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Irreducible Representations of Space Groups

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A method is presented for obtaining the matrices for the single-valued irreducible representations of any space group. Although the method is designed for computer handling of all algebraic steps, it may be easily applied for hand calculations. The procedure is based on the reduction of representations of a space group of the wave vector **k** induced by the irreducible representations of its invariant subgroup of index 2 or 3. For almost all space groups only the irreducible representations of a cyclic point group, *i.e.* the *n*th roots of unity for a generator of the group, are needed. Cubic space groups, for **k** values corresponding to high-symmetry points on the Brillouin zone boundary, are discussed in detail.

Problems in solid-state physics are greatly simplified by group-theoretical methods which require a knowledge of the irreducible representations of space groups. Although in many applications only the characters of the representations are necessary, the matrices are usually needed for numerical calculations. This is quite evident for space-group representations of high dimensionality, up to 6 for high-symmetry groups, or when only the identity element has a non-zero character.

Tables for all possible irreducible representations (hereafter 'reps' for short) of space groups have been published by several authors (Faddeyev, 1961; Kovalev, 1961; Hurley, 1966; Miller & Love, 1967; Zak, Casher, Glück & Gur, 1969; Bradley & Cracknell, 1972). Some of these tables are incomplete or contain only the characters, but it is generally true that the reps of any space group are now available with little algebraic effort. However for numerical computations it is much more convenient to have a simple method, ready to be applied as a routine in a computer program, which gives the matrices of the reps for any space group and for any value of the wave vector **k**. Such a need has already arisen in the literature (Worlton & Warren, 1972) in order to reduce the amount of input data, and possible errors, connected with group-theoretical analysis of crystal vibrations.

In this paper a method is presented for obtaining the single-valued reps of any space group, having in mind the possibilities of a digital computer for handling all the necessary algebraic steps. The procedure involves rather tedious computations for high-symmetry space groups of the cubic system. The reps for these space groups will be discussed in detail, in order to provide a procedure suitable also for hand calculations. To ease the comprehension of this paper, an effort has been made to avoid a highly sophisticated group-theoretical language in discussing the method. A knowledge of the general theory of space group representations is however assumed as presented, for instance, in Koster's (1957) review article or in the book by Lyubarskii (1960).

1. Introduction

A brief introduction, mainly intended to explain the notation used in this paper, is given here for convenience of the reader. For a complete treatment of the general theory of space groups reference is made to the classical work of Seitz (1934, 1935, 1936).

Using a notation first introduced by Seitz, the most general form for an element of a space group G is

$$\{\alpha|\mathbf{v}(\alpha)+\mathbf{R}_n\}$$

where α is a rotational element, $\mathbf{v}(\alpha)$ is a fractional translation associated with it and $\mathbf{R}_n$ is a translation of the lattice. In terms of a basis

$$\boldsymbol{t}=[\mathbf{t}_1\,\mathbf{t}_2\,\mathbf{t}_3]\,,$$

where $\mathbf{t}_1$, $\mathbf{t}_2$ and $\mathbf{t}_3$ are unit translational vectors of the direct lattice, $\mathbf{R}_n$ is given by

$$\mathbf{R}_n=n_1\mathbf{t}_1+n_2\mathbf{t}_2+n_3\mathbf{t}_3 \quad (n_1,n_2,n_3=0,\pm1,\pm2,\ldots)\,.$$

In dealing with space-group elements it will be convenient to identify $\mathbf{v}(\alpha)$ giving its three fractional components relative to the basis $\boldsymbol{t}$. These three components depend on where the origin of the coordinate system in G is taken. If $\{\alpha|\mathbf{v}(\alpha)\}$ is a space-group element written for a given origin of the coordinate system, then it becomes

$$\{\alpha|\bar{\mathbf{v}}(\alpha)\}=\{E|\mathbf{a}\}^{-1}\{\alpha|\mathbf{v}(\alpha)\}\,\{E|\mathbf{a}\} \qquad (1.1)$$

when the origin is translated by a vector $\mathbf{a}$. According to (1.1) $\mathbf{v}(\alpha)$ can be formally decomposed into two parts: a first component, $\mathbf{v}_{\parallel}(\alpha)$, is part of the definition of a space-group element; a second component, $\mathbf{v}_{\perp}(\alpha)$, depends on the choice of origin and may be put equal to zero if the origin is properly chosen. This statement will be clearer after the following discussion, based on a treatment given by Seitz (1935).

For a given $\{\alpha|\mathbf{v}(\alpha)\}$ let $\mathbf{T}(\alpha)$ be a matrix defined by

$$\alpha \boldsymbol{t} = \boldsymbol{t}\mathbf{T}(\alpha)\,.$$

$\mathbf{T}(\alpha)$ can be reduced into diagonal form by a transformation

$$\mathbf{S}^{-1}\mathbf{T}(\alpha)\mathbf{S}=\mathbf{N}$$

where $\mathbf{S}$ is a 3×3 matrix of the eigenvectors of $\mathbf{T}(\alpha)$, and $\mathbf{N}$ is a diagonal matrix of the eigenvalues $\nu_1=\pm1$, $\nu_2=\nu_3^*$. The transformation is possible because the matrices $\mathbf{T}(\alpha)$ form a 3×3 representation of the point group whose elements are the rotational parts α. According to a fundamental theorem of group theory (Wigner, 1959) a representation can always be transformed into a unitary one. Then a given unitary matrix $\mathbf{T}(\alpha)$ can be brought into diagonal form with eigenvalues of modulus 1 of the kind listed above.

If $\mathbf{s}_1$, $\mathbf{s}_2$, $\mathbf{s}_3$ are eigenvectors of $\mathbf{T}(\alpha)$, $\mathbf{v}(\alpha)$ in this new basis has components

$$\mathbf{v}(\alpha)=v_1'\mathbf{s}_1+v_2'\mathbf{s}_2+v_3'\mathbf{s}_3 \qquad (1.2)$$

obtained from the components v_1, v_2, v_3 in the basis $\boldsymbol{t}$ by the transformation

$$\begin{vmatrix}v_1'\\v_2'\\v_3'\end{vmatrix}=\mathbf{S}^{-1}\begin{vmatrix}v_1\\v_2\\v_3\end{vmatrix}\,.$$

In (1.2) the components of eigenvectors whose associated eigenvalues are $\nu=+1$ and $\nu\neq+1$ define, respectively, two vectors $\mathbf{v}_{\parallel}(\alpha)$ and $\mathbf{v}_{\perp}(\alpha)$ such that

$$\begin{aligned}\mathbf{v}(\alpha)&=\mathbf{v}_{\parallel}(\alpha)+\mathbf{v}_{\perp}(\alpha)\\ \alpha\mathbf{v}_{\parallel}(\alpha)&=\mathbf{v}_{\parallel}(\alpha)\\ \mathbf{v}_{\parallel}(\alpha)^{\dagger}\,\mathbf{v}_{\perp}(\alpha)&=0\,.\end{aligned} \qquad (1.3)$$

Any single $\mathbf{v}(\alpha)$ can then be uniquely decomposed according to (1.3). $\mathbf{v}_{\parallel}(\alpha)$ is different from zero only in two cases: $\{\alpha|\mathbf{v}(\alpha)\}$ represents a screw axis and $\mathbf{v}_{\parallel}(\alpha)$ is the component of $\mathbf{v}(\alpha)$ in the direction of the axis; $\{\alpha|\mathbf{v}(\alpha)\}$ represents a glide plane and $\mathbf{v}_{\parallel}(\alpha)$ is the component of $\mathbf{v}(\alpha)$ lying in the plane. Once $\mathbf{v}_{\parallel}(\alpha)$ and $\mathbf{v}_{\perp}(\alpha)$ are found, a vector $\mathbf{a}$ may be determined such that

$$\{E|\mathbf{a}\}^{-1}\{\alpha|\mathbf{v}(\alpha)\}\,\{E|\mathbf{a}\}=\{\alpha|\mathbf{v}_{\parallel}(\alpha)\} \qquad (1.4)$$

where $\mathbf{a}$ must obey the condition

$$[\mathbf{E}-\mathbf{T}(\alpha)]\mathbf{a}=\mathbf{v}_{\perp}(\alpha)\,.$$

It is well known (Koster, 1957; Lyubarskii, 1960) that the problem of finding the reps of a space group G associated with a given wave vector $\mathbf{k}$ reduces to the problem of obtaining the reps of the space group of $\mathbf{k}$, $G(\mathbf{k})$. Given a $\mathbf{k}=\mathbf{k}_1$ chosen from the possible arms of the star of $\mathbf{k}$, the rotational parts of the elements in $G(\mathbf{k})$ are such that

$$\alpha\mathbf{k}=\mathbf{k}+\mathbf{K}_{\alpha}$$

where $\mathbf{K}_{\alpha}$ is a translation in reciprocal space,
$\mathbf{K}_{\alpha}=m_1\mathbf{b}_1+m_2\mathbf{b}_2+m_3\mathbf{b}_3 \quad (m_1,m_2,m_3=0,\pm1,\pm2,\ldots)$, and $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$ are unit translational vectors of the reciprocal space defined by the relations

$$\mathbf{b}_i\cdot\mathbf{t}_j=\delta_{ij}\,. \qquad (1.5)$$

In what follows $\mathbf{k}$ is identified by its three fractional components in terms of $\mathbf{b}$ unit vectors. $G(\mathbf{k})$ can be decomposed into g cosets of its invariant subgroup R of the pure translations $\{E|\mathbf{R}_n\}$

$$G(\mathbf{k})=R+\{\alpha_2|\mathbf{v}(\alpha_2)\}R+\ldots+\{\alpha_g|\mathbf{v}(\alpha_g)\}R \qquad (1.6)$$

where $\{\alpha_i|\mathbf{v}(\alpha_i)\}$ is a representative of the ith coset. These coset representatives do not, in general, form a group since

$$\{\alpha_i|\mathbf{v}(\alpha_i)\}\,\{\alpha_j|\mathbf{v}(\alpha_j)\}=\{E|\mathbf{R}_n\}\,\{\alpha_l|\mathbf{v}(\alpha_l)\} \qquad (1.7)$$

where $\alpha_i\alpha_j=\alpha_l$ and $\mathbf{R}_n=\alpha_i\mathbf{v}(\alpha_j)+\mathbf{v}(\alpha_i)-\mathbf{v}(\alpha_l)$. The element on the right-hand side of (1.7) is not one of the coset representatives, and in this sense they do not form a group, unless $\mathbf{R}_n=(0,0,0)$ for all possible products. In this case $G(\mathbf{k})$ is a symmorphic space group, that is $\mathbf{v}(\alpha)=(0,0,0)$ for all α's, and its reps are simply related to those of ordinary point groups as explained by Koster (1957). In any case the elements of the factor group $G(\mathbf{k})/R$ do form a group isomorphous with the point group $G_0(\mathbf{k})$ of order g containing only the rotational parts of the elements in $G(\mathbf{k})$. Tables for the reps of $G(\mathbf{k})$ are usually given for the coset representatives only since, if

$$\mathbf{D}_{\mathbf{k}}(\{\alpha_i|\mathbf{v}(\alpha_i)\})$$

is a matrix associated with the ith coset representative in $G(\mathbf{k})$, then the matrix for any element $\{\alpha_i|\mathbf{v}(\alpha_i)+\mathbf{R}_n\}$ is simply written as

$$\exp\left(-2\pi i\mathbf{k}\cdot\mathbf{R}_n\right)\mathbf{D}_{\mathbf{k}}(\{\alpha_i|\mathbf{v}(\alpha_i)\})\,.$$

The quantity 2π is required because of the definition (1.5) of the $\mathbf{b}$ vectors; it will be omitted from now on although always implied in the exponential. The minus sign in the exponent is necessary (Altmann & Cracknell, 1965) in order to be consistent with the multiplication rule of Seitz's operators.

2. Non-cubic space groups

It is well known that every space group contains an invariant subgroup of index 2 or 3. In this section we will discuss space groups containing an invariant subgroup $G'(\mathbf{k})$ of index 2. Space groups containing an invariant subgroup of index 3 will be dealt with in the next section.

Let us decompose $G(\mathbf{k})$ as

$$G(\mathbf{k}) = G'(\mathbf{k}) + \{\alpha|\mathbf{v}(\alpha)\}G'(\mathbf{k}) \tag{2.1}$$

where $\alpha\alpha = E$ and $\{\alpha|\mathbf{v}(\alpha)\}$ does not belong to $G'(\mathbf{k})$. The reps of $G(\mathbf{k})$ can be simply derived from those of $G'(\mathbf{k})$ using an induction method very similar to that presented by Zak (1960). Let $\{\beta_i|\mathbf{v}(\beta_i)\}$ be one of the g' coset representatives of $G'(\mathbf{k})$, with respect to the pure translational group R, and let

$$\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\})$$

be a matrix associated with it in the jth rep of $G'(\mathbf{k})$ of dimensionality l'_j. If φ is a function defined in the space operated on by the operators associated with the elements of $G(\mathbf{k})$, then

$$O(\{\beta_i|\mathbf{v}(\beta_i)\})\varphi$$

will be a new function formed by operation with the operator $O(\{\beta_i|\mathbf{v}(\beta_i)\})$ associated with $\{\beta_i|\mathbf{v}(\beta_i)\}$. For the rep $D^{(j)}_{\mathbf{k}}$ of $G'(\mathbf{k})$ l'_j symmetrized functions can be written as

$$\Phi_{\nu.} = \sum_{h=1}^{g'} \mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_h|\mathbf{v}(\beta_h)\})^*_{\nu.}\, O(\{\beta_h|\mathbf{v}(\beta_h)\})\varphi\,. \tag{2.2}$$

The dot in $\Phi_{\nu.}$ remind us that a basis

$$\Phi_1, \Phi_2, \ldots, \Phi_{l'_j}$$

for the jth rep of $G'(\mathbf{k})$ was obtained using a given column of $D^{(j)}_{\mathbf{k}}$ in the projection operator and it will be omitted from now on. By acting on the l'_j functions (2.2) with the operator $O(\{\alpha|\mathbf{v}(\alpha)\})$, a set of l'_j new functions are defined as

$$\Psi_\nu = O(\{\alpha|\mathbf{v}(\alpha)\})\Phi_\nu\,. \tag{2.3}$$

The functions Ψ_ν are linearly independent among themselves; any assumption contrary to this would imply a linear dependence among the Φ's, in contrast to their definition as a basis for a rep of $G'(\mathbf{k})$. The transformation properties of these functions will now be discussed. From the definition (2.2) it is obvious that

$$O(\{\beta_i|\mathbf{v}(\beta_i)\})\Phi_\nu = \sum_{\mu=1}^{l_j'} \mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\})_{\mu\nu}\Phi_\mu\,. \tag{2.4}$$

Next, if $\alpha\beta_i\alpha = \beta_m$,

$$O(\{\beta_i|\mathbf{v}(\beta_i)\})\Psi_\nu = \omega_i \sum_{\mu=1}^{l_j'} \mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_m|\mathbf{v}(\beta_m)\})_{\mu\nu}\Psi_\mu$$

$$\omega_i = \exp\{-i\mathbf{k}\cdot[\beta_i\mathbf{v}(\alpha) + \mathbf{v}(\beta_i) - \alpha\mathbf{v}(\beta_m) - \mathbf{v}(\alpha)]\}\,. \tag{2.5}$$

Equation (2.3) through (2.5) and the following equation

$$O(\{\alpha|\mathbf{v}(\alpha)\})\Psi_\nu = \theta\Phi_\nu$$
$$\theta = \exp\{-i\mathbf{k}\cdot[\alpha\mathbf{v}(\alpha) + \mathbf{v}(\alpha)]\} \tag{2.6}$$

define a $2l'_j \times 2l'_j$ representation $D_{\mathbf{k}}$ of $G(\mathbf{k})$, induced by a rep $D^{(j)}_{\mathbf{k}}$ of $G'(\mathbf{k})$, whose basis is

$$\Phi_1, \Phi_2, \ldots, \Phi_{l'_j}, \Psi_1, \Psi_2, \ldots, \Psi_{l'_j}.$$

The matrices for this representation are

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{\alpha|\mathbf{v}(\alpha)\} \\ \begin{vmatrix} \mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\}) & \mathbf{0} \\ \mathbf{0} & \omega_i\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_m|\mathbf{v}(\beta_m)\}) \end{vmatrix} & \begin{vmatrix} \mathbf{0} & \theta\mathbf{E} \\ \mathbf{E} & \mathbf{0} \end{vmatrix} \end{array}$$

where $\mathbf{E}$ is the $l'_j \times l'_j$ identity matrix. A simple similarity transformation leads to a more convenient form for $D_{\mathbf{k}}$, namely

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{\alpha|\mathbf{v}(\alpha)\} \\ \begin{vmatrix} \mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\}) & \mathbf{0} \\ \mathbf{0} & \omega_i\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_m|\mathbf{v}(\beta_m)\}) \end{vmatrix} & \eta\begin{vmatrix} \mathbf{0} & \mathbf{E} \\ \mathbf{E} & \mathbf{0} \end{vmatrix} \end{array} \tag{2.7}$$

where $\eta = \exp\{-i\mathbf{k}/2\cdot[\alpha\mathbf{v}(\alpha) + \mathbf{v}(\alpha)]\}$, β_m and ω_i are defined in (2.5). According to Schur's lemma the representation (2.7) is reducible if a matrix $\mathbf{A} \neq c\mathbf{E}$ (c = constant) exists which commutes with all the matrices of the representation. For our purposes it is convenient to analyze the structure of an Hermitian matrix $\mathbf{H} = \mathbf{A} + \mathbf{A}^\dagger$ which commutes with all the matrices in (2.7). Since $D^{(j)}_{\mathbf{k}}$ is irreducible and $\mathbf{H}$ must commute with the matrix representing $\{\alpha|\mathbf{v}(\alpha)\}$ in (2.7), it can be written as

$$\mathbf{H} = \begin{vmatrix} c_1\mathbf{E} & \mathbf{U} \\ \mathbf{U} & c_1\mathbf{E} \end{vmatrix} \tag{2.8}$$

where $\mathbf{U}$ is a $l'_j \times l'_j$ Hermitian matrix, $\mathbf{E}$ is the identity matrix with the same dimension and c_1 is a constant.

If $\mathbf{U} = \mathbf{0}$ the representation (2.7) is irreducible and forms a rep of $G(\mathbf{k})$ of dimensionality $2l'_j$. The matrices representing $G'(\mathbf{k})$ in $D_{\mathbf{k}}$ form a representation, subduced from $D_{\mathbf{k}}$ by $G'(\mathbf{k})$ in the language of group theory, obviously reducible into two non-equivalent, conjugate reps of $G'(\mathbf{k})$ with dimensionality l'_j. That is, each pair of $l'_j \times l'_j$ reps of $G'(\mathbf{k})$, conjugate with respect to $G(\mathbf{k})$, induce one rep of $G(\mathbf{k})$ of dimensionality $2l'_j$.

If $\mathbf{U} \neq \mathbf{0}$ it can be diagonalized by a unitary transformation $\mathbf{X}$, and the unitary matrix in block form

$$\sqrt{\tfrac{1}{2}}\begin{vmatrix} \mathbf{X} & \mathbf{X} \\ \mathbf{X} & -\mathbf{X} \end{vmatrix} \tag{2.9}$$

will reduce $\mathbf{H}$ to diagonal form giving l'_j-fold degenerate eigenvalues. A transformation, obtained from (2.9) after ordering the eigenvalues and eigenvectors of $\mathbf{H}$, reduces the representation (2.7) into block-diagonal form, each block of dimensions $l'_j \times l'_j$. The two blocks correspond to two non-equivalent reps of $G(\mathbf{k})$, derived from a self-conjugate rep $D_{\mathbf{k}}^{(j)}$ of its invariant subgroup of index 2.

These conclusions lead to a particularly simple result when $\{\alpha|\mathbf{v}(\alpha)\}$ in (2.1) stands for the inversion element $\{I|\mathbf{v}(I)\}$. In what follows $G'(\mathbf{k})$ is the invariant subgroup of index 2 not containing the inversion and a representation of $G(\mathbf{k})$ is given by

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{I|\mathbf{v}(I)\} \\ \begin{vmatrix} \mathbf{D}_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) & \mathbf{0} \\ \mathbf{0} & \pm D_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) \end{vmatrix} & \begin{vmatrix} \mathbf{0} & \mathbf{E} \\ \mathbf{E} & \mathbf{0} \end{vmatrix} \end{array} \quad (2.10)$$

$\omega_l = \pm 1$, see (2.7), derives from the assumption that $I \in G_0(\mathbf{k})$; $\mathbf{k}$ and $-\mathbf{k}$ are then equivalent up to a translation of the reciprocal lattice and this is possible only if $\mathbf{k}$ has components 0 or $\frac{1}{2}$.

Since $G'_0(\mathbf{k})$ is at most of order 24, l'_j cannot exceed 4 according to a general dimensionality theorem (Hurley, 1966). However, as will be shown in the next section, no rep of dimensionality 4 exists if $G_0(\mathbf{k}) = O_h$, the full octahedral group in the Schoenflies notation. In this case $G(\mathbf{k})$ has reps of dimensionality $l_j \le 6$; since $l_j = l'_j$ or $2l'_j$, as shown above, the dimensionality of the reps of $G'(\mathbf{k})$ cannot exceed $l'_j = 3$.

It is now quite evident that, if the plus sign always holds in (2.10), $\mathbf{X} = \mathbf{E}$ in (2.9) and the representation of $G(\mathbf{k})$ reduces to

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{I|\mathbf{v}(I)\} \\ \begin{vmatrix} \mathbf{D}_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) \end{vmatrix} & \begin{vmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{0} & -\mathbf{E} \end{vmatrix} \end{array} \quad (2.11)$$

Each rep of $G'(\mathbf{k})$ is self-conjugate and produces two non-equivalent reps of $G(\mathbf{k})$ with the same dimension: an 'even' and an 'odd' rep with respect to the inversion.

If the minus sign applies in (2.10) for some $\{\beta_i|\mathbf{v}(\beta_i)\}$, the coset representatives in $G'(\mathbf{k})$ split into two sets $\delta_1, \delta_2, \ldots$ and $\gamma_1, \gamma_2, \ldots$ whose transformation properties are

$$O(\delta_i)\Psi_\nu = + \sum_{\mu=1}^{l_j'} \mathbf{D}_{\mathbf{k}}^{(j)}(\delta_i)_{\mu\nu}\Psi_\mu$$
$$O(\gamma_i)\Psi_\nu = - \sum_{\mu=1}^{l_j'} \mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)_{\mu\nu}\Psi_\mu . \quad (2.12)$$

All coset representatives of the kind δ define an invariant subgroup $S(\mathbf{k})$ of $G'(\mathbf{k})$ of index 2. This can easily be seen by checking the multiplication properties of the matrices in the representation subduced by $G'(\mathbf{k})$ from (2.10). If the representation $D_{\mathbf{k}}$ is now reducible, a $\mathbf{U}$ matrix exists such that

$$\mathbf{D}_{\mathbf{k}}^{(j)}(\delta_i)\mathbf{U} = \mathbf{U}\mathbf{D}_{\mathbf{k}}^{(j)}(\delta_i) \quad (2.13)$$
$$\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)\mathbf{U} = -\mathbf{U}\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i) \quad (2.14)$$

for all δ's and γ's. Condition (2.14) implies that

$$\det [\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)] = \det [-\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)] .$$

If l'_j is odd this requirement is satisfied only if $\det [\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)] = 0$ which is impossible since $D_{\mathbf{k}}^{(j)}$ is a rep of $G'(\mathbf{k})$. Therefore, when l'_j is odd and the minus sign applies in (2.10) for some $\{\beta_i|\mathbf{v}(\beta_i)\}$, the induced representation is already a rep of $G(\mathbf{k})$.

For l'_j even, and only $l'_j = 2$ may occur, if the representation (2.10) is reducible the $\mathbf{U}$ matrix and all $\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma)$'s have a zero character because of (2.14). From (2.13), this $\mathbf{U}$ matrix, different from $c\mathbf{E}$, commutes with all the matrices subduced from $D_{\mathbf{k}}^{(j)}$ by a subgroup $S(\mathbf{k})$. This means that all $\mathbf{D}_{\mathbf{k}}^{(j)}(\delta)$'s can be simultaneously brought to diagonal form. The possibility for all $\mathbf{D}_{\mathbf{k}}^{(j)}(\delta)$'s to be reduced to the following diagonal form

$$\mathbf{D}_{\mathbf{k}}^{(j)}(\delta_i) = c_i\mathbf{E}$$

must be ruled out. Otherwise, $S(\mathbf{k})$ being an invariant subgroup of index 2 of $G'(\mathbf{k})$, $D_{\mathbf{k}}^{(j)}$ could be reduced into two one-dimensional reps, contrary to the assumption that $l'_j = 2$.

Therefore, if all cosets representative in $G'(\mathbf{k})$ of the kind δ are represented by diagonal matrices in $D_{\mathbf{k}}^{(j)}$, a suitable $\mathbf{U}$ matrix is

$$\mathbf{U} = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \quad (2.15)$$

and every $\mathbf{D}_{\mathbf{k}}^{(j)}(\gamma_i)$ has the structure

$$\begin{vmatrix} 0 & \exp(i\Theta) \\ \pm\exp(-i\Theta) & 0 \end{vmatrix} .$$

On the other hand a different choice of basis functions in $D_{\mathbf{k}}^{(j)}$ could lead to a representation, subduced by $S(\mathbf{k})$, which is not a diagonal one. In this case the $\mathbf{H}$ matrix in (2.8) has a block

$$\mathbf{U} = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} . \quad (2.16)$$

In any case the representation (2.10) can be reduced to block-diagonal form through two consecutive similarity transformations carried out using first a matrix

$$\begin{vmatrix} \mathbf{E} & \mathbf{0} \\ \mathbf{0} & \mathbf{U} \end{vmatrix}$$

and then a matrix (2.9) where $\mathbf{X} = \mathbf{E}$. The final result is

$$\begin{array}{cc} \{\beta_i|v(\beta_i)\} & \{I|\mathbf{v}(I)\} \\ \begin{vmatrix} \mathbf{D}_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_{\mathbf{k}}^{(j)}(\{\beta_i|\mathbf{v}(\beta_i)\}) \end{vmatrix} & \begin{vmatrix} \mathbf{U} & \mathbf{0} \\ \mathbf{0} & -\mathbf{U} \end{vmatrix} \end{array} \quad (2.17)$$

where $\mathbf{U}$ is a matrix (2.15) or (2.16). The two reps of $G(\mathbf{k})$ are not equivalent; should they be equivalent, a matrix would exist which is equal to $c\mathbf{E}$ since it commutes with $D^{(j)}_{\mathbf{k}}$ but has a zero character in order to transform $\mathbf{U}$ into $-\mathbf{U}$.

In conclusion, the following procedure may be used to produce all the reps of $G(\mathbf{k})$ once the reps of $G'(\mathbf{k})$, the invariant subgroup of index 2 not containing the inversion, are known. The coset representatives $\{\beta_i|\mathbf{v}(\beta_i)\}$ in $G'(\mathbf{k})$ are classified according to the sign of $\exp(-i\mathbf{k}\cdot\mathbf{R}_n)$ where $\mathbf{R}_n=2\mathbf{v}(\beta_i)+\beta_i\mathbf{v}(I)-\mathbf{v}(I)$. One of the two following possibilities arises:

(*a*) $\exp(-i\mathbf{k}\cdot\mathbf{R}_n)>0$ for all $\{\beta_i|\mathbf{v}(\beta_i)\}$ – the reps of $G'(\mathbf{k})$ are self-conjugate and each of them produces two reps of $G(\mathbf{k})$ as shown in (2.11).

(*b*) $\exp(-i\mathbf{k}\cdot\mathbf{R}_n)<0$ for some $\{\beta_i|\mathbf{v}(\beta_i)\}$ – all coset representatives such that $\exp(-i\mathbf{k}\cdot\mathbf{R}_n)>0$ define an invariant subgroup $S(\mathbf{k})$ of index 2 of $G'(\mathbf{k})$. Reps of $G'(\mathbf{k})$ with dimensionality 1 or 3 always occur in pairs of conjugate reps, each pair easily recognized by the following rule: each coset representative in $S(\mathbf{k})$ has the same character in the two reps, any other coset representative showing characters of equal magnitude but opposite sign. Each pair of reps produces one rep of $G(\mathbf{k})$ with dimensionality $2l'_j$ as shown in (2.10). The same conclusion applies for $l'_j=2$ if a pair of conjugate reps exists. If this is not the case, each rep of $G'(\mathbf{k})$ with dimensionality 2 produces two reps (2.17) of $G(\mathbf{k})$. The $\mathbf{U}$ matrix in (2.17) is given by (2.15) if $S(\mathbf{k})$ subduces a diagonal representation from $D^{(j)}_{\mathbf{k}}$, otherwise the appropriate $\mathbf{U}$ matrix is given by (2.16).

It is now possible to simplify the process of obtaining the reps of any space group since only groups of $\mathbf{k}$ not containing the inversion need to be considered. The symbol $G(\mathbf{k})$ will be reserved for such space groups from now on. The above mentioned procedure will be applied as a final step if $G(\mathbf{k})$ is actually a subgroup of a larger group (containing the inversion).

As can be verified by inspection, almost all $G(\mathbf{k})$'s contain a cyclic invariant subgroup of index 2, with the exception of space groups belonging to the cubic system, simple and body-centred lattices, for values of $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ or $\mathbf{k}=(\frac{1}{4},\frac{1}{4},\frac{1}{4})$. This last case will be explicitly considered in the last section. Within these limits the usual induction method can be applied to $G(\mathbf{k})$, decomposed as in (2.1), bearing in mind that now $G'(\mathbf{k})$ is a cyclic invariant subgroup of index 2. The advantage of this procedure lies in the fact that it is very simple to write down the reps of a cyclic space group.

Let us first assume that the origin of the coordinate system in G coincides with the point about which all rotations in $G'(\mathbf{k})$ are defined. That is, if $\{\beta_i|\mathbf{v}(\beta_i)\}$ is any of the g' coset representatives in $G'(\mathbf{k})$, $\mathbf{v}(\beta_i)=\mathbf{v}_{\parallel}(\beta_i)$ for all β's [see (1.3)]. In this simple case the multiplier reps of $G'(\mathbf{k})$ coincide (Lyubarskii, 1960) with the ordinary point group reps of $G'_0(\mathbf{k})$, which means

$$\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\})=\exp[-i\mathbf{k}\cdot\mathbf{v}(\beta_i)]\mathbf{D}^{(j)}(\beta_i) \quad (2.18)$$

where $\mathbf{D}^{(j)}(\beta_i)$ represents β_i in the jth rep of the cyclic point group $G'_0(\mathbf{k})$.

To complete this discussion, the more general case of some coset representative in $G'(\mathbf{k})$ such that $\mathbf{v}_{\perp}(\beta_i)\neq 0$ (and $\exp[-i\mathbf{k}\cdot\mathbf{v}_{\perp}(\beta_i)]\neq 1$) must be taken into account. If β is a generator of $G'_0(\mathbf{k})$, a transformation

$$\{E|\mathbf{a}\}^{-1}\{\beta|\mathbf{v}(\beta)\}\{E|\mathbf{a}\}=\{\beta|\mathbf{v}_{\parallel}(\beta)\} \quad (2.19)$$

is always possible (see § 1). The same transformation on any other coset representative in $G'(\mathbf{k})$ gives

$$\{E|\mathbf{a}\}^{-1}\{\beta_i|\mathbf{v}(\beta_i)\}\{E|\mathbf{a}\}=\{E|\mathbf{R}^i_n\}\{\beta_i|\mathbf{v}_{\parallel}(\beta_i)\}. \quad (2.20)$$

Using (2.18) and the definitions of $\mathbf{v}_{\parallel}(\beta_i)$ and $\mathbf{R}^i_n$ connected with (2.19) and (2.20), the matrices for the jth rep of any cyclic space group of $\mathbf{k}$ are given by

$$\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\}) \\ =\exp\{-i\mathbf{k}\,.\,[\mathbf{v}_{\parallel}(\beta_i)+\mathbf{R}^i_n]\}\mathbf{D}^{(j)}(\beta_i)\,. \quad (2.21)$$

The induction method, applied now using the reps (2.21) of $G'(\mathbf{k})$, produces the following representation of the space group $G(\mathbf{k})$

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{\alpha|\mathbf{v}(\alpha)\} \\ \begin{vmatrix} b_i & 0 \\ 0 & \omega_i b_m \end{vmatrix} & \eta\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix} \end{array} \quad . \quad (2.22)$$

Here $b_i=\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_i|\mathbf{v}(\beta_i)\})$ and $b_m=\mathbf{D}^{(j)}_{\mathbf{k}}(\{\beta_m|\mathbf{v}(\beta_m)\})$ are just numbers; β_m, ω_i and η are defined in (2.5) and (2.7). A representation (2.22) is reducible if $b_i=\omega_i b_m$: two one-dimensional, non-equivalent reps of $G(\mathbf{k})$ are obtained as given below

$$\begin{array}{cc} \{\beta_i|\mathbf{v}(\beta_i)\} & \{\alpha|\mathbf{v}(\alpha)\} \\ \begin{vmatrix} b_i & 0 \\ 0 & b_i \end{vmatrix} & \eta\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix} \end{array} \quad . \quad (2.23)$$

On the other hand a rep of $G(\mathbf{k})$ with dimensionality 2 is possible only if a pair of reps of $G'(\mathbf{k})$ exists which are conjugate with respect to $G(\mathbf{k})$. Each pair of reps induces a rep (2.22) of $G(\mathbf{k})$.

3. Cubic space groups

Space groups belonging to the cubic system do not possess a cyclic invariant subgroup of index 2 and the procedure presented at the end of the previous section cannot be applied for high-symmetry points on the Brillouin zone boundary. This is the case of $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ for the simple cubic lattice and $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ or $\mathbf{k}=(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ for the body-centred cubic lattice. Any other point in $\mathbf{k}$ space defines a $G(\mathbf{k})$ which meets the requirements of § 2: $\mathbf{k}=(0,0,0)$ needs no special consideration since the reps of $G(\mathbf{0})$ coincide with those of an ordinary point group.

In this section the reps of space groups $G(\mathbf{k})$ showing tetrahedral or octahedral symmetry will be discussed explicitly. We will first analyze reps of space groups $G^T(\mathbf{k})$ whose associated point group is T, the group of the 12 rotational elements which take a regular tetrahedron into itself. $G^T(\mathbf{k})$ is contained in any space group of $\mathbf{k}$ considered in this section. Therefore, once the reps of all possible $G^T(\mathbf{k})$'s are obtained, it is simple to complete our analysis for all cubic space groups. $G^T(\mathbf{k})$ contains an invariant subgroup of index 3 and the induction method, as presented in § 2, could be extended to cover this case. However, a deeper insight into the structure of the reps of $G^T(\mathbf{k})$ can be gained if the induction method is applied in a slightly different manner. Besides, the induction method of § 2 requires first a knowledge of the reps of the invariant subgroup of index 3: that is, two steps would be necessary to obtain the reps of $G^T(\mathbf{k})$ rather than only one.

Let C_2^i, C_2^j and C_2^k be three binary axes, directed along three orthogonal unit vectors $\boldsymbol{i}, \boldsymbol{j}$ and $\boldsymbol{k}$, defining the invariant subgroup of T and let C_3 be the generator of a cyclic subgroup of order 3 of T. If $\mathbf{t}$ is a unit translational vector of the lattice in a direction not coincident with the C_3 axis, let us select three unit translational vectors $\mathbf{t}_1=\mathbf{t}$, $\mathbf{t}_2=C_3\mathbf{t}$, $\mathbf{t}_3=(C_3)^{-1}\mathbf{t}$. Or, conversely, let us choose C_3, out of the four possible threefold axes in T, such that it cyclically interchanges the three unit translational vectors of the direct lattice. If the origin of the coordinates coincides with a point about which the rotation C_3 is defined, then $\mathbf{v}(C_3)=\mathbf{v}_{\parallel}(C_3)$. These two conditions on C_3 lead to $\mathbf{v}(C_3)=(a,a,a)$ where a is equal to 0, $\frac{1}{3}$ or $\frac{2}{3}$ in order to meet the requirement $\{C_3|\mathbf{v}(C_3)\}^3=\{E|\mathbf{R}_n\}$. In any case a suitable origin shift will produce a coset representative in $G^T(\mathbf{k})$ written as $\{C_3|\mathbf{0}\}$. For instance, if $a=\frac{1}{3}$ a transformation could be applied

$$\{E|0,\tfrac{1}{3},\tfrac{2}{3}\}^{-1}\{C_3|\tfrac{1}{3},\tfrac{1}{3},\tfrac{1}{3}\}\,\{E|0,\tfrac{1}{3},\tfrac{2}{3}\} =\{E|1,0,0\}\,\{C_3|0,0,0\}$$

if $C_3\mathbf{t}_1=\mathbf{t}_2$, $C_3\mathbf{t}_2=\mathbf{t}_3$ and $C_3\mathbf{t}_3=\mathbf{t}_1$.

The reps of $G^T(\mathbf{k})$ will, of course, depend on the particular origin implied here. However, reps for different origins are simply related. Let $\{\alpha|\mathbf{v}(\alpha)\}$ be a coset representative and $D_{\mathbf{k}}^{(J)}$ a rep of $G^T(\mathbf{k})$. For any different choice of origin $\{\alpha|\mathbf{v}(\alpha)\}$ and $\{C_3|\mathbf{0}\}$ will appear as $\{\alpha|\bar{\mathbf{v}}(\alpha)\}$ and $\{C_3|\mathbf{v}(C_3)\}$ respectively, and the matrices for the new origin are given by the relationship

$$\mathbf{D}_{\mathbf{k}}^{(J)}(\{\alpha|\bar{\mathbf{v}}(\alpha)\})=\exp\,(-i\mathbf{k}\cdot\mathbf{R}_n^{\alpha})\mathbf{D}_{\mathbf{k}}^{(J)}(\{\alpha|\mathbf{v}(\alpha)\}) \quad (3.1)$$

where $\mathbf{R}_n^{\alpha}$ is such that

$$\{E|\mathbf{a}\}^{-1}\{\alpha|\bar{\mathbf{v}}(\alpha)\}\,\{E|\mathbf{a}\}=\{E|\mathbf{R}_n^{\alpha}\}\,\{\alpha|\mathbf{v}(\alpha)\}$$

and $\mathbf{a}$ is defined by the transformation

$$\{E|\mathbf{a}\}^{-1}\{C_3|\mathbf{v}(C_3)\}\,\{E|\mathbf{a}\}=\{E|\mathbf{R}_n\}\,\{C_3|\mathbf{0}\}$$

which is always possible in view of the arguments previously given.

Let β represent a binary axis in T; then

$$C_3\beta_i(C_3)^{-1}=\beta_j$$

with $\beta_i\neq\beta_j$. The corresponding multiplication of coset representatives is

$$\{C_3|\mathbf{0}\}\,\{\beta_i|\mathbf{v}(\beta_i)\}\,\{C_3|\mathbf{0})^{-1}=\{E|\mathbf{R}_n\}\,\{\beta_j|\mathbf{v}(\beta_j)\}$$

with $R_n=C_3\mathbf{v}(\beta_i)-\mathbf{v}(\beta_j)$. Since $\mathbf{v}(\beta_i)$ and $\mathbf{v}(\beta_j)$ may be written as positive fractional translations and C_3 simply interchanges the three unit translations, it must be $\mathbf{R}_n=(0,0,0)$. Let then, say,

$$\{C_3|\mathbf{0}\}\,\{C_2^i|\mathbf{v}(C_2^i)\}\,\{C_3|\mathbf{0}\}^{-1}=\{C_2^j|\mathbf{v}(C_2^j)\}\,. \quad (3.2)$$

Using this transformation property it can be shown that two possibilities arise when $G^T(\mathbf{k})$ is a non-symmorphic space group of $\mathbf{k}$:

(1) C_2^i is essentially a screw axis, that is $\mathbf{v}(C_2^i)$ has a component different from zero and equal to $a\boldsymbol{i}/2$; $\mathbf{t}_1=a\boldsymbol{i}$ is a primitive translation (simple cubic lattice) and

$$\{C_2^i|\mathbf{v}(C_2^i)\}^2=\{E|1,0,0\}\,. \quad (3.3)$$

(2) C_2^i is not a screw axis, $\mathbf{v}(C_2^i)=\mathbf{v}_{\perp}(C_2^i)$; $\mathbf{t}=a\boldsymbol{i}$ is a translation of the lattice but not a unitary one (face-centred or body-centred cubic lattices) and

$$\{C_2^i|\mathbf{v}(C_2^i)\}^2=\{E|0,0,0\}\,. \quad (3.4)$$

The following multiplication rules apply, in general, to coset representatives in $G^T(\mathbf{k})$:

$$\begin{aligned}\{C_2^i|\mathbf{v}(C_2^i)\}^2&=\{E|\mathbf{R}_n'\}\\ \{C_2^i|\mathbf{v}(C_2^i)\}\,\{C_2^j|\mathbf{v}(C_2^j)\}&=\{E|\mathbf{R}_n''\}\,\{C_2^k|\mathbf{v}(C_2^k)\}\\ \{C_2^j|\mathbf{v}(C_2^j)\}\,\{C_2^i|\mathbf{v}(C_2^i)\}&=\{E|-(C_3)^{-1}\mathbf{R}_n''\\ &\quad-\mathbf{R}_n'\}\,\{C_2^k|\mathbf{v}(C_2^k)\}\,.\end{aligned} \quad (3.5)$$

Here $\mathbf{R}_n'$ stands for $\{E|1,0,0\}$ or $\{E|0,0,0\}$ depending on the lattice under consideration. The multiplication table can be extended by applying the transformation (3.2) to (3.5). This table, and the restriction placed on the components of the wave vector $\mathbf{k}$ by symmetry requirements, will be used to obtain the reps of $G^T(\mathbf{k})$. With φ and $O(\{\ldots\})$ having the same meaning as in § 2, four basis functions for a representation of $G^T(\mathbf{k})$ are defined as

$$\begin{aligned}\Psi_1&=\varphi+\mathbf{D}^{(J)}(C_3^{-1})O(\{C_3|\mathbf{0}\})\varphi\\ &\quad+D^{(J)}(C_3)O(\{C_3|\mathbf{0}\}^{-1})\varphi\\ \Psi_2&=O(\{C_2^i|\mathbf{v}(C_2^i)\})\Psi_1\\ \Psi_3&=O(\{C_2^j|\mathbf{v}(C_2^j)\})\Psi_1\\ \Psi_4&=O(\{C_2^k|\mathbf{v}(C_2^k)\})\Psi_1\,.\end{aligned} \quad (3.6)$$

$\mathbf{D}^{(J)}(C_3)$ and $\mathbf{D}^{(J)}(C_3^{-1})$ are numbers representing elements of the ordinary cyclic point group C_3. The transformation properties for these functions, written for two generators of $G^T(\mathbf{k})$, are:

$$\begin{array}{ll}
O(\{C_3|\mathbf{0}\})\Psi_1=\mathbf{D}^{(J)}(C_3)\Psi_1 & O(\{C_2^i|\mathbf{v}(C_2^i)\})\Psi_1=\Psi_2 \\
O(\{C_3|\mathbf{0}\})\Psi_2=\mathbf{D}^{(J)}(C_3)\Psi_3 & O(\{C_2^i|\mathbf{v}(C_2^i)\})\Psi_2=\varrho\Psi_1 \\
O(\{C_3|\mathbf{0}\})\Psi_3=\mathbf{D}^{(J)}(C_3)\Psi_4 & O(\{C_2^i|\mathbf{v}(C_2^i)\})\Psi_3=\sigma\Psi_4 \\
O(\{C_3|\mathbf{0}\})\Psi_4=\mathbf{D}^{(J)}(C_3)\Psi_2 & O(\{C_2^i|\mathbf{v}(C_2^i)\})\Psi_4=\varrho^*\sigma^*\Psi_3 .
\end{array} \tag{3.7}$$

where $\varrho=\exp(-i\mathbf{k}\cdot\mathbf{R}_n')$, $\sigma=\exp(-i\mathbf{k}\cdot\mathbf{R}_n'')$, $\mathbf{R}_n'$ and $\mathbf{R}_n''$ defined in (3.5).

For the simple cubic lattice only the point $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ on the surface of the Brillouin zone shows tetrahedral symmetry. For this point $\varrho=-1$ according to (3.3) and $\sigma=+1$ or -1. The matrices for a representation of $G^T(\mathbf{k})$ are

$$\begin{array}{ccc}
 & \{C_3|\mathbf{0}\} & \{C_2^i|\mathbf{v}(C_2^i)\} \\
\mathbf{D}^{(J)}(C_3) & \begin{vmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{vmatrix} & \begin{vmatrix}0&-1&0&0\\1&0&0&0\\0&0&0&-\sigma\\0&0&\sigma&0\end{vmatrix} .
\end{array}$$

A transformation

$$\begin{vmatrix}\sigma&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{vmatrix}$$

applied to the matrices of the representation gives

$$\begin{array}{ccc}
 & \{C_3|\mathbf{0}\} & \{C_2^i|\mathbf{v}(C_2^i)\} \\
\mathbf{D}^{(J)}(C_3) & \begin{vmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{vmatrix} & \sigma\begin{vmatrix}0&-1&0&0\\1&0&0&0\\0&0&0&-1\\0&0&1&0\end{vmatrix} .
\end{array} \tag{3.8}$$

For the body-centred cubic lattice $G(\mathbf{k})$ contains $G^T(\mathbf{k})$ if $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ or $\mathbf{k}=(\frac{1}{4},\frac{1}{4},\frac{1}{4})$. For the first of these two wave vectors $\varrho=1$ and $\sigma=\pm1$ and the following representation of $G^T(\mathbf{k})$ is produced

$$\begin{array}{ccc}
 & \{C_3|\mathbf{0}\} & \{C_2^i|\mathbf{v}(C_2^i)\} \\
\mathbf{D}^{(J)}(C_3) & \begin{vmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{vmatrix} & \sigma\begin{vmatrix}0&1&0&0\\1&0&0&0\\0&0&0&1\\0&0&1&0\end{vmatrix} .
\end{array} \tag{3.9}$$

For the second value of $\mathbf{k}$ two cases are possible: $\varrho=1$ and $\sigma=\pm1$ and a representation (3.9) is obtained; $\varrho=1$ and $\sigma=\pm i$ and the corresponding representation is (3.8).

Apart from a factor σ, the representation (3.9) coincides with a representation of the point group T induced by a representation of its cyclic point group of order 3. Therefore the representation (3.9) is reducible and the reps of $G^T(\mathbf{k})$ are simply related to those of the point group T: all matrices for elements in T other than C_3 and $(C_3)^{-1}$ need to be multiplied by $\sigma=\pm1$ in order to produce a rep of $G^T(\mathbf{k})$.

Representations of the kind (3.8) are irreducible in real space and can be reduced only if a set of complex basis functions is introduced. It is simple to verify that the following Hermitian matrix commutes with all matrices in (3.8)

$$\mathbf{H}=i\begin{vmatrix}0&a&a&a\\-a&0&-a&a\\-a&a&0&-a\\-a&-a&a&0\end{vmatrix} .$$

This matrix has eigenvalues $\nu_1=\nu_2=-\nu_3=-\nu_4$ and, after ordering the eigenvalues, the matrix of the eigenvectors is

$$\begin{vmatrix}1 & i\varepsilon-\varepsilon^* & 1 & -\varepsilon-i\varepsilon^*\\ i\varepsilon-\varepsilon^* & -1 & -\varepsilon-i\varepsilon^* & -1\\ i & \varepsilon+i\varepsilon^* & -i & \varepsilon^*-i\varepsilon\\ \varepsilon+i\varepsilon^* & -i & \varepsilon^*-i\varepsilon & i\end{vmatrix} \tag{3.10}$$

where $\varepsilon=\exp(2\pi i/3)$. If a transformation (3.10), which is unitary after normalization of the eigenvectors, is now applied to (3.8), a reduction of the representation occurs. The matrix (3.10) is, of course, not unique, the reps of $G^T(\mathbf{k})$ being defined up to a similarity transformation. Our choice of the eigenvectors (3.10) produces two reps of $G^T(\mathbf{k})$, one being the complex conjugate of the other if σ is real. Using all three reps of the cyclic group C_3, a reduction of (3.8) yields three non-equivalent reps of $G^T(\mathbf{k})$ given by

$$\begin{array}{llll}
 & \{C_3|\mathbf{0}\} & \{C_2^i|\mathbf{v}(C_2^i)\} & \\
\Gamma_1 & \begin{vmatrix}D & iD\\-D & iD\end{vmatrix} & \sigma\begin{vmatrix}0&1\\-1&0\end{vmatrix} & \\
\Gamma_2 & \begin{vmatrix}D^* & -iD^*\\-D^* & -iD^*\end{vmatrix} & \sigma\begin{vmatrix}0&1\\-1&0\end{vmatrix} & \begin{array}{l}D=\sqrt{\tfrac{1}{2}}\exp(\pi i/12)\\ E=\sqrt{\tfrac{1}{2}}\exp(\pi i/4)\end{array} \\
\Gamma_3 & \begin{vmatrix}-E^* & -E\\E^* & -E\end{vmatrix} & \sigma\begin{vmatrix}0&1\\-1&0\end{vmatrix} & \begin{array}{l}D+iD=-\exp(-2\pi i/3)\\ E+E^*=1 .\end{array}
\end{array} \tag{3.11}$$

A summary of these results may be given as follows:

Let $G^T(\mathbf{k})/R$ be a factor group isomorphous with the tetrahedral point group T. If $C_3\in T$ is a threefold axis which cyclically interchanges the unit translational vectors of the direct lattice and C_2^i, $C_2^j=C_3C_2^i(C_3)^{-1}$, C_2^k are the three binary axes in T, let

$$\begin{aligned}
\varrho&=\exp\{-i\mathbf{k}\cdot[C_2^i\mathbf{v}(C_2^i)+\mathbf{v}(C_2^i)]\}\\
\sigma&=\exp\{-i\mathbf{k}\cdot[C_2^j\mathbf{v}(C_2^i)+\mathbf{v}(C_2^j)-\mathbf{v}(C_2^k)]\} .
\end{aligned}$$

The following three possibilities arise for the reps of $G^T(\mathbf{k})$:

(1) $\varrho=\sigma=1$; the reps of $G^T(\mathbf{k})$ coincide with the reps of the point group T.

(2) $\varrho=1$, $\sigma=-1$; the reps of $G^T(\mathbf{k})$ are the reps of

T after multiplication by -1 of all the matrices associated with elements other than C_3 and $(C_3)^{-1}$.

(3) for all other values of ϱ and σ, $G^T(\mathbf{k})$ has three 2×2 reps given in (3.11) for two generators of the space group.

So far our discussion is complete for cubic space groups when $G(\mathbf{k})\equiv G^T(\mathbf{k})$. If the latter is a subgroup (necessarily an invariant subgroup of index 2) of $G(\mathbf{k})$, then

$$G(\mathbf{k})=G^T(\mathbf{k})+\{\alpha|\mathbf{v}(\alpha)\}G^T(\mathbf{k}) \qquad (3.12)$$

and a further step is necessary to obtain the reps of $G(\mathbf{k})$ itself. It is worth remembering that $G(\mathbf{k})$ stands for space groups (or subgroups) of $\mathbf{k}$ not containing the inversion. At this point the reader could be referred to § 2 and our discussion concluded. However we prefer to give explicitly the reps of all cubic space groups to simplify hand calculations, as mentioned in the Introduction, and to prove a statement anticipated in the previous section. The discussion is simplified, and the reps of $G(\mathbf{k})$ can be explicitly written down, if α is chosen such that

$$\alpha\alpha=E;\quad \alpha C_3\alpha=(C_3)^{-1};\quad \alpha C_2^i\alpha=C_2^i. \qquad (3.13)$$

A general proof of the existence of an element α, with properties (3.13), can be given but it requires a rather tedious discussion. It is much simpler to verify (3.13) by inspection, since $G_0(\mathbf{k})$ here stands only for the two point groups O or T_d. If the symmetry operations of the point group O_h are described by three components of a point P' into which a point $P=(x,y,z)$ is rotated, let C_3 and C_2^i be identified by

$$C_3=(z,x,y);\quad C_2^i=(x,\bar{y},\bar{z})$$

where the bar stands for the minus sign. It follows that $C_2^j=(\bar{x},y,\bar{z})$ and the element α which meets the requirements (3.13) is

$$\alpha=(\bar{x},\bar{z},\bar{y}) \text{ if } G(\mathbf{k})=O$$
$$\alpha=(x,z,y) \text{ if } G(\mathbf{k})=T_d\,.$$

Because of the properties (3.13) and the particular choice of C_3, it must be

$$\{C_3|\mathbf{0}\}\;\{\alpha|\mathbf{v}(\alpha)\}=\{\alpha|\mathbf{v}(\alpha)\}\;\{C_3|\mathbf{0}\}^{-1}.$$

It is now possible to apply the usual induction method and obtain a representation of $G(\mathbf{k})$ induced by a rep $D_{\mathbf{k}}^{(j)}$ of $G^T(\mathbf{k})$

$$\begin{array}{c}\{C_3|\mathbf{0}\}\\ \begin{vmatrix}\mathbf{D}_{\mathbf{k}}^{(j)}(\{C_3|\mathbf{0}\}) & \mathbf{0}\\ \mathbf{0} & \mathbf{D}_{\mathbf{k}}^{(j)}(\{C_3|\mathbf{0}\}^{-1})\end{vmatrix}\end{array}$$

$$\begin{array}{cc}\{C_2^i|\mathbf{v}(C_2^i)\} & \{\alpha|\mathbf{v}(\alpha)\}\\ \begin{vmatrix}\mathbf{D}_{\mathbf{k}}^{(j)}(\{C_2^i|\mathbf{v}(C_2^i)\}) & \mathbf{0}\\ \mathbf{0} & \omega\mathbf{D}_{\mathbf{k}}^{(j)}(C_2^j|\mathbf{v}(C_2^j))\end{vmatrix} & \eta\begin{vmatrix}\mathbf{0} & \mathbf{E}\\ \mathbf{E} & \mathbf{0}\end{vmatrix}\end{array} \qquad (3.14)$$

with $\omega=\exp\{-i\mathbf{k}\cdot[C_2^j\mathbf{v}(\alpha)+\mathbf{v}(C_2^i)-\alpha\mathbf{v}(C_2^i)-\mathbf{v}(\alpha)]\}$ and $\eta=\exp\{-i\mathbf{k}/2\cdot[\alpha\mathbf{v}(\alpha)+\mathbf{v}(\alpha)]\}$. $D_{\mathbf{k}}^{(j)}$ is either very simply related to the reps of the point group T or it is one of the reps (4.14). In the first case (3.14) reduces to

$$\begin{array}{ccc}\{C_3|\mathbf{0}\} & \{C_2^i|\mathbf{v}(C_2^i)\} & \{\alpha|\mathbf{v}(\alpha)\}\\ \begin{vmatrix}\mathbf{D}^{(j)}(C_3) & \mathbf{0}\\ \mathbf{0} & \mathbf{D}^{(j)}(C_3^{-1})\end{vmatrix} & \sigma\begin{vmatrix}\mathbf{D}^{(j)}(C_2^i) & \mathbf{0}\\ \mathbf{0} & \mathbf{D}^{(j)}(C_2^j)\end{vmatrix} & \eta\begin{vmatrix}\mathbf{0} & \mathbf{E}\\ \mathbf{E} & \mathbf{0}\end{vmatrix}\end{array} \qquad (3.15)$$

where $\mathbf{D}^{(j)}(\ldots)$ are matrices in the jth rep of the point group T and $\sigma=\pm 1$. T has a 3×3 rep in which C_2^i, C_2^j and C_2^k form a class of conjugate elements with non-zero real character. If $\omega\neq 1$ in (3.14), then a 6×6 rep of $G(\mathbf{k})$ would be produced, in conflict with the dimensionality theorem. For this reason ω must be equal to 1 in (3.15). If $\sigma=\eta=1$, (3.15) is a representation of a point group $G(\mathbf{k})$ induced by a rep $D^{(j)}$ of its invariant subgroup T. Therefore (3.15) is always reducible and the reps of $G(\mathbf{k})$ are equal in number and dimension to those of either point group O or T_d. Two factors σ and η provide the only possible distinction between space-group and point-group reps.

Let now consider the second possibility, namely when $D_{\mathbf{k}}^{(j)}$ in (3.14) is one of the reps (3.11). If $D_{\mathbf{k}}^{(j)}=\Gamma_1$ (or $=\Gamma_2$) the representation (3.14) is irreducible since no matrix exists which transforms $\Gamma_1(\{C_3|\mathbf{0}\})$ into $\Gamma_1(\{C_3|\mathbf{0})^{-1})$, these two matrices having different, non-zero characters. This rep can be transformed into a real one by a transformation inverse to (3.10); that is, no extra degeneracy is produced by time-reversal symmetry, according to Herring's (1937) criterion.

The third rep Γ_3 in (3.11) is clearly self-conjugate and gives two 2×2 reps of $G(\mathbf{k})$. This is also evident from the dimensionality theorem, once a 4×4 rep of $G(\mathbf{k})$ is found. The representation induced by Γ_3 is then reducible and the appropriate $\mathbf{H}$ matrix in (2.8) has a block $\mathbf{U}$ of the kind

$$\mathbf{U}=\sqrt{\tfrac{1}{2}}\begin{vmatrix}1 & 1\\ 1 & -1\end{vmatrix}\,. \qquad (3.16)$$

Two non-equivalent reps of $G(\mathbf{k})$ are given by

$$\begin{array}{c}\{C_3|\mathbf{0}\}\\ \begin{vmatrix}\Gamma_3(\{C_3|\mathbf{0}\}) & \mathbf{0}\\ \mathbf{0} & \Gamma_3(\{C_3|\mathbf{0}\})\end{vmatrix}\end{array}$$

$$\begin{array}{cc}\{C_2^i|\mathbf{v}(C_2^i)\} & \{\alpha|\mathbf{v}(\alpha)\}\\ \begin{vmatrix}\Gamma_3(\{C_2^i|\mathbf{v}(C_2^i)\}) & \mathbf{0}\\ \mathbf{0} & \Gamma_3(\{C_2^i|\mathbf{v}(C_2^i)\})\end{vmatrix} & \eta\begin{vmatrix}\mathbf{U} & \mathbf{0}\\ \mathbf{0} & -\mathbf{U}\end{vmatrix}\end{array} \qquad (3.17)$$

where $\mathbf{U}$ is the matrix (3.16) and η is defined in (3.14).

Let $\bar{G}(\mathbf{k})$ be a space group of $\mathbf{k}$ whose associated point group is $\bar{G}_0(\mathbf{k})=O_h$. We have to prove a statement given in § 2, namely no rep of dimensionality 4 exists for $\bar{G}(\mathbf{k})$. If $\bar{G}_0(\mathbf{k})=O_h$ only a wave vector $\mathbf{k}=(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ is allowed. For the body-centred cubic lattice this value of $\mathbf{k}$ admits reps of $G^T(\mathbf{k})$ and $G(\mathbf{k})$ equal in number and dimension to those of point groups T and O respectively. Hence $G(\mathbf{k})$ has only one 2×2 rep, no 4×4 rep and cannot produce a 4×4 rep in $\bar{G}(\mathbf{k})$. The same arguments apply to the simple cubic lattice, unless $G^T(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ is a non-symmorphic space group. In this case, should $G(\mathbf{k})$ be a subgroup of index 2 of $\bar{G}(\mathbf{k})$ not containing the inversion, because of the dimensionality theorem there is only one possibility: the rep obtained from Γ_1 and Γ_2 induces two non-equivalent 4×4 reps, while the reps (3.17) induce a third 4×4 rep of $\bar{G}(\mathbf{k})$. As a consequence of the discussion in § 2, the elements of $G(\mathbf{k})$ split into two sets according to their sign in (2.12); in particular the minus sign applies for $\{\alpha|\mathbf{v}(\alpha)\}$. However, as can be verified using the properties (3.13), this is impossible. The very existence of a non-symmorphic space subgroup $G^T(\mathbf{k})$ contradicts the possibility of having a space group of $\mathbf{k}$ showing the full octahedral symmetry.

Conclusion

The single-valued reps of any space group can be evaluated using the method discussed in this paper. A limited amount of algebraic work is required for hand calculations. Except for cubic space groups, only the one-dimensional reps of cyclic point groups are needed, *i.e.* the nth roots of unity for a generator of the group. The situation is still simple for cubic space groups since the procedure of § 3 requires the reps of ordinary cubic point groups as given, for instance, by McWeeny (1963). Once the matrices for the generators are obtained, the space-group multiplication table gives a complete set of matrices for all coset representatives. The steps involved for the transformation (1.4) were discussed in detail because they must be followed in a general computer program, although the transformation is carried out by inspection in most cases.

In a computer program, based on the method given here, only one up to three generators of the space group need to be defined. It is not convenient to introduce, as input data, the reps of cubic space groups; this could cause systematic errors in the results. It is simpler to compute the representations of ordinary point groups using the induction method and then reduce them through a similarity transformation. In order to do this a matrix $\mathbf{H}$ must be computed first. This matrix, which commutes with the induced representation, is either $\mathbf{H}=\mathbf{R}$ or $\mathbf{H}=i\mathbf{C}$ where $\mathbf{R}$ and $\mathbf{C}$ are, respectively, symmetric and skew-symmetric matrices whose elements are integers and satisfy simple relationships of the kind $a=b$, $a=-b$, $a=-a$. Once a matrix $\mathbf{H}$ is found it can be diagonalized and the eigenvectors give the required transformation. This procedure may also be applied to obtain the reps (3.11) of a cubic space group, in order to have a program which uses a minimum of input data.

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