Multiparticle interpolating operators in quantum field theories with cubic symmetry

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Numerical studies of lattice quantum field theories are conducted in finite spatial volumes, typically with cubic symmetry in the spatial coordinates. Motivated by these studies, this work presents a general algorithm to construct multiparticle interpolating operators for quantum field theories with cubic symmetry. The algorithm automates the block diagonalization required to combine multiple operators of definite linear momentum into irreducible representations of the appropriate little group. Examples are given for distinguishable and indistinguishable particles including cases with both zero and nonzero spin.

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I. INTRODUCTION

The determination of energy spectra is a central task in numerical studies of lattice quantum field theories (QFTs) and is the precursor to more complex studies of the properties and interactions of the states in the theory. In strongly-coupled field theories, very little is known about the spectra *a priori*. However, analysis of the Euclidean-time dependence of two-point correlation functions between operators with the quantum numbers of the states of interest provides an avenue for first-principles determinations of spectra. This approach has been used to explore many different field theories, most notably to determine the low-energy excitations in the hadronic and nuclear spectra in quantum chromodynamics (QCD), the theory of the strong interactions. The wide-reaching goals and achievements of lattice QCD are summarized, e.g., in Refs. [1–6].

To construct correlation functions sensitive to the eigenstates of a strongly-interacting theory such as QCD requires the use of *interpolating operators*, composite objects built from products of the elementary fields of the theory. In numerical studies, the behavior of correlation functions depends sensitively on the choice of interpolating operators used in the calculation. To determine the energies of the eigenstates most effectively, it is advantageous to project these interpolating operators to particular symmetry sectors, thereby reducing the number of states that contribute to the corresponding correlation functions.

Numerical studies in lattice QFTs are usually performed in a finite cubic spatial volume. In this setting, continuous rotational symmetry is broken down to a discrete subgroup, which (combined with spatial inversions) is the cubic group, Oh. Moreover, provided translational symmetry is preserved (e.g., via the use of periodic boundary conditions), the total momentum of an energy eigenstate is a conserved quantity which further reduces the spatial symmetry. Specifically, the *little group* of rotations that leave a given total momentum $\boldsymbol{P}$ invariant is the subgroup $G_{\boldsymbol{P}} \leq O_h$. Understanding the transformation properties of states—and interpolating operators—under the cubic group and its subgroups is thus critical in analysis of lattice QFT calculations [7,8].

Multiparticle interpolating operators constructed in coordinate space or through momentum projection typically transform *reducibly* under these finite groups, obscuring the transformation properties of energy eigenstates. However, it is possible to decompose the operators into linear subspaces that do not mix with each other and only transform internally. A complete decomposition into these *irreducible representations* (irreps) is possible for any set of operators that is closed under the little group [9]. For example, suppose an interpolating operator transforms under a reducible representation labeled by s, with representation matrices

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$D^{(s)}(R)$ for $R \in G_{\boldsymbol{P}}$. Decomposing the reducible representation into a direct sum of irreps $\Gamma^{(s)} = \Gamma_a \oplus \Gamma_b \oplus \cdots$, there exist block-diagonalization (or change-of-basis) matrices $\mathrm{U}^{(s)}$ specific to $\Gamma^{(s)}$ that enact the decomposition into irrep matrices $D^{(\Gamma)}(R)$ according to

$$[\mathrm{U}^{(s)}]^\dagger D^{(s)}(R)\mathrm{U}^{(s)} = \bigoplus_i D^{(\Gamma_i)}(R). \tag{1}$$

After changing to the irrep basis, the transformation properties of multiparticle operators—and the states that they create—are then simpler to understand. Previous work has addressed the construction of lattice interpolating operators for single baryons [10,11], single mesons [12], two-hadron systems [13,14] with arbitrary spin and momenta [15,16], and three-boson systems [17]. These results cover the construction of local and extended operators with definite cubic transformation properties, as well as their combination into irreps of the relevant little group in cases of up to three local operators.

The present work provides a concrete algorithm and a numerical implementation [18] that carries out the block diagonalization for any product of N operators with definite momentum, spin, and permutation properties. Each operator can be a point-like operator, a smeared or extended operator, or an even more general construction. It is further shown that the block-diagonalization matrices can be determined for all N by enumerating a small set of examples. For spin-zero operators, only examples from $N = 1$ and $N = 2$ operators are required to specify the decomposition for general N. Additional internal symmetries such as flavor, as well as any combination of fermionic and bosonic operator-exchange symmetries, can be incorporated with a simple extension of the formalism that is also described herein.

The remainder of this article is organized as follows. Section II lays out the formalism for building the block-diagonalization matrices for the simple case of N distinguishable, spin-zero operators. Section III addresses distinguishable operators with spin, including a generic method for calculating block-diagonalization matrices; concrete results are given for several examples. Section IV presents the generalization of this construction to operators involving internal symmetries or identical particles. Section V collects the formalism of the preceding sections to give the complete block-diagonalization algorithm. Finally, Sec. VI provides an outlook. The appendices specify group-theoretical conventions, discuss the method of polarization tensors for evaluating irrep matrices, and give explicit examples of the block-diagonalization matrices appearing in Eq. (1).

II. DISTINGUISHABLE SPIN-ZERO OPERATORS

Consider a lattice QFT defined on a geometry whose spatial structure is a periodic cubic lattice Λ with volume $V = L^3$, lattice spacing a, and with associated Hilbert space $\mathcal{H}$ and vacuum state $|\Omega\rangle_{\mathcal{H}} \in \mathcal{H}$.[1] The spatial symmetry group is therefore the cubic group, O_h. In the following, all quantities will be given in lattice units with $a = 1$, where $\Lambda \sim (\mathbb{Z}_L)^3$.

Multiparticle states can be created by acting on the vacuum with interpolating operators with the quantum numbers of the desired states. Often, products of N local operators serve as useful interpolating operators for multiparticle states. Such a product may generically be written as $\mathcal{O}_1(\boldsymbol{x}_1)\cdots\mathcal{O}_N(\boldsymbol{x}_N)$, where the labels $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \in \Lambda$ indicate three-vector coordinates of spatial lattice sites. The operators $\mathcal{O}_i$ are built from the fundamental fields in the theory and need not be distinguishable. For simplicity, the initial discussion will focus on distinguishable operators transforming as scalars under spatial rotations, in which case only the coordinates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ of the operators transform under the spatial symmetry group. The extension to operators with nonzero spin or composite operators with nontrivial O_h-transformation properties is addressed in Sec. III. The extension to indistinguishable operators is addressed in Sec. IV.

For a fixed list of N local operators, $\mathcal{O}_1, \ldots, \mathcal{O}_N$, this work investigates the transformation properties of linear combinations of products constructed via

$$\sum_{\boldsymbol{x}_1 \in \Lambda} \cdots \sum_{\boldsymbol{x}_N \in \Lambda} c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)\mathcal{O}_1(\boldsymbol{x}_1)\cdots\mathcal{O}_N(\boldsymbol{x}_N), \tag{2}$$

where the $c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \in \mathbb{C}$ are V^N arbitrary coefficients.[2] Acting on the vacuum with any such linear combination yields a state

$$|\psi\rangle_{\mathcal{H}} \equiv \sum_{\boldsymbol{x}_1 \in \Lambda} \cdots \sum_{\boldsymbol{x}_N \in \Lambda} c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)\mathcal{O}_1(\boldsymbol{x}_1)\cdots\mathcal{O}_N(\boldsymbol{x}_N)|\Omega\rangle_{\mathcal{H}}. \tag{3}$$

Invariance of the vacuum state under spatial rotations means that any such $|\psi\rangle_{\mathcal{H}}$ inherits the transformation properties of the multiparticle operator itself.

The space defined by the coefficients $c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ forms a V^N-dimensional vector space which will be denoted $\mathcal{V}$. A symbolic (position-space) basis for $\mathcal{V}$ consists of the vectors $|\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\rangle$ for each choice of $\{\boldsymbol{x}_i \in \Lambda\}$. These

[1] The temporal geometry (discrete or continuous) and the spacetime metric (Euclidean or Minkowski) are left unspecified because the classification of operator representations under spatial rotations/translations is insensitive to these choices.

[2] In a continuum theory, $\sum_{\boldsymbol{x}_i \in \Lambda}$ is replaced with $\int \prod_i d^3\boldsymbol{x}_i$ and $c(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N)$ should be replaced by a continuous field over N coordinates, but otherwise the formalism developed in this work applies.

basis vectors are defined to be orthonormal with respect to the inner product on $\mathcal{V}$,

$$\langle \boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_N | \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N \rangle = \delta_{\boldsymbol{x}'_1, \boldsymbol{x}_1} \cdots \delta_{\boldsymbol{x}'_N, \boldsymbol{x}_N}. \tag{4}$$

To avoid ambiguity, elements of the abstract space $\mathcal{V}$ are written with unadorned kets, while quantum states such as $|\Omega\rangle_{\mathcal{H}}$ or $|\psi\rangle_{\mathcal{H}}$ carry a subscript. Since the list of operators is fixed, each vector in $\mathcal{V}$ is associated uniquely with an interpolating operator by the linear map $\mathcal{L}\colon\ |\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\rangle \mapsto \mathcal{O}_1(\boldsymbol{x}_1) \cdots \mathcal{O}_N(\boldsymbol{x}_N)$.

A useful starting point for the decomposition of a state $|\psi\rangle_{\mathcal{H}}$ into subspaces that transform irreducibly under spatial symmetries is the plane-wave basis of $\mathcal{V}$, defined by vectors

$$|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle \equiv \sum_{\boldsymbol{x}_1 \in \Lambda} \cdots \sum_{\boldsymbol{x}_N \in \Lambda} e^{i\frac{2\pi}{L}\boldsymbol{n}_1 \cdot \boldsymbol{x}_1} \cdots e^{i\frac{2\pi}{L}\boldsymbol{n}_N \cdot \boldsymbol{x}_N} |\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\rangle, \tag{5}$$

for each possible (ordered) set of wave vectors $\{\boldsymbol{n}_i \in (\mathbb{Z}_L)^3\}$.[3] Here, the distinction between the position-space and plane-wave bases is made by the use of the letters $\boldsymbol{x}$ and $\boldsymbol{n}$, respectively. Since there is a one-to-one mapping between wave vectors $\boldsymbol{n}_i$ and momenta $(2\pi/L)\boldsymbol{n}_i$, these terms will be used interchangeably for the wave vectors $\boldsymbol{n}_i$. Each vector $|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle$ is associated with a plane-wave interpolating operator,

$$\tilde{\mathcal{O}}_1(\boldsymbol{n}_1) \cdots \tilde{\mathcal{O}}_N(\boldsymbol{n}_N) \equiv \sum_{\boldsymbol{x}_1 \in \Lambda} \cdots \sum_{\boldsymbol{x}_N \in \Lambda} e^{i\frac{2\pi}{L}\boldsymbol{n}_1 \cdot \boldsymbol{x}_1} \mathcal{O}_1(\boldsymbol{x}_1) \cdots e^{i\frac{2\pi}{L}\boldsymbol{n}_N \cdot \boldsymbol{x}_N} \mathcal{O}_N(\boldsymbol{x}_N). \tag{6}$$

The position-space basis vectors $|\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\rangle$ and plane-wave basis vectors $|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle$ have simple transformation properties under O_h and its subgroups. Each group element $R \in O_h$ can be specified by its action on arbitrary three-vectors $\boldsymbol{x} \in \Lambda$, i.e., with each group element defined as a unique orthogonal 3×3 matrix, $R \in O_h \leq \mathrm{O}(3)$. A concrete specification of these matrices is presented in Appendix A. When acting on vectors in $\mathcal{V}$, the abstract operator associated with rotation R will be denoted $\mathcal{D}(R)$. Its action on the position-space basis vectors is given by

$$\mathcal{D}(R)|\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\rangle = |R\boldsymbol{x}_1, \ldots, R\boldsymbol{x}_N\rangle \tag{7}$$

and extends linearly to the rest of $\mathcal{V}$, including to the plane-wave basis vectors, which transform as

$$\mathcal{D}(R)|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle = |R\boldsymbol{n}_1, \ldots, R\boldsymbol{n}_N\rangle \tag{8}$$

[3] In a continuum theory, $\mathbb{Z}_L$ is replaced with $\mathbb{Z}$.

based on their definition in Eq. (5). Through the map $\mathcal{L}$ [defined following Eq. (4)], this defines the action of rotations on the corresponding interpolating operators.

The remainder of this section proceeds as follows. First, Sec. II A constructs the reducible representations associated with interpolating operators in the form of Eq. (6) for distinguishable spin-zero operators. Second, Sec. II B reviews the irreps of the cubic group and its subgroups. Section II C presents the algorithm for constructing the block-diagonalization matrices that change basis from the interpolating operators in Eq. (6) into operators that transform irreducibly. Section II D discusses a classification of cases with identical block-diagonalization matrices using the stabilizer groups of specific momenta, and finally Sec. II E presents examples of the block-diagonalization that are sufficient to implement this process for any number of spin-zero operators.

A. Momentum orbits and their representations

To construct the reducible representations associated with plane-wave interpolating operators, the space $\mathcal{V}$ is systematically decomposed into subspaces associated with *momentum orbits*, i.e., sets of plane-wave momenta closed under little-group transformations. These subspaces, labeled by s, each correspond to a definite total momentum $\boldsymbol{P}$ and carry a reducible representation $\Gamma^{(s)}$ of the little group $G_{\boldsymbol{P}}$. The representation matrices $D^{(s)}(R)$ take a simple form and are explicitly constructed below.

Given a plane wave $|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle \in \mathcal{V}$, the total momentum is $\boldsymbol{P} = \frac{2\pi}{L}\sum_i \boldsymbol{n}_i$. The ordered list of wave vectors defining the basis state $|\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N\rangle$ is denoted by $[\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]$ and will be used to define momentum orbits below. The set of such lists of wave vectors can be partitioned into disjoint subsets $K_{\boldsymbol{P}}$ of fixed total momentum $\boldsymbol{P}$,

$$K_{\boldsymbol{P}} \equiv \left\{ [\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N] \colon \frac{2\pi}{L}\sum_i \boldsymbol{n}_i = \boldsymbol{P} \right\}. \tag{9}$$

For each total momentum $\boldsymbol{P}$, the associated *little group* is defined as the subgroup $G_{\boldsymbol{P}} \leq O_h$ that leaves $\boldsymbol{P}$ invariant,

$$G_{\boldsymbol{P}} \equiv \{R \in O_h \colon R\boldsymbol{P} = \boldsymbol{P}\}. \tag{10}$$

The possible little groups, up to equivalence under rotation of the total momentum, are denoted C_{4v}, C_{3v}, C_{2v}, C_2^R, C_2^P, and C_1 following the notation of Ref. [9], where C_{nv} is the symmetry group of the n-gon with $2n$ elements and C_n is the cyclic group with n elements. The little groups C_2^R and C_2^P both have the group structure of C_2, but appear as little groups for inequivalent choices of total momenta. Details of these groups are presented in Appendix A; note that to match these definitions the little group may need to be

rotated (by conjugation) so that the total momentum aligns with the present conventions.

By construction, the space $K_{\boldsymbol{P}}$ is closed under the action of the little group $G_{\boldsymbol{P}}$. However, it can be further partitioned into minimal invariant subsets that are closed under the action of $G_{\boldsymbol{P}}$. These momentum orbits, denoted by $K_{\boldsymbol{P}}^{(s)}$, are constructed by computing the sets

$$K_{\boldsymbol{P}}^{(s)} \equiv \{R \cdot [\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N] : R \in G_{\boldsymbol{P}}\} \subseteq K_{\boldsymbol{P}}, \tag{11}$$

where $R \cdot [\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N] = [R\boldsymbol{n}_1, \ldots, R\boldsymbol{n}_N]$. Here, s is an abstract label distinguishing inequivalent subsets; the label s can also be defined concretely with one representative or *fiducial* list of wave vectors per orbit. Two examples of $K_{\boldsymbol{P}}^{(s)}$ are given by the orbits of the wave vectors $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,0,1), (0,0,-1)]$ and $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,2,1), (0,-2,-1)]$ with $G_{\boldsymbol{P}} = O_h$ as these cases both have vanishing total momentum.

It is useful to provide a conventional way of ordering the elements of a given momentum orbit. First, select a fiducial arrangement of momenta $[\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]$. With $\boldsymbol{P}$ being the total momentum defined by the fiducial momenta, let $[R_1, \ldots, R_n]$, with $n = |G_{\boldsymbol{P}}|$, denote the fixed ordering of the elements of little group $G_{\boldsymbol{P}}$ given in Appendix A.[4] The orbit $K_{\boldsymbol{P}}^{(s)}$ then inherits its ordering from the little group via Eq. (11), with the group elements acting in order on the fiducial arrangement of momenta. The mth element of $K_{\boldsymbol{P}}^{(s)}$ in this conventional ordering will be denoted by $[\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]_m^{(s)}$ so that the set can be equivalently written as

$$K_{\boldsymbol{P}}^{(s)} = \{[\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]_m^{(s)} : \; m \in \{1, 2, \ldots, |K_{\boldsymbol{P}}^{(s)}|\}\}. \tag{12}$$

The partitioning into momentum orbits gives rise to a corresponding decomposition of the space of interpolating operators. For convenience, the plane-wave vector in $\mathcal{V}$ associated with the mth list of wave vectors within the orbit labeled by s is denoted by

$$|s, m\rangle \equiv |[\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]_m^{(s)}\rangle. \tag{13}$$

It bears emphasis that each momentum orbit $K_{\boldsymbol{P}}^{(s)}$ is defined in terms of a particular total momentum $\boldsymbol{P}$ with little group $G_{\boldsymbol{P}}$; this dependence is left implicit in the notation $|s, m\rangle$. Each orbit defines an invariant subspace

$$\mathcal{V}_{\boldsymbol{P}}^{(s)} \equiv \text{span}\{|s, m\rangle : m \in \{1, 2, \ldots, |K_{\boldsymbol{P}}^{(s)}|\}\} \subset \mathcal{V} \tag{14}$$

satisfying

$$\mathcal{D}(R)\mathcal{V}_{\boldsymbol{P}}^{(s)} = \mathcal{V}_{\boldsymbol{P}}^{(s)}, \quad \text{for } R \in G_{\boldsymbol{P}}. \tag{15}$$

[4]Through the present work, $|X|$ indicates the number of elements in the set X.

These subspaces are linearly independent and jointly compose the full space,

$$\mathcal{V} = \bigoplus_{\boldsymbol{P}, s} \mathcal{V}_{\boldsymbol{P}}^{(s)}, \tag{16}$$

where the sum ranges over all possible total momenta $\boldsymbol{P}$ and (for a given $\boldsymbol{P}$) over all distinct orbits labeled by s.

The vectors in $\mathcal{V}_{\boldsymbol{P}}^{(s)}$ inherit their transformation properties from the plane waves,

$$\mathcal{D}(R)|s, m\rangle = |R \cdot [\boldsymbol{n}_1, \ldots, \boldsymbol{n}_N]_m^{(s)}\rangle = |s, m'\rangle, \tag{17}$$

which extends by linearity to the entire space. Each element $R \in G_{\boldsymbol{P}}$ permutes the basis vectors of $\mathcal{V}_{\boldsymbol{P}}^{(s)}$ due to the invariance property Eq. (15) and therefore acts as a linear operator $\mathcal{V}_{\boldsymbol{P}}^{(s)} \to \mathcal{V}_{\boldsymbol{P}}^{(s)}$ with matrix elements

$$D_{m'm}^{(s)}(R) \equiv \langle s, m'|\mathcal{D}(R)|s, m\rangle \in \{0, 1\}. \tag{18}$$

These matrices are precisely the representation matrices $D^{(s)}$ appearing in Eq. (1). The superscript on $D^{(s)}$ emphasizes the block-diagonal nature of this representation within the larger space $\mathcal{V}$, since distinct momentum orbits do not mix under the cubic group. Each such space therefore forms a (generally reducible) representation which will be denoted by $\Gamma^{(s)}$.

B. Irreducible representations

The irreps Γ of O_h and the irreps of its subgroups have been previously cataloged in many places. Following Ref. [9], such representations are completely specified by basis vectors $|B_\mu^{(\Gamma)}\rangle$, where $\mu \in \{1, \ldots, |\Gamma|\}$ labels the rows of the irrep Γ. The basis vectors can be written in an abstract coordinate space as basis functions $\langle \boldsymbol{r}|B_\mu^{(\Gamma)}\rangle = B_\mu^{(\Gamma)}(\boldsymbol{r})$ on the unit sphere, in terms of the normalized three-vector coordinate $\boldsymbol{r} \equiv (x, y, z)^T \in \mathbb{R}^3$, with $|\boldsymbol{r}| = 1$. The basis functions used in this work, for the irreps of O_h and its subgroups, are specified in Table I. Additional details related to the choice of basis functions are described in Appendix A.

For the present work, the primary utility of the basis functions is in defining the irrep matrices $D^{(\Gamma)}(R)$ appearing in the block diagonalization of Eq. (1). For instance, given the basis functions, the matrix representation associated with $R \in G_{\boldsymbol{P}}$ in irrep Γ can be computed as

$$\begin{aligned} D_{\mu'\mu}^{(\Gamma)}(R) &= \frac{1}{N^{(\Gamma)}} \langle B_{\mu'}^{(\Gamma)}|\mathcal{D}(R)|B_\mu^{(\Gamma)}\rangle \\ &= \frac{1}{N^{(\Gamma)}} \int d\Omega \langle B_{\mu'}^{(\Gamma)}|\boldsymbol{r}\rangle\langle \boldsymbol{r}|\mathcal{D}(R)|B_\mu^{(\Gamma)}\rangle \\ &= \frac{1}{N^{(\Gamma)}} \int d\Omega B_{\mu'}^{(\Gamma)*}(\boldsymbol{r}) B_\mu^{(\Gamma)}(R^{-1}\boldsymbol{r}), \end{aligned} \tag{19}$$

TABLE I. Basis functions $\langle \boldsymbol{r}|B_\mu^{(\Gamma)}\rangle = B_\mu^{(\Gamma)}(\boldsymbol{r})$ used in this work for the irreps of the cubic group O_h and its subgroups. As indicated, basis functions for the irreps of the subgroups C_{4v}, C_{3v}, C_{2v}, C_2^R, C_2^P, and C_1 can be written in terms of the basis functions of irreps of O_h. The final column indicates the z component of the SO(3) angular momentum operator modulo 4, denoted by ℓ_z.

Group	Irrep	μ	Basis function $B_\mu^{(\Gamma)}(\mathbf{r})$	Notes
O_h	A_1^+	1	$\frac{1}{\sqrt{3}}(x^2+y^2+z^2)$	$\ell_z = 0$
O_h	A_2^+	1	$\frac{1}{\sqrt{6}}[x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)]$	$\ell_z = 2$
O_h	E^+	1	$\frac{1}{\sqrt{6}}(2z^2-x^2-y^2)$	$\ell_z = 0$
O_h	E^+	2	$\frac{1}{\sqrt{2}}(x^2-y^2)$	$\ell_z = 2$
O_h	T_1^+	1	$\frac{1}{\sqrt{2}}xy(x^2-y^2)$	$\ell_z = 0$
O_h	T_1^+	2	$\frac{1}{2}[-yz(y^2-z^2)+izx(z^2-x^2)]$	$\ell_z = 1$
O_h	T_1^+	3	$\frac{1}{2}[yz(y^2-z^2)+izx(z^2-x^2)]$	$\ell_z = 3$
O_h	T_2^+	1	$\frac{1}{\sqrt{2}}(-zx+iyz)$	$\ell_z = 1$
O_h	T_2^+	2	$-ixy$	$\ell_z = 2$
O_h	T_2^+	3	$\frac{1}{\sqrt{2}}(zx+iyz)$	$\ell_z = 3$
O_h	A_1^-	1	$\frac{1}{\sqrt{6}}xyz[x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)]$	$\ell_z = 0$
O_h	A_2^-	1	xyz	$\ell_z = 2$
O_h	E^-	1	$\frac{1}{\sqrt{2}}xyz(x^2-y^2)$	$\ell_z = 0$
O_h	E^-	2	$-\frac{1}{\sqrt{6}}xyz[2z^2-x^2-y^2]$	$\ell_z = 2$
O_h	T_1^-	1	z	$\ell_z = 0$
O_h	T_1^-	2	$\frac{1}{\sqrt{2}}(-x+iy)$	$\ell_z = 1$
O_h	T_1^-	3	$\frac{1}{\sqrt{2}}(x+iy)$	$\ell_z = 3$
O_h	T_2^-	1	$\frac{1}{2}[-y(z^2-x^2)+ix(y^2-z^2)]$	$\ell_z = 1$
O_h	T_2^-	2	$-\frac{i}{\sqrt{2}}z(x^2-y^2)$	$\ell_z = 2$
O_h	T_2^-	3	$\frac{1}{2}[y(z^2-x^2)+ix(y^2-z^2)]$	$\ell_z = 3$
C_{4v}	A_1	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	
C_{4v}	A_2	1	$B_1^{(O_h,A_1^-)}(\boldsymbol{r})$	
C_{4v}	B_1	1	$B_2^{(O_h,E^+)}(\boldsymbol{r})$	
C_{4v}	B_2	1	$B_2^{(O_h,T_2^+)}(\boldsymbol{r})$	
C_{4v}	E	1	$-xz = \frac{1}{\sqrt{2}}(B_1^{(O_h,T_2^+)}(\boldsymbol{r}) - B_3^{(O_h,T_2^+)}(\boldsymbol{r}))$	
C_{4v}	E	2	$-yz = \frac{i}{\sqrt{2}}(B_1^{(O_h,T_2^+)}(\boldsymbol{r}) + B_3^{(O_h,T_2^+)}(\boldsymbol{r}))$	
C_{3v}	A_1	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	
C_{3v}	A_2	1	$B_1^{(O_h,A_2^+)}(\boldsymbol{r})$	
C_{3v}	E	1	$B_1^{(O_h,E^+)}(\boldsymbol{r})$	
C_{3v}	E	2	$B_2^{(O_h,E^+)}(\boldsymbol{r})$	
C_{2v}	A_1	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	
C_{2v}	A_2	1	$B_1^{(O_h,A_1^-)}(\boldsymbol{r})$	
C_{2v}	B_1	1	$B_1^{(O_h,A_2^-)}(\boldsymbol{r})$	
C_{2v}	B_2	1	$B_1^{(O_h,A_2^+)}(\boldsymbol{r})$	
C_2^R	A	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	
C_2^R	B	1	$B_1^{(O_h,A_1^-)}(\boldsymbol{r})$	
C_2^P	A	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	
C_2^P	B	1	$B_1^{(O_h,A_2^+)}(\boldsymbol{r})$	
C_1	A	1	$B_1^{(O_h,A_1^+)}(\boldsymbol{r})$	

where the integration is over the solid-angle measure on the unit sphere, i.e., $d\Omega \equiv d\boldsymbol{r}\delta(|\boldsymbol{r}|-1)$, and the normalization constant is

$$N^{(\Gamma)} = \int d\Omega\, B_\mu^{(\Gamma)*}(\boldsymbol{r}) B_\mu^{(\Gamma)}(\boldsymbol{r}), \tag{20}$$

with no summation over μ (by construction, all rows of a given irrep are identically normalized so $N^{(\Gamma)}$ does not carry a row index). The action of a little group transformation therefore corresponds to right multiplication of basis vectors,

$$\mathcal{D}(R)|B_\mu^{(\Gamma)}\rangle = \sum_{\mu'} |B_{\mu'}^{(\Gamma)}\rangle D_{\mu'\mu}^{(\Gamma)}(R). \tag{21}$$

In explicit calculations, it is convenient to recast the integral in Eq. (19) algebraically using polarization tensors as discussed in Appendix B.

C. Block diagonalization

Elements of the momentum orbit $K_{\boldsymbol{P}}^{(s)}$ transform in the reducible representation $\Gamma^{(s)}$, which can be decomposed into a direct sum of irreps

$$\Gamma^{(s)} = \underbrace{\Gamma_1 \oplus \ldots \oplus \Gamma_1}_{k_1 \text{ copies}} \oplus \underbrace{\Gamma_2 \oplus \ldots \oplus \Gamma_2}_{k_2 \text{ copies}} \oplus \cdots. \tag{22}$$

Above, $\Gamma_1, \Gamma_2, \ldots$ label the distinct irreps of the group $G_{\boldsymbol{P}}$, with each Γ_i appearing with multiplicity $k_i \geq 0$ in the decomposition of the momentum-orbit representation. This decomposition into irreps induces an associated decomposition of the vector space $\mathcal{V}_{\boldsymbol{P}}^{(s)}$ associated with $K_{\boldsymbol{P}}^{(s)}$ into subspaces that each transform according to a given irrep:

$$\mathcal{V}_{\boldsymbol{P}}^{(s)} = \mathcal{V}^{(\Gamma_1,s)} \oplus \mathcal{V}^{(\Gamma_2,s)} \oplus \cdots, \tag{23}$$

where dependence on $\boldsymbol{P}$ is left implicit on the right-hand side. Due to the potential for degenerate copies of irreps,[5] each summand $\mathcal{V}^{(\Gamma_i,s)}$ has dimension $k_i \cdot |\Gamma_i|$. Methods for constructing operators that project this space into particular irrep rows have been used in many previous studies [10–17]. However, only cases where irreps have relatively small multiplicities (1–2) have been considered, and general methods for consistently decomposing spaces where irreps have arbitrary multiplicities have not been discussed.

[5]Here and below, "degenerate" is used to describe situations where multiple copies of an irrep appear in a given momentum-orbit representation. In Hilbert space, the physical states associated with these operators are not necessarily degenerate in the sense of having the same energy.

To separate the k_i degenerate copies of each irrep Γ_i, it is helpful first to decompose each space $\mathcal{V}^{(\Gamma_i,s)}$ into sectors associated with the individual rows μ of the irrep Γ_i as $\mathcal{V}^{(\Gamma_i,s)} = \bigoplus_\mu \mathcal{V}_\mu^{(\Gamma_i,s)}$. Any set of k_i linearly independent vectors in $\mathcal{V}_\mu^{(\Gamma_i,s)}$, which can be labeled as

$$\{|s,\Gamma_i,\kappa,\mu\rangle : \kappa \in \{1,\ldots,k_i\}\}, \tag{24}$$

provide a basis for this space,

$$\mathcal{V}_\mu^{(\Gamma_i,s)} = \text{span}\{|s,\Gamma_i,\kappa,\mu\rangle : \kappa \in \{1,\ldots,k_i\}\}. \tag{25}$$

If a consistent set of k_i basis vectors is chosen for all μ, the transformation properties of the basis vectors follow from Eq. (21),

$$\mathcal{D}(R)|s,\Gamma_i,\kappa,\mu\rangle = \sum_{\mu'} |s,\Gamma_i,\kappa,\mu'\rangle D_{\mu'\mu}^{(\Gamma_i)}(R), \tag{26}$$

where the irrep matrices $D_{\mu'\mu}^{(\Gamma_i)}(R)$ for $R \in G_{\boldsymbol{P}}$ are defined as described in Sec. II B. The explicit construction of such a basis is detailed below. Note that the labeling of degenerate copies of irreps by κ is not unambiguously specified. A particular choice will be made in the following construction.

The unitary matrix $U^{(s)}$ that transforms from the reducible momentum-orbit basis $\{|s,m\rangle\}$ to the irrep basis $\{|s,\Gamma_i,\kappa,\mu\rangle\}$ is defined by its elements

$$\mathrm{U}_{m\mu}^{(\Gamma_i,\kappa,s)} \equiv \langle s,m|s,\Gamma_i,\kappa,\mu\rangle, \tag{27}$$

where $\kappa \in \{1,\ldots,k_i\}$, $\mu \in \{1,\ldots,|\Gamma_i|\}$, and the total momentum $\boldsymbol{P}$ is left implicit. In particular, these matrices enact the block diagonalization anticipated by Eq. (1),

$$D_{\mu\mu'}^{(\Gamma_i)}(R) = \sum_{m,m'} [U_{m\mu}^{(\Gamma_i,\kappa,s)}]^* D_{mm'}^{(s)}(R) U_{m'\mu'}^{(\Gamma_i,\kappa,s)} \tag{28}$$

$$= ([\mathrm{U}^{(s)}]^\dagger D^{(s)}(R) \mathrm{U}^{(s)})_{\mu\mu'}. \tag{29}$$

Although the labels Γ_i and κ appear as superscripts labeling the choice of irrep, $U^{(s)}$ is indeed a unitary $|K_{\boldsymbol{P}}^{(s)}| \times |K_{\boldsymbol{P}}^{(s)}|$ matrix if m is taken as a row index and the indices Γ_i, κ, and μ are enumerated jointly as a column index.

The change-of-basis matrix $U^{(s)}$ for each momentum orbit can be constructed explicitly using Schur's lemma, which says[6]

$$\frac{|\Gamma|}{|G_{\boldsymbol{P}}|} \sum_{R \in G_{\boldsymbol{P}}} D_{\mu\nu}^{(\Gamma)}(R)^* D_{\mu'\nu'}^{(\Gamma')}(R) = \delta_{\Gamma\Gamma'}\delta_{\mu\mu'}\delta_{\nu\nu'} \tag{30}$$

[6]Written in this form, Schur's lemma is sometimes referred to as the wonderful orthogonality theorem [9].

for arbitrary irreps Γ and Γ'. For each irrep Γ_i of the little group $G_{\boldsymbol{P}}$, it is convenient to define a projection operator

$$\Pi_\mu^{(\Gamma_i,s)}:\ \mathcal{V}_{\boldsymbol{P}}^{(s)} \to \mathcal{V}_\mu^{(\Gamma_i,s)}, \tag{31}$$

$$\Pi_\mu^{(\Gamma_i,s)} \equiv \frac{|\Gamma_i|}{|G_{\boldsymbol{P}}|} \sum_{R\in G_{\boldsymbol{P}}} D_{\mu\mu}^{(\Gamma_i)}(R)^* \mathcal{D}(R), \tag{32}$$

with no sum on μ implied and with matrix elements

$$(\Pi_\mu^{(\Gamma_i,s)})_{m'm} = \langle s,m'|\Pi_\mu^{(\Gamma_i,s)}|s,m\rangle \tag{33}$$

$$= \frac{|\Gamma_i|}{|G_{\boldsymbol{P}}|} \sum_{R\in G_{\boldsymbol{P}}} D_{\mu\mu}^{(\Gamma_i)}(R)^* D_{m'm}^{(s)}(R). \tag{34}$$

This projector onto a given row μ of the irrep Γ_i is closely related to the desired change-of-basis matrices:

$$(\Pi_\mu^{(\Gamma_i,s)})_{m'm} = \sum_{\kappa=1}^{k_i} \langle s,m'|s,\Gamma_i,\kappa,\mu\rangle\langle s,\Gamma_i,\kappa,\mu|s,m\rangle \tag{35}$$

$$= \sum_{\kappa=1}^{k_i} \mathrm{U}_{m'\mu}^{(\Gamma_i,\kappa,s)} [\mathrm{U}_{m\mu}^{(\Gamma_i,\kappa,s)}]^*. \tag{36}$$

The first equality follows from Schur's lemma after insertions of the identity, $\mathbb{1} = \sum_{\Gamma,\kappa,\mu} |s,\Gamma,\kappa,\mu\rangle\langle s,\Gamma,\kappa,\mu|$. By unitarity of the change-of-basis matrices, the projection operators $\Pi_\mu^{(\Gamma_i,s)}$ are idempotent.

The change-of-basis matrix elements $U_{m\mu}^{(\Gamma_i,\kappa,s)}$ can be extracted by suitable orthogonalization of the rows of $(\Pi_\mu^{(\Gamma_i,s)})_{m'm}$. The choice of an orthogonalization scheme, e.g., a Gram-Schmidt procedure, fixes the otherwise ambiguous κ labeling of degenerate copies of each irrep.

Degenerate copies must be orthogonalized consistently for all rows μ within each irrep in order to achieve the simple transformation rule in Eq. (26).[7] A natural prescription is first to orthonormalize the $\mu = 1$ rows within each irrep and then to use *transition operators* to move between the remaining rows. Schur's lemma applied to the off-diagonal elements of the rotational irrep matrices furnishes the transition operators,

$$T_{\mu\nu}^{(\Gamma_i,s)} \equiv \frac{|\Gamma_i|}{|G_{\boldsymbol{P}}|} \sum_{R\in G_{\boldsymbol{P}}} D_{\mu\nu}^{(\Gamma_i)}(R)^* \mathcal{D}(R), \tag{37}$$

$$(T_{\mu\nu}^{(\Gamma_i,s)})_{m'm} \equiv \frac{|\Gamma_i|}{|G_{\boldsymbol{P}}|} \sum_{R\in G_{\boldsymbol{P}}} D_{\mu\nu}^{(\Gamma_i)}(R)^* D_{m'm}^{(s)}(R), \tag{38}$$

$$= \sum_{\kappa=1}^{k_i} \mathrm{U}_{m'\mu}^{(\Gamma_i,\kappa,s)} [\mathrm{U}_{m\nu}^{(\Gamma_i,\kappa,s)}]^*. \tag{39}$$

By definition, $T_{\mu\mu}^{(\Gamma_i,s)} \equiv \Pi_\mu^{(\Gamma_i,s)}$. The transition operators are Hermitian, $[T_{\mu\nu}^{(\Gamma_i,s)}]^\dagger = T_{\nu\mu}^{(\Gamma_i,s)}$, and satisfy

$$\sum_{m'} (T_{\mu\nu}^{(\Gamma_i,s)})_{mm'} (T_{\rho\sigma}^{(\Gamma_i,s)})_{m'n} = \delta_{\nu\rho} (T_{\mu\sigma}^{(\Gamma_i,s)})_{mn}, \tag{40}$$

which follows from unitarity of the change-of-basis matrices. Likewise, it follows from Eq. (39) and unitarity of the change-of-basis matrices that the transition operators relate the different rows μ and ν,

$$\mathrm{U}_{m\mu}^{(\Gamma_i,\kappa,s)} = \sum_n (T_{\mu\nu}^{(\Gamma_i),s})_{mn} \mathrm{U}_{n\nu}^{(\Gamma_i,\kappa,s)}, \tag{41}$$

for fixed μ, ν, which allows all elements of the change-of-basis matrices to be determined once those with $\mu = 1$ are known.

D. Stabilizer subgroups

The block-diagonalization matrices for many different momentum orbits can be demonstrated to be identical using general arguments from group theory. The construction and ordering of a momentum orbit $K_{\boldsymbol{P}}^{(s)}$ are always performed in terms of a fiducial list of plane waves, with the associated set of wave vectors denoted by $\boldsymbol{i} \equiv [\boldsymbol{n}_1,\ldots,\boldsymbol{n}_N]$. The stabilizer subgroup of the little group $G_{\boldsymbol{P}}$ can then be defined as the subgroup of rotations $H_{\boldsymbol{P}}^{(s)} \le G_{\boldsymbol{P}}$ that leave $\boldsymbol{i}$ invariant. For any particular $\boldsymbol{i}$, the stabilizer is easily identified by acting with all elements of the (finite) little group $G_{\boldsymbol{P}}$. By construction, each stabilizer subgroup is one of the finite groups listed after Eq. (10).

The orbit-stabilizer theorem then implies that elements of the momentum orbit are in one-to-one-correspondence with the left cosets of $H_{\boldsymbol{P}}^{(s)}$ [19],

$$K_{\boldsymbol{P}}^{(s)} = \{R\cdot\boldsymbol{i} : R\in G_{\boldsymbol{P}}\} \leftrightarrow \{R_j H_{\boldsymbol{P}}^{(s)} : j\in\{1,2,\ldots|K_{\boldsymbol{P}}^{(s)}|\}\}, \tag{42}$$

because the rotations in each coset map the fiducial arrangement $\boldsymbol{i}$ to a single, unique element in $K_{\boldsymbol{P}}^{(s)}$. In Eq. (42), the jth coset is defined as $R_j H_{\boldsymbol{P}}^{(s)} \equiv \{R_j h : h\in H_{\boldsymbol{P}}^{(s)}\}$ where $R_j \in G_{\boldsymbol{P}}$ is a representative element of the coset. Acting from the left

[7] For example, applying the Gram–Schmidt procedure to each row of $(\Pi_\mu^{(\Gamma_i,s)})_{m'm}$ independently would lead to a more cumbersome transformation rule in which states $|s,\Gamma,\kappa,\mu\rangle$ are mapped by the action of $R\in G_{\boldsymbol{P}}$ to linear combinations of states $|s,\Gamma,\kappa',\mu'\rangle$ including those with $\kappa' \ne \kappa$. The coefficients of these linear combinations would need to be computed separately for each momentum orbit and would generically depend upon s, κ, and κ' as well as Γ, μ, and μ'.

with a group element R' permutes the cosets on the right of Eq. (42) in the same way as the states on the left of Eq. (42). Once $H_{\boldsymbol{P}}^{(s)}$ is determined from $\boldsymbol{i}$, the full structure of the momentum orbit is encoded in the right-hand side and the details of the fiducial state $\boldsymbol{i}$ no longer matter. This means that if two distinct momentum orbits, labeled by s and s', share the same little group $G_{\boldsymbol{P}}$ and stabilizer group $H_{\boldsymbol{P}}^{(s)} = H_{\boldsymbol{P}}^{(s')}$, they transform identically under $G_{\boldsymbol{P}}$, i.e.,

$$D_{m'm}^{(s)}(R) = D_{m'm}^{(s')}(R) \tag{43}$$

for all $m, m' \in \{1, \ldots, |K_{\boldsymbol{P}}^{(s)}|\}$ and each element $R \in G_{\boldsymbol{P}}$. As such, the block diagonalization to irreps of the cubic group can also be achieved with the same set of matrices.

Conjugating $H_{\boldsymbol{P}}^{(s)}$ by some element $R \in G_{\boldsymbol{P}}$, $H_{\boldsymbol{P}}^{(s)} \to R^{-1} H_{\boldsymbol{P}}^{(s)} R$, is equivalent to rotating the basis states to pick a different fiducial state in the same orbit, which amounts to reordering the basis states. This means that irrep decompositions need only be performed for one subgroup within each conjugacy class of subgroups of $G_{\boldsymbol{P}}$. The block-diagonalization matrices for other subgroups in the same class are related by reordering the columns.

When all operators are distinguishable, the structure of the stabilizer group $H_{\boldsymbol{P}}^{(s)}$ is also severely restricted. The stabilizer group $H_{\boldsymbol{P}}^{(s)}$ associated with products of N distinguishable operators must be the intersection of a set of individual little groups $G_{\boldsymbol{P}_1}, \ldots G_{\boldsymbol{P}_N} \subset O_h$, where each $G_{\boldsymbol{P}_j}$ is the little group of the wave vector of the jth operator. These intersections can be shown to give other—identical or smaller—finite groups in every case. Cataloging all two-operator cases, for which all of the finite groups listed after Eq. (10) appear as stabilizer groups, thus already determines the wave functions for all possible distinguishable-particle operators. For cases with $N > 2$ operators, identifying the stabilizer group $H_{\boldsymbol{P}}^{(s)}$ allows one to select the appropriate block-diagonalization matrices already constructed from specific examples in the two-operator case. The fact that two-operator cases already give rise to all possible change-of-basis matrices is specific to the case of distinguishable spin-zero operators and does not hold in the cases of nonzero spin; however, analogous stabilizer group considerations still restrict the distinct change-of-basis matrices to a finite number once the spin and permutation properties of all operators are specified, as described in Secs. III and IV below.

E. Complete classification for N distinguishable spin-zero particles

As discussed in Sec. II D, for distinguishable spin-zero particles, solving the block-diagonalization problem for two operators in fact solves the generic N-operator problem. Solution of the two-operator problem is divided into two steps:

(1) Enumerate the little groups and stabilizer groups associated with all possible two-body momenta.
(2) Compute the block-diagonalization matrices $U^{(s)}$ in each case [cf. Eq. (1)].

The remainder of this section classifies possible two-body momentum configurations and their associated little groups and stabilizers. The results of this classification are summarized in Table II. The block-diagonalization matrices $U^{(s)}$ can be computed using the method described in Sec. II C. Subsets of these results have previously been presented in Refs. [13,14].

1. Rest-frame systems

In the rest frame, all seven conjugacy classes of little groups can act as stabilizer subgroups $H_{\boldsymbol{P}}^{(s)}$ within the total symmetry group O_h. The stabilizer subgroups and representative choices of rest-frame momenta $[\boldsymbol{n}]$ or $[\boldsymbol{n}_1, \boldsymbol{n}_2]$ corresponding to $N \in \{1, 2\}$ distinguishable particles stabilized by the group are given by:

(i) $H_{\boldsymbol{P}}^{(s)} = O_h$: $[\boldsymbol{n}] = [(0,0,0)]$
(ii) $H_{\boldsymbol{P}}^{(s)} = C_{4v}$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,0,n), (0,0,-n)]$
(iii) $H_{\boldsymbol{P}}^{(s)} = C_{3v}$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(n,n,n), (-n,-n,-n)]$
(iv) $H_{\boldsymbol{P}}^{(s)} = C_{2v}$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,n,n), (0,-n,-n)]$
(v) $H_{\boldsymbol{P}}^{(s)} = C_2^R$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,m,n), (0,-m,-n)]$
(vi) $H_{\boldsymbol{P}}^{(s)} = C_2^P$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(m,n,n), (-m,-n,-n)]$
(vii) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(m,l,n), (-m,-l,-n)]$.

Examples of explicit block-diagonalization matrices for rest-frame systems are tabulated in Appendix C, following the conventions described in Appendix A.

2. Boosted systems

Boosted systems can be analyzed similarly to rest-frame systems. First, one identifies for each little group $G_{\boldsymbol{P}}$ a representative total momentum $\boldsymbol{P}$. Second, one identifies all (conjugacy classes of) subgroups $H_{\boldsymbol{P}}^{(s)}$ of the little group $G_{\boldsymbol{P}}$ which are compatible with stabilizing a set of plane waves. Representative examples for all valid choices of $G_{\boldsymbol{P}}$ and $H_{\boldsymbol{P}}^{(s)}$ can be chosen as follows:

(1) $G_{\boldsymbol{P}} = C_{4v}$: $\boldsymbol{P} = \frac{2\pi}{L}(0,0,n)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_{4v}$: $[\boldsymbol{n}] = [(0,0,n)]$
  (b) $H_{\boldsymbol{P}}^{(s)} = C_2^R$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,m,n), (0,-m,0)]$
  Note that C_2^R appears in noncanonical form here as the set of reflections of the x axis.
  (c) $H_{\boldsymbol{P}}^{(s)} = C_2^P$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(m,m,n), (-m,-m,0)]$
  (d) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(m,l,n), (-m,-l,0)]$,
(2) $G_{\boldsymbol{P}} = C_{3v}$: $\boldsymbol{P} = \frac{2\pi}{L}(n,n,n)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_{3v}$: $[\boldsymbol{n}] = [(n,n,n)]$
  (b) $H_{\boldsymbol{P}}^{(s)} = C_2^P$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(n,n,0), (0,0,n)]$
  (c) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(n+m,n,0), (-m,0,n)]$,

TABLE II. The complete solution to the N-body block diagonalization problem for distinguishable spin-zero operators. The solution follows from classifying the possible combinations of little groups $G_{\boldsymbol{P}}$ and stabilizers $H_{\boldsymbol{P}}^{(s)}$ arising in the two-body case. Example states are denoted by $|\pi(\boldsymbol{n}_1), K(\boldsymbol{n}_2)\rangle$, as πK operator construction provides a simple example of two distinguishable, spin-zero operators.

$G_{\boldsymbol{P}}$	$H_{\boldsymbol{P}}^{(s)}$	Example state	Orbit dim	Irrep decomposition
O_h	O_h	$\|\pi(0,0,0), K(0,0,0)\rangle$	1	A_1^+
O_h	C_{4v}	$\|\pi(0,0,1), K(0,0,-1)\rangle$	6	$A_1^+ \oplus E^+ \oplus T_1^-$
O_h	C_{2v}	$\|\pi(0,1,1), K(0,-1,-1)\rangle$	12	$A_1^+ \oplus E^+ \oplus T_2^+ \oplus T_1^- \oplus T_2^-$
O_h	C_2^R	$\|\pi(2,1,0), K(-2,-1,0)\rangle$	24	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus T_1^+ \oplus T_2^+ \oplus 2T_1^- \oplus 2T_2^-$
O_h	C_{3v}	$\|\pi(1,1,1), K(-1,-1,-1)\rangle$	8	$A_1^+ \oplus T_2^+ \oplus A_2^- \oplus T_1^-$
O_h	C_2^P	$\|\pi(1,1,2), K(-1,-1,-2)\rangle$	24	$A_1^+ \oplus E^+ \oplus T_1^+ \oplus 2T_2^+ \oplus A_2^- \oplus E^- \oplus 2T_1^- \oplus T_2^-$
O_h	C_1	$\|\pi(3,2,1), K(-3,-2,-1)\rangle$	48	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus 3T_1^+ \oplus 3T_2^+ \oplus A_1^- \oplus A_2^- \oplus 2E^- \oplus 3T_1^- \oplus 3T_2^-$
C_{4v}	C_{4v}	$\|\pi(0,0,1), K(0,0,0)\rangle$	1	A_1
C_{4v}	C_2^R	$\|\pi(1,0,1), K(-1,0,0)\rangle$	4	$A_1 \oplus B_1 \oplus E$
C_{4v}	C_2^P	$\|\pi(1,1,1), K(-1,-1,0)\rangle$	4	$A_1 \oplus B_2 \oplus E$
C_{4v}	C_1	$\|\pi(2,1,1), K(-2,-1,0)\rangle$	8	$A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus 2E$
C_{3v}	C_{3v}	$\|\pi(1,1,1), K(0,0,0)\rangle$	1	A_1
C_{3v}	C_2^P	$\|\pi(1,1,0), K(0,0,1)\rangle$	3	$A_1 \oplus E$
C_{3v}	C_1	$\|\pi(1,0,-1), K(0,1,2)\rangle$	6	$A_1 \oplus A_2 \oplus 2E$
C_{2v}	C_{2v}	$\|\pi(0,1,1), K(0,0,0)\rangle$	1	A_1
C_{2v}	C_2^R	$\|\pi(0,0,1), K(0,1,0)\rangle$	2	$A_1 \oplus B_2$
C_{2v}	C_2^P	$\|\pi(2,1,1), K(-2,0,0)\rangle$	2	$A_1 \oplus B_1$
C_{2v}	C_1	$\|\pi(-2,0,1), K(2,1,0)\rangle$	4	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$
C_2^R	C_2^R	$\|\pi(1,2,0), K(0,0,0)\rangle$	1	A
C_2^R	C_1	$\|\pi(1,0,1), K(0,2,-1)\rangle$	2	$A \oplus B$
C_2^P	C_2^P	$\|\pi(1,2,2), K(0,0,0)\rangle$	1	A
C_2^P	C_1	$\|\pi(1,0,0), K(0,1,2)\rangle$	2	$A \oplus B$
C_1	C_1	$\|\pi(1,2,3), K(0,0,0)\rangle$	1	A_1

(3) $G_{\boldsymbol{P}} = C_{2v}$: $\boldsymbol{P} = \frac{2\pi}{L}(0,n,n)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_{2v}$: $[\boldsymbol{n}] = [(0,n,n)]$
  (b) $H_{\boldsymbol{P}}^{(s)} = C_2^R$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(0,0,n),(0,n,0)]$
  (c) $H_{\boldsymbol{P}}^{(s)} = C_2^P$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(-m,n,n),(m,0,0)]$
  (d) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(-m,0,n),(m,n,0)]$,
(4) $G_{\boldsymbol{P}} = C_2^R$: $\boldsymbol{P} = \frac{2\pi}{L}(n,m,0)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_2^R$: $[\boldsymbol{n}_1] = [(n,m,0)]$
  (b) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(n,0,l),(0,m,-l)]$,
(5) $G_{\boldsymbol{P}} = C_2^P$: $\boldsymbol{P} = \frac{2\pi}{L}(n,n,m)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_2^P$: $[\boldsymbol{n}_1] = [(n,n,m)]$
  (b) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[\boldsymbol{n}_1, \boldsymbol{n}_2] = [(n,0,0),(0,n,m)]$,
(6) $G_{\boldsymbol{P}} = C_1$: $\boldsymbol{P} = \frac{2\pi}{L}(n,m,p)$
  (a) $H_{\boldsymbol{P}}^{(s)} = C_1$: $[(n,m,p)]$.

III. OPERATORS WITH SPIN

This section extends the discussion of the previous section to operators with nonzero spin. Since operators with half-integer spin transform in representations of SU(2) (the double cover of SO(3)) instead of SO(3) in an unbounded, continuous three-dimensional space, nonzero spin introduces the complication that the relevant symmetry group in a cubic lattice is O_h^D (the double cover of O_h), rather than O_h. Consequently, the procedures discussed above must be generalized. The approach taken here is to decompose operators into irreps of the cubic group (and its double cover) using the projection method applied to the full momentum-spin space.[8]

Extended operators involving fields evaluated at multiple lattice sites can also have nontrivial "internal" cubic transformation properties in addition to the transformation of the coordinate $\boldsymbol{x}_i$ of each operator. The same formalism presented in this section for particles with spin can be applied to the case of extended operators with such properties by replacing spinor representation matrices with

[8]An alternative approach for incorporating spin, not pursued in this work, would treat the group representation as a tensor product of the representation under transformation of the spatial coordinates $\boldsymbol{x}_i$ and the internal spin representations. The spatial representation associated with N coordinates can be decomposed as above. The problem then reduces to decomposing tensor products of the rotational-symmetry irreps with the spin representations of each operator. Computation of the Clebsch–Gordan coefficients required for this strategy is straightforward [20], and this approach has been used in practice for constructing two-nucleon operators [14]. However, a drawback is that the number of tensor products grows rapidly with the number of operators included. The number of terms in, and complexity of, the resulting block-diagonalization matrices also grow rapidly with the number of operators.

the appropriate representation matrices for such extended operators.

The remainder of this section is organized as follows. Section III A discusses the irreps of the double-cover group O_h^D. Section III B discusses the transformation properties of typical spinor operators. Section III C describes the construction of representation matrices associated with momentum-spin orbits. Section III D presents several examples of irrep decompositions for distinguishable operators with nonzero spin.

A. Double-cover irreps and basis vectors

For bosonic irreps, the irreps of O_h immediately furnish irreps of O_h^D (see Appendix A for a concrete specification of O_h^D). The key observation is that 2π rotations act trivially on states in bosonic irreps. Therefore, the O_h^D-irrep matrices for group elements differing by rotations of 2π can be identified with the relevant O_h-irrep matrix.

For fermionic irreps, note first that the Dirac spinor representation used to define the group O_h^D is a reducible representation that can be decomposed into a two-dimensional positive-parity irrep G_1^+ and a two-dimensional negative-parity irrep G_1^- of O_h^D. By convention, the Dirac spinor representation is defined in the parity eigenbasis, known as the Dirac-Pauli basis, with explicit basis states given by

$$\begin{aligned}
|1/2,+1/2,+\rangle &= (1\ \ 0\ \ 0\ \ 0)^T,\\
|1/2,-1/2,+\rangle &= (0\ \ 1\ \ 0\ \ 0)^T,\\
|1/2,-1/2,-\rangle &= (0\ \ 0\ \ 1\ \ 0)^T,\\
|1/2,+1/2,-\rangle &= (0\ \ 0\ \ 0\ \ 1)^T.
\end{aligned} \tag{44}$$

where the basis states are labeled as $|J, J_z, \pm\rangle$ in terms of their eigenvalues of total spin J, the spin z-projection J_z, and parity. These basic irreps can be used to construct the full set of fermionic irreps. Concrete basis vectors for the irreps of O_h^D and relevant subgroups are given in terms of these spin–1/2 and higher-spin basis states in Table III. Higher-spin vectors appearing in Table III are constructed in the usual way, e.g., $|\frac{3}{2},\frac{3}{2},\pm\rangle$ follows from the tensor product of three spin-$\frac{1}{2}$ vectors. Additional details related to the choice of basis vectors are given in Appendix A.

TABLE III. Basis vectors used in this work for the fermionic irreps of the double-cover group O_h^D and its subgroups. As discussed in the main text, bosonic irreps of O_h^D follow immediately from those of O_h given in Table I. The basis vectors are identical to those used in Ref. [11], and they lead to identical representation matrices to those in Ref. [15] for all fermionic irreps.

Group	Irrep	μ	Basis vector
O_h^D	$G_1^\pm$	1	$\|1/2,+1/2,\pm\rangle$
O_h^D	$G_1^\pm$	2	$\|1/2,-1/2,\pm\rangle$
O_h^D	$H^\pm$	1	$\|3/2,+3/2,\pm\rangle$
O_h^D	$H^\pm$	2	$\|3/2,+1/2,\pm\rangle$
O_h^D	$H^\pm$	3	$\|3/2,-1/2,\pm\rangle$
O_h^D	$H^\pm$	4	$\|3/2,-3/2,\pm\rangle$
O_h^D	$G_2^\pm$	1	$\sqrt{1/6}\|5/2,-5/2,\pm\rangle - \sqrt{5/6}\|5/2,+3/2,\pm\rangle$
O_h^D	$G_2^\pm$	2	$\sqrt{1/6}\|5/2,+5/2,\pm\rangle - \sqrt{5/6}\|5/2,-3/2,\pm\rangle$
Dic_4	G_1	1	$\|1/2,+1/2,+\rangle$
Dic_4	G_1	2	$\|1/2,-1/2,+\rangle$
Dic_4	G_2	1	$\sqrt{1/6}\|5/2,-5/2,+\rangle - \sqrt{5/6}\|5/2,+3/2,+\rangle$
Dic_4	G_2	2	$\sqrt{1/6}\|5/2,+5/2,+\rangle - \sqrt{5/6}\|5/2,-3/2,+\rangle$
Dic_3	G	1	$\|1/2,+1/2,+\rangle$
Dic_3	G	2	$\|1/2,-1/2,+\rangle$
Dic_3	F_1	1	Eq. (A12)
Dic_3	F_2	2	Eq. (A13)
Dic_2	G	1	$\|1/2,+1/2,+\rangle$
Dic_2	G	2	$\|1/2,-1/2,+\rangle$
C_4^R	F_1	1	$\|1/2,+1/2,+\rangle$
C_4^R	F_2	1	$\|1/2,-1/2,+\rangle$
C_4^P	F_1	1	$\sqrt{1/2}\|1/2,1/2,+\rangle + (1-i)/2\|1/2,-1/2,+\rangle$
C_4^P	F_2	1	$\sqrt{1/2}\|1/2,1/2,+\rangle - (1-i)/2\|1/2,-1/2,+\rangle$
C_1^D	F	1	$\|1/2,1/2,+\rangle$

B. Operator representations

Having defined the double-cover group structure and irreps for O_h^D and its little groups, it is useful to record the transformation properties of typical spinor interpolating operators.

Creation and annihilation operators for spin-1/2 particles, denoted $\bar{\psi}(\boldsymbol{x})$ and $\psi(\boldsymbol{x})$ respectively, transform as the spinor representation and its conjugate:

$$\begin{aligned}\hat{U}(R^D)\bar{\psi}(\boldsymbol{x})_\alpha\hat{U}^\dagger(R^D) &= \sum_\beta \bar{\psi}_\beta(R\boldsymbol{x})S_{\beta\alpha}(R^D),\\ \hat{U}(R^D)\psi(\boldsymbol{x})_\alpha\hat{U}^\dagger(R^D) &= \sum_\beta \psi_\beta(R\boldsymbol{x})S_{\beta\alpha}(R^D)^*.\end{aligned} \tag{45}$$

Here $\hat{U}(R^D)$ indicates the quantum operator that implements the O_h^D transformation R^D and $S(R^D)$ is the spinor representation matrix associated with the group element R^D,

$$S(R^D) \equiv R^D \in O_h^D, \tag{46}$$

since this is the defining representation.

Since products of $\bar{\psi}_\alpha(\boldsymbol{x})$ operators act on the vacuum to create single- and multiparticle states, the same transformation rule for $\bar{\psi}_\alpha(\boldsymbol{x})$ operators is chosen as for irrep basis vectors in Eq. (21). Spinor operators with larger spin (e.g., spin 3/2) can be constructed using tensor products of spin-1/2 operators.

With these conventions, one readily confirms the invariance of the usual kinetic terms of the Hamiltonian for free relativistic spin-1/2 fermions, $H_\psi = \int d^3\boldsymbol{x} \times \sum_j \bar{\psi}(\boldsymbol{x})\gamma^j\partial_j\psi(\boldsymbol{x})$. This invariance also applies on a discrete spatial lattice under the subgroup O_h of all rotations, meaning these conventions are compatible with familiar Hamiltonians (or actions) appearing in practical calculations in lattice gauge theory.

These transformation properties lead to a natural generalization of the space of operators introduced in Sec. II. Operators with spin can be specified in various ways; the generalized algorithm defined in the following is insensitive to this choice. Particularly for products of local operators, one useful representation arises from constructing operators with definite total spin J under SU(2). In this case, besides wave numbers $\boldsymbol{n}_i$ specifying the momenta, the extended space is defined by the total spin J, spin component J_z, and intrinsic parity $\pm$. Given the operator transformation rules above, these states transform as

$$\mathcal{D}(R)|\boldsymbol{n}, J, J_z, \pm\rangle = \sum_{J_z'=-J}^{J} |R\boldsymbol{n}, J, J_z', \pm\rangle D^{[J]}_{J_z', J_z}(R^D), \tag{47}$$

where $D^{[J]}(R^D)$ is the appropriate representation matrix for the spin-J operator. In general, one could choose operators in any reducible or irreducible representation of the little group instead of those defined by continuum spin J. Though most of the O_h^D irreps coincide with the $|J, J_z, \pm\rangle$ basis states, for large-J states and extended operators, the O_h^D representation is typically reducible.

C. Momentum-spin orbits and their representations

For operators with spin, the notion of a momentum orbit from Sec. II A is extended to a combined momentum-spin orbit. Because the spatial coordinates and spin degrees of freedom transform in distinct spaces, the combined orbit belongs to their tensor product. The spin portion of the orbit can itself be understood as the tensor product of the individual spin-J_1 through spin-J_N basis states. In other words, the extended *momentum-spin orbit* can be written as

$$\begin{aligned}\tilde{K}^{(s)}_{\boldsymbol{P}} &\equiv \{R^D\cdot[\boldsymbol{n}_1,\alpha_1\ldots,\boldsymbol{n}_N,\alpha_N] : R^D \in G^D_{\boldsymbol{P}}\}\}\\ &= \{[\boldsymbol{n}_1,\alpha_1\ldots,\boldsymbol{n}_N,\alpha_N]^{(s)}_m : m\in\{1,2,\ldots,|\tilde{K}^{(s)}_{\boldsymbol{P}}|\}\},\end{aligned} \tag{48}$$

where the α_i contain the spin and parity quantum numbers. As above, elements within this orbit are indexed by the integer label m. The value for α_i of the mth element in the orbit will be denoted $\alpha_i^{[m]}$. The dimension of the momentum-spin orbit, $|\tilde{K}^{(s)}_{\boldsymbol{p}}|$, is given by the product of the dimension of the momentum orbit with the dimensions of the individual spin representations $|J_i| = 2J_i + 1$, i.e.,

$$|\tilde{K}^{(s)}_{\boldsymbol{p}}| = |K^{(s)}_{\boldsymbol{p}}| \times \prod_{i=1}^{N} |J_i|. \tag{49}$$

Once the momentum-spin orbit has been constructed, the representation matrices $\tilde{D}^{(s)}_{m'm}(R^D)$ follow using the analog of Eq. (18) as matrix elements, labeled by m' and m, between states of the momentum-spin operators. For the case of N spin-1/2 operators, these matrix elements are explicitly given by

$$\begin{aligned}\tilde{D}^{(s)}_{m'm}(R^D) &\equiv \langle[\boldsymbol{n}_1,\alpha_1,\ldots,\boldsymbol{n}_N,\alpha_N]_{m'}\\ &\quad\times|\mathcal{D}(R^D)|[\boldsymbol{n}_1,\alpha_1,\ldots,\boldsymbol{n}_N,\alpha_N]_m\rangle.\\ &= \langle[\boldsymbol{n}_1,\ldots,\boldsymbol{n}_N]_{m'}|\mathcal{D}(R)|[\boldsymbol{n}_1,\ldots,\boldsymbol{n}_N]_m\rangle\\ &\quad\times\langle\alpha_1^{[m']}|\mathcal{D}(R^D)|\alpha_1^{[m]}\rangle\ldots\langle\alpha_N^{[m']}|\mathcal{D}(R^D)|\alpha_N^{[m]}\rangle\\ &= D^{(s)}_{m'm}(R)S_{\alpha_1^{[m']}\alpha_1^{[m]}}(R^D)\cdots S_{\alpha_N^{[m']}\alpha_N^{[m]}}(R^D),\end{aligned} \tag{50}$$

where $S(R^D)$ denotes the spinor representation matrices defined in Eq. (46) and R denotes the restriction of R^D to O_h. Expressions involving a mixture of spin-0 and spin-1/2 operators are obtained simply by removing spin labels α_i from spin-0 states and removing the corresponding transformation factors of $S(R^D)$.

For operators (e.g., spin-J operators or operators describing spatially extended objects) in a generic representation $\tilde{\Gamma}$

of the little group, the associated representation matrices are denoted $D^{[\tilde{\Gamma}]}_{\alpha\beta}(R^D)$, with $\alpha,\beta \in \{1,2,\ldots|\tilde{\Gamma}|\}$. Given these representations for the individual operator transformations, products of N such plane-wave operators transform with

$$\tilde{D}^{(s)}_{m'm}(R^D) = D^{(s)}_{m'm}(R) D^{[\tilde{\Gamma}_1]}_{\alpha_1^{[m']}\alpha_1^{[m]}}(R^D)\cdots D^{[\tilde{\Gamma}_N]}_{\alpha_N^{[m']}\alpha_N^{[m]}}(R^D). \quad (51)$$

Once the representation matrices $\tilde{D}^{(s)}_{m'm}(R^D)$ are determined, precisely the same steps described in Sec. II are used to determine block-diagonalization matrices of Eq. (1): project against the irrep matrices $D^{(\Gamma)}_{\mu'\mu}(R^D)$ using Schur's lemma, orthogonalize degenerate irreps, and fill out the remaining rows using the transition operators $T^{(\Gamma,s)}_{\mu\nu}$.

D. Examples

Unlike the spin-zero case, the irrep decompositions for products of N plane-wave operators with nonzero spin depend on the spins of the operators and cannot be cataloged completely in terms of two-body results. For a given set of spins, however, the irrep decompositions that can arise are severely restricted and can be fully classified for each of the little groups $G^D_{\boldsymbol{P}}$ and stabilizer groups $H^{D(s)}_{\boldsymbol{P}}$, where $G^D_{\boldsymbol{P}} \leq O^D_h$ and $H^{D(s)}_{\boldsymbol{P}} \leq G^D_{\boldsymbol{P}}$ indicate the little group and stabilizer group constructed from the momenta as before, now within the double cover group O^D_h. The possible $G^D_{\boldsymbol{P}}$ and $H^{D(s)}_{\boldsymbol{P}}$ can then be enumerated, and their irrep decompositions and block-diagonalization matrices can be tabulated analogously to the case of N spin-zero plane-wave operators. This section collects several explicit examples of phenomenologically relevant systems described by products of operators with nonzero spin and presents the irrep decompositions that arise during their block diagonalization. Explicit change-of-basis matrices are constructed in the accompanying code package [18].

1. np

The np system provides an example of a system with the quantum numbers of two distinguishable spin-$\frac{1}{2}$ particles. The cubic irreps of the n and p operators both correspond to G_1^+. Consideration of isospin will be deferred until discussion of internal symmetry groups in Sec. IV.

Table IV classifies the different orbit patterns in terms of little groups and stabilizer groups and shows the associated irrep decompositions of np, extending the results presented in Ref. [14]. Several general features arising in decompositions for operators with nonzero spin are illustrated by this example. In particular, the orbit dimensions are four times larger than in the spin-zero case because the two-nucleon spin space ($\frac{1}{2}\otimes\frac{1}{2} = 0\oplus 1$) has dimension four. Different patterns of irreps arise for np than for the case of distinguishable spin-zero particles.

2. pπ+

The $p\pi^+$ system is an example of a fermionic system with distinguishable operators transforming in different

TABLE IV. Combinations of irreps arising in decompositions of np operator orbits. Details are as in Table II.

$G_{\boldsymbol{P}}$	$H^{(s)}_{\boldsymbol{P}}$	Example state	Orbit dim	Irrep decomposition
O_h	O_h	$\lvert n(0,0,0), p(0,0,0)\rangle$	4	$A_1^+ \oplus T_1^+$
O_h	C_{4v}	$\lvert n(0,0,1), p(0,0,-1)\rangle$	24	$A_1^+ \oplus E^+ \oplus 2T_1^+ \oplus T_2^+ \oplus A_1^- \oplus E^- \oplus 2T_1^- \oplus T_2^-$
O_h	C_{2v}	$\lvert n(0,1,1), p(0,-1,-1)\rangle$	48	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus 3T_1^+ \oplus 3T_2^+ \oplus A_1^- \oplus A_2^- \oplus 2E^- \oplus 3T_1^- \oplus 3T_2^-$
O_h	C_{3v}	$\lvert n(1,1,1), p(-1,-1,-1)\rangle$	32	$A_1^+ \oplus A_2^+ \oplus E^+ \oplus 2T_1^+ \oplus 2T_2^+ \oplus A_1^- \oplus A_2^- \oplus E^- \oplus 2T_1^- \oplus 2T_2^-$
O_h	C_2^R	$\lvert n(2,1,0), p(-2,-1,0)\rangle$	96	$2A_1^+ \oplus 2A_2^+ \oplus 4E^+ \oplus 6T_1^+ \oplus 6T_2^+ \oplus 2A_1^- \oplus 2A_2^- \oplus 4E^- \oplus 6T_1^- \oplus 6T_2^-$
O_h	C_2^P	$\lvert n(2,1,1), p(-2,-1,-1)\rangle$	96	$2A_1^+ \oplus 2A_2^+ \oplus 4E^+ \oplus 6T_1^+ \oplus 6T_2^+ \oplus 2A_1^- \oplus 2A_2^- \oplus 4E^- \oplus 6T_1^- \oplus 6T_2^-$
O_h	C_1	$\lvert n(3,2,1), p(-3,-2,-1)\rangle$	192	$4A_1^+ \oplus 4A_2^+ \oplus 8E^+ \oplus 12T_1^+ \oplus 12T_2^+ \oplus 4A_1^- \oplus 4A_2^- \oplus 8E^- \oplus 12T_1^- \oplus 12T_2^-$
C_{4v}	C_{4v}	$\lvert n(0,0,1), p(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus E$
C_{4v}	C_2^R	$\lvert n(1,0,1), p(-1,0,0)\rangle$	16	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2 \oplus 4E$
C_{4v}	C_2^P	$\lvert n(1,1,1), p(-1,-1,0)\rangle$	16	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2 \oplus 4E$
C_{4v}	C_1	$\lvert n(2,1,1), p(-2,-1,0)\rangle$	32	$4A_1 \oplus 4A_2 \oplus 4B_1 \oplus 4B_2 \oplus 8E$
C_{3v}	C_{3v}	$\lvert n(1,1,1), p(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus E$
C_{3v}	C_2^P	$\lvert n(1,1,0), p(0,0,1)\rangle$	12	$2A_1 \oplus 2A_2 \oplus 4E$
C_{3v}	C_1	$\lvert n(1,0,-1), p(0,1,2)\rangle$	24	$4A_1 \oplus 4A_2 \oplus 8E$
C_{2v}	C_{2v}	$\lvert n(0,1,1), p(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$
C_{2v}	C_2^R	$\lvert n(0,0,1), p(0,1,0)\rangle$	8	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2$
C_{2v}	C_2^P	$\lvert n(2,1,1), p(-2,0,0)\rangle$	8	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2$
C_{2v}	C_1	$\lvert n(-2,0,1), p(2,1,0)\rangle$	16	$4A_1 \oplus 4A_2 \oplus 4B_1 \oplus 4B_2$
C_2^R	C_2^R	$\lvert n(1,2,0), p(0,0,0)\rangle$	4	$2A \oplus 2B$
C_2^R	C_1	$\lvert n(1,0,1), p(0,2,-1)\rangle$	8	$4A \oplus 4B$
C_1	C_1	$\lvert n(1,2,3), p(0,0,0)\rangle$	4	$4A$

TABLE V. Combinations of irreps arising in decompositions of $p\pi^+$ operator orbits. Details are as in Table II.

G_P	$H_P^{(s)}$	Example state	Orbit dim	Irrep decomposition
O_h	O_h	$\lvert p(0,0,0),\pi^+(0,0,0)\rangle$	2	G_1^-
O_h	C_{4v}	$\lvert p(0,0,1),\pi^+(0,0,-1)\rangle$	12	$G_1^+ \oplus H^+ \oplus G_1^- \oplus H^-$
O_h	C_{2v}	$\lvert p(0,1,1),\pi^+(0,-1,-1)\rangle$	24	$G_1^+ \oplus G_2^+ \oplus 2H^+ \oplus G_1^- \oplus G_2^- \oplus 2H^-$
O_h	C_{3v}	$\lvert p(1,1,1),\pi^+(-1,-1,-1)\rangle$	16	$G_1^+ \oplus G_2^+ \oplus H^+ \oplus G_1^- \oplus G_2^- \oplus H^-$
O_h	C_2^R	$\lvert p(2,1,0),\pi^+(-2,-1,0)\rangle$	48	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 2G_1^- \oplus 2G_2^- \oplus 4H^-$
O_h	C_2^P	$\lvert p(2,1,1),\pi^+(-2,-1,-1)\rangle$	48	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 2G_1^- \oplus 2G_2^- \oplus 4H^-$
O_h	C_1	$\lvert p(3,2,1),\pi^+(-3,-2,-1)\rangle$	96	$4G_1^+ \oplus 4G_2^+ \oplus 8H^+ \oplus 4G_1^- \oplus 4G_2^- \oplus 8H^-$
C_{4v}	C_{4v}	$\lvert p(0,0,1),\pi^+(0,0,0)\rangle$	2	G_1
C_{4v}	C_2^R	$\lvert p(1,0,1),\pi^+(-1,0,0)\rangle$	8	$2G_1 \oplus 2G_2$
C_{4v}	C_2^P	$\lvert p(1,1,1),\pi^+(-1,-1,0)\rangle$	8	$2G_1 \oplus 2G_2$
C_{4v}	C_1	$\lvert p(2,1,1),\pi^+(-2,-1,0)\rangle$	16	$4G_1 \oplus 4G_2$
C_{3v}	C_{3v}	$\lvert p(1,1,1),\pi^+(0,0,0)\rangle$	2	G
C_{3v}	C_2^P	$\lvert p(1,1,0),\pi^+(0,0,1)\rangle$	6	$F_1 \oplus F_2 \oplus 2G$
C_{3v}	C_1	$\lvert p(1,0,-1),\pi^+(0,1,2)\rangle$	12	$2F_1 \oplus 2F_2 \oplus 4G$
C_{2v}	C_{2v}	$\lvert p(0,1,1),\pi^+(0,0,0)\rangle$	2	G
C_{2v}	C_2^R	$\lvert p(0,0,1),\pi^+(0,1,0)\rangle$	4	$2G$
C_{2v}	C_2^P	$\lvert p(2,1,1),\pi^+(-2,0,0)\rangle$	4	$2G$
C_{2v}	C_1	$\lvert p(-2,0,1),\pi^+(2,1,0)\rangle$	8	$4G$
C_2^R	C_2^R	$\lvert p(1,2,0),\pi^+(0,0,0)\rangle$	2	$F_1 \oplus F_2$
C_2^R	C_1	$\lvert p(1,0,1),\pi^+(0,2,-1)\rangle$	4	$2F_1 \oplus 2F_2$
C_1	C_1	$\lvert p(1,2,3),\pi^+(0,0,0)\rangle$	2	$2F$

TABLE VI. Combinations of irreps arising in decompositions of $p\pi^+\pi^0$ operator orbits. Details are as in Table II.

G_P	$H_P^{(s)}$	Example state	Orbit dim	Irrep decomposition
O_h	O_h	$\lvert p(0,0,0),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	G_1^+
O_h	C_{4v}	$\lvert p(0,0,1),\pi^+(0,0,-1),\pi^0(0,0,0)\rangle$	12	$G_1^+ \oplus H^+ \oplus G_1^- \oplus H^-$
O_h	C_{2v}	$\lvert p(0,1,1),\pi^+(0,-1,-1),\pi^0(0,0,0)\rangle$	24	$G_1^+ \oplus G_2^+ \oplus 2H^+ \oplus G_1^- \oplus G_2^- \oplus 2H^-$
O_h	C_{3v}	$\lvert p(1,1,1),\pi^+(-1,-1,-1),\pi^0(0,0,0)\rangle$	16	$G_1^+ \oplus G_2^+ \oplus H^+ \oplus G_1^- \oplus G_2^- \oplus H^-$
O_h	C_2^R	$\lvert p(2,1,0),\pi^+(-2,-1,0),\pi^0(0,0,0)\rangle$	48	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 2G_1^- \oplus 2G_2^- \oplus 4H^-$
O_h	C_2^P	$\lvert p(2,1,1),\pi^+(-2,-1,-1),\pi^0(0,0,0)\rangle$	48	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 2G_1^- \oplus 2G_2^- \oplus 4H^-$
O_h	C_1	$\lvert p(3,2,1),\pi^+(-3,-2,-1),\pi^0(0,0,0)\rangle$	96	$4G_1^+ \oplus 4G_2^+ \oplus 8H^+ \oplus 4G_1^- \oplus 4G_2^- \oplus 8H^-$
C_{4v}	C_{4v}	$\lvert p(0,0,1),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	G_1
C_{4v}	C_2^R	$\lvert p(1,0,1),\pi^+(-1,0,0),\pi^0(0,0,0)\rangle$	8	$2G_1 \oplus 2G_2$
C_{4v}	C_2^P	$\lvert p(1,1,1),\pi^+(-1,-1,0),\pi^0(0,0,0)\rangle$	8	$2G_1 \oplus 2G_2$
C_{4v}	C_1	$\lvert p(2,1,1),\pi^+(-2,-1,0),\pi^0(0,0,0)\rangle$	16	$4G_1 \oplus 4G_2$
C_{3v}	C_{3v}	$\lvert p(1,1,1),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	G
C_{3v}	C_2^P	$\lvert p(1,1,0),\pi^+(0,0,1),\pi^0(0,0,0)\rangle$	6	$F_1 \oplus F_2 \oplus 2G$
C_{3v}	C_1	$\lvert p(1,0,-1),\pi^+(0,1,2),\pi^0(0,0,0)\rangle$	12	$2F_1 \oplus 2F_2 \oplus 4G$
C_{2v}	C_{2v}	$\lvert p(0,1,1),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	G
C_{2v}	C_2^R	$\lvert p(0,0,1),\pi^+(0,1,0),\pi^0(0,0,0)\rangle$	4	$2G$
C_{2v}	C_2^P	$\lvert p(2,1,1),\pi^+(-2,0,0),\pi^0(0,0,0)\rangle$	4	$2G$
C_{2v}	C_1	$\lvert p(-2,0,1),\pi^+(2,1,0),\pi^0(0,0,0)\rangle$	8	$4G$
C_2	C_2	$\lvert p(1,2,0),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	$F_1 \oplus F_2$
C_2	C_1	$\lvert p(1,0,1),\pi^+(0,2,-1),\pi^0(0,0,0)\rangle$	4	$2F_1 \oplus 2F_2$
C_1	C_1	$\lvert p(1,2,3),\pi^+(0,0,0),\pi^0(0,0,0)\rangle$	2	$2F$

irreps. The operator spins in this example correspond to the G_1^+ irrep for the proton and the A_1^- irrep for the pion.

Table V shows the distinct irrep decompositions of $p\pi^+$ orbits, which are again classified by the corresponding little groups and stabilizer groups. This extends the results presented in Ref. [16]. The orbit dimensions are twice as large as in the spin-zero particle case because of the nucleon spin and can be decomposed into direct sums of fermionic irreps.

3. $p\pi^+\pi^0$

The $p\pi^+\pi^0$ system provides an example with more than two distinguishable operators and nonzero spin. States with definite isospin ($I \in \{\frac{1}{2}, \frac{3}{2}\}$) involve linear combinations with $n\pi^+\pi^+$ operators and can be treated using the methods of Sec. IV below.

Table VI shows the irrep decomposition of $p\pi^+\pi^0$ orbits classified by the corresponding little groups and stabilizer groups. The patterns of little groups and stabilizer groups occurring are identical to those in Table V. The only difference in the irreps appearing in the $p\pi^+$ and $p\pi^+\pi^0$ decompositions is for the case of all operators at rest, which for $p\pi^+$ corresponds to G_1^- but for $p\pi^+\pi^0$ corresponds to G_1^+.

IV. INTERNAL SYMMETRIES AND IDENTICAL PARTICLES

In addition to the rotational transformation properties discussed so far, physical states also carry quantum numbers such as charge and flavor. Moreover, for states including identical particles, exchanging such particles leaves the state unchanged up to a possible sign. More precisely, as already exploited in Ref. [17], little-group irreps must be paired appropriately with irreps under other quantum numbers such that their combined transformations under particle exchanges are symmetric (antisymmetric) with respect to all possible exchanges of identical bosons (fermions), and are otherwise unconstrained. By identifying the definite operator-exchange properties of cubic-group irreps, the framework described above can thus be readily extended to be compatible with other quantum numbers.

A. Labeling by exchange-group irreps

Since the same rotations are applied to all operators in an N-operator basis, rotation and permutation operations commute, and Schur–Weyl duality guarantees that the rotational group irreps can be simultaneously labeled by specific irreps of the symmetric group S_N [21]. This naturally divides any space that is closed under rotations and permutations into *blocks* described by the pair (Γ, λ) of a rotational-group irrep Γ and an S_N irrep λ. In the following, Young diagrams will be used to identify particular choices of λ [22]. Note that multiple blocks may have the same Γ or the same λ, i.e., there is no one-to-one correspondence between the rotational irreps and permutation irreps.

In some cases, it is not necessary to consider definite representations under the full space of permutations. For example, operators may be distinguishable by having different total isospin or other flavor quantum number. To make this identification concrete and automatic, it is assumed that the operators $\mathcal{O}_1, \ldots, \mathcal{O}_N$ can be respectively associated with *internal labels* $\varepsilon_1, \ldots, \varepsilon_N$. In this case, the *exchange group* is taken to be the subgroup of permutations

$$S \equiv S_{N_1} \times S_{N_2} \times \cdots \leq S_N \tag{52}$$

corresponding to exchanges among subsets of identically labeled particles of size $N_1, N_2, \cdots$ with $N_1 + N_2 + \ldots = N$. In this case, the categorization of rotational irreps can be given by the rotational representation and the individual $S_{N_1}, S_{N_2}, \ldots$ irreps as $(\Gamma, \lambda_1, \lambda_2, \ldots)$.

B. Extended orbits

Orbits constructed as in Secs. II A and III C may not necessarily be closed under the exchange group S. To ensure states can always be constructed with definite permutation properties, the orbit must be extended to include all states generated by applying permutations in S. The labeling s of orbits and the indices m of basis states will continue to be used for these *extended orbits*, which will be denoted as $\hat{K}_{\boldsymbol{P}}^{(s)}$:

$$\begin{aligned}\hat{K}_{\boldsymbol{P}}^{(s)} &\equiv \{g \cdot [\boldsymbol{n}_1, \alpha_1, \varepsilon_1, \ldots, \boldsymbol{n}_N, \alpha_N, \varepsilon_N] : g \in G_{\boldsymbol{P}}^D \times S\} \\ &= \{[\boldsymbol{n}_1, \alpha_1, \varepsilon_1, \ldots, \boldsymbol{n}_N, \alpha_N, \varepsilon_N]_m^{(s)} : \\ &\quad m \in \{1, 2, \ldots, |\hat{K}_{\boldsymbol{P}}^{(s)}|\}\},\end{aligned} \tag{53}$$

where α_i label the spin and parity of the ith particle and where ε_i labels its internal quantum numbers. Orbits then furnish representations of exchange-group elements $\sigma \in S$ in the usual way

$$D_{m'm}^{(s)}(\sigma) = \langle s, m' | \mathcal{D}(\sigma) | s, m \rangle. \tag{54}$$

Since σ corresponds to identical-operator exchange, $D_{m'm}^{(s)}(\sigma) \in \{0, 1\}$.

C. Projection to exchange-group irreps

Just as Schur's lemma was applied in Eq. (36) to project into a basis with specific rotational-group irrep Γ, it can be applied to project simultaneously into a basis with a specific permutation-group irrep. The representation theory of the permutation group has been well studied (see Ref. [23] for guidance on standard textbooks). Each irrep of S_n is labeled by a Young diagram consisting of n boxes in left-justified rows with row lengths in nonincreasing order. Closely related is the notion of a Young tableau, in which the n boxes in a given Young diagram are filled with the numbers $\{1, \ldots, n\}$ distributed such that each row and each column is strictly ascending. Let $\mathcal{Y}_n$ denote the set of Young tableaux with n boxes. For example, $\mathcal{Y}_3 = \{\ytableaushort{123}, \ytableaushort{12,3}, \ytableaushort{13,2}, \ytableaushort{1,2,3}\}$.

The connection to the internal symmetry group follows from the fact that products of operators can be taken to transform as (a row of) an irrep of the exchange group, labeled by a Young tableau $\Theta \in \mathcal{Y}_n$. For each Young tableau Θ, there exists a projection operator in the group algebra

Π_Θ which projects onto the relevant row [23–25]. In fact, mirroring the construction in Sec. II C, the group algebra can be decomposed completely into a basis of idempotents Π_Θ and Hermitian ($T^\dagger_{\Theta\Phi} = T_{\Phi\Theta}$) transition operators [24] $T_{\Theta\Phi}$ such that, for fixed $\Theta, \Theta', \Phi, \Phi'$,

$$\Pi_\Theta \equiv T_{\Theta\Theta}, \tag{55}$$

$$T_{\Theta\Phi} T_{\Phi'\Theta'} = \delta_{\Phi\Phi'} T_{\Theta\Theta'}, \tag{56}$$

$$\sum_{\Theta \in \mathcal{Y}_n} \Pi_\Theta = \mathbb{1}. \tag{57}$$

Eq. (56) is analogous to the product rule for the transition operators of the cubic group in Eq. (40).

When multiple instances of the same irrep row Θ appear in the decomposition of a space acted on by the exchange group, they can often be distinguished by letting $T_{\Theta\Phi}$ act on a fiducial vector for different Φ. All such products are left invariant by Π_Θ. In this way, the transition operators acting on fiducial vectors give a way to construct relevant multiparticle operators. Concrete examples are discussed below.

For arbitrary S_n, recursive formulas for Hermitian projection are given in Refs. [23–25] and for Hermitian transition operators in Ref. [24]. Generic projection and transition operators are elements of the group algebra,

$$\Pi_\Theta = \sum_{\sigma \in S_n} c_\sigma^{(\Theta)} \sigma, \tag{58}$$

$$T_{\Theta\Phi} = \sum_{\sigma \in S_n} c_\sigma^{(\Theta\Phi)} \sigma, \tag{59}$$

with $c_\sigma^{(\Theta\Theta)} \equiv c_\sigma^{(\Theta)}$. As indicated, the coefficients $c_\sigma^{(\Theta\Phi)}$ depend explicitly on $\Theta, \Phi \in \mathcal{Y}_n$. A concrete example illustrates the important features of the general case. Consider the permutation group S_3, for which Table VII summarizes the irreps. The projectors Π_Θ, with $\Theta \in \mathcal{Y}_3$, are [24]

$$\Pi_{\begin{array}{|c|c|c|}\hline 1&2&3\\\hline\end{array}} = \frac{1}{6}\left[(1) + (1,2,3) + (1,3,2) + (1,2) + (1,3) + (2,3)\right], \tag{60a}$$

$$\Pi_{\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}} = \frac{1}{6}\left[(1) + (1,2,3) + (1,3,2) - (1,2) - (1,3) - (2,3)\right], \tag{60b}$$

$$\Pi_{\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}} = \frac{1}{6}\left[2\,(1) - (1,2,3) - (1,3,2) + 2\,(1,2) - (1,3) - (2,3)\right], \tag{60c}$$

$$\Pi_{\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}} = \frac{1}{6}\left[2\,(1) - (1,2,3) - (1,3,2) - 2\,(1,2) + (1,3) + (2,3)\right]. \tag{60d}$$

Here and below, cycle notation $(i, j, k, \ldots, z)$ is used to indicate permutations mapping the elements cyclically $i \to j \to k \ldots \to z \to i$. The transition operators between the two rows of the two-dimensional standard irrep are [24]

$$T_{\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}\;\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}} = \frac{1}{\sqrt{12}}\left[(2,3) + (1,2,3) - (1,3) - (1,3,2)\right], \tag{61a}$$

$$T_{\begin{array}{|c|c|}\hline 1&3\\\hline 2\\\cline{1-1}\end{array}\;\begin{array}{|c|c|}\hline 1&2\\\hline 3\\\cline{1-1}\end{array}} = \frac{1}{\sqrt{12}}\left[(2,3) - (1,2,3) - (1,3) + (1,3,2)\right], \tag{61b}$$

where the normalization factors follow from Eq. (56).

The projection matrix acting on the extended orbit then follows from linearity, with components:

$$D^{(s)}_{m'm}(\Pi_\Theta) = \sum_{\sigma \in S} c_\sigma^{(\Theta)} D^{(s)}_{m'm}(\sigma). \tag{62}$$

The symmetric-group projection matrices are applied to the orbit representation matrices in Eq. (51) to construct projected orbit representation matrices

$$\begin{aligned}\hat{D}^{(s,\Theta)}(R^D) &\equiv D^{(s)}(\Pi_\Theta) \cdot \tilde{D}^{(s)}(R^D) \cdot D^{(s)}(\Pi_\Theta) \\ &= \tilde{D}^{(s)}(R^D) \cdot D^{(s)}(\Pi_\Theta).\end{aligned} \tag{63}$$

The equality in the second line follows from the fact that the permutations commute with rotations and that $D^{(s)}(\Pi_\Theta)$ is idempotent. Subsequent application of block diagonalization using Schur's lemma, orthogonalization, and rotational transition operators—needed to construct the block-diagonalization matrices in the analog of Eq. (1)—remains unchanged.

TABLE VII. Irreps of the symmetric group S_3.

Name	Dimension	Young diagram	Young tableaux
Trivial	1		
Sign	1		
Standard	2		

D. Examples

1. Identical fermions: nn and nnn

Identical fermions provide a first example with internal symmetry. Operators constructed from products of identical fermions such as neutrons, e.g., *nn* or *nnn*, must be totally antisymmetric under simultaneous exchange of the spins and momenta of any two particles. For *nn*, the exchange group is S_2. Fermion antisymmetry implies *nn* operators

transform in the sign irrep ($\begin{smallmatrix}1\\2\end{smallmatrix}$) of S_2. Irrep decomposition proceeds as in the distinguishable np case summarized Table IV, with the additional projection step of Eq. (63) using the projection operator for the sign irrep of S_2,

$$\Pi_{\begin{smallmatrix}1\\2\end{smallmatrix}} = \frac{1}{2}\left[(1) - (1,2)\right]. \tag{64}$$

Table VIII summarizes the irrep decompositions for nn operators.

Operators constructed from products of more neutrons can be decomposed analogously. For nnn, the exchange group is S_3. Fermion antisymmetry requires that nnn operators transform in the sign irrep of S_3, corresponding to the projection operator in Eq. (60b). Table IX summarizes the irrep decompositions for nnn operators. Note that, in this case, specification of the little group and stabilizer group does *not* suffice to specify the irrep decomposition uniquely—whether certain permutations correspond to little-group transformations affects the resulting irrep decomposition. These results illustrate the general fact that the irrep decomposition of a multiparticle operator depends on the little group $G_{\boldsymbol{P}}$, the stabilizer group $H_{\boldsymbol{P}}^{(s)}$, and on the irrep of the exchange group S. It is also noteworthy that in this case the application of the exchange group projects away the orbit with $\boldsymbol{n}_1 = \boldsymbol{n}_2 = \boldsymbol{n}_3 = 0$; fermion antisymmetry dictates that this orbit vanishes from the irrep decomposition.

2. Three pions with isospin

The three-pion system provides an example of the interplay between the cubic group and nontrivial internal symmetries. Since each pion transforms as an isotriplet with $I = 1$, the three-pion system has the isospin decomposition

$$1 \otimes 1 \otimes 1 = 3 \oplus 2 \oplus 2 \oplus 1 \oplus 1 \oplus 1 \oplus 0. \tag{65}$$

TABLE VIII. Combinations of irreps arising in decompositions of nn operator orbits. Details are as in Table II.

$G_{\boldsymbol{P}}$	$H_{\boldsymbol{P}}^{(s)}$	S_2 irrep	Example state	Orbit dim	Irrep decomposition
O_h	O_h	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,0,0), n(0,0,0)\rangle$	1	A_1^+
O_h	C_{4v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,0,1), n(0,0,-1)\rangle$	12	$A_1^+ \oplus E^+ \oplus A_1^- \oplus E^- \oplus T_1^- \oplus T_2^-$
O_h	C_{2v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,1,1), n(0,-1,-1)\rangle$	24	$A_1^+ \oplus E^+ \oplus T_2^+ \oplus A_1^- \oplus A_2^- \oplus 2E^- \oplus 2T_1^- \oplus 2T_2^-$
O_h	C_{3v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,1), n(-1,-1,-1)\rangle$	16	$A_1^+ \oplus T_2^+ \oplus A_1^- \oplus E^- \oplus T_1^- \oplus 2T_2^-$
O_h	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,0), n(-2,-1,0)\rangle$	48	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus T_1^+ \oplus T_2^+ \oplus 2A_1^- \oplus 2A_2^- \oplus 4E^- \oplus 4T_1^- \oplus 4T_2^-$
O_h	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,1), n(-2,-1,-1)\rangle$	48	$A_1^+ \oplus E^+ \oplus T_1^+ \oplus 2T_2^+ \oplus 2A_1^- \oplus A_2^- \oplus 3E^- \oplus 4T_1^- \oplus 5T_2^-$
O_h	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(3,2,1), n(-3,-2,-1)\rangle$	96	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus 3T_1^+ \oplus 3T_2^+ \oplus 3A_1^- \oplus 3A_2^- \oplus 6E^- \oplus 9T_1^- \oplus 9T_2^-$
C_{4v}	C_{4v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,0,1), n(0,0,1)\rangle$	1	A_1
C_{4v}	C_{4v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,0,1), n(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus E$
C_{4v}	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,0,1), n(-1,0,1)\rangle$	8	$2A_1 \oplus A_2 \oplus 2B_1 \oplus B_2 \oplus E$
C_{4v}	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,0,1), n(-1,0,0)\rangle$	16	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2 \oplus 4E$
C_{4v}	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,1), n(-1,-1,1)\rangle$	8	$2A_1 \oplus A_2 \oplus B_1 \oplus 2B_2 \oplus E$
C_{4v}	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,1), n(-1,-1,0)\rangle$	16	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2 \oplus 4E$
C_{4v}	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,1), n(-2,-1,1)\rangle$	16	$3A_1 \oplus 3A_2 \oplus 3B_1 \oplus 3B_2 \oplus 2E$
C_{4v}	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,1), n(-2,-1,0)\rangle$	32	$4A_1 \oplus 4A_2 \oplus 4B_1 \oplus 4B_2 \oplus 8E$
C_{3v}	C_{3v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,1), n(1,1,1)\rangle$	1	A_1
C_{3v}	C_{3v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,1), n(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus E$
C_{3v}	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,1,0), n(0,0,1)\rangle$	12	$2A_1 \oplus 2A_2 \oplus 4E$
C_{3v}	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,0,-1), n(0,1,2)\rangle$	24	$4A_1 \oplus 4A_2 \oplus 8E$
C_{2v}	C_{2v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,1,1), n(0,1,1)\rangle$	1	A_1
C_{2v}	C_{2v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,1,1), n(0,0,0)\rangle$	4	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$
C_{2v}	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,0,1), n(0,1,0)\rangle$	4	$2A_1 \oplus A_2 \oplus B_1$
C_{2v}	C_{2v}	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(0,2,2), n(0,-1,-1)\rangle$	4	$A_1 \oplus A_2 \oplus B_1 \oplus B_2$
C_{2v}	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,1), n(-2,1,1)\rangle$	4	$2A_1 \oplus A_2 \oplus B_2$
C_{2v}	C_2^P	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(2,1,1), n(-2,0,0)\rangle$	8	$2A_1 \oplus 2A_2 \oplus 2B_1 \oplus 2B_2$
C_{2v}	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(-2,0,1), n(2,1,0)\rangle$	8	$3A_1 \oplus 3A_2 \oplus B_1 \oplus B_2$
C_{2v}	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,2,1), n(-1,-1,0)\rangle$	16	$4A_1 \oplus 4A_2 \oplus 4B_1 \oplus 4B_2$
C_2^R	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,2,0), n(1,2,0)\rangle$	1	A
C_2^R	C_2^R	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,2,0), n(0,0,0)\rangle$	4	$2A \oplus 2B$
C_2^R	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,0,1), n(0,2,-1)\rangle$	8	$4A \oplus 4B$
C_1	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,2,3), n(1,2,3)\rangle$	1	A
C_1	C_1	$\begin{smallmatrix}1\\2\end{smallmatrix}$	$\lvert n(1,2,3), n(0,0,0)\rangle$	4	$4A$

TABLE IX. Combinations of irreps arising in decompositions of *nnn* operator orbits. Details are as in Table II.

G_P	$H_P^{(s)}$	S_3 irrep	Example state	Orbit dim	Irrep decomposition
O_h	C_{4v}	▯▯▯	$\lvert n(0,0,1), n(0,0,-1), n(0,0,0)\rangle$	24	$G_1^+ \oplus H^+ \oplus 2G_1^- \oplus G_2^- \oplus 3H^-$
O_h	C_{4v}	▯▯▯	$\lvert n(0,0,1), n(0,0,2), n(0,0,-3)\rangle$	48	$3G_1^+ \oplus G_2^+ \oplus 4H^+ \oplus 3G_1^- \oplus G_2^- \oplus 4H^-$
O_h	C_{2v}	▯▯▯	$\lvert n(0,1,1), n(0,-1,-1), n(0,0,0)\rangle$	48	$G_1^+ \oplus G_2^+ \oplus 2H^+ \oplus 3G_1^- \oplus 3G_2^- \oplus 6H^-$
O_h	C_{2v}	▯▯▯	$\lvert n(0,-1,-1), n(0,-2,-2), n(0,3,3)\rangle$	96	$4G_1^+ \oplus 4G_2^+ \oplus 8H^+ \oplus 4G_1^- \oplus 4G_2^- \oplus 8H^-$
O_h	C_{3v}	▯▯▯	$\lvert n(1,1,1), n(-1,-1,-1), n(0,0,0)\rangle$	32	$G_1^+ \oplus G_2^+ \oplus H^+ \oplus 2G_1^- \oplus 2G_2^- \oplus 4H^-$
O_h	C_{3v}	▯▯▯	$\lvert n(1,1,1), n(2,2,2), n(-3,-3,-3)\rangle$	64	$3G_1^+ \oplus 3G_2^+ \oplus 5H^+ \oplus 3G_1^- \oplus 3G_2^- \oplus 5H^-$
O_h	C_2^R	▯▯▯	$\lvert n(2,1,0), n(-2,-1,0), n(0,0,0)\rangle$	96	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 6G_1^- \oplus 6G_2^- \oplus 12H^-$
O_h	C_2^R	▯▯▯	$\lvert n(0,1,1), n(0,-1,0), n(0,0,-1)\rangle$	96	$4G_1^+ \oplus 4G_2^+ \oplus 8H^+ \oplus 4G_1^- \oplus 4G_2^- \oplus 8H^-$
O_h	C_2^R	▯▯▯	$\lvert n(2,1,0), n(-2,0,0), n(0,-1,0)\rangle$	192	$8G_1^+ \oplus 8G_2^+ \oplus 16H^+ \oplus 8G_1^- \oplus 8G_2^- \oplus 16H^-$
O_h	C_2^P	▯▯▯	$\lvert n(2,1,1), n(-2,-1,-1), n(0,0,0)\rangle$	96	$2G_1^+ \oplus 2G_2^+ \oplus 4H^+ \oplus 6G_1^- \oplus 6G_2^- \oplus 12H^-$
O_h	C_2^P	▯▯▯	$\lvert n(1,1,1), n(-1,-1,0), n(0,0,-1)\rangle$	192	$8G_1^+ \oplus 8G_2^+ \oplus 16H^+ \oplus 8G_1^- \oplus 8G_2^- \oplus 16H^-$
O_h	C_1	▯▯▯	$\lvert n(0,-1,1), n(2,1,0), n(-2,0,-1)\rangle$	192	$8G_1^+ \oplus 8G_2^+ \oplus 16H^+ \oplus 8G_1^- \oplus 8G_2^- \oplus 16H^-$
O_h	C_1	▯▯▯	$\lvert n(2,1,1), n(-2,-1,0), n(0,0,-1)\rangle$	384	$16G_1^+ \oplus 16G_2^+ \oplus 32H^+ \oplus 16G_1^- \oplus 16G_2^- \oplus 32H^-$

The relevant exchange group is S_3, for which the irreps and projectors have been summarized above. As in Sec. II, Schur's lemma provides the means to decompose the product-state isospin representation into irreps of S_3. Since I_z is conserved by permutations, it suffices to work at fixed I_z. Permutations of the states with a given I_z furnish the reducible representation matrices $D^{(I_z)}_{m'm}(\sigma)$. For example, the seven states with $I_z = 0$ yield 7×7 representation matrices $D^{(I_z=0)}_{m'm}(\sigma)$. Irrep matrices $D^{(\lambda)}$ for S_3 are also readily obtained. For the trivial irrep they are simply unity, while for the sign representation they are equal to the permutation signature. Irrep matrices for the two-dimensional standard representation of S_3 are given in Ref. [17].

Table X shows the result of applying Schur's lemma, i.e., using Eq. (30) in terms of the $D^{(\lambda)}$ and $D^{(I_z)}$ matrices, to extract the overlap of the reducible I_z representation onto the irrep λ. As expected, $I = 3$ corresponds to the trivial representation of S_3 for each $I_z \in \{-3, \ldots, 3\}$, which is totally symmetric. The doublets of states with $I = 2$ for each I_z fall in the standard representation of S_3. The three copies with $I = 1$ split into a doublet from the standard representation and a trivial representation for each I_z. Finally, the isosinglet transforms in the sign representation of S_3, which is totally antisymmetric. Explicit expressions for the associated states have been given in Ref. [17].

Combining these results with block diagonalization for the cubic group amounts to applying Eq. (62), where Π_Θ is selected to project onto the rows of Table X with the desired isospin. Applying these projectors in Eq. (63) reproduces the cubic-group irrep decompositions given in Appendix D of Ref. [17] for the rest frame.

As discussed in Sec. IV C, the transition operators $T_{\Theta\Phi}$ can be used to construct multiparticle operators with definite S_n transformation properties. For the case at hand, consider three-pion operators with $I_z = 0$ and $I \in \{0, 1, 2, 3\}$. These operators can be built from permutations of the fiducial ordering of single-pion operators, say, $\lvert\pi^+\pi^-\pi^0\rangle$. Letting permutations act in the natural way, e.g., $(1,2,3)\lvert\pi^+\pi^-\pi^0\rangle = \lvert\pi^0\pi^+\pi^-\rangle$, gives the seven three-pion states with $I_z = 0$ constructed in Ref. [17]:

$$\Pi_{\boxed{1}\boxed{2}\boxed{3}} \left(6\lvert\pi^+\pi^-\pi^0\rangle + 2\lvert\pi^0\pi^0\pi^0\rangle\right) \propto \lvert\chi_s\rangle_{I=3}, \tag{66a}$$

$$\Pi_{\boxed{1}\boxed{2}\boxed{3}} \left(6\lvert\pi^+\pi^-\pi^0\rangle - 3\lvert\pi^0\pi^0\pi^0\rangle\right) \propto \lvert\chi_s\rangle_{I=1}, \tag{66b}$$

TABLE X. Decomposition of the $\pi\pi\pi$ system into irreps of S_3 given in Table VII. For each column of fixed I_z, the number of check marks equals the sum of the dimensions in the irrep decomposition.

	I_z							
I	+3	+2	+1	0	−1	−2	−3	S_3 irrep
3	✓	✓	✓	✓	✓	✓	✓	▯▯▯
2		✓	✓	✓	✓	✓		⎫ ▯▯
2		✓	✓	✓	✓	✓		⎭ ▯▯
1			✓	✓	✓			⎫ ▯▯
1			✓	✓	✓			⎭ ▯▯
1			✓	✓	✓			▯▯▯
0				✓				▯ / ▯ / ▯

$$\Pi_{\begin{smallmatrix}1&2\\3\end{smallmatrix}}|\pi^+\pi^-\pi^0\rangle \propto |\chi_1\rangle_{I=1}, \tag{66c}$$

$$T_{\begin{smallmatrix}1&2\\3\end{smallmatrix}\begin{smallmatrix}1&3\\2\end{smallmatrix}}|\pi^+\pi^-\pi^0\rangle \propto |\chi_1\rangle_{I=2}, \tag{66d}$$

$$\Pi_{\begin{smallmatrix}1&3\\2\end{smallmatrix}}|\pi^+\pi^-\pi^0\rangle \propto |\chi_2\rangle_{I=2}, \tag{66e}$$

$$T_{\begin{smallmatrix}1&3\\2\end{smallmatrix}\begin{smallmatrix}1&2\\3\end{smallmatrix}}|\pi^+\pi^-\pi^0\rangle \propto |\chi_2\rangle_{I=1}, \tag{66f}$$

$$\Pi_{\begin{smallmatrix}1\\2\\3\end{smallmatrix}}|\pi^+\pi^-\pi^0\rangle \propto |\chi_a\rangle_{I=0}. \tag{66g}$$

The totally symmetric cases (Eqs. (66a) and (66b)) contain a component proportional to $|\pi^0\pi^0\pi^0\rangle$, which vanishes in all other representations; the relative coefficient between the $|\pi^+\pi^-\pi^0\rangle$ and $|\pi^0\pi^0\pi^0\rangle$ terms is related to the isospin Clebsch–Gordan decomposition. As in Ref. [17], the two-dimensional standard irrep is spanned by a basis denoted by $|\chi_1\rangle$ and $|\chi_2\rangle$, with a final subscript outside the ket giving the total isospin. As expected, Eqs. (66c) and (66d) are invariant under Eq. (60c) and associated with degenerate copies of the first row $|\chi_1\rangle$ of the irrep $\begin{smallmatrix}\square&\square\\\square\end{smallmatrix}$. Similarly, Eqs. (60e) and (66f) are invariant under Eq. (60d) and associated with degenerate copies of the second row $|\chi_2\rangle$.

Three pions in boosted frames provide examples where the full S_3 exchange group influences the cubic-group irrep decomposition. A minimal example is the system with momenta $[\boldsymbol{n}_1,\boldsymbol{n}_2,\boldsymbol{n}_3]=[(1,0,0),(0,1,0),(0,0,1)]$, for which the momenta can all be permuted by little group operations. The little group of the total momentum is C_{3v}, while the stabilizer is C_1. Without projecting under the exchange group, the resulting irreps can be seen from the relevant row of Table II to be

$$A_1 \oplus A_2 \oplus 2E. \tag{67}$$

Applying the various S_3 projectors Π_Θ with $\Theta \in \mathcal{Y}_3$ restricts to the following irreps:

$$\begin{aligned}
\begin{smallmatrix}1&2&3\end{smallmatrix}&: \quad A_1 \oplus A_2 \oplus 2E \mapsto A_1,\\
\begin{smallmatrix}1\\2\\3\end{smallmatrix}&: \quad A_1 \oplus A_2 \oplus 2E \mapsto A_2,\\
\begin{smallmatrix}1&2\\3\end{smallmatrix}&: \quad A_1 \oplus A_2 \oplus 2E \mapsto E,\\
\begin{smallmatrix}1&3\\2\end{smallmatrix}&: \quad A_1 \oplus A_2 \oplus 2E \mapsto E.
\end{aligned} \tag{68}$$

Comparison with Table X determines which combinations of cubic group and isospin irreps are compatible with bosonic statistics for this set of momenta. For example, total $I=0$ must be combined with the cubic group irrep A_2, while total $I=1$ or $I=3$ must be combined with the cubic group irrep A_1. Both $I=1$ and $I=2$ may be combined with the cubic group irrep E, but the correct degenerate copy of this irrep must be chosen.

3. $DD\pi$

Decay channels with resonances are also categorized by isospin and provide examples of internal symmetry where not all particles are identical. For instance, the doubly charmed tetraquark $T_{cc}(3875)^+$ has been observed just below threshold for $D^{\star+}D^0$ in the decay mode $D^0D^0\pi^+$ with charmness $C=+2$ and charge $Q=+1$, corresponding to $I_z=0$ [26]. The isospin decomposition of the $DD\pi$ system is

$$\frac{1}{2}\otimes\frac{1}{2}\otimes 1 = 2\oplus 1\oplus 1\oplus 0, \tag{69}$$

where the D-meson isodoublet is $(D^+,D^0)^T$. Similar to the preceding example, for each fixed I_z the direct sum is decomposed into irreps of S_2 (permutations of the two D-meson operators) using projectors $\Pi_{\begin{smallmatrix}1\\2\end{smallmatrix}}$ (defined in Eq. (64) above) and

$$\Pi_{\begin{smallmatrix}1&2\end{smallmatrix}} = \frac{1}{2}\left[(1)+(1,2)\right]. \tag{70}$$

The four states with $I_z=0$ are constructed from linear combinations of the states $|D^+D^+\pi^-\rangle$, $|D^+D^0\pi^+\rangle$, $|D^0D^+\pi^+\rangle$, and $|D^0D^0\pi^+\rangle$. In terms of fiducial orderings,

$$\begin{aligned}
|\psi_{00}\rangle &\equiv |D^0D^0\pi^+\rangle,\\
|\psi_{++}\rangle &\equiv |D^+D^+\pi^-\rangle,\\
|\psi_{+0}\rangle &\equiv |D^+D^0\pi^+\rangle,
\end{aligned} \tag{71}$$

states of definite isospin with $I_z=0$ are given by

$$\begin{aligned}
|(DD)_1\pi\rangle_2 &\propto \Pi_{\begin{smallmatrix}1&2\end{smallmatrix}}\left(|\psi_{00}\rangle+|\psi_{++}\rangle+2\sqrt{2}|\psi_{+0}\rangle\right)\\
|(DD)_1\pi\rangle_{1,a} &\propto \Pi_{\begin{smallmatrix}1&2\end{smallmatrix}}\left(|\psi_{++}\rangle-|\psi_{00}\rangle\right)\\
|(DD)_1\pi\rangle_{1,b} &\propto \Pi_{\begin{smallmatrix}1\\2\end{smallmatrix}}|\psi_{+0}\rangle\\
|(DD)_1\pi\rangle_0 &\propto \Pi_{\begin{smallmatrix}1&2\end{smallmatrix}}\left(\sqrt{2}(|\psi_{00}\rangle+|\psi_{++}\rangle)-2|\psi_{+0}\rangle\right),
\end{aligned} \tag{72}$$

where the left-hand side uses the notation of Ref. [27]. In the state $|(DD)_{I_{DD}}\pi\rangle_I$, I is the total isospin, and I_{DD} is the isospin of the DD subsystem. As expected, the states with $I=2$ and $I=0$ transform in the symmetric representation of S_2. Of the two copies of $I=1$, one is symmetric, while the other is antisymmetric. Results for irrep decompositions of $DD\pi$ operators are summarized in Table XI, where the orbit dimension refers to the rank of the projected orbit-representation matrices $\hat{D}^{(s,\Theta)}$. The trivial and sign irreps of

TABLE XI. Combinations of irreps arising in decompositions of $DD\pi$ operator orbits. In the example states, the label D refers collectively to D^0 and D^+ and the pion is either π^0 or π^+. Details are as in Table II.

G_P	$H_P^{(s)}$	S_2 Irrep	Example state	Orbit dim	Irrep decomposition
O_h	O_h	▭	$\lvert D(0,0,0), D(0,0,0), \pi(0,0,0)\rangle$	1	A_1^-
O_h	C_4^v	▭	$\lvert D(0,0,1), D(0,0,-1), \pi(0,0,0)\rangle$	3	$A_1^- \oplus E^-$
O_h	C_4^v	▯▯	$\lvert D(0,0,1), D(0,0,-1), \pi(0,0,0)\rangle$	3	T_1^+
O_h	C_2^v	▭	$\lvert D(0,1,1), D(0,-1,-1), \pi(0,0,0)\rangle$	6	$A_1^- \oplus E^- \oplus T_2^-$
O_h	C_2^v	▯▯	$\lvert D(0,1,1), D(0,-1,-1), \pi(0,0,0)\rangle$	6	$T_1^+ \oplus T_2^+$
O_h	C_3^v	▭	$\lvert D(1,1,1), D(-1,-1,-1), \pi(0,0,0)\rangle$	4	$A_1^- \oplus T_2^-$
O_h	C_3^v	▯▯	$\lvert D(1,1,1), D(-1,-1,-1), \pi(0,0,0)\rangle$	4	$A_2^+ \oplus T_1^+$
O_h	C_2^R	▭	$\lvert D(2,1,0), D(-2,-1,0), \pi(0,0,0)\rangle$	12	$A_1^- \oplus A_2^- \oplus 2E^- \oplus T_1^- \oplus T_2^-$
O_h	C_2^R	▯▯	$\lvert D(2,1,0), D(-2,-1,0), \pi(0,0,0)\rangle$	12	$2T_1^+ \oplus 2T_2^+$
O_h	C_2^P	▭	$\lvert D(2,1,1), D(-2,-1,-1), \pi(0,0,0)\rangle$	12	$A_1^- \oplus E^- \oplus T_1^- \oplus 2T_2^-$
O_h	C_2^P	▯▯	$\lvert D(2,1,1), D(-2,-1,-1), \pi(0,0,0)\rangle$	12	$A_2^+ \oplus E^+ \oplus 2T_1^+ \oplus T_2^+$
O_h	C_1	▭	$\lvert D(3,2,1), D(-3,-2,-1), \pi(0,0,0)\rangle$	24	$A_1^- \oplus A_2^- \oplus 2E^- \oplus 3T_1^- \oplus 3T_2^-$
O_h	C_1	▯▯	$\lvert D(3,2,1), D(-3,-2,-1), \pi(0,0,0)\rangle$	24	$A_1^+ \oplus A_2^+ \oplus 2E^+ \oplus 3T_1^+ \oplus 3T_2^+$

S_2 correspond to odd- and even-parity irreps in the decomposition of the cubic group, respectively, such that the overall exchange of two identical D mesons is symmetric.

4. H-dibaryon

The H-dibaryon provides an example where flavor and operator-exchange symmetry come together to satisfy bosonic symmetry or fermionic antisymmetry. The H-dibaryon is a hypothetical two-baryon bound state with strangeness $S=-2$ that corresponds to an SU(3)-flavor singlet when the up, down, and strange quark masses are equal. Interpolating operators with these quantum numbers can be constructed from two flavor-octet baryon interpolating operators using the SU(3)-flavor irrep decomposition

$$\mathbf{8}\otimes\mathbf{8}=\mathbf{1}\oplus\mathbf{8}_A\oplus\mathbf{8}_S\oplus\mathbf{10}\oplus\overline{\mathbf{10}}\oplus\mathbf{27}, \tag{73}$$

where $\mathbf{8}_A$ ($\mathbf{8}_S$) denotes an SU(3) octet irrep where the two-baryon flavor state is antisymmetric (symmetric) under exchange. The singlet irrep 1 corresponds to a symmetric flavor state associated with the operator $B^aB^b\delta_{ab}$ where B^a is a baryon octet field with SU(3) adjoint index a. Writing explicitly the baryon spin representation indices α_1, α_2 and the momentum labels $\boldsymbol{n}_1,\ldots$ for each field, fermion antisymmetry implies $B^a_{\alpha_1}(\boldsymbol{n}_1)B^b_{\alpha_2}(\boldsymbol{n}_2)=-B^b_{\alpha_2}(\boldsymbol{n}_2)B^a_{\alpha_1}(\boldsymbol{n}_1)$. This implies that the momentum-spin states $\lvert\boldsymbol{n}_1,\alpha_1,\boldsymbol{n}_2,\alpha_2\rangle$ associated with $\delta_{ab}B^a_{\alpha_1}(\boldsymbol{n}_1)B^b_{\alpha_2}(\boldsymbol{n}_2)$ will be antisymmetric under the exchange of momentum-spin pairs $(\boldsymbol{n}_1,\alpha_1)\leftrightarrow(\boldsymbol{n}_2,\alpha_2)$. These states therefore transform in the sign irrep of S_2, and the permutation projector defined in Eq. (64) should be applied. These two-baryon operators, which are linear combinations of $\Lambda\Lambda$, $\Sigma\Sigma$, and $N\Xi$, therefore have identical irrep decompositions to the case of nn operators summarized in Table VIII.

Operators with the same quantum numbers can be constructed from products of two octet baryon operators and one pseudoscalar octet meson operator. This corresponds to the product of SU(3) irreps $\mathbf{8}\otimes\mathbf{8}\otimes\mathbf{8}$, which includes two copies of the 1 irrep relevant for the H-dibaryon. Tensor operators describing these products are given by

$$d_{abc}B^aB^bM^c, \qquad f_{abc}B^aB^bM^c, \tag{74}$$

where a, b, c are SU(3) adjoint indices, M^a is a pseudoscalar octet meson operator, and d_{abc} (f_{abc}) are totally symmetric (antisymmetric) structure constants. Although these operators involve linear combinations of several different products of meson and baryon flavors, for example $\Lambda\Lambda\pi^0$, ΛpK^-, and $\Sigma^+\Sigma^0\pi^-$, their cubic irrep decompositions and block-diagonalization matrices only depend on the permutation transformation properties of the flavor tensors d_{abc} and f_{abc} as well as the fermionic nature of the baryon fields.

Because B^a and M^a fields represent distinct types of SU(3)-octet particles while B^a and B^b are identical besides their SU(3) flavor indices, the relevant exchange group for this case is S_2. Writing explicitly the baryon spin representation indices α_1, α_2 and the momentum labels $\boldsymbol{n}_1,\ldots,\boldsymbol{n}_3$ for each field, fermion antisymmetry implies $B^a_{\alpha_1}(\boldsymbol{n}_1)B^b_{\alpha_2}(\boldsymbol{n}_2)M^c(\boldsymbol{n}_3)=-B^b_{\alpha_2}(\boldsymbol{n}_2)B^a_{\alpha_1}(\boldsymbol{n}_1)M^c(\boldsymbol{n}_3)$. When contracted with the totally symmetric tensor d_{abc}, momentum-spin states $\lvert\boldsymbol{n}_1,\alpha_1,\boldsymbol{n}_2,\alpha_2,\boldsymbol{n}_3\rangle$ associated with these operators will be antisymmetric under the exchange of momentum-spin pairs $(\boldsymbol{n}_1,\alpha_1)\leftrightarrow(\boldsymbol{n}_2,\alpha_2)$. These states therefore transform in the sign irrep of S_2, and the permutation projector defined in Eq. (64) should be applied. Conversely, when contracted with the totally antisymmetric tensor f_{abc}, momentum-spin states created by these operators will be symmetric under the exchange of

TABLE XII. Permutation irreps of S_2 or S_3 for SU(3)-singlet operators arising from products of three meson octet M^a and baryon octet B^a operators.

Flavor tensor	$M^aM^bM^c$	$M^aM^bB^c$	$B^aB^bM^c$	$B^aB^bB^c$
d_{abc}	$\boxed{1}\boxed{2}\boxed{3}$	$\boxed{1}\boxed{2}$	$\begin{array}{|c|}\hline 1\\\hline 2\\\hline\end{array}$	$\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}$
f_{abc}	$\begin{array}{|c|}\hline 1\\\hline 2\\\hline 3\\\hline\end{array}$	$\begin{array}{|c|}\hline 1\\\hline 2\\\hline\end{array}$	$\boxed{1}\boxed{2}$	$\boxed{1}\boxed{2}\boxed{3}$

momentum-spin pairs $(\boldsymbol{n}_1,\alpha_1)\leftrightarrow(\boldsymbol{n}_2,\alpha_2)$. These states therefore transform in the trivial irrep of S_2, and the permutation projector defined in Eq. (70) should be applied.

Similar considerations apply to other SU(3)-singlet operators built from different combinations of three meson- and baryon-octet operators, $M^aM^bB^c$, $M^aM^bM^c$, and $B^aB^bB^c$, which provide further examples of the interplay between identical-particle labels and flavor-transformation properties. Table XII summarizes the possible combinations with irreps of the particle-exchange group S_2 or S_3.

5. $\pi\pi KK$

An illustrative example of how the exchange group and extended orbit dimension depend on the configuration of the momentum orbit is provided by the $\pi\pi KK$ and $\pi\pi\pi\pi$ systems with two pairs of particles moving back to back. This also provides an example where the exchange group is a direct product of nontrivial subgroups. Table XIII shows the irrep decomposition for four spin-zero particles moving pairwise back-to-back with momenta $\boldsymbol{n}_1=(0,0,1)$, $\boldsymbol{n}_2=(0,2,0)$, $-\boldsymbol{n}_1$, and $-\boldsymbol{n}_2$. Depending on how many operators correspond to identical bosons, different permutation projectors are used and lead to different cubic-group irrep decompositions.

The simplest case is $\pi^+\pi^-K^+K^-$, which has no identical particles. The (extended) orbits for all momentum configurations have the standard irrep decomposition for distinguishable spin-zero operator products with stabilizer group C_2^R.

When there are two pairs of identical bosons such as $\pi^+\pi^+K^+K^+$, the exchange group is $S_2\times S_2$. States are invariant under exchange of both the first two momenta and the last two momenta and therefore transform in the trivial irrep of both S_2 factors. The appropriate projector is a product of the S_2 trivial irrep projectors given in Eq. (70),

$$\begin{aligned}\Pi_{\boxed{1}\boxed{2}}\Pi_{\boxed{3}\boxed{4}} &= \left(\frac{1}{2}[(1)+(1,2)]\right)\left(\frac{1}{2}[(1)+(3,4)]\right)\\ &= \frac{1}{4}[(1)+(1,2)+(3,4)+(1,2)(3,4)].\end{aligned} \tag{75}$$

In this case, the dimensionality of the extended orbit, i.e., the rank of the projected orbit-representation matrices $\hat{D}^{(s,\Theta)}$, and the irrep decomposition depend on the momentum configuration.

With four identical bosons such as $\pi^+\pi^+\pi^+\pi^+$, states transform in the trivial representation of the exchange group S_4. The appropriate permutation projector is therefore obtained from the normalized sum of all $4!=24$ elements of S_4, that is

$$\Pi_{\boxed{1}\boxed{2}\boxed{3}\boxed{4}} = \tfrac{1}{4!}[(1)+(1,2)+(1,3)+(1,4)+\cdots]. \tag{76}$$

The irrep decompositions for each of these cases are shown in Table XIII. For a fixed exchange group, the size of the irrep is related to the size of the orbit. In the second row, identical particles are moving back-to-back, which reduces the size of the decomposition compared to the third row, where exchange group elements only affect operators with momenta that cannot be related by cubic transformations.

V. ALGORITHM SUMMARY

To collect details spread across several sections, the steps of the full algorithm are reproduced here, including for the case of identical particles with nonzero spin. The algorithm begins by selecting a fiducial state $\boldsymbol{i}=[\boldsymbol{n}_1,\alpha_1,\varepsilon_1,\ldots,\boldsymbol{n}_N,\alpha_N,\varepsilon_N]$ (in terms of the momentum $\boldsymbol{n}_i$, spin and parity α_i, and internal quantum numbers ε_i of the ith particle) and specifying its permutation properties as corresponding to a row Θ of an exchange-group irrep. Given the fiducial state $\boldsymbol{i}$ and desired exchange-group irrep row Θ, the algorithm proceeds as follows:

(1) Compute the little group $G_{\boldsymbol{P}}$, defined in Eq. (10), of the total momentum.

TABLE XIII. Combinations of irreps arising in the decomposition of momentum orbits with four spin-zero operators, where $\boldsymbol{n}_1=(0,0,1)$ and $\boldsymbol{n}_2=(0,2,0)$. Projection from symmetrization over identical operators generically reduces the number of irreps appearing in the decomposition.

$G_{\boldsymbol{P}}$	$H_{\boldsymbol{P}}^{(s)}$	Exchange	Example state	Orbit dim	Irrep decomposition
O_h	C_2^R	–	$\lvert\pi^+(\boldsymbol{n}_1),\pi^-(-\boldsymbol{n}_1),K^+(\boldsymbol{n}_2),K^-(-\boldsymbol{n}_2)\rangle$	24	$A_1^+\oplus A_2^+\oplus 2E^+\oplus T_1^+\oplus T_2^+\oplus 2T_1^-\oplus 2T_2^-$
O_h	C_2^R	$\square\square\times\square\square$	$\lvert\pi^+(\boldsymbol{n}_1),\pi^+(-\boldsymbol{n}_1),K^+(\boldsymbol{n}_2),K^+(-\boldsymbol{n}_2)\rangle$	6	$A_1^+\oplus A_2^+\oplus 2E^+$
O_h	C_2^R	$\square\square\times\square\square$	$\lvert\pi^+(\boldsymbol{n}_1),\pi^+(\boldsymbol{n}_2),K^+(-\boldsymbol{n}_1),K^+(-\boldsymbol{n}_2)\rangle$	24	$A_1^+\oplus A_2^+\oplus 2E^+\oplus T_1^+\oplus T_2^+\oplus 2T_1^-\oplus 2T_2^-$
O_h	C_2^R	$\square\square\square\square$	$\lvert\pi^+(\boldsymbol{n}_1),\pi^+(-\boldsymbol{n}_1),\pi^+(\boldsymbol{n}_2),\pi^+(-\boldsymbol{n}_2)\rangle$	6	$A_1^+\oplus A_2^+\oplus 2E^+$

(2) Compute irrep matrices of the little group $D^{(\Gamma)}_{\mu'\mu}(R)$ via Eq. (B5).
(3) Compute the extended orbit $\hat{K}^{(s)}_{\boldsymbol{P}}$ of the fiducial state under the action of the little group and the exchange group via Eq. (53).
(4) Compute the momentum-orbit representation matrices $D^{(s)}_{m'm}(R)$, Eq. (18).
(5) Compute the spin-representation matrices $D^{[J]}_{J'_z J_z}(R^D)$ associated with each interpolating operator, defined generically in Eq. (47) or specifically for spin-half (G_1^+) operators in Eq. (46).
(6) Construct the combined momentum-spin-orbit representation matrices via Eq. (51).
(7) Compute the exchange-group projector Π_Θ, Eq. (58), as described in Refs. [23–25].
(8) Construct projected orbit-representation matrices via Eq. (62).
(9) Apply Schur's lemma in the form of Eq. (34) to the projected orbit representation matrices in order to compute the first row for each irrep in the block-diagonalization matrices. Orthogonalize any degenerate copies which appear.
(10) Construct transition operators via Eq. (38) and use Eq. (41) to fill the remaining rows of each irrep. The result is the complete set of block-diagonalization matrices $U^{(\Gamma,\kappa,s)}_{m\mu}$.

VI. OUTLOOK

This work presents a general algorithm with which to construct multiparticle interpolating operators for quantum field theories with cubic symmetry, including both lattice and continuum theories. The algorithm, together with the implementation in Ref. [18], automates the block diagonalization to build multiparticle interpolating operators transforming under irreps of the relevant little group. Automating this technical component allows the focus of interpolating-operator construction to shift to the design of local and extended operators to access multiparticle states of interest. It also helps facilitate construction of large operator sets in variational calculations aiming to constrain finite-volume spectra precisely.

These or similar methods can be expected to play an increasingly important role in lattice QCD studies of multiparticle systems. Especially for systems with multiple baryons, the field has developed rapidly over the past several years as algorithmic advances (e.g., Refs. [28–34]) have rendered variational studies a practical reality [14,35–37].

An implementation of the algorithm is publicly available at [38].

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APPENDIX A: GROUP CONVENTIONS

This appendix describes the conventions for the groups O_h, O_h^D, and their subgroups, giving the concrete forms used in the numerical implementation of the algorithm presented in this work, available in Ref. [18]. Connections to conventions in the literature are also discussed.

1. The cubic group O_h

For the cubic group O_h, any element $R \in O_h$ may be written as a product of a reflection r and a permutation p [8],

$$R = rp, \tag{A1}$$

with r and p given by

$$\begin{aligned} r &\in \{e, r_z, r_y, r_y r_z, r_x, r_x r_z, r_x r_y, r_x r_y r_z\} \\ p &\in \{e, p_{xy}, p_{yz}, p_{xz}, p_{xyz}, p_{xzy}\}, \end{aligned} \tag{A2}$$

where e is the identity matrix, r_k acts on 3-vectors by multiplying the kth component by -1, p_{ij} acts on 3-vectors by permuting their ith and jth components, and the cyclic permutations are defined by $p_{xyz} = p_{xy}p_{yz}$ and $p_{xzy} = p_{yz}p_{xy}$. For example,

$$p_{xy} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad r_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{A3}$$

An ordering for the 48 elements of O_h can be established by labeling permutations and reflections as r_a and p_b with $a \in \{1, \ldots, 8\}$ and $b \in \{1, \ldots, 6\}$ ordered as shown in Eq. (A2) and $R_c = r_a p_b$ labeled by $c = 6(a-1) + b$ with

$c \in \{1, \ldots, 48\}$. For completeness, the elements are enumerated as:

$$
\begin{aligned}
R_1 &= e, & R_2 &= p_{xy}, \\
R_3 &= p_{yz}, & R_4 &= p_{xz}, \\
R_5 &= p_{xyz}, & R_6 &= p_{xzy}, \\
R_7 &= r_z, & R_8 &= r_z p_{xy}, \\
R_9 &= r_z p_{yz}, & R_{10} &= r_z p_{xz}, \\
R_{11} &= r_z p_{xyz}, & R_{12} &= r_z p_{xzy}, \\
R_{13} &= r_y, & R_{14} &= r_y p_{xy}, \\
R_{15} &= r_y p_{yz}, & R_{16} &= r_y p_{xz}, \\
R_{17} &= r_y p_{xyz}, & R_{18} &= r_y p_{xzy}, \\
R_{19} &= r_y r_z, & R_{20} &= r_y r_z p_{xy}, \\
R_{21} &= r_y r_z p_{yz}, & R_{22} &= r_y r_z p_{xz}, \\
R_{23} &= r_y r_z p_{xyz}, & R_{24} &= r_y r_z p_{xzy}, \\
R_{25} &= r_x, & R_{26} &= r_x p_{xy}, \\
R_{27} &= r_x p_{yz}, & R_{28} &= r_x p_{xz}, \\
R_{29} &= r_x p_{xyz}, & R_{30} &= r_x p_{xzy}, \\
R_{31} &= r_x r_z, & R_{32} &= r_x r_z p_{xy}, \\
R_{33} &= r_x r_z p_{yz}, & R_{34} &= r_x r_z p_{xz}, \\
R_{35} &= r_x r_z p_{xyz}, & R_{36} &= r_x r_z p_{xzy}, \\
R_{37} &= r_x r_y, & R_{38} &= r_x r_y p_{xy}, \\
R_{39} &= r_x r_y p_{yz}, & R_{40} &= r_x r_y p_{xz}, \\
R_{41} &= r_x r_y p_{xyz}, & R_{42} &= r_x r_y p_{xzy}, \\
R_{43} &= r_x r_y r_z, & R_{44} &= r_x r_y r_z p_{xy}, \\
R_{45} &= r_x r_y r_z p_{yz}, & R_{46} &= r_x r_y r_z p_{xz}, \\
R_{47} &= r_x r_y r_z p_{xyz}, & R_{48} &= r_x r_y r_z p_{xzy}.
\end{aligned} \tag{A4}
$$

The basis functions for the irreps of O_h used in this work are specified in Table I. Irreps are classified by their dimension and eigenvalue (± 1) under the parity operation $R_{43}: \boldsymbol{r} \mapsto -\boldsymbol{r}$. The basis functions for the irreps A_1^+, T_1^-, T_2^+, E^+, A_2^- are chosen to match those used in Ref. [11] and correspond to linear combinations of spherical harmonics with ℓ_z equal to 0, 1, 2, 2, and 3, respectively. The basis vectors for the remaining irreps A_1^-, T_1^+, T_2^-, E^-, and A_2^+ are taken to be linear combinations of the corresponding basis vectors in Ref. [9]. The linear combinations are chosen so that the same Clebsch-Gordan coefficients presented in Ref. [11] can be used for positive and negative parity irreps in all cases. Note however that the rows of the $T_1^\pm$ irreps are ordered differently here than in Ref. [11] and Clebsch-Gordan coefficient results must be transposed accordingly (cf. conventions in Appendix A 3 below). A different set of basis vectors was used for O_h irreps in Ref. [15], and the explicit representation matrices obtained in the present work therefore differ from those in Ref. [15] by a change of basis.

The subgroups of O_h are summarized in Table XIV. The present work follows the naming scheme of Ref. [9] which labels one-dimensional irreps as variants of A or B and two-dimensional irreps as variants of E. It bears emphasizing that irreps of different groups may have identical names, but should be distinguished. The Clebsch-Gordan coefficients for little-group irreps below can be deduced from the corresponding Clebsch-Gordan results in Ref. [11] for the O_h basis vectors identified with the little-group basis vectors, or they can be calculated directly from the little-group irrep matrices as described for example in Ref. [20]. As shown in Table I, basis functions for all irreps follow from the irreps of O_h.

It is useful to make several notes regarding the conventions in Table I.

(i) For C_{4v}, the irrep names and the coefficients appearing in the E irrep definition are chosen so that identical representation matrices for little group transformations are obtained as those presented in Ref. [15].

(ii) For C_{4v}, the basis functions for irreps of O_h in Table I are eigenstates of L_z, which singles out the $\hat{e}_z$–axis. Other choices for the reference momentum, e.g., $\boldsymbol{P}' = \frac{2\pi}{L}(n, 0, 0)$, remain valid but less convenient, since the associated basis functions for C_{4v} must then be permuted.

(iii) For C_{3v}, the A_1 and A_2 representation matrices built from these basis vectors using Eq. (19) match those explicitly presented in Ref. [15]. The E representation matrices corresponding to this definition differ from those of Ref. [15] by interchange of the rows/columns [equivalent to $B_1^{(C_{3v},E)}(\boldsymbol{r}) \leftrightarrow B_2^{(C_{3v},E)}(\boldsymbol{r})$] for consistency with the convention of increasing ℓ_z with μ applied here to irreps of O_h. The conventions adopted here permit the Clebsch-Gordan coefficients for the A_1, A_2, and E irreps of Ref. [11] to be applied to the corresponding irreps of C_{3v}.

(iv) For C_{2v}, the irrep names are chosen so that the representation matrices match those explicitly presented in Ref. [15]. Clebsch-Gordan coefficients for this and other little groups with only one-dimensional irreps are equal to the Clebsch-Gordan coefficients in Ref. [11] for the irreps corresponding to the same basis vectors.

2. The double-cover group O_h^D

In the present work, the group O_h^D is defined using the Dirac spinor representation consisting of the direct sum of a positive-parity and a negative-parity spin-1/2 state, which provides a faithful representation of the full group of spatial transformations.

TABLE XIV. Explicit forms for groups appearing in this work for O_h, O_h^D, and their subgroups. Basis functions for irreps of O_h (and its subgroups) are given in Table I. Basis functions for the fermionic irreps of O_h^D (and its subgroups) are given in Table III. Group parametrizations for the subgroups of O_h^D follow from those of O_h by the replacements $r_i \to r_i^D$, $p_{ij} \to p_{ij}^D$ and the inclusion of inversions.

Momentum	$G_{\boldsymbol{P}}$	Order	Irreps	Group parametrization rp	Group elements
$\frac{2\pi}{L}(0,0,0)$	O_h	48	$\{A_1^\pm, A_2^\pm, E^\pm, T_1^\pm, T_2^\pm\}$	Eq. (A2)	Eq. (A4)
$\frac{2\pi}{L}(0,0,n)$	C_{4v}	8	$\{A_1, A_2, B_1, B_2, E\}$	$\{e, r_x, r_y, r_x r_y\} \times \{e, p_{xy}\}$	$\{1,2,13,14,25,26,37,38\}$
$\frac{2\pi}{L}(n,n,n)$	C_{3v}	6	$\{A_1, A_2, E\}$	$\{e\} \times \{e, p_{xy}, p_{yz}, p_{zx}, p_{xyz}, p_{xzy}\}$	$\{1,2,3,4,5,6\}$
$\frac{2\pi}{L}(0,n,n)$	C_{2v}	4	$\{A_1, A_2, B_1, B_2\}$	$\{e, r_x\} \times \{e, p_{yz}\}$	$\{1,3,25,27\}$
$\frac{2\pi}{L}(n,m,0)$	C_2^R	2	$\{A, B\}$	$\{e, r_z\} \times \{e\}$	$\{1,7\}$
$\frac{2\pi}{L}(n,n,m)$	C_2^P	2	$\{A, B\}$	$\{e\} \times \{e, p_{xy}\}$	$\{1,2\}$
$\frac{2\pi}{L}(n,m,p)$	C_1	1	$\{A\}$	$\{e\} \times \{e\}$	$\{1\}$
$\frac{2\pi}{L}(0,0,0)$	O_h^D	96	$\{G_1^\pm, G_2^\pm, H^\pm\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled Eq. (A2))	$\{1,2,\ldots,96\}$
$\frac{2\pi}{L}(0,0,n)$	Dic_4	16	$\{G_1, G_2\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_{4v})	(doubled C_{4v})
$\frac{2\pi}{L}(n,n,n)$	Dic_3	12	$\{G, F_1, F_2\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_{3v})	(doubled C_{3v})
$\frac{2\pi}{L}(0,n,n)$	Dic_2	8	$\{G\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_{2v})	(doubled C_{2v})
$\frac{2\pi}{L}(n,m,0)$	C_4^R	4	$\{F_1, F_2\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_2^R)	(doubled C_2^R)
$\frac{2\pi}{L}(n,n,m)$	C_4^P	4	$\{F_1, F_2\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_2^P)	(doubled C_2^P)
$\frac{2\pi}{L}(n,m,p)$	C_1^D	2	$\{F\}$	$\{e^D, R_{2\pi}^D\} \times$ (doubled C_1)	(doubled C_1)

The group elements of O_h can be mapped to (half of) the group elements of O_h^D by replacing rotation operators in the defining representations of SO(3) with the corresponding rotation operators in the Dirac spinor representation. To do so, first note that the explicit matrix representation of O_h in terms of permutations and reflections in Eqs. (A2) and (A3) can be (nonuniquely) related to a matrix representation in terms of rotations and the parity operator $P = \mathrm{diag}(-1,-1,-1)$ by

$$\begin{aligned} r_k &= P \cdot R(\pi \hat{e}_k), \\ p_{ij} &= P \cdot R(\pi \hat{e}_i) \cdot R\left(\frac{\pi}{2} \hat{e}_i \times \hat{e}_j\right). \end{aligned} \tag{A5}$$

Above, the $\hat{e}_i$ are unit vectors in the ith direction and $R(\vec{\omega}) \equiv R(\sum_k \omega_k \hat{e}_k)$ describes a rotation by angle $|\vec{\omega}|$ about the $\hat{\omega}$ axis,

$$R(\vec{\omega}) = \exp\left(-\sum_k \omega_k t_k\right) \tag{A6}$$

in terms of the $\mathfrak{so}(3)$ generators $[t_k]_{ij} = \varepsilon_{ijk}$.

The Dirac spinor representation of the corresponding element of the double cover is given by

$$R^D(\vec{\omega}) = \exp\left(-\frac{1}{8}\sum_{i,j,k} \omega_k \varepsilon_{ijk} [\gamma_i, \gamma_j]\right), \tag{A7}$$

where the γ_i are the spatial gamma matrices satisfying $\{\gamma_i, \gamma_j\} = 2\delta_{ij}$ and $\gamma_i^\dagger = \gamma_i$ (this choice coincides with both the Euclidean and mostly-positive Minkowski gamma matrices). The superscript D is used to denote double-cover group elements here and below. The definition in Eq. (A7) implies the transformation property

$$R^D \gamma^j (R^D)^\dagger = \sum_i \gamma^i R_{ij}. \tag{A8}$$

The Dirac spinor representation of the parity element P^D is given by the temporal gamma matrix up to an overall phase. The Euclidean γ_4 and Minkowski γ_0 are equivalent up to a phase choice. The present work takes $P^D = \gamma_4$, which satisfies $\{\gamma_i, \gamma_4\} = 0$, $\gamma_4^\dagger = \gamma_4$, and $\gamma_4^2 = 1$.

The double-cover permutations and reflections are then defined in the Dirac spinor representation by

$$\begin{aligned} r_k^D &= P^D \cdot R^D(\pi \hat{e}_k) = \gamma_5 \gamma_k, \\ p_{ij}^D &= P^D \cdot R^D(\pi \hat{e}_i) \cdot R^D\left(\frac{\pi}{2} \hat{e}_i \times \hat{e}_j\right) \\ &= \frac{1}{\sqrt{2}} \gamma_5 (\gamma_i - \gamma_j), \end{aligned} \tag{A9}$$

where $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4$ is the fifth Euclidean gamma matrix. The set of products of r_k^D and p_{ij}^D analogous to Eq. (A4) provides an explicit matrix representation of the first 48 elements of O_h^D. Note that this set is not closed under group multiplication; O_h is not a subgroup of O_h^D. The remaining 48 elements can be obtained by multiplying these elements by a 2π rotation,

$$R_{2\pi}^D = \mathrm{diag}(-1,-1,-1,-1), \tag{A10}$$

where the form above holds for a 2π rotation about any axis.

The numerical implementation in Ref. [18] uses the Dirac-Pauli basis, in which the γ-matrices are represented in 2×2 block form as

$$\gamma_k = \begin{pmatrix} 0 & -i\sigma_k \\ i\sigma_k & 0 \end{pmatrix}, \qquad \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \gamma_5 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}, \tag{A11}$$

where the σ_k are the usual Pauli matrices and I is the 2×2 identity matrix; for more details and relations to other common bases see Ref. [11].[9]

To distinguish the notion of abstract group elements $R^D \in O_h^D$ from the specific spinor representation in this basis, the action of the group on these spinors is denoted by $S(R^D)$, following the convention of Ref. [15]. Because this is the defining representation, the matrix representations are simply given by $S(R^D) = R^D$ using the definitions in Eq. (A9) and the Dirac-Pauli basis above.

Basis vectors for irreps of O_h^D and its subgroups are summarized in Table III. The naming convention in the present work follows Ref. [15] in denoting 1, 2, and 4 dimensional fermionic irreps by F, G, and H, respectively. For alternative strategies involving subduction of O_h^D irreps into little-group irreps, see Refs. [15,45].

The only nontrivial basis vectors are associated with 1-dimensional irreps F_1 and F_2 of Dic_3, which serves as the little group for the momentum $\boldsymbol{P} = \frac{2\pi}{L}(n,n,n)$ for any $n \in \mathbb{Z}\backslash\{0\}$. Basis vectors for F_1 and F_2 may be obtained by projecting to the linear combinations of $\{|\frac{3}{2},\frac{3}{2},+\rangle, |\frac{3}{2},\frac{1}{2},+\rangle, |\frac{3}{2},-\frac{1}{2},+\rangle, |\frac{3}{2},-\frac{3}{2},+\rangle\}$ transforming in these irreps using Schur's lemma (see Eq. (30) and the characters of F_1 and F_2 given in Ref. [15]. It is also possible to identify these irreps from first principles by determining the two-dimensional orthogonal complement of the G irrep contained in the $J = 3/2$ representation using Gram-Schmidt orthonormalization, then solving for linear combinations that diagonalize the representation matrices for this orthogonal compliment. The basis vectors used in this work are:

$$B_1^{(\mathrm{Dic}_3,F_1)} = \frac{1}{2}\left|\frac{3}{2},\frac{3}{2},+\right\rangle - \frac{(1-i)(\sqrt{2}-2i)}{4\sqrt{3}}\left|\frac{3}{2},\frac{1}{2},+\right\rangle + \frac{\sqrt{2}+i}{2\sqrt{3}}\left|\frac{3}{2},-\frac{1}{2},+\right\rangle - \frac{1+i}{2\sqrt{2}}\left|\frac{3}{2},-\frac{3}{2},+\right\rangle, \tag{A12}$$

$$B_1^{(\mathrm{Dic}_3,F_2)} = \frac{1}{2}\left|\frac{3}{2},\frac{3}{2},+\right\rangle + \frac{(1+i)(2-i\sqrt{2})}{4\sqrt{3}}\left|\frac{3}{2},\frac{1}{2},+\right\rangle - \frac{\sqrt{2}-i}{2\sqrt{3}}\left|\frac{3}{2},-\frac{1}{2},+\right\rangle + \frac{1+i}{2\sqrt{2}}\left|\frac{3}{2},-\frac{3}{2},+\right\rangle. \tag{A13}$$

3. Phase conventions

The block-diagonalization matrices in Eq. (1) are only defined up to an overall phase. This appendix records the phase conventions used in Ref. [18].

For each irrep *except* $T_2^{\pm}$ of the cubic group, the overall phase within each irrep is selected such that the first nonzero entry of $U^{(\Gamma_i,\kappa,s)}_{m,\mu=1}$ is real and positive. For $T_2^{\pm}$ of the cubic group, the overall phase is selected such that $U^{(\Gamma_i,\kappa,s)}_{m,\mu=2}$ is purely imaginary with negative imaginary part. This choice matches the basis-vector conventions of Ref. [11], where the combination of spherical harmonics $Y_2^2 - Y_2^{-2}$ is used as the $\mu = 2$ basis vector for T_2. This choice ensures that the Clebsch-Gordan coefficients presented in Ref. [11] are applicable to operators constructed using the methods of the present work (noting the different ordering of the rows of the $T_1^{\pm}$ irreps discussed above).

APPENDIX B: POLARIZATION TENSORS

This appendix recasts the computation of irrep matrices $D^{(\Gamma)}_{\mu'\mu}(R)$ (see Eq. (19)) algebraically using polarization tensors. For a given irrep Γ, the basis functions are homogeneous polynomials of fixed degree d, i.e., $B_\mu^{(\Gamma)}(\lambda \boldsymbol{r}) = \lambda^d B_\mu^{(\Gamma)}(\boldsymbol{r})$ for $\lambda \in \mathbb{R}$. Homogenous polynomials $B_\mu^{(\Gamma)}(\boldsymbol{r})$ can be expressed in terms of so-called *polarizations* $\mathcal{P}B_\mu^{(\Gamma)}$, symmetric rank-$d$ tensors defined via [46]

$$\begin{aligned}[\mathcal{P}B_\mu^{(\Gamma)}](\boldsymbol{r}_{(1)},\ldots,\boldsymbol{r}_{(d)}) &\equiv (\mathcal{P}B_\mu^{(\Gamma)})_{a_1a_2\ldots a_d} r^{a_1}_{(1)} r^{a_2}_{(2)} \cdots r^{a_d}_{(d)} \\ &\equiv \frac{1}{d!}\frac{\partial}{\partial\lambda_1}\cdots\frac{\partial}{\partial\lambda_d} B_\mu^{(\Gamma)}(\lambda_1\boldsymbol{r}_{(1)} + \cdots + \lambda_d \boldsymbol{r}_{(d)})\Big|_{\lambda_i=0}, \end{aligned} \tag{B1}$$

where $\{\boldsymbol{r}_{(i)} \in \mathbb{R}^3, 1 \le i \le d\}$ are arbitrary auxiliary vectors.[10] In the second line, summation is implied over the repeated indices $a_i \in \{1,2,3\}$. The polarization is symmetric and tensorial due to the symmetry and linearity of the derivatives. Evaluated diagonally (i.e., contracted with

[9]Note that the change-of-basis matrix relating the Dirac-Pauli and DeGrand-Rossi bases denoted $U^{(\mathrm{DR})}$ in Ref. [11] should be $\mathrm{U}^{(\mathrm{DR})} = (-i\gamma_2 + i\gamma_1\gamma_3)/\sqrt{2}$ in terms of Dirac-Pauli matrices.

[10]The identification between basis functions and symmetric tensors amounts to a map between the polynomial ring $K(\{x,y,z\})$ and the symmetric tensor space $S(\mathbb{R}^{3*})$. Such a relationship is quite general. In fact, for any vector space V with basis B and dual space V^*, the two spaces are canonically isomorphic: $K(B) \simeq S(V^*)$ [46].

the same vector $\boldsymbol{r}$ along all d indices), the polarization returns the original homogeneous polynomial:

$$[\mathcal{P}B_\mu^{(\Gamma)}](\boldsymbol{r},\ldots,\boldsymbol{r}) = B_\mu^{(\Gamma)}(\boldsymbol{r}). \tag{B2}$$

This relationship can provide a useful consistency check in explicit calculations. In this work, polarizations are normalized with respect to the tensor inner product

$$\langle\!\langle X, Y\rangle\!\rangle \equiv (X^*)^{a_1 a_2 \ldots a_d}(Y)_{a_1 a_2 \ldots a_d}. \tag{B3}$$

Polarizations normalized with respect to this inner product are denoted by $\bar{B}_\mu^{(\Gamma)}$.

The transformation of $\bar{B}_\mu^{(\Gamma)}$ under rotations follows immediately from the definition in Eq. (B1),

$$\begin{aligned}&\bar{B}_\mu^{(\Gamma)}(R^{-1}\boldsymbol{r},\ldots,R^{-1}\boldsymbol{r})\\ &\quad= (\bar{B}_\mu^{(\Gamma)})_{a_1\ldots a_d} R_{b_1}{}^{a_1}\cdots R_{b_d}{}^{a_d} r^{b_1}\cdots r^{b_d}\\ &\quad\equiv (R\circ\bar{B}_\mu^{(\Gamma)})_{b_1\ldots b_d} r^{b_1}\cdots r^{b_d},\end{aligned} \tag{B4}$$

where the second line uses $R^{-1} = R^T$ and the final line defines $R\circ\bar{B}_\mu^{(\Gamma)}$. Given this transformation property, the inner product in Eq. (19) reduces to

$$D_{\mu'\mu}^{(\Gamma)}(R) = \langle\!\langle \bar{B}_{\mu'}^{(\Gamma)}, R\circ\bar{B}_\mu^{(\Gamma)}\rangle\!\rangle. \tag{B5}$$

The tensorial method for computing the matrix elements via Eq. (B5) generalizes easily to particles with spin (see Section III), since spin vectors can be viewed as basis vectors for the double-cover of the relevant little group with transformation properties analogous to Eq. (21).

An explicit example of polarization tensors in this context follows. Table I gives the basis function for $\ell_z = 1$ row of the irrep T_2^+ of O_h: $B_1^{(T_2^+)}(\boldsymbol{r}) = (-zx + iyz)/\sqrt{2}$. This function is a homogeneous degree-2 polynomial, so the polarization will be a rank-2 tensor. Using the coordinates $\boldsymbol{r}_{(i)} = (x_{(i)}, y_{(i)}, z_{(i)})$ for auxiliary vectors, the polarization is

$$\begin{aligned}&[\mathcal{P}\bar{B}_1^{(T_2^+)}](\boldsymbol{r}_{(1)},\boldsymbol{r}_{(2)})\\ &\quad= \frac{1}{2\sqrt{2}}[-z_{(1)}x_{(2)} - x_{(1)}z_{(2)} + iy_{(1)}z_{(2)} + iz_{(1)}y_{(2)}].\end{aligned} \tag{B6}$$

The nonzero components of the normalized basis tensor are

$$\begin{aligned}(\bar{B}_1^{(T_2^+)})_{13} &= (\bar{B}_1^{(T_2^+)})_{31} = -\frac{1}{2},\\ (\bar{B}_1^{(T_2^+)})_{23} &= (\bar{B}_1^{(T_2^+)})_{32} = \frac{i}{2}.\end{aligned} \tag{B7}$$

As an example of the algebraic setup, consider the transformation about the y-axis sending $x\to z$ and $z\to -x$:

$$R = \begin{pmatrix} 0 & 0 & 1\\ 0 & 1 & 0\\ -1 & 0 & 0\end{pmatrix}. \tag{B8}$$

The matrix element of this rotation between $\bar{B}_1^{(T_2^+)}$ and itself is given by

$$D_{11}^{(T_2^+)}(R) = \langle\!\langle \bar{B}_1^{(T_2^+)}, R\circ\bar{B}_1^{(T_2^+)}\rangle\!\rangle \tag{B9}$$

$$= \mathrm{tr}\left[\begin{pmatrix} 0 & 0 & -1/2\\ 0 & 0 & -i/2\\ -1/2 & -i/2 & 0\end{pmatrix}\begin{pmatrix} 0 & i/2 & 1/2\\ i/2 & 0 & 0\\ 1/2 & 0 & 0\end{pmatrix}\right] \tag{B10}$$

$$= -1/2. \tag{B11}$$

The equivalent calculation in the integral setup is

$$D_{11}^{(T_2^+)}(R) = \frac{8}{\pi^2}\int d\Omega\left(\frac{-zx+iyz}{\sqrt{2}}\right)^*\left(\frac{xz+iyx}{\sqrt{2}}\right) \tag{B12}$$

$$\begin{aligned}&= \frac{-4}{\pi^2}\int d\Omega\, e^{i\varphi}\sin^2\theta\cos\theta\cos\varphi(\cos\theta + i\sin\theta\sin\varphi)\\ &= -1/2.\end{aligned} \tag{B13}$$

Although the integral in the second line is elementary, evaluating many such integrals is cumbersome when compared to tensor algebra.

APPENDIX C: EXPLICIT BLOCK-DIAGONALIZATION MATRICES

This appendix presents examples of block-diagonalization matrices in the rest frame in a few illustrative cases. The results in Tables XV–XVII employ the phase conventions in Appendix A 3.

TABLE XV. Table of $U^{(\Gamma,\kappa,s)}_{m\mu}$ for the orbit of $[\boldsymbol{n}_1,\boldsymbol{n}_2]=[(0,0,1),(0,0,-1)]$. Columns of the tables are listed in order of increasing $m\in\{1,\ldots,6\}$. Only the momentum of the first operator is shown in the column header.

Γ,κ	μ	(0, 0, 1)	(0, 1, 0)	(1, 0, 0)	(0, 0, −1)	(0, −1, 0)	(−1, 0, 0)
$A_1^+,1$	1	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$\frac{1}{\sqrt{6}}$
$E^+,1$	1	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$\frac{1}{\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$	$-\frac{1}{2\sqrt{3}}$
	2	0	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$	$\frac{1}{2}$
$T_1^-,1$	1	$\frac{1}{\sqrt{2}}$	0	0	$-\frac{1}{\sqrt{2}}$	0	0
	2	0	$\frac{i}{2}$	$-\frac{1}{2}$	0	$-\frac{i}{2}$	$\frac{1}{2}$
	3	0	$\frac{i}{2}$	$\frac{1}{2}$	0	$-\frac{i}{2}$	$-\frac{1}{2}$

TABLE XVI. Table of $U^{(\Gamma,\kappa,s)}_{m\mu}$ for the orbit of $[\boldsymbol{n}_1,\boldsymbol{n}_2]=[(0,1,1),(0,-1,-1)]$. Columns of the tables are listed in order of increasing $m\in\{1,\ldots,12\}$. Only the momentum of the first operator is shown in the column header.

Γ,κ	μ	(1, 1, 0)	(1, 0, 1)	(0, 1, 1)	(1, 0, −1)	(0, 1, −1)	(1, −1, 0)	(0, −1, 1)	(0, −1, −1)	(−1, 1, 0)	(−1, 0, 1)	(−1, 0, −1)	(−1, −1, 0)
$A_1^+,1$	1	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$	$\frac{1}{2\sqrt{3}}$
$E^+,1$	1	$\frac{1}{\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$-\frac{1}{2\sqrt{6}}$	$\frac{1}{\sqrt{6}}$
	2	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0
$T_2^+,1$	1	0	$-\frac{1}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	0	$-\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0
	2	$-\frac{i}{2}$	0	0	0	0	$\frac{i}{2}$	0	0	$\frac{i}{2}$	0	0	$-\frac{i}{2}$
	3	0	$\frac{1}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	0	$-\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	0	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	0
$T_1^-,1$	1	0	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	0
	2	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}$	$\frac{i}{4}$	$-\frac{1}{4}$	$\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$-\frac{i}{4}$	$-\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}-\frac{i}{4}$
	3	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}$	$\frac{i}{4}$	$\frac{1}{4}$	$\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{i}{4}$	$-\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}-\frac{i}{4}$
$T_2^-,1$	1	$\frac{1}{4}+\frac{i}{4}$	$-\frac{i}{4}$	$-\frac{1}{4}$	$-\frac{i}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}-\frac{i}{4}$	$\frac{i}{4}$	$\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$
	2	0	$-\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	0	$\frac{i}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	0	$-\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	0
	3	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{i}{4}$	$\frac{1}{4}$	$-\frac{i}{4}$	$\frac{1}{4}$	$\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{i}{4}$	$\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$

TABLE XVII. Table of $U^{(\Gamma,\kappa,s)}_{m\mu}$ for the orbit of $[\boldsymbol{n}_1,\boldsymbol{n}_2]=[(1,1,1),(-1,-1,-1)]$. Columns of the tables are listed in order of increasing $m\in\{1,\ldots,8\}$. Only the momentum of the first operator is shown in the column header.

Γ,κ	μ	(1, 1, 1)	(1, 1, −1)	(1, −1, 1)	(1, −1, −1)	(−1, 1, 1)	(−1, 1, −1)	(−1, −1, 1)	(−1, −1, −1)
$A_1^+,1$	1	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$
$T_2^+,1$	1	$-\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$
	2	$-\frac{i}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$\frac{i}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$	$-\frac{i}{2\sqrt{2}}$
	3	$\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$
$A_2^-,1$	1	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$
$T_1^-,1$	1	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$	$\frac{1}{2\sqrt{2}}$	$-\frac{1}{2\sqrt{2}}$
	2	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$
	3	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}+\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}+\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$	$-\frac{1}{4}-\frac{i}{4}$

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