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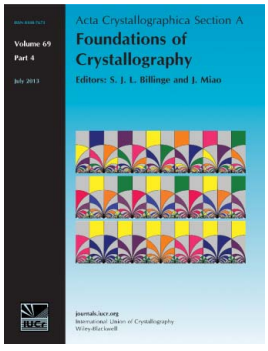

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Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions

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New tables of irreducible representations (IRs) are introduced for the 230 crystallographic space groups (SGs) in three-dimensional space, at both special and non-special **k** vectors, and for their extensions to $(3 + d)$-dimensional superspace ('superspace-extended SGs' or SSESGs). Neither a tabulation of SG IR matrices for non-special **k** vectors nor a tabulation of SSESG IR matrices for $d > 1$ have been previously published. These tabulations are made possible by a new form in which the IR matrices of SGs are separated as a product of a translation part T and a point-operation part P, and where the IR matrices of SSESGs are separated as a product of a phase-shift part Q and a point-operation part P_s. Both T and Q have a simple prescribed form that does not need to be tabulated. Also, the new IR matrices are in a convenient block form which allows one to see by inspection which parts of the matrices and the associated order parameters belong to which arm of the star of **k**. In addition to complex IR matrices, real physically irreducible representation (PIR) matrices are tabulated. The new IR and PIR tables are available on the ISO-IR website (http://stokes.byu.edu/iso/irtables.php) in both convenient human-readable and computer-readable forms.

1. Introduction

The methods of group-representation theory have been applied with much success to many different areas of crystallography. One application of special interest is the exploration and interpretation of distortions in crystals, including those that appear in real structural phase transitions. By distortion, we include any change in the crystal that breaks its symmetry, such as lattice strains, atomic displacements, atomic ordering, magnetic ordering *etc*. The centerpiece of these group-theoretical methods is the irreducible representation (IR) which maps the operators of a symmetry group onto a set of matrices.

Tables of IR matrices have been published mainly for the little group of **k** (Kovalev, 1965, 1993; Miller & Love, 1967; Zak, 1969; Bradley & Cracknell, 1972; Cracknell *et al.*, 1979; *etc.*). The IR matrices for the complete space group can be induced from those for the little group of **k**, but the process is tedious if done by hand. Tabulations of the IR matrices for the complete space group have only been available at Kovalev (1993) and Stokes & Hatch (1988), and these are restricted to special **k** vectors.

In addition to the tables of Stokes & Hatch (1988), for IRs of three-dimensional space groups (SGs) at special **k** points, matrices for complete IRs at non-special **k** points have been available for many years, individually on demand, *via* real-time calculations performed within the interactive *ISOTROPY* program. The *ISOTROPY* website (http://stokes.byu.edu/iso/) has now grown to include an extensive suite of related programs, utilities and data tables. In 2007, matrices for IRs of SGs extended to (3 + 1)-dimensional superspace ('superspace-extended SGs' or SSESGs) were made available *via* the ISO(3+1)D tables on the *ISOTROPY* website (Stokes *et al.*, 2007), which are important when dealing with incommensurate distortions. We refer to these sources collectively as the '1988 version' of the IR matrices.

Until now, no practical way of tabulating complete-SG IR matrices for non-special **k** vectors has been established. This problem is due in part to the fact that the IR matrices depend in a non-trivial way on the free components of the non-special **k** vectors, which can take on an infinite number of values. The problem is further compounded by the fact that the IR matrices are only unique to within a similarity transformation, which may also depend on **k**.

Here, we report a new separated form for the IR matrices for complete SGs that allows their tabulation at both special and non-special **k** vectors. In addition, we put the matrices into a block form that makes the interpretation of order parameters easier. IR matrices for SSESGs have also been included. We call the result the '2011 version' of the IR matrices, which are now available *via* the ISO-IR tables on the *ISOTROPY* website (http://stokes.byu.edu/iso/irtables.php),

both in convenient human-readable form and also in computer-readable form. The 2011 IRs are accessible on a case-by-case basis through the *ISOTROPY* suite. But because they are tabulated in ISO-IR, they can also be used by other software packages now.

The matrices tabulated in the ISO(3+1)D tables for (3 + 1)-dimensional SSESGs actually have a separated form as well. However, these were not the full IR matrices but only the upper left block which takes the $\mathbf{k}$ vector in $\pm\mathbf{k}$. The separated form in ISO(3+1)D was an intermediate step to the final separated form of the full IR matrices presented here.

Note that the IRs used by tools within the *ISOTROPY* software suite have always been based on the tables of Miller & Love (1967) and the extension of Cracknell *et al.* (1979) (hereafter denoted as CDML). We use their notation and we build the SG IR matrices using IRs of the little groups of $\mathbf{k}$ from their tables. From the very start, however, we have generated our own similarity transformations to bring the IR matrices into a form that we desire.

2. Induced IRs in block form

We begin with the usual method for inducing IRs of SG G from the IRs of G^k, its little group of $\mathbf{k}$ (see, for example, Bradley & Cracknell, 1972). The little group of $\mathbf{k}$ consists of all operators $g = \{R|\mathbf{v}\} \in G$ for which $\mathbf{k}R^{-1} = \mathbf{k}$ (modulo a reciprocal-lattice vector $\mathbf{K}$). We express operators g in Seitz notation $\{R|\mathbf{v}\}$ to denote a point operation R followed by a translation $\mathbf{v}$.

Note that we consider R to represent a matrix such that the operation of R on a vector $\mathbf{v}$ results in a vector $R\mathbf{v}$. This requires that the operation of R on a $\mathbf{k}$ vector results in $\mathbf{k}R^{-1}$ so that the dot product $(\mathbf{k}R^{-1}) \cdot (R\mathbf{v}) = \mathbf{k} \cdot \mathbf{v}$ remains invariant.

We obtain the IR matrices for G^k from CDML and express them in a form that separates the dependencies on R and $\mathbf{v}$:

$$D^k(\{R|\mathbf{v}\}) = \exp(i2\pi\mathbf{k} \cdot \mathbf{v})P^k(R). \quad (1)$$

The matrices $P^k(R)$ are called 'loaded IRs' by Kovalev (1993) and 'weighted IRs' by Lyubarskii (1960). Let n_k be the dimension of $D^k(g)$.

It is useful at this point to also define what we call $G^{k\overline{k}}$, the 'little group of $\pm\mathbf{k}$', which consists of all operators $g = \{R|\mathbf{v}\} \in G$ for which $\mathbf{k}R^{-1} = \pm\mathbf{k}$ (mod $\mathbf{K}$). If no operator in G takes $\mathbf{k}$ into $-\mathbf{k}$ or if $\mathbf{k} = -\mathbf{k}$ (mod $\mathbf{K}$), then $G^{k\overline{k}} = G^k$.

We first decompose $G^{k\overline{k}}$ into cosets with respect to G^k:

$$G^{k\overline{k}} = \sum_{i'=1}^{e} h_{i'}^k G^k, \quad (2)$$

where e is the number of cosets, $h_{i'}^k = \{R_{i'}^k|\mathbf{v}_{i'}^k\}$ are coset representatives (coset reps) and the first coset rep h_1^k is chosen to be the identity operator. If $G^{k\overline{k}} = G^k$, then $e = 1$, and there is only one term in this decomposition; otherwise $e = 2$, and there are two terms with $\mathbf{k}(R_2^k)^{-1} = -\mathbf{k}$ (mod $\mathbf{K}$).

Next, we decompose G into cosets with respect to $G^{k\overline{k}}$:

$$G = \sum_{i=1}^{d} h_i^{k\overline{k}} G^{k\overline{k}}, \quad (3)$$

where d is the number of cosets, $h_i^{k\overline{k}} = \{R_i^{k\overline{k}}|\mathbf{v}_i^{k\overline{k}}\}$ are coset reps and the first coset rep $h_1^{k\overline{k}}$ is chosen to be the identity operator. These coset reps generate a set of $\mathbf{k}$ vectors, $\{\mathbf{k}_1 = \mathbf{k}, \mathbf{k}_2 = \mathbf{k}(R_2^{k\overline{k}})^{-1}, \ldots, \mathbf{k}_d = \mathbf{k}(R_d^{k\overline{k}})^{-1}\}$, which we call the 'star of $\pm\mathbf{k}$'. This formalism will make it easier to generalize to the case of superspace extensions in the next section.

We combine equations (2) and (3) to obtain the usual decomposition of G into cosets with respect to G^k:

$$G = \sum_{i=1}^{d} \sum_{i'=1}^{e} h_{ii'} G^k, \quad (4)$$

where $h_{ii'} = h_i^{k\overline{k}} h_{i'}^k = \{R_{ii'}|\mathbf{v}_{ii'}\}$. These coset reps $h_{ii'}$ generate the usual star of $\mathbf{k}$:

$$\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_d \quad (5)$$

if $e = 1$, and

$$\mathbf{k}_1, -\mathbf{k}_1, \mathbf{k}_2, -\mathbf{k}_2, \ldots \mathbf{k}_d, -\mathbf{k}_d \quad (6)$$

if $e = 2$.

Finally, we induce the IRs of G from the IRs of G^k using

$$D_{iji'j'}(g) = \begin{cases} D^k(h_{ii'}^{-1} g h_{jj'}), & \text{if } h_{ii'}^{-1} g h_{jj'} \in G^k; \\ 0, & \text{otherwise.} \end{cases} \quad (7)$$

The IR matrices $D(g)$ are in block form, with de rows and columns of n_k-dimensional matrix blocks $D_{iji'j'}(g)$. Each row and each column contains one nonzero block.

For a pure lattice translation, the IR matrix is diagonal ($i = j$ and $i' = j'$). Using $h_{ii'}^{-1}\{1|\mathbf{v}\}h_{ii'} = \{1|R_{ii'}^{-1}\mathbf{v}\}$, we obtain $D_{iii'i'}(\{1|R_{ii'}^{-1}\mathbf{v}\}) = D^k(\{1|R_{ii'}^{-1}\mathbf{v}\})$. Since $\mathbf{k} \cdot (R_{ii'}^{-1}\mathbf{v}) = (\mathbf{k}R_{ii'}^{-1}) \cdot \mathbf{v}) = \pm\mathbf{k}_i \cdot \mathbf{v}$ (the plus sign for $i' = 1$ and the minus sign for $i' = 2$), we finally obtain

$$D_{iii'i'}(\{1|\mathbf{v}\}) = \begin{cases} \mathbf{1}_{n_k} \exp(2\pi i\mathbf{k}_i \cdot \mathbf{v}), & \text{if } i' = 1; \\ \mathbf{1}_{n_k} \exp(-2\pi i\mathbf{k}_i \cdot \mathbf{v}), & \text{if } i' = 2, \end{cases} \quad (8)$$

where $\mathbf{1}_{n_k}$ is an n_k-dimensional unit matrix.

3. IRs of SSESGs in block form

The essential properties of superspace groups (SSGs) are reviewed in Appendix *A*. For non-special $\mathbf{k}$ vectors, the vectors in the star of $\pm\mathbf{k}$ can be treated as modulation vectors. The phase shifts Δ_i of these modulations become internal coordinates in the $(3 + d)$-dimensional superspace extension of G that we call G_s. We express these phase shifts as components of a vector $\mathbf{\Delta} = \{\Delta_1, \Delta_2, \ldots, \Delta_d\}$ and we write the operators in G_s as $\{R, \varepsilon|\mathbf{v}, \mathbf{\Delta}\}$ (using the unmixed setting).

Just as for three-dimensional SGs, we can induce IRs of an SSESG G_s from the IRs of G_s^k, the little group of $\mathbf{k}$ in superspace. The operators $\{R, \varepsilon|\mathbf{v}, 0\}$ in G_s^k are isomorphic to the corresponding operators $\{R|\mathbf{v}\}$ in G^k. Thus, we can map them onto the same IR matrices:

$$D_s^k(\{R, \varepsilon|\mathbf{v}, 0\}) = D^k(\{R|\mathbf{v}\}) = \exp(i2\pi\mathbf{k} \cdot \mathbf{v})P^k(R). \quad (9)$$

Pure phase shifts are mapped onto simple exponentials (Perez-Mato *et al.*, 1984*a*,*b*):

$$D_s^k(\{(1,1)|0,\mathbf{\Delta}\}) = \mathbf{1}_{n_k}\exp(2\pi i\Delta_1). \quad (10)$$

Note that we include only Δ_1 in the IR since the little group of $\mathbf{k}$ only involves the first arm of the star of $\pm\mathbf{k}$. Combining equations (9) and (10), we obtain

$$\begin{aligned} D_s^k(\{R,\varepsilon|\mathbf{v},\mathbf{\Delta}\}) &= D_s^k(\{(1,1)|0,\mathbf{\Delta}\})D_s^k(\{R,\varepsilon|\mathbf{v},0\}) \\ &= \exp(2\pi i\Delta_1)\exp(i2\pi\mathbf{k}\cdot\mathbf{v})P^k(R) \\ &= \exp(2\pi i[\Delta_1+\mathbf{k}\cdot\mathbf{v}])P^k(R). \end{aligned} \quad (11)$$

This is the result for the unmixed setting. In the SSG lattice setting, we obtain

$$D_s^k(\{R_s|\mathbf{v},\boldsymbol{\delta}\}) = \exp(2\pi i\delta_1)P^k(R), \quad (12)$$

where $\delta_1 = \Delta_1 + \mathbf{k}\cdot\mathbf{v}$. We note that $D_s^k(\{R_s|\mathbf{v},\boldsymbol{\delta}\})$ does not depend on $\mathbf{v}$. The IR maps SSG lattice vectors onto the unit matrix.

Once we have the IR matrices of G_s^k, we can induce the IR matrices of G_s. We decompose $G_s^{k\bar{k}}$ into cosets of G_s^k as in equation (2) and we decompose G_s into cosets of $G_s^{k\bar{k}}$ as in equation (3). Finally, we induce the IR as in equation (7):

$$D_{sij\bar{i}'\bar{j}'}(g_s) = \begin{cases} D_s^k(h_{si\bar{i}'}^{-1}g_s h_{sj\bar{j}'}), & \text{if } h_{si\bar{i}'}^{-1}g_s h_{sj\bar{j}'} \in G_s^k; \\ 0, & \text{otherwise.} \end{cases} \quad (13)$$

As for SGs, this complete SSESG IR is also in block form, having de rows and columns of n_k-dimensional blocks.

4. A separated matrix form

For superspace extensions, we can separate out the contribution from the phase shifts:

$$h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},\boldsymbol{\delta}\}h_{sj\bar{j}'} = \{1|0,(\varepsilon_{si'}^k)^{-1}(\varepsilon_{si}^{k\bar{k}})^{-1}\boldsymbol{\delta}\}h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},0\}h_{sj\bar{j}'}. \quad (14)$$

Using $(\varepsilon_{si}^{k\bar{k}})^{-1}(\delta_1,\ldots) = (\delta_i,\ldots)$ and $(\varepsilon_{si'}^k)^{-1}(\delta_i,\ldots) = (\pm\delta_i,\ldots)$ (the plus sign for $i'=1$ and the minus sign for $i'=2$), we obtain

$$\begin{aligned} &D_s^k(h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},\boldsymbol{\delta}\}h_{sj\bar{j}'}) = \\ &\quad\begin{cases} \exp(2\pi i\delta_i)D_s^k(h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},0\}h_{sj\bar{j}'}), & \text{if } i'=1; \\ \exp(-2\pi i\delta_i)D_s^k(h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},0\}h_{sj\bar{j}'}), & \text{if } i'=2. \end{cases} \end{aligned} \quad (15)$$

Putting this into equation (13), we obtain a complete separation of the IR matrix into a phase-shift part and a point-operation part:

$$D_s(\{R_s|\mathbf{v},\boldsymbol{\delta}\}) = Q(\boldsymbol{\delta})P_s(R_s), \quad (16)$$

where

$$\begin{aligned} &P_{sij\bar{i}'\bar{j}'}(R_s) = \\ &\quad\begin{cases} D_s^k(h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},0\}h_{sj\bar{j}'}), & \text{if } h_{si\bar{i}'}^{-1}\{R_s|\mathbf{v},0\}h_{sj\bar{j}'} \in G_s^k; \\ 0, & \text{otherwise,} \end{cases} \end{aligned} \quad (17)$$

and

$$Q_{ii\bar{i}'\bar{i}'}(\boldsymbol{\delta}) = \begin{cases} \mathbf{1}_{n_k}\exp(2\pi i\delta_i), & \text{if } i'=1; \\ \mathbf{1}_{n_k}\exp(-2\pi i\delta_i), & \text{if } i'=2, \end{cases} \quad (18)$$

which is diagonal. Note that the IR matrices $D_s(\{R_s|\mathbf{v},\boldsymbol{\delta}\})$ do not depend on the free parameters in the $\mathbf{k}$ vector. For SSESGs, it is the phase shifts δ_i that have arbitrary values, and they are separated out into a function $Q(\boldsymbol{\delta})$ which is known analytically. This fact makes the tabulation of the IR matrices possible. We only need to tabulate the point-operation part $P_s(R_s)$, one matrix for each point operator R_s in the translation factor group.

We can now obtain SG IR matrices with similar separation properties. In the unmixed setting, equation (16) becomes

$$D_{sij\bar{i}'\bar{j}'}(\{R,\varepsilon|\mathbf{v},\mathbf{\Delta}\}) = Q_{ii\bar{i}'\bar{i}'}(\Delta_i+\mathbf{k}_i\cdot\mathbf{v})P_{sij\bar{i}'\bar{j}'}(R). \quad (19)$$

Since the operators $\{R,\varepsilon|\mathbf{v},0\}$ in G_s are isomorphic to the corresponding operators $\{R|\mathbf{v}\}$ in G, we can map them onto the same IR matrices:

$$D_{ij\bar{i}'\bar{j}'}(\{R|\mathbf{v}\}) = D_{sij\bar{i}'\bar{j}'}(\{R,\varepsilon|\mathbf{v},0\}) = Q_{ii\bar{i}'\bar{i}'}(\mathbf{k}_i\cdot\mathbf{v})P_{sij\bar{i}'\bar{j}'}(R). \quad (20)$$

We now define a translational part of the IR matrix,

$$T_{ii\bar{i}'\bar{i}'}(\mathbf{v}) = Q_{ii\bar{i}'\bar{i}'}(\mathbf{k}_i\cdot\mathbf{v}) = \begin{cases} \mathbf{1}_{n_k}\exp(2\pi i\mathbf{k}_i\cdot\mathbf{v}), & \text{if } i'=1; \\ \mathbf{1}_{n_k}\exp(-2\pi i\mathbf{k}_i\cdot\mathbf{v}), & \text{if } i'=2, \end{cases} \quad (21)$$

which is diagonal and identical to the expression in equation (8) for a pure lattice translation. Recalling that $P(R) = P_s(R_s)$, we finally obtain

$$D(\{R|\mathbf{v}\}) = T(\mathbf{v})P(R). \quad (22)$$

The complicated detour through superspace was necessary to obtain the IRs in the separated form, which does not arise naturally from equation (7). This separation property of $D(g)$ now enables us to tabulate complete IRs for non-special $\mathbf{k}$ vectors, which contain one or more free parameters that can take on arbitrary values. These free parameters are contained only in the translation part $T(\mathbf{v})$, which is known analytically and has the same form for every IR. We only need to tabulate the point-operation part $P(R)$, one matrix for each point operator R in the translational factor group.

The idea of separating the translational and point-operation parts of an IR matrix is evident in Kovalev's work on 'loaded' IRs of the little group of $\mathbf{k}$. Kovalev also uses an apparently separated form for his IRs of complete SGs only at special $\mathbf{k}$ vectors where the separated form has little or no value. Here, we obtain a highly useful separated form for the case of non-special $\mathbf{k}$ vectors, and simply use equation (7) instead for special $\mathbf{k}$ vectors.

5. IRs in real form

The complex-conjugation type of an IR describes the relationship between the IR and its complex conjugate (Bradley & Cracknell, 1972). Type 1: the IR is intrinsically real (*i.e.* equivalent *via* a similarity transformation to a set of real matrices); in real form, the IR and its complex conjugate are

identical. Type 2: the IR is intrinsically complex (*i.e.* not equivalent to a set of real matrices) but equivalent to its own complex conjugate; this requires that the characters of the IR be real. Type 3: the IR is intrinsically complex and also inequivalent to its own complex conjugate; this requires that some of the IR characters be complex.

When an IR is of type 2 or 3, we form a 'physically' irreducible representation (PIR) by forming the direct sum of the true IR with its complex conjugate,

$$\begin{bmatrix} D_{\rm IR}(g) & \mathbf{0} \\ \mathbf{0} & D_{\rm IR}(g)^* \end{bmatrix}, \tag{23}$$

which can be brought to real form by a similarity transformation. The PIR is convenient for projecting out real basis functions. In Appendix *B*, we describe a straightforward method for constructing the PIR matrices in real form.

We must also bring type-1 IRs to real form. In general, the form generated by equations (7) or (13) is not real. The strategies that we use to bring them to real form are also discussed in Appendix *B*.

In their real form, all of our IR and PIR matrices (types 1, 2, 3) have the following properties:

(i) Separated form for non-special $\mathbf{k}$ vectors: $D\{R|\mathbf{v}\} = T(\mathbf{v})P(R)$ for SGs and $D_s\{R_s|\mathbf{v},\boldsymbol{\delta}\} = Q(\boldsymbol{\delta})P_s(R_s)$ for SSESGs. The matrices $T(\mathbf{v})$ and $Q(\boldsymbol{\delta})$ have a standard form [see (iii) below], so that we only need to tabulate the $P(R)$ or $P_s(R_s)$ matrices.

(ii) Block form: in complex form, our IR matrices have *de* rows and columns of n_k-dimensional blocks. Upon conversion to real form, however, the blocks associated with $\mathbf{k}$ and $-\mathbf{k}$ become mixed, so that we then obtain d rows and columns of (en_kt)-dimensional blocks, where $t = 1$ for type-1 IRs and $t = 2$ for PIRs of type 2 and 3 IRs. Each row and column contains one nonzero block. The ith row and the ith column are associated with $\mathbf{k}_i$, the ith vector in the star of $\pm\mathbf{k}$.

(iii) Standard real form for translation matrices in SGs [$D(\{1|\mathbf{v}\})$ in equation (8) and $T(\mathbf{v})$ in equation (21)] and phase-shift matrices in SSESGs [$Q(\boldsymbol{\delta})$ in equation (18)]. The form is block diagonal, with the ith matrix block of dimension $b = en_kt$ given by

$$U_b(x_i) = \begin{bmatrix} \mathbf{1}_{b/2}\cos(2\pi x_i) & \mathbf{1}_{b/2}\sin(2\pi x_i) \\ -\mathbf{1}_{b/2}\sin(2\pi x_i) & \mathbf{1}_{b/2}\cos(2\pi x_i) \end{bmatrix}, \tag{24}$$

where $x_i = \mathbf{k}_i \cdot \mathbf{v}$ for translation matrices and $x_i = \delta_i$ for phase-shift matrices.

Note that ISO-IR contains separate tables for IR matrices in both the real form and the complex form. From the upper left-hand matrix block of the complex form, users can easily obtain IR matrices for G^k and G_s^k.

As an example, consider the Δ_1 (DT1) IR of SG No. 90 $P42_12$. The star of $\pm\mathbf{k}$ consists of two $\mathbf{k}$ vectors: $\mathbf{k}_1 = (0, \beta, 0)$ and $\mathbf{k}_2 = (\beta, 0, 0)$. Because $d = 2$, $e = 2$ and $n_k = 1$, the IR matrices are four-dimensional, each constructed in real form with two-dimensional matrix blocks. For $g = \overline{x} + \frac{1}{2}, y + \frac{1}{2}, \overline{z}$ (180° screw rotation about $\mathbf{b}$), we obtain

$$\begin{aligned} D(g) &= T(\tfrac{1}{2},\tfrac{1}{2},0)P(\overline{x}, y, \overline{z}) \\ &= \begin{bmatrix} \cos(\pi\beta) & \sin(\pi\beta) & 0 & 0 \\ -\sin(\pi\beta) & \cos(\pi\beta) & 0 & 0 \\ 0 & 0 & \cos(\pi\beta) & \sin(\pi\beta) \\ 0 & 0 & -\sin(\pi\beta) & \cos(\pi\beta) \end{bmatrix} \\ &\quad \times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \end{aligned} \tag{25}$$

where we obtained the T matrix for $\mathbf{v} = (\frac{1}{2}, \frac{1}{2}, 0)$ using $\mathbf{k}_1 \cdot \mathbf{v} = \mathbf{k}_2 \cdot \mathbf{v} = \frac{1}{2}\beta$, and we obtained the P matrix from ISO-IR. Note that $T(\frac{1}{2}, \frac{1}{2}, 0)$ alone is not an IR matrix since $\{1|\frac{1}{2}, \frac{1}{2}, 0\}$ alone is not an operator in the SG. Similarly, $P(\overline{x}, y, \overline{z})$ alone is not an IR matrix.

Now suppose we want to consider incommensurate modulations. We choose β to take an irrational value. Since there are two $\mathbf{k}$ vectors in the star of $\pm\mathbf{k}$ ($d = 2$), the symmetry operators of the group act in $(3 + 2)$-dimensional superspace. The IR matrix for $g = \overline{x}_1 + \frac{1}{2}, x_2 + \frac{1}{2}, \overline{x}_3, x_4 + \delta_1, x_5 + \delta_2$ is given by

$$\begin{aligned} D(g) &= Q(\delta_1,\delta_2)P_s(\overline{x}_1, x_2, \overline{x}_3, x_4, x_5) \\ &= \begin{bmatrix} \cos(2\pi\delta_1) & \sin(2\pi\delta_1) & 0 & 0 \\ -\sin(2\pi\delta_1) & \cos(2\pi\delta_1) & 0 & 0 \\ 0 & 0 & \cos(2\pi\delta_2) & \sin(2\pi\delta_2) \\ 0 & 0 & -\sin(2\pi\delta_2) & \cos(2\pi\delta_2) \end{bmatrix} \\ &\quad \times \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \end{aligned} \tag{26}$$

where we again obtain the P_s matrix from ISO-IR.

6. Order parameters and the new block form

An order parameter $\boldsymbol{\eta}$ is a multi-dimensional vector which is associated with an IR. SG operators act on an order parameter *via* the IR matrix, *i.e.* $g\boldsymbol{\eta} = D(g)\boldsymbol{\eta}$. In most applications, the order parameter describes how the SG symmetry of a structure is broken by a distortion. The symmetry of the distorted structure consists of all operators $g \in G$ which keep $\boldsymbol{\eta}$ invariant, *i.e.* $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$. The set of these operators is called an isotropy subgroup of G.

To see how the form of the IR matrix affects the form of $\boldsymbol{\eta}$, consider the (en_k)-dimensional block $D_{11}(g)$ of the IR matrix. Since $h_1^{k\overline{k}}$ is the identity operator, this block is nonzero only if $g \in G^{k\overline{k}}$. Recall that these are the operators that take $\mathbf{k}$ into $\pm\mathbf{k}$. If an order parameter is zero except for the first en_k components, then only IR matrices with a nonzero $D_{11}(g)$ block can satisfy $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$, and the resulting symmetry group contains only operators that take $\mathbf{k}$ into $\pm\mathbf{k}$. Such a structure will be characterized by a single modulation vector $\mathbf{k}$.

Next consider the ith block $D_{ii}(g)$ along the diagonal of the IR matrix. This block is nonzero only if $(h_i^{k\bar{k}})^{-1} g h_i^{k\bar{k}} \in G^{k\bar{k}}$, *i.e.*, $\mathbf{k}R_i^{-1}RR_i = \pm\mathbf{k}$. Since $\mathbf{k}R_i^{-1} = \mathbf{k}_i$, this condition becomes $\mathbf{k}_i R^{-1} = \pm\mathbf{k}_i$. These are the operators g that take $\mathbf{k}_i$ into $\pm\mathbf{k}_i$. If an order parameter is zero except for the ith set of en_k components [components $(i-1)en_k+1$ through ien_k], then only IR matrices with a nonzero block $D_{ii}(g)$ can satisfy $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$, and the resulting symmetry group contains only operators that take $\mathbf{k}_i$ into $\pm\mathbf{k}_i$. Such a structure will be characterized by a modulation vector $\mathbf{k}_i$.

In summary, the first en_k components of $\boldsymbol{\eta}$ describe distortions belonging to $\mathbf{k}_1$, the next en_k components describe distortions belonging to $\mathbf{k}_2$ *etc.* As a result, we can determine which $\mathbf{k}$ vectors are involved in a particular distortion simply by inspecting its order parameter.

As an example, consider the X_1 IR of SG No. 90 $P42_12$. The star of $\pm\mathbf{k}$ consists of two $\mathbf{k}$ vectors: $\mathbf{k}_1 = (0, \frac{1}{2}, 0)$ and $\mathbf{k}_2 = (\frac{1}{2}, 0, 0)$. Because $d = 2$, $e = 1$ and $n_k = 2$, the IR matrices are four-dimensional, each constructed in real form with two-dimensional matrix blocks. The IR matrix for $g = \{R|\mathbf{v}\} = \overline{x}+\frac{1}{2}, y+\frac{1}{2}, \overline{z}$ (180° screw rotation about **b**) is given by (from the ISO-IR tables)

$$D(g) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{27}$$

Note that the blocks,

$$\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

lie on the diagonal of D, since $\mathbf{k}_1 R^{-1} = \mathbf{k}_1$ and $\mathbf{k}_2 R^{-1} = -\mathbf{k}_2$. The IR matrix for $g = \{R|\mathbf{v}\} = y+\frac{1}{2}, \overline{x}+\frac{1}{2}, z$ (270° rotation about **c**) is given by

$$D(g) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{28}$$

In this case, the blocks,

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

are off-diagonal in D, since $\mathbf{k}_1 R^{-1} = \mathbf{k}_2$ and $\mathbf{k}_2 R^{-1} = -\mathbf{k}_1$.

If we use the *ISODISTORT* package (Campbell *et al.*, 2006) of the *ISOTROPY* software suite to find displacive distortions in $P42_12$ for the X_1 IR, we find nine possible nonequivalent distortions, each described by a four-dimensional order parameter $\boldsymbol{\eta}$. The first and second components of $\boldsymbol{\eta}$ describe distortions belonging to $\mathbf{k}_1$, and the third and fourth components describe distortions belonging to $\mathbf{k}_2$. Thus, $\boldsymbol{\eta} = (0, 0, a, 0)$ describes a distortion involving $\mathbf{k}_2 = (\frac{1}{2}, 0, 0)$ and results in the monoclinic isotropy subgroup $P2_1$ with a cell doubling in the **a** direction. On the other hand, $\boldsymbol{\eta} = (a, a, a, a)$ describes a distortion involving equal contributions from both $\mathbf{k}_1$ and $\mathbf{k}_2$ and results in an orthorhombic isotropy subgroup with $C222$ symmetry and a cell doubling in both the **a** and **b** directions.

For the 1988 version of the matrices, the interpretation of the order parameter is generally not so simple. Consider the distortion that takes us from the $P42_12$ parent symmetry to the monoclinic subgroup $P2_1$. The 180° screw rotation about **b** in the setting of $P2_1$ is $g = \overline{x}, y+\frac{1}{2}, \overline{z}$. In the setting of the parent $P42_12$, this operator is $g = \overline{x}+\frac{1}{2}, y+\frac{1}{2}, \overline{z}$. Using the 2011 version of the matrices, the IR matrix for this operator is given by

$$D(g) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{29}$$

Solving $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$ for $\boldsymbol{\eta}$, we obtain the order parameter $\boldsymbol{\eta} = (0, 0, 0, a)$, *i.e.*

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ a \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ a \end{pmatrix}. \tag{30}$$

In the 1988 version of the matrices, the IR matrix for this operator is given by

$$D(g) = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{31}$$

Solving $D(g)\boldsymbol{\eta} = \boldsymbol{\eta}$ for $\boldsymbol{\eta}$, we now obtain $\boldsymbol{\eta} = (a, 0, \overline{a}, 0)$ as the order parameter. Immediately, we can see a difference in the form of the matrix and the order parameter. This matrix is not block diagonal, even though $\mathbf{k}_1 R^{-1} = \mathbf{k}_1$ and $\mathbf{k}_2 R^{-1} = -\mathbf{k}_2$. Thus, there is no easy way to tell from this order parameter that the distortion involves only $\mathbf{k}_2$.

The unfortunate form used in the 1988 version was the result of a broad emphasis on transforming isomorphic IRs to have the same matrix images whenever possible. That strategy proved to be inconvenient in ways that were not foreseen at the time.

7. Dependence on setting

By definition, an IR is not intrinsically tied to a specific setting of the SG or SSESG that it represents. Consider a transformation S that takes a symmetry group from 'setting 1' to 'setting 2'. The operators in the two settings are related by $g^{(2)} = Sg^{(1)}S^{-1}$. Since the groups $\{g_i^{(1)}\}$ and $\{g_i^{(2)}\}$ are isomorphic, they can be mapped onto the same IR matrices. Therefore, if the IR matrices $D^{(1)}(g^{(1)})$ for operators in setting 1 are known, we can easily assign the IR matrices for operators in setting 2:

$$D^{(2)}(g^{(2)}) = D^{(1)}(S^{-1}g^{(2)}S). \tag{32}$$

We do this to ensure that the IR matrices are the same regardless of setting, so that order parameters are identical in different settings.

We constructed the 2011 version of IR matrices using the SG settings of CDML. These matrices are stored in our

database, which also contains the transformations that take operators in the CDML settings to all of the settings in *International Tables for Crystallography*, Vol. A (2002) (denoted by IT). Implementing equation (32) to obtain IR matrices for operators in the IT settings is straightforward.

In the ISO-IR tables, we display the IR matrices for operators in the settings of IT. The transformations from CDML settings to IT settings cause some issues relating to the appearance of the entries in the tables.

7.1. IRs of SGs

Consider a simple example using SG No. 48 *Pnnn*. IT gives this space group in two different settings: origin choices 1 and 2. To change the setting from origin choice 1 to origin choice 2, we move the origin by $\boldsymbol{\tau} = (\bar{\frac{1}{4}}, \bar{\frac{1}{4}}, \bar{\frac{1}{4}})$. (The transformation S in terms of its action on x, y, z is given by $S = x + \frac{1}{4}, y + \frac{1}{4}, z + \frac{1}{4}$.) In origin choice 2, the glide reflection through the *bc* plane is given by $g^{(2)} = \overline{x}, y + \frac{1}{2}, z + \frac{1}{2}$. That same operator in origin choice 1 is given by $g^{(1)} = S^{-1}g^{(2)}S = \overline{x} - \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}$. Thus, from equation (32), we obtain

$$D^{(2)}(\overline{x}, y + \tfrac{1}{2}, z + \tfrac{1}{2}) = D^{(1)}(\overline{x} - \tfrac{1}{2}, y + \tfrac{1}{2}, z + \tfrac{1}{2}). \quad (33)$$

If the IR matrices are chosen so that they have the form of equation (22) for setting 1, we obtain for setting 2

$$D^{(2)}(x, y + \tfrac{1}{2}, z + \tfrac{1}{2}) = T(\bar{\tfrac{1}{2}}, \tfrac{1}{2}, \tfrac{1}{2})P^{(1)}(\overline{x}, y, z), \quad (34)$$

which is clearly not the expected form of equation (22), where the translation part would normally have been $T(0, \frac{1}{2}, \frac{1}{2})$.

Entries in the ISO-IR tables reflect these departures from the form of equation (22). For example, the CDML setting of SG No. 48 uses origin choice 1, and we use origin choice 2 in the tables. The A_1 IR matrix for $\overline{x}, y + \frac{1}{2}, z + \frac{1}{2}$ is listed in the table as

$$T(\bar{\tfrac{1}{2}}, \tfrac{1}{2}, \tfrac{1}{2}) \begin{pmatrix} 0 & 0 & 0 & \overline{1} \\ 0 & 0 & 1 & 0 \\ 0 & \overline{1} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (35)$$

As another example, consider SG No. 4 $P2_1$ which IT lists in several different settings. Consider the two settings that use (1) unique axis *b* and (2) unique axis *c* (both with cell choice 1). The transformation from setting 1 to 2 is simply a transformation of axes, $S = z, x, y$. The 180° screw rotation is given by $g^{(2)} = \overline{x}, \overline{y}, z + \frac{1}{2}$ in setting 2 and $g^{(1)} = S^{-1}g^{(2)}S = \overline{x}, y + \frac{1}{2}, \overline{z}$ in setting 1. Thus, we obtain from equation (32),

$$D^{(2)}(\overline{x}, \overline{y}, z + \tfrac{1}{2}) = D^{(1)}(\overline{x}, y + \tfrac{1}{2}, \overline{z}) = T^{(1)}(0, \tfrac{1}{2}, 0)P^{(1)}(\overline{x}, y, \overline{z}). \quad (36)$$

Now, $T^{(1)}(\mathbf{v^{(1)}})$ contains dot products of $\mathbf{v}$ in setting 1 with $\mathbf{k}$ vectors in setting 1, and $T^{(2)}(\mathbf{v^{(2)}})$ contains dot products of $\mathbf{v}$ in setting 2 with $\mathbf{k}$ vectors in setting 2. Since vector dot products are the same in every setting, we find that $T^{(1)}(\mathbf{v^{(1)}}) = T^{(2)}(\mathbf{v^{(2)}})$ and

$$D^{(2)}(\overline{x}, \overline{y}, z + \tfrac{1}{2}) = T^{(2)}(0, 0, \tfrac{1}{2})P^{(2)}(\overline{x}, \overline{y}, z), \quad (37)$$

where $P^{(2)}(\overline{x}, \overline{y}, z) = P^{(1)}(\overline{x}, y, \overline{z})$, as desired. No special notation is required in the ISO-IR tables for IT settings that are related to the CDML setting by a simple transformation of axes.

7.2. IRs of SSESGs

For SSESGs, the situation is simpler than that of SGs. Let us consider again the example of SG No. 48 *Pnnn* extended to $(3 + 1)$-dimensional superspace with the modulation vector $\mathbf{k} = (\alpha, 0, \frac{1}{2})$. In origin choice 2, the glide reflection followed by an arbitrary phase shift δ is given by $g^{(2)} = \overline{x}_1, x_2 + \frac{1}{2}, x_3 + \frac{1}{2}, x_3 - x_4 + \delta$. The transformation that takes origin choice 1 into origin choice 2 is given by $S = x_1 + \frac{1}{4}, x_2 + \frac{1}{4}, x_3 + \frac{1}{4}, x_4$, and therefore the same glide reflection in origin choice 1 is given by $g^{(2)} = S^{-1}g^{(1)}S = x_1 - \frac{1}{2}, x_2 + \frac{1}{2}, x_3 + \frac{1}{2}, x_3 - x_4 + \frac{1}{4} + \delta$. Now we can write an expression for the IR matrix using equation (32):

$$D^{(2)}(g^{(2)}) = D^{(1)}(S^{-1}g^{(2)}S) = Q(\tfrac{1}{4} + \delta)P_s^{(1)}(\overline{x}_1, x_2, x_3, \overline{x}_4). \quad (38)$$

Since $Q(\frac{1}{4} + \delta) = Q(\frac{1}{4})Q(\delta)$, we can obtain the prescribed form in equation (16),

$$D^{(2)}(g^{(2)}) = Q(\delta)P_s^{(2)}(\overline{x}_1, x_2, x_3, \overline{x}_4), \quad (39)$$

where

$$P_s^{(2)}(\overline{x}_1, x_2, x_3, \overline{x}_4) = Q(\tfrac{1}{4})P_s^{(1)}(\overline{x}_1, x_2, x_3, \overline{x}_4). \quad (40)$$

In the example of SG No. 48, the A_1 IR matrix for $\overline{x}, y + \frac{1}{2}, z + \frac{1}{2}$ is listed in the ISO-IR tables as

$$Q(\delta) \begin{pmatrix} 0 & \overline{1} & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & \overline{1} & 0 \end{pmatrix}. \quad (41)$$

Note that the matrices $P_s^{(2)}$ in the above equation and $P_s^{(1)} = P^{(1)}$ in equation (35) are related by the expression in equation (40).

8. Conclusions

The 2011 version of our IR matrices include some important improvements.

(i) For three-dimensional SGs, IR matrices are separated into a translation part T and a point-operation part P. The T matrix has a simple prescribed form that depends on the free parameters in $\mathbf{k}$, while the P matrix does not depend on the free parameters in $\mathbf{k}$. The separation of IR matrices into T and P makes the tabulation of these matrices possible for non-special $\mathbf{k}$ vectors.

(ii) For $(3 + d)$-dimensional SSESGs, IR matrices are separated into a phase-shift part Q and a point-operation part P_s. The Q matrix has a simple prescribed form, and neither the Q nor P_s matrices depend on the free parameters in $\mathbf{k}$. The separation of IR matrices into Q and P_s makes the tabulation of these matrices possible.

(iii) The IR matrices are brought to a block form which allows one to see by inspection which parts of the matrices and

the associated order parameters belong to which **k** vector in the star of $\pm\mathbf{k}$.

In the *ISODISTORT* software package, we now allow users to choose which version of the IR matrices they use. The 2011 version is expected to become the default within the *ISOTROPY* suite in the future. But because many published papers are based on the 1988 version, we plan to continue to support it. Some features in *ISODISTORT* already require the 2011 version, and many new features implemented in the future will require the 2011 version as well. We strongly encourage those who work with either version to explicitly state which version they use in published work.

APPENDIX *A*
Superspace groups

If any of the components of a non-special **k** point are irrational, then the resulting distortion will be incommensurate with the lattice. These types of distortions are best described by extending G to $(3+d)$-dimensional superspace, resulting in isotropy subgroups with SSG symmetry. The additional d dimensions in superspace are phase shifts Δ_i of the modulations along the directions of each of the d **k** vectors, respectively, in the star of $\pm\mathbf{k}$.

The coordinates in three-dimensional space are called 'external coordinates', while the phase shifts Δ_i are called 'internal coordinates'. The SSG point operators are denoted by (R, ε), where R operates on the external coordinates and ε operates on the internal coordinates. The point operator is represented by a block-diagonal matrix,

$$(R, \varepsilon) = \begin{pmatrix} R & \mathbf{0} \\ \mathbf{0} & \varepsilon \end{pmatrix}. \tag{42}$$

We call this the *unmixed* setting because its operators never mix external and internal coordinates.

The lattice of the SSG is defined by the following basis vectors, each given in terms of coordinates in the unmixed setting:

$$\begin{aligned}
a_1 &= (1, 0, 0, -\mathbf{k}_1\cdot\mathbf{a}, -\mathbf{k}_2\cdot\mathbf{a}, \ldots, -\mathbf{k}_d\cdot\mathbf{a}),\\
a_2 &= (0, 1, 0, -\mathbf{k}_1\cdot\mathbf{b}, -\mathbf{k}_2\cdot\mathbf{b}, \ldots, -\mathbf{k}_d\cdot\mathbf{b}),\\
a_3 &= (0, 0, 1, -\mathbf{k}_1\cdot\mathbf{c}, -\mathbf{k}_2\cdot\mathbf{c}, \ldots, -\mathbf{k}_d\cdot\mathbf{c}),\\
a_4 &= (0, 0, 0, 1, 0, \ldots, 0),\\
a_5 &= (0, 0, 0, 0, 1, \ldots, 0),\\
&\ldots\\
a_{3+d} &= (0, 0, 0, 0, 0, \ldots, 1).
\end{aligned} \tag{43}$$

These lattice vectors define another setting that we refer to as the *SSG-lattice* setting. In the SSG-lattice setting, a point operator, denoted by R_s, is no longer represented by a block-diagonal matrix:

$$R_s = \begin{pmatrix} R & \mathbf{0} \\ M & \varepsilon \end{pmatrix}. \tag{44}$$

The off-diagonal portion M is a $d \times 3$ matrix defined by

$$M_{mj} = \sum_{i=1}^{3} k_{mi} R_{ij} - \sum_{n=1}^{d} \varepsilon_{mn} k_{nj}, \tag{45}$$

where k_{mi} is the ith component of the mth **k** vector in the star of $\pm\mathbf{k}$. The same $(3+d)$-dimensional vector will have different coordinate components depending on which setting is used (unmixed coordinates or SSG-lattice coordinates). But in either case, the first three and the last d components are loosely referred to as the 'external' and 'internal' coordinates, respectively. We see that operators in the SSG-lattice setting can mix external coordinates onto internal coordinates, but not the other way around.

Consider a vector $\mathbf{v}_s$ expressed in the SSG-lattice setting:

$$\mathbf{v}_s = v_1 a_1 + v_2 a_2 + v_3 a_3 + \delta_1 a_4 + \delta_2 a_5 + \cdots + \delta_d a_{3+d}. \tag{46}$$

Substituting equations (43) into this expression, we obtain $\mathbf{v}_s$ expressed in the unmixed setting:

$$\mathbf{v}_s = (v_1, v_2, v_3, \delta_1 - \mathbf{k}_1\cdot\mathbf{v}, \delta_2 - \mathbf{k}_2\cdot\mathbf{v}, \ldots, \delta_d - \mathbf{k}_d\cdot\mathbf{v}). \tag{47}$$

Extracting the phase shifts Δ_i from the above expression, we obtain

$$\Delta_i = \delta_i - \mathbf{k}_i\cdot\mathbf{v}, \tag{48}$$

where Δ_i are the internal coordinates in the unmixed setting and δ_i are the internal coordinates in the SSG-lattice setting.

APPENDIX *B*
IR and PIR matrices in real form

We obtain the real form of IR and PIR matrices such that all translation matrices in SGs and all phase-shift matrices in SSESGs have a standard form: d matrix blocks along the diagonal with the ith block equal to $U_b(\mathbf{k}_i\cdot\mathbf{v})$ for SGs and $U_b(\boldsymbol{\delta}_i)$ for SSESGs. Here, the matrix $U_b(x_i)$ of dimension $b = en_k t$ is given by equation (24), where $t = 1$ for type-1 IRs and $t = 2$ for PIRs of type-2 and type-3 IRs.

B1. Type-2 and 3 PIRs

We form a PIR from the direct sum of the IR and its complex conjugate, as in equation (23), resulting in matrices of dimension $n = 2den_k$. Then we apply three consecutive similarity transformations.

(i) A permutation transformation S_1 composed of (en_k)-dimensional matrix blocks,

$$S_{1IJ} = \begin{cases} \mathbf{1}_{en_k}, & \text{if } I \text{ is odd and } J = \frac{1}{2}(I+1);\\ \mathbf{1}_{en_k}, & \text{if } I \text{ is even and } J = d + \frac{1}{2}I;\\ \mathbf{0}_{en_k}, & \text{otherwise,} \end{cases} \tag{49}$$

where I and J are hybrid indices that combine i with i' and j with j', and therefore run from 1 to $2d$.

(ii) A transformation S_2 with identical $(2en_k)$-dimensional matrix blocks on the diagonal,

$$S_{2ii} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1}_{en_k} & \mathbf{1}_{en_k} \\ i\mathbf{1}_{en_k} & -i\mathbf{1}_{en_k} \end{pmatrix}. \tag{50}$$

(iii) If $e = 2$, another permutation transformation S_3 with identical $(2en_k)$-dimensional matrix blocks on the diagonal,

$$S_{3ii} = \begin{pmatrix} \mathbf{1}_{n_k} & \mathbf{0}_{n_k} & \mathbf{0}_{n_k} & \mathbf{0}_{n_k} \\ \mathbf{0}_{n_k} & \mathbf{0}_{n_k} & \mathbf{0}_{n_k} & \mathbf{1}_{n_k} \\ \mathbf{0}_{n_k} & \mathbf{0}_{n_k} & \mathbf{1}_{n_k} & \mathbf{0}_{n_k} \\ \mathbf{0}_{n_k} & \mathbf{1}_{n_k} & \mathbf{0}_{n_k} & \mathbf{0}_{n_k} \end{pmatrix}. \quad (51)$$

We obtain the real form of the PIR matrix using

$$D_{\rm PIR}(g) = S_3 S_2 S_1 \begin{bmatrix} D_{\rm IR}(g) & 0 \\ 0 & D_{\rm IR}(g)^* \end{bmatrix} S_1^{-1} S_2^{-1} S_3^{-1}. \quad (52)$$

We can also obtain the block-diagonal complex form from the real form using the inverse transformation. Some applications require this transformation (for example, the algorithm for projecting distortion mode vectors; Stokes *et al.*, 1991). ISO-IR contains tables of $D_{\rm PIR}(g)$ as well as tables of $D_{\rm IR}(g)$.

B2. Type-1 IRs

We begin by bringing IR matrices for pure translations $\{1|\mathbf{v}\}$ in SGs and pure phase shifts $\{1, 1|0, \boldsymbol{\delta}\}$ in SSESGs to the standard real form.

If $e = 1$, these matrices are already in standard real form. This happens because, for type-1 IRs, the condition $e = 1$ only occurs if the $\mathbf{k}$ vector is special and if $\mathbf{k} = -\mathbf{k}$ (mod $\mathbf{K}$), resulting in $\mathbf{k}_i \cdot \mathbf{v} = \frac{1}{2}$ (mod 1) and

$$D_{ii}(\{1|\mathbf{v}\}) = \mathbf{1}_{n_k} \cos(2\pi \mathbf{k}_i \cdot \mathbf{v}). \quad (53)$$

If $e = 2$, we simply apply the transformation S_2 with identical (en_k)-dimensional matrix blocks on the diagonal,

$$S_{2ii} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1}_{en_k} & \mathbf{1}_{en_k} \\ i\mathbf{1}_{en_k} & -i\mathbf{1}_{en_k} \end{pmatrix}. \quad (54)$$

This transformation often brings the remaining IR matrices to real form as well. If not, then we need to find a transformation S_4 to complete the task:

$$D_{\rm PIR}(g) = S_4 S_2 D_{\rm IR}(g) S_2^{-1} S_4^{-1}. \quad (55)$$

The task of finding S_4 is not straightforward, but we can make one simplification: S_4 can be chosen to be block diagonal with identical (en_k)-dimensional matrix blocks on the diagonal. We also require that S_4 does not change the matrices for translations in SGs or for phase shifts in SSESGs, which, at this point, are already in the desired standard form. The S_4 transformations used here were determined on a case-by-case basis, a process that required a significant effort and involved a rather long history.

Once the IR matrices have been obtained in real form, S_2^{-1} can be used to transform them back to a complex form,

$$D'_{\rm IR}(g) = S_2^{-1} D_{\rm PIR}(g) S_2, \quad (56)$$

although generally only the matrices for translations in SGs and phase shifts in SSESGs will be the same as those we began with since we omitted S_4 from the inverse transformation. ISO-IR contains tables of the real form $D_{\rm PIR}(g)$ as well as tables of the complex form $D'_{\rm IR}(g)$ that are obtained by the transformation in equation (56).

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