is defined analogously.

Below, rotations by angle \(\pi\) about the three axes \(x\), \(y\), and \(z\), which are called signature operators, will be of particular interest:

\[
\hat{r}_x(r's't', r, st) = \hat{a}^{\alpha\beta\gamma}(r's't', r, st),
\]

\[
\hat{r}_y(r's't', r, st) = \hat{a}^{\alpha\beta\gamma}(r's't', r, st),
\]

\[
\hat{r}_z(r's't', r, st) = \hat{a}^{\alpha\beta\gamma}(r's't', r, st).
\]

Products of signature operators and the space-inversion operator, which are called simplex operators, correspond to reflections with respect to the \(y-z\), \(z-x\), and \(x-y\) planes, respectively:

\[
\hat{s}_x = \hat{r}_x \bullet \hat{p},
\]

\[
\hat{s}_y = \hat{r}_y \bullet \hat{p},
\]

\[
\hat{s}_z = \hat{r}_z \bullet \hat{p}.
\]

Symmetry operations \([43]\) form well-known group structures:

- Proper rotations \([43a]\): they belong to the orthogonal unimodular group in three dimensions \(SO(3)\).

- Improper (or mirror) rotations, i.e., rotations \([43a]\) combined with space inversion \([43b]\): they belong to the full orthogonal group \(O(3)\).

- Improper rotations supplemented by time reversal \([43c]\): they form the group called \(O^T(3)\).

- Together with the group of isorotations \([43d]\), the symmetry operations \([43]\) constitute the group \(O^T(3) \times SO(3)\).

- Space-inversion \([43b]\) together with three signatures \([45]\) and three simplexes \([46]\) constitute the point group of symmetries of a parallelepiped, called \(D_{2h}\), which is of interest for triaxial nuclei.

Due to the fact that the rotation of a spin-\(\frac{1}{2}\) system by \(2\pi\) changes sign of the wave function, one has to, in fact, double these groups (see Refs. [22, 23] for details). The doubling of groups has no bearing on the results of the present study; hence, in what follows we do not refer to it.

Although strong nuclear forces are charge-independent, i.e., invariant under rotations in isospace, the nuclear Hamiltonian is not, at least because of electromagnetic forces. Within the HFB theory, the charge independence is additionally broken by the auxiliary condition \([21]\) which is manifestly isovector. This constraint gives rise to HFB product states which violate isospin even for charge-independent Hamiltonians (see Ref. [31] for a recent discussion). If the density matrix in the p-p channel does not vanish, particle number is also violated in the HFB theory. The local energy density \(H(r)\) is usually constructed under assumption that it should be invariant \([1]\) with respect to the time reversal \(T\) and isorotations \(D_\tau\), and covariant \([2]\) with respect to the space symmetries \(D\) and \(P\), see Appendix A in Ref. [16]. All these symmetries are often spontaneously broken in mean-field theories. As discussed in the Introduction, the problem of symmetries that are conserved by \(H\) and internally broken by \(H\) is, in fact, one of the most important elements of a mean-field description of many-body systems.

### A. Symmetries in the isotopic space

As has been discussed in I, the standard case of no explicit p-n mixing can be described by the conserved p-n symmetry given by

\[
\hat{c}_3 = -i\hat{a}(\hat{r}, \pi, 00) = \hat{r}^{(3)}.
\]

That is, \(\hat{c}_3\) does not change the third isospin component but it reverses the sign of \(\hat{r}^{(1)}\) and \(\hat{r}^{(2)}\). Since \(\hat{c}_3 = -\hat{r}^{(3)}\), we obtain from Eq. [31] that

\[
\hat{c}_3 \hat{p} \hat{c}_3 = \hat{p},
\]

\[
\hat{c}_3 \hat{p} \hat{c}_3 = -\hat{p}.
\]

Consequently, in the absence of the explicit p-n mixing, the p-h density matrices have only the \(k=0\) and 3 isospin components, while the p-p densities have only the \(k=1\) and 2 isospin components.
In the presence of an additional p-n exchange symmetry (charge-reversal transformation \(C\) of Eq. (I-5) multiplied by \(i\)), defined as
\[
\hat{c}_2 = -i\hat{a}(\hat{T}, 0\pi 0) = \hat{T}^{(2)},
\]
only the \(k=0\) isospin component remains for p-h density matrix whereas the p-p has only a \(k=1\) non-vanishing isospin component. In other words, in this case proton and neutron densities are equal to each other.

B. Symmetries in the position-spin space

In this section, we discuss transformation properties of the generalized density matrices \(\hat{\mathcal{R}}\) under \(D(\alpha\beta\gamma)\), \(P\), and \(T\). In the case of rotations, the general transformation matrix \((58)\) is given by \(d\) of Eq. \((13a)\). Since the single-particle orbital angular-momentum operator is imaginary, \(\mathbf{I}(\mathbf{r}) = -\mathbf{I}(\mathbf{r})\), by applying \((21)\) to Eqs. \((13a)\) and \((34)\), one obtains:
\[
\hat{d}^{\alpha\beta\gamma}(\mathbf{r}'s't', \mathbf{r}st) = \hat{d}^{\alpha\beta\gamma}(\mathbf{r}'s't', \mathbf{r}st),
\]
i.e., the density matrices in both channels, \(\hat{\mathbf{d}}\) and \(\hat{\mathbf{d}}\), transform under rotations in the same way, and the generalized rotation matrix has a simple form:
\[
\hat{\mathcal{D}}(\alpha\beta\gamma) = \begin{pmatrix}
\hat{d}^{\alpha\beta\gamma} & 0 \\
0 & \hat{d}^{\beta\gamma}\end{pmatrix}.
\]
When applying this symmetry operation to the generalized density matrix \((54)\), we need to use the Hermitian-conjugate matrix, \((\hat{d}^{\alpha\beta\gamma})^\dagger\):

and Pauli matrices that transform as vectors under the spin matrix \(\hat{a}\), i.e.,
\[
\hat{a}(\hat{\sigma}, \alpha\beta\gamma) \hat{a}^\dagger(\hat{\sigma}, \alpha\beta\gamma) = \sum_b a_{ab}(\alpha\beta\gamma) \hat{a}^b,
\]
for \(a, b = x, y, z\), where the Cartesian rotation matrix reads
\[
a(\alpha\beta\gamma) = \begin{pmatrix}
cos \alpha \cos \beta \cos \gamma & -\cos \alpha \cos \beta \sin \gamma & \cos \alpha \sin \beta \\
\cos \alpha \cos \beta \sin \gamma & -\cos \alpha \cos \beta \cos \gamma & -\cos \alpha \sin \beta \\
-\sin \alpha \cos \gamma & \sin \alpha \cos \gamma & \sin \alpha \sin \beta
\end{pmatrix}.
\]
Similarly, the rotation matrix \((53)\) also rotates the position arguments, \(\mathbf{r}\) and \(\mathbf{r}'\), of the density matrices. Finally, we have
\[
\hat{\rho}^D(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{8} \rho_0(\mathbf{a}r, \mathbf{a}r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{a}r, \mathbf{a}r') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{a}r, \mathbf{a}r') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{55a}
\]
\[
\hat{\rho}^D(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{8} \rho_0(\mathbf{a}r, \mathbf{a}r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{a}r, \mathbf{a}r') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{a}r, \mathbf{a}r') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{55b}
\]

The inversion matrix \((43b)\) is evidently real and symmetric, and it does not depend on \(\hat{\sigma}\) and \(\hat{T}\). Thus, we also have \(\hat{\rho}(\mathbf{r}'s't', \mathbf{r}st) = \hat{\rho}(\mathbf{r}'s't', \mathbf{r}st)\), and
\[
\hat{\rho}^P(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{4} \rho_0(\mathbf{a}r, \mathbf{a}r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(-\mathbf{r}, -\mathbf{r}') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(-\mathbf{r}, -\mathbf{r}') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{56a}
\]
\[
\hat{\rho}^P(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{4} \rho_0(\mathbf{a}r, \mathbf{a}r') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(-\mathbf{r}, -\mathbf{r}') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(-\mathbf{r}, -\mathbf{r}') \circ \hat{T}_{tt'} + \frac{1}{4} \delta_{0}(\mathbf{a}r, \mathbf{a}r') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{56b}
\]

The time reversal \(T\) is an antilinear operation and has the form given in Eq. \((30)\) with the corresponding single-particle time-reversal density matrix \(\hat{\mathbf{t}}\) given in Eq. \((13c)\). It transforms all the position-dependent densities and the isospin Pauli matrices \(\hat{T}\) to their complex conjugate partners and changes signs of \(\hat{\sigma}\). Therefore, \(\hat{\mathbf{t}}(\mathbf{r}'s't', \mathbf{r}st) = \hat{\mathbf{t}}(\mathbf{r}'s't', \mathbf{r}st)\), and the time-reversal densities are:
\[
\hat{\rho}^T(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{4} \rho_0(\mathbf{r}, \mathbf{r}') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{r}, \mathbf{r}') \circ \hat{T}_{tt'} - \frac{1}{4} \delta_{0}(\mathbf{r}, \mathbf{r}') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} - \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{r}, \mathbf{r}') \circ \hat{T}_{tt'} - \frac{1}{4} \delta_{0}(\mathbf{r}, \mathbf{r}') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{57a}
\]
\[
\hat{\rho}^T(\mathbf{r}st, \mathbf{r}'s't') = \frac{1}{4} \rho_0(\mathbf{r}, \mathbf{r}') \delta_{ss'} \delta_{tt'} + \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{r}, \mathbf{r}') \circ \hat{T}_{tt'} - \frac{1}{4} \delta_{0}(\mathbf{r}, \mathbf{r}') \cdot (a\hat{\sigma})_{ss'} \delta_{tt'} - \frac{1}{4} \delta_{ss'} \hat{\rho}(\mathbf{r}, \mathbf{r}') \circ \hat{T}_{tt'} - \frac{1}{4} \delta_{0}(\mathbf{r}, \mathbf{r}') \cdot (a\hat{\sigma})_{ss'} \circ \hat{T}_{tt'}\tag{57b}
\]
From Eqs. \((55b), (56b),\) and \((57b)\) we conclude that the density matrix \(\hat{\rho}\) in the p-p channel transforms under
all position-spin transformations considered here in the same way as the p-h density matrix \( \hat{\rho} \). In other words, the generalized transformation matrices of \( \hat{P} \) and \( \hat{T} \) have the same general structures as that of rotations, \( \hat{D} \), given in Eq. \( \text{(61)} \).

IV. SYMMETRY PROPERTIES OF DENSITIES

We begin by recalling general symmetry properties of nonlocal densities, which have been given in I. Since the p-h density matrix \( \text{(58a)} \) and the Pauli matrices are both Hermitian, all the p-h densities are Hermitian as well:

\[
\rho_k(r, r') = \rho_k^\ast(r', r), \quad (58a)
\]

\[
s_k(r, r') = s_k^\ast(r', r), \quad (58b)
\]

for \( k = 0, 1, 2, 3 \); hence, their real parts are symmetric, while the imaginary parts are antisymmetric, with respect to exchanging \( r \) and \( r' \).

Similarly, transformation properties of Pauli matrices under \( TC \) \( \text{(81)} \) imply that 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:

\[
\tilde{\rho}_k(r, r') = (-1)^{t_0 + 1} \tilde{\rho}_k(r', r), \quad (59a)
\]

\[
\tilde{s}_k(r, r') = (-1)^{t_0} \tilde{s}_k(r', r), \quad (59b)
\]

for \( k = 0, 1, 2, 3 \), where \( t_0 = 0 \) (isoscalars) and \( t_{1,2,3} = 1 \) (isovectors). Equations \( \text{(58a)} \) and \( \text{(59a)} \) are fulfilled independently of any other symmetries conserved by the system; they result from definitions of density matrices \( \hat{\rho} \) and \( \hat{\tilde{\rho}} \).

A. Spherical symmetry

1. Spherical and space-inversion symmetries

Let us suppose that the generalized density matrix is invariant under the transformations of Eqs. \( \text{(65a)} \) and \( \text{(65b)} \) forming the full orthogonal group \( O(3) = \text{P} \otimes \text{SO}(3) \otimes \text{SO}(3) \), which is the direct product of the group of proper rotations \( \text{SO}(3) \) and the two-element group \( \text{P} \) of the space inversion. It means that \( \hat{R}^D = \hat{R}^P = \hat{R}^{DP} = \hat{R} \), and these symmetries impose the following conditions on nonlocal densities:

\[
\rho_k(r, r') = \rho_k(\varsigma r, \varsigma r'), \quad (60a)
\]

\[
\tilde{\rho}_k(r, r') = \tilde{\rho}_k(\varsigma r, \varsigma r'), \quad (60b)
\]

\[
s_k(r, r') = a^\ast s_k(\varsigma r, \varsigma r'), \quad (60c)
\]

\[
\tilde{s}_k(r, r') = a^\ast \tilde{s}_k(\varsigma r, \varsigma r'), \quad (60d)
\]

for \( k = 0, 1, 2, 3 \), and for arbitrary Euler angles \( \alpha, \beta, \gamma \) that are arguments of the rotation matrix \( a \). The factor \( c \) is equal to +1 for rotations and −1 for improper rotations.

The full \( O(3) \) symmetry imposes quite strong conditions on the nonlocal densities. Equations \( \text{(60a)} \) and \( \text{(60b)} \) tell us that, due to the Generalized Cayley-Hamilton (GCH) theorem (see Appendix A), scalar densities, \( \rho_k \) and \( \tilde{\rho}_k \), depend on \( r \) and \( r' \) through rotational invariants \( r \cdot r' = r^2 \), \( r' \cdot r' = r'^2 \), and \( r \cdot r' \), i.e.,

\[
\rho_k(r, r') = \rho_k(r^2, r' \cdot r', r'^2), \quad (61a)
\]

\[
\tilde{\rho}_k(r, r') = \tilde{\rho}_k(r^2, r' \cdot r', r'^2), \quad (61b)
\]

for \( k = 0, 1, 2, 3 \).

Similarly, from Eqs. \( \text{(60c)} \) and \( \text{(60d)} \), we see that vector densities, \( s_k \) and \( \tilde{s}_k \), are pseudovectors. At the same time, they are functions of two vectors, \( r \) and \( r' \). The only pseudovector that can be constructed from two vectors is their vector product \( r \times r' \) — therefore, all pseudovector densities, \( s_k \) and \( \tilde{s}_k \), for \( k = 0, 1, 2, 3 \), have the form

\[
s_k(r, r') = i(r \times r') s_k(r^2, r' \cdot r', r'^2), \quad (62a)
\]

\[
\tilde{s}_k(r, r') = (r \times r') \tilde{s}_k(r^2, r' \cdot r', r'^2). \quad (62b)
\]

For the sake of convenience, in the definition \( \text{(62a)} \), we have introduced the imaginary unit \( i \).

Due to the general symmetry properties \( \text{(58a)} \) and \( \text{(59a)} \), scalar functions that define the nonlocal densities must obey the following conditions:

\[
\rho_k(r^2, r' \cdot r', r'^2) = \rho_k(r'^2, r \cdot r', r^2), \quad (63a)
\]

\[
\tilde{\rho}_k(r^2, r' \cdot r', r'^2) = (-1)^{t_0 + 1} \tilde{\rho}_k(r'^2, r \cdot r', r^2), \quad (63b)
\]

and

\[
s_k(r^2, r' \cdot r', r'^2) = s_k(r'^2, r \cdot r', r^2), \quad (64a)
\]

\[
\tilde{s}_k(r^2, r' \cdot r', r'^2) = (-1)^{t_0 + 1} \tilde{s}_k(r'^2, r \cdot r', r^2). \quad (64b)
\]

This means that nonlocal p-h densities \( \rho_k \) and \( \tilde{\rho}_k \), are Hermitian, while nonlocal isoscalar and isovector p-p densities \( \rho_k \) and \( \tilde{\rho}_k \) are antisymmetric and symmetric functions of \( r \) and \( r' \), respectively.

The above symmetry properties of densities imply strong conditions on local densities. For instance, Eqs. \( \text{(61a)} \) – \( \text{(61b)} \) imply that

\[
\rho_k(r) = \rho_k(r, r) = \rho_k(r) = \rho_k^*(r), \quad (65a)
\]

\[
\tilde{\rho}(r) = \tilde{\rho}(r, r) = \tilde{\rho}(r), \quad (65b)
\]

and

\[
s_k(r) \equiv s_k(r, r) = 0, \quad (66a)
\]

\[
\tilde{s}_0(r) \equiv \tilde{s}_0(r, r) = 0, \quad (66b)
\]

i.e., the scalar local p-h densities \( \rho_k \), and isovector scalar local p-p densities \( \tilde{\rho} \), depend on the radial variable \( r \) only, \( \rho_k \) are real, and all vector local p-h densities \( s_k \) and the isovector vector local p-p density \( \tilde{s}_0 \) vanish. At this point, we remind the reader that conditions \( \text{(59a)} \) imply that
local p-p densities $\tilde{\rho}_0$ and $\tilde{\tau}$ always vanish, irrespective of any other symmetries being imposed or not, see Table IV in I.

All local derivative densities can be derived from Eqs. (61) and (62) by using expressions for gradients of scalar functions, e.g.,

$$\nabla \rho(r^2, r \cdot r', r'^2) = 2 \frac{\partial \rho}{\partial (r^2)} r + \frac{\partial \rho}{\partial (r \cdot r')} r', \quad (67a)$$

$$\nabla' \rho(r^2, r \cdot r', r'^2) = \frac{\partial \rho}{\partial (r^2)} r + 2 \frac{\partial \rho}{\partial (r^2')} r', \quad (67b)$$

which are linear combinations of vectors $r$ and $r'$ with scalar coefficients (again illustrating the GCH theorem). In this way, all local derivative densities can be expressed through derivatives of the scalar functions $\rho_k$, $\tilde{\rho}_k$, $s_k$, and $\tilde{s}_k$. Alternatively, one can employ the GCH theorem to build local scalar, pseudoscalar, vector, pseudovector, and symmetric-traceless-pseudotensor densities from the single position vector $r$, and we follow this path below.

Pseudoscalar, pseudovector, and pseudotensor densities cannot be built from the position vector $r$. Therefore, they must all vanish:

$$T_k(r) = 0, \quad (68a)$$
$$\tilde{T}_0(r) = 0, \quad (68b)$$
$$F_k(r) = 0, \quad (68c)$$
$$\tilde{F}_0(r) = 0, \quad (68d)$$
$$J_k(r) = 0, \quad (68e)$$
$$\tilde{J}_0(r) = 0, \quad (68f)$$
$$\tilde{J}_{ab}(r) = 0, \quad (68g)$$
$$\tilde{J}_0(r) = 0, \quad (68h)$$

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

The local scalar kinetic densities must have properties analogous to those of scalar densities in Eqs. (65), i.e.,

$$\tau_k(r) \equiv \tau_k(r, r) = \tau_k(r), \quad (69a)$$
$$\tilde{\tau}(r) = \tilde{\tau}(r, r) = \tilde{\tau}(r), \quad (69b)$$

and all local vector densities must be proportional to $r$, i.e.,

$$J_k(r) = J_{kr}(r)e_r = J_{kr}^*(r)e_r, \quad (70a)$$
$$\tilde{J}_0(r) = \tilde{J}_0^*(r)e_r, \quad (70b)$$
$$J_k(r) = J_{kr}(r)e_r = J_{kr}^*(r)e_r, \quad (70c)$$
$$\tilde{J}(r) = \tilde{J}(r)e_r. \quad (70d)$$

where $e_r = \frac{\hat{r}}{r}$ is the unit vector in radial direction. In addition, the radial components $j_k^*$ and $J_{kr}$ are real.

Conditions on local densities, presented in this section, can be further restricted by imposing the time-reversal and/or p-n symmetries, see Table IV of I. The conditions on local time-even and proton-neutron-symmetric p-h and p-p densities are exactly those as in Ref. [32], whereupon properties of the p-p densities exactly mirror those of the p-h densities. Such a mirroring does not hold if time-reversal or p-n symmetries are broken.

For a broken time-reversal symmetry and conserved p-n symmetry two modifications occur: (i) the isovector p-p densities $\tilde{\rho}(r), \tilde{\tau}(r)$, and $\tilde{J}_0(r)$ become complex, while the p-h densities $\rho_k(r), \tau_k(r)$, and $J_{kr}(r)$ still remain real [32], and (ii) the current p-h density $\tilde{j}_k(r)$ does not vanish. It is interesting to see that in this case the only non-zero time-odd density is the current density, i.e., spin polarizations are not allowed and only the flow of particles in the radial direction (a breathing mode) is permitted if the spherical and space-inversion symmetries are present.

It is also interesting to see that the spherical and space-inversion symmetries impose very strong restrictions on the isoscalar pairing densities. Indeed, the isoscalar pairing density $\tilde{s}_0(r)$ must then vanish [33]. The only allowed isoscalar-pairing channel can be related to the p-p current density $\tilde{j}_0(r)$, which represents a radial flow of isoscalar pairs within a nucleus. Such a flow can be, in fact, non-zero either in the time-even or time-odd case, represented by $\tilde{R}(\tilde{j}_0)(r)$ or $\tilde{3}(\tilde{j}_0)(r)$, respectively. It corresponds to the situation in which p-n pairs locally change into the neutron-proton pairs, or vice versa, while the sum of densities thereof remains constant.

2. Spherical symmetry alone

Let us consider the unusual case of the SO(3)$\subset O(3)$ symmetry, in which the spherical symmetry of the generalized density matrix is conserved, whereas the space inversion symmetry is broken. As compared to the results presented in the previous section IV A 1, here, properties of scalar nonlocal densities, Eqs. (60), remain the same. However, in Eqs. (60) $\varsigma$ is always equal to +1, meaning that there is no difference between vectors and pseudovectors. Thus, vector nonlocal densities can now have structures that are richer than those of Eqs. (62). Indeed, due to the GCH theorem, these densities can be linear combinations of the pseudovector $\mathbf{r} \times \mathbf{r}'$ and vectors $\mathbf{r}$ and $\mathbf{r}'$.

Hence, vector densities in the p-h and p-p channels can now be presented in the form:

$$s_k(r, r') = i(r \times r')s_k(r^2, r \cdot r', r'^2) + r's_k^*(r^2, r \cdot r', r'^2), \quad (71a)$$
$$\tilde{s}_k(r, r') = (r \times r')\tilde{s}_k(r^2, r \cdot r', r'^2) + r's_k^*\tilde{s}_k^*(r^2, r \cdot r', r'^2), \quad (71b)$$

where scalar functions $s_k$ and $\tilde{s}_k$ obey previous conditions [34], while scalar functions $s_k^*$ and $\tilde{s}_k^*$ are arbitrary.

Breaking the parity does not affect the local scalar densities in both channels and Eqs. (60) and (60) are still valid. The same is true for vector current densities of Eqs. (70a) and (70b) being gradients of scalar densities.
On the other hand, the local spin densities no longer vanish. The isoscalar and isovector components of the p-h spin density are

\[ s_k(r) = s_{kr}(r)e_r, \quad (72) \]

where their radial components \( s_{kr} \) are real for \( k = 0, 1, 2, 3 \). The p-p isoscalar spin density has a complex radial component and reads:

\[ \tilde{s}_0(r) = \tilde{s}_{0r}(r)e_r. \quad (73) \]

Spin-kinetic and tensor-kinetic densities have the same structures as the spin densities of Eqs. (72) and (73), namely

\[
\begin{align*}
T_k(r) &= T_{kr}(r) e_r, \quad (74a) \\
F_k(r) &= F_{kr}(r) e_r, \quad (74b)
\end{align*}
\]

for all \( k \)'s and

\[
\begin{align*}
\tilde{T}_0(r) &= \tilde{T}_{0r}(r) e_r, \quad (75a) \\
\tilde{F}_0(r) &= \tilde{F}_{0r}(r) e_r. \quad (75b)
\end{align*}
\]

When the parity is not conserved, the tensor densities have, apart from the antisymmetric parts represented by vectors of Eqs. (70c) and (70d), also non-vanishing traces, namely

\[
\begin{align*}
J_k(r) &= J_{kr}(r) = J_k^*(r), \quad (76a) \\
\tilde{J}(r) &= \tilde{J}(r), \quad (76b)
\end{align*}
\]

and symmetric traceless parts have the following structure:

\[
\begin{align*}
\jmath_{ab}(r) &= \frac{1}{2} \jmath_{arr}(r) \mathcal{S}_{ab} = \frac{1}{2} \jmath_{arr}(r) \mathcal{S}_{ab}, \quad (77a) \\
\tilde{\jmath}_{ab}(r) &= \frac{1}{2} \tilde{\jmath}_{arr}(r) \mathcal{S}_{ab}. \quad (77b)
\end{align*}
\]

where the standard symmetric traceless tensor function of the space vector \( r \) is defined as

\[ \mathcal{S}_{ab} = 3 \frac{r_ar_b}{r^2} - \delta_{ab}. \quad (78) \]

3. Spherical symmetry - summary

When the spherical O(3) symmetry is conserved, all the local densities can be treated as fields depending on the O(3) vector \( r \) (see Appendix A). Then, vector \( r \) itself is the only one elementary vector and its length squared \( r^2 \) is the only one elementary scalar. The scalar densities are functions of \( r^2 \). The vector densities are pointing along \( r \), and their radial components depend on \( r^2 \) only.

The pseudoscalar, pseudovector, and pseudotensor densities all vanish. They can become non-vanishing when the parity is broken and only the rotational SO(3) symmetry remains conserved. Then, they have properties of the scalar, vector, and tensor densities, respectively. The symmetric tensor densities are proportional to outer product \( r \otimes r \).

In general, the p-h densities are real whereas the p-p densities are complex. Additional symmetries (space inversion, time-reversal, p-n symmetry), when conserved, can cause additionally some isoscalars or isovector p-h densities to vanish, and those in the p-p channel become either purely real or purely imaginary, or vanish. In Tables II and III we list all the local SO(3)-invariant densities in cases when additional symmetries are broken or conserved.

B. Axial symmetry

While the spherical symmetry of the mean field is often broken, the axial symmetry is usually conserved in the presence of time reversal. Here we discuss consequences of conserved symmetry of Eq. (43a) with \( \beta = 0 \) and \( \gamma = 0 \), and the transformation of Eq. (46a), forming together group \( O(2) = S_z \otimes O(2) \subset O(3) \), which is the direct product of the rotations \( SO(2) \) about the \( z \)-axis and the reflection \( S_z \) in the plane perpendicular to this axis. For rotations about the \( z \)-axis, the Cartesian rotation matrix (54) takes the form:

\[ a(\alpha 00) = \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (79) \]

It is now convenient to decompose the position vectors as

\[ r = r_\perp + z, \quad (80) \]

where \( r_\perp \) is a two-dimensional vector perpendicular to the \( z \)-axis and \( z \) is the \( z \)-component vector of \( r \).

Since \( -a^+(\alpha) = a^+(\alpha + \pi) \), the \( O^+(2) = S_z \otimes O^+(2) \) symmetry of the generalized density matrix implies the following conditions for the nonlocal densities:

\[
\begin{align*}
\rho_k(r, r') &= \rho_k(a^+r_\perp + cz, a^+r'_\perp + cz'), \quad (81a) \\
\tilde{\rho}_k(r, r') &= \tilde{\rho}_k(a^+r_\perp + cz, a^+r'_\perp + cz'), \quad (81b) \\
s_k(r, r') &= s_k(a^+r_\perp + cz, a^+r'_\perp + cz') \\
+ &s_{k\parallel}(a^+r_{\perp} + cz, a^+r'_{\perp} + cz')e_z, \quad (81c) \\
\tilde{s}_k(r, r') &= \tilde{s}_k(a^+r_\perp + cz, a^+r'_\perp + cz') \\
+ &\tilde{s}_{k\parallel}(a^+r_{\perp} + cz, a^+r'_{\perp} + cz')e_z, \quad (81d)
\end{align*}
\]

where \( e_z \) is the unit vector \( (z = ze_z) \) and \( \varsigma \) is the sign of the determinant of the orthogonal \( O^+(2) \) transformation.
### TABLE I: Properties of local particle-hole rotationally symmetric (SO(3)-invariant) densities, depending on the conserved (C) or broken (B) space-inversion (P), proton-neutron (p-n), or time-reversal (T) symmetries. Generic real, imaginary, or complex functions of the radial variable \( r \) are denoted by \( f_R(r) \), \( f_I(r) \), or \( f_C(r) \), respectively.

| symmetry | \( P \) | \( p-n \) | \( T \) | conserved (C) | broken (B) |
|----------|--------|----------|------|-------------|------------|
| \( \rho_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( \rho_1 \) | \( f_R(r) \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) |
| \( \rho_2 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( \tau_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( \tau_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( J_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( J_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( J_2 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( s_{0,3} \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( s_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( s_2 \) | \( f_R(r) \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) |
| \( T_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) |
| \( T_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( F_0 \) | \( f_R(r) \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) |
| \( F_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( F_2 \) | \( f_R(r) \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) |
| \( J_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( J_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( J_2 \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( L_{0,3} \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) | \( f_R(r) \) |
| \( L_1 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |
| \( L_2 \) | \( f_R(r) \) | 0 | 0 | \( f_R(r) \) | 0 | 0 |

### TABLE II: Similar to Table I except for the particle-particle densities.

| symmetry | \( P \) | \( p-n \) | \( T \) | conserved (C) | broken (B) |
|----------|--------|----------|------|-------------|------------|
| \( \rho_{1} \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( \rho_2 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( \rho_3 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( \tau_1 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( \tau_2 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( \tau_3 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( J_1 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( J_2 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( J_3 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( s_0 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( T_0 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( F_0 \) | \( f_C(r) \) | \( f_C(r) \) | 0 | 0 | \( f_C(r) \) |
| \( J_1 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( J_2 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( J_3 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( L_1 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
| \( L_2 \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) | \( f_C(r) \) |
In this case, Eqs. (81a) and (81b) imply that the scalar densities \( p_k \) and \( \tilde{p}_k \) depend on \( r \) and \( r' \) through the \( O^{\perp}(2) \) invariants \( z \cdot z = z^2 \), \( z' \cdot z' = z'^2 \), \( z \cdot z' = z z' \), \( r_\perp \cdot r_\perp = r^2 \), \( r'_\perp \cdot r'_\perp = r'^2 \), and \( r_\perp \cdot r'_\perp \). Apart from the invariants, there are two \( O^{\perp}(2) \) pseudoscalars: \( z \cdot (r_\perp \times r'_\perp) \) and \( z' \cdot (r_\perp \times r'_\perp) = (z' / z^2) z \cdot (r_\perp \times r'_\perp) \). The spin nonlocal densities have the following transformation properties under the \( O^{\perp}(2) \). Their \( z \)-components are the \( O^{\perp}(2) \) scalars. Their perpendicular components are the \( S_2 \) pseudoscalars (i.e., they change sign under \( S_2 \)). Because the spin densities are the \( O(3) \) pseudovectors, their components that are parallel to the \( z \)-axis should be linear combinations of \( r_\perp \times r'_\perp \), \([z \cdot (r_\perp \times r'_\perp)]z\), and \([z' \cdot (r_\perp \times r'_\perp)]z'\), while the perpendicular components should be linear combinations of \( z \times r_\perp \), \( z' \times r'_\perp \), \([z \cdot (r_\perp \times r'_\perp)]r_\perp \), and \([z' \cdot (r_\perp \times r'_\perp)]r'_\perp \). Consequently, the Hermitian nonlocal spin densities in the \( p-h \) channel should have the following structure:

\[
s_{kz}(r, r')e_z = i(r_\perp \times r'_\perp)\theta_{kz}(r, r')
+ [z \cdot (r_\perp \times r'_\perp)]z\phi_{kz}(r, r')
- [z' \cdot (r_\perp \times r'_\perp)]z'\bar{\phi}_{kz}(r, r'),
\]

\[
s_{k\perp}(r, r') = (z \times r_\perp)\theta_{k\perp}(r, r')
+ (z' \times r'_\perp)\bar{\phi}_{k\perp}(r, r')
- [z \cdot (r_\perp \times r'_\perp)]r_\perp\phi_{k\perp}(r, r')
- [z' \cdot (r_\perp \times r'_\perp)]r'_\perp\bar{\phi}_{k\perp}(r, r'),
\]

where \( \theta_{kz} \), \( \phi_{kz} \), \( \theta_{k\perp} \), and \( \bar{\phi}_{k\perp} \) are scalar functions. The pseudovector nonlocal densities in the \( p-h \) channel are either symmetric or antisymmetric in \( r \) and \( r' \). Therefore, we have

\[
s_{0z}(r, r')e_z = (r_\perp \times r'_\perp)\bar{\theta}_{0z}(r, r')
+ [z \cdot (r_\perp \times r'_\perp)]z\bar{\phi}_{0z}(r, r')
- [z' \cdot (r_\perp \times r'_\perp)]z'\phi_{0z}(r, r'),
\]

\[
\bar{s}_z(r, r')e_z = (r_\perp \times r'_\perp)\bar{\phi}_{0z}(r, r')
+ [z \cdot (r_\perp \times r'_\perp)]z\bar{\theta}_{0z}(r, r')
- [z' \cdot (r_\perp \times r'_\perp)]z'\phi_{0z}(r, r'),
\]

\[
s_{0\perp}(r, r') = (z \times r_\perp)\phi_{0\perp}(r, r')
+ (z' \times r'_\perp)\bar{\theta}_{0\perp}(r, r')
- [z \cdot (r_\perp \times r'_\perp)]r_\perp\phi_{0\perp}(r, r')
- [z' \cdot (r_\perp \times r'_\perp)]r'_\perp\bar{\theta}_{0\perp}(r, r'),
\]

where \( \bar{\theta}_{0z} \), \( \bar{\phi}_{0z} \), \( \phi_{0\perp} \), and \( \bar{\theta}_{0\perp} \) are arbitrary scalar functions, while \( \bar{\phi}_{0z} \) and \( \bar{\theta}_{0\perp} \) are antisymmetric and symmetric scalars, respectively.

The local scalar \( p-h \) and \( p-p \) densities are functions of two invariants, \( z^2 \) and \( r^2 \). The particle density \( \rho_k(z^2, r^2) \) for \( k = 0, 1, 2, 3 \) is real whereas the pairing density \( \tilde{\rho}(z^2, r^2) \) is complex in general; hence,

\[
\rho_k(r) \equiv \rho_k(r, r) = \rho_k(z^2, r^2) = \rho_k(z^2, r^2),
\]

\[
\tilde{\rho}(r) \equiv \tilde{\rho}(r, r) = \tilde{\rho}(z^2, r^2).
\]

Differentiable operators \( \nabla_z \) and \( \nabla_\perp \) have the same transformation properties under the \( O^{\perp}(2) \) transformations as \( z \) and \( r_\perp \), respectively. That is, \( \nabla_z \) and \( z \) are \( S_2 \) pseudo-invariants and \( SO^{\perp}(2) \) invariants, whereas \( \nabla_\perp \) and \( r_\perp \) are \( S_2 \) invariants and \( SO^{\perp}(2) \) vectors. Counters of Eqs. (67a) and (67b) for gradients of scalar functions are now linear combinations of vectors \( z \), \( z' \), \( r_\perp \), and \( r'_\perp \) with scalar coefficients:

\[
(\nabla_z + \nabla_\perp)\rho(z^2, z', z^2, r^2, r_\perp \cdot r'_\perp, r_\perp \cdot r'_\perp) = 2\frac{\partial \rho}{\partial (z^2)} + \frac{\partial \rho}{\partial (z' z)} \frac{\partial}{\partial (z' z)}
+ 2\frac{\partial \rho}{\partial (r_\perp \cdot r'_\perp)} + \frac{\partial \rho}{\partial (r_\perp \cdot r'_\perp)} r_\perp \cdot r'_\perp.
\]

Both terms of the operator:

\[
\nabla \cdot \nabla' = \nabla_z \cdot \nabla_\perp + \nabla_\perp \cdot \nabla_\perp
\]

are \( O^{\perp}(2) \) scalars. Therefore, the local scalar kinetic densities:

\[
\tau_k(z^2, r^2) = [(\nabla_z \cdot \nabla'_z + \nabla_\perp \cdot \nabla'_\perp)\rho_k(r, r')]|_{r=r'}
\]

\[
\tilde{\tau}(z^2, r^2) = [(\nabla_z \cdot \nabla'_z + \nabla_\perp \cdot \nabla'_\perp)\tilde{\rho}(r, r')]|_{r=r'}
\]

can be expressed as sums of the two \( O^{\perp}(2) \) scalars. Since the operator \( \mathbf{S}_0 \) is Hermitian, again the \( p-h \) densities are real and the \( p-p \) ones are complex.

It is seen from Eqs. (82) and (83) that the spin densities in both channels are parallel to the vector product \( z \times r_\perp \) and take the form:

\[
s_k(r) = \theta_{k\perp}(z^2, r^2) (z \times r_\perp),
\]

\[
\bar{s}_0 = \phi_{0\perp}(z^2, r^2) (z \times r_\perp),
\]

with real \( \theta_{k\perp} \) and complex \( \phi_{0\perp} \). Applying Eq. (53) to Eqs. (82) and (83), we find that the spin-kinetic and tensor-kinetic densities in both channels can be written as:

\[
T_k(r) = [(\nabla_z \cdot \nabla'_z + \nabla_\perp \cdot \nabla'_\perp) s_k(r, r')]|_{r=r'}
= \theta_{k}(z^2, r^2) (z \times r_\perp),
\]

\[
\bar{T}_0(r) = [(\nabla_z \cdot \nabla'_z + \nabla_\perp \cdot \nabla'_\perp) \bar{s}_0(r, r')]|_{r=r'}
= \phi_{0}(z^2, r^2) (z \times r_\perp),
\]
\[ F_k(r) = \frac{1}{2} \left\{ (\nabla_z \times \nabla_{r}) \cdot \left( (\nabla_z \times \nabla_{r}) \cdot s_k(r, r') \right) \right\}_{r=r'}^r \]

\[ + \left\{ (\nabla_z \times \nabla_{r}) \cdot \left( (\nabla_z + \nabla_{r}) \cdot s_k(r, r') \right) \right\}_{r=r'}^r \]

\[ = \varphi_k (z^2, r_{\perp}^2) (z \times r_{\perp}), \quad (90a) \]

\[ \tilde{F}_0(r) = \frac{1}{2} \left\{ (\nabla_z \times \nabla_{r}) \cdot \left( (\nabla_z + \nabla_{r}) \cdot \bar{s}_0(r, r') \right) \right\}_{r=r'}^r \]

\[ + \left\{ (\nabla_z \times \nabla_{r}) \cdot \left( (\nabla_z + \nabla_{r}) \cdot \bar{s}_0(r, r') \right) \right\}_{r=r'}^r \]

\[ = \bar{\varphi}_0 (z^2, r_{\perp}^2) (z \times r_{\perp}), \quad (90b) \]

The scalar functions \( \varphi_k \) and \( \varphi_0 \) are real whereas \( \bar{\varphi}_0 \) and \( \bar{\varphi}_0 \) are, in general, complex. Equations \( (90a) \) and \( (90b) \) imply that the vector current densities in both channels are spanned by vectors \( z \) and \( r_{\perp} \), and read

\[ \tilde{j}_k(r) = i_{\perp k} (z^2, r_{\perp}^2) z + i_{k,\perp} (z^2, r_{\perp}^2) r_{\perp}, \quad (91a) \]

\[ \tilde{j}_0(r) = i_{b z} (z^2, r_{\perp}^2) z + i_{z, \perp} (z^2, r_{\perp}^2) r_{\perp}, \quad (91b) \]

where \( i_{k,\perp}, i_{k,\perp}, i_{b z}, \) and \( i_{z, \perp} \) are scalar functions. The p-h currents are real and the p-p current is complex.

The spin-current pseudotensor densities can be decomposed according to:

\[ j_k(r) = j_k^r(r) + j_k^z(r), \quad (92a) \]

\[ \tilde{j}(r) = \tilde{j}^r(r) + \tilde{j}^z(r), \quad (92b) \]

where

\[ j_k^r(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \otimes s_k(r, r') \right\}_{r=r'}^r, \quad (93a) \]

\[ j_k^z(r) = \frac{1}{2i} \left\{ (\nabla_{r} \times \nabla_{r}) \otimes s_k(r, r') \right\}_{r=r'}^r, \quad (93b) \]

\[ j_k^{\perp}(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \otimes s_k(r, r') \right\}_{r=r'}^r \]

\[ + (\nabla_{r} \times \nabla_{r}) \otimes s_k(r, r') \right\}_{r=r'}^r, \quad (93c) \]

\[ \tilde{j}^z(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \otimes \bar{s}_z(r, r') \right\}_{r=r'}^r, \quad (93d) \]

\[ \tilde{j}^{\perp}(r) = \frac{1}{2i} \left\{ (\nabla_{r} \times \nabla_{r}) \otimes \bar{s}_z(r, r') \right\}_{r=r'}^r, \quad (93e) \]

\[ \tilde{j}^{\perp}(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \otimes \bar{s}_{\perp}(r, r') \right\}_{r=r'}^r \]

\[ + (\nabla_{r} \times \nabla_{r}) \otimes \bar{s}_{\perp}(r, r') \right\}_{r=r'}^r. \quad (93f) \]

The traces of the spin-current pseudotensors:

\[ j_k(r) = j_k^r(r) + j_k^z(r), \quad (94a) \]

\[ \tilde{j}(r) = \tilde{j}^r(r) + \tilde{j}^z(r), \quad (94b) \]

where

\[ j_k^r(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \cdot s_k(r, r') \right\}_{r=r'}^r, \quad (95a) \]

\[ j_k^z(r) = \frac{1}{2i} \left\{ (\nabla_{r} \times \nabla_{r}) \cdot s_k(r, r') \right\}_{r=r'}^r, \quad (95b) \]

\[ \tilde{j}^z(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \cdot \bar{s}_z(r, r') \right\}_{r=r'}^r, \quad (95c) \]

\[ \tilde{j}^{\perp}(r) = \frac{1}{2i} \left\{ (\nabla_{r} \times \nabla_{r}) \cdot \bar{s}_{\perp}(r, r') \right\}_{r=r'}^r. \quad (95d) \]

are the scalar products of gradient operators and spin densities. Since \( j_k \) and \( \tilde{j} \) are sums of \( O(2) \) pseudo-scalars, they cannot be constructed from two vectors \( z \) and \( r_{\perp} \); hence, all spin currents \( \tilde{j}(r) \) must vanish. On the other hand, the \( O(3) \) vectors coming from the anti-symmetric parts of spin-current pseudotensors:

\[ j_k(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \cdot s_k(r, r') \right\}_{r=r'}^r \]

\[ + (\nabla_{r} \times \nabla_{r}) \cdot s_k(r, r') \right\}_{r=r'}^r, \quad (96a) \]

\[ \tilde{j}(r) = \frac{1}{2i} \left\{ (\nabla_z \times \nabla_{r}) \cdot \bar{s}_z(r, r') \right\}_{r=r'}^r \]

\[ + (\nabla_{r} \times \nabla_{r}) \cdot \bar{s}_z(r, r') \right\}_{r=r'}^r, \quad (96b) \]

do not vanish. They can be decomposed in the same way as the current vectors \( (81) \):

\[ j_k(r) = v_{k,\perp} (z^2, r_{\perp}^2) z + v_{k,\perp} (z^2, r_{\perp}^2) r_{\perp}, \quad (97a) \]

\[ \tilde{j}(r) = \tilde{v}_z (z^2, r_{\perp}^2) z + \tilde{v}_{\perp} (z^2, r_{\perp}^2) r_{\perp}. \quad (97b) \]

The scalar functions \( v_{k,\perp} \) and \( v_{k,\perp} \) are real whereas \( \tilde{v}_z \) and \( \tilde{v}_{\perp} \) are complex. Finally, the traceless symmetric parts of the spin-current densities \( (92) \) are:

\[ j_k^r(r) = 0, \quad (98a) \]

\[ \tilde{j}^r(r) = 0, \quad (98b) \]

\[ j_k^{\perp}(r) = k_{k,\perp} (z^2, r_{\perp}^2) (r_{\perp} \otimes (z \times r_{\perp})), \quad (98c) \]

\[ j_k^{\perp}(r) = \tilde{k}_{k,\perp} (z^2, r_{\perp}^2) (r_{\perp} \otimes (z \times r_{\perp})), \quad (98d) \]

\[ \tilde{j}^{\perp}(r) = \tilde{k}_{k,\perp} (z^2, r_{\perp}^2) (r_{\perp} \otimes (z \times r_{\perp})), \quad (98e) \]

\[ \tilde{j}^{\perp}(r) = \tilde{k}_{k,\perp} (z^2, r_{\perp}^2) (z \otimes (z \times r_{\perp})), \quad (98f) \]

where

\[ r_{\perp} \otimes (z \times r_{\perp}) = \frac{1}{2} \left[ r_{\perp} \otimes (z \times r_{\perp}) \right. \]

\[ + (z \times r_{\perp}) \otimes r_{\perp} \right\] \]

\[ z \otimes (z \times r_{\perp}) = \frac{1}{2} \left[ z \otimes (z \times r_{\perp}) \right. \]

\[ + (z \times r_{\perp}) \otimes z \right\] \]

are the symmetrized outer products of the vector product \( z \times r_{\perp} \), and vectors \( r_{\perp} \) and \( z \), respectively. As usual, the scalar functions \( k_{k,\perp} \) are real, whereas \( \tilde{k} \) are complex.

2. Axial symmetry alone

From the above discussion we see that the mirror symmetry imposes quite strong conditions on the nonlocal and local density functions. When the generalized density matrix is invariant only under the \( SO^\perp(2) \subset SO(3) \) group of rotations about the z-axis, the transformation rules of Eqs. \( (81) \) with \( c = +1 \) are fulfilled. This means that coordinate \( r_z = z \) is the \( SO^\perp(2) \) invariant, and there
is no difference between the SO(3) pseudovectors and vectors. The scalar nonlocal densities are thus functions of $z, r_\perp, z', r_\perp',$ and $r_\perp \cdot r_\perp'.$

The spin densities are SO(3) vectors and can take more general forms than those of Eqs. (82) and (83); namely, the Hermitian spin densities in the $p$-$p$ channel are:

$$s_{kz}(r, r')e_z = i(r \times r')\tilde{g}_{kz}(r, r') + z'\tilde{g}_{kz}^* (r', r),$$

$$s_{k\perp}(r, r') = (z \times r)\tilde{g}_{k\perp}(r, r') + (z' \times r')\tilde{g}_{k\perp}^* (r', r)' + r_\perp \tilde{g}_{k\perp}^* (r', r),$$

where $\tilde{g}_{kz}$ is Hermitian and $\tilde{g}_{k\perp}$, $g_{k\perp}$, and $\tilde{g}_{k\perp}$ are arbitrary scalars.

The spin nonlocal densities in the $p$-$p$ channel are either symmetric or antisymmetric in $r$ and $r'$:

$$\tilde{s}_0(r, r')e_z = (r \times r')\tilde{g}_{0z}(r, r') + z'\tilde{g}_{0z}^* (r', r),$$

$$\tilde{s}_z(r, r')e_z = (r \times r')\tilde{g}_{z}(r, r') + z'\tilde{g}_{z}^* (r', r),$$

$$\tilde{s}_{0\perp}(r, r') = (z \times r)\tilde{g}_{0\perp}(r, r') + (z' \times r')\tilde{g}_{0\perp}^* (r', r) + r_\perp \tilde{g}_{0\perp}^* (r', r),$$

$$\tilde{s}_{\perp}(r, r') = (z \times r)\tilde{g}_{\perp}(r, r') - (z' \times r')\tilde{g}_{\perp}^* (r', r) + r_\perp \tilde{g}_{\perp}^* (r', r),$$

where $\tilde{g}_{0z}$ is antisymmetric, $\tilde{g}_{z}$ is symmetric, and $\tilde{g}_{0\perp}$, $\tilde{g}_{0\perp}$, $\tilde{g}_{\perp}$, $\tilde{g}_{\perp}$, and $\tilde{g}_{\perp}$ are arbitrary complex scalar functions.

In the case of broken mirror symmetry, the real local $p$-$p$ densities $\rho_k(z, r_\perp) = \rho_k^*(z, r_\perp)$ and the complex local isovector $p$-$p$ density $\tilde{\rho}(z, r_\perp)$ are functions of the two cylindrical coordinates, $z$ and $r_\perp$, i.e., they depend on the sign of $z$. The same is true for the scalar kinetic densities (77), i.e., the real $p$-$p$ densities $\tau_k(z, r_\perp) = \tau_k^*(z, r_\perp)$ and complex $p$-$p$ isovector kinetic density $\tilde{\tau}(z, r_\perp)$.

At this point, it becomes convenient to use the cylindrical coordinates $z, \phi$, and $z$, and the corresponding unit vectors $e_z, e_\phi$, and $e_z$. The $p$-$p$ isoscalar and isovector real spin densities and the $p$-$p$ isoscalar complex spin density are:

$$s_k(r) = s_{kz}(z, r_\perp)e_z + s_{k\phi}(z, r_\perp)e_\phi + s_{kz}(z, r_\perp)e_z \quad (102)$$

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

$$\tilde{s}_0(r) = \tilde{s}_{0z}(z, r_\perp)e_z + \tilde{s}_{0\phi}(z, r_\perp)e_\phi + \tilde{s}_{0z}(z, r_\perp)e_z \quad (103)$$

All differential local densities can be calculated by using the gradient formula:

$$\nabla_z + \nabla_{\perp} \rho(z, r_\perp, r_\perp', r_\perp') = \frac{\partial \rho}{\partial z} e_z + \frac{\partial \rho}{\partial r_\perp} e_{r_\perp} + \frac{1}{r_\perp} \frac{\partial \rho}{\partial r_\perp'} e_{r_\perp'} \quad (104a)$$

$$\nabla_z + \nabla_{\perp} \rho(z, r_\perp, r_\perp', r_\perp') = \frac{\partial \rho}{\partial z} e_z + \frac{\partial \rho}{\partial r_\perp} e_{r_\perp} + \frac{1}{r_\perp} \frac{\partial \rho}{\partial r_\perp'} e_{r_\perp'} \quad (104b)$$

The spin-kinetic densities (89) have all non-vanishing cylindrical components:

$$T_k(r) = T_{kr_\perp}(z, r_\perp)e_z + T_{kz}(z, r_\perp)e_z, \quad (105a)$$

$$\tilde{T}_0(r) = \tilde{T}_{0z}(z, r_\perp)e_z + T_{0z}(z, r_\perp)e_z. \quad (105b)$$

As usual, the $p$-$p$ spin-kinetic densities are real and the $p$-$p$ ones are complex.

The tensor-kinetic densities (101a) and (101b) have the same structure as the vectors (105):

$$F_k(r) = F_{kr_\perp}(z, r_\perp)e_z + F_{kz}(z, r_\perp)e_z, \quad (106a)$$

$$\tilde{F}_0(r) = \tilde{F}_{0z}(z, r_\perp)e_z + F_{0z}(z, r_\perp)e_z. \quad (106b)$$

The current densities, being proportional to the gradients of scalar functions, have only the $r_\perp$- and $z$-components:

$$j_k(r) = j_{kz}(z, r_\perp)e_z + j_{kr_\perp}(z, r_\perp)e_z, \quad (107a)$$

$$\tilde{j}_0(r) = \tilde{j}_{0z}(z, r_\perp)e_z + \tilde{j}_{0r_\perp}(z, r_\perp)e_z. \quad (107b)$$

Finally, due to the breaking of mirror symmetry, the spin-current densities can have rich structures. The traces of spin-current tensors (35) do not vanish, and they decompose into the sums of two SO(3) scalars:

$$J_k(r) = J_{kz}(z, r_\perp) + J_{kr_\perp}(z, r_\perp), \quad (108a)$$

$$\tilde{J}(r) = \tilde{J}_{z}(z, r_\perp) + \tilde{J}_{r_\perp}(z, r_\perp). \quad (108b)$$

The antisymmetric parts (36) of the spin-current tensors (33) form the vectors with nonzero transverse components:

$$J_k(r) = J_{kz}(r_\perp) = J_{kr_\perp}(z, r_\perp)e_z + J_{z}(z, r_\perp)e_z, \quad (109a)$$

$$\tilde{J}_{r_\perp}(r) = \tilde{J}_{r_\perp}(z, r_\perp)e_z + \tilde{J}_{z}(z, r_\perp)e_z. \quad (109b)$$

The symmetric traceless parts of the tensors (33) vanish:

$$\tilde{J}_{zz} = 0, \quad (110a)$$

$$\tilde{J}_{zz} = 0. \quad (110b)$$
The remaining traceless symmetric tensors are:
\[
\begin{align*}
\mathbb{J}_{ab}^\perp &= \mathbb{J}_{ab}^\perp + \mathbb{J}_{ab}^\perp \\
&= K_{\pm}(z,r_{\perp}) P_{ab}^\pm + J_{\perp}(z,r_{\perp}) S_{ab}^\perp,
\end{align*}
\]
(111a)
\[
\mathbb{J}_b^\perp = K_{\pm}(z,r_{\perp}) P_{ab}^\pm + J_{\perp}(z,r_{\perp}) S_{ab}^\perp
\]
(111b)
for \(a, b = x, y, z\), where
\[
S_{ab}^\perp = 2 r_{\perp} \delta_{ab} - \delta_{ab}
\]
(112)
is the standard symmetric traceless SO\(^{(2)}\) tensor and
\[
P_{ab}^\perp = \frac{z}{2|z| r_{\perp}^2} (r_{\perp} \epsilon_{bcz} + r_{\perp} \epsilon_{azz}) r_{\perp}.
\]
(113)
is a symmetric pseudotensor. The tensor \(J_{ab}^\perp\) is traceless by definition. Its symmetric part has the following structure:
\[
\mathbb{J}_{az}^\perp = \mathbb{J}_{az}^\perp = K_{\pm}(z,r_{\perp}) P_{az}^\pm + J_{\perp}(z,r_{\perp}) S_{az}^\perp
\]
(114)
for \(a = x, y, z\), where non-vanishing components of the normalized and symmetrized outer products \(z \otimes r_{\perp}\) and \(z \otimes (z \times r_{\perp})\) are:
\[
S_{az}^\perp = \frac{r_{\perp} a}{r_{\perp} |z|}
\]
(115)
and
\[
P_{az}^\perp = \frac{z a c r_{\perp}}{r_{\perp}}.
\]
(116)
Similarly,
\[
\mathbb{J}_{az}^\perp = K_{\pm}(z,r_{\perp}) P_{az}^\pm + J_{\perp}(z,r_{\perp}) S_{az}^\perp.
\]
(117)
All components of the spin-current tensor in the p-h channel are real whereas those in the p-p channel are complex.

3. Axial symmetry – summary

In the case of the axial O\(^{(2)}\) symmetry, the position vector \(r\) can be decomposed into two vectors \(z\) and \(r_{\perp}\) having different transformation properties under rotations and mirror rotations about the \(z\)-axis. Vector \(r_{\perp}\) is the SO\(^{(2)}\) vector, whereas \(z\) is the O\(^{(2)}\) pseudoscalar. There are two O\(^{(2)}\) scalars: \(z^2\) and \(r_{\perp}^2\), and all the local scalar densities are functions thereof. In this study, we are not concerned with the question whether the densities are analytical functions of the invariants. Therefore, it does not matter whether the argument of densities is \(r_{\perp}^2\) or just \(r_{\perp}\).

The local vector densities are linear combinations of vectors \(z\) and \(r_{\perp}\) with scalar coefficients. The pseudovector densities are proportional to vector product \(z \times r_{\perp}\) and thus have the azimuthal direction. While it is not possible to build pseudoscalar densities from elementary vectors \(z\) and \(r_{\perp}\), pseudotensor densities can be constructed. The symmetric pseudotensor densities are linear combinations of the symmetrized outer products \(r_{\perp} \otimes (z \times r_{\perp})\) and \(z \otimes (z \times r_{\perp})\). The symmetry properties of local axially symmetric (O\(^{(2)}\)-invariant) densities are listed in Tables III and IV.

If the mirror symmetry is broken, the two SO\(^{(2)}\)-invariants are \(z\) and \(r_{\perp}\). The scalar and pseudoscalar densities are now functions thereof. The vector and pseudovector densities now have non-vanishing components along all three vectors, \(e_{\perp}\), \(e_{\perp}\), and \(e_z\). The traceless symmetric tensor densities are linear combinations of the pseudotensors \(P^\perp\) and \(P^\perp\), and tensors \(S^\perp\) and \(S^\perp\). Properties of the SO\(^{(2)}\)-invariant local densities are listed in Tables VI and VII.

C. Symmetry D\(_{2h}\)

The identity, inversion, three signatures, three simples, and their negative partners form the symmetry group D\(_{2h}\). The Cartesian rotation matrices of Eq. (101) for the identity (labeled by \(u\)) and signature operations are all diagonal:
\[
a^u = \begin{pmatrix} a^u_z & 0 & 0 \\ 0 & a^u_y & 0 \\ 0 & 0 & a^u_z \end{pmatrix}
\]
(118)
for \(a = u, x, y, z\). They can be written explicitly as:
\[
a^u = a(000) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},
\]
(119a)
\[
a^x = a(00\pi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},
\]
(119b)
\[
a^y = a(0\pi0) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},
\]
(119c)
\[
a^z = a(\pi00) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\]
(119d)
Let us suppose that the generalized density matrix is invariant under the generalized transformation matrix \(\tilde{U}^a\), \((a = u, x, y, z)\), belonging to the D\(_{2h}\) of transformations. According to Eqs. (60), the transformation rules for non-local densities are:
\[
\rho_k(r, r') = \rho_k(\varsigma^a r, \varsigma^a r'),
\]
(120a)
\[
\tilde{\rho}_k(r, r') = \tilde{\rho}_k(\varsigma^a r, \varsigma^a r'),
\]
(120b)
\[
s_{kk}(r, r') = a^2_k s_{kk}(\varsigma^a r, \varsigma^a r'),
\]
(120c)
\[
\tilde{s}_{kk}(r, r') = a^2_k \tilde{s}_{kk}(\varsigma^a r, \varsigma^a r').
\]
(120d)
TABLE III: Properties of the local axial and mirror-symmetric \((O^{+1/2}(2))-\)invariant\) particle-hole densities, depending on the conserved \((C)\) or broken \((B)\) proton-neutron \((p-n)\), and time-reversal \((T)\) symmetries. The \(z\)-simplex \((S_z)\) symmetry is conserved. Vector and pseudovector densities can be expanded in a basis of three vectors: \(r_\perp, z\) and \(z \times r_\perp\). The symmetrized outer products \(r_\perp \otimes (z \times r_\perp)\) and \(z \otimes (z \times r_\perp)\) form a basis for the pseudotensor densities. The expansion coefficients are real, imaginary, and complex functions of the two \(O^{+1/2}(2)\) scalars: \(z^2\) and \(r_\perp^2\). Generic real, imaginary, and complex coefficients are denoted by \(f_R(z^2, r_\perp^2)\), \(f_I(z^2, r_\perp^2)\), and \(f_C(z^2, r_\perp^2)\), respectively.

| \(S_z\) | \(p-n\) | \(T\) | \(C\) | \(B\) | \(C\) | \(B\) |
|---|---|---|---|---|---|---|
| \(\rho_0,3\) | 1 | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |
| \(\rho_1\) | 1 | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(\rho_2\) | 1 | 0 | 0 | 0 | 0 | 0 |
| \(\tau_{0,3}\) | 1 | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |
| \(\tau_1\) | 1 | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(\tau_2\) | 1 | 0 | 0 | 0 | 0 | 0 |
| \(J_0,3\) | 0 | 0 | 0 | 0 | 0 | 0 |
| \(J_1\) | 0 | 0 | 0 | 0 | 0 | 0 |
| \(J_2\) | 0 | 0 | 0 | 0 | 0 | 0 |
| \(s_{0,3}\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | \(f_R(z^2, r_\perp^2)\) | 0 | 0 |
| \(s_1\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(s_2\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 |
| \(T_{0,3}\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(T_1\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(T_2\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 |
| \(F_{0,3}\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | \(f_R(z^2, r_\perp^2)\) | 0 | 0 |
| \(F_1\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(F_2\) | \(z \times r_\perp\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 |
| \(J_{0,3}\) | \(r_\perp, z\) | \(f_R(z^2, r_\perp^2)\) | 0 | \(f_R(z^2, r_\perp^2)\) | 0 | 0 |
| \(J_1\) | \(r_\perp, z\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 | 0 |
| \(J_2\) | \(r_\perp, z\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | 0 | 0 | 0 |
| \(s_{0,3}\) | \(r_\perp \otimes (z \times r_\perp), z \otimes (z \times r_\perp)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |
| \(J_1\) | \(r_\perp \otimes (z \times r_\perp), z \otimes (z \times r_\perp)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |
| \(J_2\) | \(r_\perp \otimes (z \times r_\perp), z \otimes (z \times r_\perp)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |
| \(s_{0,3}\) | \(r_\perp \otimes (z \times r_\perp), z \otimes (z \times r_\perp)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) | \(f_R(z^2, r_\perp^2)\) |

The differential local densities in both channels should now be classified according to irreducible representations of the point group \(D_{2h}\). Therefore, the vector notation used so far is no longer useful. Instead, in this section we rely on definitions \([18]\), where the Cartesian components are explicitly shown.

The \(p-h\) isoscalar and isovector kinetic densities \([17a]\) transform according to:

\[
\tau_{kbc}(r) = \tau_{kbc}(r) = a^a_b a^c_d \tau_{kbc}(\sigma^a r). \tag{123}\]

The complex isovector component of \(p-p\) kinetic densities \([17b]\) obeys analogous symmetry conditions:

\[
\tilde{\tau}_{bc}(r) = a^a_b a^c_d \tilde{\tau}_{bc}(\sigma^a r). \tag{124}\]

The symmetries of the kinetic scalar densities \([11]\) can be obtained from Eqs. \([18a]\) and \([18b]\).

The spin-kinetic and tensor-kinetic densities \([17c]\) and \([17d]\) fulfill the symmetry conditions:

\[
T_{kbed}(r) = T_{kbed}(r) = a^a_b a^c_d T_{kbed}(\sigma^a r), \tag{125a}\]

\[
\tilde{T}_{obed}(r) = a^a_b a^c_d \tilde{T}_{obed}(\sigma^a r). \tag{125b}\]
The transformation properties of the spin-kinetic densities [126] and tensor-kinetic densities [127] are obtained by contractions defined by Eqs. 130c–130f.

Finally, the symmetry conditions of the current and the spin-current densities in both channels are:

\[ j_{kh}(r) = j_{kh}(r) = \zeta a^2 j_{kh}(\zeta a^2 r), \]
\[ \tilde{j}_{kh}(r) = \zeta a^2 \tilde{j}_{kh}(\zeta a^2 r), \]
\[ J_{kh}(r) = J_{kh}(r) = \zeta a^2 J_{kh}(\zeta a^2 r), \]
\[ \tilde{J}_{kh}(r) = \zeta a^2 \tilde{J}_{kh}(\zeta a^2 r). \]

V. SYMMETRIES OF MULTI-REFERENCE TRANSITION DENSITIES

In analogy to Eqs. 33 and 35, the transition p-h and p-p density matrices are defined, respectively, as

\[ \tilde{\hat{\rho}}^{(t)}(rst, r's't') = \langle \Psi_1 | a_{r's't'}^+ a_{rst} | \Psi_2 \rangle, \]
\[ \hat{\rho}^{(t)}(rst, r's't') = 4s's't't' \langle \Psi_2 | a_{r's't'}^+ a_{rst} | \Psi_1 \rangle, \]

where |\Psi_1\rangle and |\Psi_2\rangle are two different independent-quasiparticle states. The corresponding spin-isospin scalar and vector transition densities \(\rho_k^{(t)}(r, r')\) and \(\hat{s}_k^{(t)}(r, r')\) and \(\hat{\rho}_k^{(t)}(r, r')\) and \(\tilde{s}_k^{(t)}(r, r')\) with \(k = 0, \ldots, 3\) are defined by the relations analogous to Eqs. 10. The local transition densities are defined in an identical way as the local densities Eqs. 10 and are denoted with the same respective symbols but with the superscript \(l\).

What are the differences in the symmetry properties of the transition density matrices from those of the density matrices discussed above? First of all, the p-h transition density matrix is not Hermitian:

\[ \tilde{\hat{\rho}}^{(t)}(rst, r's't') = \langle \Psi_1 | a_{r's't'}^+ a_{rst} | \Psi_2 \rangle \neq \langle \Psi_2 | a_{r's't'}^+ a_{rst} | \Psi_1 \rangle. \]

Consequently, Eqs. 58 for the p-h nonlocal transition densities are not fulfilled. On the other hand, the antisymmetry property of the p-p density matrix is preserved:

\[ \tilde{\hat{\rho}}^{(t)}(rst, r's't') = -16ss't't' \tilde{\hat{\rho}}^{(t)}(r' - s' - t', r - s - t). \]

Hence, the p-p nonlocal transition densities obey relations 79.

The transformation rules for the transition matrices under the single-particle unitary (and antiunitary) transformations \(U (U_{\psi})\) follow the transformation rules 27 for the creation and annihilation operators and are given by Eqs. 30, namely:

\[ \tilde{\hat{\rho}}^{(t)U} = \hat{u} \cdot \tilde{\hat{\rho}}^{(t)} \cdot \hat{u}^+, \]
\[ \hat{\rho}^{(t)U} = \hat{u} \cdot \hat{\rho}^{(t)} \cdot \hat{u}^+. \]

Therefore, the discussion of density matrix symmetries presented in Sec. [IV] applies to transition densities with the only difference being that the p-h transition densities are, in general, complex, unless the time-reversal in-
TABLE V: Properties of local axially symmetric (SO₄(2)-invariant) particle-hole densities, depending on the conserved (C) or broken (B) p-n and time-reversal symmetries. The $z$-simplex ($S_z$) symmetry is broken. The vector, pseudovector, or pseudotensor densities can be expanded in the vector $(e_\parallel, e_\perp, e_z)$ or tensor $(P^\parallel, P^\perp, S_z, S^\perp)$ bases. The expansion coefficients are real, imaginary, and complex functions of cylindrical coordinates $r_\perp$ and $z$. Generic real, imaginary, and complex coefficients are denoted by $f_R(z, r_\perp)$, $f_I(z, r_\perp)$, or $f_C(z, r_\perp)$, respectively.

| symmetry | conserved (C) or broken (B) |
|----------|----------------------------|
| $S_z$    | B  | B  | B  | B  |
| p-n      | B  | B  | C  | C  |
| $T$      | C  | C  | B  | B  |

| basis | coefficients |
|-------|--------------|
| $p_{0,3}$ | 1  | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ |
| $p_1$ | 1  | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | 0  | 0  |
| $p_2$ | 1  | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $p_{7,3}$ | 1  | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ |
| $p_1$ | 1  | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $p_2$ | 1  | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $p_{7,3}$ | 1  | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ | $f_R(z, r_\perp)$ |
| $s_{0,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | $f_R(z, r_\perp)$ |
| $s_1$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $s_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $s_{7,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $s_{1}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $s_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $s_{7,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_1$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_{0,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_1$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_{0,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_1$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_{0,3}$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_1$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $j_2$ | $e_\parallel, e_\perp, e_z$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $l_{0,3}$ | $P^\parallel, P^\perp, S_z, S^\perp$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $l_1$ | $P^\parallel, P^\perp, S_z, S^\perp$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $l_2$ | $P^\parallel, P^\perp, S_z, S^\perp$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |
| $l_3$ | $P^\parallel, P^\perp, S_z, S^\perp$ | $f_R(z, r_\perp)$ | 0  | 0  | 0  |

Variance introduces some restrictions. The time-reversal-invariant non-local p-h transition densities obey the following relations:

\[
\rho_k^{(t)}(\mathbf{r}, \mathbf{r}') = \rho_{k}^{(t)*}(\mathbf{r}, \mathbf{r}'), \quad (132a)
\]

\[
s_k^{(t)}(\mathbf{r}, \mathbf{r}') = -s_k^{(t)*}(\mathbf{r}, \mathbf{r}'), \quad (132b)
\]

for $k = 0, 1, 3$,

and

\[
\rho_k^{(t)}(\mathbf{r}, \mathbf{r}') = -\rho_{k}^{(t)*}(\mathbf{r}, \mathbf{r}'), \quad (132c)
\]

\[
s_k^{(t)}(\mathbf{r}, \mathbf{r}') = s_k^{(t)*}(\mathbf{r}, \mathbf{r}'), \quad (132d)
\]

which means that some transition densities are real while others are purely imaginary. Symmetry properties of the local p-h transition densities are catalogued in Tables VII, VIII, and IX. For the local p-p transition densities, the results of Tables III, IV, and VI apply.

VI. DISCUSSION OF PAIRING CHANNELS AND EXAMPLES OF PREVIOUS APPROACHES

The form of the most general EDF that is quadratic in local isovector and isovector densities has been proposed in Ref. I, where the expressions for the p-h and p-p mean fields can be found. In current applications, pairing interaction is often approximated by the zero-range pairing force $34, 35, 36, 37$,

\[
V_{\text{pair}}(\mathbf{r}, \mathbf{r}') = f_{\text{pair}}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'), \quad (133)
\]

where the density-dependent form factor reads

\[
f_{\text{pair}}(\mathbf{r}) = V_0 \left\{ 1 + x_0 \hat{P}^\sigma - \frac{\rho_0(\mathbf{r})}{\rho_c} \right\} \{1 + x_3 \hat{P}^\sigma\}, \quad (134)
\]

and $\hat{P}^\sigma$ is the usual spin-exchange operator. When only the isovector pairing is studied, the exchange parameters $x_0$ and $x_3$ are usually set to zero. However, in the general case of coexisting isoscalar and isovector pairing correlations, nonzero values of $x_0$ and $x_3$ have to be used.

In Ref. 35, the density-independent, zero-range pairing force,

\[
V_{\text{pair}}(\mathbf{r}, \mathbf{r}') = \sum_{\sigma} \left[ p_0^T \delta(\mathbf{r} - \mathbf{r}') + p_1^T k' \delta(\mathbf{r} - \mathbf{r}')k \right] \hat{\Pi}_{TS}, \quad (135)
\]

has been employed to study the interplay between isoscalar and isovector pairing within an axially symmetric HF+BCS scheme. In Eq. 135, $\hat{\Pi}_{TS}$ stands for the
TABLE VI: Similar to Table \[\text{IV}\] except for the particle-particle densities.

| symmetry | \( S_\lambda \) | \( p-n \) | \( T \) | conserved (C) or broken (B) |
|----------|----------------|---------|-------|-----------------------------|
|          | \( \bar{B} \) | \( \bar{B} \) | \( \bar{B} \) | \( \bar{B} \) |
| \( p-n \) | \( \bar{B} \) | \( \bar{B} \) | \( C \) | \( C \) |
| \( T \)  | \( \bar{B} \) | \( C \)  | \( B \)  | \( B \)  |

spin-isospin projection operator, and \( p_0^T \) and \( p_2^T \) are coupling strengths adjusted to the data.

As seen in (I-84) and (I-89), for the commonly used pairing force \[\text{[133]},\] only two pairing densities come into play: the isovector density \( \bar{\rho} \) and the isoscalar \( p-p \) spin density \( \bar{s}_0 \). The corresponding isovector \( p-p \) potential \( \bar{U}(r) \) is simply proportional to \( \bar{\rho} \) while the isoscalar \( p-p \) field \( \bar{\Sigma}_0(r) \) is proportional to the scalar product of the quasiparticle’s spin \( \vec{\sigma} \) and \( \bar{s}_0 \). Physically, \( \bar{\rho} \) represents the density of \( S=0 \), neutron-neutron, proton-proton, and p-n pairs while the vector field \( \bar{s}_0 \) describes the spin distribution of \( S=1 \) isoscalar p-n pairs. Indeed, when expressing Eq. (125) directly in terms of the p-n pairs, one can see that \( \bar{s}_{0z} \) contains the \( S=0, M_S=0 \) component while \( \bar{s}_{0x} \) and \( \bar{s}_{0y} \) contain combinations of \( M_S=1 \) and \( M_S=-1 \) pairs. The physical interpretation of the isoscalar p-p mean-field Hamiltonian

\[
\bar{h}_0(r) = \bar{\Sigma}_0 \cdot \vec{\sigma} \propto \bar{s}_0 \cdot \vec{\sigma}
\]  

(136)
is the projection of the quasiparticle’s spin on the spin of the p-n pairing field, its local magnitude determined by the HFB equations; hence, the SCSs are present in the problem.

It is important to emphasize that the isoscalar density \( \bar{s}_0 \) contains all magnetic components of the \( S=1 \) p-n pairing field. When studying an individual component separately, e.g., in the context of the so-called \( \alpha - \bar{\alpha} \) or \( \alpha - \alpha \) pairing \[\text{[39]},\] one may arrive at erroneous conclusions that the presence of isoscalar pairing must be associated with breaking certain SCSs, such as axial symmetry or signature. The usual argument, made originally in Ref. \[\text{[39]},\] and then repeated in the literature \[\text{[40, 41, 42]}\], is that the individual components of the \( S=1 \) pair field are not invariant under rotations. For instance, the pairing tensor \( \kappa_{1M} \) does not commute with signature \( R_a \) \( \text{(a=x, y, z)} \)

\[
R_a^{-1} \kappa_{1M_a} R_a = (-1)^{M_a} \kappa_{1M_a},
\]  

(137)
and this has led to a conclusion that the isoscalar pairing must break signature.

Let us consider axial and mirror symmetry as SCS. As seen in Table \[\text{IV}\] the isoscalar pairing density \( \bar{s}_0 \) vanishes only if the p-n symmetry is conserved. In the generalized pairing theory that mixes proton and neutron orbits, the solenoidal field \( \bar{s}_0 \) is nonzero. The lines of field \( \bar{s}_0 \) are schematically shown in the left panel of Fig. 1. The right panel shows that while an individual vector \( \bar{s}_0 \) at a given point is not invariant with respect to symmetries \( S \) such as rotations around the third axis or signature \( R_x \), the field \( \bar{s}_0 \) is perfectly covariant \[\text{[2]}\):

\[
\bar{s}_0^S(r) = \bar{s}_0(S^+ r S),
\]  

(138)
TABLE VII: Properties of local particle-hole rotationally symmetric (SO(3)-invariant) transition densities, depending on the conserved (C) or broken (B) space-inversion (P), proton-neutron (p-n), or time-reversal (T) symmetries. Generic real, imaginary, or complex functions of the radial variable $r$ are denoted by $f_R(r)$, $f_I(r)$, or $f_C(r)$, respectively.

| $\nu$ | $\tau$ | $\nu$ | $\tau$ | $\nu$ | $\tau$ | $\nu$ | $\tau$ | $\nu$ | $\tau$ | $\nu$ | $\tau$ |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|       |       |       |       |       |       |       |       |       |       |       |       |
| $\rho_0$ | $\rho_1$ | $\rho_2$ | $\tau_0$ | $\tau_1$ | $\tau_2$ | $J_0$ | $J_1$ | $J_2$ | $J_3$ | $J_4$ | $\tilde{J}_0$ |
|       |       |       |       |       |       |       |       |       |       |       |       |
| $f_C(r)$ | $f_B(r)$ | $f_C(r)$ | $f_R(r)$ | $f_C(r)$ | $f_B(r)$ | $f_C(r)$ | $f_R(r)$ | $f_C(r)$ | $f_B(r)$ | $f_C(r)$ | $f_R(r)$ |
| $f_B(r)$ | $f_C(r)$ | $f_B(r)$ | $f_R(r)$ | $f_B(r)$ | $f_C(r)$ | $f_B(r)$ | $f_R(r)$ | $f_B(r)$ | $f_C(r)$ | $f_B(r)$ | $f_R(r)$ |

Indeed, according to Table II, the densities $\tilde{s}_0$ and $\tilde{J}_0(r)$ are perpendicular to $\tilde{s}_0$. It is interesting to note that when the mirror symmetry is broken, the densities $\tilde{s}_0$ and $\tilde{J}_0$ have all components (radial, azimuthal, and vertical) nonzero but their geometries will differ in general.

In the absence of spin polarization, i.e., for time-reversal invariant systems, the isoscalar pairing field $\tilde{s}_0$ is purely imaginary. In the presence of rotation, the time-reversal symmetry is internally broken. In this case, the pairing field is generally complex. Consequently, assuming the real Bogoliubov transformation and real pairing tensor may limit the domain of self-consistent solutions.

Another factor that may impact the generality of conclusions of Ref. [40] is the lack of the p-n symmetry-breaking on the HF level. Such an approximation does not seem to be justified as the self-consistent polarization between p-h and p-p channels is well known in the isovector pairing case. Originally, the condition that the p-h density matrix preserves the p-n symmetry has been pro-

The isoscalar vector current density is solely responsible for the isoscalar pairing field in the spherical, mirror symmetric case when time-reversal symmetry is broken. Indeed, according to Table II the L=0 density $\tilde{s}_0$ vanishes in this limit. It is only when the mirror symmetry is broken that $\tilde{s}_0$ becomes nonzero in spherical nuclei. Such a scenario could be an interesting possibility in very neutron-rich nuclei, in which, e.g., the $1\tau d_{5/2}$ and $1\nu d_{5/2}$ or $1\tau f_{7/2}$ and $1\nu g_{7/2}$ orbitals could appear near the Fermi surface. The isovector density $\tilde{J}(r)$ is generally nonzero in spherical nuclei, and it has radial character.
TABLE VIII: Properties of local axially and mirror symmetric \( (O^+)^2 \)-invariant \) particle-hole 
transition densities depending on the conserved \( (C) \) or broken \( (B) \) proton-neutron \( (p-n) \), or time-reversal \( (T) \) symmetries. 
The \( z \)-simplex \( (S_z) \) symmetry is conserved. The vector and pseudovector densities take the form of an expansion in a basis of some of the three vectors: 
\( r_\perp, z \) and \( z \times r_\perp \). The pseudotensor densities are linear 
combinations of the two symmetric pseudotensors: 
\( r_\perp \otimes (z \times r_\perp) \) and \( z \otimes (z \times r_\perp) \). The expansion coefficients are real, imaginary, or complex functions of the two \( O^+ \)-\( (2) \) scalars, \( z^2 \) and \( r_\perp^2 \). Generic real, imaginary, or complex coefficients are denoted by \( f_R(z^2, r_\perp^2) \), \( f_I(z^2, r_\perp^2) \), or \( f_C(z^2, r_\perp^2) \), respectively.

| symmetry | basis | conserved (C) or broken (B) | coefficients |
|----------|-------|-----------------------------|--------------|
| \( S_z \) | \( p-n \) | C | C | C | C |
| \( T \) | | B | B | C | C |

| \( \rho_0^{(1)} \) | 1 | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) |
| \( \rho_1^{(1)} \) | 1 | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) | 0 | 0 |
| \( \rho_2^{(1)} \) | 1 | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) | 0 | 0 |
| \( z_0^{(1)} \) | 1 | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) |
| \( r_\perp^{(1)} \) | 1 | \( f_C(z^2, r_\perp^2) \) | \( f_R(z^2, r_\perp^2) \) | 0 | 0 |
| \( j_0^{(1)} \) | 0 | 0 | 0 | 0 | 0 |
| \( j_1^{(1)} \) | 0 | 0 | 0 | 0 | 0 |
| \( s_0^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( s_1^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( s_2^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( T_0^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( T_1^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( T_2^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( F_0^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( F_1^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( F_2^{(1)} \) | \( z \times r_\perp \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( j_0^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( j_1^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( j_2^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( J_0^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( J_1^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( J_2^{(1)} \) | \( r_\perp \), \( z \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( J_0^{(2)} \) | \( r_\perp \otimes (z \times r_\perp) \), \( z \otimes (z \times r_\perp) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) |
| \( J_1^{(2)} \) | \( r_\perp \otimes (z \times r_\perp) \), \( z \otimes (z \times r_\perp) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |
| \( J_2^{(2)} \) | \( r_\perp \otimes (z \times r_\perp) \), \( z \otimes (z \times r_\perp) \) | \( f_C(z^2, r_\perp^2) \) | \( f_I(z^2, r_\perp^2) \) | 0 | 0 |

posed in Ref. [39] in the context of BCS calculations for \( N-Z \) nuclei where it was postulated that the expectation value of isospin in the quasiparticle vacuum is zero:

\[
\langle \Psi | \hat{T} | \Psi \rangle = 0. \tag{139}
\]

We note that while the absence of the \( p-n \) mixing in the \( p-h \) sector automatically guarantees the condition \ref{139} for the \( N-Z \) nuclei in the absence of isospin-breaking interactions, the three constraints \ref{139} are in general not sufficient for all the \( t' = -t \) matrix elements of \( \hat{\rho} \) to vanish.

In addition, the independent treatment of time-reversal and isospin symmetries as done in Ref. \cite{39} is not justified. Indeed, as pointed out in Ref. \cite{21}, the time-reversal and the isospin rotations do not commute. This implies that the relative phases between proton and neutron wave functions in a \( p-n \) broken quasiparticle state cannot be chosen arbitrarily.

VII. CONCLUSIONS

In this study, we investigated the symmetries of nucleonic densities of the generalized nuclear DFT that allows for the arbitrary mixing of protons and neutrons. We considered the most important self-consistent symmetries: spherical, axial, space-inversion, and mirror symmetries. The main conclusions of our work can be summarized as follows:

1. The local pairing densities \( \tilde{\rho}_0 \) (isoscalar pairing density) and \( \tilde{\sigma} \) (isovector spin density) always vanish.
2. One can always construct a phase convention for
TABLE IX: Properties of local axially symmetric (SO\(^+\)(2)-invariant) particle-hole transition densities depending on the conserved (C) or broken (B) proton-neutron (p-n), or time-reversal (T) symmetries. The z-simplex (S\(_z\)) symmetry is broken. The vector, pseudovector, or pseudoscalar densities take the form of an expansion in the vector \((e_\perp, e_\phi, e_z)\) or tensor \((e_\perp, e_\phi, S_\perp, S_z)\) basis. The expansion coefficients are real, imaginary, or complex functions of cylindrical coordinates \(r_\perp\) and \(\phi\). Generic real, imaginary, or complex coefficients are denoted by \(f_R(z, r_\perp)\), \(f_I(z, r_\perp)\), or \(f_C(z, r_\perp)\), respectively.

| Symmetry | \(S_z\) | \(T\) | B | B | C | B | B | C | C |
|----------|---------|--------|---|---|---|---|---|---|---|
| Basis    |         |        |   |   |   |   |   |   |   |
| \(p_{0,3}^{(1)}\) | 1       | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{0,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{1,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{2,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{3,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{4,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{5,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |
| \(j_{6,3}^{(1)}\) | \(e_\perp, e_\phi, e_z\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) | \(f_C(z, r_\perp)\) | \(f_R(z, r_\perp)\) |

which the local p-h densities are purely real \(^{22}\). In the presence of particular SCSs, some p-h densities vanish.

3. In the absence of SCSs, the local p-p densities are complex. If time reversal is SCS, p-p densities become either purely real or purely imaginary.

4. If p-n symmetry is SCS (no explicit p-n mixing), the \(k=1\) and 2 isospin components of p-h densities and \(k=0\) and 3 isospin components of p-p densities vanish.

5. When O(3) is SCS (spherical, mirror-symmetric case), the local pseudoscalar, pseudovector, and pseudotensor densities vanish. The only nonzero isoscalar-pairing density is the current density \(j_0(r)\). All these densities can become nonzero in the SO(3) limit when the parity is broken. See Tables \(^{11}\) and \(^{10}\) for a summary.

6. When SO(2) and \(S_z\) are SCS (axial, mirror-symmetric case), pseudoscalar and pseudotensor densities vanish. If time reversal is SCS, p-p densities become either purely real or purely imaginary. Properties of local axially symmetric (O\(^\perp\)(2)-invariant) densities are listed in Tables \(^{11}\) and \(^{10}\).

7. When SO(2) is SCS (axial case), all densities are generally present. Properties of the SO(2)-invariant local densities are listed in Tables \(^{14}\) and \(^{11}\).

8. When space inversion, three signatures, and three simplexes are SCSs (D\(_{2h}\) group), all densities are generally present. Symmetry properties of p-h densities have been previously discussed in Refs. \(^{22}\) \(^{23}\). The analogous expressions for p-p densities are given in Sec. IV.C.C.

9. The symmetry properties of the transition densi-
The symmetry properties discussed in this work provide the necessary, but not sufficient, conditions for the presence of isoscalar pairing in nuclei. Whether such fields will appear or not depends, of course, on the actual form of the EDF and the values of coupling constants. In general, similar to the isovector pairing channel, a strong dynamical coupling between p-h and p-p channels is expected. Consequently, in order to fully benefit from the p-n symmetry-breaking mechanism, p-n symmetry should be broken already on the level of p-h mean field. This is not what has usually been done in existing calculations.

The main results of this paper, summarized in Tables I-IX and in relations in Sec. IV C are symmetry properties of the local p-h and p-p densities that are building blocks of the generalized nuclear DFT formalism. These results can be useful when building a microscopic framework, rooted in the LDA, to describe various phenomena occurring in $N\sim Z$ nuclei.

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APPENDIX A: GENERALIZATION OF THE CAYLEY-HAMILTON THEOREM

When analyzing symmetries, we often meet the problem of how to construct a tensor quantity in terms of another tensor. Such a situation has been first encountered in investigations of phenomenological constituent equations for macroscopic systems (see, e.g., [43]). The starting point in the analysis is the Cayley-Hamilton theorem [44, 45] by which an arbitrary function $f(A)$ of a $3\times 3$ matrix $A$ can be expressed as

$$f(A)_{ab} = C_0(A)\delta_{ab} + C_1(A)A_{ab} + C_2(A)A^2_{ab}, \quad (A1)$$

where the scalar functions $C_i(A) = C_i(a_1, a_2, a_3) \ (i=0, 1, \text{ or } 2)$ depend only on three independent invariants of $A$: $a_1$ (trace of $A$), $a_2$ (trace of $A^2$), and $a_3$ (determinant of $A$). In this case, matrix $A$ is a rank-2 (reducible) tensor ($\lambda = 2$) and the tensor field $f(A)$ is also a rank-2 (reducible) tensor ($L = 2$). Coupling of rank-2 tensors to $L = 2$ simply corresponds to multiplying matrices, and then Eq. (A1) can be derived from the Taylor expansion of $f(A)$ combined with the observation that every matrix obeys its own characteristic equation (any power $A^n \ (n > 2)$ can be written as a linear combination of $A^0$, $A^1$, and $A^2$).

In applications presented in this study, we are interested in spherical (irreducible) tensors and tensor fields corresponding to the rotation group $O(3)$,

$$\hat{d}(\alpha\beta\gamma) = e^{i\gamma\hat{J}_z}e^{i\beta\hat{J}_y}e^{i\alpha\hat{J}_x}, \quad (A2)$$

cf. Eq. [43a]. In this case, $\chi^\mu_\lambda$ is called irreducible spherical tensor of rank $\lambda$ [46] if in the rotated reference frame
it can be expressed as:

\[ \chi'_{\lambda\mu} \equiv \left[ \hat{d}^+(\alpha\beta\gamma)\chi\hat{d}(\alpha\beta\gamma) \right]_{\lambda\mu} = \sum_{\mu=-\lambda}^{\lambda} D^\lambda_{\mu\rho}(\alpha\beta\gamma)\chi_{\lambda\rho}, \]

where \( D^\lambda_{\mu\rho}(\alpha\beta\gamma) \) are the Wigner functions [46].

Now let \( \Phi_{LM} \) be a tensor field of \( \chi_{\lambda\mu} \):

\[ \Phi'_{LM'} = \sum_{M=-L}^{L} D^L_{M,M'}(\alpha\beta\gamma)\Phi_{LM}, \]

which is a function of \( 2\lambda + 1 \) components of \( \chi_{\lambda\mu} \),

\[ \Phi_{LM} = \Phi_{LM}(\chi_{\lambda\mu}), \]

such that

\[ \Phi'_{LM'} = \Phi_{LM'}(\chi'_{\lambda\mu}). \]

In other words, we are interested only in tensor fields being the isotropic functions of \( \chi_{\lambda\mu} \).

Condition (A6) is essential: it states that the rotated tensor field \( \Phi'_{LM'} \) can be obtained by calculating the original tensor field \( \Phi_{LM} \) at arguments which are the rotated tensor components \( \chi'_{\lambda\mu} \) of \( \chi_{\lambda\mu} \). It means that functions \( \Phi_{LM} \), apart from depending on \( \chi_{\lambda\mu} \), do not depend on any other tensor object (fixed material tensor). If they did, values of rotated tensor field \( \Phi'_{LM'} \) could have been obtained by rotating the arguments \( \chi_{\lambda\mu} \) and all material tensors simultaneously, but otherwise the rotation of arguments suffices.

From Eq. (A1) we derive the general form of the quadrupole \((L = 2)\) field \( \Phi_{2M} \) being an isotropic function of the quadrupole tensor \( \chi_2 \) [17]:

\[ \Phi_{2M}(\chi_2) = C_1(\chi_2 \times \chi_2)_0, \chi_2 \times \chi_2 \times \chi_2)_0 \chi_{2M} + C_2(\chi_2 \times \chi_2)_0, \chi_2 \times \chi_2 \times \chi_2)_0 \chi_2 \times \chi_2)_{2M}. \]

The notation \([ \times ]_L\) means the vector coupling to multipolarity \(L\). Symbols \(\times\) and \(\cdot\) for the vector and scalar products of vectors used previously in the paper are, up to coefficients, equivalent to \( \[ \times \]_1 \) and \( \[ \times \]_0 \), respectively.

To generalize Eq. (A7) to arbitrary values of \( L \) and \( \lambda \), one should first establish a (finite) complete system of \( \nu \lambda \) irreducible elementary tensors \( \varepsilon_{lm} \) characteristic for a given \( \lambda \). (Irreducible means that none of them can be expressed rationally and integrally in terms of the others.) The highest components \((m = l)\) of the elementary tensors are called elementary factors. The elementary tensors are constructed by successive vector couplings of \( n \lambda \)'s to different intermediate \( l \)'s (meaning that \( l < n \lambda \)):

\[ \varepsilon_{lm} = \varepsilon_{lm}^{(n)}(l) = \left[ \chi_\lambda \times \cdots \times \chi_\lambda \right]_{lm}^{(n)}, \]

for \( i = 1, \ldots, \lambda \), where symbol \([c]\), redundant in most cases, stands for a specific coupling scheme. Tensor \( \chi_\lambda = \varepsilon_\lambda^{(1)} \) is itself an elementary tensor. In the particular case of \( l = 0 \), all independent scalars are elementary factors. Completeness of the system of elementary factors does not exclude the relations (syzygies) between them. The syzygies can be written in the form:

\[ S_j(\varepsilon_1^1, \ldots, \varepsilon_{j\lambda}^\lambda) = 0, \]

for \( j = 1, \ldots, j_\lambda \), where \( S_j \) are rational integral functions. Again, the number of independent syzygies is finite and depends on \( \lambda \).

Having determined the elementary tensors, we align them (i.e., couple to the maximal multipolarity) to get a tensor of rank \( L \):

\[ [\varepsilon_1^1 \times \varepsilon_{j\lambda}^{\lambda'} \times \ldots ]_{L=l+l'+\ldots} \]

Alignment of the elementary tensors means multiplication for the elementary factors. Because of the existence of syzygies (A9), some aligned tensors can be expressed in terms of others. Using syzygies, we find a finite number \( k_{LM} \) of independent aligned tensors \( \varphi_{LM}^\lambda(\varepsilon) \), \((k = 1, \ldots, k_{LM})\) called fundamental tensors. It turns out that an arbitrary tensor field of rank \( L \) being the isotropic function of tensor \( \chi_\lambda \) can always be presented in the form:

\[ \Phi_{LM}(\chi_\lambda) = \sum_{k=1}^{k_{LM}} C_k(\varepsilon_0)\varphi_{LM}^k(\varepsilon), \]

where argument \( \varepsilon_0 \) of \( C_k \) stands for all the independent scalars. Scalar functions \( C_k \) can be, in general, arbitrary. However, the form of some \( C_k \) can be restricted. For instance, high powers of some scalars \( \varepsilon_0 \) do not appear. This is because that a syzygy can make an expression \( (\varepsilon_0)^{i_1}(\varepsilon_{i'\lambda'}^{i'}\varepsilon_1^{i_1})^{i_2}\varepsilon_{i_1}^{i_2}\varepsilon_{i_2}^{i_3}\varepsilon_{i_3}^{i_4}\varepsilon_1^{i_4} \) for some \( i \) and \( i', \), \( i'' \), and \( n \) and \( n', \), \( \ldots, n'' \) dependent on other elementary factors. We refer to Eq. (A11) as the Generalized Cayley-Hamilton (GCH) theorem.

An explanation of the procedure presented above can be traced back to the theory of covariants of algebraic forms given by Dickson [18], which, however, uses quite different notations than those used here. Let us sketch the main points of the theory [11]. Let the \( 2\lambda\)-ic (of order \( 2\lambda \)) algebraic form, binary in variables \( x_1, x_2 \), be given by:

\[ F_{2\lambda}(x_1, x_2; \chi_\lambda \ldots, \chi_\lambda) = \sum_{\mu=-\lambda}^{\lambda} \left( \frac{2\lambda}{\lambda - \mu} \right)^{1/2} \chi_{\lambda\mu}x_1^{\lambda+\mu}x_2^{\lambda-\mu}, \]

with \( \chi_{\lambda\mu} \) \((\mu = -\lambda, \ldots, \lambda)\) being the set of coefficients. Replacing the variables by a linear non-singular transformation

\[ x_i = \sum_{k=1}^{2} A_{ik}y_k \]

(A13)
for $i = 1, 2$, in the form of Eq. (A12), one obtains:

$$F_{2\lambda}(x_1, x_2; \chi_\lambda) = G_{2\lambda}(y_1, y_2; \chi_\lambda)$$

$$= \sum_{\mu=-\lambda}^{\lambda} \left( \frac{2\lambda}{\lambda - \mu} \right)^{1/2} \psi_{\lambda \mu}(\chi_\lambda) y_1^{\lambda + \mu} y_2^{\lambda - \mu},$$

(A14)

where $\psi_{\lambda \mu}$ is a new set of coefficients. The 2$l$-ic form,

$$H_2^{(n)}(x_1, x_2; \chi_\lambda) = \sum_{m=-l}^{l} \left( \frac{2l}{l - m} \right)^{1/2} h_{lm}^{(n)}(\chi_\lambda)x_1^{l+m}x_2^{-m},$$

(A15)

such that

$$H_2^{(n)}(y_1, y_2; \psi_\lambda) = (\det(A_{ik}))^w H_2^{(n)}(x_1, x_2; \chi_\lambda)$$

(A16)

we call a (homogeneous) covariant of weight $w$ of $F$. Coefficients $h_{lm}^{(n)}$ are homogeneous polynomials of order $n$ (called the degree of the covariant) such that $\lambda n = l + w$. When $l = 0$, $H_0^{(n)} = h_0^{(n)}$ is an invariant of $F$. The polynomial in front of the highest power of $x_1$ in Eq. (A15), $h_{l}^{(n)}$ is called a semi-invariant of $F$. The theory of covariants of algebraic forms shows that an arbitrary covariant can be expressed rationally and integrally in terms of a finite, irreducibly complete set of covariants, which can be related rationally and integrally to each other by a finite system of independent syzygies (Gordan-Hilbert Finiteness Theorem, see [44]). The number of basis covariants for a few lowest $\lambda$’s is listed by Olver [49].

What do the covariants of algebraic forms have in common with the tensor fields as functions of tensors? It turns out that semi-invariant $h_{lm}^{(n)}(\chi_\lambda)$ forms the highest projection of a tensor of rank $l$ dependent on the tensor of rank $\lambda$ (the heaviest state of an irreducible representation of $SO(3)$ embedded in an irreducible representation of $SU(2\lambda + 1)$). The remaining polynomials in Eq. (A15) $h_{lm}^{(n)}(\chi_\lambda)$ are other components of the same tensor. Proof of this statement is outlined in Ref. [50]. Constructive proof of Eq. (A11) can be performed by an explicit construction of a basis in the space of functions of $\chi_\lambda$ and demonstration that it has the structure of Eq. (A11). In case of $\lambda = 1$, we know that an arbitrary tensor field of rank $L$ as a function of the position vector $r$, takes the form:

$$\Phi_{LM}(r) = C_L(r) Y_{LM} \left( \frac{r}{r} \right),$$

(A17)

where $r^2 = r \cdot r$ and $Y_{LM}$ is the spherical harmonic. From Eq. (A17) we see immediately that in case of $\lambda = 1$, there are two elementary tensors ($i_1 = 2$), namely vector $r$ and scalar $r^2$, and no syzygy ($j_1 = 0$). For every given $L$ there is only one fundamental tensor ($kL = 1$) of the form [46]:

$$\varphi^{(1)}_{LM}(r) = r^L Y_{LM} \left( \frac{r}{r} \right).$$

(A18)

In particular, Eq. (A17) tells that an arbitrary isotropic vector field takes the form:

$$\Phi(r) = C(r)r.$$  

(A19)

Other examples are constructions of the oscillator bases in cases of $\lambda = 2$ (see Ref. [47] and references quoted therein) and $\lambda = 3$ [50].

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