Tensor fields on crystals

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A new method is presented to determine the irreducible representations of the space group of a crystal contained in the representation whose basis functions are the components of a tensor field defined on the atoms of a crystal. This reducible representation is the direct product of a tensor representation, dependent only on the tensor, and a permutation representation dependent only on how the atoms permute under elements of the space group. The permutation representation is first separately reduced prior to the reduction of the direct product. The permutation representation is shown to be an induced representation and its reduction is facilitated using the theory of induced representations. Examples and tables of results of applying this method are given in the case of a polar vector tensor field, applicable to lattice vibrational problems, and crystals, as the diamond structure, of space group symmetry 0_h^7.

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I. INTRODUCTION

In many problems in solid-state physics it is often necessary to determine the irreducible representations of the space group of a crystal contained in a tensor field representation, a reducible representation of the space group whose basis functions are components of a tensor defined on the atoms of the crystal. In lattice vibrational problems[1,2] the basis functions of the tensor field representation are components of a three component tensor defined on each atom, the displacements of each atom. In classifying magnetic ordering in crystals by irreducible representations of a nonmagnetic space group,[3–5] one reduces a tensor field representation whose basis functions are the components of the atomic spins. Also, in applying the tensor-field criterion[6] in the Landau theory of continuous phase transitions, one reduces a tensor field representation, as in the case of magnetostructural phase transitions where the basis functions are components of a six-component tensor[7] defined on each atom.

The tensor field representation is the direct product of a permutation representation of the atoms of the crystal, representing how the atoms of the crystal permute under the space group elements of the crystal, and a tensor representation associated with the transformation of the tensor components defined on the atoms. In the case of lattice vibrational problems, the tensor representation is the polar vector representation, in the case of classification of magnetic ordering, it is the axial vector representation, and in the case of magnetostructural phase transitions, it is the direct product of the polar and axial vector representations.

To determine the irreducible representations contained in the tensor field representation one could use the standard group theoretical projection operator method[8] as has been done, for example, in the case of lattice vibrational problems.[1] Such a method, while of course giving the correct irreducible representations, does not take into account the common property of all tensor field representations defined on a specific crystal: The permutation representation component of the tensor field representation is the same for all tensor field representations defined on the crystal. This commonality has led to an alternate method to determine the irreducible representations contained in the tensor field representation: First determine the irreducible representations contained in the permutation representation, and then those contained in the tensor field representation.

Lulek[9] has considered the lattice vibrational problem of molecules using such a method. The irreducible representation of the point group of the molecule contained in the permutational representation, there called the positional representation, are determined using the theory of representations of permutation groups. Kuzma, Kupolowski, and Lulek[10] have applied this method to the cases of the lattice vibrations of a regular tetrahedron and cube. Birman, Kotzev, and Litvin,[11] in the context of the tensor-field criterion of the Landau theory of continuous phase transitions, have also used such a method. They have derived using the theory of color groups the $k = 0$ irreducible representations of a space group contained in the permutation representation for all possible crystals. Berenson, Kotzev, and Litvin[12] have then tabulated the $k = 0$ irreducible representations of a space group in the tensor field representation, for all possible crystals in the cases where the tensor representation is taken to be the polar vector representation, the axial vector representation, the product of the polar and axial vector representations, and the symmetrized square of the polar vector representation.

In this paper we shall consider the problem of determining all irreducible representations of the space group of a crystal contained in a tensor field representation defined on a crystal. In Sec. II we show that the tensor field representation defined on an arbitrary crystal is the direct sum of the tensor field representations defined on the arbitrary crystal's constituent simple crystals. The structure of the permutation representation of a simple crystal is derived in Sec. III. In Sec. IV, using the theory of induced representations, a general method is derived to determine all irreducible representations of the space group of a crystal contained in the permutation representation of a simple crystal. As an example, all irreducible representations contained in the permutation representations of all simple crystals of a crystal of space group symmetry O_h^7 are derived and tabulated. Finally, in Sec. V, we discuss determining all irreducible representations of the space group of a crystal contained in a tensor field representation defined on a simple crystal. As an example we consider the polar vector tensor-field representation of the diamond structure in conjunction with the lattice vibrational problem in this structure.

II. TENSOR FIELD REPRESENTATION

Consider a crystal of space group symmetry **G** and let $\mathbf{r}_i$, $i = 1,2\cdots$, denote the atomic position vectors of the atoms of the crystal. To each atom of the crystal we associate a q-component tensor $\mathscr{T}$ with components $\mathscr{T}_s$, $s = 1,2,...,q$. The q-component function $\mathscr{T}(\mathbf{r}_i)_s$, $s = 1,2,...,q$ defined on the atomic positions $\mathbf{r}_i$, $i = 1,2,\cdots$, is called a q-component tensor field on the crystal. The corresponding tensor field representaion $D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys})$ of the space group **G** is that representation of **G** whose basis functions are the components $\mathscr{T}(\mathbf{r}_i)_s$, $s = 1,2,...,q$, $i = 1,2,\cdots$, of the tensor field.

The tensor field representation $D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys})$ can be written as

$$D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys}) = D_{\mathbf{G}}^{\mathrm{PERM}}(\mathrm{Crys}) \times D_{\mathbf{G}}^{T}, \tag{1}$$

where $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathrm{Crys})$ is the permutation representation of the atoms of the crystal, representing how the atoms of the crystal permute under elements of the space group of the crystal, and $D_{\mathbf{G}}^{T}$ is the representation of **G** called the tensor representation whose basis functions are the q components of the tensor $\mathscr{T}$. It is the purpose of this paper to derive a method to determine the irreducible representations of **G** contained in a tensor field representation $D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys})$ defined by Eq. (1).

A crystal of space group symmetry **G** can be partitioned into "simple crystals."[13] Each simple crystal consists of all atoms whose atomic position vectors can be obtained by applying all elements of the space group **G** to any one atomic position vector **r**, and is said to be generated by **G** from **r**. A crystal can be considered as consisting of a certain number of simple crystals, no two simple crystals have atoms in common, and the elements of **G** permute the atoms of each simple crystal among themselves.

Let the tensor field be defined on a crystal consisting of m simple crystals generated by **G** from $\mathbf{r}_j$, $j = 1,2,...,m$. Because the elements of **G** permute the atoms of each simple crystal among themselves,

$$D_{\mathbf{G}}^{\mathrm{PERM}}(\mathrm{Crys}) = D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_1) + D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_2) + \cdots + D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_m), \tag{2}$$

that is, the permutation representation of the atoms of the crystal is the direct sum of the permutation representations $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_j)$, $j = 1,2,...,m$, of each of the simple crystals. Substituting Eq. (2) into Eq. (1), the tensor field representation is written

$$D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys}) = [D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_1) + D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_2) + \cdots + D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_m)] \times D_{\mathbf{G}}^{T}, \tag{3}$$

and subsequently as

$$D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys}) = D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_1) + D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_2) + \cdots + D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_m), \tag{4}$$

where $D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_j)$, the tensor field representation of the jth simple crystal, is defined by

$$D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_j) = D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}_j) \times D_{\mathbf{G}}^{T}. \tag{5}$$

The tensor field representation of the crystal is, by Eq (4), the direct sum of the tensor field representations associated with each simple crystal. To determine the irreducible representation of **G** contained in $D_{\mathbf{G}}^{\mathrm{TF}}(\mathrm{Crys})$ is then equivalent to determining the irreducible representations of **G** contained in each of the tensor field representations $D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}_j)$, $j = 1,2,...,m$, of each simple crystal. Consequently, in what follows, we shall restrict ourselves to the case of a crystal consisting of a single simple crystal. We shall consider a single simple crystal generated by **G** from the atomic position vector **r**, and the tensor field representation $D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r})$ defined on this simple crystal:

$$D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r}) = D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}) \times D_{\mathbf{G}}^{T}. \tag{6}$$

Common to all tensor field representations $D_{\mathbf{G}}^{\mathrm{TF}}(\mathbf{r})$ defined on a specific simple crystal generated by **G** from **r**, is the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ of the atoms of the simple crystal.

III. PERMUTATION REPRESENTATION $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$

Let $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ be the permutation representation of the atoms of a simple crystal generated by a space group **G** from the atom position vector **r**. The position vector **r** can be characterized by its site space group $\mathbf{G}(\mathbf{r})$, the subgroup of elements G of **G** such that

$$G\mathbf{r} = \mathbf{r} + \mathbf{t}, \tag{7}$$

where **t** is a primitive translation of the space group **G**. The point group $\mathbf{R}(\mathbf{r})$ of $\mathbf{G}(\mathbf{r})$ is called the "site point group" of **r**. One can expand the space group **G** into a coset decomposition with respect to $\mathbf{G}(\mathbf{r})$,

$$\mathbf{G} = \mathbf{G}(\mathbf{r}) + G_2\mathbf{G}(\mathbf{r}) + \cdots + G_n\mathbf{G}(\mathbf{r}), \tag{8}$$

and define the set of atom positions $G_i\mathbf{r}$, $i = 1,2,...,n$, where G_i is a coset representative in Eq. (8). The coordinates of this set of atom positions, for one or two of each class of space groups **G**, each **r**, and a specific choice of coset representatives, are given in the *International Tables for X-Ray Crystallography*.[14] They are called there the "coordinates of equivalent positions" and the site point group $\mathbf{R}(\mathbf{r})$ is called the "point symmetry" of each of the equivalent positions.

In addition, we characterize the position vector **r** from which a simple crystal is generated by **G** by the "site subgroup" $\mathbf{H}(\mathbf{r})$, the subgroup of elements of the space group **G** such that

$$G\mathbf{r} = \mathbf{r}. \tag{9}$$

Elements of the site subgroup $\mathbf{H}(\mathbf{r})$ are, in general, of the form $(R\,|\mathbf{v}(R) + \mathbf{t}_R)$ where R is an element of the site point group $\mathbf{R}(\mathbf{r})$, $\mathbf{v}(R)$ the nonprimitive translation associated with R, and $\mathbf{t}_R$ a specific primitive translation. The site subgroup $\mathbf{H}(\mathbf{r})$ is isomorphic to the site point group $\mathbf{R}(\mathbf{r})$. However, if the choice of the origin of the space group **G** is taken to be that given in the *International Tables for X-Ray Crystallography*,[14] then the site point group $\mathbf{R}(\mathbf{r})$ is not necessarily a subgroup of the space group **G**. As we shall show below, it is the site subgroup $\mathbf{H}(\mathbf{r})$ of the position vector **r** from which the simple crystal is generated by **G** which plays a central role in determining the irreducible representations of G contained in the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$.

To determine the structure of the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ we expand the space group **G** into a coset decomposition with respect to the site subgroup $\mathbf{H}(\mathbf{r})$:

$$\mathbf{G} = \mathbf{H}(\mathbf{r}) + G_2\mathbf{H}(\mathbf{r}) + G_3\mathbf{H}(\mathbf{r}) + \cdots. \quad (10)$$

Since all elements $\mathbf{H}(\mathbf{r})$ leave **r** invariant, the atomic position vectors of the simple crystal generated by **G** from **r** are in a one-to-one correspondence with the cosets of Eq. (10). That is, the atomic position vectors $\mathbf{r}_i$, $i = 1,2,3,\cdots$, of the simple crystal are such that $\mathbf{r}_i = G_i\mathbf{r}$, $i = 1,2,3,\cdots$, where G_i is a coset representative of Eq. (10). Since the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ is the representation of **G** whose basis functions are the atomic position vectors $\mathbf{r}_i = G_i\mathbf{r}$, $i = 1,2,3,\cdots$, the (i,j)th component of the matrix $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ is one if $G\mathbf{r}_j = \mathbf{r}_i$ or zero if $G\mathbf{r}_j \neq \mathbf{r}_i$. Consequently, the matrices of the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ are defined by

$$D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})[G]_{ij} = \begin{cases} 1 & \text{if } G_i^{-1}GG_j \in \mathbf{H}(\mathbf{r}), \\ 0 & \text{otherwise,} \end{cases} \quad (11)$$

where $i,j = 1,2,3,\cdots$, and G_i and G_j are coset representatives of Eq. (10). It follows from Eq. (11) that the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ is the representation of the space group **G** "induced" by the identity representation $D_{\mathbf{H}(\mathbf{r})}^{1}$ of the site subgroup $\mathbf{H}(\mathbf{r})$.[15] We shall write

$$D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}) = D_{\mathbf{H}(\mathbf{r})}^{1} \uparrow \mathbf{G} \quad (12)$$

to denote the permutation representation as the representation of **G** induced by the identity representation of the site subgroup $\mathbf{H}(\mathbf{r})$.

IV. REDUCTION OF PERMUTATION REPRESENTATION

A. General reduction

We determine the irreducible representations of a space group **G** contained in the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$: Let $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ denote the $(\mathbf{k}^*,\nu)$th irreducible representation of the space group **G**, and $D_{\mathbf{G}(\mathbf{k})}^{\nu}$ the νth irreducible representation of the group $\mathbf{G}(\mathbf{k})$ of the wave vector **k**.[16] We have

$$D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)} = D_{\mathbf{G}(\mathbf{k})}^{\nu} \uparrow \mathbf{G}, \quad (13)$$

that is, the irreducible representation $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ of **G** is induced by the irreducible representation $D_{\mathbf{G}(\mathbf{k})}^{\nu}$ of $\mathbf{G}(\mathbf{k})$. We decompose the permutation representation

$$D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r}) = \sum_{(\mathbf{k}^*,\nu)} d(\mathbf{k}^*,\nu) D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}, \quad (14)$$

where $d(\mathbf{k}^*,\nu)$ is the number of times the irreducible representation $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ of the space group **G** is contained in the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$. We shall determine the coefficients $d(\mathbf{k}^*,\nu)$ of Eq. (14) using the theory of induced representations.[17,18]

The number of times the irreducible representation $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ is contained in $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ is called the "intertwining number of $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ with $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$" and is denoted by the symbol $\mathrm{I}[D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}, D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})]$. From Eq. (14) we have then that

$$d(\mathbf{k}^*,\nu) = \mathrm{I}[D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}, D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})]. \quad (15)$$

Using Eqs. (12) and (13) we can rewrite this as

$$d(\mathbf{k}^*,\nu) = \mathrm{I}[D_{\mathbf{G}(\mathbf{k})}^{\nu} \uparrow \mathbf{G}, D_{\mathbf{H}(\mathbf{r})}^{1} \uparrow \mathbf{G}]. \quad (16)$$

To evaluate the intertwining number on the right-hand side of Eq. (16) using the Intertwining Number Theorem[18] requires the introduction of a double coset decomposition of **G**: We expand the space group **G** into a double coset decomposition[17] with respect to the site subgroup $\mathbf{H}(\mathbf{r})$ and the group $\mathbf{G}(\mathbf{k})$ of the wavevector **k**,

$$\mathbf{G} = \sum_i \mathbf{H}(\mathbf{r}) G_i \mathbf{G}(\mathbf{k}), \quad (17)$$

where the $\mathbf{G}_i$ are double coset representatives. For each double coset representative in Eq. (17) we define the group $\mathbf{L}_i$,

$$\mathbf{L}_i = \mathbf{H}(\mathbf{r}) \cap G_i \mathbf{G}(\mathbf{k}) G_i^{-1}, \quad (18)$$

and the representation D_i^{ν} of the group $G_i\mathbf{G}(\mathbf{k})G_i^{-1}$:

$$D_i^{\nu}(G_i G(\mathbf{k}) G_i^{-1}) \equiv D_{\mathbf{G}(\mathbf{k})}^{\nu}(G(\mathbf{k})). \quad (19)$$

Using the Intertwining Number Theorem,[18] Eq. (16) can be rewritten as

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}[D_i^{\nu} \downarrow \mathbf{L}_i, D_{\mathbf{H}(\mathbf{r})}^{1} \downarrow \mathbf{L}_i], \quad (20)$$

where the summation is over all "i" corresponding to double coset representatives G_i of Eq. (17), with $\mathbf{L}_i$ and D_i^{ν} defined, respectively, by Eqs. (18) and (19). A symbol $D_{\mathbf{A}}^{\alpha} \downarrow \mathbf{B}$ denotes the representation of the subgroup **B** of **A** subduced onto **B** from the representation $D_{\mathbf{A}}^{\alpha}$ of **A**,[15] the representation of **B** found by restricting the representation $D_{\mathbf{A}}^{\alpha}(A)$ to elements $A \in \mathbf{B}$. Equation (20) can be rewritten as

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}[D_{\mathbf{L}_i}^{1}, (D_i^{\nu} \downarrow \mathbf{L}_i) \times (D_{\mathbf{H}(\mathbf{r})}^{1} \downarrow \mathbf{L}_i)], \quad (21)$$

where $D_{\mathbf{L}_i}^{1}$ is the identity representation of $\mathbf{L}_i$. Finally, since by Eq. (18), $\mathbf{L}_i$ is a subgroup of $\mathbf{H}(\mathbf{r})$, $D_{\mathbf{H}(\mathbf{r})}^{1} \downarrow \mathbf{L}_i = D_{\mathbf{L}_i}^{1}$, and

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}[D_{\mathbf{L}_i}^{1}, D_i^{\nu} \downarrow \mathbf{L}_i]. \quad (22)$$

Consequently, the number $d(\mathbf{k}^*,\nu)$ of times the irreducible representation $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ of the space group **G** is contained in the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ is equal to the sum, over the index i, of the number of times the identity representation of $\mathbf{L}_i$ is contained in the subduced representation $D_i^{\nu} \downarrow \mathbf{L}_i$.

Equation (22) can be reformulated in terms of the irreducible representations $D_{\mathbf{G}(\mathbf{k})}^{\nu}$ of the group $\mathbf{G}(\mathbf{k})$ of the wavevector **k**: an intertwining number on the right-hand side of Eq. (22) is defined by

$$\mathrm{I}[D_{\mathbf{L}_i}^{1}, D_i^{\nu} \downarrow \mathbf{L}_i] = \frac{1}{|\mathbf{L}_i|} \sum_{\mathbf{L}_i} \chi_i^{\nu}(L_i), \quad (23)$$

where $|\mathbf{L}_i|$ is the order of the group $\mathbf{L}_i$ and $\chi_i^{\nu}(L_i)$ is the character of $D_i^{\nu}(L_i)$ defined by Eq. (19), $D_i^{\nu}(L_i) = D_i^{\nu}(G_i G(\mathbf{k}) G_i^{-1}) \equiv D_{\mathbf{G}(\mathbf{k})}^{\nu}(G(\mathbf{k}))$ for the elements $G(\mathbf{k}) = G_i^{-1} L_i G_i^{-1}$ of $\mathbf{G}(\mathbf{k})$. Since $D_i^{\nu}(L_i) = D_{\mathbf{G}(\mathbf{k})}^{\nu}(G_i^{-1} L_i G_i)$, $|\mathbf{L}_i| = |G_i^{-1}\mathbf{L}_i G_i|$, and

$G_i^{-1}\mathbf{L}_i G_i$ is a subgroup of $\mathbf{G(k)}$, we may rewrite Eq. (23) as

$$\mathrm{I}[D^1_{\mathbf{L}_i}, D^\nu_i \downarrow \mathbf{L}_i] = \frac{1}{|G_i^{-1}\mathbf{L}_i G_i|} \sum_{\mathbf{L}_i} \chi^\nu_{\mathbf{G(k)}}(G_i^{-1}L_i G_i), \quad (24)$$

and subsequently,

$$\mathrm{I}[D^1_{\mathbf{L}_i}, D^\nu_i \downarrow \mathbf{L}_i] = \mathrm{I}[D^1_{G_i^{-1}\mathbf{L}_i G_i}, D^\nu_{\mathbf{G(k)}} \downarrow G_i^{-1}\mathbf{L}_i G_i]. \quad (25)$$

Substituting Eq. (25) into Eq. (22), the coefficients $d(\mathbf{k}^*,\nu)$ of Eq. (14) are given in terms of the irreducible representation $D^\nu_{\mathbf{G(k)}}$ by

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}[D^1_{G_i^{-1}\mathbf{L}_i G_i}, D^\nu_{\mathbf{G(k)}} \downarrow G_i^{-1}\mathbf{L}_i G_i]. \quad (26)$$

Consequently, the number $d(\mathbf{k}^*,\nu)$ of times the irreducible representation $D^{(\mathbf{k}^*,\nu)}_{\mathbf{G}}$ of the space group $\mathbf{G}$ is contained in the permutation representation $D^{\mathrm{PERM}}_{\mathbf{G}}(\mathbf{r})$ is equal to the sum, over the index i, of the number of times the identity representation of $G_i^{-1}\mathbf{L}_i G_i$, a subgroup of $\mathbf{G(k)}$, is contained in the representation $D^\nu_{\mathbf{G(k)}}$. Equation (25) provides a three-step method to determine the number $d(\mathbf{k}^*,\nu)$ of times in an irreducible representation $D^{(\mathbf{k}^*,\nu)}_{\mathbf{G}}$ is contained in the permutation representation $D^{\mathrm{PERM}}_{\mathbf{G}}(\mathbf{r})$:

(1) Determine the double coset representatives G_i of Eq. (17).

(2) Determine for each i the subgroup $G_i^{-1}\mathbf{L}_i G_i$ of $\mathbf{G(k)}$ using Eq.(18).

(3) Determine for each subgroup $G_i^{-1}\mathbf{L}_i G_i$ the number of times the identity representation is contained in $D^\nu_{\mathbf{G(k)}} \downarrow G_i^{-1}\mathbf{L}_i G_i$ using Eq. (24). The coefficient $d(\mathbf{k}^*,\nu)$ of Eq. (14), is given by Eq. (26) as the sum of the numbers determined in the above third step.

The calculation of the number of times the identity representation is contained in $D^\nu_{\mathbf{G(k)}} \downarrow G_i^{-1}\mathbf{L}_i G_i$, Eq. (24), can be simplified by taking into account the structure of the irreducible representations $D^\nu_{\mathbf{G(k)}}$ of the group $\mathbf{G(k)}$ of the wave vector $\mathbf{k}$.

B. k inside the Brillouin zone

Let $(R|\mathbf{v}(R)+\mathbf{t})$ denote an element of the group $\mathbf{L}_i$ defined by Eq. (18), $\mathbf{R}(\mathbf{L}_i)$ the point group of $\mathbf{L}_i$, and $(R_i|\mathbf{v}(R_i))$ the double coset representatives G_i of Eq. (17). Since $(R|\mathbf{v}(R)+\mathbf{t})$ is contained in $\mathbf{H}(\mathbf{r})$,

$$\mathbf{v}(R) + \mathbf{t} = \mathbf{r} - R\mathbf{r}, \quad (27)$$

and since $(R|\mathbf{v}(R)+\mathbf{t})$ is also contained in $G_i^{-1}\mathbf{G(k)}G_i$,

$$R_i^{-1}RR_i\mathbf{k} = \mathbf{k} + \mathbf{K}, \quad (28)$$

where $\mathbf{K}$ is a reciprocal lattice vector. If $\mathbf{k}$ is inside the Brillouin Zone $\mathbf{K}=0$ and the matrix of the irreducible representation $D^\nu_{\mathbf{G(k)}}(G_i^{-1}L_iG_i)$ can be written as[19]

$$D^\nu_{\mathbf{G(k)}}(G_i^{-1}L_iG_i) = \exp\{i\mathbf{k}\cdot R_i^{-1}[\mathbf{v}(R) + \mathbf{t} - \mathbf{v}(R_i) + R\mathbf{v}(R_i)]\} D^\nu_{\mathbf{R(k)}}(R_i^{-1}RR_i), \quad (29)$$

where $D^\nu_{\mathbf{R(k)}}$ is the νth irreducible representation of the point group $\mathbf{R(k)}$ of $\mathbf{G(k)}$. Using Eqs. (27) and (28) one finds that the exponential term equals one, and

$$D^\nu_{\mathbf{G(k)}}(G_i^{-1}L_iG_i) = D^\nu_{\mathbf{R(k)}}(R_i^{-1}RR_i). \quad (30)$$

Consequently, for wavevectors $\mathbf{k}$ within the Brillouin Zone, Eq. (26) becomes

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}[D^1_{R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i}, D^\nu_{\mathbf{R(k)}} \downarrow R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i], \quad (31)$$

where $\mathbf{R}(\mathbf{L}_i)$ is the point group of $\mathbf{L}_i$, R_i the rotational part of a double coset representative, $\mathbf{R(k)}$ the point group of the wavevector $\mathbf{k}$, and $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$ a subgroup of $\mathbf{R(k)}$.

To determine $d(\mathbf{k}^*,\nu)$ is then a point group problem entailing three steps analogous to the three steps given in the preceding subsection:

(1) Determine the double coset representatives R_i in

$$\mathbf{R} = \sum_i \mathbf{R}(\mathbf{r})R_i\mathbf{R}(\mathbf{k}), \quad (32)$$

where $\mathbf{R}$ is the point group of the space group $\mathbf{G}$, $\mathbf{R(k)}$ of $\mathbf{G(k)}$, and $\mathbf{R}(\mathbf{r})$ is the site point group, the point group of $\mathbf{H}(\mathbf{r})$.

(2) Determine for each double coset representative R_i the subgroup $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$ of $\mathbf{R(k)}$ from

$$R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i = R_i^{-1}\mathbf{R}(\mathbf{r})R_i \cap \mathbf{R}(\mathbf{k}). \quad (33)$$

(3)Determine for each subgroup $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$ the number of times the identity representation is contained in $D^\nu_{\mathbf{R(k)}}$ subduced onto $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$. The coefficient $d(\mathbf{k}^*,\nu)$, Eq. (31), is the sum of the numbers calculated in step three above.

For the special case of $\mathbf{k}=0$, $\mathbf{R(k)}=\mathbf{R}$, there is only one double coset representative in Eq. (32), $R_1=E$, and $R_1^{-1}\mathbf{R}(\mathbf{L}_1)R_1 = \mathbf{R}(\mathbf{r})$. From Eq. (31) we have

$$d(0,\nu) = \mathrm{I}[D^1_{\mathbf{R}(\mathbf{r})}, D^\nu_{\mathbf{R}} \downarrow \mathbf{R}(\mathbf{r})], \quad (34)$$

and the number $d(0,\nu)$ of times $D^{(0,\nu)}_{\mathbf{G}}$ is contained in the permutation representation $D^{\mathrm{PERM}}_{\mathbf{G}}(\mathbf{r})$ is equal to the number of times the identity representation is contained in $D^\nu_{\mathbf{R}}$ subduced onto the site point group $\mathbf{R}(\mathbf{r})$. Tables of $d(0,\nu)$ for all space groups $\mathbf{G}$ and site point groups $\mathbf{R}(\mathbf{r})$ are given by Kotzev, Litvin, and Birman.[11]

As an example we consider the space group $\mathbf{G}=0^7_h$ and the simple crystal generated by 0^7_h from $\mathbf{r}=(\frac{1}{8},\frac{1}{8},\frac{1}{8})$, Wyckoff (c) position in the notation of Ref. 14. The site point group is $\mathbf{R}(\mathbf{r}) = D^{(xyz)}_{3d}$. We shall determine the number of times an irreducible representation $D^{(\mathbf{k}^*,\nu)}_{\mathbf{G}}$ of the space group $\mathbf{G}$, with $\mathbf{k}=(k_x,k_x,k_x)\equiv\mathbf{\Lambda}$, is contained in the permutation representation $D^{\mathrm{PERM}}_{\mathbf{G}}(\mathbf{r})$.

The point group $\mathbf{R(k)} = C^{(xyz)}_{3v}$, and there are two double coset representatives, in this case, in Eq. (32), $R_1=E$ and $R_2=C_{2y}$. The corresponding subgroups, Eq. (33), are $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_1 = C^{(xyz)}_{3v}$ and $R_2^{-1}\mathbf{R}(\mathbf{L}_2)R_2 = C^{(x\bar{z})}_m$. For this wavevector $\mathbf{k}=\mathbf{\Lambda}$, the only nonzero intertwining numbers in Eq. (31) are

$$\begin{aligned} &\mathrm{I}[D^1_{C_{3v}}, D^1_{C_{3v}} \downarrow C_{3v}] = 1,\\ &\mathrm{I}[D^1_{C_m}, D^1_{C_{3v}} \downarrow C_m] = 1,\\ &\mathrm{I}[D^1_{C_m}, D^3_{C_{3v}} \downarrow C_m] = 1, \end{aligned} \quad (35)$$

where for the index ν of the irreducible representation $D^\nu_{\mathbf{R(k)}}$ we have used the conventions of Zak, Casher, Gluck, and Gur.[19] From Eqs. (32) and (35), we have that the only nonzero coefficients $d(\mathbf{k}^*,\nu)$ with $\mathbf{k}=\mathbf{\Lambda}$ are

$$\begin{aligned} &d(\mathbf{\Lambda}^*,1) = 2,\\ &d(\mathbf{\Lambda}^*,3) = 1. \end{aligned} \quad (36)$$

TABLE I. Irreducible representations $G_G^{(k^*,\nu)}$ contained in the permutation representation $D_G^{\mathrm{PERM}}(r)$ of a simple crystal generated by $G = O_h^7$ from a point r: The points r are denoted in the Wyckoff position notation of Ref. 14: (a) = (0,0,0), (b) = $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, (c) $(\frac{1}{8},\frac{1}{8},\frac{1}{8})$, (d) = $(\frac{5}{8},\frac{5}{8},\frac{5}{8})$, (e) = (x,x,x), (f) = $(x,0,0)$, (g) = (x,x,z), (h) = $(\frac{1}{8},x,\frac{1}{4}-x)$, and (i) = (x,y,z). The number $d(k^*,\nu)$ of times $D_G^{(k^*,\nu)}$ is contained in $D_G^{\mathrm{PERM}}(r)$ is found at the intersection of the νth row of the kth subtable, and the column under the Wycokoff notation for the point r. The notation for k and indexation of ν is that of Ref. 20.

Γ	(a)	(b)	(c)	(d)	(e)	(f)	(g)	(h)	(i)
1	1	1	1	1	1	1	1	1	1
2									1
3						1	1	1	2
4			1	1	1	1	2	2	2
5							1	1	3
6								1	1
7	1	1			1	1	1		1
8						1	1	1	2
9							1	2	3
10					1	1	2	1	3
Δ									
1	1	1	1	1	2	3	4	3	6
2						1	2	3	6
3						1	3	3	6
4	1	1	1	1	2	3	3	3	6
5			1	1	2	2	6	6	12
Σ									
1	1	1	1	1	3	4	7	7	12
2			1	1	1	2	5	5	12
3			1	1	1	2	5	7	12
4	1	1	1	1	3	4	7	5	12
Λ									
1	2	2	2	2	4	4	5	4	8
2							3	4	8
3			1	1	2	4	8	8	16
Ξ									
1	1	1	2	2	4	6	12	12	24
2	1	1	2	2	4	6	12	12	24
Θ									
1	2	2	2	2	6	8	14	12	24
2			2	2	2	4	10	12	24
X									
1	1	1	1	1	2	2	4	3	6
2						2	2	3	6
3			1	1	1	1	3	4	6
4					1	1	3	2	6
W									
1	1		1	1	2	3	6	6	12
2		1	1	1	2	3	6	6	12
K									
1	1	1	2	2	3	4	7	7	12
2					1	2	5	5	12
3	1	1	1	1	3	4	7	5	12
4			1	1	1	2	5	7	12
L									
1	1	1	1	1	2	2	3	2	4
2							1	2	4
3				1	1	2	4	4	8
4			1	1	1	2	3	2	4
5	1	1			1		1	2	4
6			1		1	2	4	4	8
U									
1	1	1	1	1	3	4	7	5	12
2	1	1	2	2	3	4	7	7	12
3			1	1	1	2	5	7	12
4					1	2	5	5	12
Z									
1	1	1	2	2	4	6	12	12	24
Q									
1	1	1	2	2	4	6	12	12	24
2	1	1	2	2	4	6	12	12	24
S									
1	1	1	1	1	3	4	7	5	12
2	1	1	2	2	3	4	7	7	12
3			1	1	1	2	5	7	12
4					1	2	5	5	12
A									
1	1	1	2	2	4	6	12	12	24
2	1	1	2	2	4	6	12	12	24
B									
1	1	1	2	2	4	6	12	12	24
2	1	1	2	2	4	6	12	12	24
M									
1	2	2	3	3	6	8	14	12	24
2			1	1	2	4	10	12	24
N									
1	1	1	2	2	4	6	12	12	24
2	1	1	2	2	4	6	12	12	24

Consequently, the permutation representation $D_G^{\mathrm{PERM}}(\mathbf{r})$ for $\mathbf{G} = O_h^7$ and $\mathbf{r} = (\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$, contains the irreducible representation $D_{\mathbf{G}}^{(\Lambda^*,1)}$ twice and $D_{\mathbf{G}}^{(\Lambda^*,3)}$ once, and no other irreducible representations of the space group $\mathbf{G} = O_h^7$ with the wavevector $\mathbf{k} = \Lambda$. This information can be found in Table I at the intersection of the "c" column and the first and third rows of subtable Λ.

C. k on the Brillouin Zone

For wavevectors **k** on the Brillouin Zone, in place of Eq. (29), one writes[19]

$$D_{\mathbf{G(k)}}^{\nu}(G_i^{-1}L_iG_i) = e^{i\mathbf{k}\cdot\mathbf{t}(R_i^{-1}R(L_i)R_i)}\bar{D}_{\mathbf{R(k)}}^{\nu}(R_i^{-1}R(L_i)R_i), \tag{37}$$

where the primitive translation $\mathbf{t}(R_i^{-1}R(L_i)R_i)$ is determined by

$$G_i^{-1}L_iG_i = (R_i^{-1}R(L_i)R_i|\mathbf{v}(R_i^{-1}R(L_i)R_i) + \mathbf{t}(R_i^{-1}R(L_i)R_i)) \tag{38}$$

and $\bar{D}^{\nu}_{\mathbf{R}(\mathbf{k})}$ is the νth irreducible ray representation[19] of the point group $\mathbf{R}(\mathbf{k})$ of the wavevector $\mathbf{k}$.

Using Eq. (37), Eq. (26) can be rewritten for wavevectors $\mathbf{k}$ on the Brillouin Zone, as

$$d(\mathbf{k}^*,\nu) = \sum_i \mathrm{I}\left[D^{1}_{R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i}, e^{i\mathbf{k}\cdot\mathbf{t}}\bar{D}^{\nu}_{\mathbf{R}(\mathbf{k})}\downarrow R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i\right], \tag{39}$$

where $\bar{D}^{\nu}_{\mathbf{R}(\mathbf{k})}$ is the νth irreducible ray representation of $\mathbf{R}(\mathbf{k})$, and $\mathbf{t} = \mathbf{t}(R_i^{-1}R(L_i)R_i)$ is defined by Eq. (38).

The coefficients $d(\mathbf{k}^*,\nu)$ are determined again by a three-step procedure:

(1) The double coset representatives G_i are determined from Eq. (17).

(2) The subgroups $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$ of $\mathbf{R}(\mathbf{k})$ are determined from Eq. (33), and the translations $\mathbf{t}(R_i^{-1}\mathbf{R}(L_i)R_i)$ from Eq. (38).

(3) Determine for each subgroup $R_i\mathbf{R}(\mathbf{L}_i)R_i$ the number of times the identity representation is contained in $e^{i\mathbf{k}\cdot\mathbf{t}}\bar{D}^{\nu}_{\mathbf{R}(\mathbf{k})}$ subduced onto $R_i^{-1}\mathbf{R}(\mathbf{L}_i)R_i$. The coefficient $d(\mathbf{k}^*,\nu)$, Eq. (39), is the sum of the numbers calculated in step three above.

As an example we again consider the space group $\mathbf{G} = O_h^7$ and the simple crystal generated by O_h^7 from the (c) position $\mathbf{r} = (\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$. We shall determine the number of times irreducible representations $D_{\mathbf{G}}^{(\mathbf{k}^*,\nu)}$ with $\mathbf{k} = (3\pi/2a, 3\pi/2a, 0) \equiv \mathbf{K}$ are contained in the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$. The site subgroup $\mathbf{H}(\mathbf{r}) = (C_{3v}^{(xyz)}|0,0,0) + (\bar{1}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})(C_{3v}^{(xyz)}|0,0,0)$ and $\mathbf{G}(\mathbf{k})$ consists of the elements $(E|0,0,0)$, $(m^{(z)}|\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$, $(m^{(\bar{x}y)}|0,0,0)$, $(C_2^{(xy)}|0,0,0)$ and all primitive translations of $\mathbf{G} = O_h^7$. There are two double coset representatives, Eq. (17), $G_1 = (E|0,0,0)$ and $G_2 = (C_2^x|0,0,0)$. The corresponding subgroups of $\mathbf{R}(\mathbf{k}) = C_{2v}^{(xy,\bar{x}y,z)}$ are $R_1^{-1}\mathbf{R}(\mathbf{L}_1)R_1 = C_2^{\bar{x}y}$ with $\mathbf{t}(E) = \mathbf{t}(m^{\bar{x}y}) = 0$, and $R_2^{-1}\mathbf{R}(\mathbf{L}_2)R_2 = C_2^{xy}$ with $\mathbf{t}(E) = 0$ and $\mathbf{t}(C_2^{xy}) = (0, -\frac{1}{2}, -\frac{1}{2})$. Using Eq. (39) and the numbering of Ref. 19 for the index ν of irreducible ray representations, the nonzero coefficients $d(\mathbf{k}^*,\nu)$ for $\mathbf{k} = \mathbf{K}$, are in this example:

$$\begin{aligned} d(\mathbf{K}^*,1) &= 2, \\ d(\mathbf{K}^*,3) &= 1, \\ d(\mathbf{K}^*,4) &= 1. \end{aligned} \tag{40}$$

Consequently, the permutation representation $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ for $\mathbf{G} = O_h^7$ and $\mathbf{r} = (\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$ contains the irreducible representation $D_{\mathbf{G}}^{(\mathbf{K}^*,1)}$ twice, the irreducible representations $D_{\mathbf{G}}^{(\mathbf{K}^*,3)}$ and $D_{\mathbf{G}}^{(\mathbf{K}^*,4)}$ each once, and no other irreducible representations with the wavevector $\mathbf{k} = \mathbf{K}$. This information is found in Table I at the intersection of the (c) column and rows of subtable $\mathbf{K}$.

In Table I we have tabulated all irreducible representations of the space group $\mathbf{G} = O_h^7$ contained in the permutation representations $D_{\mathbf{G}}^{\mathrm{PERM}}(\mathbf{r})$ for all simple crystals generated by $\mathbf{G} = O_h^7$.

TABLE II. The irreducible representations $D^{\nu}_{R(k)}$ contained in the direct product $D^{\bar{\nu}}_{R(k)} \times (D^{T}_{G}\downarrow R(k))$ for $G = O_h^7$ and the polar vector tensor representation $D^{T}_{G} = D^{V}_{G}$: The irreducible representations $D^{\nu}_{R(k)}$ contained in the direct product are listed to the right of the irreducible representation $D^{\bar{\nu}}_{R(k)}$. Irreducible representations $D^{\nu}_{R(k)}$ are denoted by k_ν in the notation and indexation of Ref. 20.

Γ_1	Γ_{10}	Θ_1	$2\Theta_1 + \Theta_2$	Z_1	$3Z_1$
Γ_2	Γ_9	Θ_2	$\Theta_1 + 2\Theta_2$		
Γ_3	$\Gamma_9 + \Gamma_{10}$			Q_1	$Q_1 + 2Q_2$
Γ_4	$\Gamma_7 + \Gamma_8 + \Gamma_9 + \Gamma_{10}$			Q_2	$2Q_1 + Q_2$
Γ_5	$\Gamma_6 + \Gamma_8 + \Gamma_9 + \Gamma_{10}$				
Γ_6	Γ_5	X_1	$X_1 + X_3 + X_4$	S_1	$S_1 + S_2 + S_3$
Γ_7	Γ_4	X_2	$X_2 + X_3 + X_4$	S_2	$S_1 + S_2 + S_4$
Γ_8	$\Gamma_4 + \Gamma_5$	X_3	$X_1 + X_2 + X_4$	S_3	$S_1 + S_3 + S_4$
Γ_9	$\Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5$	X_4	$X_1 + X_2 + X_3$	S_4	$S_2 + S_3 + S_4$
Γ_{10}	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_5$				
				A_1	$2A_1 + A_2$
		W_1	$W_1 + 2W_2$	A_2	$A_1 + 2A_2$
Δ_1	$\Delta_1 + \Delta_5$	W_2	$2W_1 + W_2$		
Δ_2	$\Delta_2 + \Delta_5$			B_1	$2B_1 + B_2$
Δ_3	$\Delta_3 + \Delta_5$			B_2	$B_1 + 2B_2$
Δ_4	$\Delta_4 + \Delta_5$	K_1	$K_1 + K_2 + K_3$		
Δ_5	$\Delta_1 + \Delta_2 + \Delta_3 + \Delta_4 + \Delta_5$	K_2	$K_1 + K_2 + K_4$	M_1	$M_1 + 2M_2$
		K_3	$K_1 + K_3 + K_4$	M_2	$2M_1 + M_2$
		K_4	$K_2 + K_3 + K_4$		
Σ_1	$\Sigma_1 + \Sigma_2 + \Sigma_4$			N_1	$2N_1 + N_2$
Σ_2	$\Sigma_1 + \Sigma_2 + \Sigma_3$			N_2	$N_1 + 2N_2$
Σ_3	$\Sigma_2 + \Sigma_3 + \Sigma_4$	L_1	$L_5 + L_6$		
Σ_4	$\Sigma_1 + \Sigma_3 + \Sigma_4$	L_2	$L_4 + L_6$		
		L_3	$L_4 + L_5 + 2L_6$		
		L_4	$L_2 + L_3$		
Λ_1	$\Lambda_1 + \Lambda_3$	L_5	$L_1 + L_3$		
Λ_2	$\Lambda_2 + \Lambda_3$	L_6	$L_1 + L_2 + 2L_3$		
Λ_3	$\Lambda_1 + \Lambda_2 + 2\Lambda_3$				
		U_1	$U_1 + U_2 + U_3$		
Ξ_1	$2\Xi_1 + \Xi_2$	U_2	$U_1 + U_2 + U_4$		
Ξ_2	$\Xi_1 + 2\Xi_2$	U_3	$U_1 + U_3 + U_4$		
		U_4	$U_2 + U_3 + U_4$		

V. REDUCTION OF TENSOR FIELD REPRESENTATION

The tensor field representation $D_G^{TF}(\mathbf{r})$ of a simple crystal is defined by Eq. (6)

$$D_G^{TF}(\mathbf{r}) = D_G^{PERM}(\mathbf{r}) \times D_G^T, \tag{6}$$

where $D_G^{PERM}(\mathbf{r})$ is the permutation representation of the atomic positions of the simple crystal, and D_G^T is the tensor representation. In the preceding section we have derived a method to reduce the permutation representation and here shall assume that the coefficients $d(\mathbf{k}^*,\nu)$ of Eq. (13) are known. Substituting Eq. (13) into Eq. (6) we have

$$D_G^{TF}(\mathbf{r}) = \sum_{\mathbf{k}^*,\nu} d(\mathbf{k}^*,\nu)[D_G^{(\mathbf{k}^*,\nu)} \times D_G^T]. \tag{41}$$

To determine the irreducible representations in $D_G^{TF}(\mathbf{r})$ one must reduce the direct product of irreducible representations $D_G^{(\mathbf{k}^*,\nu)}$ and the tensor representation D_G^T. If

$$D_G^{(\mathbf{k}^*,\nu)} \times D_G^T = \sum_{\bar{\mathbf{k}}^*,\bar{\nu}} C(\mathbf{k}^*,\nu;\bar{\mathbf{k}}^*,\bar{\nu}) D_G^{(\bar{\mathbf{k}}^*,\bar{\nu})}, \tag{42}$$

then the reduced form of the tensor field representation is

$$D_G^{TF}(\mathbf{r}) = \sum_{\mathbf{k}^*,\nu} b(\mathbf{k}^*,\nu) D_G^{(\mathbf{k}^*,\nu)}, \tag{43}$$

where

$$b(\mathbf{k}^*,\nu) = \sum_{\bar{\mathbf{k}}^*,\bar{\nu}} d(\bar{\mathbf{k}}^*,\bar{\nu}) C(\bar{\mathbf{k}}^*,\bar{\nu};\mathbf{k}^*,\nu). \tag{44}$$

We shall consider here tensor representations D_G^T which are independent of the translational components of the elements of $\mathbf{G}$, that is, which are $\mathbf{k} = 0$ representations of $\mathbf{G}$. Consequently, in Eq. (42), $\bar{\mathbf{k}}^* = \mathbf{k}^*$. Abbreviating $C(\mathbf{k}^*,\nu;\mathbf{k}^*,\bar{\nu})$ by $C(\mathbf{k}^*,\nu,\bar{\nu})$, we can write Eqs. (42) and (44), respectively, as

$$D_G^{(\mathbf{k}^*,\nu)} \times D_G^T = \sum_{\bar{\nu}} C(\mathbf{k}^*,\nu,\bar{\nu}) D_G^{(\mathbf{k}^*,\bar{\nu})} \tag{45}$$

and

$$b(\mathbf{k}^*,\nu) = \sum_{\bar{\nu}} d(\mathbf{k}^*,\bar{\nu}) C(\mathbf{k}^*,\bar{\nu},\nu), \tag{46}$$

where the coefficients $C(\mathbf{k}^*,\bar{\nu},\nu)$ are defined as the intertwining numbers

$$C(\mathbf{k}^*,\bar{\nu},\nu) = \mathrm{I}[D_G^{(\mathbf{k}^*,\nu)}, D_G^{(\mathbf{k}^*,\bar{\nu})} \times D_G^T]. \tag{47}$$

Using Eq. (3), this can be rewritten as

$$C(\mathbf{k}^*,\bar{\nu},\nu) = \mathrm{I}[D_{\mathbf{G}(\mathbf{k})}^{\nu}, D_{\mathbf{G}(\mathbf{k})}^{\bar{\nu}} \times (D_G^T \downarrow \mathbf{G}(\mathbf{k}))] \tag{48}$$

and since D_G^T is a $\mathbf{k} = 0$ representation of $\mathbf{G}$,

$$C(\mathbf{k}^*,\bar{\nu},\nu) = \mathrm{I}[D_{\mathbf{R}(\mathbf{k})}^{\nu}, D_{\mathbf{R}(\mathbf{k})}^{\bar{\nu}} \times (D_G^T \downarrow \mathbf{R}(\mathbf{k}))], \tag{49}$$

where, if $\mathbf{k}$ is a wavevector inside the Brillouin Zone, $D_{\mathbf{R}(\mathbf{k})}^{\nu}$ and $D_{\mathbf{R}(\mathbf{k})}^{\bar{\nu}}$ are irreducible representations of the point group $\mathbf{R}(\mathbf{k})$, and if $\mathbf{k}$ is on the Brillouin Zone, $D_{\mathbf{R}(\mathbf{k})}^{\nu}$ and $D_{\mathbf{R}(\mathbf{k})}^{\bar{\nu}}$ are replaced by $\bar{D}_{\mathbf{R}(\mathbf{k})}^{\nu}$ and $\bar{D}_{\mathbf{R}(\mathbf{k})}^{\bar{\nu}}$, irreducible ray representations of $\mathbf{R}(\mathbf{k})$. For the space group $\mathbf{G} = 0_h^7$ and $D_G^T = D_G^V$, the polar vector representation, the irreducible representations $D_{\mathbf{R}(\mathbf{k})}^{\nu}$ contained in $D_{\mathbf{R}(\mathbf{k})}^{\bar{\nu}} \times (D_G^T \downarrow \mathbf{R}(\mathbf{k}))$ have been calculated and are tabulated in Table II. From this table the coefficients $C(\mathbf{k}^*,\bar{\nu},\nu)$ can be found for the case $\mathbf{G} = 0_h^7$ and $D_G^T = D_G^V$. For example, for $\mathbf{k} = \Lambda$ from Table II one finds the nonzero coefficients $C(\Lambda^*,\bar{\nu},\nu)$:

$$\begin{aligned} &C(\Lambda^*,1,1) = C(\Lambda^*,1,3) = 1,\\ &C(\Lambda^*,2,2) = C(\Lambda^*,2,3) = 1,\\ &C(\Lambda^*,3,1) = C(\Lambda^*,3,2) = 1,\\ &C(\Lambda^*,3,3) = 2. \end{aligned} \tag{50}$$

The number $b(\mathbf{k}^*,\nu)$, Eq. (43), of times an irreducible representation $D_G^{(\mathbf{k}^*,\nu)}$ is contained in a tensor field representation $D_G^{TF}(\mathbf{r})$ is determined from Eq. (46), with the coefficients $d(\mathbf{k}^*,\bar{\nu})$ calculated from Eq. (31) and $C(\mathbf{k}^*,\bar{\nu},\nu)$ from Eq. (49). For $\mathbf{k} = \Lambda$, the nonzero coefficients $d(\Lambda^*,\bar{\nu})$ are given in Eq. (36) and the nonzero coefficients $C(\Lambda^*,\bar{\nu},\nu)$ in Eq. (50). Using Eq. (45) we have

$$\begin{aligned} &b(\Lambda^*,1) = 3,\\ &b(\Lambda^*,2) = 1,\\ &b(\Lambda^*,3) = 4. \end{aligned} \tag{51}$$

Consequently, the tensor field representation $D_G^{TF}(\mathbf{r})$ for $\mathbf{G} = 0_h^7$, $\mathbf{r} = (\frac{1}{8}, \frac{1}{8}, \frac{1}{8})$, $D_G^T = D_G^V$, and $\mathbf{k} = \Lambda$, contains the irreducible representation $D_G^{(\Lambda^*,1)}$ three times, $D_G^{(\Lambda^*,2)}$ once, and $D_G^{(\Lambda^*,3)}$ four times.

For this case, where $D_G^T = D_G^V$, is the polar vector representation, the irreducible representations contained in the tensor field representation $D_G^{TF}(\mathbf{r})$, Eq. (6), are the lattice vibration irreducible representations of the simple crystal generated by $\mathbf{G}$ from $\mathbf{r}$. For the diamond structure, $\mathbf{G} = 0_h^7$, $\mathbf{r} = (0,0,0)$, the (a) position according to Ref. 14, we find for $\mathbf{k} = \Lambda$, from Eq. (46) and Tables I and II, the nonzero coefficients are $b(\Lambda^*,1) = b(\Lambda^*,3) = 2$. That is, the lattice vibration decomposition for the diamond structure at $\mathbf{k} = \Lambda$ is $2D_G^{(\Lambda^*,1)} + 2D_G^{(\Lambda^*,3)}$, in agreement with Ref. 20.

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[1]A. A. Maradudin and S. H. Vosko, Rev. Mod. Phys. **40**, 1 (1958).
[2]J. L. Birman, *Theory of Crystal Space Groups and Infra-Red and Raman Lattice Processes of Insulating Crystals* (Springer, Berlin, 1974).
[3]I. E. Dzialoshinsky, Z. Eksp. Teoret. Fiz. **32**, 1547 (1957) [Sov. Phys. JETP **5**, 1259 (1957)].
[4]S. Alexander, Phys. Rev. **127**, 420 (1962).
[5]E. F. Bertaut, J. Phys. (Paris), Suppl. A **24**, 217 (1968).
[6]J. L. Birman, Phys. Rev. Lett. **17**, 1216 (1966).
[7]J. L. Birman and Y. A. Izyumov, Phys. Rev. B **21**, 1089 (1980).
[8]L. Jansen and M. Boon, *Theory of Finite Groups. Applications in Physics* (North-Holland, Amsterdam, 1967), p. 223.
[9]T. Lulek, Acta Phys. Pol. A **57**, 407 (1980).
[10]M. Kuzma, I. Kuplowski, and T. Lulek, Acta Phys. Pol. A **57**, 415 (1980).
[11]J. N. Kotzev, D. B. Litvin, and J. L. Birman, to be published.
[12]R. Berenson, J. N. Kotzev, and D. B. Litvin, to be published.
[13]W. Opechowski and R. Guccione, in *Magnetism*, edited by G. T. Rado and H. Suhl (Academic, New York, 1965), Vol. IIA, p. 105.

[14]*International Tables for X-Ray Crystallography*, edited by N. F. M. Henry and K. Lonsdale (Kynoch, Birmingham, England, 1952), Vol. I.
[15]Reference 8, Sec. II.6.
[16]Reference 8, p. 252.
[17]C. J. Bradley, J. Math. Phys. 7, 1145 (1966).
[18]A. J. Coleman, in *Group Theory and Its Applications*, edited by M. Loebl (Academic, New York, 1968).
[19]J. Zak, A. Casher, M. Gluck, and Y. Gur, *The Irreducible Representations of Space Groups* (Benjamin, New York, 1969).
[20]J. L. Warren and T. G. Worlton, *Symmetry Properties of the Lattice Dynamics of Twenty-Three Crystals*, ANL-8053 (Argonne National Laboratory, Chicago, 1973), p. 508.