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Generalized relativistic cubic harmonics

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Generalized relativistic cubic harmonics are constructed by methods based on purely group-theoretical considerations. Noncentered states localized either at primitive cubic or fcc or bcc sites or fractions thereof are symmetry adapted simultaneously to the full cubic point group O_h. The noncentered states are needed, for example, to define off-diagonal Green's functions describing fully relativistic scattering in real space.

I. INTRODUCTION

Relativistic effects play an important role in solid-state physics, not only because there are quite a few systems of considerable interest containing heavy elements, but also because some physical properties do require a relativistic description, such as, for example, transitions to core levels or nuclear-spin relaxation. In particular, with the help of the fully relativistic versions of the Korringa-Kohn-Rostoker (KKR) method (Onodera and Okazaki[1]), the KKR Green's-function (GF) method (Holzwarth,[2] Weinberger[3]), and the KKR coherent-potential approximation (CPA) (Staunton *et al.*[4]), it is possible to solve the band-structure problem not only for pure systems, but also for single isolated impurities such as Ni in a Au host (Weinberger[3]) and for concentrated alloys with $5d$ metal components such as $\mathrm{Ni}_x\mathrm{Pt}_{1-x}$ (Staunton *et al.*[4]). In the KKR GF, as well as in the KKR-CPA method, only the site-diagonal Green's function in real space is required, from which not only the density of states, charge densities, etc. can be calculated, but also the Bloch spectral functions (Faulkner,[5] Faulkner and Stocks,[6] Weinberger *et al.*[7]).

In all these applications it is sufficient to use the central-site double-group symmetrization given by Onodera and Okazaki.[8] However, there are rather important problems for which the off-diagonal Green's functions are needed, most prominently the problem of short-range order in disordered alloys. Here one must consider a cluster embedded in the CPA effective medium. By studying different configurations of atoms at the sites of the cluster, important insights are gained into short-range ordering. A similar problem must be solved when the cluster-variation method (de Fontaine[9]) is applied to calculate parameter-free phase diagrams.

In a different context, off-diagonal Green's functions are also needed whenever the local environment is of importance for a physical property or when the case of delocalized atoms is studied (Gonis *et al.*[10]). Obviously, in all these different cases the off-diagonal Green's functions must calculated relativistically, whenever heavy elements are involved, but what is meant by "heavy" in this context depends slightly on the physical property studied. In some cases, $4d$ elements already have to be studied relativistically. For systems involving $4f$, $5d$, and $5f$ elements, however, a fully relativistic description is of crucial importance.

Turning to the most intriguing problem, namely to the question of short-range order, one can easily check that the consideration of systems of d-only elements requires a matrix for the relativistic Green's function of order $18\times(N+1)$, where N is the number of neighboring sites included. For an octahedral cluster this implies the calculation of a matrix of order 126 in terms of 8001 Brillouin-zone integrals for each energy point on an appropriate energy scale, which is prohibitive. Use of symmetry, however, can bring the work into manageable limits.

In the present paper, methods are discussed and applied to produce tables such that, independently of the highest angular momentum used and of the number of shells of neighbors considered, the appropriate site symmetry can be taken into account. It should be kept in mind that without this symmetrization a discussion of short-range order in such prominent systems as, for example, $\mathrm{Cu}_3\mathrm{Au}$, is virtually impossible, even with the most powerful supercomputers available.

Onodera and Okazaki[8] have obtained spinors centered on a single site that are symmetry-adapted to the double group corresponding to the full cubic point group O_h. The problem that we must handle is, starting from these centered spinors, to obtain spinors that are centered around bcc or fcc crystal sites or any fraction thereof and that are correctly symmetrized. A method to do this work has recently been given by Altmann and Dirl,[11] and it will be used here. Because of the widespread use of the Onodera-Okazaki expansions, we shall use precisely the definitions for the operations and representations of the point group O_h used by these authors.

II. O_h-SYMMETRIZED CENTERED DIRAC STATES

We follow closely the notation and definitions of Altmann and Dirl[11] as well as of Onodera and Okazaki.[8] In particular, we use exactly the same O_h-symmetrized spinors that have been calculated and tabulated by Onodera and Okazaki.[8] We denote these states as follows:

$$\begin{aligned} &|(lJ)\Gamma\sigma a\rangle=\phi_a^{(lJ)\Gamma\sigma} ,\\ &\Gamma\in\mathscr{A}_O ,\\ &\sigma=\pm ,\\ &a=1,2,\ldots,n_\Gamma , \end{aligned} \tag{2.1}$$

where $\mathscr{A}_O$ is the set of labels defining irreducible projective representations of the octahedral group O, σ is the parity, and a is the row index of the projective irreducible representation D^Γ of O. These are well-defined linear combinations of the spinors (3.9) which have been introduced in Ref. 11. Following Altmann and Dirl[11] or Messiah,[12] the centered O_h-adapted spinors are of the form

$$|(J)\tilde{\omega}\pm;\Gamma\sigma a\rangle=\sum_\lambda(\pm i)^{1/2-\lambda}R_\lambda\,|(\bar{\lambda}J)\Gamma\sigma_\lambda a\rangle\,|\lambda\rangle , \tag{2.2}$$

$$\bar{\lambda}=J+(-1)^{1/2-\lambda}(\tilde{\omega}/2) , \tag{2.3}$$

where R_λ is a radial function, $|\lambda\rangle$ is a two-spinor, and $\tilde{\omega}$ is the eigenvalue of the four-inversion operator I [defined in Eq. (3.5) of Ref. 11]. On account of (4.1)–(4.3) of Ref. 11, we define

$$\sigma_\lambda=\begin{cases}\sigma & \text{if } \lambda=\frac{1}{2} ,\\ -\sigma & \text{if } \lambda=-\frac{1}{2}\end{cases} \tag{2.4}$$

in order to achieve the following transformation law of (2.2) under a function-space operator $W(R)$, for $R\in O_h$,

$$W(R)\,|(J)\tilde{\omega}\pm;\Gamma\sigma a\rangle=\sum_b D_{ba}^{\Gamma,\sigma}(R)\,|(J)\tilde{\omega}\pm;\Gamma\sigma b\rangle , \tag{2.5}$$

because of the specific form of the four-inversion operator [see (3.4) and (3.3) of Ref. 11]. However, any other basis is equally well suited for our purposes. For instance, the states

$$|(\tilde{\omega}J)\Gamma\sigma a;\lambda\rangle=R_\lambda\,|(\bar{\lambda}J)\Gamma\sigma_\lambda a\rangle\,|\lambda\rangle \tag{2.6}$$

transform according to

$$W(R)\,|(\tilde{\omega}J)\Gamma\sigma a;\lambda\rangle=\sum_b D_{ba}^{\Gamma,\sigma}(R)\,|(\tilde{\omega}J)\Gamma\sigma b;\lambda\rangle , \quad R\in O_h \tag{2.7}$$

and, hence, verify (2.5). However, one must be aware that the states (2.6) are either given by Table I of Ref. 8 or they do not exist. For convenience, we give some examples:

$$|(+\tfrac{1}{2})\Gamma_6+a;\lambda\rangle=\begin{cases}|(1\,\tfrac{1}{2})\Gamma_6+a\rangle\,|\tfrac{1}{2}\rangle=0\\ |(0\,\tfrac{1}{2})\Gamma_6-a\rangle\,|-\tfrac{1}{2}\rangle=0\end{cases} , \tag{2.8}$$

$$|(-\tfrac{1}{2})\Gamma_6+a;\lambda\rangle=\begin{cases}|(0\,\tfrac{1}{2})\Gamma_6+a\rangle\,|\tfrac{1}{2}\rangle\\ |(1\,\tfrac{1}{2})\Gamma_6-a\rangle\,|-\tfrac{1}{2}\rangle\end{cases} , \tag{2.9}$$

$$|(+\tfrac{1}{2})\Gamma_6-a;\lambda\rangle=\begin{cases}|(1\,\tfrac{1}{2})\Gamma_6-a\rangle\,|\tfrac{1}{2}\rangle\\ |(0\,\tfrac{1}{2})\Gamma_6+a\rangle\,|-\tfrac{1}{2}\rangle\end{cases} , \tag{2.10}$$

$$|(-\tfrac{1}{2})\Gamma_6-a;\lambda\rangle=\begin{cases}|(0\,\tfrac{1}{2})\Gamma_6-a\rangle\,|\tfrac{1}{2}\rangle=0\\ |(1\,\tfrac{1}{2})\Gamma_6+a\rangle\,|-\tfrac{1}{2}\rangle=0\end{cases} . \tag{2.11}$$

Henceforward, we shall use the states (2.6).

III. CUBIC ORBITS, SHIFTED STATES, AND PERMUTATIONAL REPRESENTATIONS OF O_h

Given the centered O_h-adapted spinors, we must construct from them shifted states, as defined in Ref. 11, under translations that belong to the fcc Bravais lattice or that are well-defined fractions of such translations. However, as fcc lattices and bcc lattices—being associated with a given lattice constant—can be embedded in a primitive cubic lattice having a lattice constant of half of the former, we can do our job for the three different cubic lattices simultaneously. Moreover, we assume that our point group is the full cubic point group O_h. According to our approach,[13] we prefer to use vector and projective representations of the point group O_h, depending on whether the states belong to integral or half-integral quantum numbers of the angular momentum, instead of vector representations of the corresponding double point group O_h^*.

We note that in a crystal, as in a molecular system, identical atoms must occupy equivalent sites, i.e., positions that can be transformed among themselves by means of space-group operations, if the space group is the symmetry group of the given crystal structure. However, as we are only interested in the neighbors of a given atom (being located at a specific position that need not be the origin), we admit positions that can be reached by pure point-group operations of O_h. Hence we assume that our crystal structure is invariant under a symmorphic space group having O_h as its point group. The point-group operations are assumed to be assigned to a well-defined origin.

A set of equivalent sites is called an orbit (star) and the group of configuration-space operations that leaves a site invariant is called the stabilizer or little group. We accordingly write the little group $G(\mathbf{t})$ corresponding to the site denoted by $\mathbf{t}$ as follows,

$$G(\mathbf{t})=\{R\in O_h\,|\,R\mathbf{t}=\mathbf{t}\}\ , \tag{3.1}$$

where $\mathbf{t}\in\mathbb{R}^3$ need not necessarily belong to the Bravais lattice. Let

$$K(\mathbf{t})=O_h{:}G(\mathbf{t}) \tag{3.2}$$

be a set of left coset representatives that decompose O_h with respect to $G(\mathbf{t})$. Whenever possible, we choose $K(\mathbf{t})$ to be also a subgroup of O_h. Fortunately, for all the cases that occur we are able to choose $K(\mathbf{t})$ to be a subgroup of O_h.

Since fcc lattices, $T_{\text{fcc}}(a)$, as well as bcc lattices, $T_{\text{bcc}}(a)$, associated with a given lattice constant a, can be embedded in a primitive-cubic (pc) lattice, $T_{\text{pc}}(a/2)$, that has a lattice constant which is half of the former, we confine our considerations to the latter. For convenience, we denote the primitive cubic translations as follows:

$$\mathbf{p}=\sum_j m_j\mathbf{p}_j\ ,\quad m_j\in\mathbb{Z}\ ,\quad \{\mathbf{p}_j\}_l=(a/2)\delta_{jl}\ , \tag{3.3}$$

where the $\mathbf{p}_j$ are the basic translations. In order to distinguish translations with different lattice constants, we denote by capital letters translations that belong to Bravais lattices having a as lattice constant. We accordingly denote

$$\mathbf{P}_j=2\mathbf{p}_j\ ,\quad j=1,2,3 \tag{3.4}$$

as basic translations of a primitive-cubic lattice with a as lattice constant. Face-centered and body-centered (basic) translations are indicated by the symbols $\mathbf{F}$ and $\mathbf{B}$, respectively. As is well known from textbooks, we have

$$\mathbf{F}_j=\tfrac{1}{2}\sum_l(1-\delta_{jl})\mathbf{P}_l\ , \tag{3.5}$$

$$\mathbf{P}_l=\sum_j(-1)^{\delta_{jl}}\mathbf{F}_j\ , \tag{3.6}$$

$$\mathbf{B}_j=\tfrac{1}{2}\sum_l(-1)^{\delta_{jl}}\mathbf{P}_l\ , \tag{3.7}$$

$$\mathbf{P}_l=\sum_j(1-\delta_{jl})\mathbf{B}_j\ , \tag{3.8}$$

which shows that any $\mathbf{F}_j$ or $\mathbf{B}_j$ is an integral linear combination of $\mathbf{p}_l$ because of (3.4). Hence not every $\mathbf{p}\in T_{\text{pc}}(a/2)$ belongs to $T_{\text{fcc}}(a)$ and/or $T_{\text{bcc}}(a)$, respectively. Therefore,

$$\mathbf{p}=\sum_j N_j\mathbf{F}_j\quad\text{with } N_j\in\mathbb{Z}\ , \tag{3.9}$$

$$\mathbf{p}=\sum_j M_j\mathbf{B}_j\quad\text{with } M_j\in\mathbb{Z} \tag{3.10}$$

constrains the $m_j\in\mathbb{Z}$. Inserting (3.3), (3.6), (3.8), and (3.4) into (3.9) and (3.10), respectively, we obtain

$$N_j=\tfrac{1}{2}\sum_l(-1)^{\delta_{jl}}m_l\ , \tag{3.11}$$

$$M_j=\tfrac{1}{2}\sum_l(1-\delta_{jl})m_l\ , \tag{3.12}$$

where we additionally demand $N_j\in\mathbb{Z}$ and $M_j\in\mathbb{Z}$. This imposes constraints on the possible m_j values. For obvious reasons we restrict the m_j values as follows:

$$m_1\geq m_2\geq m_3\geq 0\ . \tag{3.13}$$

Hence for N_j to be an integer, we must require that $m_1+m_2+m_3$ be an even integer. For M_j to be an integer, likewise, we must require that m_i+m_j (i and j cyclically permuted) be even integers. In Table I we give the first 30 integer linear combinations of the $\mathbf{p}_j$'s and also write the corresponding $\mathbf{F}\in T_{\text{fcc}}(a)$ and/or $\mathbf{B}\in T_{\text{bcc}}(a)$ if they are integer linear combinations of the $\mathbf{F}_j$ and $\mathbf{B}_j$, respectively.

Now we easily infer from Table I that in taking (3.13) into account, only six different cases may occur. Clearly, at this stage we are allowed to skip the constraint that $m_j\in\mathbb{Z}$ ($j=1,2,3$), since the corresponding $G(\mathbf{p})$ are not affected whether the m_j are integers or not. The following cases occur:

$$\text{Case 1:}\quad m_1=m>0\ ,\quad m_2=m_3=0\ ,\quad m\in\mathbb{Z} \tag{3.14}$$

$$\text{Case 2:}\quad m_1=m_2=m>0\ ,\quad m_3=0\ ,\quad m\in\mathbb{Z} \tag{3.15}$$

$$\text{Case 3:}\quad m_1=m_2=m_3=m>0\ ,\quad m\in\mathbb{Z} \tag{3.16}$$

$$\text{Case 4:}\quad m_1=m>m_2=n>0\ ,\quad m_3=0\ ,\quad m,n\in\mathbb{Z} \tag{3.17}$$

$$\text{Case 5:}\quad m_1=m>m_2=m_3=n>0\ ,\quad m,n\in\mathbb{Z} \tag{3.18}$$

$$\text{Case 5}'\text{:}\quad m_1=m_2=m>m_3=n>0\ ,\quad m,n\in\mathbb{Z} \tag{3.19}$$

$$\text{Case 6:}\quad m_1>m_2>m_3>0\ ,\quad m_j\in\mathbb{Z}\ . \tag{3.20}$$

Clearly, cases 5 and 5′ are equivalent; nevertheless, we discuss them separately and show later that they are correlated in a simple manner.

The next task is to define, for a given case, the shifted states by means of appropriately defined translation operators. Before doing this, we list $G(\mathbf{p})$ and $K(\mathbf{p})$ for the various cases:

$$\text{Case 1:}\quad G(m\,0\,0)=\{E,C_{4x}^{+},C_{2x},C_{4x}^{-}\}\circledS\{E,\sigma_z\}\cong C_{4v}\ , \tag{3.21}$$

$$K(m\,0\,0)=\{E,C_{31}^{+},C_{31}^{-}\}\times\{E,I\}\cong C_{3i}\ , \tag{3.22}$$

$$\text{Case 2:}\quad G(m\,m\,0)=\{E,C_{25}\}\times\{E,\sigma_z\}\ , \tag{3.23}$$

$$K(m\,m\,0)=T\quad\text{(tetrahedral point group)}\ , \tag{3.24}$$

$$\text{Case 3:}\quad G(m\,m\,m)=\{E,C_{31}^{+},C_{31}^{-}\}\circledS\{E,\sigma_{22}\}\cong C_{3v}\ , \tag{3.25}$$

$$K(m\,m\,m)=\{E,C_{4z}^{+},C_{2z},C_{4z}^{-}\}\times\{E,I\}\cong C_{4i}\ , \tag{3.26}$$

$$\text{Case 4:}\quad G(m\,n\,0)=\{E,\sigma_z\}\ , \tag{3.27}$$

$$K(m\,n\,0)=O\quad\text{(octahedral point group)}\ , \tag{3.28}$$

$$\text{Case 5:}\quad G(m\,n\,n)=\{E,\sigma_{22}\}\ , \tag{3.29}$$

$$K(m\,n\,n)=O\ , \tag{3.30}$$

$$\text{Case 5}'\text{:}\quad G(m\,m\,n)=\{E,\sigma_{26}\}\ , \tag{3.31}$$

$$K(m\,m\,n)=O\ , \tag{3.32}$$

TABLE I. “Cubic” neighbors.

pc($a/2$)			fcc(a)			bcc(a)				
m_1	m_2	m_3	N_1	N_2	N_3	M_1	M_2	M_3	$d(\mathbf{p},\mathbf{0})$	Star of $\mathbf{t}$ vector
1	0	0							$1/2$	6 1
1	1	0	0	0	1				$1/\sqrt{2}$	12 2
1	1	1				1	1	1	$\sqrt{3}/2$	8 3
2	0	0	−1	1	1	0	1	1	1	6 1
2	1	0							$\sqrt{5}/2$	24 4
2	1	1	0	1	1				$\sqrt{6}/2$	24 5
2	2	0	0	0	2	1	1	2	$\sqrt{2}$	12 2
2	2	1							$3/2$	24 5′
3	0	0							$3/2$	6 1
3	1	0	−1	1	2				$\sqrt{10}/2$	24 4
3	1	1							$\sqrt{11}/2$	24 5
2	2	2	1	1	1	2	2	2	$\sqrt{3}$	8 3
3	2	0							$\sqrt{13}/2$	24 4
3	2	1							$\sqrt{14}/2$	48 6
4	0	0	−2	2	2	0	2	2	2	6 1
3	2	2							$\sqrt{17}/2$	24 5
4	1	0							$\sqrt{17}/2$	24 4
3	3	0	0	0	3				$3/\sqrt{2}$	12 2
4	1	1	−1	2	2				$3/\sqrt{2}$	24 5
3	3	1				2	2	3	$19/2$	24 5′
4	2	0	−1	1	3	1	2	3	$\sqrt{5}$	24 4
4	2	1							$\sqrt{21}/2$	48 6
3	3	2	1	1	2				$\sqrt{11/2}$	24 5′
4	2	2	0	2	2	2	3	3	$\sqrt{6}$	24 5
4	3	0							$5/2$	24 4
5	0	0							$5/2$	6 1
4	3	1	0	1	3				$\sqrt{13}/2$	48 6
5	1	0	−2	2	3				$\sqrt{13}/2$	24 4
3	3	3				3	3	3	$3\sqrt{3}/2$	8 3
5	1	1				1	3	3	$3\sqrt{3}/2$	24 5

Case 6: $G(m\,n\,0)=\{E\}$, (3.33)

$$K(m\,n\,0)=O_h=O\times\{E,I\}$$

(full octahedral point group) . (3.34)

Regarding the notation of point-group elements, we follow Ref. 11, which differs from Ref. 14. The point-group element R of Onodera and Okazaki[8] is defined in their Table II by the action of R on the components of a position vector $\mathbf{r}$, a point that must be borne in mind since it can easily lead into error.

It should be noted that O_h can be written for each case as a product of $K(m\,n\,0)$ times $G(m\,n\,0)$, but only in cases 2, 4, 5, 5′, and 6 is it a semidirect product, whereas in the other cases we are confronted with more general products.

As in Ref. 11, we define, as shifted states,

$$\Psi_{a;\lambda}^{(\tilde{\omega}J)\Gamma\sigma}(\mathbf{p};Z)=W(E\mid Z\mathbf{p})\,|\,(\tilde{\omega}J)\Gamma\sigma a;\lambda\rangle\ ,\quad Z\in K(\mathbf{p}) \tag{3.35}$$

where $W(E\mid Z\mathbf{p})$ acts in a nontrivial way on the spatial part of (2.6) by transforming $\mathbf{x}\in\mathbb{R}^3$ into $\mathbf{x}-Z\mathbf{p}\in\mathbb{R}^3$. Exploiting the definitions (3.35) we obtain

$$W(R\mid\mathbf{0})\Psi_{a;\lambda}^{(\tilde{\omega}J)\Gamma\sigma}(\mathbf{p};Z)=\sum_{Z'}P_{Z',Z}(\mathbf{p};R)\sum_{a'}D_{a'a}^{\Gamma,\sigma}(R)\Psi_{a';\lambda}^{(\tilde{\omega}J)\Gamma\sigma}(\mathbf{p};Z')\ ,$$

$$R\in O_h \text{ and } Z,Z'\in K(\mathbf{p}) \tag{3.36}$$

where the transformation law of the basis vectors $\mathbf{p}_j$, $j=1,2,3$, is defined by

$$R\,\mathbf{p}_j=\sum_l D_{lj}(R)\mathbf{p}_l . \tag{3.37}$$

The 3×3 matrix $D(R),R\in O_h$, are the so-called Jones symbols.[14]

The $|K(\mathbf{p})|$-dimensional representation $P(\mathbf{p})$ of O_h is given by

$$P_{Z',Z}(\mathbf{p};Y)=\delta_{Z',YZ}\ \text{ for all } Y\in K(\mathbf{p})\ , \tag{3.38}$$

$$P_{Z',Z}(\mathbf{p};H)=\begin{Bmatrix}1 & \text{if } Z'^{-1}HZ\in G(\mathbf{p})\\ 0 & \text{otherwise}\end{Bmatrix}$$

$$\text{for all } H\in G(\mathbf{p})\ . \tag{3.39}$$

In those cases where $K(\mathbf{p})$ is a normal subgroup of O_h, $P(\mathbf{p};H)$, for $H\in G(p)$, specializes to

$$P_{Z',Z}(\mathbf{p};H)=\delta_{Z',HZH^{-1}}\ \text{ if } K(\mathbf{p})\lhd O_h\ . \tag{3.40}$$

The property of $P(\mathbf{p})$ to be factorized into (3.38) and (3.39) will be exploited later,

$$P(\mathbf{p};YH)=P(\mathbf{p};Y)P(\mathbf{p};H)\ ,\quad Y\in K(\mathbf{p}),\quad H\in G(\mathbf{p})\ . \tag{3.41}$$

It is important to note that the orthogonal permutational representation (3.41) is defined by linear independent, but not orthogonal, states. Besides this, our only task is to decompose $P(\mathbf{p})$ into a direct sum of its irreducible constituents. Hence we must compute for each of the six cases an appropriate (unitary) similarity transformation satisfying

$$S(\mathbf{p})^{\dagger}P(\mathbf{p};R)S(\mathbf{p})=\bigoplus_{\Gamma,\sigma} m_{\mathbf{p};\Gamma\sigma}D^{\Gamma,\sigma}(R)\ ,\quad R\in O_h\ . \tag{3.42}$$

The quantity $m_{\mathbf{p};\Gamma\sigma}$ is called multiplicity and indicates how often $D^{\Gamma,\sigma}$ is contained in $P(\mathbf{p})$.

IV. REDUCTION OF THE PERMUTATIONAL REPRESENTATIONS

As already pointed out in the preceding section, we must determine appropriate unitary similarity transformations $S(\mathbf{p})$ satisfying (3.42). Following closely the method described in Ref. 15, (3.42) can be rewritten as

$$P(\mathbf{p};R)\mathbf{S}_j^{\Gamma\sigma;m}(\mathbf{p})=\sum_l D_{lj}^{\Gamma,\sigma}(R)\mathbf{S}_l^{\Gamma\sigma;m}(\mathbf{p})\ ,$$
$$\Gamma\in A_O\ ,\quad m=1,2,\ldots,m_{\mathbf{p};\Gamma\sigma}\ ,\quad j=1,2,\ldots,n_\Gamma \tag{4.1}$$

where A_O is the set of labels defining irreducible vector representations of the octahedral point group O, and m denotes the multiplicity index, which is necessary if an irreducible representation $D^{\Gamma,\sigma}$ of O_h occurs more than once. To clarify our notation, we write

$$\{\mathbf{S}_j^{\Gamma\sigma;m}(\mathbf{p})\}_Y=\{\mathbf{S}_j^{\Gamma\sigma;m}\}_Y=S_{Y;\Gamma\sigma mj}$$

where

$$Y\in K(\mathbf{p})\ ,$$

for the row index of $S(\mathbf{p})=S$, and

$$\Gamma\in A_O\ ,\quad \sigma=\pm\ ,\quad m=1,2,\ldots,m_{\mathbf{p};\Gamma\sigma}\ ,\quad j=1,2,\ldots,n_\Gamma \tag{4.2}$$

for the column index of S, where the label $\mathbf{p}$ is suppressed. Accordingly, the vectors $\mathbf{S}_j^{\Gamma\sigma;m}$ distinguish the various columns of the $|K(\mathbf{p})|$-dimensional subduction matrix S. The lexicographical sequence of the columns is fixed by conventions which must always be retained. Any change of the sequence would lead to erroneous results.

Regarding the irreducible representations, we use henceforward the projective representations of Onodera and Okazaki[8] given in Table II. For convenience the irreducible projective representations of the octahedral point group O are listed in Table III. On account of the fact that the irreducible representations of the point group O_h factorize into the irreducible representations of the point group O and of S_2 (C_i), we only tabulate the vector and projective representations of the point group O. Although the form of tabulation we prefer is uncommon, it is compact and informative and will be very useful in what follows. Because of the relation $R=XS$, with $X\in O$ and $S\in S_2=\{E,I\}$ (I being the inversion), we have

$$D^{\Gamma,\sigma}(R)=D^{\Gamma}(X)D^{\sigma}(S)\ ,\quad \Gamma\in A_O\cup\mathscr{A}_O\ ,\quad \sigma=\pm\ . \tag{4.3}$$

Accordingly, the irreducible representations of the octahedral point group O must be multiplied by ± 1 if an improper rotation, XI with $X\in O$, is taken, depending on the parity we want to consider. The notation we use is as follows. The columns are lexicographically enumerated by $\Gamma\in A_O\cup\mathscr{A}_O$, $v=1,2,\ldots,n_\Gamma$ and $j=1,2,\ldots,n_\Gamma$. The rows are indexed by the group elements $X\in O$ in consecutive order. Moreover, it should be noted that the irreducible vector representations of the point group O are chain-adapted to the tetrahedral point group T, i.e., they subduce the irreducible representations in block-diagonal form.

The next step in our method is to carry out the decompositions of the various cases that we have listed in Sec. III. Clearly, since every $P(\mathbf{p})$ is a vector representation of the point group O_h, we only need Table II. However, as the Clebsch-Gordan coefficients for O_h, which can easily be obtained from the Clebsch-Gordan coefficients of O (see, e.g., Ref 16), are representation dependent, one must be very cautious when using tables of Clebsch-Gordan coefficients given in the literature. Accordingly, the only task is to decompose properly the various permutation representations. We shall try to avoid as much as possible a computer calculation since, apart from two cases, the decompositions can be carried out elegantly without using a computer. The reason for doing this is to provide a method that can be generally applied in similar problems. A brief outline of the present approach is also given in Ref. 17. The task of decomposing a permutational representation is, of course, a special case of the reduction of reducible representations.

Case 1: $(m,0,0)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$ if fractions of integers are admitted; $\mathbb{Z}$ denotes the set of integers, $\mathbb{Q}$ the set of rationals). First of all one must determine $P(\mathbf{p};R)$, $R\in O_h$, for this case. Taking (3.21), (3.22) and (3.38), (3.39) into account, one readily obtains a six-dimensional permutational representation of the point group O_h. The row and column indices are enumerated by the $Y\in K(\mathbf{p})$ in the same sequence as they occur in (3.22).

The following decomposition is readily verified:

$$P(\mathbf{p},R)\cong D^{A_{1g}}(R)\oplus D^{E_g}(R)\oplus D^{T_{1u}}(R)\ . \tag{4.4}$$

Because of $|K(\mathbf{p})|=6$ we have to compute a 6-dimensional unitary matrix S satisfying (4.1). This was performed by means of a computer employing the projection-operator technique. Our result reads

TABLE II. Irreducible vector representations of the octahedral point group of O. $\{\mathbf{D}_j^{\Gamma v}\}_X = D_{jv}(X)$, $X \in O$; $\omega = e^{i\pi/3}$.

	A_1	A_2	E				T_1									T_2									
	1	1	1		2		1			2			3			1			2			3			
	1	1	1	2	1	2	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3	
E	1	1	1	0	0	1	1	0	0	0	1	0	0	0	1	1	0	0	0	1	0	0	0	1	1
C_{2x}	1	1	1	0	0	1	$\bar{1}$	0	0	0	$\bar{1}$	0	0	0	1	$\bar{1}$	0	0	0	$\bar{1}$	0	0	0	1	2
C_{2y}	1	1	1	0	0	1	1	0	0	0	$\bar{1}$	0	0	0	$\bar{1}$	1	0	0	0	$\bar{1}$	0	0	0	$\bar{1}$	3
C_{2z}	1	1	1	0	0	1	$\bar{1}$	0	0	0	1	0	0	0	$\bar{1}$	$\bar{1}$	0	0	0	1	0	0	0	$\bar{1}$	4
C^+_{4x}	1	$\bar{1}$	0	ω^*	ω	0	0	$\bar{i}$	0	$\bar{i}$	0	0	0	0	1	0	i	0	i	0	0	0	0	$\bar{1}$	5
C^-_{4x}	1	$\bar{1}$	0	ω^*	ω	0	0	i	0	i	0	0	0	0	1	0	$\bar{i}$	0	$\bar{i}$	0	0	0	0	$\bar{1}$	6
C^+_{4y}	1	$\bar{1}$	0	ω	ω^*	0	1	0	0	0	0	$\bar{1}$	0	1	0	$\bar{1}$	0	0	0	0	1	0	$\bar{1}$	0	7
C^-_{4y}	1	$\bar{1}$	0	ω	ω^*	0	1	0	0	0	0	1	0	$\bar{1}$	0	$\bar{1}$	0	0	0	0	$\bar{1}$	0	1	0	8
C^+_{4z}	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	0	0	$\bar{i}$	0	1	0	$\bar{i}$	0	0	0	0	i	0	$\bar{1}$	0	$\bar{i}$	0	0	9
C^-_{4z}	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	0	0	i	0	1	0	i	0	0	0	0	$\bar{i}$	0	$\bar{1}$	0	$\bar{i}$	0	0	10
C_{21}	1	$\bar{1}$	0	ω^*	ω	0	0	$\bar{i}$	0	$\bar{i}$	0	0	0	0	$\bar{1}$	0	i	0	$\bar{i}$	0	0	0	0	1	11
C_{22}	1	$\bar{1}$	0	ω^*	ω	0	0	i	0	$\bar{i}$	0	0	0	0	$\bar{1}$	0	$\bar{i}$	0	i	0	0	0	0	1	12
C_{23}	1	$\bar{1}$	0	ω	ω^*	0	$\bar{1}$	0	0	0	0	$\bar{1}$	0	$\bar{1}$	0	1	0	0	0	0	1	0	1	0	13
C_{24}	1	$\bar{1}$	0	ω	ω^*	0	$\bar{1}$	0	0	0	0	1	0	1	0	1	0	0	0	0	$\bar{1}$	0	$\bar{1}$	0	14
C_{25}	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	0	0	i	0	$\bar{1}$	0	$\bar{i}$	0	0	0	0	$\bar{i}$	0	1	0	i	0	0	15
C_{26}	1	$\bar{1}$	0	$\bar{1}$	$\bar{1}$	0	0	0	$\bar{i}$	0	$\bar{1}$	0	i	0	0	0	0	i	0	1	0	$\bar{i}$	0	0	16
C^+_{31}	1	1	$\bar{\omega}^*$	0	0	$\bar{\omega}$	0	$\bar{i}$	0	0	0	$\bar{1}$	$\bar{i}$	0	0	0	$\bar{i}$	0	0	0	$\bar{1}$	$\bar{i}$	0	0	17
C^-_{31}	1	1	$\bar{\omega}$	0	0	$\bar{\omega}^*$	0	0	i	i	0	0	0	$\bar{1}$	0	0	0	i	i	0	0	0	$\bar{1}$	0	18
C^-_{32}	1	1	$\bar{\omega}$	0	0	$\bar{\omega}^*$	0	0	$\bar{i}$	$\bar{i}$	0	0	0	$\bar{1}$	0	0	0	$\bar{i}$	$\bar{i}$	0	0	0	$\bar{1}$	0	19
C^+_{32}	1	1	$\bar{\omega}^*$	0	0	$\bar{\omega}$	0	i	0	0	0	$\bar{1}$	i	0	0	0	i	0	0	0	$\bar{1}$	i	0	0	20
C^-_{33}	1	1	$\bar{\omega}$	0	0	$\bar{\omega}^*$	0	0	$\bar{i}$	i	0	0	0	1	0	0	0	$\bar{i}$	i	0	0	0	1	0	21
C^+_{33}	1	1	$\bar{\omega}^*$	0	0	$\bar{\omega}$	0	$\bar{i}$	0	0	0	1	i	0	0	0	$\bar{i}$	0	0	0	1	i	0	0	22
C^+_{34}	1	1	$\bar{\omega}^*$	0	0	$\bar{\omega}$	0	i	0	0	0	1	$\bar{i}$	0	0	0	i	0	0	0	1	$\bar{i}$	0	0	23
C^-_{34}	1	1	$\bar{\omega}$	0	0	$\bar{\omega}^*$	0	0	i	$\bar{i}$	0	0	0	1	0	0	0	i	$\bar{i}$	0	0	0	1	0	24

$$\begin{array}{cccccc|c} A_{1g} & E_g & & & T_{1u} & & \Gamma,\sigma \\ 1 & 1 & 2 & 1 & 2 & 3 & j \\ \hline \end{array}$$

$$S=\left[\begin{array}{cccccc} \delta & \delta & \delta\omega & 0 & 0 & i\alpha \\ \delta & \bar{\omega} & \bar{\delta} & \bar{\alpha} & 0 & 0 \\ \delta & \bar{\delta}\omega^* & \omega^* & 0 & i\bar{\alpha} & 0 \\ \delta & \delta & \omega & 0 & 0 & i\bar{\alpha} \\ \delta & \bar{\omega} & \bar{\delta} & \alpha & 0 & 0 \\ \delta & \bar{\delta}\omega^* & \omega^* & 0 & i\alpha & 0 \end{array}\right] \begin{array}{|c} E \\ C^+_{31} \\ C^-_{31} \\ I \\ S^-_{61} \\ S^+_{61} \end{array} \tag{4.5}$$

where the columns of S are enumerated by $(\Gamma,\sigma) = A_{1g}, E_g, T_{1u}$ and $j=1,2,\ldots,n_\Gamma$ in lexicographical order. The rows are indexed (by E, C^+_{31}, C^-_{31}, I, S^-_{61}, S^+_{61}) in the same manner as they occur in $K(\mathbf{p})$. Since each irreducible vector representation of the point group O_h that occurs appears only once, we suppress the multiplicity index. It should be noted that the column vectors assigned to a particular irreducible representation of the point group O_h are uniquely defined up to an arbitrary phase factor. The abbreviations used in (4.5) are defined as $\delta = 1/\sqrt{6}$, $\omega = \exp(i\pi/3)$, and $\alpha = 1/\sqrt{2}$.

Case 2. $(m,m,0) \in \mathbb{Z}^3$ (or $\mathbb{Q}^3$). As in case 1 the first task is to compute $P(\mathbf{p};R)$, $R \in O_h$. Again we take (3.38) and (3.39), but now we must insert (3.23) and (3.24). The subduction matrix can now be determined by induction rather than by a computer calculation. As already pointed out, the point group O_h can be written as a semidirect product of $K(\mathbf{p})$ times $G(\mathbf{p})$, i.e.,

$$O_h = K(\mathbf{p}) \circledS G(\mathbf{p})\ , \quad K(\mathbf{p}) \lhd O_h\ . \tag{4.6}$$

We reorder this semidirect product as follows, for convenience,

$$O_h = [K(\mathbf{p}) \circledS \{E, C_{25}\}] \times \{E, I\}\ . \tag{4.7}$$

Because of (3.38), $P(\mathbf{p};Y)$, for $Y \in K(\mathbf{p}) = T$, is the regular matrix representation of T (see Ref. 18). The first task now is to decompose the regular representation of T into its irreducible constituents, i.e., to bring the matrix into block-diagonal form. Hence we want to find a $|T|$-dimensional matrix B whose columns satisfy

TABLE III. Irreducible projective representations of the octahedral point group of O. $\{\mathbf{D}_j^{\Gamma v}\}_X = D_{jv}^{\Gamma}(X)$, $X \in O$; $a = 1/\sqrt{2}$, $A = a(1+i)$, and $\underset{\sim}{A} = A/\sqrt{2}$; $b = \sqrt{3/8}$ and $c = \sqrt{2}/4$; $D = (1+i)/4$ and $E = \sqrt{3}(1+i)/4$.

	$E_{1/2}$				$E_{5/2}$				$G_{3/2}$																
	1		2		1		2		1				2				3				4				
	1	2	1	2	1	2	1	2	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4	
E	1	0	0	1	1	0	0	1	1	0	0	0	0	1	0	0	0	0	1	0	0	0	0	1	1
C_{2x}	0	$\bar{i}$	$\bar{i}$	0	0	$\bar{i}$	$\bar{i}$	0	0	0	0	i	0	0	i	0	0	i	0	0	i	0	0	0	2
C_{2y}	0	1	$\bar{1}$	0	0	1	$\bar{1}$	0	0	0	0	1	0	0	$\bar{1}$	0	0	1	0	0	$\bar{1}$	0	0	0	3
C_{2z}	$\bar{i}$	0	0	i	$\bar{i}$	0	0	i	i	0	0	0	0	$\bar{i}$	0	0	0	0	i	0	0	0	0	i	4
C_{4x}^+	a	$i\bar{a}$	$i\bar{a}$	a	$\bar{a}$	ia	ia	$\bar{a}$	c	$i\bar{b}$	$\bar{b}$	ic	$i\bar{b}$	$\bar{c}$	$i\bar{c}$	$\bar{b}$	$\bar{b}$	$i\bar{c}$	$\bar{c}$	$i\bar{b}$	ic	$\bar{b}$	$i\bar{b}$	c	5
C_{4x}^-	a	ia	ia	a	$\bar{a}$	$i\bar{a}$	$i\bar{a}$	$\bar{a}$	c	ib	$\bar{b}$	$i\bar{c}$	ib	$\bar{c}$	ic	$\bar{b}$	$\bar{b}$	ic	$\bar{c}$	ib	$i\bar{c}$	$\bar{b}$	ib	c	6
C_{4y}^+	a	a	$\bar{a}$	a	$\bar{a}$	$\bar{a}$	a	$\bar{a}$	c	b	b	c	$\bar{b}$	$\bar{c}$	c	b	b	$\bar{c}$	$\bar{c}$	b	$\bar{c}$	b	$\bar{b}$	c	7
C_{4y}^-	a	$\bar{a}$	a	a	$\bar{a}$	a	$\bar{a}$	$\bar{a}$	c	$\bar{b}$	b	$\bar{c}$	b	$\bar{c}$	$\bar{c}$	b	b	c	$\bar{c}$	$\bar{b}$	c	b	b	c	8
C_{4z}^+	A^*	0	0	A	$\bar{A}^*$	0	0	$\bar{A}$	$\bar{A}$	0	0	0	0	A^*	0	0	0	0	A	0	0	0	0	$\bar{A}^*$	9
C_{4z}^-	A	0	0	A^*	$\bar{A}$	0	0	$\bar{A}^*$	$\bar{A}^*$	0	0	0	0	A	0	0	0	0	A^*	0	0	0	0	$\bar{A}$	10
C_{21}	$i\bar{a}$	a	$\bar{a}$	ia	ia	$\bar{a}$	a	$i\bar{a}$	ic	$\bar{b}$	$i\bar{b}$	c	b	ic	c	ib	$i\bar{b}$	$\bar{c}$	$i\bar{c}$	$\bar{b}$	$\bar{c}$	ib	b	$i\bar{c}$	11
C_{22}	ia	a	$\bar{a}$	$i\bar{a}$	$i\bar{a}$	$\bar{a}$	a	ia	$i\bar{c}$	$\bar{b}$	ib	c	b	$i\bar{c}$	c	$i\bar{b}$	ib	$\bar{c}$	ic	$\bar{b}$	$\bar{c}$	$i\bar{b}$	b	ic	12
C_{23}	$i\bar{a}$	$i\bar{a}$	$i\bar{a}$	ia	ia	ia	ia	$i\bar{a}$	ic	ib	ib	ic	ib	ic	$i\bar{c}$	$i\bar{b}$	ib	$i\bar{c}$	$i\bar{c}$	ib	ic	$i\bar{b}$	ib	$i\bar{c}$	13
C_{24}	$i\bar{a}$	ia	ia	ia	ia	$i\bar{a}$	$i\bar{a}$	$i\bar{a}$	ic	$i\bar{b}$	ib	$i\bar{c}$	$i\bar{b}$	ic	ic	$i\bar{b}$	ib	ic	$i\bar{c}$	$i\bar{b}$	$i\bar{c}$	$i\bar{b}$	$i\bar{b}$	$i\bar{c}$	14
C_{25}	0	A^*	$\bar{A}$	0	0	$\bar{A}^*$	A	0	0	0	0	$\bar{A}$	0	0	$\bar{A}^*$	0	0	A	0	0	A^*	0	0	0	15
C_{26}	0	$\bar{A}$	A^*	0	0	A	$\bar{A}^*$	0	0	0	0	A^*	0	0	A	0	0	$\bar{A}^*$	0	0	$\bar{A}$	0	0	0	16
C_{31}^+	$\underset{\sim}{A}^*$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}$	$\bar{D}$	$\bar{E}$	$\bar{E}$	$\bar{D}$	$\bar{E}^*$	$\bar{D}^*$	D^*	E^*	E	$\bar{D}$	$\bar{D}$	E	D^*	$\bar{E}^*$	E^*	$\bar{D}^*$	17
C_{31}^-	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\bar{D}^*$	$\bar{E}$	E^*	D	$\bar{E}^*$	$\bar{D}$	$\bar{D}^*$	$\bar{E}$	$\bar{E}^*$	D	$\bar{D}^*$	E	$\bar{D}^*$	E	E^*	$\bar{D}$	18
C_{32}^-	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\bar{D}$	$\bar{E}^*$	E	D^*	$\bar{E}$	$\bar{D}^*$	$\bar{D}$	$\bar{E}^*$	$\bar{E}$	D^*	$\bar{D}$	E^*	$\bar{D}$	E^*	E	$\bar{D}^*$	19
C_{32}^+	$\underset{\sim}{A}$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}^*$	$\bar{D}^*$	$\bar{E}^*$	$\bar{E}^*$	$\bar{D}^*$	$\bar{E}$	$\bar{D}$	D	E	E^*	$\bar{D}^*$	$\bar{D}^*$	E^*	D	$\bar{E}$	E	$\bar{D}$	20
C_{33}^-	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\bar{D}$	E^*	E	$\bar{D}^*$	E	$\bar{D}^*$	D	$\bar{E}^*$	$\bar{E}$	$\bar{D}^*$	$\bar{D}$	$\bar{E}^*$	D	E^*	$\bar{E}$	$\bar{D}^*$	21
C_{33}^+	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}^*$	$\bar{D}^*$	E^*	$\bar{E}^*$	D^*	E	$\bar{D}$	$\bar{D}$	E	E^*	D^*	$\bar{D}^*$	$\bar{E}^*$	$\bar{D}$	$\bar{E}$	$\bar{E}$	$\bar{D}$	22
C_{34}^+	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}$	$\bar{D}$	E	$\bar{E}$	D	E^*	$\bar{D}^*$	$\bar{D}^*$	E^*	E	D	$\bar{D}$	$\bar{E}$	$\bar{D}^*$	$\bar{E}^*$	$\bar{E}^*$	$\bar{D}^*$	23
C_{34}^-	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\underset{\sim}{A}$	$\underset{\sim}{A}^*$	$\bar{\underset{\sim}{A}}$	$\underset{\sim}{A}^*$	$\bar{D}^*$	E	E^*	$\bar{D}$	E^*	$\bar{D}$	D^*	$\bar{E}$	$\bar{E}^*$	$\bar{D}$	$\bar{D}^*$	$\bar{E}$	D^*	E	$\bar{E}^*$	$\bar{D}$	24

$$P(\mathbf{p};Y)\mathbf{B}_j^{\tau v} = \sum_l D_{lj}^{\tau}(Y)\mathbf{B}_l^{\tau v}, \quad Y \in T \tag{4.8}$$

where the irreducible representation labels of the tetrahedral point group T are denoted by τ. Firstly, one must note that, due to Burnside's theorem,[18] each irreducible representation occurs n_τ times, when $n_\tau = \dim D^\tau$. It has been shown[17] that this task can easily be implemented if a complete set of irreducible representations of $K(\mathbf{p})$ is known. Since this is the case, we define the column vectors $\mathbf{B}_j^{\tau v}$, $\tau \in A_T$, $v = 1,2,\ldots,n_\tau$, $j = 1,2,\ldots,n_\tau$, as follows:

$$\{\mathbf{B}_j^{\tau v}\}_Y = (n_\tau/12)^{1/2} D_{jv}^{\tau}(Y)^*, \quad Y \in T. \tag{4.9}$$

Hence the multiplicity index v can be chosen as the column index of $D^\tau(Y)$, $Y \in T$. It is readily verified that (4.8) holds. One must only specify $\mathbf{B}_j^{\tau v}$ by (4.9) and insert (3.38) by taking the multiplication law of the irreducible matrix representations into account. The proof is straightforward and need not be given here. The irreducible vector representations of T are easily extracted from the vector representations of O by deleting, in Table II, the rows associated with the group elements 5–16 and by confining oneself to the columns assigned to $\{A_1,1,1\}$, $\{E,1,1\}$, $\{E,2,2\}$, and $\{T_1,v,j\}$, with $v = 1,2,3$ and $j = 1,2,3$. This can be done because the irreducible vector representations of the octahedral point group O are $T \lhd O$ chain-adapted. This means that the irreducible vector representations of the point group O decompose into the block-diagonal form without any further similarity transformation, if restricted to the group elements of $K(\mathbf{p}) = T$. Although, in principle, the irreducible representations of the tetrahedral point group T can be taken from Table II, we give them separately in Table IV.

Clearly, the next step is to determine O-adapted states that are appropriate linear combinations of the vectors, $\mathbf{B}_j^{\tau v}$ $\tau \in A_T$, $v = 1,2,\ldots,n_\tau$ and $j = 1,2,\ldots,n_\tau$. Before doing this, it is useful to determine the irreducible constituents of $P(\mathbf{p};R)$, $R \in O_h$. We obtain

$$P(\mathbf{p};R)\cong D^{A_{1g}}(R)\oplus D^{E_g}(R)\oplus D^{T_{1u}}(R)$$
$$\oplus D^{T_{2g}}(R)\oplus D^{T_{2u}}(R)\ ,\quad R\in O_h \qquad (4.10)$$

which indicates that $P(\mathbf{p};X)$, $X\in O$, contains T_2 twice, whereas the other irreducible representations of the octahedral point group O occur only once. Even though this might cause some trouble when decomposing the representation $P(\mathbf{p};X)$, $X\in O$, into the irreducible representations of the point group O, it turns out to be handled easily,

$$P(\mathbf{p};X)\cong D^{A}(X)\oplus D^{E}(X)\oplus D^{T_1}(X)\oplus 2D^{T_2}(X)\ ,\quad X\in O. \qquad (4.11)$$

To obtain O-adapted vectors it suffices to know, in accordance with the chain (4.7), the action of $P(p;C_{25})$ on the vectors $\mathbf{B}_j^{\tau v}$. Because of (3.40), we have

$$P_{Z',Z}(\mathbf{p};C_{25})=\delta_{Z',C_{25}ZC_{25}}\ ,\quad Z,Z'\in K(\mathbf{p})=T \qquad (4.12)$$

which leads to

$$\{P(\mathbf{p};C_{25})\mathbf{B}_j^{\tau v}\}_Z=(n_\tau/12)^{1/2}D_{jv}^{\tau}(C_{25}ZC_{25})^*\ . \qquad (4.13)$$

We must hence, distinguish two different cases. Either the outer automorphism C_{25} maps τ onto τ, i.e.,

$$C_{25}(\tau)=\tau\in A_T\ , \qquad (4.14)$$

or it maps τ onto an inequivalent τ', i.e.,

$$C_{25}(\tau)=\tau'\neq\tau. \qquad (4.15)$$

Since we assume the actual form of the irreducible vector representations of the tetrahedral point group T (Table IV) in both situations we must expect nontrivial similarity transformations (i.e., n_τ-dimensional unitary matrices) satisfying

$$C_{25}(\tau)=\tau\colon\ D^{\tau}(C_{25}ZC_{25})=A^{\tau}(C_{25})D^{\tau}(Z)[A^{\tau}(C_{25})]^{\dagger}\ , \qquad (4.16)$$

$$C_{25}(\tau)=\tau'\colon\ D^{\tau}(C_{25}ZC_{25})=A^{\tau}(C_{25})D^{\tau'}(Z)[A^{\tau}(C_{25})]^{\dagger}. \qquad (4.17)$$

A simple manipulation yields

$$C_{25}(\tau)=\tau \ \text{ if } \tau=E,T\ ,$$
$$C_{25}(E_1)=E_2\ ,\quad C_{25}(E_2)=E_1\ , \qquad (4.18)$$

which is in agreement with the irreducible representations subduced from O, $D^{\Gamma}\downarrow T$. But, irrespective of which case of (4.18) is realized, we have the transformation property

$$P(\mathbf{p};C_{25})\mathbf{B}_j^{\tau v}=\sum_{w,l}A_{lj}^{\tau}(C_{25})A_{wv}^{\tau}(C_{25})\mathbf{B}_l^{C_{25}(\tau),w}\ . \qquad (4.19)$$

In deriving this formula, we utilized $A^{\tau}(C_{25})^2=\mathbb{1}_{n_\tau}$, since $P(\mathbf{p};C_{25})P(\mathbf{p};C_{25})=P(\mathbf{p};E)$ must be satisfied. We see that the action of $P(\mathbf{p};C_{25})$ on $\mathbf{B}_j^{\tau v}$ affects j as well as the multiplicity index v. On the other hand, we know that O-adapted vectors can only be linear combinations of the $\mathbf{B}_j^{\tau v}$ concerning only the multiplicity index v, since we want to retain their transformation law (4.8) with respect to the tetrahedral point group T. This, of course, drastically limits the possible transformations. We determine (4.19) for every case by direct manipulations. In detail, (4.19) turns out to be

$$P(C_{25})\mathbf{B}^{A}=\mathbf{B}^{A}\ , \qquad (4.20)$$

$$P(C_{25})\mathbf{B}^{E_1}=\mathbf{B}^{E_2}\ , \qquad (4.21)$$

$$P(C_{25})\mathbf{B}^{E_2}=\mathbf{B}^{E_1}\ , \qquad (4.22)$$

$$P(C_{25})\mathbf{B}_1^{T,2}=-i\mathbf{B}_3^{T,2}\ , \qquad (4.23)$$

$$P(C_{25})\mathbf{B}_2^{T,2}=\mathbf{B}_2^{T,2}\ , \qquad (4.24)$$

$$P(C_{25})\mathbf{B}_3^{T,2}=i\mathbf{B}_1^{T,2}\ , \qquad (4.25)$$

$$P(C_{25})\mathbf{B}_1^{T,1}=\mathbf{B}_3^{T,3}\ , \qquad (4.26)$$

$$P(C_{25})\mathbf{B}_2^{T,1}=i\mathbf{B}_2^{T,3}\ , \qquad (4.27)$$

$$P(C_{25})\mathbf{B}_3^{T,1}=-\mathbf{B}_1^{T,3}\ , \qquad (4.28)$$

$$P(C_{25})\mathbf{B}_1^{T,3}=-\mathbf{B}_3^{T,1}\ , \qquad (4.29)$$

$$P(C_{25})\mathbf{B}_2^{T,3}=-i\mathbf{B}_2^{T,1}\ , \qquad (4.30)$$

$$P(C_{25})\mathbf{B}_3^{T,3}=\mathbf{B}_1^{T,1}\ , \qquad (4.31)$$

TABLE IV. Irreducible vector representations of the tetrahedral point group T. $\{\mathbf{D}_j^{\lambda v}\}_Y=D_{jv}^{\lambda}(Y)$, $Y\in T$; $\omega=e^{i\pi/3}$.

	A	E_1	E_2	T									
	1	1	1	1			2			3			
	1	1	1	1	2	3	1	2	3	1	2	3	
E	1	1	1	1	0	0	0	1	0	0	0	1	1
C_{2x}	1	1	1	$\bar{1}$	0	0	0	$\bar{1}$	0	0	0	1	2
C_{2y}	1	1	1	1	0	0	0	$\bar{1}$	0	0	0	$\bar{1}$	3
C_{2z}	1	1	1	$\bar{1}$	0	0	0	1	0	0	0	$\bar{1}$	4
C_{31}^{+}	1	$\bar{\omega}^*$	$\bar{\omega}$	0	$\bar{i}$	0	0	0	$\bar{1}$	$\bar{i}$	0	0	17
C_{31}^{-}	1	$\bar{\omega}$	$\bar{\omega}^*$	0	0	i	i	0	0	0	$\bar{1}$	0	18
C_{32}^{-}	1	$\bar{\omega}$	$\bar{\omega}^*$	0	0	$\bar{i}$	$\bar{i}$	0	0	0	$\bar{1}$	0	19
C_{32}^{+}	1	$\bar{\omega}^*$	$\bar{\omega}$	0	i	0	0	0	$\bar{1}$	i	0	0	20
C_{33}^{-}	1	$\bar{\omega}$	$\bar{\omega}^*$	0	0	$\bar{i}$	i	0	0	0	1	0	21
C_{33}^{+}	1	$\bar{\omega}^*$	$\bar{\omega}$	0	$\bar{i}$	0	0	0	1	i	0	0	22
C_{34}^{+}	1	$\bar{\omega}^*$	$\bar{\omega}$	0	i	0	0	0	1	$\bar{i}$	0	0	23
C_{34}^{-}	1	$\bar{\omega}$	$\bar{\omega}^*$	0	0	i	$\bar{i}$	0	0	0	1	0	24

where again we omit the index **p** of the matrices $P(\mathbf{p};X)$, $X \in O$. Note that the multiplicity and row indices are omitted where they can take only one value. Equations (4.29)–(4.31) are an immediate consequence of (4.26)–(4.28), because of $P(C_{25})^2 = \mathbb{1}$, and are therefore redundant.

From (4.20)–(4.31), we infer that with respect to the basis **B** the permutational representation $P(X)$, $X \in O$, decomposes into three irreducible representations, and a reducible representation, of O. The group element C_{25} is represented with respect to $\mathbf{B}^A$ by the unity [see (4.20)]. With respect to $\mathbf{B}^{E_1}$ and $\mathbf{B}^{E_2}$, we obtain the following matrix:

$$C_{25} \rightarrow \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = F^E(C_{25}) \; . \tag{4.32}$$

Analogously, we have

$$C_{25} \rightarrow \begin{bmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ \bar{i} & 0 & 0 \end{bmatrix} = F^T(C_{25}) \; , \tag{4.33}$$

$$C_{25} \rightarrow \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & \bar{i} & 0 \\ 0 & 0 & 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} = E^T(C_{25}) \tag{4.34}$$

when taking into account (4.23)–(4.25) and (4.26)–(4.31) respectively. It is worth noting that the specific form of the matrices $F^T(C_{25})$ and $E^T(C_{25})$ is achieved by means of the definitions

$$P(C_{25})\mathbf{B}^{E_j} = \sum_k F^E_{kj}(C_{25})\mathbf{B}^{E_k} \; , \tag{4.35}$$

$$P(C_{25})\mathbf{B}^{T,2}_j = \sum_k F^T_{kj}(C_{25})\mathbf{B}^{T,2}_k \; , \tag{4.36}$$

$$P(C_{25})\mathbf{B}^{T,v}_j = \sum_{k,w} E^T_{kw,jv}(C_{25})\mathbf{B}^{T,w}_k \; , \quad v,w = 1,3 \; . \tag{4.37}$$

When adopting now the notation $\mathbf{C}^{\Gamma w}_j$, $\Gamma \in A_O$, $w = 1,2,3,\ldots,m_{\mathbf{p};\Gamma}$ (equal to the multiplicity of Γ), $j = 1,2,\ldots,n_\Gamma$ for O-adapted vectors, they satisfy the definition

$$P(X)\mathbf{C}^{\Gamma;w}_j = \sum_l D^\Gamma_{lj}(X)\mathbf{C}^{\Gamma;w}_l \; , \quad X \in O \; . \tag{4.38}$$

As already pointed out, the **C**'s must be appropriate linear combinations of the **B**'s. Hence, we must take linear transformations of the **B**'s where only the multiplicity index of the **B**'s is affected, since the **C**'s must satisfy (4.8) simultaneously. From (4.20), we may infer that

$$\mathbf{C}^{A_1} = \mathbf{B}^{A_1} \; . \tag{4.39}$$

However, since $F^E(C_{25}) = -D^E(C_{25})$ (see Table II), we are forced to take

$$\mathbf{C}^E_1 = \mathbf{B}^{E_1} \quad \text{and} \quad \mathbf{C}^E_2 = -\mathbf{B}^{E_2} \tag{4.40}$$

in order to achieve the desired transformation law (4.38). Of course, the vectors $\mathbf{C}^E_j$, $j = 1,2$, are unique up to an arbitrary overall phase factor. We choose this factor to be unity, but any other choice is equally well suited to satisfy (4.38). Because of

$$F^T(C_{25}) = D^{T_2}(C_{25}) \; , \tag{4.41}$$

the vectors $\mathbf{B}^{T,2}_j$, $j = 1,2,3$, are already O-adapted, i.e.,

$$\mathbf{C}^{T_2;1}_j = \mathbf{B}^{T,2}_j \; , \quad j = 1,2,3 \; . \tag{4.42}$$

It must be noted that a multiplicity index must be added since T_2 occurs twice in $P(\mathbf{p};X)$, $X \in O$.

The next task consists of the decomposition of (4.34) into its irreducible constituents T_1 and T_2, which are two inequivalent irreducible representations of the point group O. We immediately infer this result from (4.11). A simple manipulation shows that the following states,

$$\mathbf{C}^{T_2;2}_j = \frac{1}{\sqrt{2}}(\mathbf{B}^{T;1}_j + i\mathbf{B}^{T;3}_j) \; , \quad j = 1,2,3 \tag{4.43}$$

$$\mathbf{C}^{T_1}_j = \frac{1}{\sqrt{2}}(\mathbf{B}^{T;1}_j - i\mathbf{B}^{T;3}_j) \; , \quad j = 1,2,3 \tag{4.44}$$

transform properly under the action of $P(\mathbf{p};X)$, $X \in O$. Note that we have suppressed in (4.44) a multiplicity index, since T_1 occurs only once.

Finally, the remaining problem is to construct O_h-adapted vectors out of the **C**'s [Eqs. (4.40)–(4.44)]. We only need to know for this purpose the action of $P(I)$ on the **C**'s, i.e., on the **B**'s. Using $I = C_{2z}\sigma_z$, we obtain, from (3.38) and (3.40), the following matrix for I:

$$P_{Z',Z}(I) = \delta_{Z',ZC_{2z}} \; , \quad Z,Z' \in T \; . \tag{4.45}$$

We thus obtain, from (4.9),

$$P(I)\mathbf{B}^{\tau v}_j = \sum_w D^\tau_{wv}(C_{2z})^* \mathbf{B}^{\tau w}_j \; , \tag{4.46}$$

which means that only the multiplicity index is concerned. This is in total agreement with our assumptions. Taking $D^\tau(C_{2z})$ from Table IV, we immediately obtain

$$P(I)\mathbf{C}^{A_1} = +\mathbf{C}^{A_1} \; , \tag{4.47}$$

$$P(I)\mathbf{C}_j^{E}=+\mathbf{C}_j^{E}\ ,\quad j=1,2 \tag{4.48}$$

$$P(I)\mathbf{C}_j^{T_1}=-\mathbf{C}_j^{T_1}\ ,\quad j=1,2,3 \tag{4.49}$$

$$P(I)\mathbf{C}_j^{T_2;1}=-\mathbf{C}_j^{T_2,1}\ ,\quad j=1,2,3 \tag{4.50}$$

$$P(I)\mathbf{C}_j^{T_2;2}=+\mathbf{C}_j^{T_2;2}\ ,\quad j=1,2,3 \tag{4.51}$$

which implies that the **C**'s are already eigenvectors of the parity operator $P(I)$. Thus, no further similarity transformation is necessary to achieve the initial constraint, namely (4.1). Hence our subduction matrix S is composed of the column vectors **C** that are given by (4.39), (4.40), and (4.42)–(4.44). We summarize, for convenience, our results in Table V. It is worth noting that the structure of (4.47)–(4.49) is immediate, since the irreducible representations A_1, E, and T_1 occur once in (4.11). However, the irreducible representation T_2 appears twice in (4.11), which means that the action of $P(I)$ on $\mathbf{C}_j^{T_2;w}$ could be, in the most general case, a 2×2 matrix. The matrix then would have to be diagonalized in order to fulfill (4.1). Fortunately, such a transformation is not necessary. The columns of S are unique up to arbitrary phase factors within every irreducible representation of O_h. As a precaution, we also calculated S by means of computer and gained total agreement up to the phase factors previously mentioned.

Case 3. $(m,m,m)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$). As in the preceding case, one must determine $P(\mathbf{p};R)$, $R\in O_h$. This situation is completely comparable with case 1, since $K(\mathbf{p})$ does not form a normal subgroup of O_h. Hence it requires the use of (3.39) instead of (3.40) apart from (3.38). Character theory yields

$$P(\mathbf{p};R)\cong D^{A_{1g}}(R)\oplus D^{A_{2u}}(R)\oplus D^{T_{1u}}(R)\oplus D^{T_{2g}}(R)\ ,\qquad R\in O_h \tag{4.52}$$

i.e., the irreducible vector representations of O_h appear only once. This implies that the corresponding column vectors satisfying (4.1) are unique up to an arbitrary phase factor within every irreducible representation. The corresponding subduction matrix has been calculated by means of a computer by using projection-operator techniques:

$$\begin{array}{c|cccccccc|c}
 & A_{1g} & A_{2u} & & T_{1u} & & & T_{2g} & & \Gamma,\sigma \\
 & 1 & 1 & 1 & 2 & 3 & 1 & 2 & 3 & j \\
\hline
 & \xi & \xi & \xi & i\xi & i\bar{\xi} & \xi & i\xi & i\bar{\xi} & E \\
 & \xi & \xi & \bar{\xi} & i\xi & i\xi & \bar{\xi} & i\xi & i\xi & C_{4z}^{+} \\
 & \xi & \bar{\xi} & \xi & i\xi & i\xi & \bar{\xi} & i\bar{\xi} & i\bar{\xi} & C_{2z} \\
S= & \xi & \bar{\xi} & \bar{\xi} & i\xi & i\bar{\xi} & \xi & i\bar{\xi} & i\xi & C_{4z}^{-} \\
 & \xi & \bar{\xi} & \bar{\xi} & i\bar{\xi} & i\xi & \xi & i\xi & i\bar{\xi} & I \\
 & \xi & \bar{\xi} & \xi & i\bar{\xi} & i\bar{\xi} & \bar{\xi} & i\xi & i\xi & IC_{4z}^{+} \\
 & \xi & \xi & \bar{\xi} & i\bar{\xi} & i\bar{\xi} & \bar{\xi} & i\bar{\xi} & i\bar{\xi} & IC_{2z} \\
 & \xi & \xi & \xi & i\bar{\xi} & i\xi & \xi & i\bar{\xi} & i\xi & IC_{4z}^{-}
\end{array} \tag{4.53}$$

Here, $\xi=1/\sqrt{8}$ is a normalization factor, and the columns of S are enumerated by $(\Gamma,\sigma)=A_{1g}$, A_{2u}, T_{1u}, T_{2g}, and $j=1,2,\ldots,n_\Gamma$ in lexicographical order. The rows are labeled in the same manner as the group elements occur in $K(\mathbf{p})$. Obviously any change of the sequence would lead to erroneous subduction matrices. Hence the introduced sequences must be retained without any change. One peculiar property of (4.53) should be noted, namely that each matrix element of S is different from zero.

Case 4. $(m,n,0)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$). We determine the columns of the corresponding subduction matrix by induction as in case 2. For simplicity, we rearrange the semidirect product so that it becomes a direct-product group,

$$O_h=K(\mathbf{p})\circledS G(\mathbf{p})=K(\mathbf{p})\times\{E,I\}\ . \tag{4.54}$$

Because of $K(\mathbf{p})=O$, the permutational representation $P(\mathbf{p};X)$, $X\in O=K(\mathbf{p})$, represents the regular representation of the point group O. Hence we start to decompose

TABLE V. Subduction matrix $S(m,m,0)$; $\omega=e^{i\pi/3}$.

A_{1g}	E_g			T_{1u}			T_{2g}			T_{2u}		
1	1	2	1	2	3	1	2	3	1	2	3	
1	1	$\bar{1}$	1	0	$\bar{i}$	0	1	0	1	0	i	E
1	1	$\bar{1}$	$\bar{1}$	0	$\bar{i}$	0	$\bar{1}$	0	$\bar{1}$	0	i	C_{2x}
1	1	$\bar{1}$	1	0	i	0	$\bar{1}$	0	1	0	$\bar{i}$	C_{2y}
1	1	$\bar{1}$	$\bar{1}$	0	i	0	1	0	$\bar{1}$	0	$\bar{i}$	C_{2z}
1	ϖ	ω^*	1	i	0	0	0	$\bar{1}$	$\bar{1}$	i	0	C_{31}^{+}
1	ϖ^*	ω	0	i	$\bar{i}$	$\bar{i}$	0	0	0	$\bar{i}$	$\bar{i}$	C_{31}^{-}
1	ϖ^*	ω	0	i	i	i	0	0	0	$\bar{i}$	i	C_{32}^{-}
1	ϖ	ω^*	$\bar{1}$	$\bar{i}$	0	0	0	$\bar{1}$	1	$\bar{i}$	0	C_{32}^{+}
1	ϖ^*	ω	0	$\bar{i}$	i	$\bar{i}$	0	0	0	i	i	C_{33}^{-}
1	ϖ	ω^*	$\bar{1}$	i	0	0	0	1	1	i	0	C_{33}^{+}
1	ϖ	ω^*	1	$\bar{i}$	0	0	0	1	$\bar{1}$	$\bar{i}$	0	C_{34}^{+}
1	ϖ^*	ω	0	$\bar{i}$	$\bar{i}$	i	0	0	0	i	$\bar{i}$	C_{34}^{-}

it into a direct sum of its irreducible constituents. Exploiting our general result,[17] we make the ansatz

$$\{\mathbf{B}_j^{\Gamma v}\}_Y=(n_\Gamma/24)^{1/2}[D_{jv}^{\Gamma}(Y)]^* ,$$
$$\Gamma\in A_O ,\quad v=1,2,\ldots,n_\Gamma ,\quad j=1,2,\ldots,n_\Gamma ,\quad Y\in O \tag{4.55}$$

which automatically satisfies

$$P(X)\mathbf{B}_j^{\Gamma v}=\sum_l D_{lj}^{\Gamma}(X)\mathbf{B}_l^{\Gamma v} ,\quad X\in O . \tag{4.56}$$

Before constructing O_h-adapted vectors, we give the O_h decomposition of $P(\mathbf{p};R)$, $R\in O_h$,

$$P(\mathbf{p};R)\cong D^{A_{1g}}(R)\oplus D^{A_{2g}}(R)\oplus 2D^{E_g}(R)\oplus D^{T_{1g}}(R)$$
$$\oplus 2D^{T_{1u}}(R)\oplus 2D^{T_{2g}}(R)\oplus D^{T_{2u}}(R) , \tag{4.57}$$

which shows that three inequivalent irreducible representations of the point group O_h occur twice. Hence the corresponding multiplicity problem seems to be nontrivial at first glance.

All that remains, in fact, is to find systematically and, in as simple as possible a manner, O_h-adapted vectors that transform according to (4.1) and are linear combinations of the **B**'s, (4.55). Clearly, the similarity transformation must not affect the index j (because of Schur's lemma with respect to O) any may only concern the multiplicity index v assigned to the **B**'s. Again, because of $I=C_{2z}\sigma_z$, we obtain, from (3.38) and (3.40), the following matrix for I:

$$P_{Z'Z}(\mathbf{p};I)=\delta_{Z',ZC_{2z}} ,\quad Z,Z'\in O . \tag{4.58}$$

Together with (4.55), we arrive at the result

$$P(I)\mathbf{B}_j^{\Gamma v}=\sum_w [D_{wv}^{\Gamma}(C_{2z})]^*\mathbf{B}_j^{\Gamma w} , \tag{4.59}$$

which is again in agreement with Schur's lemma with respect to O. Owing to the fact that $D^{\Gamma}(C_{2z})$ is diagonal (with diagonal matrix elements ± 1), the **B**'s already define S.

How the columns associated with the parity must be identified follows in an obvious manner from the irreducible representations $D^{\Gamma}(C_{2z})$ of O. We have

$$\mathbf{S}^{A_{1g}}=\mathbf{B}^{A_1} , \tag{4.60}$$

$$\mathbf{S}^{A_{2g}}=\mathbf{B}^{A_2} , \tag{4.61}$$

$$\mathbf{S}_j^{E_g;v}=\mathbf{B}_j^{E;v} ,\quad v=1,2 ,\quad j=1,2 \tag{4.62}$$

$$\mathbf{S}_j^{T_{1g}}=\mathbf{B}_j^{T_1;2} ,\quad j=1,2,3 \tag{4.63}$$

$$\mathbf{S}_j^{T_{1u};v}=\mathbf{B}_j^{T_1;v} ,\quad v=1,3 ,\quad j=1,2,3 \tag{4.64}$$

$$\mathbf{S}_j^{T_{2g};v}=\mathbf{B}_j^{T_2;v} ,\quad v=1,2 ,\quad j=1,2,3 \tag{4.65}$$

$$\mathbf{S}_j^{T_{2u}}=\mathbf{B}_j^{T_2;3} ,\quad j=1,2,3 . \tag{4.66}$$

Finally, the columns of s are indexed in lexicographical order by $(\Gamma,\sigma)=A_{1g}, A_{2g}, T_{1g}, T_{1u}, T_{2g}, T_{2u}$, the corresponding multiplicity index v, and $j=1,2,\ldots,n_\Gamma$. The rows are labeled by $X\in O$ in consecutive order.

Case 5: $(m,n,n)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$). Again we start with the corresponding semidirect product of O_h in terms of $K(\mathbf{p})$ and $G(\mathbf{p})$ and simplify the task by rearranging this product to a direct product,

$$O_h=K(\mathbf{p})\circledS G(\mathbf{p})=K(\mathbf{p})\times\{E,I\} . \tag{4.67}$$

By virtue of $K(\mathbf{p})=O$, the permutational representation $P(\mathbf{p};X)$, $X\in O$, forms the regular representation of this group. Accordingly, we can start from the same bases, $\mathbf{B}_j^{\Gamma v}$, as in the preceding case. The O_h decomposition of $P(\mathbf{p};R)$, $R\in O_h$, is given by

$$P(\mathbf{p};R)\cong D^{A_{1g}}(R)\oplus D^{A_{2u}}(R)\oplus D^{E_g}(R)\oplus D^{E_u}(R)$$
$$\oplus D^{T_{1g}}(R)\oplus 2D^{T_{1u}}(R)\oplus 2D^{T_{2g}}(R)\oplus D^{T_{2u}}(R) . \tag{4.68}$$

Hence two irreducible representations of the point group O_h occur twice, whereas all the others appear only once. It is worth mentioning that (4.68) differs from (4.57) even though we start from the same normal subgroup.

Our task is to determine O_h-adapted vectors $\mathbf{S}_j^{\Gamma\sigma;w}$ out of the **B**'s. By application of Schur's lemma to O, the desired vectors $\mathbf{S}_j^{\Gamma\sigma;w}$ are linear combinations of the **B**'s where the transformation coefficients only may concern the multiplicity index being associated with the **B**'s. Because of $I=C_{22}\sigma_{22}$ $[\sigma_{22}\in G(\mathbf{p})]$, we obtain from (3.38) and (3.40),

$$P_{Z',Z}(I)=\delta_{Z',ZC_{22}} ,\quad Z,Z'\in O . \tag{4.69}$$

Together with (4.55), we arrive at the result

$$P(I)\mathbf{B}_j^{\Gamma v}=\sum_w [D_{wv}^{\Gamma}(C_{22})]^*\mathbf{B}_j^{\Gamma w} . \tag{4.70}$$

However, in contrast to case 4, the irreducible representations $D^{\Gamma}(C_{22})$ of the point group O, in general, are not diagonal, so that nontrivial similarity transformations must be carried out. In the following we list all $D^{\Gamma}(C_{22})$, $\Gamma\in A_O$:

$$D^{A_1}(C_{22})=1, \tag{4.71}$$

$$D^{A_2}(C_{22})=-1 , \tag{4.72}$$

$$D^{E}(C_{22})=\begin{bmatrix}0 & \omega\\ \omega^* & 0\end{bmatrix} ,\quad \omega=e^{i\pi/3} \tag{4.73}$$

$$D^{T_1}(C_{22})=\begin{bmatrix}0 & \bar{i} & 0\\ i & 0 & 0\\ 0 & 0 & 1\end{bmatrix} , \tag{4.74}$$

$$D^{T_2}(C_{22})=\begin{bmatrix}0 & i & 0\\ \bar{i} & 0 & 0\\ 0 & 0 & 1\end{bmatrix} . \tag{4.75}$$

In the cases of (4.73)–(4.75), we need similarity transformations V^{Γ} that satisfy

$$(V^{\Gamma})^{\dagger}[D^{\Gamma}(C_{22})]^* V^{\Gamma}=\{D^{\Gamma}(C_{22})\}^{\text{diag}} , \tag{4.76}$$

where the superscript (diag) on the right-hand side indicates a diagonal matrix. Obviously, the eigenvalues of

$D^{\Gamma}(C_{22})$ can only be ±1. Hence the desired O_h-adapted vectors $\mathbf{S}_j^{\Gamma\sigma;w}$ are defined by

$$\mathbf{S}_j^{\Gamma\sigma;w}=\sum_v V_{v;\sigma w}\mathbf{B}_j^{\Gamma v} , \tag{4.77}$$

where σ defines the parity and w is the multiplicity index. We always ignore this index if the corresponding irreducible representation of the point group O_h occurs only once. Accordingly, only in two cases this additional index is needed. The first two situations (4.71)—(4.72), are obvious:

$$\mathbf{S}^{A_{1g}}=\mathbf{B}^{A_1}, \tag{4.78}$$

$$\mathbf{S}^{A_{2u}}=\mathbf{B}^{A_2} . \tag{4.79}$$

For the remaining three cases, we arrive at the results

$$\mathbf{S}_j^{E_g}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{E;1}+\omega\mathbf{B}_j^{E;2}) , \quad j=1,2 \tag{4.80}$$

$$\mathbf{S}_j^{E_u}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{E;1}-\omega\mathbf{B}_j^{E;2}) , \quad j=1,2 \tag{4.81}$$

$$\mathbf{S}_j^{T_{1g}}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{T_1;1}-i\mathbf{B}_j^{T_1;2}) , \quad j=1,2,3 \tag{4.82}$$

$$\mathbf{S}_j^{T_{1u};1}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{T_1;1}+i\mathbf{B}_j^{T_1;2}) , \quad j=1,2,3 \tag{4.83}$$

$$\mathbf{S}_j^{T_{1u};2}=\mathbf{B}_j^{T_1;3} , \quad j=1,2,3 \tag{4.84}$$

$$\mathbf{S}_j^{T_{2g};1}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{T_2;1}+i\mathbf{B}_j^{T_2;2}) , \quad j=1,2,3 \tag{4.85}$$

$$\mathbf{S}_j^{T_{2g};2}=\mathbf{B}_j^{T_2;3} , \quad j=1,2,3 \tag{4.86}$$

$$\mathbf{S}_j^{T_{2u}}=\frac{1}{\sqrt{2}}(\mathbf{B}_j^{T_2;1}-i\mathbf{B}_j^{T_2;2}) , \quad j=1,2,3 . \tag{4.87}$$

Again, the columns of S are labeled in consecutive order, as listed in (4.78)—(4.87). Finally, it should be noted that the symmetrized O_h states (4.60)—(4.66) are different from those belonging to (4.78)—(4.87). What is common to both is that we must start from the same **B**'s.

Case 5′: $(m,m,n)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$). The situation here is entirely equivalent to Case 5. The only difference is the sequence of the components. This property can also be seen from

$$\utilde{\mathbf{p}}=C_{31}^{-}\mathbf{p} , \tag{4.88}$$

$$G(\utilde{\mathbf{p}})=C_{31}^{-}G(\mathbf{p})C_{31}^{+} , \tag{4.89}$$

which means nothing else than that they belong to the same orbit. Accordingly, the corresponding permutational representations of the point group O_h are equivalent. Without going into further details, we have verified that

$$\utilde{\mathbf{B}}_j^{\Gamma v}=\sum_w D_{wv}^{\Gamma}(C_{31}^{-})\mathbf{B}_j^{\Gamma w} \tag{4.90}$$

holds where the wavy underlined $\utilde{\mathbf{B}}$'s belong to $P(\mathbf{p};X)$, $X\in O$. This has, as a consequence,

$$\utilde{\mathbf{S}}^{A_{1g}}=\mathbf{S}^{A_{1g}} , \tag{4.91}$$

$$\utilde{\mathbf{S}}^{A_{2u}}=\mathbf{S}^{A_{2u}} , \qquad 4.92)$$

$$\utilde{\mathbf{S}}_j^{E_g}=(-\omega)\mathbf{S}_j^{E_g} , \quad j=1,2 \tag{4.93}$$

$$\utilde{\mathbf{S}}_j^{E_u}=(-\omega)\mathbf{S}_j^{E_u} , \quad j=1,2 \tag{4.94}$$

$$\utilde{\mathbf{S}}_j^{T_{1g}}=-\mathbf{S}_j^{T_{1g}} , \quad j=1,2,3 \tag{4.95}$$

$$\utilde{\mathbf{S}}_j^{T_{1u};1}=(-i)\mathbf{S}_j^{T_{1u};2} , \quad j=1,2,3 \tag{4.96}$$

$$\utilde{\mathbf{S}}_j^{T_{1u};2}=\mathbf{S}_j^{T_{1u};1} , \quad j=1,2,3 \tag{4.97}$$

$$\utilde{\mathbf{S}}_j^{T_{2g};1}=\mathbf{S}_j^{T_{2g};1} , \quad j=1,2,3 \tag{4.98}$$

$$\utilde{\mathbf{S}}_j^{T_{2g};2}=(-i)\mathbf{S}_j^{T_{2g};2} , \quad j=1,2,3 \tag{4.99}$$

$$\utilde{\mathbf{S}}_j^{T_{2u}}=-\mathbf{S}_j^{T_{2u}} , \quad j=1,2,3 . \tag{4.100}$$

The interchange of the multiplicity indices in (4.96) and (4.97) is merely due to the enumeration of the states we have introduced. As in all preceding cases, the columns are indexed as the states are listed and the rows are labeled in the same manner as the elements of the point group O.

Case 6. $(m,n,0)\in\mathbb{Z}^3$ (or $\mathbb{Q}^3$). Although this is the most involved problem, it is the simplest case. Clearly, $P(\mathbf{p};R)$, $R\in O_h$, forms the 48-dimensional regular representation of O_h. Owing to our general result,[17] we only have to know the irreducible vector representations of the point group O_h. They are given by

$$D^{\Gamma,\sigma}(R)=D^{\Gamma,\sigma}(XS)=D^{\Gamma}(X)D^{\sigma}(S) , \quad X\in O, \quad S\in\{E,I\} , \tag{4.101}$$

where $D^{\sigma}(I)=(-1)^{\sigma}$. Using Table III, we introduce the following enumeration in Table VI.

Therefore, the columns of S are given by

$$\{\mathbf{S}_j^{\Gamma\sigma;v}\}_R=(n_{\Gamma}/48)^{1/2}[D_{jv}^{\Gamma,\sigma}(R)]^* , \quad R=XS\in O_h \tag{4.102}$$

and they automatically satisfy (4.1). Now all possible cases are covered, so that the symmetry adaptation of the Dirac states can be carried out immediately, irrespective of whether equivalent atoms occupy lattice sites or fractions thereof. In the latter case, one merely has to replace $(m,n,0)\in\mathbb{Z}^3$ by $(x,y,z)\in\mathbb{Q}^3$.

V. O_h-ADAPTED SHIFTED STATES

In our approach[11] the complete O_h adaptation of our shifted states is achieved if the corresponding Clebsch-Gordan coefficients of the point group O_h are known. However, as they are well known and given for half a dozen equivalent irreducible representations of O_h, our job is, in principle, done. The Clebsch-Gordan coeffi-

TABLE VI. Irreducible representations of the full cubic point group O_h, $X\in O$.

$\Gamma,+$	$\Gamma,-$	
v	v	
j	j	
$D_{jv}^{\Gamma}(X)$	$D_{jv}^{\Gamma}(X)$	X
$D_{jv}^{\Gamma}(X)$	$-D_{jv}^{\Gamma}(X)$	IX

TABLE VII. Clebsch-Gordan matrices for the octahedral point group O. $\alpha=1/\sqrt{2}$, $\beta=1/\sqrt{3}$, and $\gamma=1/2$. $\delta=1/\sqrt{6}$ and $\epsilon=1/\sqrt{12}$.

a

			$A_2\otimes E_{1/2}$	
		Γ''	$E_{5/2}$	
		v	1	
j	a	l	1	2
1	1		1	0
1	2		0	1

b

			$A_2\otimes E_{5/2}$	
		Γ''	$E_{1/2}$	
		v	1	
j	a	l	1	2
1	1		1	0
1	2		0	1

c

			$A_2\otimes G_{3/2}$			
		Γ''	$G_{3/2}$			
		v	1			
j	a	l	1	2	3	4
1	1		0	0	$\bar{1}$	0
1	2		0	0	0	1
1	3		1	0	0	0
1	4		0	$\bar{1}$	0	0

d

			$E\otimes E_{1/2}$			
		Γ''	$G_{3/2}$			
		v	1			
j	a	l	1	2	3	4
1	1		0	$i\alpha$	0	$\bar{\alpha}$
1	2		α	0	$i\bar{\alpha}$	0
2	1		0	$i\bar{\alpha}$	0	$\bar{\alpha}$
2	2		α	0	$i\alpha$	0

e

			$E\otimes E_{5/2}$			
		Γ''	$G_{3/2}$			
		v	1			
j	a	l	1	2	3	4
1	1		0	$i\alpha$	0	$\bar{\alpha}$
1	2		α	0	$i\bar{\alpha}$	0
2	1		0	$i\alpha$	0	α
2	2		$\bar{\alpha}$	0	$i\bar{\alpha}$	0

f

			$E\otimes G_{3/2}$							
		Γ''	$E_{1/2}$		$E_{5/2}$		$G_{3/2}$			
		v	1		1		1			
j	a	l	1	2	1	2	1	2	3	4
1	1		0	$i\bar{\gamma}$	0	$i\bar{\gamma}$	γ	0	$i\gamma$	0
1	2		γ	0	γ	0	0	$\bar{\gamma}$	0	$i\gamma$
1	3		0	$\bar{\gamma}$	0	$\bar{\gamma}$	$i\gamma$	0	$\bar{\gamma}$	0
1	4		$i\gamma$	0	$i\gamma$	0	0	$i\gamma$	0	γ
2	1		0	$i\bar{\gamma}$	0	$i\gamma$	$\bar{\gamma}$	0	$i\gamma$	0
2	2		$\bar{\gamma}$	0	γ	0	0	γ	0	$i\gamma$
2	3		0	γ	0	$\bar{\gamma}$	$i\gamma$	0	γ	0
2	4		$i\gamma$	0	$i\bar{\gamma}$	0	0	$i\gamma$	0	$\bar{\gamma}$

TABLE VII. (*Continued*).

g

			$T_1\otimes E_{1/2}$					
		Γ''	$E_{1/2}$		$G_{3/2}$			
		v	1		1			
j	a	l	1	2	1	2	3	4
1	1		0	$\bar{\beta}$	α	0	δ	0
1	2		β	0	0	δ	0	α
2	1		$\bar{\beta}$	0	0	β/α	0	0
2	2		0	β	0	0	β/α	0
3	1		0	β	α	0	$\bar{\delta}$	0
3	2		β	0	0	δ	0	$\bar{\alpha}$

h

			$T_1\otimes E_{5/2}$					
		Γ''	$E_{5/2}$		$G_{3/2}$			
		v	1		1			
j	a	l	1	2	1	2	3	4
1	1		0	$\bar{\beta}$	δ	0	$\bar{\alpha}$	0
1	2		β	0	0	$\bar{\alpha}$	0	δ
2	1		$\bar{\beta}$	0	0	0	0	β/α
2	2		0	β	β/α	0	0	0
3	1		0	β	$\bar{\delta}$	0	$\bar{\alpha}$	0
3	2		β	0	0	α	0	δ

i

			$T_1\otimes G_{3/2}$															
		Γ''	$E_{1/2}$		$E_{5/2}$		$G_{3/2}$				$G_{3/2}$			
		v	1		1		1				2			
j	a	l	1	2	1	2	1	2	3	4	1	2	3	4
1	1		γ	0	ϵ	0	0	$\bar{\gamma}$	0	$\bar{\epsilon}$	0	0	0	$\bar{\beta}$
1	2		0	ϵ	0	$\bar{\gamma}$	γ	0	$\bar{\epsilon}$	0	0	0	β	0
1	3		ϵ	0	$\bar{\gamma}$	0	0	ϵ	0	$\bar{\gamma}$	0	$\bar{\beta}$	0	0
1	4		0	γ	0	ϵ	ϵ	0	γ	0	β	0	0	0
2	1		0	0	0	$\bar{\beta}$	$\bar{\beta}$	0	0	0	β	0	0	0
2	2		$\bar{\beta}$	0	0	0	0	$\bar{\beta}$	0	0	0	$\bar{\beta}$	0	0
2	3		0	$\bar{\beta}$	0	0	0	0	β	0	0	0	β	0
2	4		0	0	$\bar{\beta}$	0	0	0	0	β	0	0	0	$\bar{\beta}$
3	1		$\bar{\gamma}$	0	ϵ	0	0	γ	0	$\bar{\epsilon}$	0	0	0	$\bar{\beta}$
3	2		0	$\bar{\epsilon}$	0	$\bar{\gamma}$	γ	0	ϵ	0	0	0	$\bar{\beta}$	0
3	3		ϵ	0	γ	0	0	ϵ	0	γ	0	$\bar{\beta}$	0	0
3	4		0	γ	0	$\bar{\epsilon}$	$\bar{\epsilon}$	0	γ	0	$\bar{\beta}$	0	0	0

TABLE VII. (*Continued*).

j

			$T_2 \otimes E_{1/2}$					
		Γ''	$E_{5/2}$		$G_{3/2}$			
		v	1		1			
j	a	l	1	2	1	2	3	4
1	1		0	$\bar{\beta}$	δ	0	$\bar{\alpha}$	0
1	2		β	0	0	$\bar{\alpha}$	0	δ
2	1		$\bar{\beta}$	0	0	0	0	β/α
2	2		0	β	β/α	0	0	0
3	1		0	β	$\bar{\delta}$	0	$\bar{\alpha}$	0
3	2		β	0	0	α	0	δ

k

			$T_2 \otimes E_{5/2}$					
		Γ''	$E_{1/2}$		$G_{3/2}$			
		v	1		1			
j	a	l	1	2	1	2	3	4
1	1		0	$\bar{\beta}$	α	0	δ	0
1	2		β	0	0	δ	0	α
2	1		$\bar{\beta}$	0	0	β/α	0	0
2	2		0	β	0	0	β/α	0
3	1		0	β	α	0	$\bar{\delta}$	0
3	2		β	0	0	δ	0	$\bar{\alpha}$

l

			$T_2 \otimes G_{3/2}$											
		Γ''	$E_{1/2}$		$E_{5/2}$		$G_{3/2}$				$G_{3/2}$			
		v	1		1		1				2			
j	a	l	1	2	1	2	1	2	3	4	1	2	3	4
1	1		ϵ	0	γ	0	0	ϵ	0	$\bar{\gamma}$	0	$\bar{\beta}$	0	0
1	2		0	$\bar{\gamma}$	0	ϵ	$\bar{\epsilon}$	0	$\bar{\gamma}$	0	$\bar{\beta}$	0	0	0
1	3		$\bar{\gamma}$	0	ϵ	0	0	γ	0	ϵ	0	0	0	β
1	4		0	ϵ	0	γ	γ	0	$\bar{\epsilon}$	0	0	0	β	0
2	1		0	$\bar{\beta}$	0	0	0	0	$\bar{\beta}$	0	0	0	β	0
2	2		0	0	$\bar{\beta}$	0	0	0	0	$\bar{\beta}$	0	0	0	β
2	3		0	0	0	$\bar{\beta}$	β	0	0	0	$\bar{\beta}$	0	0	0
2	4		$\bar{\beta}$	0	0	0	0	$\bar{\beta}$	0	0	0	$\bar{\beta}$	0	0
3	1		ϵ	0	$\bar{\gamma}$	0	0	ϵ	0	γ	0	$\bar{\beta}$	0	0
3	2		0	$\bar{\gamma}$	0	$\bar{\epsilon}$	ϵ	0	$\bar{\gamma}$	0	β	0	0	0
3	3		γ	0	ϵ	0	0	$\bar{\gamma}$	0	ϵ	0	0	0	β
3	4		0	$\bar{\epsilon}$	0	γ	γ	0	ϵ	0	0	0	$\bar{\beta}$	0

cients, however, are representation dependent and we need those that are associated with the irreducible representations we use (see Tables III and IV). Since we wanted to use the centered states precisely as computed by Onodera and Okazaki,[8] we were forced to recompute the Clebsch-Gordan coefficients for the irreducible representations used by them. We have done this by a computer routine that exploits the projection-operator technique. Unfortunately, some Clebsch-Gordan coefficients are complex.

For brevity, we only list the Clebsch-Gordan coefficients that belong to Kronecker products that are composed of an irreducible vector representation and a projective representation of the point group O as it occurs for our shifted states. This is so because the resulting states must always belong to irreducible projective representations of O_h. To extend the Clebsch-Gordan coefficients from O to O_h is straightforward and hence omitted. One merely has to take into account the parity selection rule.

One must proceed in detail as follows:

(1) Define the shifted states

$$\Psi_{a;\lambda}^{(\tilde{\omega}J)\Gamma'\sigma'}(\mathbf{p};Z)\,,\qquad \Gamma'\in\mathscr{A}_O\,,\quad \sigma'=\pm,\quad a=1,2,\ldots,n_{\Gamma'}\,,\quad Z\in K(\mathbf{p}) \tag{5.1}$$

by means of (3.35), (2) construct the linear combinations

$$\Phi_{j;a;\lambda}^{(\tilde{\omega}J)\Gamma\sigma m;\Gamma'\sigma'}=\sum_{Z\in K(\mathbf{p})} S_{Z;\Gamma\sigma mj}\Psi_{a;\lambda}^{(\tilde{\omega}J)\Gamma'\sigma'}(\mathbf{p};Z)\,, \tag{5.2}$$

which, due to their definition, transform, for fixed λ, according to the Kronecker product $(\Gamma,\sigma)\otimes(\Gamma',\sigma')$ of O_h, and (3) form the linear combinations

$$\Phi_{l;\lambda}^{(\tilde{\omega}J)(\Gamma,\sigma;m;\Gamma',\sigma')\Gamma'',\sigma+\sigma';v}=\sum_{j,a}\left\{\begin{array}{cc|cc}\Gamma & \Gamma' & \Gamma'' & v\\ j & a & l & \end{array}\right]\Phi_{j;a;\lambda}^{(\tilde{\omega}J)\Gamma\sigma m;\Gamma'\sigma'}\,, \tag{5.3}$$

where the bracket symbol denotes the Clebsch-Gordan coefficients of O. Since the parity selection rule is already taken into account in the states on the left-hand side, only the Clebsch-Gordan coefficients of O are necessary. The states (5.3) transform by definition according to the irreducible representations of $O_h(\Gamma'',\sigma+\sigma')$, where the parity selection rule has to be understood modulo 2.

The states (5.3) are the desired states. To simplify the use of (5.1)–(5.3) for practical calculations, let us recall the definitions

$$S_{Z;\Gamma\sigma mj}=\{\mathbf{S}_j^{\Gamma\sigma;m}(\mathbf{p})\}_Z\,,\quad Z\in K(\mathbf{p}) \tag{5.4}$$

$$\left\{\begin{array}{cc|c}\Gamma & \Gamma' & \Gamma''\\ j & a & l\end{array}\right]=\{\mathbf{C}_l^{\Gamma\otimes\Gamma';\Gamma''v}\}_{ja}\,,\qquad j=1,2,\ldots,n_\Gamma\,,\quad a=1,2,\ldots,n_{\Gamma'} \tag{5.5}$$

where the **C**'s are the columns of the corresponding Clebsch-Gordan matrices listed in Table VII. Thus we can obtain all the information required from the various $S(\mathbf{p})$ and Clebsch-Gordan matrices.

As an example, we show our procedure for fcc(a) nearest-neighbor states (case 2):

(1) Take the centered states of Table I of Onodera and Okazaki.[8] The order of this set of states is 42. $(\Gamma_6,+)$ occurs three times, $(\Gamma_6,-)$, $(\Gamma_7,+)$, and $(\Gamma_7,-)$ occur twice, and $(\Gamma_8,+)$ and $(\Gamma_8,-)$ occur three times, which is in agreement with the order of the set.

(2) Shift all states by means of (5.1). We thus obtain a total set of $12\times42=504$ states.

(3) Implement step 2, i.e., construct the corresponding vectors (5.2) by inserting the S matrix given in Table V.

(4) Finally, take (5.3) by utilizing Table VII. Thus we obtain 504 states that are O_h-adapted and can be exploited for practical calculations.

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