Point symmetries in the Hartree-Fock approach. II. Symmetry-breaking schemes

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We analyze breaking of symmetries that belong to the double point group D_{2h}^{TD} (three mutually perpendicular symmetry axes of the second order, inversion, and time reversal). Subgroup structure of the D_{2h}^{TD} group indicates that there can be as many as 28 physically different, broken-symmetry mean-field schemes — starting with solutions obeying all the symmetries of the D_{2h}^{TD} group, through 26 generic schemes in which only a nontrivial subgroup of D_{2h}^{TD} is conserved, down to solutions that break all of the D_{2h}^{TD} symmetries. Choices of single-particle bases and the corresponding structures of single-particle Hermitian operators are discussed for several subgroups of D_{2h}^{TD}.

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I. INTRODUCTION

One of the salient features of the mean-field approach to many-fermion (e.g., nuclear) systems is the spontaneous symmetry breaking. The symmetry of a mean-field state is called broken, if the solution of the Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) self-consistent equations do not obey symmetries of the original many-body Hamiltonian [1]. This happens when the calculated mean-field energy of the system is lower for states which break a symmetry than that for unbroken symmetries. Such a mechanism depends on the physical situation and is governed by the Jahn-Teller effect [2]. Without going into details, let us recall that the spontaneous breaking of an original symmetry is usually accompanied by a significant decrease in the single-particle level density at the Fermi energy. Hence, the doubly magic nuclei can be safely described by imposing conservation of the spherical symmetry, while this symmetry should be allowed to be broken in the open-shell systems.

One of the simplest examples in this context is that of the breaking of the translational symmetry. The related mechanism is present, e.g., in the nuclear shell model. Indeed, within the framework of the shell model, interacting nucleons are assumed to move in a common mean field that is localized in space and consequently they cannot be described by eigenstates of the momentum operator (plane waves). In other words, the wave functions of a nucleus cannot be approximated by uncorrelated single-particle plane waves—this can only be attempted for an infinite system, i.e., for the nuclear matter. The use of a shell-model, space-localized wave function simply reflects the correlations present in the system. In this example, the correlations ensure that it is improbable to find two nucleons of a nucleus at large relative distances apart.

In nuclear structure physics one can easily identify the use of various broken symmetries in a description of well-defined, observable effects. For instance the rotational, parity, time-reversal, and gauge symmetry breaking were introduced to describe the deformations, octupole correlations, nuclear rotation and pair correlations, and combined effects thereof. At present, we approach the situation where the mean-field calculations can be performed without explicitly using any of the mean-field symmetries. Several such approaches have already been implemented [3–5], although very few calculations for specific physical problems have been done to date.

One could, in principle, perform the mean-field calculations without assuming *a priori* any symmetry, and let the dynamics choose those discrete symmetries which are, in a specific situation, broken, and those which remain obeyed. Obviously, by choosing such an approach we cannot profit from simplifications possible when it is known beforehand that some symmetries are obeyed or disobeyed. However, following the general guidelines provided by the Jahn-Teller mechanism one usually can make a reasonable choice of obeyed or disobeyed symmetries. Such a choice is dictated by the properties of the many-body Hamiltonian and by the classes of phenomena which one wants to describe—it usually facilitates the calculations markedly. In all those cases the analysis presented in this article provides us with the mathematical means for constructing the algorithms optimally adapted to the symmetries of the problem in question.

In the preceding article [6], we have presented properties of the single point group D_{2h}^{T} and double point group D_{2h}^{TD}, that can be built from operators related to the three mutually perpendicular symmetry axes of the second order, inversion, and time reversal. We have also discussed their roles in the description of even and odd fermion systems, respectively, their representations, and the symmetry conditions induced by the conserved D_{2h}^{T} or D_{2h}^{TD} symmetries on the local densities and electromagnetic moments.

By considering the D_{2h}^{TD} double point group we focus on quantum objects that are in general nonspherical, but can have one or more symmetry axes and/or symmetry planes. Obviously, any nuclear many-body Hamiltonian of an isolated system is time-even and rotationally invariant. In the present paper we do not aim at analyzing the conditions under which these symmetries are broken spontaneously, with one or another symmetry element of the D_{2h}^{TD} group still being conserved in the HF solution. Instead, we present a classification of all such possibilities, and discuss the resulting properties of the mean-field Hamiltonians and single-particle wave functions. For a review of applications of point symmetries to a description of rotating nuclei see the recent study in Ref. [7].

Our goal is thus twofold. First, in Sec. II we discuss all possible physically meaningful subgroups of D_{2h}^{TD}, and classify the corresponding physical situations from the view point of the conserved D_{2h}^{TD} symmetries. In many applications to date, specific choices of conserved and broken D_{2h}^{TD} symmetries have been made [8–14], however, here we aim at a complete description of all achievable symmetry-breaking schemes. Second, in Sec. III we review and discuss practical aspects of structure of the mean-field operators under specific D_{2h}^{TD} group operations. This essential question has been explicitly or tacitly addressed in most approaches using the deformed mean-field theory; our aim here is to present exhaustive list of options pertaining to all the D_{2h}^{TD} symmetry conditions. Finally, conclusions are presented in Sec. IV.

II. SUBGROUPS OF D_{2h}^{T} AND D_{2h}^{TD} AND THE SYMMETRY BREAKING

The single group D_{2h}^{T} and double group D_{2h}^{TD} [6] can be built from three rotations through angle π about the coordinate axes $k=x,y,z$, called the signature operators

$$\hat{R}_k = e^{-i\pi\hat{I}_k}, \tag{1}$$

to which one adds the inversion operator $\hat{P}$ and the time reversal

$$\hat{T} = \bigotimes_{n=1}^{A} (-i\hat{\sigma}_y^{(n)})\hat{K}, \tag{2}$$

where $\hat{I}_k = \Sigma_{n=1}^{A} \hat{j}_k^{(n)}$ is the total angular momentum operator, $\hat{j}_k^{(n)}$ and $\hat{\sigma}_k^{(n)}$ are the angular momenta and the Pauli spin matrices for the particle number n, respectively, and $\hat{K}$ is the complex-conjugation operator in the coordinate representation.

Following the convention introduced in Ref. [6], with roman symbols, like $\hat{U}=\hat{R}_k$ or $\hat{T}$, we denote operators acting in the Fock space $\mathcal{H}\equiv\mathcal{H}_0\oplus\mathcal{H}_1\oplus\ldots\oplus\mathcal{H}_A\oplus\ldots$. Moreover, in order to help the reader in distinguishing between properties of these operators when they act in even, $\mathcal{H}_+\equiv\mathcal{H}_0\oplus\mathcal{H}_2\oplus\cdots\oplus\mathcal{H}_{A=2p}\oplus\cdots$, or odd, $\mathcal{H}_-\equiv\mathcal{H}_1\oplus\mathcal{H}_3\oplus\cdots\oplus\mathcal{H}_{A=2p+1}\oplus\cdots$, fermion spaces, we denote the former ones with bold symbols, and the latter ones with script symbols, i.e., we formally split the Fock-space operators $\hat{U}=\hat{\mathbf{U}}+\hat{\mathcal{U}}$ into two parts according to their domains.

It follows Refs. [15,16,6] that D_{2h}^{T} is an Abelian group of 16 elements, which contains: the identity $\hat{\mathbf{E}}$, inversion $\hat{\mathbf{P}}$, time-reversal $\hat{\mathbf{T}}$, their product $\hat{\mathbf{P}}^T=\hat{\mathbf{P}}\hat{\mathbf{T}}$, three signatures $\hat{\mathbf{R}}_k$, three simplexes $\hat{\mathbf{S}}_k=\hat{\mathbf{P}}\hat{\mathbf{R}}_k$, three T signatures $\hat{\mathbf{R}}_k^T=\hat{\mathbf{T}}\hat{\mathbf{R}}_k$, and three T simplexes $\hat{\mathbf{S}}_k^T=\hat{\mathbf{T}}\hat{\mathbf{S}}_k$, i.e.,

$$D_{2h}^{T}: \quad \{\hat{\mathbf{E}},\hat{\mathbf{P}},\hat{\mathbf{R}}_k,\hat{\mathbf{S}}_k,\hat{\mathbf{T}},\hat{\mathbf{P}}^T,\hat{\mathbf{R}}_k^T,\hat{\mathbf{S}}_k^T\}, \tag{3}$$

where all these operators act in even-fermion-number space $\mathcal{H}_+$.

Similarly, the Fock-space operators $\hat{U}$, as well as the odd-fermion-number operators $\hat{\mathcal{U}}$, form the group D_{2h}^{TD} which is a non-Abelian group of 32 elements. Apart from the 16 operators enumerated for D_{2h}^{T}, it contains their partners obtained by multiplying every one of them by the operators $\overline{E}$ or $\overline{\mathcal{E}}$, respectively. These operators can be identified with the rotation operators through angle 2π about an arbitrary axis. The partner operators are denoted by replacing the hats with bars, i.e., the group of operators acting in $\mathcal{H}_-$ reads

$$D_{2h}^{TD}: \quad \{\hat{\mathcal{E}},\hat{\mathcal{P}},\hat{\mathcal{T}},\hat{\mathcal{P}}^T,\hat{\mathcal{R}}_k,\hat{\mathcal{S}}_k,\hat{\mathcal{R}}_k^T,\hat{\mathcal{S}}_k^T,\overline{\mathcal{E}},\overline{\mathcal{P}},\overline{\mathcal{T}},\overline{\mathcal{P}^T},\overline{\mathcal{R}}_k,\overline{\mathcal{S}}_k,\overline{\mathcal{R}}_k^T,\overline{\mathcal{S}}_k^T\}. \tag{4}$$

The complete D_{2h}^{T} and D_{2h}^{TD} multiplication tables have been given and discussed in Ref. [6], and will not be repeated here. We only recall a few properties of the D_{2h}^{TD} group that are essential in the following analysis, namely,

$$\hat{\mathcal{R}}_k^2=\hat{\mathcal{S}}_k^2=\hat{\mathcal{T}}^2=\overline{\mathcal{E}}, \tag{5a}$$

$$(\hat{\mathcal{R}}_k^T)^2=(\hat{\mathcal{S}}_k^T)^2=\hat{\mathcal{P}}^2=\hat{\mathcal{E}}, \tag{5b}$$

for $k=x,y,z$,

$$\hat{\mathcal{R}}_k\hat{\mathcal{R}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{S}}_l=\hat{\mathcal{R}}_k^T\hat{\mathcal{R}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{S}}_l^T=\hat{\mathcal{R}}_m, \tag{6}$$

for (k,l,m) being an *even* permutation of (x,y,z), and

$$\hat{\mathcal{R}}_k\hat{\mathcal{R}}_l=\hat{\mathcal{S}}_k\hat{\mathcal{S}}_l=\hat{\mathcal{R}}_k^T\hat{\mathcal{R}}_l^T=\hat{\mathcal{S}}_k^T\hat{\mathcal{S}}_l^T=\overline{\mathcal{R}}_m, \tag{7}$$

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

The multiplication table of D_{2h}^{T} is obtained by replacing $\overline{\mathcal{E}}$ and $\overline{\mathcal{R}}_m$ by $\hat{\mathbf{E}}$ and $\hat{\mathbf{R}}_m$, respectively, and using all bold symbols in Eqs. (5)–(7). Obviously, a product of conserved symmetries is a conserved symmetry, and consequently, the conserved symmetries form groups that are subgroups of D_{2h}^{T} or D_{2h}^{TD}. Therefore, in order to analyze various physically meaningful subsets of the conserved D_{2h}^{T} or D_{2h}^{TD} operators, we should first consider the subgroup structure of these groups.

Suppose that in a given physical problem, the mean-field states obey the symmetries of a given subgroup rather than those of the whole D_{2h}^{T} or D_{2h}^{TD} groups. In such a case that subgroup contains the maximal set of operators representing the symmetry of the problem, i.e., all D_{2h}^{T} and D_{2h}^{TD} operators which do not belong to such subgroup are the broken symmetries. From the view point of physics, we are more interested in the symmetries which are broken (which is related to interesting dynamical correlations), than in those which are conserved. It then follows that the physically interesting information will be attached to the operators that *do not* belong to the subgroup studied, but *do belong* to D_{2h}^{T} or D_{2h}^{TD}; those latter ones do not necessarily form a group.

First we consider the single group D_{2h}^{T}, because (i) it is a smaller and simpler group than D_{2h}^{TD} and (ii) the operator $\overline{\mathcal{E}}$

TABLE I. Nontrivial subgroups of the single D_{2h}^T group, classified according to the types described in the text. The second column gives the generators. The third column gives numbers of different subgroups irrespective of names of Cartesian axes, and the fourth column gives the total number of subgroups in each type.

Type	Generators	Generic	Total
1-0_A:	$\{\hat{\mathbf{T}}\}$, $\{\hat{\mathbf{P}}\}$, $\{\hat{\mathbf{P}}^T\}$	3	3
1-I_A:	$\{\hat{\mathbf{R}}_k^T\}$, $\{\hat{\mathbf{S}}_k\}$, $\{\hat{\mathbf{S}}_k^T\}$	3	9
1-I_B:	$\{\hat{\mathbf{R}}_k\}$	1	3
	Total number of one-generator subgroups:	7	15
2-0_A:	$\{\hat{\mathbf{T}},\hat{\mathbf{P}}\}$	1	1
2-I_A:	$\{\hat{\mathbf{S}}_k,\hat{\mathbf{T}}\}$, $\{\hat{\mathbf{S}}_k^T,\hat{\mathbf{P}}\}$, $\{\hat{\mathbf{R}}_k^T,\hat{\mathbf{P}}^T\}$	3	9
2-I_B:	$\{\hat{\mathbf{R}}_k,\hat{\mathbf{T}}\}$, $\{\hat{\mathbf{R}}_k,\hat{\mathbf{P}}\}$, $\{\hat{\mathbf{R}}_k,\hat{\mathbf{P}}^T\}$	3	9
2-III_A:	$\{\hat{\mathbf{S}}_l,\hat{\mathbf{S}}_m^T\}$	1	6
2-III_B:	$\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m^T\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{S}}_m\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{S}}_m^T\}$	3	9
2-III_D:	$\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m\}$	1	1
	Total number of two-generator subgroups:	12	35
3-I_B:	$\{\hat{\mathbf{R}}_k,\hat{\mathbf{T}},\hat{\mathbf{P}}\}$	1	3
3-III_B:	$\{\hat{\mathbf{R}}_l,\hat{\mathbf{S}}_m,\hat{\mathbf{T}}\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{S}}_m^T,\hat{\mathbf{P}}\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m^T,\hat{\mathbf{P}}^T\}$	3	9
3-III_D:	$\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m,\hat{\mathbf{T}}\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m,\hat{\mathbf{P}}\}$, $\{\hat{\mathbf{R}}_l,\hat{\mathbf{R}}_m,\hat{\mathbf{P}}^T\}$	3	3
	Total number of three-generator subgroups:	7	15
	Total number of subgroups:	26	65

which makes the difference between the single and the double group is always a conserved symmetry. The analysis below is based on identifying sets of the so-called subgroup generators, i.e, operators from which the whole given subgroup can be obtained by their successive multiplications. Choices of generators are, of course, nonunique, and hence in each case we discuss and enumerate all the available possibilities.

A. Subgroups of D_{2h}^T

Since the square of every element of D_{2h}^T is proportional to the identity operator $\hat{\mathbf{E}}$, we have fifteen two-element, one-generator subgroups, each of them composed of the identity and one of the other D_{2h}^T operators. We denote these subgroups by $\{\hat{\mathbf{G}}_1\}$, where $\hat{\mathbf{G}}_1$ is the generic symbol corresponding to one of the nonidentity elements of D_{2h}^T. Obviously, only one choice of the generator is possible for every of the two-element subgroups.

Similarly, group D_{2h}^T has 35 different four-element subgroups, which can be called the two-generator subgroups, and are denoted by symbols $\{\hat{\mathbf{G}}_1,\hat{\mathbf{G}}_2\}$. pertaining to their generators. The two-generator subgroups contain, in addition to $\hat{\mathbf{G}}_1$ and $\hat{\mathbf{G}}_2$, also the identity $\hat{\mathbf{E}}$ and the product $\hat{\mathbf{G}}_1\hat{\mathbf{G}}_2$. Since this product is also one of the D_{2h}^T operators, we have in each of the four-element, two-generator subgroups three possibilities to select the generators.

Finally, there are 15 different eight-element, three-generator subgroups of D_{2h}^T, denoted by $\{\hat{\mathbf{G}}_1,\hat{\mathbf{G}}_2,\hat{\mathbf{G}}_3\}$. Each of these subgroups contains the identity $\hat{\mathbf{E}}$, the three generators, three products of pairs of generators, and the product of all three generators. Hence, to choose the generators we may first pick any pair out of seven nonidentity elements (21 possibilities), and next pick any other subgroup element, except the product of the first two (four possibilities). Since the order in which we pick the generators is irrelevant, one has altogether 28 possibilities of choosing the three generators in each of the eight-element, three-generator subgroups of D_{2h}^T.

In the same way one can calculate that there are 168 different choices of the four generators of the whole D_{2h}^T group; one of them is, e.g., the set $\{\hat{\mathbf{T}},\hat{\mathbf{P}},\hat{\mathbf{R}}_x,\hat{\mathbf{R}}_y\}$. This illustrates the degree of arbitrariness in implementing calculations for which the whole group D_{2h}^T is conserved. Similar freedom, although to a lesser degree, is available when conserving any of the subgroups of D_{2h}^T. Of course, the freedom of choosing generators cannot influence the final results, however, it allows using different quantum numbers, phase conventions, and structure of matrix elements, as discussed in Sec. III.

A classification of all the 65 nontrivial subgroups of D_{2h}^T (we do not include trivial subgroups $\{\hat{\mathbf{E}}\}$ and D_{2h}^T itself) is presented in Table I. Every subgroup is assigned to a certain type, and described by a symbol given in the first column of the table. The types are defined according to (i) the number of generators in the subgroup (1, 2, or 3), (ii) the number of Cartesian axes involved in the subgroup (0, I, or III standing for 0, 1, or 3), and (iii) the number of signature operators in the subgroup (A, B, or D standing for 0, 1, or 3).

The classification is based on two important characteristics of each subgroup. As shown in Ref. [6], every conserved symmetry, labeled by one of the Cartesian directions x, y, or

TABLE II. Same as in Table I, but for additional subgroups of the double D_{2h}^{TD} group.

Type	Generators	Generic	Total
2-0_A:	$\{\hat{\mathcal{P}},\overline{\mathcal{E}}\}$	1	1
2-I_A:	$\{\hat{\mathcal{R}}_k^T,\overline{\mathcal{E}}\}$, $\{\hat{\mathcal{S}}_k^T,\overline{\mathcal{E}}\}$	2	6
Total number of two-generator subgroups:		3	7
3-I_A:	$\{\hat{\mathcal{S}}_k^T,\hat{\mathcal{P}},\overline{\mathcal{E}}\}$	1	3
Total number of three-generator subgroups:		1	3
Total number of subgroups:		4	10

z, induces a specific symmetry of local densities, related to this particular direction. Therefore, the number of Cartesian axes involved in the subgroup gives us the number of symmetries of local densities induced by the given subgroup. In addition, the number of signature operators illustrates the way in which the given subgroup is located with respect to the standard D_2 subgroup, which is composed of the three signatures.

Classification of the subgroups of the single group D_{2h}^T allows us to discuss conserved and broken-symmetry schemes in even-fermion systems.

B. Subgroups of D_{2h}^{TD}

In order to discuss the conserved and broken symmetries in odd-fermion systems, we now proceed to the discussion of the subgroups of the double group D_{2h}^{TD}. In fact, the classification of Table I can now be repeated almost without change. Indeed, whenever a given D_{2h}^T subgroup contains the time reversal $\hat{\mathbf{T}}$, signature $\hat{\mathbf{R}}_k$, or simplex $\hat{\mathbf{S}}_k$, at least one of those, the corresponding subgroup of D_{2h}^{TD} contains $\hat{\mathcal{T}}$, $\hat{\mathcal{R}}_k$, or $\hat{\mathcal{S}}_k$, and it automatically becomes a doubled D_{2h}^{TD} subgroup, with exactly the same generators. This is so, because in the D_{2h}^{TD} group the squares of the time reversal, signature, and simplex operators are equal to $\overline{\mathcal{E}}$, Eq. (5a), and hence whenever one of these operators is present in the subgroup, it generates the appropriate double subgroup of the double group D_{2h}^{TD}. On the other hand, when none of these generators are present in a given D_{2h}^T subgroup, this subgroup becomes the subgroup of D_{2h}^{TD} without doubling.

Therefore, all the D_{2h}^T subgroups listed in Table I are simultaneously subgroups of D_{2h}^{TD}, provided the generators denoted with bold symbols are replaced by the corresponding script generators. Most of the D_{2h}^{TD} subgroups have twice more elements than the corresponding D_{2h}^T subgroups, with few exceptions: subgroups $\{\hat{\mathcal{P}}\}$, $\{\hat{\mathcal{R}}_k^T\}$, $\{\hat{\mathcal{S}}_k^T\}$, $\{\hat{\mathcal{S}}_k^T,\hat{\mathcal{P}}\}$ do not double, and contain the same number of elements as the corresponding subgroups of D_{2h}^T.

In addition, these few exceptional subgroups can be doubled explicitly by adding $\overline{\mathcal{E}}$ to the set of generators. For completeness, these additional subgroups of D_{2h}^{TD} are enumerated in Table II. However, the physical contents of the additional, and of the corresponding not doubled subgroups from Table I, are the same. For example, they lead to exactly the same symmetry properties of the density matrices [6]. The difference between them consists in the fact that the latter ones have no irreps in the spinor space, whereas the former ones have one-dimensional irreps with spinor bases (see Ref. [15]). However, from the viewpoint of the symmetry breaking, they lead to exactly the same schemes, and thus the additional subgroups shown in Table II can be called trivial. Note, that the single-particle operators (e.g., the mean-field Hamiltonian) are classified according to one-dimensional representations [6], and hence, from the viewpoint of the symmetry breaking it is irrelevant whether or not a given subgroup has spinor representations.

Apart from the phase relations of electromagnetic moments [6] (note that the standard multipole operators are defined by singling out the z axis), the three Cartesian directions are, of course, entirely equivalent. Therefore, even though changing names of axes leads to different subgroups of D_{2h}^T or D_{2h}^{TD}, they are identical from the point of view of physically important features. In Tables I and II, we give in the third columns the numbers of generic subgroups, i.e., those which are different irrespective of names of axes, and in the fourth column—the total numbers of subgroups of each type. Index k always denotes one of the axes, i.e., k can be equal to x, y, or z, while indices l and m, $l\neq m$, denote one of the three pairs of different axes.

Subgroups in type 0 do not depend on the Cartesian axes and, therefore, for them the numbers of generic subgroups are equal to the total numbers of subgroups. Those in type I have one generic form each, and three forms in total, depending on which Cartesian axis is chosen. Finally, for subgroups in type III, the total numbers of subgroups can be the same, three times larger, or six times larger (2-III_A) than the numbers of generic subgroups.

In practical applications, conservation of different D_{2h}^T or D_{2h}^{TD} subgroups may require considering either only the generic subgroup, or all the subgroups with changed names of axes. For example, if one considers a triaxially deformed system with $0°\leqslant\gamma\leqslant 60°$, the lengths of principal axes $a_y \leqslant a_x \leqslant a_z$ define the orientation of the nucleus. Then, conserved D_{2h}^T or D_{2h}^{TD} subgroups with different names of axes may lead to different physical consequences. On the other hand, it can be advantageous to consider only one generic subgroup, with a fixed orientation, and allow for various orientations of the physical system by extending allowed values of γ deformation beyond the standard first sector of $0°\leqslant\gamma \leqslant 60°$.

III. SINGLE-PARTICLE BASES AND MATRIX STRUCTURE OF THE SINGLE-PARTICLE HERMITIAN OPERATORS

Throughout this section we restrict our analysis to Hermitian single-particle operators, and we study their matrix elements in the single-particle space. Therefore, we are here concerned with the odd number of particles (one), and hence we have to consider the double group D_{2h}^{TD}. As discussed in Ref. [6], the D_{2h}^{TD} operators are either linear or antilinear, and they can have squares equal to either unity or minus unity, as

summarized in Table II of Ref. [6]. This gives us four categories of operators with markedly different properties, which here will be used for different purposes.

In the discussion which follows, we assume that the single-particle basis is composed of pairs of time-reversed states, and in addition we assume that the spatial wave functions are real, i.e., not affected by the time reversal

$$\hat{\mathcal{T}}\,|\boldsymbol{n}\zeta\rangle=\zeta|\boldsymbol{n}-\zeta\rangle, \tag{8}$$

where $\zeta=\pm1$ represents the intrinsic-spin degree of freedom and $\boldsymbol{n}$ represents the set of quantum numbers corresponding to space coordinates. In particular, for the harmonic-oscillator (HO) basis, $\boldsymbol{n}=(n_x,n_y,n_z)$ are the numbers of quanta in three Cartesian directions. Assumption (8) does not preclude whether or not the time-reversal is a conserved operator; it only defines the property of the single-particle basis in which the dynamic problem is to be solved. (In principle, the discussion below can be *mutatis mutandis* repeated with $\hat{\mathcal{T}}$ replaced by $\hat{\mathcal{P}}^T$, however, the use of the time-reversal operator is more appropriate in practical applications.)

From now on we also assume that the basis is ordered in such a way that its first half corresponds to the $\zeta=+1$ states, and the second half is composed of their time-reversed $\zeta=-1$ partners. In fact, we are entirely free to choose states in the first half of the basis ($\zeta=+1$), and then Eq. (8) defines those which belong to the second half ($\zeta=-1$). In such basis, the single-particle matrix elements corresponding to an arbitrary Hermitian operator $\hat{\mathcal{O}}$ have the form

$$\mathcal{O}=\begin{pmatrix} A & Y \\ Y^\dagger & B \end{pmatrix}, \tag{9}$$

where A and B are Hermitian matrices, Y is arbitrary, and all submatrices are, in general, complex.

A. Single-particle bases for conserved D_{2h}^{TD} operators

We may now separately consider several cases corresponding to different subgroups of conserved D_{2h}^{TD} operators, Table I, and to the four different categories of operators (linear or antilinear, and Hermitian or anti-Hermitian). In Secs. III A 1–III A 4, we consider cases of various D_{2h}^{TD} generators being separately conserved, and in Secs. III A 5–III A 8, cases of pairs of generators being simultaneously conserved. Three-generator subgroups are briefly discussed in Sec. III A 9.

1. Time reversal

Let us first consider operators $\hat{\mathcal{O}}$ which are either even (invariant) or odd (anti-invariant) with respect to the time reversal:

$$\hat{\mathcal{T}}^\dagger\hat{\mathcal{O}}\hat{\mathcal{T}}=\epsilon_T\hat{\mathcal{O}},\quad \epsilon_T=\pm1. \tag{10}$$

From Eqs. (8) and (10) one gets

$$\langle\boldsymbol{n}\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'\zeta'\rangle=\epsilon_T\zeta\zeta'\langle\boldsymbol{n}-\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'-\zeta'\rangle^*. \tag{11}$$

It follows, that the matrix corresponding to $\hat{\mathcal{O}}$ reads

$$\mathcal{O}=\begin{pmatrix} A & Y \\ -\epsilon_T Y^* & \epsilon_T A^* \end{pmatrix}, \tag{12}$$

where A is Hermitian, and Y is antisymmetric or symmetric for $\epsilon_T=+1$ and $\epsilon_T=-1$, respectively. No block-diagonal structure appears. Nevertheless, only two, instead of four, submatrices A and Y, complex in general, have to be calculated.

2. T signature or T simplex

As is well known [17,6], for each of the six antilinear D_{2h}^{TD} operators, i.e., for T signature $\hat{\mathcal{R}}_k^T$ or T simplex $\hat{\mathcal{S}}_k^T$, $k=x,y,z$, which have squares equal to unity ($\hat{\mathcal{Z}}^2=\hat{\mathcal{E}}$, where $\hat{\mathcal{Z}}$ denotes one of them), one can construct a basis composed of eigenvectors of $\hat{\mathcal{Z}}$ with eigenvalue equal to 1,

$$\hat{\mathcal{Z}}|\boldsymbol{n}\zeta\rangle=|\boldsymbol{n}\zeta\rangle. \tag{13}$$

Moreover, since every operator $\hat{\mathcal{Z}}$ commutes with the time-reversal $\hat{\mathcal{T}}$, such basis can always be chosen so as to fulfill condition (8) at the same time. Table III lists examples of such bases, constructed for the HO states $|n_xn_yn_z,s_z=\pm\frac{1}{2}\rangle$. A similar construction is possible for any other single-particle basis, and has the explicit form shown in Table III provided the space and spin degrees of freedom are separated. Note that any linear combination of states $|\boldsymbol{n}\zeta=+1\rangle$ and $|\boldsymbol{n}\zeta=-1\rangle$, with real coefficients, is another valid eigenstate of $\hat{\mathcal{Z}}$ with eigenvalue 1.

For operators even or odd with respect to $\hat{\mathcal{Z}}$,

$$\hat{\mathcal{Z}}^\dagger\hat{\mathcal{O}}\hat{\mathcal{Z}}=\epsilon_Z\hat{\mathcal{O}},\quad \epsilon_Z=\pm1, \tag{14}$$

one then has

$$\langle\boldsymbol{n}\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'\zeta'\rangle=\epsilon_Z\langle\boldsymbol{n}\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'\zeta'\rangle^*. \tag{15}$$

Hence, in bases fulfilling Eqs. (8) and (13), matrix $\mathcal{O}$ is purely real ($\epsilon_Z=+1$) or purely imaginary ($\epsilon_Z=-1$). This gives matrix $\mathcal{O}$ in the form (tilde stands for the transposition)

$$\begin{pmatrix} A & Y \\ \tilde{Y} & B \end{pmatrix}\quad\text{or}\quad i\begin{pmatrix} A' & Y' \\ -\tilde{Y}' & -B' \end{pmatrix}, \tag{16}$$

for $\epsilon_Z=+1$ and $\epsilon_Z=-1$, respectively, where all submatrices are real, A and B are symmetric, A' and B' are antisymmetric, and Y and Y' are arbitrary. Note that in order to diagonalize $\mathcal{O}$ one only needs to diagonalize a real matrix with unrestricted eigenvalues (for $\epsilon_Z=+1$), or an imaginary matrix with pairs of opposite nonzero eigenvalues (for $\epsilon_Z=-1$).

3. Signature or simplex

Let us now consider operator $\hat{\mathcal{O}}$ which is even or odd with respect to one of the six linear D_{2h}^{TD} operators, signatures $\hat{\mathcal{R}}_k$

TABLE III. Examples of eigenstates $|n_x n_y n_z \zeta\rangle_k^T$ of the T signature $\hat{\mathcal{R}}_k^T$, or T simplex $\hat{\mathcal{S}}_k^T$ operators, $k=x$, y, or z, with eigenvalue 1 [see Eqs. (8) and (13)], determined for the harmonic oscillator states $|n_x n_y n_z, s_z=\pm\frac{1}{2}\rangle$. Symbols (N_x, N_y, N_z) refer to (n_x, n_y, n_z) for $\hat{\mathcal{S}}_k^T$ operators, and to $(n_y+n_z, n_x+n_z, n_x+n_y)$ for $\hat{\mathcal{R}}_k^T$ operators.

k	ζ	$\lvert n_x n_y n_z \zeta\rangle_k^T$
x	$+1$	$(+i)^{N_x}\exp\left(-i\frac{\pi}{4}\right)\lvert n_x n_y n_z, s_z=+\frac{1}{2}\rangle$
x	-1	$(-i)^{N_x}\exp\left(+i\frac{\pi}{4}\right)\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle$
y	$+1$	$(+i)^{N_y+1}\lvert n_x n_y n_z, s_z=+\frac{1}{2}\rangle$
y	-1	$(-i)^{N_y+1}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle$
z	$+1$	$\frac{1}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle + i(-1)^{N_z}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$
z	-1	$\frac{i(-1)^{N_z}}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle - i(-1)^{N_z}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$

or simplexes $\hat{\mathcal{S}}_k$, $k=x,y,z$, which have squares equal to minus unity ($\hat{\mathcal{X}}^2=\overline{\mathcal{E}}=-\hat{\mathcal{E}}$, where $\hat{\mathcal{X}}$ denotes one of them), i.e.,

$$\hat{\mathcal{X}}^\dagger \hat{\mathcal{O}} \hat{\mathcal{X}} = \epsilon_X \hat{\mathcal{O}}, \quad \epsilon_X = \pm 1. \tag{17}$$

Since every operator $\hat{\mathcal{X}}$ commutes with the time-reversal $\hat{\mathcal{T}}$, one can always choose a basis in which Eq. (8) holds, and

$$\hat{\mathcal{X}}|\boldsymbol{n}\zeta\rangle = i\zeta|\boldsymbol{n}\zeta\rangle, \tag{18}$$

where again $\zeta=\pm 1$, so $r=\zeta i=\pm i$ is the signature (for $\hat{\mathcal{X}}=\hat{\mathcal{R}}_k$) or simplex $s=\zeta i=\pm i$ (for $\hat{\mathcal{X}}=\hat{\mathcal{S}}_k$) quantum number. Table IV lists such bases constructed for the HO states $|n_x n_y n_z, s_z=\pm\frac{1}{2}\rangle$. A similar construction is possible for any other single-particle basis. Note that one can arbitrarily change the phases of states $|\boldsymbol{n}\zeta=+1\rangle$, and still fulfill Eqs. (8) and (18); we shall use this freedom in Secs. III A 8 and III B.

From Eqs. (17) and (18) one gets

$$\langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'\zeta'\rangle = \epsilon_X \zeta\zeta' \langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}|\boldsymbol{n}'\zeta'\rangle, \tag{19}$$

TABLE IV. Eigenstates $|n_x n_y n_z \zeta\rangle_k$ of the signature or simplex operators, $\hat{\mathcal{R}}_k$ or $\hat{\mathcal{S}}_k$ for $k=x$, y, or z, [see Eqs. (8) and (18)], determined for the harmonic oscillator states $|n_x n_y n_z, s_z=\pm\frac{1}{2}\rangle$. Symbols (N_x, N_y, N_z) refer to (n_x, n_y, n_z) for $\hat{\mathcal{S}}_k$ operators, and to $(n_y+n_z, n_x+n_z, n_x+n_y)$ for $\hat{\mathcal{R}}_k$ operators. Phases of eigenstates are fixed so as to fulfill condition (36).

k	ζ	$\lvert n_x n_y n_z \zeta\rangle_k$
x	$+1$	$\frac{1}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle - (-1)^{N_x}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$
x	-1	$\frac{(-1)^{N_x}}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle + (-1)^{N_x}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$
y	$+1$	$\frac{i^{N_y}}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle - i(-1)^{N_y}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$
y	-1	$\frac{i^{N_y-1}}{\sqrt{2}}(\lvert n_x n_y n_z, s_z=\frac{1}{2}\rangle + i(-1)^{N_y}\lvert n_x n_y n_z, s_z=-\frac{1}{2}\rangle)$
z	$+1$	$+i^{N_z}\exp\left(-i\frac{\pi}{4}\right)\lvert n_x n_y n_z, s_z=+\frac{1}{2}(-1)^{N_z+1}\rangle$
z	-1	$-i^{N_z}\exp\left(+i\frac{\pi}{4}\right)\lvert n_x n_y n_z, s_z=-\frac{1}{2}(-1)^{N_z+1}\rangle$

so the matrix $\mathcal{O}$ has the form

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & Y \\ Y^{\dagger} & 0 \end{pmatrix} \tag{20}$$

for $\epsilon_X=+1$ and $\epsilon_X=-1$, respectively, with A and B Hermitian, and Y arbitrary complex matrix. Note that in order to diagonalize $\mathcal{O}$ one only needs to diagonalize: (i) for $\epsilon_X=+1$, two Hermitian matrices with complex, in general, submatrices in twice smaller dimension, which gives real eigenvalues with no additional restrictions or (ii) for $\epsilon_X=-1$, one Hermitian matrix $Y^{\dagger}Y$, again with complex submatrices in twice smaller dimension, which gives pairs of real nonzero eigenvalues with opposite signs.

Comparing result (20) with that obtained in Sec. III A 2, one sees that the antilinear symmetries allow for using real matrices, while linear symmetries give special block-diagonal forms for complex matrices.

4. Parity

Standard simplification always occurs for operators which are even with respect to the parity operator $\hat{\mathcal{P}}$,

$$\hat{\mathcal{P}}^{\dagger}\hat{\mathcal{O}}\hat{\mathcal{P}}=\hat{\mathcal{O}}. \tag{21}$$

All matrices and submatrices introduced above or below acquire a block-diagonal form, provided the single-particle bases consist of states with well defined parity (such as, e.g., bases listed in Tables III or IV). Therefore, apart from Sec. III A 7, we do not separately discuss cases when the parity is one of the conserved D_{2h}^{TD} operators, and we note that the effect of the parity conservation can be easily included on top of any other symmetry conditions.

5. Time reversal, and T signature or T simplex

For operators $\hat{\mathcal{O}}$, for which both Eqs. (10) and (14) hold, matrix $\mathcal{O}$ in Eq. (12) can be additionally simplified, and reads

$$\begin{pmatrix} A & Y \\ -\epsilon_T Y & \epsilon_T A \end{pmatrix} \quad \text{or} \quad i\begin{pmatrix} A' & Y' \\ \epsilon_T Y' & -\epsilon_T A' \end{pmatrix}, \tag{22}$$

for $\epsilon_Z=+1$ and $\epsilon_Z=-1$, respectively, where all submatrices are real, A is symmetric, A' is antisymmetric, $\tilde{Y}=-\epsilon_T Y$, and $\tilde{Y}'=-\epsilon_T Y'$.

In particular, with $\epsilon_T=\epsilon_Z=+1$, the matrix from Eq. (22) reduces to

$$\mathcal{O}=\begin{pmatrix} A & Y \\ -Y & A \end{pmatrix}, \tag{23}$$

where A is symmetric, Y antisymmetric, and both are real. In order to diagonalize such matrix, one can consider a smaller problem, by constructing a complex matrix $\mathcal{O}_C=A-iY$ which has the size twice smaller than the original matrix $\mathcal{O}$. After diagonalizing $\mathcal{O}_C$, and separating real and imaginary parts of its complex eigenvectors,

$$\mathcal{O}_C(u+iv)=\omega(u+iv), \tag{24}$$

one gets two degenerate real eigenvectors of $\mathcal{O}$:

$$\begin{pmatrix} u \\ v \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} v \\ -u \end{pmatrix}.$$

If $\hat{\mathcal{O}}$ is the mean-field Hamiltonian, such a form of eigenvectors simplifies expressions for densities.

6. Time reversal, and signature or simplex

For operators $\hat{\mathcal{O}}$, for which both Eqs. (10) and (17) hold, matrix $\mathcal{O}$ in Eq. (12) can be additionally simplified, and reads

$$\begin{pmatrix} A & 0 \\ 0 & \epsilon_T A^{*} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} 0 & Y \\ -\epsilon_T Y^{*} & 0 \end{pmatrix} \tag{25}$$

for $\epsilon_X=+1$ and $\epsilon_X=-1$, respectively, with A Hermitian, and Y antisymmetric ($\epsilon_T=+1$) or symmetric ($\epsilon_T=-1$). Of course, this case is identical to that described in Sec. III A 5, because whenever the time reversal, and signature or simplex are conserved, the corresponding T signature or T simplex are also conserved, and $\epsilon_X=\epsilon_Z\epsilon_T$. Therefore, we may now use two different bases, and obtain two different forms of the matrix $\mathcal{O}$, Eqs. (22) or (25), which lead either to real, or to block-diagonal matrices. Note that in order to diagonalize matrix $\mathcal{O}$ for $\epsilon_X=+1$, one has to diagonalize only its Hermitian submatrix A, which has dimension twice smaller than $\mathcal{O}$, similarly as in Eq. (24).

7. Parity, and signature or simplex

In the D_{2h}^{TD} group, the possibility of having at one's disposal two different quantum numbers simultaneously is very limited. Indeed in D_{2h}^{TD} one has only three pairs of commuting linear operators, namely, $(\hat{\mathcal{R}}_k,\hat{\mathcal{P}})$ for $k=x$, y, or z. For each such pair, the corresponding simplex operator $\hat{\mathcal{S}}_k$ is also conserved, but it does not give any additional quantum number. Only one generic two-generator subgroup, $\{\hat{\mathcal{R}}_k,\hat{\mathcal{P}}\}$, see 2-$I_B$ in Table I, allows, therefore, for two quantum numbers. Similarly, only three generic three-generator subgroups allow for two quantum numbers, namely, (i) $\{\hat{\mathcal{R}}_k,\hat{\mathcal{T}},\hat{\mathcal{P}}\}$, which allows only for stationary solutions, (ii) $\{\hat{\mathcal{R}}_l,\hat{\mathcal{R}}_m,\hat{\mathcal{P}}\}$, which does not allow for nonzero average values of the angular-momentum, and (iii) $\{\hat{\mathcal{R}}_l,\hat{\mathcal{S}}_m^T,\hat{\mathcal{P}}\}$, which is the only two-quantum-number subgroup which allows for rotating mean-field states. Needless to say, this latter case is most often used in cranking calculations to date, see Sec. III C.

8. T signature or T simplex, and signature or simplex

Let us now consider operator $\hat{\mathcal{O}}$ which is even or odd with respect to one of the six antilinear, $\hat{\mathcal{Z}}^2=\hat{\mathcal{E}}$, operators (see Sec. III A 2), and simultaneously even or odd with respect to one of the six linear, $\hat{\mathcal{X}}^2=\overline{\hat{\mathcal{E}}}=-\hat{\mathcal{E}}$, operators (see Sec. III A 3). In such a case, simplification of the single-particle

basis is possible only for pairs of $\hat{\mathcal{Z}}$ and $\hat{\mathcal{X}}$ operators which correspond to two *different* Cartesian directions. Indeed, focusing our attention on signatures, $\hat{\mathcal{R}}_k^T$ *commutes* with $\hat{\mathcal{R}}_k$, and therefore (being antilinear) it flips the $\hat{\mathcal{R}}_k$ signature quantum number. Therefore, the eigenstates of $\hat{\mathcal{R}}_k$ cannot be eigenstates of $\hat{\mathcal{R}}_k^T$. We may then only work either in the basis of eigenstates of $\hat{\mathcal{R}}_k^T$, Sec. III A 2, or in the basis of eigenstates of $\hat{\mathcal{R}}_k$, Sec. III A 3. On the other hand, for $l \neq k$ $\hat{\mathcal{R}}_l^T$ *anticommutes* with $\hat{\mathcal{R}}_k$, and therefore, it conserves the $\hat{\mathcal{R}}_k$ signature quantum number. Hence, the eigenstates of $\hat{\mathcal{R}}_k$ can be rendered the eigenstates of $\hat{\mathcal{R}}_l^T$ by a suitable choice of phases.

It is easy to check that after multiplying eigenstates listed in Table IV by the following phase factors:

$$\Phi_{lk} = \exp\left\{ i\zeta \frac{\pi}{2}(N_l + 1) \right\}, \quad \text{for } k < l, \tag{26a}$$

$$\Phi_{lk} = \exp\left\{ i\zeta \frac{\pi}{4} + i\zeta \frac{\pi}{2}(N_l + N_k + 1) \right\}, \quad \text{for } l < k, \tag{26b}$$

one obtains the basis states

$$|\boldsymbol{n}\zeta\rangle_{lk} = \Phi_{lk} |\boldsymbol{n}\zeta\rangle_k, \tag{27}$$

which simultaneously fulfill Eqs. (8), (13), and (18), i.e.,

$$\hat{\mathcal{T}} |\boldsymbol{n}\zeta\rangle_{lk} = \zeta |\boldsymbol{n} - \zeta\rangle_{lk}, \tag{28a}$$

$$\hat{\mathcal{Z}}_l |\boldsymbol{n}\zeta\rangle_{lk} = |\boldsymbol{n}\zeta\rangle_{lk}, \tag{28b}$$

$$\hat{\mathcal{X}}_k |\boldsymbol{n}\zeta\rangle_{lk} = i\zeta |\boldsymbol{n}\zeta\rangle_{lk}. \tag{28c}$$

Here, $\hat{\mathcal{Z}}_l$ stands for $\hat{\mathcal{R}}_l^T$ or $\hat{\mathcal{S}}_l^T$, and $\hat{\mathcal{X}}_k$ stands for $\hat{\mathcal{R}}_k$ or $\hat{\mathcal{S}}_k$. In Eqs. (26), symbols (N_x, N_y, N_z) refer to (n_x, n_y, n_z) for the $\hat{\mathcal{S}}_l^T$ or $\hat{\mathcal{S}}_k$ operators, and to $(n_y + n_z, n_x + n_z, n_x + n_y)$ for the $\hat{\mathcal{R}}_l^T$ or $\hat{\mathcal{R}}_k$ operators. Moreover, a circular ordering of Cartesian directions is assumed, i.e., $x < y < z < x$, in order to define conditions $l < k$ and $k < l$.

For operators $\hat{\mathcal{O}}$ even or odd simultaneously with respect to $\hat{\mathcal{Z}}_l$ and $\hat{\mathcal{X}}_k$, see Eqs. (14) and (17), bases defined by Eq. (27) allow for a very simple forms of matrices $\mathcal{O}$. Combining conditions (16) and (20) one obtains block diagonal *and* real matrix elements, e.g., for $\epsilon_Z = +1$,

$$\begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \text{ or } \begin{pmatrix} 0 & Y \\ \tilde{Y} & 0 \end{pmatrix}, \tag{29}$$

for $\epsilon_X = +1$ and $\epsilon_X = -1$, respectively, with A and B real symmetric, and Y arbitrary real matrix.

9. Three-generator subgroups

Apart from the unique case of the whole D_{2h}^{TD} group being conserved, which amounts to conserving its four generators, we also have 15 different three-generator subgroups (Table I), which when conserved, may lead to physically different mean-field solutions. Conserved three-generator subgroups are exceptional in that they do not lead to further simplifications of the matrix elements of mean-field Hamiltonians.

This is so, because cases enumerated in Secs. III A 1–III A 8 exhaust different possibilities of using conserved D_{2h}^{TD} operators to simplify the structure of operators by suitable choices of the single-particle bases. Indeed, the type III subgroups of D_{2h}^{TD}, Table I, which involve operators for three different Cartesian axes, do not induce any new simplifications. The signature or simplex operators for different axes (the $\hat{\mathcal{X}}$ operators of Sec. III A 3) do not commute, and hence cannot give independent quantum numbers of single-particle states. Similarly, T signature or T simplex operators for different axes (the $\hat{\mathcal{Z}}$ operators of Sec. III A 2) do not commute either, and hence cannot simultaneously define phases of single-particle states.

One should stress, however, that even if a given conserved symmetry does not allow for any further simplification of the matrix elements of a mean-field Hamiltonian (such as each third generator of a three-generator subgroup), its conservation or its nonconservation may induce entirely different solutions of the mean-field problem.

B. Phase conventions

In Sec. III A we have shown how one can simplify the matrix elements of operators by using a given phase convention, i.e, by fixing phases of single-particle basis states in a given way. Whenever an antilinear D_{2h}^{TD} operator is conserved, one can always construct a phase convention for which the matrix elements of the mean-field Hamiltonian are real numbers. However, from technical point of view, it can be more advantageous to fix the phase convention in yet another way. Indeed, whenever the calculation of matrix elements is more time consuming than the diagonalization of the Hamiltonian matrix, one may use the phase convention to facilitate the former task, at the expense of diagonalizing complex matrices. Moreover, such a strategy allows for keeping the simplicity of performing the former task even in cases when there is no antilinear conserved symmetry available, and when one has to diagonalize complex matrices anyhow. In the present section we show constructions of phase conventions which facilitate calculations of the space-spin matrix elements.

Representation (8), which separates space and spin degrees of freedom, is convenient in applications pertaining to deformed single-particle states, as those discussed in the present study. This is because, each Hermitian operator can be represented as a sum of four components of the form

$$\hat{\mathcal{O}}^{(\mu)} = \hat{O}_r^{(\mu)} \hat{\sigma}_\mu, \quad \mu = 0,1,2,3, \tag{30}$$

where $\hat{O}_r^{(\mu)}$ acts in the coordinate space, and $\hat{\sigma}_\mu$ are the Pauli

TABLE V. Antilinear spin operators $\hat{\mathcal{K}}_l$, which can be used to fix convenient phase conventions leading to conditions (35).

l	$\hat{\mathcal{K}}_l$	ϵ_{0l}	ϵ_{1l}	ϵ_{2l}	ϵ_{3l}
x	$\hat{\mathcal{T}}i\hat{\sigma}_x=i\hat{\sigma}_z\hat{\mathcal{K}}$	$+1$	$+1$	-1	-1
y	$\hat{\mathcal{T}}i\hat{\sigma}_y=\hat{\mathcal{K}}$	$+1$	-1	$+1$	-1
z	$\hat{\mathcal{T}}i\hat{\sigma}_z=-i\hat{\sigma}_x\hat{\mathcal{K}}$	$+1$	-1	-1	$+1$

matrices acting in the spin space, with $\hat{\sigma}_0$ defined as the 2×2 identity matrix. Then, the matrix elements of $\hat{\mathcal{O}}^{(\mu)}$ can be factorized into space and spin parts

$$\langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}^{(\mu)}|\boldsymbol{n}'\zeta'\rangle=\langle \boldsymbol{n}|\hat{O}_r^{(\mu)}|\boldsymbol{n}'\rangle\cdot\langle\zeta|\hat{\sigma}_\mu|\zeta'\rangle, \tag{31}$$

and the spin part can be computed once for all. Usually many of the spin matrix elements $\langle\zeta|\hat{\sigma}_\mu|\zeta'\rangle$ vanish, thus making it unnecessary to calculate the corresponding coordinate-space matrix elements $\langle \boldsymbol{n}|\hat{O}_r^{(\mu)}|\boldsymbol{n}'\rangle$.

Matrix elements of operators $\hat{\mathcal{O}}^{(\mu)}$ can be made purely real or purely imaginary if phases of single-particle basis states are chosen in such a way that, for one Cartesian direction $l=x$, y, or z, one has

$$\hat{\mathcal{K}}_l|\boldsymbol{n}\zeta\rangle=|\boldsymbol{n}\zeta\rangle, \tag{32}$$

where $\hat{\mathcal{K}}_l^2=\hat{\mathcal{E}}$ is the antilinear spin operator defined by

$$\hat{\mathcal{K}}_l=\hat{\mathcal{T}}i\hat{\sigma}_l=i\hat{\sigma}_l\hat{\mathcal{T}}. \tag{33}$$

Indeed, for time-even ($\epsilon_T=+1$) or time-odd ($\epsilon_T=-1$) operators one obtains that

$$\hat{\mathcal{K}}_l^\dagger\hat{\mathcal{O}}^{(\mu)}\hat{\mathcal{K}}_l=\epsilon_{\mu l}\hat{\mathcal{T}}^\dagger\hat{\mathcal{O}}^{(\mu)}\hat{\mathcal{T}}=\epsilon_{\mu l}\epsilon_T\hat{\mathcal{O}}^{(\mu)},\quad \epsilon_{\mu l}=\pm1, \tag{34}$$

where coefficients $\epsilon_{\mu l}$ are given in Table V. Using Eqs. (32) and (34), one gets for matrix elements of $\hat{\mathcal{O}}^{(\mu)}$

$$\langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}^{(\mu)}|\boldsymbol{n}'\zeta'\rangle=\epsilon_{\mu l}\epsilon_T\langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}^{(\mu)}|\boldsymbol{n}'\zeta'\rangle^*, \tag{35a}$$

$$\langle \boldsymbol{n}\zeta|\hat{\mathcal{O}}^{(\mu)}|\boldsymbol{n}'\zeta'\rangle=\epsilon_{\mu l}\zeta\zeta'\langle \boldsymbol{n}-\zeta|\hat{\mathcal{O}}^{(\mu)}|\boldsymbol{n}'-\zeta'\rangle, \tag{35b}$$

where Eq. (35a) tells us which elements are real, and which are imaginary, while Eq. (35b) gives the matrix elements, e.g., for $\zeta=-1$ expressed through those for $\zeta=+1$.

As is usual for antilinear operators, there is a lot of freedom in finding bases (32) of eigenstates of $\hat{\mathcal{K}}_l$. We can use this freedom to fulfill other useful conditions. For example, since $\hat{\mathcal{K}}_l$ and $\hat{\mathcal{R}}_k$ anticommute for $l\neq k$, one can find bases (32) which are at the same time the eigenstates of signature or simplex operators. In fact, phases of eigenstates listed in Table IV, has been chosen in such a way that,

$$\hat{\mathcal{K}}_l|\boldsymbol{n}\zeta\rangle_k=|\boldsymbol{n}\zeta\rangle_k,\quad \text{for}\quad k<l, \tag{36}$$

where again the circular ordering of Cartesian directions, $x<y<z<x$, is assumed to define $k<l$.

C. Examples of previous cranking approaches

As argued in Sec. III A 7, there are good reasons to use in cranking calculations the subgroup $\{\hat{\mathcal{R}}_l,\hat{\mathcal{S}}_m^T,\hat{\mathcal{P}}\}$ (Table I) of conserved D_{2h}^{TD} symmetries. This generic three-generator subgroup appears in three space orientations, i.e., for $l=x$, y, or z, and each of these possibilities was employed in one of the HF(B) or phenomenological-mean-field cranking analyses to date.

In particular, traditionally the x axis was chosen as the direction of the cranking angular momentum, see, e.g., Ref. [11], and therefore, the standard Goodman basis [10] corresponds to the $l=x$ subgroup, with phases of single-particle states (and quasiparticle states, for that matter) fixed by using the $\hat{\mathcal{R}}_z^T$ operator. Then, by dropping the parity operator from the symmetry group $\{\hat{\mathcal{R}}_x,\hat{\mathcal{S}}_z^T,\hat{\mathcal{P}}\}$, most octupole-cranking calculations were performed within the 2-III$_A$ subgroup $\{\hat{\mathcal{S}}_x,\hat{\mathcal{S}}_y^T\}$ of Table I.

Another choice was made in the HO basis [9] and coordinate-space [12,13] HF(B) calculations, where the z axis was used as the cranking axis. Such choice was motivated by the standard representation of spinors, that are eigenstates of $\hat{\sigma}_z$, and hence the $l=z$ subgroup $\{\hat{\mathcal{R}}_z,\hat{\mathcal{S}}_y^T,\hat{\mathcal{P}}\}$ was employed. In these approaches, phases of single-particle states were fixed by using the $\hat{\mathcal{S}}_y^T$ operator, and the parity-broken calculations were done within the $\{\hat{\mathcal{S}}_z,\hat{\mathcal{S}}_y^T\}$ subgroup.

Finally, in the recent Cartesian HO-basis HF approach of Ref. [14], the code HFODD was constructed for the conserved $l=y$ subgroup $\{\hat{\mathcal{R}}_y,\hat{\mathcal{S}}_x^T,\hat{\mathcal{P}}\}$, and the y direction was used for the cranking axis. The choice of this symmetry, and the resulting choice of the y cranking axis, was motivated by the fact that it allows for using real electric multipole moments, see Ref. [6]. Phases of single-particle states were in Ref. [14] fixed by using the $\hat{\mathcal{K}}_z$ operator (33), and calculations were performed within the basis of the $\hat{\mathcal{S}}_y$ eigenstates, Table IV. The HFODD code allows for calculations with one symmetry plane, and this is done within the $\{\hat{\mathcal{S}}_y\}$ conserved symmetry group of Table I. The code can also optionally perform the two-symmetry-plane cranking calculations for the 2-III$_A$ subgroups $\{\hat{\mathcal{S}}_y,\hat{\mathcal{S}}_x^T\}$ and $\{\hat{\mathcal{S}}_y,\hat{\mathcal{S}}_z^T\}$.

IV. CONCLUSIONS

We have analyzed the ''far end'' of the symmetry breaking chain, namely, symmetries of mean-field nuclear states which range from time-even, parity-even, signature conserving states (nevertheless breaking the rotational and axial symmetry), to those which do not conserve any symmetries at all. We have shown that intermediate cases, between such two extremes, correspond to conserved subgroups of the D_{2h}^T or D_{2h}^{TD} point symmetry groups. A classification of all the

subgroups has been proposed, and we have shown that there are 26 different nontrivial symmetry-breaking schemes, when names of Cartesian axes are irrelevant, and 65 different nontrivial symmetry-breaking schemes when names of axes are distinguished in the intrinsic frame of reference.

Consequences of conserving individual D_{2h}^{TD} symmetries have been enumerated for the construction of single-particle bases in which mean-field operators may have special simplified forms. We point out that the same forms of the mean-field Hamiltonian may correspond to different conserved symmetries, and hence to different physical consequences for observables obtained in the mean-field methods. We have also analyzed and compared various options for defining phase conventions of single-particle basis states.

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