SPATIAL SYMMETRIES OF THE LOCAL DENSITIES

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Spatial symmetries of the densities appearing in the nuclear Density Functional Theory are discussed. General forms of the local densities are derived by using methods of construction of isotropic tensor fields. The spherical and axial cases are considered.

1. Introduction

The nuclear Density Functional Theory (DFT) has become a conventional approach to describing complex nuclei. In nuclear theory, the nuclear DFT is closely linked with the Hartree-Fock-Bogoliubov (HFB) approximation to the nuclear many-body problem formulated in the position space. The mean value of the system’s energy can here be expressed as a functional of the single-particle density matrices in the particle-hole (p-h) and particle-particle (p-p or pairing) channels. The density matrices in both channels are expressed through the scalar-isoscalar, scalar-isovector, vector-isoscalar and vector-isovector densities, which are nonlocal, i.e., they depend on two position vectors. In the local theory, e.g., the local density approximation, the nonlocal densities can be represented in the energy density
through local densities and their derivatives.

The nuclear self-consistent mean field resulting from the DFT may spontaneously break the symmetry of the original many-body Hamiltonian. The symmetry-breaking phenomenon allows for capturing important physics effects and for including essential correlations in the many-body system. The existence of a self-consistent symmetry (SCS), i.e., a symmetry obeyed by the mean-field Hamiltonian, reflects physical properties of the system. Due to the self-consistency, the SCS of the mean field is also the symmetry of the density matrix. This has a number of important consequences. First of all, to understand SCSs of DFT, it is sufficient to study symmetries of the density matrix without considering the specific form of the density functional and resulting mean-field Hamiltonian. We also realize that if the initial density matrix used at the first iteration of the self-consistent procedure has a certain SCS, then this symmetry will propagate through to the final DFT solution. This means that the choice of the initial density matrix is crucial for the proper physical content of the DFT results. Sometimes, e.g., to simplify numerical calculations, a SCS of the initial density matrix is \textit{ad hoc} assumed. Such an assumption may lead to overestimation of the DFT energy and incorrect prediction of many properties of the system. Finally, assuming a SCS, one should know the general form of the density matrix possessing that symmetry.

Some point symmetries and the associated symmetry-breaking schemes of the p-h densities have been investigated in Refs.\textsuperscript{4,5} A detailed analysis of SCSs of the DFT densities in both channels has recently been presented in Ref.\textsuperscript{6} which will be referred to as I in the following. The present paper is a comment to I, with the main goal of detailing the consequences of spatial symmetries discussed therein. Although our discussion remains rigorous, in this contribution we simplify the notation so as to make the results more transparent and understandable.

As in I, we treat the nonlocal and local densities as isotropic tensor fields, i.e., functions of the position vector(s) independent of other tensor quantities (material tensors).\textsuperscript{7} Under this assumption, in Refs.\textsuperscript{6,8} we introduced the Generalized Cayley-Hamilton (GCH) theorem for tensor fields, and we used it as a tool to study general forms of local densities. Since many different generalizations of the Cayley-Hamilton theorem exist in the literature, in Sec.\textsuperscript{6} we give a brief explanation of the present version.

In Sec.\textsuperscript{2} we recall definitions of the density matrices and nonlocal and local densities. The spherical symmetry with and without space inversion is discussed in Sec.\textsuperscript{3} In Sec.\textsuperscript{4} we consider the axial symmetry with and without space reflection. The summary of our study is contained in Sec.\textsuperscript{5}

### 2. Density matrices and densities

Within the HFB approach to the nuclear many-body problem, the mean value of a many-body Hamiltonian is a functional (the energy functional) of the p-h and p-p
density matrices defined, respectively, as

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

where \( a_{rst}' \) and \( a_{rst} \) 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 properties of density matrices that directly result from their definitions are the following:

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

The dependence on the spin and isospin variables in the density matrices can be easily separated by expanding in the spin and isospin Pauli matrices \( \hat{\sigma}_{ss'} \) and \( \hat{\tau}_{tt'} \), \( (k = 1, 2, 3) \), respectively:

\[ \hat{\rho}(rst, r's't') = \frac{1}{2} (\rho_0(r, r') \delta_{ss'} + s_0(r, r') \cdot \hat{\sigma}_{ss'}) \delta_{tt'} + \frac{1}{2} \sum_k (\delta_{ss'} \rho_k(r, r') + s_k(r, r') \cdot \hat{\sigma}_{ss'}) \hat{\tau}_{tt'}^k, \]
\[ \hat{\rho}(rst, r's't') = \frac{1}{2} (\rho_0(r, r') \delta_{ss'} + s_0(r, r') \cdot \hat{\sigma}_{ss'}) \delta_{tt'} + \frac{1}{2} \sum_k (\delta_{ss'} \rho_k(r, r') + s_k(r, r') \cdot \hat{\sigma}_{ss'}) \hat{\tau}_{tt'}^k, \]

where \( k = 0, 1, 2, 3 \). The spin-isospin components of the p-h \( (\rho_k, s_k) \) and p-p \( (\tilde{\rho}_k, \tilde{s}_k) \) nonlocal densities are functions of two position vectors \( r \) and \( r' \) and have the following symmetry properties that result from Eqs. \( 3 \) and \( 4 \):

\[ \rho_k(r, r') = \rho_k^*(r', r), \]
\[ s_k(r, r') = s_k^*(r', r), \]

for \( k = 0, 1, 2, 3 \), and:

\[ \tilde{\rho}_k(r, r') = \pm \tilde{\rho}_k(r', r), \]
\[ \tilde{s}_k(r, r') = \pm \tilde{s}_k(r', r), \]

where the upper sign is for \( k = 0 \) (isoscalars) and the lower for \( k = 1, 2, 3 \) (isovectors).

In general, the p-h and p-p density matrices transform differently under the single-particle unitary transformations. However, it is proved in I that for the spatial transformations such as rotations, space-inversion, etc., the transformation rules for the p-p density matrix are the same as those for the p-h density matrix. These rules are obviously the same for all the isospin components. Therefore, in further discussion of the space symmetries, we shall omit the accent “breve” and the index \( k \). Also, we shall not take into account conditions \( 7 \) and \( 8 \), i.e., the hermiticity of the p-h densities and the symmetry or antisymmetry of the p-p densities. We mention only that the former condition ensures the reality of all the p-h local
densities, whereas the latter one results in vanishing of either the isoscalar or the isovector p-p local densities.

Within the local density approximation, the energy functional is built from the local densities \( r = r' \) and derivatives thereof. The exact definitions of all used local densities are given, e.g., in Refs. \[9\], \[10\]. Here we only provide schematic definitions that clearly expose the corresponding spatial properties. The densities of interest are:

- **zero-order local densities**
  - particle or pairing density
    \[
    \rho(r) = \rho(r, r')_{r=r'}
    \] (9)
  - spin density
    \[
    s(r) = s(r, r')_{r=r'}
    \] (10)

- **first-order local densities**
  - current density
    \[
    j(r) = \frac{1}{2i} \left[ (\nabla - \nabla') \rho(r, r') \right]_{r=r'}
    \] (11)
  - spin-current density
    \[
    J(r) = \frac{1}{2i} \left[ (\nabla - \nabla') \otimes s(r, r') \right]_{r=r'}
    \] (12)
    which is decomposed into the spin-divergence (trace of \( J \)) density \( J \), the spin-curl (antisymmetric part of \( J \)) density \( \mathcal{J} \), and the traceless symmetric spin-current density \( \mathcal{J} \):
    \[
    J(r) = \frac{1}{2i} \left[ (\nabla - \nabla') \cdot s(r, r') \right]_{r=r'}
    \] (13)
    \[
    J(r) = \frac{1}{2i} \left[ (\nabla - \nabla') \times s(r, r') \right]_{r=r'}
    \] (14)
    \[
    \mathcal{J}(r) = \frac{1}{2i} \left[ (\nabla - \nabla') \otimes s(r, r') \right]_{r=r'}
    \] (15)

- **second-order local densities**
  - kinetic density
    \[
    \tau(r) = \left[ (\nabla \cdot \nabla') \rho(r, r') \right]_{r=r'}
    \] (16)
  - spin-kinetic density
    \[
    T(r) = \left[ (\nabla \cdot \nabla') s(r, r') \right]_{r=r'}
    \] (17)
  - spin-tensor density
    \[
    F(r) = \frac{1}{2} \left[ (\nabla \otimes \nabla' + \nabla' \otimes \nabla) \cdot s(r, r') \right]_{r=r'}.
    \] (18)

We confine ourselves to the second-order derivatives as is usually done. But our analysis can also be extended to higher-order derivatives of the nonlocal densities that have recently been considered\[11\].

*Underlined symbols stand for tensors after symmetrizing and subtracting the trace, e.g., \( \mathcal{J}_{ab} = \frac{1}{2} (J_{ab} + J_{ba}) - \frac{1}{4} \delta_{ab} \sum_c J_{cc}. \)
3. Spherical symmetry

3.1. Nonlocal and local fields

Let \( \mathbf{r} \) and \( \mathbf{r}' \) be two arbitrary, linearly independent position vectors. Then the vector product \( \mathbf{r} \times \mathbf{r}' \) is the third linearly independent vector, and all three form a basis in the three-dimensional space of positions. The scalar products: \( \mathbf{r} \cdot \mathbf{r} = r^2 \), \( \mathbf{r}' \cdot \mathbf{r}' = r'^2 \), and \( \mathbf{r} \cdot \mathbf{r}' \) form three independent scalars quadratic in \( \mathbf{r} \), \( \mathbf{r}' \). It is impossible to form a cubic scalar because \( \mathbf{r} \cdot (\mathbf{r} \times \mathbf{r}') = 0 \) and \( \mathbf{r}' \cdot (\mathbf{r} \times \mathbf{r}') = 0 \). Six possible outer products of the three vectors in question form the following second rank Cartesian tensors:

- three quadratic tensors — \( \mathbf{r} \otimes \mathbf{r} \), \( \mathbf{r}' \otimes \mathbf{r}' \), and \( \mathbf{r} \otimes \mathbf{r}' \):
  - the first two tensors are symmetric and their traces are \( r^2 \) and \( r'^2 \), respectively;
  - the vector antisymmetric part of the third tensor is \( \mathbf{r} \times \mathbf{r}' \) and its trace is \( \mathbf{r} \cdot \mathbf{r}' \).
- two traceless cubic tensors — \( \mathbf{r} \otimes (\mathbf{r} \times \mathbf{r}') \) and \( \mathbf{r}' \otimes (\mathbf{r} \times \mathbf{r}') \) with the vector antisymmetric parts equal to \( \mathbf{r} \times (\mathbf{r} \times \mathbf{r}') = (\mathbf{r} \cdot \mathbf{r}') \mathbf{r} - r^2 \mathbf{r}' \) and \( \mathbf{r}' \times (\mathbf{r} \times \mathbf{r}') = -(\mathbf{r} \cdot \mathbf{r}') \mathbf{r}' - r'^2 \mathbf{r} \), respectively.
- one fourth-order tensor \( (\mathbf{r} \times \mathbf{r}') \otimes (\mathbf{r} \times \mathbf{r}') \) which can be expressed as a linear combination of the quadratic tensors with scalar coefficients:

\[
(r \times r') \otimes (r \times r') = (r \cdot r')(r \otimes r' + r' \otimes r) - (r \cdot r')^2 1
- r'^2(r' \otimes r') - r^2(r \otimes r) + r^2 r'^2 1,
\]

where \( (1)_{ab} = \delta_{ab} \) (\( a, b = x, y, z \)) is the unit tensor.

Having listed all the independent scalars, vectors, and tensors that can be constructed from vectors \( \mathbf{r} \) and \( \mathbf{r}' \), we are able to give general expressions for the nonlocal isotropic fields depending on the two position vectors. We note that (i) any scalar field must be an arbitrary function of the independent scalar functions:

\[
Q(\mathbf{r}, \mathbf{r}') = q_0(r^2, \mathbf{r} \cdot \mathbf{r}', r'^2);
\]

(ii) any vector field must be a linear combination of \( \mathbf{r} \), \( \mathbf{r}' \), and \( \mathbf{r} \times \mathbf{r}' \) with scalar coefficients:

\[
Q(\mathbf{r}, \mathbf{r}') = q_{11}(r^2, \mathbf{r} \cdot \mathbf{r}', r'^2) \mathbf{r} + q_{12}(r^2, \mathbf{r} \cdot \mathbf{r}', r'^2) \mathbf{r}' + q_{13}(r^2, \mathbf{r} \cdot \mathbf{r}', r'^2) \mathbf{r} \times \mathbf{r}';
\]
and (iii) any symmetric traceless tensor field must be a linear combination of the five basic tensors:

\[ \mathbf{Q}(r, r') = q_{21}(r^2, r \cdot r', r'^2) \mathbf{r} \otimes \mathbf{r} + q_{22}(r^2, r \cdot r', r'^2) \mathbf{r}' \otimes \mathbf{r}' + q_{23}(r^2, r \cdot r', r'^2) \mathbf{r} \otimes \mathbf{r}' + q_{24}(r^2, r \cdot r', r'^2) \mathbf{r} \otimes (\mathbf{r} \times \mathbf{r}') + q_{25}(r^2, r \cdot r', r'^2) \mathbf{r}' \otimes (\mathbf{r} \times \mathbf{r}') \]

\[ = q_{21}(r^2, r \cdot r', r'^2)(\mathbf{r} \otimes \mathbf{r} - \frac{1}{3} r^2 \mathbf{1}) + q_{22}(r^2, r \cdot r', r'^2)(\mathbf{r}' \otimes \mathbf{r}' - \frac{1}{3} r'^2 \mathbf{1}) + q_{23}(r^2, r \cdot r', r'^2) \frac{1}{2} (\mathbf{r} \otimes (\mathbf{r} \times \mathbf{r}') + (\mathbf{r} \times \mathbf{r}') \otimes \mathbf{r}) + q_{24}(r^2, r \cdot r', r'^2) \frac{1}{2} (\mathbf{r} \otimes (\mathbf{r} \times \mathbf{r}') + (\mathbf{r} \times \mathbf{r}') \otimes \mathbf{r}'). \] (22)

In the expressions above, all \( q \)'s are arbitrary scalar functions. Scalar fields always have the positive parity. The parities of vector and tensor fields are, in general, indefinite. However, since each independent vector or tensor field does have a definite parity, the vector and tensor fields of definite parities can be easily defined.

It is readily seen from Eqs. (20), (21), and (22) that the corresponding local fields, which depend on one position vector \( r = r' \), only take very simple forms (cf. Appendix A in I):

\[ Q(r) = q_0(r^2), \] (23)
\[ Q(r) = q_1(r^2) \mathbf{r}, \] (24)
\[ Q(r) = q_2(r^2)(\mathbf{r} \otimes \mathbf{r} - \frac{1}{3} r^2 \mathbf{1}). \] (25)

3.2. Nonlocal and local densities

3.2.1. Rotational symmetry SO(3)

If we assume that the density matrices \( \hat{\rho} \) and \( \hat{\tilde{\rho}} \), Eqs. (11) and (12), are invariant under the three-dimensional rotations forming the SO(3) group, it immediately follows from Eqs. (13) and (16) that the densities of type \( \rho \) are the SO(3) scalars while the densities of type \( s \) are the SO(3) vectors (note that the spin Pauli matrices are the SO(3) vectors). Therefore, the nonlocal density of type \( \rho \) takes a form of Eq. (20):

\[ \rho(r, r') = \rho_0(r^2, r \cdot r', r'^2), \] (26)

while the nonlocal density of type \( s \) has a form of Eq. (21):

\[ s(r, r') = s_{11}(r^2, r \cdot r', r'^2) \mathbf{r} + s_{12}(r^2, r \cdot r', r'^2) \mathbf{r}' + s_{13}(r^2, r \cdot r', r'^2) \mathbf{r} \times \mathbf{r}', \] (27)

where \( \rho_0, s_{11}, s_{12}, \) and \( s_{13} \) are arbitrary scalar functions. All local differential densities (11)–(18) can be calculated by differentiating Eqs. (20) and (21), like it was done in I. But to establish general forms of all local densities, it is sufficient to realize that all of them are local isotropic fields with definite transformation rules under SO(3) rotations. These rules can be deduced from the definitions (19)–(18).

We see that the local densities \( \rho(r), \tau(r), \) and \( J(r) \) are scalar fields and all take the form of Eq. (23). Similarly, the densities \( s(r) \), \( j(r) \), \( T(r) \), and \( F(r) \) are the SO(3) vectors; hence, are given by the form of Eq. (24). Finally, the spin-current density \( \mathbf{j}(r) \) is the traceless symmetric tensor of the form (24).
3.2.2. Rotational and mirror symmetry $O(3)$

When the density matrices are also invariant under mirror reflections, it follows from Eqs. (5), (6), and (26) that $\rho(r, r')$ should have positive parity. The spin Pauli matrices form an $O(3)$ pseudovector and thus the nonlocal spin density should be a pseudovector as well. On the right-hand side of Eq. (27), only the last term is a pseudovector. Therefore, in the case of the $O(3)$ symmetry, the spin nonlocal density takes the form:

$$s(r, r') = g''(r^2, r \cdot r', r'^2)(r \times r'),$$  \hspace{1cm} (28)$$

meaning that the local spin density $s(r) = 0$. It is impossible to build a pseudovector from one vector $r$; therefore, local densities $T(r)$ and $F(r)$, being pseudovectors, must vanish, as well as pseudoscalar $J(r) = 0$ and pseudotensor $J(r) = 0$. On the other hand, vectors $j(r)$ and $J(r)$ do not vanish and take the form (24).

4. Axial symmetry

Let us suppose that rotations and mirror rotations around one axis (say $z$-axis) are SCSs. This symmetry group will be denoted as $O_z(2) \subset O(3)$. It is the direct product $O_z(2) = S_z \otimes SO_z(2)$ of the $SO_z(2)$ group of rotations around the $z$-axis and the two-element group $S_z$ consisting of the reflection in the plane perpendicular to the symmetry axis and the identity. To investigate the axial symmetry, it is convenient to decompose the position vector $r$ into the components parallel and perpendicular to the symmetry axis:

$$r = r_z + r_\perp,$$  \hspace{1cm} (29)$$

which have different transformation properties under the $O_z(2)$ transformations. The component $r_\perp$ is a $SO_z(2)$ vector whereas $r_z$ is not affected by the $SO_z(2)$ rotations; hence, it is invariant under $SO_z(2)$. On the other hand, $r_z$ changes its sign under the reflection $S_z$, while $r_\perp$ is $S_z$-invariant.

4.1. Two-dimensional rotational symmetry $SO_z(2)$

If the density matrices $\hat{\rho}$ and $\hat{\bar{\rho}}$ possess the $SO_z(2)$ symmetry, it follows from Eqs. (5) and (26) that all densities of type $\rho$ should be $SO_z(2)$ scalars. Now it is convenient to decompose densities of type $s$ into components perpendicular and parallel to the symmetry axis:

$$s(r, r') = s_\perp(r, r') + s_z(r, r').$$  \hspace{1cm} (30)$$

The perpendicular components $s_\perp(r, r')$ are $SO_z(2)$ vectors and the parallel components $s_z(r, r')$ are $SO_z(2)$ invariants.

The following $SO_z(2)$ scalars can be constructed from the perpendicular and parallel components of the position vectors $r$ and $r'$: $z$, $z'$, the $z$-coordinates of $r_z$ and $r_z'$, respectively, $r_\perp^2 = r_\perp \cdot r_\perp$, $r_\perp' = r_\perp' \cdot r_\perp'$, $r_\perp'^2 = r_\perp'^2 \cdot r_\perp'^2$, and $r_z \cdot (r_\perp \times r_\perp')$ and...
\( \rho(r, r') = g_0(z, z', r_2^2, r_\perp \cdot r'_\perp, r_\perp^2, r_z \cdot (r_\perp \times r'_\perp)) \),

where \( g_0 \) is an arbitrary scalar function, linear in the last argument. There are three vectors invariant under \( SO^\perp(2) \) parallel to the symmetry axis, namely \( r_z, r'_z \), and \( r_\perp \times r'_\perp \). Consequently, the \( z \)-component of \( s(r, r') \) is of the form

\[
s_z(r, r') = g_z(z, z', r_2^2, r_\perp \cdot r'_\perp, r_\perp^2, r_z \cdot (r_\perp \times r'_\perp)) r_z
+ \varphi_z(z, z', r_2^2, r_\perp \cdot r'_\perp, r_\perp^2, r_z \cdot (r_\perp \times r'_\perp))(r_z \times r'_\perp),
\]

where \( g_z, \varphi_z \) are scalar functions. General forms of the local zero-order densities are obtained from Eqs. (31), (32), and (33) by putting \( r_z = r'_z \) and \( r_\perp = r'_\perp \). This gives:

\[
\rho(r) = \rho_0(z, r_\perp),
\]

\[
s_z(r) = \rho_z(z, r_\perp) r_z,
\]

\[
s_\perp(r) = \rho_\perp(z, r_\perp) + \phi_\perp(z, r_\perp)(r_z \times r_\perp),
\]

where \( \rho_0, \rho_z, \rho_\perp, \) and \( \phi_\perp \) are arbitrary scalar functions of \( z \) and \( r_\perp = \sqrt{r_\perp^2} \). The general form of the remaining scalar densities \( \tau(r) \) and \( J(r) \) is the same as that of Eq. (31).

The components of the differential operator,

\[
\nabla = \nabla_z + \nabla_\perp,
\]

have the same transformation properties under \( SO^\perp(2) \) rotations as the corresponding components of the position vector \( \mathbf{r} \). Hence, the densities \( \mathbf{j}(r), \mathbf{J}(r), \mathbf{T}(r) \), and \( \mathbf{F}(r) \) have the components parallel to the \( z \)-axis that are invariant under \( SO^\perp(2) \) and the \( SO^\perp(2) \) vector components that are perpendicular to the symmetry axis. Therefore, they all take general forms given by Eqs. (35) and (36).

It follows from the definitions (12), (15), and (37) that the components \( \varphi_{\perp a} \) \((a = x, y)\) of the symmetric traceless spin-current density form the \( SO^\perp(2) \) vector
while the components \((\underline{J})_{ab}\) \((a, b = x, y)\) form the SO\(^{\perp}(2)\) symmetric traceless tensor. The following four symmetric traceless tensors can be formed with vectors \(r_z\) and \(r_{\perp}\):

\[
\begin{align}
\underline{r}_z \otimes \underline{r}_{\perp} &= \frac{1}{2}(\underline{r}_z \otimes \underline{r}_{\perp} + \underline{r}_{\perp} \otimes \underline{r}_z), \\
\underline{r}_z \otimes (\underline{r}_z \times \underline{r}_{\perp}) &= \frac{1}{2}(\underline{r}_z \otimes (\underline{r}_z \times \underline{r}_{\perp}) + (\underline{r}_z \times \underline{r}_{\perp}) \otimes \underline{r}_z), \\
\underline{r}_{\perp} \otimes \underline{r}_{\perp} &= \underline{r}_{\perp} \otimes \underline{r}_{\perp} - \frac{1}{2} \underline{1}_{\perp}, \\
\underline{r}_{\perp} \otimes (\underline{r}_z \times \underline{r}_{\perp}) &= \frac{1}{2}(\underline{r}_{\perp} \otimes (\underline{r}_z \times \underline{r}_{\perp}) + (\underline{r}_z \times \underline{r}_{\perp}) \otimes \underline{r}_{\perp}),
\end{align}
\]

where \((\underline{1}_{\perp})_{ab} = (1 - \delta_{az})\delta_{ab}\) \((a, b = x, y, z)\) is the unit tensor in the plane perpendicular to the symmetry axis. Two tensors \((38)\) and \((39)\) transform under SO\(^{\perp}(2)\) like vectors perpendicular to the \(z\)-axis. The tensors \((40)\) and \((41)\) are the SO\(^{\perp}(2)\) tensors. Consequently, the general form of the symmetric traceless spin-current density is:

\[
\underline{J}(\underline{r}) = \theta_{z\perp}(z, \underline{r}_{\perp})\underline{r}_z \otimes \underline{r}_{\perp} + \theta_{zz}(z, \underline{r}_{\perp})\underline{r}_z \otimes (\underline{r}_z \times \underline{r}_{\perp}) + \theta_{\perp\perp}(z, \underline{r}_{\perp})\underline{r}_{\perp} \otimes \underline{r}_{\perp} + \theta_{\perp z}(z, \underline{r}_{\perp})\underline{r}_{\perp} \otimes (\underline{r}_z \times \underline{r}_{\perp}),
\]

where \(\theta_{z\perp}, \theta_{zz\perp}, \theta_{\perp\perp},\) and \(\theta_{\perp z}\) are scalar functions. We note in passing that in the case of the axial symmetry, all local densities formally look like the spherical symmetric nonlocal fields \((20), (21)\), and \((22)\) with \(\underline{r} = \underline{r}_z\) and \(\underline{r}' = \underline{r}_{\perp}\), provided that \(\underline{r}_z \cdot \underline{r}_{\perp} = 0\).

**4.2. Two-dimensional rotational and mirror symmetry \(O_{zz\perp}(2)\)**

It follows from the \(S_z\) invariance of the density matrices \((11)\) and \((2)\) that \(\rho(\underline{r}, \underline{r}')\) and \(s_z(\underline{r}, \underline{r}')\) do not change signs under \(S_z\), while \(s_{\perp}(\underline{r}, \underline{r}')\) does. All scalar functions invariant under \(S_z\) depend on \(z, z'\) only through \(z^2 = r_z \cdot r_z, z'^2 = r_z' \cdot r_z'\), and \(z'z = r_z \cdot r_z'\). For instance, Eq. \((31)\) for the nonlocal scalar density now takes the form

\[
\rho(\underline{r}, \underline{r}') = \varrho_0(z^2, z'z, z'^2, r_z^2, r_z'^2, r_{\perp}^2, r_{\perp}'^2).
\]

There exist two pseudoscalars formed from \(r_z, r_z', r_{\perp}, r_{\perp}'\), namely \(r_z \cdot (r_{\perp} \times r'_{\perp})\) and \(r_{\perp}' \cdot (r_{\perp} \times r'_{\perp})\) \((zz'/z^2)r_z \cdot (r_{\perp} \times r'_{\perp})\) equal to each other up to the scalar factor \(zz'/z^2\). The square \((r_z \cdot (r_{\perp} \times r'_{\perp}))^2 = z^2(r_{\perp}^2r_{\perp}'^2 - (r_{\perp} \cdot r'_{\perp})^2)\) is, of course, a scalar.

To fulfill the transformation rules, the general forms of the components of the nonlocal spin density should be modified in the following way:

\[
\begin{align}
\underline{s}_z(\underline{r}, \underline{r}') &= (r_z \cdot (r_{\perp} \times r'_{\perp}))\varrho_z(z^2, z'z, z'^2, r_z^2, r_z'^2, r_{\perp}^2, r_{\perp}'^2)\underline{r}_z \\
+ (r_{\perp}' \cdot (r_{\perp} \times r'_{\perp}))\varrho'_z(z^2, z'z, z'^2, r_z^2, r_z'^2, r_{\perp}^2, r_{\perp}'^2)\underline{r}_{\perp}' \\
+ \varphi_z(z^2, z'z, z'^2, r_z^2, r_z'^2, r_{\perp}^2, r_{\perp}'^2)\underline{r}_z \otimes (r_{\perp} \times r'_{\perp}),
\end{align}
\]
and

\[ s_{\perp}(r, r') = (r_z \cdot (r_\perp \times r'_\perp))q_\perp(z^2, z'z', r_\perp^2, r'_\perp \cdot r'^2_\perp)r_\perp \]
\[ + (r'_z \cdot (r_\perp \times r'_\perp))d'_\perp(z^2, z'z', r_\perp^2, r'_\perp \cdot r'^2_\perp)r'_\perp \]
\[ + \varphi_\perp(z^2, zz', r_\perp^2, r'_\perp \cdot r'^2_\perp)(r_z \times r_\perp) \]
\[ + \varphi'_\perp(z^2, zz', r_\perp^2, r'_\perp \cdot r'^2_\perp)(r'_z \times r'_\perp). \]  

(45)

It follows from Eqs. (43), (44), and (45) that the local zero-order densities for \( r_z = r'_z \) and \( r_\perp = r'_\perp \) can be written in the general form:

\[ \rho(r) = \rho_0(z^2, r^2_\perp), \]
\[ s_z(r) = 0, \]
\[ s_\perp(r) = \phi_\perp(z^2, r^2_\perp)(r_z \times r_\perp). \]

(46)  
(47)  
(48)

The local kinetic density \( \tau(r) \) is of the form (46) too. On the other hand, the pseudoscalar density \( J(r) \) vanishes. The densities \( T(r) \) and \( F(r) \), are pseudovectors; hence, they take the form (48). On the other hand, vectors \( j(r) \) and \( J(r) \) are linear combinations of the components of the position vector:

\[ j(r) = \iota_z(z^2, r^2_\perp)r_z + \iota_\perp(z^2, r^2_\perp)r_\perp. \]

(49)

The spin-curl \( J(r) \) takes a similar form to that of (49). Finally, \( \underline{J}(r) \) is a pseudotensor. Therefore, as follows from (25), its general form is given by:

\[ \underline{J}(r) = \theta_{zz}(z^2, r^2_\perp)r_z \otimes (r_z \times r_\perp) \]
\[ + \theta_{z\perp}(z^2, r^2_\perp)r_\perp \otimes (r_z \times r_\perp). \]

(50)

5. Summary

In the DFT, for both theoretical and practical reasons, it is important to know what general forms of densities are which obey SCS of interest. In the case of the space symmetries, such general forms can be established by means of methods of constructing the isotropic tensor fields.

For the spherical symmetry, the local densities are the isotropic scalar, vector, or (the second rank) tensor fields, depending on the position vector \( r \). The form of an isotropic field with given rank is unique and determined through one arbitrary scalar function. In particular, the parity of the field is unique for a given rank. Pseudoscalar, pseudovector, and pseudotensor fields do not exist. This is why in the case of the rotational and mirror symmetry, the pseudoscalar (spin-divergence), pseudovector (spin, spin-kinetic and tensor-kinetic), and pseudotensor (symmetric spin-current) local densities vanish.

For the axial symmetry, the local densities are isotropic fields depending on two components of the position vector: \( r_z \) and \( r_\perp \). The case of \( SO^+(2) \) is interesting as it allows us to better understand the assumption of the isotropy of a field. Indeed, in this case it might seem that the local densities are fields, depending on the \( SO^+(2) \)
vector \( \mathbf{r}_\perp \). However, such fields are not isotropic. There is another vector, \( \mathbf{r}_z \), which plays the role of a material vector fixed by the direction of the symmetry axis of the system.

6. Appendix: The Generalized Cayley-Hamilton Theorem

The original Cayley-Hamilton Theorem states that every square matrix satisfies its own characteristic equation (cf. e.g. [12][13]). It immediately follows from the theorem that the second rank SO(3) Cartesian tensor \( \mathbf{q} \) satisfies the equation

\[
-q^3 + q_1q^2 - q_2q + q_3 = 0,
\]

(51)

where \( q_1 \) is the trace, \( q_2 \) is the sum of the principal subdeterminants, and \( q_3 \) is the determinant of \( \mathbf{q} \). Hence, a second rank tensor field \( \mathbf{Q}(\mathbf{q}) \) being the power series of the tensor \( \mathbf{q} \)

\[
\mathbf{Q}(\mathbf{q}) = c_0 + c_1q + c_2q^2 + c_3q^3 + \ldots
\]

(52)

can be summed up to the form:

\[
\mathbf{Q}(\mathbf{q}) = \rho_0(q_1, q_2, q_3)\mathbf{1} + \rho_1(q_1, q_2, q_3)\mathbf{q} + \rho_2(q_1, q_2, q_3)\mathbf{q}^2,
\]

(53)

where \( \rho_1 \), \( \rho_2 \) and \( \rho_3 \) are functions of scalars \( q_1 \), \( q_2 \) and \( q_3 \). The power series is an isotropic function of \( \mathbf{q} \) because it does not contain any other tensor. For a symmetric traceless \((q_1 = 0)\) tensor \( \mathbf{Q} \) (a quadrupole tensor) Eq. (53) takes the form:

\[
\mathbf{Q}(\mathbf{q}) = \varrho_1(q_2, q_3)\mathbf{1} + \varrho_2(q_2, q_3)\mathbf{q}^2
\]

(54)

with two functions \( \varrho_1 \) and \( \varrho_2 \) of the two scalars \( q_2 \) and \( q_3 \). Eq. (54) is a direct consequence of the Cayley-Hamilton theorem for the quadrupole tensors. It can be generalized for the isotropic tensor field \( \mathbf{Q}^{(L)}(q^{(\lambda)}, q^{(\lambda')}, \ldots) \) with an arbitrary multipolarity \( L \) being a function of one or a few spherical tensors \( q^{(\lambda)}, q^{(\lambda')}, \ldots \) of ranks \( \lambda, \lambda', \ldots \), respectively. The Generalized Cayley-Hamilton Theorem has the following general form:

\[
\mathbf{Q}^{(L)}(q^{(\lambda)}, q^{(\lambda')}, \ldots) = \sum_{k=1}^{k(L, \lambda, \lambda', \ldots)} R_k(q)T_k^{(L)}(q^{(\lambda)}, q^{(\lambda')}, \ldots),
\]

(55)

where \( q \) stands for the set of independent scalars, \( T_k^{(L)} \) are some definite fundamental tensors, all constructed from \( q^{(\lambda)}, q^{(\lambda')}, \ldots \), and \( R_k \) are arbitrary scalar functions. The number \( k(L, \lambda, \lambda', \ldots) \) depends on the ranks of the all involved tensors. To find the number and the forms of the fundamental tensors in a general case may appear to be a difficult task. A systematic method of constructing them in the case of the tensor fields depending on one tensor are presented in Refs. [18][19] Eqs. (20)–(22) are examples of the GCH theorem for \( \lambda = \lambda' = 1 \) and \( L = 0, 1, 2, \) whereas Eqs. (23)–(24) — for \( \lambda = 1 \) and \( L = 0, 1, 2 \). In the nuclear collective model the GCH theorem was used for \( \lambda = 2 \) and \( \lambda = 3 \) [4][15].
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