Point symmetries in the Hartree-Fock approach. I. Densities, shapes, and currents

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Three mutually perpendicular symmetry axes of the second order, inversion, and time reversal can be used to construct a double point group denoted by D_{2h}^{TD}. Properties of this group are analyzed in relation to the symmetry and symmetry-breaking effects within the mean-field (Hartree-Fock) theories, both in even and odd fermion systems. We enumerate space symmetries of local one-body densities, and symmetries of electromagnetic moments, that appear when some or all of the D_{2h}^{TD} elements represent self-consistent mean-field symmetries.

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I. INTRODUCTION

Point-group symmetries play a very important role in nuclear mean-field theories. Two distinct aspects of this role can be singled out. First, the point symmetries of a Hamiltonian provide good quantum numbers that can conveniently be used to label its eigenstates. They help to formulate selection rules for electromagnetic and/or other types of transitions, and allow for solving the stationary problems in subspaces rather than in the complete Hilbert space of the problem in question. In that respect the use of point symmetries in nuclear physics resembles their use in other branches of physics. Second, however, and this aspect is more specific to nuclear structure domain, the use of the self-consistent Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) mean field approximations invariably leads to the problem of self-consistent symmetries and related spontaneous symmetry-breaking mechanisms [1].

In this article we aim at describing properties of nuclear one-body densities under the action of point symmetries. For the time-even densities we calculate the electric multipole moments which give information about nuclear shapes. Various point symmetries obeyed by the Hamiltonian lead then to various types of allowed shapes. In addition, for the time-odd densities we calculate magnetic multipole moments which give information about current distributions in nuclei, i.e., about the ''shapes'' of matter flow. Again, various conserved symmetries restrict these flow patterns in different ways that are studied in this paper.

Numerous experiments indicate that a great number of nuclei are deformed in their ground states. Interpretation of the corresponding results shows that most often the shapes involved are axially symmetric. Many realistic calculations, e.g., those based on the nuclear mean-field approximation, reproduce these experimental data. However, the same calculations suggest that the excited nuclear states often correspond to the nucleonic mass distributions that have the so-called triaxial shapes. It thus becomes clear that in a realistic description of the nuclear properties, the spontaneous symmetry breaking leading to the triaxially symmetric objects must be given attention.

The classical point group that contains three mutually perpendicular symmetry axes of the second order passing through a common point is denoted D_2 (see, e.g., Refs. [2–5]). Attaching to D_2 the three mutually perpendicular symmetry planes spanned on the symmetry axes gives the D_{2h} point group which contains all the spatial symmetries of interest in the present paper.

As is well known, the classical (single) point groups can be applied to spinless particles and/or systems of an even number of fermions, and thus to even-even nuclei. However, for odd fermion systems and, in particular, in the single-nucleon space, these have no faithful irreducible representations. There exist two methods to remedy this problem. One is to extend the notion of the group representation and to introduce projective or ray representations [2,6,7]. Another one, which is employed in the present work, is to enlarge the single groups by adjoining the rotation through angle 2π and all its products with the original group elements, and to double in this way the order of the group [5].

Physically, the need of such an extension is related to the fact that in the space of spinors the rotation through angle of 2π necessarily changes the sign of the wave function of an odd-fermion system. Since within the group theory a multiplication of a group element by a number is not defined, the change of sign must be introduced as an extra group element. The point group enlarged in this way is called the *double* point group and usually denoted with the superscript D (see, e.g., Refs. [4,5]), although some authors (see, e.g., Ref. [3]), denote single and double point groups by the same symbols. Here we follow the former convention, and thus the double group corresponding to single group D_{2h} is denoted by D_{2h}^{D}.

In the case of classical objects the elements of a symmetry point group are real orthogonal coordinate transformations. In quantum mechanics it is often of advantage to take into consideration both the spatial symmetries and the time-reversal operator explicitly and treat them as elements of a common ensemble of symmetry operators. Time-reversal symmetry operator (antilinear) and the space symmetries (linear) have usually been considered separately (cf., e.g., Ref. [3]). Here we follow Ref. [8] and add the time-reversal operator to the set of group elements, thus obtaining new groups denoted D_{2h}^{T} and D_{2h}^{DT}. Hence, the D_{2h} group is a subgroup of D_{2h}^{T} composed of its linear elements, and similarly, the D_{2h}^{D} group is composed of the linear elements of D_{2h}^{TD}.

Gauge symmetries, which pertain to pairing correlations of nucleons, can be added independently and are not considered in the present study. In particular, neutron-proton correlations are not discussed. Therefore, the isospin degree of freedom is irrelevant in the discussion and can be disregarded to simplify the notation.

In this paper our goal is threefold. First, in Sec. II, we present and discuss properties of the single group D_{2h}^{T} and double group D_{2h}^{TD} that are appropriate for a description of even and odd fermion systems, respectively. In particular, we recall the classification of representations of both groups, and classify properties of the group elements when they are represented in fermion Fock space. Second, in Sec. III, we present explicit symmetry properties of local densities with respect to the operators in the D_{2h}^{TD} group. This problem has been solved in particular applications [9,10]; however, it can be solved in many different ways, and it is useful to have a systematic approach which enumerates all available options. Although the local densities are most important for applications using the local density approximation (LDA), or those using the Skyrme effective interaction (see, respectively, Refs. [11,12] or Ref. [13] for reviews), they also define general properties of average values of any local one-body operator. Finally, in Sec. IV, we discuss symmetries of multipole moments which define the nuclear shapes and currents, and in Sec. V we present conclusions which can be drawn from our study. In the companion paper [14], we discuss physical aspects of the symmetry-breaking schemes pertaining to the point groups in question.

II. SYMMETRY OPERATORS

The point groups of interest in this paper can be introduced in two ways. The first one consists in defining an abstract point group by giving its table of multiplication, and then classifying the states and operators in the fermion Fock space according to the relevant irreducible representations (irreps). The second one, which we follow below, is more intuitive, and consists in defining the symmetry operators in the Fock space first, and then identifying their multiplication tables and the corresponding group structures.

A. Fock-space representations

It will be convenient to use the Cartesian representation of the symmetry operators. Let $\hat{I}_k$ for $k=x,y,z$ denote the Cartesian components of the total angular momentum operator (generators of the group of rotations). In the coordinate-space representation these operators read ($\hbar=1$)

$$\hat{I}_k \equiv \sum_{n=1}^{A} \hat{j}_k^{(n)} = \hat{L}_k + \hat{\Sigma}_k = \sum_{n=1}^{A} (\hat{l}_k^{(n)} + \tfrac{1}{2}\hat{\sigma}_k^{(n)}), \tag{1}$$

where $\hat{j}_k^{(n)}$, $\hat{l}_k^{(n)}$, and $\frac{1}{2}\hat{\sigma}_k^{(n)}$ are operators of the total, orbital, and intrinsic angular momenta, respectively, of particle number n. By definition, operators (1) act in the Hilbert space $\mathcal{H}_A$ of A-particle states, and the number of particles A appears explicitly in their definitions.

One can use another representation of $\hat{I}_k$, the so-called second quantized, or Fock-space form

$$\hat{I}_k = \sum_{\mu\nu} \langle \mu | \hat{j}_k | \nu \rangle a_\mu^+ a_\nu, \tag{2}$$

where $\langle \mu | \hat{j}_k | \nu \rangle$ are the matrix elements of the angular-momentum operators in the single-particle basis defined by the fermion creation and annihilation operators a_μ^+ and a_ν. Operators $\hat{I}_k$ in the form of Eq. (2) do not explicitly depend on A, and act simultaneously in all the A-particle spaces, i.e., they act in the Fock space $\mathcal{H}$,

$$\mathcal{H} \equiv \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_A \oplus \cdots. \tag{3}$$

In each subspace $\mathcal{H}_A$, operators (2) are equal to Eq. (1). Since both act in different domains, one should, in principle, denote them with different symbols. However, one usually understands definition (1) as a prescription to construct $\hat{I}_k$ for all values of A simultaneously (adjoined by $\hat{I}_k \equiv 0$ for $A=0$). With this extension, operators (1) and (2) are equal. In this section we understand that all operators act in the Fock space (3), while the corresponding definitions are given in the coordinate-space representation.

We introduce three standard transformations of rotation around three mutually perpendicular axes, $\mathcal{O}x$, $\mathcal{O}y$, and $\mathcal{O}z$, through the angles of π as

$$\hat{R}_k \equiv e^{-i\pi\hat{I}_k} = \bigotimes_{n=1}^{A} e^{-i\pi\hat{j}_k^{(n)}}. \tag{4}$$

Similarly, we introduce three operators of reflection in planes yz, zx, and xy, for $k=x,y,z$, respectively, which can be written as

$$\hat{S}_k \equiv \hat{P}\hat{R}_k, \tag{5}$$

where the inversion operator is denoted by $\hat{P}$. The order of operators in Eq. (5) is unimportant because

$$[\hat{P}, \hat{R}_k] = 0. \tag{6}$$

Finally, the (antilinear) time-reversal operator in the coordinate-space representation is defined as [15]

$$\hat{T} \equiv \bigotimes_{n=1}^{A} (-i\hat{\sigma}_y^{(n)})\hat{K}, \tag{7}$$

where $\hat{K}$ is the complex conjugation operator associated with the coordinate representation.

In what follows it will be convenient to denote with separate symbols the products of $\hat{T}$ with $\hat{P}$, $\hat{R}_k$, and $\hat{S}_k$ [16], i.e., the seven additional (apart from $\hat{T}$ itself) antilinear operators read

$$\hat{P}^T \equiv \hat{P}\hat{T} \tag{8a}$$

$$\hat{R}_k^T \equiv \hat{R}_k\hat{T}, \tag{8b}$$

$$\hat{S}_k^T \equiv \hat{S}_k \hat{T}. \tag{8c}$$

The order of multiplications in the above definitions is irrelevant since

$$[\hat{P},\hat{T}]=[\hat{R}_k,\hat{T}]=[\hat{S}_k,\hat{T}]=0. \tag{9}$$

In nuclear physics applications the linear operators $\hat{P}$, $\hat{R}_k$, and $\hat{S}_k$ are usually referred to as inversion, signature, and simplex. The antilinear operators $\hat{P}^T$, $\hat{R}_k^T$, and $\hat{S}_k^T$ will be called T inversion, T signature, and T simplex, respectively.

For completeness, yet two other operators must be added to the above symmetry operators. One of them is, of course, the identity operator $\hat{E}$, which can be treated as the rotation through angle equal to 0 or 4π about an arbitrary axis. The second one is the rotation through angle 2π about an arbitrary axis, i.e.,

$$\overline{E} \equiv e^{-i2\pi\hat{I}_k} = e^{-i2\pi\hat{L}_k} \bigotimes_{n=1}^{A} (-\hat{\sigma}_0^{(n)}) = (-1)^A \hat{E}, \tag{10}$$

where $\hat{\sigma}_0$ is the unity 2×2 matrix. We see that only for even systems $\overline{E}$ is equal to identity, while for odd systems it is equal to the minus identity. We should keep in mind, that in the group theory there is no such notion as a change of sign. Operators such as $(-1)^A$ may appear in representations, as they appear in the Fock-space representation here, however, one cannot use them when defining the group structures in Secs. II B and II C below.

To investigate multiplication rules of the symmetry operators introduced above one explicitly calculates products of them. For example, the products of two signatures are

$$\hat{R}_k \hat{R}_m = e^{-i\pi\hat{L}_k} e^{-i\pi\hat{L}_m} \bigotimes_{n=1}^{A} (-\hat{\sigma}_k^{(n)} \hat{\sigma}_m^{(n)}), \tag{11}$$

and the square of the time reversal reads

$$\hat{T}^2 = \bigotimes_{n=1}^{A} [-(\hat{\sigma}_y^{(n)})^2] = \overline{E}. \tag{12}$$

It is obvious that these results depend on whether A is even or odd.

Therefore, in what follows we introduce notation which explicates whether the operators act in even or odd fermion spaces $\mathcal{H}_+$ or $\mathcal{H}_-$,

$$\mathcal{H}_+ \equiv \mathcal{H}_0 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_{A=2p} \oplus \cdots, \tag{13a}$$

$$\mathcal{H}_- \equiv \mathcal{H}_1 \oplus \mathcal{H}_3 \oplus \cdots \oplus \mathcal{H}_{A=2p+1} \oplus \cdots. \tag{13b}$$

Any Fock-space operator $\hat{U}:\mathcal{H}\to\mathcal{H}$, which conserves the particle number, is split into two parts with different domains, i.e.,

$$\hat{U} = \hat{\mathbf{U}} + \hat{\mathcal{U}}, \tag{14}$$

where the bold symbols denote operators which act in the even-A spaces, while the script symbols denote those acting in the odd-A spaces, i.e.,

$$\hat{\mathbf{U}}:\mathcal{H}_+ \to \mathcal{H}_+, \tag{15a}$$

$$\hat{\mathcal{U}}:\mathcal{H}_- \to \mathcal{H}_-. \tag{15b}$$

With these definitions we are now in a position to investigate the group structures appearing for the introduced operators.

B. Single group D_{2h}^T for even systems

For even fermion numbers we consider the Fock-space operators defined in Sec. II A, and restrict them to $\mathcal{H}_+$, Eqs. (14) and (15a). Then, the complete multiplication table reads

$$\hat{\mathbf{R}}_k^2 = \hat{\mathbf{S}}_k^2 = \hat{\mathbf{T}}^2 = \hat{\mathbf{E}}, \tag{16a}$$

$$(\hat{\mathbf{R}}_k^T)^2 = (\hat{\mathbf{S}}_k^T)^2 = \hat{\mathbf{P}}^2 = \hat{\mathbf{E}}, \tag{16b}$$

$$\hat{\mathbf{R}}_k \hat{\mathbf{S}}_k = \hat{\mathbf{S}}_k \hat{\mathbf{R}}_k = \hat{\mathbf{P}}, \tag{16c}$$

$$\hat{\mathbf{R}}_k^T \hat{\mathbf{S}}_k^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{R}}_k^T = \hat{\mathbf{P}}, \tag{16d}$$

$$\hat{\mathbf{R}}_k \hat{\mathbf{R}}_k^T = \hat{\mathbf{R}}_k^T \hat{\mathbf{R}}_k = \hat{\mathbf{S}}_k \hat{\mathbf{S}}_k^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{S}}_k = \hat{\mathbf{T}}, \tag{16e}$$

$$\hat{\mathbf{R}}_k \hat{\mathbf{S}}_k^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{R}}_k = \hat{\mathbf{R}}_k^T \hat{\mathbf{S}}_k = \hat{\mathbf{S}}_k \hat{\mathbf{R}}_k^T = \hat{\mathbf{P}}^T, \tag{16f}$$

for $k=x,y,z$, and

$$\hat{\mathbf{R}}_k \hat{\mathbf{R}}_l = \hat{\mathbf{S}}_k \hat{\mathbf{S}}_l = \hat{\mathbf{R}}_k^T \hat{\mathbf{R}}_l^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{S}}_l^T = \hat{\mathbf{R}}_m, \tag{17a}$$

$$\hat{\mathbf{R}}_k \hat{\mathbf{S}}_l = \hat{\mathbf{S}}_k \hat{\mathbf{R}}_l = \hat{\mathbf{R}}_k^T \hat{\mathbf{S}}_l^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{R}}_l^T = \hat{\mathbf{S}}_m, \tag{17b}$$

$$\hat{\mathbf{R}}_k \hat{\mathbf{R}}_l^T = \hat{\mathbf{R}}_k^T \hat{\mathbf{R}}_l = \hat{\mathbf{S}}_k \hat{\mathbf{S}}_l^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{S}}_l = \hat{\mathbf{R}}_m^T, \tag{17c}$$

$$\hat{\mathbf{R}}_k^T \hat{\mathbf{S}}_l = \hat{\mathbf{S}}_k \hat{\mathbf{R}}_l^T = \hat{\mathbf{R}}_k \hat{\mathbf{S}}_l^T = \hat{\mathbf{S}}_k^T \hat{\mathbf{R}}_l = \hat{\mathbf{S}}_m^T, \tag{17d}$$

for (k,l,m) being an *arbitrary* permutation of (x,y,z).

We see that the 16 operators acting in the even-A fermion spaces constitute an Abelian single group which we denote by D_{2h}^T,

$$D_{2h}^T: \quad \{\hat{\mathbf{E}},\hat{\mathbf{P}},\hat{\mathbf{R}}_k,\hat{\mathbf{S}}_k,\hat{\mathbf{T}},\hat{\mathbf{P}}^T,\hat{\mathbf{R}}_k^T,\hat{\mathbf{S}}_k^T\}, \tag{18}$$

for $k=x,y,z$. The half of the elements in Eq. (18) are linear operators and the other half are antilinear.

It follows from the multiplication table of the D_{2h}^T operators, Eqs. (16) and (17), that the whole group can be generated by its four elements only. These elements are called the group generators. Various possibilities of choosing the generators are discussed in Ref. [14]; here we only mention that, e.g., the subset $\{\hat{\mathbf{T}}, \hat{\mathbf{P}}, \hat{\mathbf{R}}_x, \hat{\mathbf{R}}_y\}$ can be used to obtain all the operators that belong to D_{2h}^T.

The D_{2h}^T group has two important subgroups, the eight-element Abelian group D_{2h} composed of all the linear D_{2h}^T operators

$$D_{2h}: \quad \{\hat{\mathbf{E}}, \hat{\mathbf{P}}, \hat{\mathbf{R}}_k, \hat{\mathbf{S}}_k\}, \tag{19}$$

and the four-element Abelian group D_2,

$$D_2: \quad \{\hat{\mathbf{E}}, \hat{\mathbf{R}}_k\}. \tag{20}$$

Obviously, the D_{2h} subgroup of D_{2h}^T, being an Abelian group of order eight, has eight one-dimensional irreps. These can be labeled by eigenvalues equal to either $+1$ or -1 of three of its generators, say, $\hat{\mathbf{P}}$, $\hat{\mathbf{R}}_x$, and $\hat{\mathbf{R}}_y$.

We introduce names for the (one-dimensional) bases of the associated irreps according to the following convention. First, a basis is called *invariant* if it remains unchanged (belongs to eigenvalue $+1$) under all three signature operators $\hat{\mathbf{R}}_k$, and it is called either *x*, or *y*, or *z covariant* if it transforms under the signature operators like the *x*, *y*, or *z* coordinates, respectively. Secondly, prefix *pseudo* is added for bases which are odd, i.e., belong to eigenvalue -1 with respect to the inversion $\hat{\mathbf{P}}$.

Since $\hat{\mathbf{T}}$ is an antilinear operator and also an involutive operator [i.e., its square is equal to identity, Eq. (16a)], we can always choose the phases of all the basis states so that they belong to the eigenvalue $T=+1$ of $\hat{\mathbf{T}}$ [15] (see Sec. II E below). In this way we construct eight irreducible one-dimensional corepresentations (ircoreps) of D_{2h}^T, all being even with respect to the time reversal. After Wigner [8], we call the representations of a group containing antilinear operators *corepresentations* to emphasize the fact that they are *not* the representations in the usual sense (see the Appendix for details). By a suitable change of phases of the basis states we can obtain another set of eight ircoreps of D_{2h}^T, all of them odd (i.e., belonging to the eigenvalue $T=-1$) with respect to the time reversal. We use prefix *anti* to name these time-odd ircoreps. Obviously, time-even and time-odd ircoreps are pairwise equivalent (see Ref. [3]).

Note that all operators acting in the even fermion spaces $\mathcal{H}_+$ can also be classified according to the same set of sixteen ircoreps of D_{2h}^T. All these ircoreps are listed in Table III together with explicit transformation properties of several examples of one-particle operators belonging to each ircorep.

C. Double group D_{2h}^{TD} for odd systems

For odd fermion numbers we consider the Fock-space operators defined in Sec. II A, and restrict them to $\mathcal{H}_-$, Eqs. (14) and (15b). Since operator $\overline{\mathcal{E}}$ [odd-fermion-number part of $\overline{E}$ of Eq. (10)] is now an independent group element, additional *partner* operators should be introduced in order to construct the double group D_{2h}^{TD}, i.e.,

$$\overline{\mathcal{P}}=\overline{\mathcal{E}}\hat{\mathcal{P}}, \quad \overline{\mathcal{T}}=\overline{\mathcal{E}}\hat{\mathcal{T}}, \quad \overline{\mathcal{P}^T}=\overline{\mathcal{E}}\hat{\mathcal{P}}^T, \tag{21}$$

and

$$\overline{\mathcal{R}}_k=\overline{\mathcal{E}}\hat{\mathcal{R}}_k, \quad \overline{\mathcal{S}}_k=\overline{\mathcal{E}}\hat{\mathcal{S}}_k, \quad \overline{\mathcal{R}}_k^T=\overline{\mathcal{E}}\hat{\mathcal{R}}_k^T, \quad \overline{\mathcal{S}}_k^T=\overline{\mathcal{E}}\hat{\mathcal{S}}_k^T, \tag{22}$$

for $k=x,y,z$. Now the group multiplication table reads

$$\hat{\mathcal{R}}_k^2=\hat{\mathcal{S}}_k^2=\hat{\mathcal{T}}^2=\overline{\mathcal{E}}, \tag{23a}$$

$$(\hat{\mathcal{R}}_k^T)^2=(\hat{\mathcal{S}}_k^T)^2=\hat{\mathcal{P}}^2=\hat{\mathcal{E}}, \tag{23b}$$

$$\hat{\mathcal{R}}_k\hat{\mathcal{S}}_k=\hat{\mathcal{S}}_k\hat{\mathcal{R}}_k=\overline{\mathcal{P}}, \tag{23c}$$

$$\hat{\mathcal{R}}_k^T\hat{\mathcal{S}}_k^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{R}}_k^T=\hat{\mathcal{P}}, \tag{23d}$$

$$\hat{\mathcal{R}}_k\hat{\mathcal{R}}_k^T=\hat{\mathcal{R}}_k^T\hat{\mathcal{R}}_k=\hat{\mathcal{S}}_k\hat{\mathcal{S}}_k^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{S}}_k=\overline{\mathcal{T}}, \tag{23e}$$

$$\hat{\mathcal{R}}_k\hat{\mathcal{S}}_k^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{R}}_k=\hat{\mathcal{R}}_k^T\hat{\mathcal{S}}_k=\hat{\mathcal{S}}_k\hat{\mathcal{R}}_k^T=\overline{\mathcal{P}}^T \tag{23f}$$

for $k=x,y,z$, and

$$\hat{\mathcal{R}}_k\hat{\mathcal{R}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{S}}_l=\hat{\mathcal{R}}_k^T\hat{\mathcal{R}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{S}}_l^T=\overline{\mathcal{R}}_m, \tag{24a}$$

$$\hat{\mathcal{R}}_k\hat{\mathcal{S}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{R}}_l=\hat{\mathcal{R}}_k^T\hat{\mathcal{S}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{R}}_l^T=\overline{\mathcal{S}}_m, \tag{24b}$$

$$\hat{\mathcal{R}}_k\hat{\mathcal{R}}_l^T=\hat{\mathcal{R}}_k^T\hat{\mathcal{R}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{S}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{S}}_l=\overline{\mathcal{R}}_m^T, \tag{24c}$$

$$\hat{\mathcal{R}}_k^T\hat{\mathcal{S}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{R}}_l^T=\hat{\mathcal{R}}_k\hat{\mathcal{S}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{R}}_l=\overline{\mathcal{S}}_m^T \tag{24d}$$

for (k,l,m) being an *odd* permutation of (x,y,z), while relations identical to Eq. (17) hold for an *even* permutation of (x,y,z). After multiplying relations (23) and (24) by $\overline{\mathcal{E}}$ once or twice, one can easily obtain the remaining elements of the multiplication table, i.e., those which pertain to products involving one or two partner operators (22).

The D_{2h}^{TD} group is thus composed of 32 operators:

$$D_{2h}^{TD}: \quad \{\hat{\mathcal{E}}, \hat{\mathcal{P}}, \hat{\mathcal{T}}, \hat{\mathcal{P}}^T, \hat{\mathcal{R}}_k, \hat{\mathcal{S}}_k, \hat{\mathcal{R}}_k^T, \hat{\mathcal{S}}_k^T, \overline{\mathcal{E}}, \overline{\mathcal{P}}, \overline{\mathcal{T}}, \overline{\mathcal{P}^T}, \overline{\mathcal{R}}_k, \overline{\mathcal{S}}_k, \overline{\mathcal{R}}_k^T, \overline{\mathcal{S}}_k^T\}. \tag{25}$$

One can see that this double group is not Abelian, because relations (24) now do depend on whether the permutation (k,l,m) of (x,y,z) is even or odd, whereas for the single group, relations (17) are independent of that.

One may note that the Fock-space operators $\hat{U}$ of Sec. II A and the odd-fermion-space operators $\hat{\mathcal{U}}$ of Eqs. (14) and (15b) obey exactly the same multiplication rules of the double D_{2h}^{TD} group. Therefore, one might, in principle, consider only the double group D_{2h}^{TD} and refrain from studying the group structures in even and odd spaces separately. However, at the level of representations, one would then have been deprived of important properties of operators such as $\hat{\mathbf{T}}^2=\hat{\mathbf{E}}$ or $\hat{\mathcal{T}}^2=-\hat{\mathcal{E}}$ (see Sec. II E), neither of which holds in the whole Fock space, see Eqs. (12) and (10).

Since the squares of the time reversal, signatures, and simplexes, Eq. (23a), are equal to $\overline{E}$, the whole double group D_{2h}^{TD} can be generated by the same operators which generate the single group in even systems, Sec. II B. So the double group also needs four generators; for instance, the set of four elements, $\hat{\mathcal{T}}$, $\hat{\mathcal{P}}$, $\hat{\mathcal{R}}_x$, and $\hat{\mathcal{R}}_y$, can be used to obtain the entire double group of the D_{2h}^{TD} operators.

The linear operators of the D_{2h}^{TD} double group form the 16-element double group D_{2h}^{D},

$$D_{2h}^{D}: \quad \{\hat{\mathcal{E}},\hat{\mathcal{P}},\hat{\mathcal{R}}_k,\hat{\mathcal{S}}_k,\overline{\mathcal{E}},\overline{\mathcal{P}},\overline{\mathcal{R}}_k,\overline{\mathcal{S}}_k\}. \tag{26}$$

This group has ten equivalence classes (see Refs. [2,3,5]). There are six classes composed of two elements each, i.e., $\{\hat{\mathcal{R}}_k,\overline{\mathcal{R}}_k\}$ and $\{\hat{\mathcal{S}}_k,\overline{\mathcal{S}}_k\}$ for $k=x,y,z$, while the remaining elements $\{\hat{\mathcal{E}}\}$, $\{\overline{\mathcal{E}}\}$, $\{\hat{\mathcal{P}}\}$, and $\{\overline{\mathcal{P}}\}$ form four one-element classes by themselves. The group is not Abelian and possesses, apart from the 8 one-dimensional irreps already known for the single group, another two two-dimensional spinor irreps. The spinor irreps can be labeled by the parities (the eigenvalues $\pi=+1$ or -1 of the inversion operators $\hat{\mathcal{P}}$), see the Appendix.

The time reversal $\hat{\mathcal{T}}$ is an antilinear and also an antiinvolutive operator [i.e., its representations give the minus identity when squared, Eq. (23a)], and therefore it cannot be diagonalized [15] (see Sec. II E below), and used for labeling the D_{2h}^{TD} ircoreps. A Hermitian antilinear involutive operator, i.e., either a T signature or a T simplex [see Eq. (23b)] should be chosen to serve this purpose. For instance, a pair of commuting Hermitian operators $\hat{\mathcal{P}}$ and $\hat{\mathcal{R}}_y^T$ can be used to label the D_{2h}^{TD} ircoreps. As for the single group D_{2h}^{T}, ircoreps being either even or odd with respect to $\hat{\mathcal{R}}_y^T$ can be obtained one from another by a suitable change of phase, and are therefore equivalent. In analogy to the one-dimensional ircoreps, the bases of spinor ircoreps belonging to pairs of eigenvalues of $\{\hat{\mathcal{P}},\hat{\mathcal{R}}_y^T\}$ equal to $\{+1,+1\}$, $\{-1,+1\}$, $\{+1,-1\}$, and $\{-1,-1\}$ can be called the spinor, pseudospinor, antispinor, and antipseudospinor bases, respectively.

Note that only spinor ircoreps of D_{2h}^{TD} appear in the classification of states of systems with odd numbers of fermions. However, the operators acting in $\mathcal{H}_-$ can all be classified according to the one-dimensional ircoreps of D_{2h}^{TD}, similarly as operators acting in $\mathcal{H}_+$ can all be classified according to the corresponding one-dimensional ircoreps of D_{2h}^{T}. (This is completely analogous to the fact that fermion-number conserving operators can carry only integer angular momenta, i.e., they are integer-rank tensors.) Therefore, whenever we consider the action of the D_{2h}^{T} or D_{2h}^{TD} operators on fermion states we always specify whether they act in even $\mathcal{H}_+$ or odd $\mathcal{H}_-$ spaces, and use for them the corresponding notations $\hat{\mathbf{U}}$ and $\hat{\mathcal{U}}$ of Eqs. (15a) and (15b). On the other hand, whenever we consider transformation properties $\hat{U}^\dagger\hat{O}\hat{U}$ of operators $\hat{O}$ with respect to the D_{2h}^{TD} group, we do not make this distinction, and use for them notation $\hat{U}$ of Sec. II A.

D. Cartesian harmonic oscillator basis

One often uses the Cartesian harmonic oscillator (HO) basis to solve the self-consistent equations when neither spherical nor axial symmetry is assumed, see, e.g., Refs. [17,10]. The Cartesian HO states are identified by the numbers of oscillator quanta, n_x, n_y, and n_z, in the three Cartesian directions, and by the spin projection $s_z=\pm\frac{1}{2}$ on the z axis. For the standard HO phase convention, this basis is real, $\hat{\mathcal{K}}|n_xn_yn_z,s_z\rangle=|n_xn_yn_z,s_z\rangle$, where according to our standard convention the script symbol $\hat{\mathcal{K}}$ denotes the coordinate-space complex-conjugation operator acting in the odd-fermion-number space $\mathcal{H}_-$, see Sec. II A.

TABLE I. Properties of the D_{2h}^{T} operators $\hat{\mathbf{U}}$ in even fermion spaces.

	Linear	Antilinear
Hermitian ($\hat{\mathbf{U}}^2=\hat{\mathbf{E}}$)	$\hat{\mathbf{P}}$, $\hat{\mathbf{R}}_k$, $\hat{\mathbf{S}}_k$	$\hat{\mathbf{R}}_k^T$, $\hat{\mathbf{S}}_k^T$, $\hat{\mathbf{T}}$, $\hat{\mathbf{P}}^T$

For the HO states the following relations hold [18]:

$$\hat{\mathcal{P}}|n_xn_yn_z,s_z\rangle=(-1)^{n_x+n_y+n_z}|n_xn_yn_z,s_z\rangle, \tag{27a}$$

$$\hat{\mathcal{T}}|n_xn_yn_z,s_z\rangle=(-1)^{\frac{1}{2}-s_z}|n_xn_yn_z,-s_z\rangle, \tag{27b}$$

$$\hat{\mathcal{R}}_x|n_xn_yn_z,s_z\rangle=i(-1)^{n_y+n_z+1}|n_xn_yn_z,-s_z\rangle, \tag{27c}$$

$$\hat{\mathcal{R}}_y|n_xn_yn_z,s_z\rangle=(-1)^{n_x+n_z+\frac{1}{2}-s_z}|n_xn_yn_z,-s_z\rangle, \tag{27d}$$

$$\hat{\mathcal{R}}_z|n_xn_yn_z,s_z\rangle=i(-1)^{n_x+n_y+\frac{1}{2}+s_z}|n_xn_yn_z,s_z\rangle, \tag{27e}$$

$$\overline{\mathcal{E}}|n_xn_yn_z,s_z\rangle=-|n_xn_yn_z,s_z\rangle, \tag{27f}$$

from where one can find similar equations for all the remaining operators of group D_{2h}^{TD}. Since the HO Hamiltonian is symmetric under D_{2h}^{TD}, its eigenstates can be classified according to the ircoreps of D_{2h}^{TD}. It is easily seen that the HO states $|n_xn_yn_z,s_z\rangle$ form bases of the spinor, pseudospinor, antispinor, and antipseudospinor ircoreps for $\{N=n_x+n_y+n_z,\ N_y=n_x+n_z\}$ being {even, odd}, {odd, odd}, {even, even}, and {odd, even}, respectively (see the Appendix). The entire HO basis would have belonged to the spinor and pseudospinor ircoreps only, if the basis states and phase convention were chosen differently, see Ref. [14].

E. Properties of the D_{2h}^{T} and D_{2h}^{TD} operators

In this section we recall properties of the D_{2h}^{T} and D_{2h}^{TD} operators when they are represented in the fermion Fock space. Within representations, apart from the corresponding multiplication tables, Eqs. (16)–(17) and (23)–(24), these operators are characterized by their Hermitian-conjugation properties. Since all the Fock-space representations of the D_{2h}^{T} and D_{2h}^{TD} operators are unitary, they are Hermitian or

TABLE II. Properties of the D_{2h}^{TD} operators $\hat{\mathcal{U}}$ in odd fermion spaces.

	Linear	Antilinear
Hermitian ($\hat{\mathcal{U}}^2=\hat{\mathcal{E}}$)	$\hat{\mathcal{P}}$	$\hat{\mathcal{R}}_k^T$, $\hat{\mathcal{S}}_k^T$
Anti-Hermitian ($\hat{\mathcal{U}}^2=-\hat{\mathcal{E}}$)	$\hat{\mathcal{R}}_k$, $\hat{\mathcal{S}}_k$	$\hat{\mathcal{T}}$, $\hat{\mathcal{P}}^T$

anti-Hermitian depending on whether they are involutive or anti-involutive, respectively. Properties of these operators are very different depending on whether they are linear or antilinear. These characteristics are summarized in Tables I and II, where the D_{2h}^{T} and D_{2h}^{TD} operators are split into two or four subsets, respectively. Below we review the properties of operators in each such subset.

For each linear D_{2h}^{T} or D_{2h}^{TD} operator one can attribute quantum numbers to fermion states. These quantum numbers can be equal to ± 1 or $\pm i$ for Hermitian (involutive) or anti-Hermitian (anti-involutive) operators, respectively. Therefore, the parity operators $\hat{\mathbf{P}}$ or $\hat{\mathcal{P}}$ give the parity quantum numbers, $\pi = \pm 1$, the signature operators $\hat{\mathbf{R}}_k$ give the signature quantum numbers, $r = \pm 1$, in even systems and the signature operators $\hat{\mathcal{R}}_k$ give $r = \pm i$ in odd systems. Likewise, the simplex operators $\hat{\mathbf{S}}_k$ and $\hat{\mathcal{S}}_k$ give the simplex quantum numbers, $s = \pm 1$ and $s = \pm i$, respectively.

Antilinear operators do not give good quantum numbers, and their role is very different, depending on whether they are Hermitian or anti-Hermitian, Tables I and II. For each Hermitian antilinear D_{2h}^{T} or D_{2h}^{TD} operator, i.e., for $\hat{\mathbf{R}}_k^T$, $\hat{\mathbf{S}}_k^T$, $\hat{\mathbf{T}}$, $\hat{\mathbf{P}}^T$, $\hat{\mathcal{R}}_k^T$, or $\hat{\mathcal{S}}_k^T$ one can find a basis consisting solely of its eigenstates with the common eigenvalue equal to 1 [15]. Indeed, if state $|\Psi\rangle$ is an eigenstate of, e.g., $\hat{R}_k^T$, the corresponding eigenvalue must be a phase, i.e., $\hat{R}_k^T|\Psi\rangle = e^{2i\phi}|\Psi\rangle$. In such a case, state $|\Psi'\rangle = e^{i\phi}|\Psi\rangle$ is an eigenstate of $\hat{R}_k^T$ with eigenvalue 1. This demonstrates explicitly that properties of eigenstates of $\hat{R}_k^T$ are, of course, phase dependent. In the case when state $|\Psi\rangle$ is not an eigenstate of $\hat{R}_k^T$, one can transform the two linearly independent states $|\Psi\rangle$ and $\hat{R}_k^T|\Psi\rangle$ into eigenstates of $\hat{R}_k^T$ with eigenvalue 1 by symmetrization and antisymmetrization of the two:

$$|\Psi_s\rangle = |\Psi\rangle + \hat{R}_k^T|\Psi\rangle, \tag{28a}$$

$$|\Psi_a\rangle = i|\Psi\rangle - i\hat{R}_k^T|\Psi\rangle, \tag{28b}$$

which also requires a specific phase. Therefore, phase-convention properties of states are essential for a discussion of bases of eigenstates of the Hermitian antilinear operators, and in Ref. [14] a special discussion is devoted to this problem.

One should also remember, that only linear combinations of basis states with *real* coefficients remain eigenstates of any Hermitian antilinear operator. This is in contrast to properties of linear operators, for which a linear combination of eigenstates, corresponding to the same eigenvalue, with *arbitrary* coefficients, is also an eigenstate with the same eigenvalue.

Very special properties characterize the anti-Hermitian antilinear operators. Within the D_{2h}^{T} or D_{2h}^{TD} groups only the $\hat{\mathcal{T}}$ and $\hat{\mathcal{P}}^T$ operators in odd systems belong to such a subset (Table II). For each anti-Hermitian antilinear D_{2h}^{TD} operator the space of fermion states can be arranged in pairs of orthogonal states $(|\Psi(+)\rangle, |\Psi(-)\rangle)$ [15], such that, for example,

$$\hat{\mathcal{T}}\,|\Psi(\pm)\rangle = \pm|\Psi(\mp)\rangle \tag{29}$$

or

$$\hat{\mathcal{P}}^T|\Psi(\pm)\rangle = \pm|\Psi(\mp)\rangle. \tag{30}$$

Therefore, the $\hat{\mathcal{T}}$ and $\hat{\mathcal{P}}^T$ operators cannot be diagonalized. In particular, there is no odd fermion state which would be invariant with respect to $\hat{\mathcal{T}}$ or $\hat{\mathcal{P}}^T$.

III. SYMMETRIES OF LOCAL DENSITIES

Suppose that the Fock-space operator $\hat{\mathbf{U}}$ or $\hat{\mathcal{U}}$, belonging to D_{2h}^{T} or D_{2h}^{TD}, respectively, represents a symmetry conserved by a mean-field many-particle state $|\Psi_+\rangle$ or $|\Psi_-\rangle$, in even or odd fermion spaces, i.e.,

$$\hat{\mathbf{U}}|\Psi_+\rangle = u|\Psi_+\rangle, \tag{31a}$$

$$\hat{\mathcal{U}}|\Psi_-\rangle = u|\Psi_-\rangle. \tag{31b}$$

As discussed in Sec. II E, eigenvalue u can be equal to ± 1 or $\pm i$, and moreover, in odd fermion systems $\hat{U}$ cannot be equal to either $\hat{\mathcal{T}}$ or $\hat{\mathcal{P}}^T$, i.e., neither the time reversal nor the product of inversion and time reversal can be a conserved symmetry in odd systems. According to conventions introduced in Sec. II C, in odd systems the hat always denotes one of the D_{2h}^{TD} operators introduced in Sec. II A, and not one of their partners [Eqs. (21) and (22)]. Of course, if $\hat{\mathcal{U}}$ is a symmetry of $|\Psi_-\rangle$ then $\overline{\mathcal{U}}$ is a symmetry as well, so from the point of view of conserved symmetries, any extra study of partner operators is unnecessary.

Mean-field state $|\Psi\rangle$ can be characterized by the single-particle density matrix ρ (see Ref. [1] for the definition), for which the symmetry properties (31) imply

$$\hat{U}^\dagger \rho \hat{U} = \rho, \tag{32}$$

independently of eigenvalue u. [Symmetry property (32) does not depend on whether the mean-field state belongs to the even or odd fermion space, and therefore, we use the Fock-space notation $\hat{U}$ for the symmetry operators, see definitions in Sec. II A and discussion in Sec. II C.] It then follows that the single-particle self-consistent Hamiltonian $h[\rho]$ is also symmetric with respect to operator $\hat{U}$ [1], namely,

$$\hat{U}^\dagger h[\rho]\hat{U} = h[\rho]. \tag{33}$$

Equation (33) implies that if φ is a normalized single-particle eigenfunction of $h[\rho]$, then $\hat{U}\varphi$ is also a normalized eigenfunction, both belonging to the same eigenvalue. As a consequence, it can be shown [19] that the symmetry is preserved during the standard self-consistent iteration, provided the entire multiplets of states belonging to the same eigenvalue of $\hat{U}$ are either fully occupied, or fully empty. In such

TABLE III. Symmetry properties of space-spin one-particle operators $\hat{O}$ belonging to different one-dimensional ircoreps of the D_{2h}^{T} and D_{2h}^{TD} groups. The first column gives names of different ircoreps, the second column lists examples of operators $\hat{O}$, and the remaining columns give signs in the expression $\hat{U}^{\dagger}\hat{O}\hat{U}=\pm\hat{O}$, for operators $\hat{U}$ given in the column headers. Note that these results do not depend on whether operators $\hat{U}$ act in even or odd spaces, and therefore the Fock-space notation is used for them.

Ircorep	Space-spin one-particle operators $\hat{O}$	$\hat{T}$	$\hat{P}$	$\hat{R}_x$	$\hat{R}_y$
invariants	$x^2,y^2,z^2,\nabla_x^2,\nabla_y^2,\nabla_z^2;xi\nabla_y\hat{\sigma}_z,yi\nabla_z\hat{\sigma}_x,zi\nabla_x\hat{\sigma}_y$	+	+	+	+
pseudoinvariants	$xyz,xi\nabla_y i\nabla_z,yi\nabla_z i\nabla_x,zi\nabla_x i\nabla_y;i\nabla_x\hat{\sigma}_x,i\nabla_y\hat{\sigma}_y,i\nabla_z\hat{\sigma}_z$	+	−	+	+
anti-invariants	$xi\nabla_x,yi\nabla_y,zi\nabla_z;xy\hat{\sigma}_z,yz\hat{\sigma}_x,zx\hat{\sigma}_y$	−	+	+	+
antipseudoinvariants	$xyi\nabla_z,yzi\nabla_x,zxi\nabla_y;x\hat{\sigma}_x,y\hat{\sigma}_y,z\hat{\sigma}_z$	−	−	+	+
x covariants	$x;i\nabla_y\hat{\sigma}_z,i\nabla_z\hat{\sigma}_y$	+	−	+	−
y covariants	$y;i\nabla_x\hat{\sigma}_z,i\nabla_z\hat{\sigma}_x$	+	−	−	+
z covariants	$z;i\nabla_x\hat{\sigma}_y,i\nabla_y\hat{\sigma}_x$	+	−	−	−
x pseudocovariants	$yz;xi\nabla_y\hat{\sigma}_y,i\nabla_x y\hat{\sigma}_y,\hat{\sigma}_x yi\nabla_y$	+	+	+	−
y pseudocovariants	$xz;yi\nabla_z\hat{\sigma}_z,i\nabla_y z\hat{\sigma}_z,\hat{\sigma}_y zi\nabla_z$	+	+	−	+
z pseudocovariants	$xy;zi\nabla_x\hat{\sigma}_x,i\nabla_z x\hat{\sigma}_x,\hat{\sigma}_z xi\nabla_x$	+	+	−	−
x anticovariants	$i\nabla_x;y\hat{\sigma}_z,z\hat{\sigma}_y$	−	−	+	−
y anticovariants	$i\nabla_y;x\hat{\sigma}_z,z\hat{\sigma}_x$	−	−	−	+
z anticovariants	$i\nabla_z;x\hat{\sigma}_y,y\hat{\sigma}_x$	−	−	−	−
x antipseudocovariants	$yi\nabla_z,zi\nabla_y;\hat{\sigma}_x$	−	+	+	−
y antipseudocovariants	$xi\nabla_z,zi\nabla_x;\hat{\sigma}_y$	−	+	−	+
z antipseudocovariants	$xi\nabla_y,yi\nabla_x;\hat{\sigma}_z$	−	+	−	−

a case Eqs. (32) and (33) are fulfilled repeatedly in the successive steps of iteration, and $\hat{U}$ is a self-consistent symmetry.

Since the one-body density is a fermion-number conserving one-body operator, it can be classified according to one-dimensional ircoreps of D_{2h}^{T} or D_{2h}^{TD}, and this can be done both in even and odd systems. This means that either the given operator $\hat{U}$ is a conserved symmetry, Eqs. (31) and (32), and the density matrix belongs to the given one-dimensional ircorep of the subgroup generated by $\hat{U}$, or $\hat{U}$ is a broken symmetry and the density matrix has two nonzero components in two different such one-dimensional ircoreps. It follows that in odd systems the density matrix has always nonzero components in two ircoreps corresponding to the time reversal.

This classification procedure is used below to enumerate properties of the density matrix when one or more D_{2h}^{T} or D_{2h}^{TD} operators are conserved symmetries. Note also, that unlike for the many-body states $|\Psi\rangle$, one does not have a freedom to change the phase of the density matrix, because it is a Hermitian operator independent of the phase of the mean-field state it corresponds to. Therefore, if the density matrix has non-zero components in two ircoreps corresponding to two different eigenvalues of an antilinear D_{2h}^{T} or D_{2h}^{TD} operator, it cannot be transformed to the form in which it would have been either even or odd with respect to this operator.

A definite symmetry of the density matrix, Eq. (32), implies certain symmetries for local densities and their derivatives. These symmetries are discussed and enumerated in the present section.

The spin structure of the density matrix is given by

$$\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma')=\tfrac{1}{2}\rho(\boldsymbol{r},\boldsymbol{r}')\,\delta_{\sigma\sigma'}+\tfrac{1}{2}\sum_{k=x,y,z}s_k(\boldsymbol{r},\boldsymbol{r}')\langle\sigma|\hat{\sigma}_k|\sigma'\rangle, \tag{34}$$

where $\boldsymbol{r}=(x,y,z)$ and $\boldsymbol{r}'=(x',y',z')$ represent three-dimensional position vectors. When the rotational symmetry is preserved one often refers to $\rho(\boldsymbol{r},\boldsymbol{r}')$ and $s_k(\boldsymbol{r},\boldsymbol{r}')$ as the *scalar* and *vector* densities, respectively. In our case, the rotational symmetry is broken, and we will avoid using these terms. Instead, we classify the densities according to the ircoreps of the D_{2h}^{T} or D_{2h}^{TD} group. As discussed above, for the one-body operators only the one-dimensional ircoreps are relevant for the classification. There are 16 characteristic transformation properties of the bases for one-dimensional ircoreps. In Table III we list all these ircoreps, illustrated by examples of space-spin operators of interest, e.g., powers of coordinates, x, y, z and gradients, ∇_x, ∇_y, ∇_z.

The table also lists explicitly the transformation properties of operators belonging to every type of symmetry. For example, the minus sign which appears in row denoted by y covariants and column denoted by $\hat{R}_x$ means that $\hat{R}_x^{\dagger}y\hat{R}_x=-y$. It can be easily checked that the Pauli matrices $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ transform under the signatures as the x,y,z coordinates, respectively, do not change under the inversion, and change their signs under the time reversal. Therefore, these can be classified as k-antipseudocovariants for $k=x,y,z$, respectively. Spin-dependent operators belonging to other ircoreps can also be constructed from the Pauli matrices. Therefore,

TABLE IV. Symmetry properties of various local densities belonging to different one-dimensional ircoreps of the D_{2h}^{T} or D_{2h}^{TD} groups. For instructions on using the table see the text explaining Eq. (41).

Ircorep	Local densities		$\hat{P}$	$\hat{P}^T$	$\hat{R}_k$	$\hat{R}_k^T$	$\hat{S}_k$	$\hat{S}_k^T$	$\hat{R}_l$	$\hat{R}_l^T$	$\hat{S}_l$	$\hat{S}_l^T$	$\hat{R}_m$	$\hat{R}_m^T$	$\hat{S}_m$	$\hat{S}_m^T$
invariants	$\rho,\tau_{ii},\nabla_i^2\rho,\nabla_k J_{lm}$	$\rho,\tau,\Delta\rho,\boldsymbol{\nabla}\cdot\boldsymbol{J}$	+	+	+	+	+	+	+	+	+	+	+	+	+	+
pseudoinvariants	J_{ii}	J	−	−	+	+	−	−	+	+	−	−	+	+	−	−
anti-invariants	$T_{klm},\nabla_i j_i,\nabla_k\nabla_l s_m$	$\boldsymbol{\nabla}\cdot\boldsymbol{j}$	+	−	+	−	+	−	+	−	+	−	+	−	+	−
antipseudoinvariants	$\nabla_i s_i$	$\boldsymbol{\nabla}\cdot\boldsymbol{s}$	−	+	+	−	−	+	+	−	−	+	+	−	−	+
k covariants	$J_{lm},\nabla_k\rho$	$(\boldsymbol{J})_k,(\vec{J})_{lm},(\boldsymbol{\nabla}\rho)_k$	−	−	+	+	−	−	−	−	+	+	−	−	+	+
k pseudocovariants	$\tau_{lm},\nabla_l\nabla_m\rho,\nabla_k J_{ii},$ $\nabla_i J_{ki},\nabla_i J_{ik}$	$(\boldsymbol{\nabla}J)_k,$ $(\boldsymbol{\nabla}\cdot\vec{J})_k,(\boldsymbol{\nabla}\times\boldsymbol{J})_k$	+	+	+	+	+	+	−	−	−	−	−	−	−	−
k anticovariants	$j_k,\nabla_l s_m$	$(\boldsymbol{j})_k,(\boldsymbol{\nabla}\times\boldsymbol{s})_k$	−	+	+	−	−	+	−	+	+	−	−	+	+	−
k antipseudocovariants	$s_k,T_{iik},T_{kii},\nabla_l j_m,$ $\nabla_k\nabla_i s_i,\nabla_i^2 s_k$	$(\boldsymbol{s})_k,(\boldsymbol{T})_k,(\boldsymbol{\nabla}\times\boldsymbol{j})_k$ $(\boldsymbol{\nabla}(\boldsymbol{\nabla}\cdot\boldsymbol{s}))_k,(\Delta\boldsymbol{s})_k$	+	−	+	−	+	−	−	+	−	+	−	+	−	+
		$(\epsilon_k,\epsilon_l,\epsilon_m)=$	(−−−)	(+−−)	(−++)	(−+−)	(+−+)	(−−+)	(++−)							

examples of spin-dependent operators are also listed in the table. In Table III we have introduced the same names for operators as for the bases of one-dimensional ircoreps (see Sec. II B).

Similarly as in Ref. [20], we consider the following local densities:
particle and spin densities:

$$\rho(\boldsymbol{r})=\rho(\boldsymbol{r},\boldsymbol{r}), \tag{35a}$$

$$s_k(\boldsymbol{r})=s_k(\boldsymbol{r},\boldsymbol{r}); \tag{35b}$$

kinetic and spin-kinetic densities:

$$\tau_{kl}(\boldsymbol{r})=[\nabla_k\nabla'_l\rho(\boldsymbol{r},\boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}, \tag{36a}$$

$$T_{klm}(\boldsymbol{r})=[\nabla_k\nabla'_l s_m(\boldsymbol{r},\boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}; \tag{36b}$$

current and spin-current densities:

$$j_k(\boldsymbol{r})=\frac{1}{2i}[\nabla_k-\nabla'_k)\rho(\boldsymbol{r},\boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}, \tag{37a}$$

$$J_{kl}(\boldsymbol{r})=\frac{1}{2i}[(\nabla_k-\nabla'_k)s_l(\boldsymbol{r},\boldsymbol{r}')]_{\boldsymbol{r}=\boldsymbol{r}'}; \tag{37b}$$

where each index k, l, or m may refer to either of x, y, or z. It follows from the Hermiticity of the density matrix ρ that all the above local densities are real functions of $\boldsymbol{r}$. Usually only the traces of kinetic densities,

$$\tau(\boldsymbol{r})=\sum_k \tau_{kk}(\boldsymbol{r}), \tag{38a}$$

$$T_m(\boldsymbol{r})=\sum_k T_{kkm}(\boldsymbol{r}), \tag{38b}$$

are used in applications.

When operator $\hat{U}$ represents a conserved symmetry of the density matrix, Eq. (32), the transformation rules for gradients and spin operators, given in Table III, imply definite transformation rules for the local densities. These are listed in Table IV, for all the one-dimensional ircoreps of D_{2h}^{T} or D_{2h}^{TD} as indicated in the first column. In the second column we show the local densities in forms defined by Eqs. (35)–(37), while the third column gives, when possible, the local densities in the traditional vector-tensor notation, e.g.,

$$\boldsymbol{s}=(s_x,s_y,s_z), \tag{39a}$$

$$\boldsymbol{T}=(T_x,T_y,T_z), \tag{39b}$$

$$J=\sum_k J_{kk}, \tag{40a}$$

$$(\vec{J})_{kl}=\frac{1}{2}(J_{kl}+J_{lk})-\frac{1}{3}J\delta_{kl}, \tag{40b}$$

$$(\boldsymbol{J})_k=\sum_{lm}\varepsilon_{klm}J_{lm}. \tag{40c}$$

Derivatives of densities up to the second order are also included in the table.

From Table IV one can read off the symmetry properties of various densities. Suppose $d(x,y,z)$ is a generic name of one of the densities listed in the second or third column, and $\hat{U}$ is a generic name of one of the D_{2h}^{T} or D_{2h}^{TD} operators listed in the first row. We use the convention that index i may take any value among x, y or z, while indices $k\neq l\neq m$ are arbitrary permutations of x, y, and z. If $\hat{U}$ represents a conserved symmetry, one has the following symmetry rule for the density $d(x,y,z)$:

$$d(\epsilon_x x,\epsilon_y y,\epsilon_z z)=\epsilon d(x,y,z), \tag{41}$$

where ϵ is the sign listed in Table IV in the row denoted by d and column denoted by $\hat{U}$. Signs $(\epsilon_x,\epsilon_y,\epsilon_z)$ are given in the last row of Table III, and pertain to two D_{2h}^{T} or D_{2h}^{TD} operators (viz. $\hat{U}$ and $\hat{U}^T$) in two adjacent columns. These latter signs give changes of coordinates (x,y,z) under the action of $\hat{U}$. As the time reversal does not affect spatial coordinates, these signs are the same for any pair of operators

TABLE V. Symmetry properties of electric multipole operators $\hat{Q}_{\lambda\mu}$ with respect to operators of the D_{2h}^{T} or D_{2h}^{TD} groups. The results of the symmetry operator $\hat{U}^{\dagger}\hat{Q}_{\lambda\mu}\hat{U}$ are given for three spatial directions $k=x, y, z$. Where applicable, the upper part of the table gives expressions in terms of changed signs of magnetic components, and the lower part gives the equivalent expressions in terms of the complex conjugation.

k	$\hat{R}_k$	$\hat{R}_k^T$	$\hat{S}_k$	$\hat{S}_k^T$
x	$(-1)^{\lambda}\hat{Q}_{\lambda,-\mu}$	$(-1)^{\lambda+\mu}\hat{Q}_{\lambda\mu}$	$\hat{Q}_{\lambda,-\mu}$	$(-1)^{\mu}\hat{Q}_{\lambda\mu}$
y	$(-1)^{\lambda-\mu}\hat{Q}_{\lambda,-\mu}$	$(-1)^{\lambda}\hat{Q}_{\lambda\mu}$	$(-1)^{-\mu}\hat{Q}_{\lambda,-\mu}$	$\hat{Q}_{\lambda\mu}$
z	$(-1)^{\mu}\hat{Q}_{\lambda\mu}$	$\hat{Q}_{\lambda,-\mu}$	$(-1)^{\lambda+\mu}\hat{Q}_{\lambda\mu}$	$(-1)^{\lambda}\hat{Q}_{\lambda,-\mu}$
x	$(-1)^{\lambda+\mu}\hat{Q}^{*}_{\lambda\mu}$	$(-1)^{\lambda+\mu}\hat{Q}_{\lambda\mu}$	$(-1)^{\mu}\hat{Q}^{*}_{\lambda\mu}$	$(-1)^{\mu}\hat{Q}_{\lambda\mu}$
y	$(-1)^{\lambda}\hat{Q}^{*}_{\lambda\mu}$	$(-1)^{\lambda}\hat{Q}_{\lambda\mu}$	$\hat{Q}^{*}_{\lambda\mu}$	$\hat{Q}_{\lambda\mu}$
z	$(-1)^{\mu}\hat{Q}_{\lambda\mu}$	$(-1)^{\mu}\hat{Q}^{*}_{\lambda\mu}$	$(-1)^{\lambda+\mu}\hat{Q}_{\lambda\mu}$	$(-1)^{\lambda+\mu}\hat{Q}^{*}_{\lambda\mu}$

$\hat{U}$ and $\hat{U}^T$. One generic table of signs determines, therefore, symmetry properties of any local density for any of the D_{2h}^{T} or D_{2h}^{TD} symmetries being preserved.

For example, symmetry properties of density J_{xy} can be found by using indices $l=x$ and $m=y$ (which requires $k=z$) in the row pertaining to k covariants. For the conserved $\hat{R}_z=\hat{R}_k$ symmetry we then find in the corresponding column $\epsilon=+$ and $\epsilon_x=\epsilon_l=-$, $\epsilon_y=\epsilon_m=-$, and $\epsilon_z=\epsilon_k=+$, which gives $J_{xy}(-x,-y,z)=J_{xy}(x,y,z)$.

It is worth noting that symmetry properties (41) which correspond to various D_{2h}^{T} or D_{2h}^{TD} operators, are related to one another only by the corresponding group multiplication rules. Therefore, a specific choice of the conserved generators, either for the complete D_{2h}^{T} or D_{2h}^{TD} groups or for any of their subgroups [14], leads to a specific set of symmetry properties of local densities.

Symmetry properties (41) can be used for the purpose of a continuation of densities from one semispace into the second semispace, i.e., one can use only space points for, e.g., $x\geqslant 0$. For two symmetry properties (41), coming from two different symmetry operators (but not from the pair $\hat{U}$ and $\hat{U}^T$), one can restrict the space to a quarter-space, where two coordinates have definite signs, e.g., $x\geqslant 0$ and $y\geqslant 0$. Finally, three conserved symmetries allow for a restriction to one eighth of the full space with all the coordinates having definite signs, e.g., $x\geqslant 0$, $y\geqslant 0$, and $y\geqslant 0$. The time-reversal symmetry does not lead to restrictions on the space properties of densities, but, when conserved, gives the vanishing of all the anti-invariant, antipseudoinvariant, anticovariant, and antipseudocovariant densities, viz., s_k, j_k, T_{klm} for arbitrary k,l,m as well as their derivatives (see Table IV). The possibilities of simultaneously conserving one, two, three, or four symmetry operators from the D_{2h}^{T} or D_{2h}^{TD} groups will be discussed in Ref. [14].

Since density matrix ρ and single-particle Hamiltonian $h[\rho]$ are always simultaneously invariant under any conserved symmetry $\hat{U}$, Eqs. (32) and (33), the discussion above can be repeated for self-consistent local fields appearing in a local mean-field Hamiltonian. Explicit formulas for symmetry properties of local fields are identical to those listed in Table IV, and will not be repeated here. In applications, these symmetries appear automatically when the self-consistent mean fields are calculated in terms of densities, see Ref. [20].

IV. SYMMETRIES OF SHAPES, CURRENTS, AND AVERAGE ANGULAR MOMENTA

In this section we discuss properties of average values of various operators, calculated for the HF many-particle state $|\Psi\rangle$. In particular, we consider the electromagnetic multipole operators and the total angular momentum; the quantities which are used to characterize properties of investigated systems. First of all, we enumerate transformation properties of these operators under the D_{2h}^{T} or D_{2h}^{TD} operators. Similarly as for the density matrix (Sec. III), the one-body operators discussed in this section belong to one-dimensional ircoreps of D_{2h}^{T} or D_{2h}^{TD}, and therefore, their properties do not depend on whether the system contains even or odd number of fermions.

A. Transformation properties of angular momentum and multipole operators

The k component of total angular momentum $\hat{I}_k$ transforms obviously as k antipseudocovariant under D_{2h}^{T} or D_{2h}^{TD}, and its transformation rules can be easily read off from Table III.

For λ even (odd), the electric multipole operators $\hat{Q}_{\lambda\mu}$ are even (odd), respectively, under the action of the inversion, and are all even with respect to the time reversal, i.e.,

$$\hat{P}^{\dagger}\hat{Q}_{\lambda\mu}\hat{P}=(-1)^{\lambda}\hat{Q}_{\lambda\mu}, \tag{42a}$$

$$\hat{T}^{\dagger}\hat{Q}_{\lambda\mu}\hat{T}=\hat{Q}^{*}_{\lambda\mu}. \tag{42b}$$

The magnetic multipole operators $\hat{M}_{\lambda\mu}$ have opposite transformation properties

$$\hat{P}^{\dagger}\hat{M}_{\lambda\mu}\hat{P}=-(-1)^{\lambda}\hat{M}_{\lambda\mu}, \tag{43a}$$

$$\hat{T}^{\dagger}\hat{M}_{\lambda\mu}\hat{T}=-\hat{M}^{*}_{\lambda\mu}. \tag{43b}$$

Table V gives transformation properties [21] of $\hat{Q}_{\lambda\mu}$ with respect to operators of the D_{2h}^{T} or D_{2h}^{TD} groups, other than $\hat{T}$

TABLE VI. Conditions fulfilled by the electric and magnetic multipole moments $Q_{\lambda\mu}$ and $M_{\lambda\mu}$, for conserved D_{2h}^{T} or D_{2h}^{TD} operators. Where applicable, the upper part of the table gives expressions in terms of changed signs of magnetic components, and the lower part gives equivalent expressions in terms of the complex conjugation.

k	$\hat{R}_k$	$\hat{R}_k^T$	$\hat{S}_k$	$\hat{S}_k^T$
x	$Q_{\lambda\mu}=(-1)^{\lambda}Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda}Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=Q_{\lambda,-\mu}$
x	$M_{\lambda\mu}=(-1)^{\lambda}M_{\lambda,-\mu}$	$M_{\lambda\mu}=-(-1)^{\lambda}M_{\lambda,-\mu}$	$M_{\lambda\mu}=-M_{\lambda,-\mu}$	$M_{\lambda\mu}=M_{\lambda,-\mu}$
y	$Q_{\lambda\mu}=(-1)^{\lambda-\mu}Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda-\mu}Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=(-1)^{-\mu}Q_{\lambda,-\mu}$	$Q_{\lambda\mu}=(-1)^{-\mu}Q_{\lambda,-\mu}$
y	$M_{\lambda\mu}=(-1)^{\lambda-\mu}M_{\lambda,-\mu}$	$M_{\lambda\mu}=-(-1)^{\lambda-\mu}M_{\lambda,-\mu}$	$M_{\lambda\mu}=-(-1)^{-\mu}M_{\lambda,-\mu}$	$M_{\lambda\mu}=(-1)^{-\mu}M_{\lambda,-\mu}$
z	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}$
z	$M_{\lambda\mu}=(-1)^{\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=-(-1)^{\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=-(-1)^{\lambda+\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=(-1)^{\lambda+\mu}M_{\lambda\mu}$
x	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}^{*}$
x	$M_{\lambda\mu}=(-1)^{\lambda+\mu}M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=-(-1)^{\lambda+\mu}M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=-(-1)^{\mu}M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=(-1)^{\mu}M_{\lambda\mu}^{*}$
y	$Q_{\lambda\mu}=(-1)^{\lambda}Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=(-1)^{\lambda}Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=Q_{\lambda\mu}^{*}$	$Q_{\lambda\mu}=Q_{\lambda\mu}^{*}$
y	$M_{\lambda\mu}=(-1)^{\lambda}M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=-(-1)^{\lambda}M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=-M_{\lambda\mu}^{*}$	$M_{\lambda\mu}=M_{\lambda\mu}^{*}$
z	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}$	$Q_{\lambda\mu}=(-1)^{\lambda+\mu}Q_{\lambda\mu}$
z	$M_{\lambda\mu}=(-1)^{\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=-(-1)^{\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=-(-1)^{\lambda+\mu}M_{\lambda\mu}$	$M_{\lambda\mu}=(-1)^{\lambda+\mu}M_{\lambda\mu}$

and $\hat{P}$. One may note that the electric multipole operators are invariant with respect to the $\hat{S}_y^T$ symmetry. This is of course a consequence of the standard phase convention for the rotational irreducible tensor operators [21,22],

$$\hat{Q}_{\lambda\mu}^{*}=(-1)^{-\mu}\hat{Q}_{\lambda,-\mu}, \tag{44a}$$

$$\hat{M}_{\lambda\mu}^{*}=(-1)^{-\mu}\hat{M}_{\lambda,-\mu}, \tag{44b}$$

which ensures that the antilinear operator $\hat{S}_y^T$ acts as an identity upon any irreducible spherical tensor operator.

B. Average values

The electric and magnetic moments are defined as

$$Q_{\lambda\mu}=\langle\Psi|\hat{Q}_{\lambda\mu}|\Psi\rangle=\int q_{\lambda\mu}(\boldsymbol{r})\,d^3\boldsymbol{r}, \tag{45a}$$

$$M_{\lambda\mu}=\langle\Psi|\hat{M}_{\lambda\mu}|\Psi\rangle=\int m_{\lambda\mu}(\boldsymbol{r})\,d^3\boldsymbol{r}, \tag{45b}$$

where $|\Psi\rangle$ is a many-body mean-field state, and $q_{\lambda\mu}(\boldsymbol{r})$ and $m_{\lambda\mu}(\boldsymbol{r})$ are the corresponding moment densities:

$$q_{\lambda\mu}(\boldsymbol{r})=e\rho(\boldsymbol{r})Q_{\lambda\mu}(\boldsymbol{r}), \tag{46a}$$

$$m_{\lambda\mu}(\boldsymbol{r})=\mu_N\sum_{k=x,y,z}\left(g_s s_k\nabla_k Q_{\lambda\mu}(\boldsymbol{r})-\frac{2}{\lambda+1}g_l j_k[\boldsymbol{r}\times\boldsymbol{\nabla}Q_{\lambda\mu}(\boldsymbol{r})]_k\right), \tag{46b}$$

and e, g_s, and g_l are the elementary charge, and the spin and orbital gyromagnetic factors, respectively [1]. In definitions (46), multipole functions [21] (solid harmonics) have the standard form $Q_{\lambda\mu}(\boldsymbol{r})=r^{\lambda}Y_{\lambda\mu}(\theta,\phi)$.

Similarly, the mean value of the k-component of total angular momentum (in units of $\hbar$) reads

$$I_k=\langle\Psi|\hat{I}_k|\Psi\rangle=\int[\varepsilon_{klm}r_l j_m(\boldsymbol{r})+\tfrac{1}{2}s_k(\boldsymbol{r})]d^3\boldsymbol{r}. \tag{47}$$

We may now combine symmetry properties of densities ρ, $\boldsymbol{s}$, and $\boldsymbol{j}$, Table III, with those of multipole operators, Table V, to obtain symmetry conditions obeyed by the electric and magnetic moments, and by the average angular momenta, for given conserved symmetries of the D_{2h}^{T} or D_{2h}^{TD} groups. In doing so, we have to remember that since the electric multipole operators are time even, the corresponding electric moments depend only on the time-even component of the density matrix, as given in Eq. (46a). This is so irrespective of whether the time reversal is, or is not a conserved symmetry, or whether the system contains even or odd number of fermions. Therefore, the time reversal does not impose any condition on the electric multipole moments. On the other hand, with the time-reversal symmetry conserved, which may occur only for even systems, all magnetic moments and average angular momenta must vanish, because they depend only on the time-odd component of the density matrix, Eqs. (46b) and (47).

For the conserved parity, one obtains the standard conditions

$$Q_{\lambda\mu}=(-1)^{\lambda}Q_{\lambda\mu}, \tag{48a}$$

$$M_{\lambda\mu}=-(-1)^{\lambda}M_{\lambda\mu}, \tag{48b}$$

i.e., odd electric and even magnetic moments must vanish. Similar symmetry properties with respect to other symmetries of the D_{2h}^{T} or D_{2h}^{TD} groups are collected in Table VI.

Within the standard phase convention of Eq. (44), only a conservation of the y-T-simplex symmetry $\hat{S}_y^T$ enforces the reality of all multipole electric and magnetic moments. In such a case, the lower part of Table VI gives at a glance all

TABLE VII. Properties of electric multipole moments $Q_{\lambda\mu}$, magnetic multipole moments $M_{\lambda\mu}$, and average angular momenta I_k for conserved D_{2h}^T or D_{2h}^{TD} operators. Symbols *C*, *R*, *I*, or 0 denote values which can be, in general, complex, real, imaginary, or zero, respectively.

	$\hat{E}$	$\hat{T}$	$\hat{P}$	$\hat{P}^T$	$\hat{R}_x$	$\hat{R}_x^T$	$\hat{S}_x$	$\hat{S}_x^T$	$\hat{R}_y$	$\hat{R}_y^T$	$\hat{S}_y$	$\hat{S}_y^T$	$\hat{R}_z$	$\hat{R}_z^T$	$\hat{S}_z$	$\hat{S}_z^T$
$Q_{10},Q_{30},Q_{50}\ldots$	R	R	0	0	0	0	R	R	0	0	R	R	R	R	0	0
$Q_{11},Q_{31},Q_{33}\ldots$	C	C	0	0	R	R	I	I	I	I	R	R	0	0	C	C
$Q_{20},Q_{40},Q_{60}\ldots$	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R
$Q_{21},Q_{41},Q_{43}\ldots$	C	C	C	C	I	I	I	I	R	R	R	R	0	0	0	0
$Q_{22},Q_{42},Q_{44}\ldots$	C	C	C	C	R	R	R	R	R	R	R	R	C	C	C	C
$Q_{32},Q_{52},Q_{54}\ldots$	C	C	0	0	I	I	R	R	I	I	R	R	C	C	0	0
$M_{10},M_{30},M_{50}\ldots$	R	0	R	0	0	R	0	R	0	R	0	R	R	0	R	0
$M_{11},M_{31},M_{33}\ldots$	C	0	C	0	R	I	R	I	I	R	I	R	0	C	0	C
$M_{20},M_{40},M_{60}\ldots$	R	0	0	R	R	0	0	R	R	0	0	R	R	0	0	R
$M_{21},M_{41},M_{43}\ldots$	C	0	0	C	I	R	R	I	R	I	I	R	0	C	C	0
$M_{22},M_{42},M_{44}\ldots$	C	0	0	C	R	I	I	R	R	I	I	R	C	0	0	C
$M_{32},M_{52},M_{54}\ldots$	C	0	C	0	I	R	R	R	I	R	I	R	C	0	C	0
I_x	R	0	R	0	R	0	R	0	0	R	0	R	0	R	0	R
I_y	R	0	R	0	0	R	0	R	R	0	R	0	0	R	0	R
I_z	R	0	R	0	0	R	0	R	0	R	0	R	R	0	R	0

the multipole moments which must vanish whenever any other symmetry is additionally conserved; these are those for which the phase factors are negative. On the other hand, a conservation of the *x*-*T*-simplex symmetry $\hat{S}_x^T$ enforces the equality of negative and positive magnetic components. In this case, a conservation of any additional symmetry puts to zero the multipole moments with negative phase factors appearing in the upper part of the table. Of course, numerous other combinations of conserved symmetries can be considered, for example, a conservation of the *y*-simplex symmetry $\hat{S}_y$ gives real electric moments and imaginary magnetic moments.

Since conditions listed in Table VI depend only on the parity of λ and on the parity of μ, and since condition (44) allows us to consider only non-negative values of μ, one has only six types of the symmetry properties of multipole moments with respect to the D_{2h}^T or D_{2h}^{TD} operators. These six types are listed in Table VII for electric and magnetic moments. Column denoted by the identity operator $\hat{E}$ gives the properties resulting solely from condition (44), while the remaining columns give properties of moments when one of the nonidentity D_{2h}^T or D_{2h}^{TD} operators is conserved.

In the same table we also give symmetry properties of the Cartesian components of the average angular momenta I_k (47). Although the symmetry properties of the angular momentum are identical to those of the dipole magnetic moment, explicit values shown for its Cartesian components allow for a simple visualization of a direction taken by the angular-momentum vector when various D_{2h}^T or D_{2h}^{TD} operators are conserved. In particular, one can see that a conservation of any of the signature or simplex operators for a given axis enforces the angular-momentum direction along that axis, while a conservation of any *T*-signature or *T*-simplex operators allows for a tilted angular momentum in the plane perpendicular to the given axis, see Ref. [23]. On the other hand, none of these operators may be conserved if the angular momentum is to be tilted beyond any of the *x*-*y*, *y*-*z*, and *z*-*x* planes. Note, however, that the above tilting conditions pertain to the reference frame, and not to the principal axes of the mass distribution. An appropriate choice of the reference frame, as discussed below, has to be performed in order to relate the conserved D_{2h}^T or D_{2h}^{TD} operators to the direction of I_k with respect to the mass principal axes.

Independently of any D_{2h}^T or D_{2h}^{TD} symmetry breaking, the reference frame in the space coordinates can be chosen in such way that some of the moments have simple forms. For example, a shift of the reference frame can bring all electric dipole moments to zero (this corresponds to using the center-of-mass system of reference), i.e.,

$$\mathrm{Re}\, Q_{10} = \mathrm{Re}\, Q_{11} = \mathrm{Im}\, Q_{11} = 0. \tag{49}$$

Similarly, a suitable rotation of the reference frame can bring the electric quadrupole moments $Q_{2\mu}$ to the principal axes, where

$$\mathrm{Re}\, Q_{21} = \mathrm{Im}\, Q_{21} = \mathrm{Im}\, Q_{22} = 0. \tag{50}$$

On the other hand, for some conserved symmetries, these conditions can be automatically satisfied. For example, conservation of the D_{2h} group (i.e., simultaneous invariance with respect to operators $\hat{P}$, $\hat{R}_x$, and $\hat{R}_y$) ensures that the center-of-mass (49) and principal-axes (50) conditions are automatically satisfied, see Table VII. Therefore, the breaking of the D_{2h}^T or D_{2h}^{TD} symmetries may have nontrivial physical consequences only for higher electric moments; starting from Q_{30}, if the parity is broken, or starting from Q_{41}, for example, if the parity is conserved. In other words, the D_{2h}^T or D_{2h}^{TD} symmetry breaking will not lead to new classes of low-multipolarity shapes. Nevertheless, such sym-

metry breaking will immediately be reflected in values of magnetic moments, whenever the time reversal is broken too.

V. CONCLUSIONS

In the present study we have presented applications of point groups based on the three mutually perpendicular symmetry axes of the second order, inversion, and time reversal, to nuclear structure problems. We have discussed properties of the corresponding single D_{2h}^{T} and double D_{2h}^{TD} groups in describing even and odd fermion systems, respectively. We have enumerated their representations, both for many-body states and for the single-particle operators, and reviewed properties of group operators when they are represented in the fermion Fock space.

Consequences of conserving individual D_{2h}^{T} or D_{2h}^{TD} symmetries have been enumerated for (i) space symmetries of local one-body densities, (ii) electric and magnetic multipole moments, and (iii) average values of the angular-momentum operators. This gives information about the nuclear shapes and matter-flow currents in states obeying one or more of the D_{2h}^{T} or D_{2h}^{TD} symmetries, and allows for selecting appropriate conserved symmetries in descriptions aiming at various physical phenomena.

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APPENDIX

In this appendix we explicitly construct irreducible representations of the D_{2h}^{TD} group by using the example of the HO basis (Sec. II D), and we illustrate the Wigner classification of groups that contain antilinear operators (see Chap. 26 of Ref. [8]). The results of such an analysis were used in Sec. II.

We consider here only the two-dimensional spinor representations, appropriate for the odd-fermion systems and in particular for the single-particle states. From Eqs. (27) one finds representation matrices $\Gamma(\hat{\mathcal{U}})$ (where operators $\hat{\mathcal{U}} \in D_{2h}^{D}$ of Sec. II C form the double group D_{2h}^{D}), in the two-dimensional invariant subspace spanned by $|n_x n_y n_z, s_z = +\frac{1}{2}\rangle$ and $|n_x n_y n_z, s_z = -\frac{1}{2}\rangle$. We have

$$\Gamma(\hat{\mathcal{E}}) = -\Gamma(\overline{\mathcal{E}}) = \sigma_0, \tag{A1a}$$

$$\Gamma(\hat{\mathcal{P}}) = -\Gamma(\overline{\mathcal{P}}) = (-1)^{n_x+n_y+n_z}\sigma_0, \tag{A1b}$$

$$\Gamma(\hat{\mathcal{R}}_k) = -\Gamma(\overline{\mathcal{R}}_k) = -i(-1)^{N_k}\sigma_k, \tag{A1c}$$

$$\Gamma(\hat{\mathcal{S}}_k) = -\Gamma(\overline{\mathcal{S}}_k) = -i(-1)^{n_k}\sigma_k, \tag{A1d}$$

where σ_0 is the identity 2×2 matrix, σ_k for $k = x,y,z$ are the standard Pauli matrices, and symbols N_x, N_y, and N_z refer to n_y+n_z, n_x+n_z, and n_x+n_y, respectively.

The characters of the classes are

$$\chi(\hat{\mathcal{E}}) = -\chi(\overline{\mathcal{E}}) = 2, \tag{A2a}$$

$$\chi(\hat{\mathcal{P}}) = -\chi(\overline{\mathcal{P}}) = 2(-1)^{n_x+n_y+n_z}, \tag{A2b}$$

$$\chi(\{\hat{\mathcal{R}}_x, \overline{\mathcal{R}}_x\}) = \chi(\{\hat{\mathcal{S}}_x, \overline{\mathcal{S}}_x\}) = 0, \tag{A2c}$$

$$\chi(\{\hat{\mathcal{R}}_y, \overline{\mathcal{R}}_y\}) = \chi(\{\hat{\mathcal{S}}_y, \overline{\mathcal{S}}_y\}) = 0, \tag{A2d}$$

$$\chi(\{\hat{\mathcal{R}}_z, \overline{\mathcal{R}}_z\}) = \chi(\{\hat{\mathcal{S}}_z, \overline{\mathcal{S}}_z\}) = 0. \tag{A2e}$$

One can see, that only the characters of $\hat{\mathcal{P}}$ and $\overline{\mathcal{P}}$ depend on quantum numbers n_x, n_y, and n_z that define the invariant subspaces; more precisely, they depend only on the parity of the sum $n_x+n_y+n_z$, i.e., on the total parity of basis states. Therefore, the only two spinor representations of D_{2h}^{TD} can be labeled by the eigenvalues of the parity operator $\hat{\mathcal{P}}$. Let us also note that all characters are real.

If we introduce the time reversal, $\hat{\mathcal{T}}$, into the ensemble of the linear operators belonging to D_{2h}^{D} we obtain the D_{2h}^{TD} group with 16 new antilinear elements $\hat{\mathcal{U}}^{T} \equiv \hat{\mathcal{U}}\hat{\mathcal{T}}$, Sec. II C. To study properties of the representations of the D_{2h}^{TD} group, one has to consider representations provided by matrices

$$\check{\Gamma}(\hat{\mathcal{U}}) = \Gamma(\hat{\mathcal{A}}^{-1}\hat{\mathcal{U}}\hat{\mathcal{A}})^*, \tag{A3}$$

where $\hat{\mathcal{A}}$ is one of the antilinear elements of D_{2h}^{TD} (see Ref. [8]). It is most convenient to take $\hat{\mathcal{T}}$ itself as $\hat{\mathcal{A}}$; we then have simply

$$\check{\Gamma}(\hat{\mathcal{U}}) = \Gamma(\hat{\mathcal{U}})^*, \tag{A4}$$

as $\hat{\mathcal{T}}$ commutes with all $\hat{\mathcal{U}} \in D_{2h}^{D}$. In such a case, matrices $\check{\Gamma}(\hat{\mathcal{U}})$ are just complex conjugates of $\Gamma(\hat{\mathcal{U}})$, and therefore the characters of representation $\check{\Gamma}$ are exactly the same as those of Γ, because they are all real, see Eqs. (A2). Therefore these two representations are equivalent, and a matrix β exists which brings by a similarity transformation all matrices $\Gamma(\hat{\mathcal{U}})$ to $\check{\Gamma}(\hat{\mathcal{U}}) = \Gamma(\hat{\mathcal{U}})^*$,

$$\beta^{-1}\Gamma(\hat{\mathcal{U}})\beta = \Gamma(\hat{\mathcal{U}})^*, \quad \hat{\mathcal{U}} \in D_{2h}^{D}. \tag{A5}$$

Now, as shown by Wigner [8], there are only two cases possible: either

$$\beta\beta^* = +\Gamma(\hat{\mathcal{T}}^2) \tag{A6}$$

or

$$\beta\beta^* = -\Gamma(\hat{\mathcal{T}}^2). \tag{A7}$$

Matrix β can easily be found from the explicit expressions for matrices $\Gamma(\hat{\mathcal{U}})$ given in Eqs. (A1), and it reads

$$\beta = e^{i\phi}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -ie^{i\phi}\sigma_y . \tag{A8}$$

Choosing the phase factor $e^{i\phi} \neq 1$ in Eq. (A8) is equivalent to a change of phase of the $|n_x n_y n_z, s_z = +\frac{1}{2}\rangle$ states, and to a change in the phase convention in Eq. (27b).

It is easy to demonstrate that with this form of the matrix β, Eq. (A6), and not Eq. (A7) holds. In Wigner's classification this case leads to what is called the corepresentations of the ''first kind'': any representation Γ of the group D_{2h}^{D} can be completed to a corepresentation of the full D_{2h}^{TD} group by defining

$$\Gamma(\hat{\mathcal{U}}^T) = \Gamma(\hat{\mathcal{U}})\beta. \tag{A9}$$

Note that taking $\hat{\mathcal{U}} = \hat{\mathcal{E}}$ one gets $\Gamma(\hat{\mathcal{T}}) = \beta$, so β is, of course, just the matrix representing $\hat{\mathcal{T}}$ itself.

After Wigner, the term *corepresentation* is used here because the representations of groups containing antilinear operators are *not* representations in the usual sense. To see this, let us consider an orthonormal set of states $\{|\phi_i\rangle\}$ constituting a basis of a representation Γ. Let $\hat{\mathcal{U}}$ be any linear, and $\hat{\mathcal{U}}'$ any element of the group. Then, because of antilinearity of $\hat{\mathcal{U}}^T$ one has

$$\begin{aligned}(\hat{\mathcal{U}}^T \cdot \hat{\mathcal{U}}')|\phi_j\rangle &= \sum_i \hat{\mathcal{U}}^T \Gamma(\hat{\mathcal{U}}')_{ij}|\phi_i\rangle = \sum_i \Gamma(\hat{\mathcal{U}}')^*_{ij}\hat{\mathcal{U}}^T|\phi_i\rangle \\ &= \sum_{ik} \Gamma(\hat{\mathcal{U}}')^*_{ij}\Gamma(\hat{\mathcal{U}}^T)_{ki}|\phi_k\rangle \\ &= \sum_k [\Gamma(\hat{\mathcal{U}}^T)\Gamma(\hat{\mathcal{U}}')^*]_{kj}|\phi_k\rangle \end{aligned} \tag{A10}$$

and, consequently,

$$\Gamma(\hat{\mathcal{U}}^T \cdot \hat{\mathcal{U}}') = \Gamma(\hat{\mathcal{U}}^T)\Gamma(\hat{\mathcal{U}}')^*, \tag{A11}$$

to be compared with

$$\Gamma(\hat{\mathcal{U}} \cdot \hat{\mathcal{U}}') = \Gamma(\hat{\mathcal{U}})\Gamma(\hat{\mathcal{U}}'), \tag{A12}$$

which holds for the ''usual'' representations. The presence of complex conjugation on the right-hand side of Eq. (A11) implies that the homomorphism between the group multiplication and the multiplication of representation matrices no longer holds when the group contains antilinear operators. This is not surprising in view of the fact that matrices, by construction, always act on vectors (columns of numbers) linearly. In conclusion, there are only two spinor corepresentations of D_{2h}^{TD}, and they can be labeled, as is also the case for the D_{2h}^{D} group, by one quantum number only (parity).

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