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The crystallographic fast Fourier transform. II. One-step symmetry reduction

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An algorithm for evaluation of the crystallographic FFT for 67 crystallographic space groups is presented. The symmetry is reduced in such a way that it is enough to calculate $P1$ FFT in the asymmetric unit only and then, in a computationally simpler step, recover the final result. The algorithm yields the maximal symmetry reduction for every space group considered. For the central step in the calculation consisting of general $P1$ FFTs, any generic fast Fourier subroutine can be used. The approach developed in this paper is an extension of the scheme derived for $p3$-symmetric data [Rowicka, Kudlicki & Otwinowski (2002). *Acta Cryst.* A**58**, 574–579]. Algorithms described here will also be used in our forthcoming papers [Rowicka, Kudlicki & Otwinowski (2003). *Acta Cryst* A**59**, 183–192; Rowicka, Kudlicki & Otwinowski (2003), in preparation], where more complicated groups will be considered.

1. Introduction

Taking full advantage of crystallographic symmetries in computation of the Fourier transform would yield much more efficient fast Fourier transform (FFT) routines for crystallographic data processing. However, there has been no general space-group-efficient implementation of fast Fourier transform so far. Such algorithms should operate only in the asymmetric unit and should have speeds comparable to $P1$ FFT transforms of the same amount of data. This will be called a maximal symmetry reduction.

This problem has already been partially solved by Ten Eyck (1973). Subsequently, it has attracted lots of attention and more than 20 research papers have been devoted to the issue. In particular, an elegant approach has been proposed by Bricogne (1993), but without a prescription how to design algorithms.

Our work has resulted in a set of easy-to-implement algorithms for all 230 crystallographic groups. For every one of them, we can achieve maximal symmetry reduction. Moreover, at all times only a region of memory corresponding to the asymmetric unit has to be allocated.

Recently, we have presented an explicit scheme for the $p3$ symmetry group (Rowicka *et al.*, 2002). The present paper is the second in a series of articles describing our approach. Here we deal with 67 crystallographic groups for which it is possible to reduce crystallographic symmetry in one step. For each of these groups, we find a computational grid without points in special positions. It means that in such a computational grid data points do not lie on symmetry elements (such as rotation axes or mirror planes). Implementation of this algorithm already exists and yields expected gains in speed and reduction in memory usage.

Our approach differs from that of Ten Eyck. We do not factorize the one-dimensional Fourier transform, nor do symmetry elements of order 2 play a special role in our scheme. This makes our algorithm versatile and easy to combine with other algorithms we developed. The approach we use in this paper is a generalization of an approach proposed by Bricogne, (1993). However, our forthcoming papers (Rowicka *et al.*, 2003*a*,*b*) (where we will discuss all crystallographic groups not covered here) will be very different in spirit.

We based our approach on the Cooley–Tukey decomposition (Cooley & Tukey, 1965), which has the advantage of a simple geometric interpretation, unlike the widely discussed Winograd scheme (Auslander & Shenefelt, 1987; Auslander *et al.*, 1988; Bricogne & Tolimieri, 1990; An *et al.*, 1992; Bricogne, 1993). In the Cooley–Tukey algorithm, data are divided into subsets consisting of points regularly distributed in space. Regular spacing has an additional implementation advantage of an easy to optimize memory access pattern. Another advantage of the approach presented here and in our other papers (Rowicka *et al.*, 2002, 2003*a*) over the Winograd scheme is that our algorithms generally do not depend on the prime-factor decomposition of the grid size. In the Winograd-based approach, each group and each grid size leads to a different algorithm. We will also cope with the limited sensitivity to the prime-factor decomposition of the grid size in the last portion of algorithms, which will be presented in Rowicka *et al.* (2003*b*).

The paper is organized as follows. In §2, we introduce mathematical notions and notation we will use later on. In §3, the symmetry-reduction formula is derived. Following that, in §4, we explain by examples how the symmetry-reduction formula works. The purpose of these examples is twofold: they

are intended to provide insight into how our algorithm works in practice; reading them will also aid in understanding the formalism introduced in §§2 and 3. In §5, we discuss requirements, limitations and future development and application of our algorithms. In Appendix *A*, we provide a detailed description of the algorithm and requirements on the grid size for specific crystallographic groups.

2. Mathematical notions and notation

Throughout this paper, we will follow the spirit of the modern mathematical approach of Bricogne (1993), we will also use a similar notation. Let $\mathbb{Z}$ denote the set of all integers and $\mathbb{Z}^3$ denote $\mathbb{Z}\times\mathbb{Z}\times\mathbb{Z}$, where $\times$ is the Cartesian product. Matrices and vectors will be written in bold type.

Our goal is to compute the discrete Fourier transform of a periodic function f defined on $\mathbb{Z}^3$. Such a function will have the periodicity of the underlying crystal structure. The crystal periodicity can be described in many ways, for example by listing three primitive translation vectors. These vectors will be denoted by $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. In the standard basis of $\mathbb{Z}^3$, consisting of basis vectors $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$:

$$\mathbf{e}_1 = \begin{bmatrix}1\\0\\0\end{bmatrix},\ \mathbf{e}_2 = \begin{bmatrix}0\\1\\0\end{bmatrix},\ \mathbf{e}_3 = \begin{bmatrix}0\\0\\1\end{bmatrix},$$

the primitive translation vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ can be written as

$$\begin{aligned}\mathbf{a}_1 &= a_{11}\mathbf{e}_1 + a_{21}\mathbf{e}_2 + a_{31}\mathbf{e}_3\\ \mathbf{a}_2 &= a_{12}\mathbf{e}_1 + a_{22}\mathbf{e}_2 + a_{32}\mathbf{e}_3\\ \mathbf{a}_3 &= a_{13}\mathbf{e}_1 + a_{23}\mathbf{e}_2 + a_{33}\mathbf{e}_3,\end{aligned}$$

where all a_{ij} are integer. Let $\mathbf{A}$ denote the matrix whose columns are vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$:

$$\mathbf{A} = \begin{bmatrix}a_{11} & a_{12} & a_{13}\\ a_{21} & a_{22} & a_{23}\\ a_{31} & a_{32} & a_{33}\end{bmatrix}.$$

Note that, since the primitive translation vectors $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are linearly independent, it follows that the matrix $\mathbf{A}$ is invertible (that is, its determinant is not equal to zero: $\det\mathbf{A}\neq 0$).

Periodicity of the crystal can be also encoded by lattice Λ defined as a set of linear combinations of primitive translation vectors, with integer coefficients:

$$\Lambda = \{\boldsymbol{\lambda} :\ \boldsymbol{\lambda} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3,\ m_1, m_2, m_3 \in \mathbb{Z}\},$$

or in shorthand notation

$$\Lambda = \mathbf{A}\mathbb{Z}^3.$$

Following Bricogne (1993), we will call $\mathbf{A}$ the period matrix of the crystal and Λ its period lattice. Lattice types encountered in this paper are graphically depicted in Fig. 1, the period lattice Λ is coloured blue.

The periodicity of the function f can be encoded by the period lattice Λ, as follows:

$$f(\mathbf{x}+\mathbf{t}) = f(\mathbf{x}) \quad \text{for} \quad \mathbf{t}\in\Lambda \quad \text{and} \quad \mathbf{x}\in\mathbb{Z}^3.$$

Observe that the function f has the same values in points $\mathbf{x}$ and $\mathbf{y}$ if $\mathbf{x}-\mathbf{y}\in\Lambda$. To build a formalism convenient for describing such periodic functions, we will use the notion of an equivalence relation, which naturally arises in crystallography. Let X be a set and let $x, y \in X$. We say that *x is in relation $\mathcal{R}$ with y* and we write $x\mathcal{R}y$ whenever a certain condition is fulfilled. This condition can have a fairly general nature. A relation is called an *equivalence relation* if it is reflexive ($x\mathcal{R}x$ for every $x\in X$), symmetric (if $x\mathcal{R}y$ then $y\mathcal{R}x$) and transitive (if $x\mathcal{R}y$ and $y\mathcal{R}z$ then $x\mathcal{R}z$). Equivalence relations are of great importance to us, since they induce a decomposition of a set, on which they are defined, into equivalence classes. The *equivalence class* of an element $x\in X$ with respect to relation $\mathcal{R}$ is a set of all elements $y\in X$ such that y is in relation $\mathcal{R}$ with x. It will be denoted by $[x]_{\mathcal{R}}$:

$$[x]_{\mathcal{R}} = \{y\in X : y\mathcal{R}x\}.$$

A useful example of an equivalence relation is given by

$$\mathbf{y}\mathcal{R}_\Lambda\mathbf{x} \Leftrightarrow \mathbf{y}-\mathbf{x}\in\Lambda.$$

That means that $\mathbf{x}$ and $\mathbf{y}$ are in the relation $\mathcal{R}_\Lambda$ if and only if they have the same crystallographic coordinates. The equivalence class of $\mathbf{x}$ will be

$$[\mathbf{x}]_\Lambda = \{\mathbf{y}\in\mathbb{Z}^3\ :\ \mathbf{y}-\mathbf{x}\in\Lambda\}.$$

In other words, the equivalence class of a point $\mathbf{x}$ is the set of all points that are related to $\mathbf{x}$ by a combination of primitive translations, with integer coefficients. For example, in fractional coordinates (that is if $\mathbf{A}$ is an identity matrix), the equivalence class with respect to the relation $\mathcal{R}_\Lambda$ of the point $(0,0,0)$ is the set of all points with integer coordinates. Generally, in fractional coordinates, the equivalence class of the point (x,y,z) consists of all points $(\tilde{x},\tilde{y},\tilde{z})$ such that fractional parts of x, y and z equal those of $\tilde{x}$, $\tilde{y}$ and $\tilde{z}$, respectively. Another useful notion will be that of a *quotient space*. The quotient space of a vector space X by a vector space Y is a set of all equivalence classes of the elements of X with respect to the relation $\mathcal{R}_Y$, defined by

$$\mathbf{x}_1\mathcal{R}_Y\mathbf{x}_2 \Leftrightarrow \mathbf{x}_1-\mathbf{x}_2\in Y,$$

for $\mathbf{x}_1, \mathbf{x}_2\in X$. Such a quotient is a vector space and it is denoted by X/Y. In this article, we deal with the quotient space of $\mathbb{Z}^3$ by Λ (by definition, the lattice Λ is a vector space, too):

$$\mathbb{Z}^3/\Lambda = \{[\mathbf{x}]_\Lambda :\ \mathbf{x}\in\mathbb{Z}^3\}.$$

One can think of this quotient space as a unit cell, with one difference: every point from $\mathbb{Z}^3/\Lambda$ represents an infinite number of points related by lattice translations. In fractional coordinates, this quotient space is a set of representatives of all points with coordinates greater than or equal to zero and smaller than 1 (fractional parts of real numbers). One of the reasons why equivalence classes are very useful is that they are invariant under lattice translations. This clarifies the picture and allows us to focus on meaningful symmetry operations. More detailed examples will be discussed later on, when

application of our algorithm to the specific crystallographic groups will be presented.

The notion of a quotient space allows us to describe periodicity conditions in a very convenient way. Instead of viewing f as a Λ-periodic function, it can be equivalently considered as defined on the set of the equivalence classes, $\mathbb{Z}^3/\Lambda$. Let us introduce the notation

$$\Gamma = \mathbb{Z}^3/\mathbf{A}\mathbb{Z}^3 = \mathbb{Z}^3/\Lambda \tag{1}$$

and

$$\Gamma^* = \mathbb{Z}^3/\mathbf{A}^T\mathbb{Z}^3,$$

where $\mathbf{A}^T$ denotes the transposition of the matrix $\mathbf{A}$. The space Γ^* is a space dual to Γ. Its elements are covectors, that is objects dual to vectors. Covectors will be also printed in bold type and they will be, when there is no risk of confusion, also called vectors. However, covectors will be usually depicted as 'horizontal' vectors. Let $\mathbf{h} \in \Gamma^*$. Then,

$$\mathbf{h} = \begin{bmatrix} h_1 & h_2 & h_3 \end{bmatrix}.$$

Covectors can also be expressed using a standard dual basis $\mathbf{e}_1^*$, $\mathbf{e}_2^*$, $\mathbf{e}_3^*$:

$$\mathbf{h} = h_1\mathbf{e}_1^* + h_2\mathbf{e}_2^* + h_3\mathbf{e}_3^*,$$

where

$$\mathbf{e}_1^* = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}, \quad \mathbf{e}_2^* = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}, \quad \mathbf{e}_3^* = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}.$$

The scalar product is always defined between a covector and a vector. For example, the scalar products of a basis covector and a basis vector is

$$\mathbf{e}_i^* \cdot \mathbf{e}_j = \delta_{ij},$$

where δ_{ij} is the Kronecker delta:

$$\delta_{ij} = \begin{cases} 0 & \text{for} \quad i \neq j \\ 1 & \text{for} \quad i = j. \end{cases}$$

Consequently, the scalar product of a covector $\mathbf{h}$ and a vector $\mathbf{x}$ expressed in standard bases reads

$$\begin{aligned} \mathbf{h} \cdot \mathbf{x} &= (h_1\mathbf{e}_1^* + h_2\mathbf{e}_2^* + h_3\mathbf{e}_3^*) \cdot (x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + x_3\mathbf{e}_3) \\ &= h_1x_1 + h_2x_2 + h_3x_3 \end{aligned}$$

or

$$\mathbf{h} \cdot \mathbf{x} = \begin{bmatrix} h_1 & h_2 & h_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = h_1x_1 + h_2x_2 + h_3x_3.$$

We will use a shorthand notation $e_{\mathbf{A}}(\mathbf{h}, \mathbf{x})$ for a coefficient (also called 'twiddle factor') that will occur frequently in considered formulae:

$$e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}) = \exp(-2\pi i \mathbf{h} \cdot \mathbf{A}^{-1}\mathbf{x}).$$

This symbol has the following properties:

$$\begin{aligned} e_{\mathbf{A}}(\mathbf{g} + \mathbf{h}, \mathbf{x}) &= e_{\mathbf{A}}(\mathbf{g}, \mathbf{x})e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}) \\ e_{\mathbf{A}}(\mathbf{h}, \mathbf{x} + \mathbf{y}) &= e_{\mathbf{A}}(\mathbf{h}, \mathbf{x})e_{\mathbf{A}}(\mathbf{h}, \mathbf{y}) \end{aligned}$$

for any $\mathbf{g}, \mathbf{h} \in \Gamma^*$ and $\mathbf{x}, \mathbf{y} \in \Gamma$. Moreover,

$$e_{\mathbf{A}}(\mathbf{h}, \mathbf{A}\mathbf{x}) = 1 \quad \text{for any } \mathbf{h} \in \Gamma^* \text{ and } \mathbf{x} \in \Gamma. \tag{2}$$

Let f be a complex-valued function on Γ, where Γ is given by (1). The Fourier transform of function f will be denoted by F and for any $\mathbf{h} \in \Gamma^*$ defined by

$$F(\mathbf{h}) = \sum_{\mathbf{x} \in \Gamma} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{h}, \mathbf{x}). \tag{3}$$

For simplicity, in the above formula, we have omitted the normalization constant $1/|\det \mathbf{A}|$.

2.1. Multidimensional Cooley–Tukey factorization

Assume that $\mathbf{A}_0$ and $\mathbf{A}_1$ are matrices with integer entries, such that

$$\mathbf{A} = \mathbf{A}_0\mathbf{A}_1. \tag{4}$$

Let us define

$$X_0 = \mathbb{Z}^3/\mathbf{A}_0\mathbb{Z}^3 \quad \text{and} \quad X_1 = \mathbb{Z}^3/\mathbf{A}_1\mathbb{Z}^3.$$

Observe that every element $\mathbf{x} \in \Gamma$ can be expressed uniquely as

$$\mathbf{x} = \mathbf{x}_0 + \mathbf{A}_0\mathbf{x}_1, \tag{5}$$

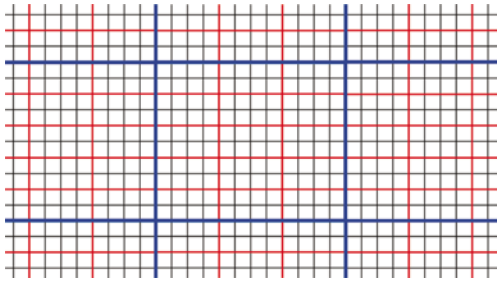

Figure 1
Lattices used in crystallographic Fourier transform calculations. For simplicity, we depict an example in two dimensions. The standard lattice $\mathbb{Z}^2$ is coloured black. The period lattice Λ is spanned in this case by the vectors $\mathbf{a}_1 = \left[\begin{smallmatrix} 12 \\ 0 \end{smallmatrix}\right]$ and $\mathbf{a}_2 = \left[\begin{smallmatrix} 0 \\ 10 \end{smallmatrix}\right]$ and it is coloured blue. The asymmetric lattice $\mathbf{A}_0\mathbb{Z}^2$ is spanned here by vectors $\left[\begin{smallmatrix} 4 \\ 0 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} 0 \\ 2 \end{smallmatrix}\right]$ and it is coloured red.

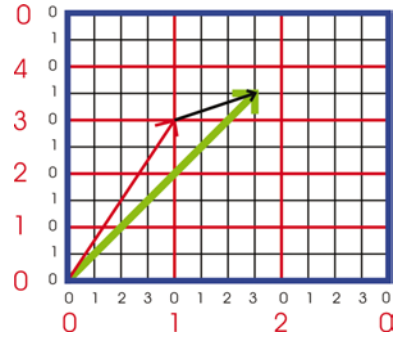

Figure 2
Decomposition (5) in the real space. Here, $\mathbf{A} = \left[\begin{smallmatrix} 12 & 0 \\ 0 & 10 \end{smallmatrix}\right]$ and $\mathbf{A}_0 = \left[\begin{smallmatrix} 4 & 0 \\ 0 & 2 \end{smallmatrix}\right]$. The vector $\mathbf{x} = \left[\begin{smallmatrix} 7 \\ 7 \end{smallmatrix}\right]$ is represented as $\left[\begin{smallmatrix} 3 \\ 1 \end{smallmatrix}\right] + \left[\begin{smallmatrix} 4 & 0 \\ 0 & 2 \end{smallmatrix}\right]\left[\begin{smallmatrix} 1 \\ 3 \end{smallmatrix}\right]$, that is $\mathbf{x}_0 = \left[\begin{smallmatrix} 3 \\ 1 \end{smallmatrix}\right]$ and $\mathbf{x}_1 = \left[\begin{smallmatrix} 1 \\ 3 \end{smallmatrix}\right]$.

where $\mathbf{x}_0 \in X_0$ and $\mathbf{x}_1 \in X_1$. An example of such a decomposition (for clarity again in two dimensions) is illustrated in Fig. 2. Decompositions of this type are also common in real life, for example, instead of saying 'I am 75 inches tall', one would rather say 'I am 6 feet 3 inches tall' *etc*.

Analogously, let us define

$$X_0^* = \mathbb{Z}^3/\mathbf{A}_0^T\mathbb{Z}^3 \quad \text{and} \quad X_1^* = \mathbb{Z}^3/\mathbf{A}_1^T\mathbb{Z}^3.$$

Then, in the reciprocal space there is a similar unique decomposition for every $\mathbf{h} \in \Gamma^*$:

$$\mathbf{h} = \mathbf{h}_1 + \mathbf{A}_1^T\mathbf{h}_0, \tag{6}$$

where $\mathbf{h}_0 \in X_0^*$ and $\mathbf{h}_1 \in X_1^*$ (see Fig. 3).

We introduce a shorthand notation

$$F(\mathbf{h}_0, \mathbf{h}_1) = F(\mathbf{h}_1 + \mathbf{A}_1^T\mathbf{h}_0) = F(\mathbf{h}).$$

Let us insert the decomposition of $\mathbf{h}$ given by equation (6) into equation (3):

$$F(\mathbf{h}_0, \mathbf{h}_1) = \sum_{\mathbf{x} \in \Gamma} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{x}) e_{\mathbf{A}}(\mathbf{h}_1, \mathbf{x}).$$

Using the decomposition of $\mathbf{x}$, given by equation (5), we obtain

$$e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{x}) = e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{x}_0) e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{A}_0\mathbf{x}_1).$$

Since $e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{A}_0\mathbf{x}_1) = e_{\mathbf{A}}(\mathbf{h}_0, \mathbf{A}\mathbf{x}_1)$, we can skip the last factor because (2) implies $e_{\mathbf{A}}(\mathbf{h}_0, \mathbf{A}\mathbf{x}_1) = 1$. It follows that

$$F(\mathbf{h}_0, \mathbf{h}_1) = \sum_{\mathbf{x} \in \Gamma} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{x}_0) e_{\mathbf{A}}(\mathbf{h}_1, \mathbf{x})$$

or

$$F(\mathbf{h}) = \sum_{\mathbf{x}_0 \in X_0} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0, \mathbf{x}_0) \sum_{\mathbf{x}_1 \in X_1} f(\mathbf{x}) e_{\mathbf{A}}(\mathbf{h}_1, \mathbf{x}). \tag{7}$$

The above formula is the well known multidimensional Cooley–Tukey factorization, here we use it in the form presented by Bricogne (1993). The main idea of this decomposition is to replace the Fourier transform of $|\det \mathbf{A}|$ points with $|\det \mathbf{A}_1|$ Fourier transforms of $|\det \mathbf{A}_0|$ points each. How the Cooley–Tukey decomposition can be combined with the underlying crystallographic symmetry will be shown in §3.

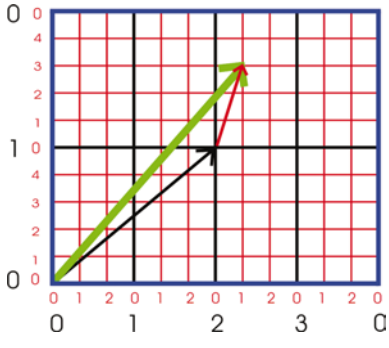

Figure 3
Decomposition (6) in the reciprocal space. Here, $\mathbf{A}$ and $\mathbf{A}_0$ are the same as in Fig. 2. Hence, $\mathbf{A}^T = \left[\begin{smallmatrix}12 & 0\\ 0 & 10\end{smallmatrix}\right]$ and $\mathbf{A}_1^T = \left[\begin{smallmatrix}3 & 0\\ 0 & 5\end{smallmatrix}\right]$. Consequently, the vector $\mathbf{h} = \left[\begin{smallmatrix}7\\ 8\end{smallmatrix}\right]$ is represented as $\left[\begin{smallmatrix}1\\ 3\end{smallmatrix}\right] + \left[\begin{smallmatrix}3 & 0\\ 0 & 5\end{smallmatrix}\right]\left[\begin{smallmatrix}2\\ 1\end{smallmatrix}\right]$, that is $\mathbf{h}_1 = \left[\begin{smallmatrix}1\\ 3\end{smallmatrix}\right]$ and $\mathbf{h}_0 = \left[\begin{smallmatrix}2\\ 1\end{smallmatrix}\right]$.

2.2. Crystallographic group action

Let $\mathcal{G}$ denote the crystallographic space group. All the crystallographic space groups have an infinite number of elements (Bricogne, 1993), since they contain all linear combinations of primitive translations, with integer coefficients. As we remarked while discussing equivalency classes, this is not a desirable feature for our purpose, since we are not interested in lattice translations. Therefore, we shall consider quotient crystallographic groups (also called factor groups), that is crystallographic space groups without lattice translations. To this end, we will recall the quotient group construction and then, in order to obtain the quotient group, we 'divide' the crystallographic group by a subgroup spanned by lattice translations. Observe that the period lattice Λ with addition of vectors as group operation is a subgroup of $\mathcal{G}$. In fact, Λ is even a normal subgroup of $\mathcal{G}$. Thus, we can consider a quotient group $G = \mathcal{G}/\Lambda$ obtained by dividing the crystallographic group by its normal subgroup Λ. The group operation on G is induced from $\mathcal{G}$. It can be thought of as 'collapsing' the subgroup Λ to the identity operator. The elements of G are the symmetry operators as listed in *International Tables for Crystallography* (ITC) (Hahn, 1995). The group operation on G is a usual symmetry-operator composition. We will call the resulting quotient group G a *quotient crystallographic group* G. It may not be obvious that $\mathcal{G}/\Lambda$ is a group. However, this becomes clear when one keeps in mind that elements of G are not individual operators but their equivalence classes. The equivalence relation here is that the difference of two operators is an integer linear combination of the primitive translations. Therefore, G defined in such a way is a group. There are many advantages of using a quotient crystallographic group instead of a usual crystallographic space group. For example, since all space groups have an infinite number of elements, one cannot derive any useful information from comparing the number of elements in these groups. The number of elements of the quotient crystallographic group is useful in many aspects, also it is a convenient measure of the redundancy of the data.

We represent the action of an element $g \in G$ in the real space as follows:

$$S_g(\mathbf{x}) = \mathbf{R}_g\mathbf{x} + \mathbf{t}_g, \tag{8}$$

where $\mathbf{x} \in \Gamma$. We will call $\mathbf{R}_g$ the rotational part of the symmetry operator related to g. Since $\det \mathbf{R}_g = \pm 1$, it follows that $\mathbf{R}_g$ can be a proper ($\det \mathbf{R}_g = 1$) or an improper ($\det \mathbf{R}_g = -1$) rotation. We will call $\mathbf{t}_g$ a (non-primitive) translational part of the symmetry operator. We stress again that, since $\mathbf{x} \in \Gamma = \mathbb{Z}^3/\Lambda$, the symbol $\mathbf{x}$ in the formula above is in fact the equivalence class $[\mathbf{x}]_\Lambda$, that is a set of all elements from $\mathbb{Z}^3$, which are equal to $\mathbf{x}$ modulo Λ. The action equation (8) defines an action $S^\#$ on a function f on space Γ by

$$(S_g^\# f)(\mathbf{x}) = f(S_g^{-1}(\mathbf{x})) = f(\mathbf{R}_g^{-1}(\mathbf{x} - \mathbf{t}_g)).$$

This action $S^\#$ on the functions in the real space extends to the action S^* on their Fourier transforms in reciprocal space

$$S_g^* F(\mathbf{h}) = e_{\mathbf{A}}(\mathbf{h}\cdot\mathbf{t}_g)F(\mathbf{R}_g^T\mathbf{h}). \quad (9)$$

3. Symmetry reduction

Now we will combine the multidimensional Cooley–Tukey factorization with crystallographic symmetry. In this section, we will derive a symmetry-reduction formula. This formula will allow us to evaluate the Fourier transform in the whole unit cell by computing $P1$ Fourier transform of the asymmetric unit only. Then, in a computationally simpler step, the final result will be recovered. Of course, such algorithms have to be group specific. Let $\mathbf{A}$ be a matrix describing the periodic computational grid. Then $|\det\mathbf{A}|$ equals the number of points in the unit cell. Suppose that for the quotient crystallographic group G there exist matrices $\mathbf{A}_0$ and $\mathbf{A}_1$ satisfying (4). Suppose also that these matrices are such that the number of elements of G, denoted by $|G|$, equals $|\det\mathbf{A}_1|$:

$$|G| = |\det\mathbf{A}_1|.$$

Let Γ_0 denote

$$\Gamma_0 = \mathbf{A}_0 X_1. \quad (10)$$

The lattice Γ_0 is depicted in Fig. 1, where it is referred to as an asymmetric lattice. Let f be any function on Γ that respects the crystallographic symmetry, that is such that

$$f(\mathbf{x}) = f(S_g\mathbf{x}) \quad (11)$$

for any $\mathbf{x}\in\Gamma$ and $g\in G$.

We will require that the following assumptions are satisfied:

Assumption 1. Grid Γ can be expressed as a sum of $|G|$ mutually disjoint sets $S_{g_i}\Gamma_0$, where $g_i\in G$, that is

$$S_{g_1}\Gamma_0 \cap S_{g_2}\Gamma_0 = \emptyset \quad \text{for} \quad g_1 \neq g_2$$

and

$$\Gamma = \bigcup_{g\in G} S_g\Gamma_0. \quad (12)$$

Then,

$$|\Gamma| = |G||\Gamma_0|.$$

Assumption 2. For every $g\in G$, we have:

$$S_g(\Gamma_0) = [\mathbf{t}_g]_{\Gamma_0} = \{\mathbf{x}\in\Gamma \;:\; \mathbf{x} = \boldsymbol{\gamma} + \mathbf{t}_g \quad \text{and} \quad \boldsymbol{\gamma}\in\Gamma_0\}.$$

Assumption 3. Matrix $\mathbf{A}$ commutes with $\mathbf{R}_g$ for every $g\in G$:

$$\mathbf{A}\mathbf{R}_g = \mathbf{R}_g\mathbf{A}.$$

We proceed to the derivation of the symmetry-reduction formula. In what follows, Γ_0 plays the role of the asymmetric unit. Assumption 1 means that any element of Γ can be obtained by some symmetric transformation of some element of Γ_0. It follows that, for every $\mathbf{x}$, there exist a $\boldsymbol{\gamma}\in\Gamma_0$ and a $g\in G$ such that

$$\mathbf{x} = S_g\boldsymbol{\gamma}. \quad (13)$$

From Assumption 2, it follows that for every $\mathbf{x}\in\Gamma$ there exists $g\in G$ such that

$$\mathbf{x}\in[\mathbf{t}_g]_{\Gamma_0}.$$

Moreover, for every $\mathbf{x}\in\Gamma$, by the decomposition (5) and since $\mathbf{A}_0\mathbf{x}_1\in\Gamma_0$, it follows that $\mathbf{x}_0$ belongs to the same equivalence class as $\mathbf{x}$, namely

$$\mathbf{x}_0\in[\mathbf{t}_g]_{\Gamma_0}.$$

Now we can rewrite $e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{x}_0)$ as follows:

$$e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{x}_0) = e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g+\boldsymbol{\gamma}) = e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\boldsymbol{\gamma})$$

and

$$\begin{aligned} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\boldsymbol{\gamma}) &= e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{A}_0\mathbf{x}_1) = \exp(-2\pi i\mathbf{h}_0\cdot\mathbf{A}_1\mathbf{A}^{-1}\mathbf{A}_0\mathbf{x}_1)\\ &= 1.\end{aligned}$$

Therefore,

$$e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{x}_0) = e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g+\boldsymbol{\gamma}) = e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g).$$

After substituting (13) and the above into (7), we obtain

$$F(\mathbf{h}) = \sum_{\mathbf{x}_0\in X_0} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)\sum_{\boldsymbol{\gamma}\in\Gamma_0} f(S_g\boldsymbol{\gamma})e_{\mathbf{A}}(\mathbf{h}_1,S_g\boldsymbol{\gamma}).$$

By equation (11), the function f is invariant under the action of $g\in G$:

$$F(\mathbf{h}) = \sum_{\mathbf{x}_0\in X_0} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)\sum_{\boldsymbol{\gamma}\in\Gamma_0} f(\boldsymbol{\gamma})e_{\mathbf{A}}(\mathbf{h}_1,S_g\boldsymbol{\gamma}).$$

From formula (8), describing the action of the symmetry operator in terms of its rotational and translational components, we obtain

$$e_{\mathbf{A}}(\mathbf{h}_1,S_g\boldsymbol{\gamma}) = e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{t}_g)e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{R}_g\boldsymbol{\gamma}).$$

Assumption 3 implies that $\mathbf{A}^{-1}\mathbf{R}_g = \mathbf{R}_g\mathbf{A}^{-1}$. Hence,

$$\begin{aligned} e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{R}_g\boldsymbol{\gamma}) &= \exp(-2\pi i\mathbf{h}_1\cdot\mathbf{A}^{-1}\mathbf{R}_g\boldsymbol{\gamma})\\ &= \exp(-2\pi i\mathbf{R}_g^T\mathbf{h}_1\cdot\mathbf{A}^{-1}\boldsymbol{\gamma})\\ &= e_{\mathbf{A}}(\mathbf{R}_g^T\mathbf{h}_1,\boldsymbol{\gamma}). \quad (14)\end{aligned}$$

From the formulae derived above and (14), it follows that

$$F(\mathbf{h}) = \sum_{g\in G} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{t}_g)\sum_{\boldsymbol{\gamma}\in\Gamma_0} f(\boldsymbol{\gamma})e_{\mathbf{A}}(\mathbf{R}_g^T\mathbf{h}_1,\boldsymbol{\gamma}).$$

Let us introduce the symbol $Y(\mathbf{h}_1)$ as the Fourier transform of data in the asymmetric unit Γ_0:

$$Y(\mathbf{h}_1) = \sum_{\boldsymbol{\gamma}\in\Gamma_0} f(\boldsymbol{\gamma})e_{\mathbf{A}}(\mathbf{h}_1,\boldsymbol{\gamma}).$$

With this notation,

$$F(\mathbf{h}) = \sum_{g\in G} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{t}_g)Y(\mathbf{R}_g^T\mathbf{h}_1).$$

Let us introduce the notation

$$Z(\mathbf{h}_1,\mathbf{t}_g) = e_{\mathbf{A}}(\mathbf{h}_1,\mathbf{t}_g)Y(\mathbf{R}_g^T\mathbf{h}_1).$$

Finally,

$$F(\mathbf{h}_1+\mathbf{A}_1^T\mathbf{h}_0) = \sum_{g\in G} e_{\mathbf{A}}(\mathbf{A}_1^T\mathbf{h}_0,\mathbf{t}_g)Z(\mathbf{h}_1,\mathbf{t}_g). \quad (15)$$

The above formula shows how to compute the Fourier transform of the unit cell using only $P1$ Fourier transform of the asymmetric unit (Y). This way one performs FFT on $1/|G|$ of the starting number of points. This is the maximal possible reduction as one cannot use fewer points than in the asymmetric unit. We will show later on that such a symmetry reduction is possible for a large number of space groups.

A similar reasoning, leading to the same final formula (15), has been performed by Bricogne (1993). However, he built it on a more restrictive assumption that $\mathbf{A}$, $\mathbf{A}_0$ and $\mathbf{A}_1$ all commute with $\mathbf{R}_g$ for every $g \in G$. Such a strict assumption is not necessary and, what is more important, it cannot be satisfied for some of the most interesting cases [*e.g.* the $p3$ symmetry (Rowicka *et al.*, 2002)].

3.1. Finding a FFT-friendly asymmetric unit

Formula (15) gives the desired symmetry reduction provided that Assumptions 1–3 are fulfilled by the chosen grid Γ, symmetry operators from the considered group G and the asymmetric unit Γ_0. To find asymmetric units satisfying these conditions is a non-trivial task. They do not exist for all the space groups.

Algorithms for all the space groups for which it is practical to apply formula (15) are presented below. The choice of an appropriate coordinate system is a crucial step in our scheme. To derive solutions, we work in a new coordinate system, which we call a *grid coordinate system*. Let $\mathbf{x}^c$ and $\mathbf{x}$ denote coordinates of the same point in the crystallographic and grid coordinate systems, respectively. Let $\mathbf{A}$ be a 3×3 matrix with integer entries and let $\mathbf{b}$ be a vector from $\mathbb{R}^3$. The transformation between the grid coordinate system and the standard crystallographic coordinate systems is an affine transformation

$$\mathbf{x} = \mathbf{A}\mathbf{x}^c + \mathbf{b}. \tag{16}$$

The matrix $\mathbf{A}$ here is the same matrix that described the period lattice Λ and the grid Γ [see equation (1)]. The vector $\mathbf{b}$ corresponds to the shift of the origin of the coordinate system. We will require $\mathbf{b}$ to be such that all our data points will have integer coordinates ($|\det \mathbf{A}|$ corresponds to the number of data points in the unit cell). The transformation equation (16) will be described later by giving $\mathbf{A}$ and $\mathbf{b}$ only.

By Assumption 3, $\mathbf{A}$ commutes with $\mathbf{R}_g$ for any $g \in G$. Then, the relation between the symmetry operator $(\mathbf{R}_g^c, \mathbf{t}_g^c)$ in the crystallographic coordinate system and in the grid coordinate system $(\mathbf{R}_g, \mathbf{t}_g)$ is the following:

$$\mathbf{R}_g = \mathbf{R}_g^c \quad \text{and} \quad \mathbf{t}_g = (\mathbf{I} - \mathbf{R}_g^c)\mathbf{b} + \mathbf{A}\mathbf{t}_g^c.$$

As will be shown in the next section, the shift introduced by $\mathbf{b}$ will induce phase shifts in formulae for symmetry operators in the reciprocal space. We will compute the Fourier transform in the grid coordinate system only.

4. Examples of algorithms

Particular complexities of the algorithm will now be illustrated by a few examples. The examples given will cover all types of algorithms that appear in Appendix *A*. The first one is the $p4$ group. It is then followed by a primitive orthorhombic or tetragonal space group. The example of $p3$ has already been described in Rowicka *et al.* (2002). There, however, we strove to avoid heavy mathematics. In the present paper, this example is described in a different way, it introduces an issue of a subgrid described by a non-diagonal matrix. We will also sketch out the algorithm for the $P\bar{6}$ group.

4.1. Plane group $p4$

This class of algorithms is denoted by 2x2y in Appendix *A*. The plane group $p4$ is the simplest plane group with a fourfold symmetry axis. The symmetry operators in the crystallographic coordinates are x, y and $-x, -y$ and $-y, x$ and $y, -x$.

In this case, the grid coordinate system is described by

$$\mathbf{A} = \begin{bmatrix} 2N & 0 \\ 0 & 2N \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix},$$

where N is a positive integer related to the number of points in the unit cell. Let

$$\mathbf{A}_0 = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \quad \text{and} \quad \mathbf{A}_1 = \begin{bmatrix} N & 0 \\ 0 & N \end{bmatrix}.$$

Observe that $\mathbf{A} = \mathbf{A}_0\mathbf{A}_1$. The grid Γ, defined as $\Gamma = \mathbb{Z}^2/\mathbf{A}\mathbb{Z}^2$, has in this case the form

$$\Gamma = \left\{ \left[\left[\begin{bmatrix} x \\ y \end{bmatrix} \right]\right]_{\mathbf{A}} : x, y \in \{0, 1, 2, \ldots, 2N-1\} \right\}.$$

The subspace $X_0 = \mathbb{Z}^2/\mathbf{A}_0\mathbb{Z}^2$ consists of four vectors:

$$X_0 = \left\{ \left[\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\right]_{\mathbf{A}_0}, \left[\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \right]\right]_{\mathbf{A}_0}, \left[\left[\begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]\right]_{\mathbf{A}_0}, \left[\left[\begin{bmatrix} 1 \\ 1 \end{bmatrix} \right]\right]_{\mathbf{A}_0} \right\}.$$

Here, $\left[\left[\begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right]\right]_{\mathbf{A}_0}$ denotes an equivalence class of the vector $\left[\begin{smallmatrix} 0 \\ 0 \end{smallmatrix}\right]$, defined as

$$\left[\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\right]_{\mathbf{A}_0} = \left\{ \mathbf{x} \in \Gamma : \mathbf{x} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} n \\ m \end{bmatrix} = \begin{bmatrix} 2n \\ 2m \end{bmatrix},\ n, m \in \mathbb{Z} \right\}.$$

It means that this equivalence class consists of these elements of Γ whose x and y coordinates are both even. By analogy,

$$\left[\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix} \right]\right]_{\mathbf{A}_0} = \left\{ \mathbf{x} \in \Gamma : \mathbf{x} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} n \\ m \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2n+1 \\ 2m \end{bmatrix},\ n, m \in \mathbb{Z} \right\}.$$

All elements of this equivalence class have their x coordinate odd and y coordinate even. The other two equivalence classes contain points with x coordinate even and y coordinate odd, and with both x and y coordinates odd, respectively.

On the other hand,

$$X_1 = \mathbb{Z}^2/\mathbf{A}_1\mathbb{Z}^2 = \left\{ \left[\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix} \right]\right]_{\mathbf{A}_1}, \left[\left[\begin{bmatrix} 0 \\ 1 \end{bmatrix} \right]\right]_{\mathbf{A}_1}, \ldots, \left[\left[\begin{bmatrix} N-1 \\ N-2 \end{bmatrix} \right]\right]_{\mathbf{A}_1}, \left[\left[\begin{bmatrix} N-1 \\ N-1 \end{bmatrix} \right]\right]_{\mathbf{A}_1} \right\}.$$

Here, the equivalence classes are taken with respect to a different relation. For example, if $N > 7$,

$$\left[\begin{bmatrix}3\\7\end{bmatrix}\right]_{\mathbf{A}_1} = \left\{\mathbf{x}\in\Gamma : \mathbf{x} = \begin{bmatrix}N & 0\\0 & N\end{bmatrix}\begin{bmatrix}n\\m\end{bmatrix} + \begin{bmatrix}3\\7\end{bmatrix} = \begin{bmatrix}nN+3\\mN+7\end{bmatrix},\ n,m\in\mathbb{Z}\right\}.$$

Since $\mathbf{x}$ is also an equivalence class itself (its coordinates are understood to be modulo $2N$), then there are only four elements in this equivalence class:

$$\left[\begin{bmatrix}3\\7\end{bmatrix}\right]_{\mathbf{A}_1} = \left\{\begin{bmatrix}3\\7\end{bmatrix}, \begin{bmatrix}3\\N+7\end{bmatrix}, \begin{bmatrix}N+3\\7\end{bmatrix}, \begin{bmatrix}N+3\\N+7\end{bmatrix}\right\}.$$

The number of elements of X_1 is $|\det\mathbf{A}|/|G| = (2N)^2/4 = N^2$. Every element $\mathbf{x}\in\Gamma$ has a unique decomposition

$$\mathbf{x} = \mathbf{x}_0 + \begin{bmatrix}2 & 0\\0 & 2\end{bmatrix}\mathbf{x}_1,$$

where $\mathbf{x}_0\in X_0$ and $\mathbf{x}_1\in X_1$. The asymmetric unit is $\Gamma_0 = \mathbf{A}_0 X_1$.

$$\Gamma_0 = \left\{\begin{bmatrix}2 & 0\\0 & 2\end{bmatrix}\begin{bmatrix}\xi\\\eta\end{bmatrix} = \begin{bmatrix}2\xi\\2\eta\end{bmatrix} : \begin{bmatrix}\xi\\\eta\end{bmatrix}\in X_1\right\} = \left[\begin{bmatrix}0\\0\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Observe that the number of points in the asymmetric unit Γ_0 is N^2 and it is the same as the number of points in X_1.

The asymmetric unit Γ_0 is depicted in Fig. 4, it consists of points lying in the centres of red squares. In this figure, the black outline denotes a traditional choice of the unit cell. Observe that, owing to the affine change of coordinate system, there are no points in special positions, not only in the asymmetric unit but also in the entire unit cell.

Let the clockwise rotation by 90° around the origin of the crystallographic coordinate system be denoted by α. Then, in the grid coordinate system,

$$\mathbf{R}_\alpha = \begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix} \quad\text{and}\quad \mathbf{t}_\alpha = \begin{bmatrix}0\\-1\end{bmatrix}\in\left[\begin{bmatrix}0\\1\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Let us check how the group G acts on the elements of Γ_0:

$$S_\alpha\left(\begin{bmatrix}2\xi\\2\eta\end{bmatrix}\right) = \begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix}\begin{bmatrix}2\xi\\2\eta\end{bmatrix} + \begin{bmatrix}0\\-1\end{bmatrix} = \begin{bmatrix}2\eta\\-2\xi-1\end{bmatrix}.$$

This means that the image under the action of symmetry group element α on any point with both even coordinates belongs to the equivalence class of vector $\mathbf{t}_\alpha$:

$$S_\alpha\left(\begin{bmatrix}2\xi\\2\eta\end{bmatrix}\right) = \begin{bmatrix}2\eta\\-2\xi-1\end{bmatrix}\in\left[\begin{bmatrix}0\\1\end{bmatrix}\right]_{\mathbf{A}_0}.$$

By analogy,

$$\mathbf{R}_{\alpha^2} = \begin{bmatrix}-1 & 0\\0 & -1\end{bmatrix} \quad\text{and}\quad \mathbf{t}_{\alpha^2} = \begin{bmatrix}-1\\-1\end{bmatrix}\in\left[\begin{bmatrix}1\\1\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Hence,

$$S_{\alpha^2}\left(\begin{bmatrix}2\xi\\2\eta\end{bmatrix}\right) = \begin{bmatrix}-1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}2\xi\\2\eta\end{bmatrix} + \begin{bmatrix}-1\\-1\end{bmatrix} = \begin{bmatrix}-2\xi-1\\-2\eta-1\end{bmatrix}\in\left[\begin{bmatrix}1\\1\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Finally,

$$\mathbf{R}_{\alpha^3} = \begin{bmatrix}0 & -1\\1 & 0\end{bmatrix} \quad\text{and}\quad \mathbf{t}_{\alpha^3} = \begin{bmatrix}-1\\0\end{bmatrix}\in\left[\begin{bmatrix}1\\0\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Then,

$$S_{\alpha^3}\left(\begin{bmatrix}2\xi\\2\eta\end{bmatrix}\right) = \begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}\begin{bmatrix}2\xi\\2\eta\end{bmatrix} + \begin{bmatrix}-1\\0\end{bmatrix} = \begin{bmatrix}-2\eta-1\\2\xi\end{bmatrix}\in\left[\begin{bmatrix}1\\0\end{bmatrix}\right]_{\mathbf{A}_0}.$$

Let us prepare to apply the symmetry reduction formula (15). Let $\mathbf{h}$ be any element of the reciprocal lattice Γ^*. Γ^* is defined as follows:

$$\Gamma^* = \mathbb{Z}^2/\mathbf{A}^T\mathbb{Z}^2 = \left\{\begin{bmatrix}x\\y\end{bmatrix} : x,y\in\{0,1,2,\ldots,2N-1\}\right\}.$$

Every such $\mathbf{h}\in\Gamma^*$ has a unique decomposition

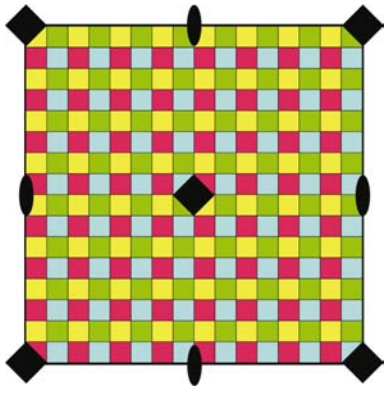

Figure 4
Example of the 2x2y subgrid decomposition for $p4$ symmetry group and for $N = 8$, that is for a 16×16 grid Γ. The asymmetric unit consists of centres of red coloured squares. Equivalently, one can choose squares of any other colour as an asymmetric unit as well.

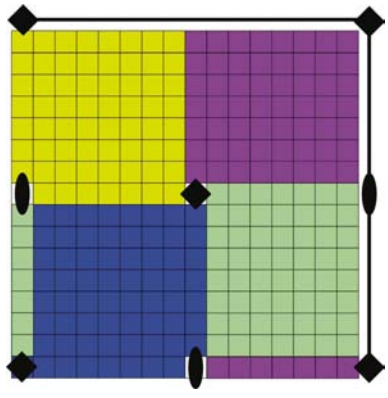

Figure 5
The FFT-asymmetric unit in the reciprocal space for $p4$ symmetry is coloured blue. The other colours denote its symmetric copies (up to the phase shift). Here we use the same symbols for symmetry elements, but actual formulae for symmetry operators in the reciprocal space differ from those in the real space by phase shifts.

$$\mathbf{h} = \mathbf{h}_1 + \begin{bmatrix} N & 0 \\ 0 & N \end{bmatrix}\mathbf{h}_0,$$

where

$$\mathbf{h}_0 \in X_0^* = \mathbb{Z}^2/\mathbf{A}_0^T\mathbb{Z}^2 = \left\{\left[\begin{bmatrix}0\\0\end{bmatrix}\right]_{\mathbf{A}_0}, \left[\begin{bmatrix}1\\0\end{bmatrix}\right]_{\mathbf{A}_0}, \left[\begin{bmatrix}0\\1\end{bmatrix}\right]_{\mathbf{A}_0}, \left[\begin{bmatrix}1\\1\end{bmatrix}\right]_{\mathbf{A}_0}\right\}$$

and

$$\mathbf{h}_1 \in X_1^* = \mathbb{Z}^2/\mathbf{A}_1^T\mathbb{Z}^2 = X_1 = \left\{\left[\begin{bmatrix}0\\0\end{bmatrix}\right]_{\mathbf{A}_1}, \left[\begin{bmatrix}0\\1\end{bmatrix}\right]_{\mathbf{A}_1}, \ldots, \left[\begin{bmatrix}N-1\\N-2\end{bmatrix}\right]_{\mathbf{A}_1}, \left[\begin{bmatrix}N-1\\N-1\end{bmatrix}\right]_{\mathbf{A}_1}\right\}.$$

Note that in this case $\mathbf{A} = \mathbf{A}^T$ and the same holds for $\mathbf{A}_0$ and $\mathbf{A}_1$. By (9), the symmetry operator in the reciprocal space S_α^* in this case is

$$\begin{aligned} S_\alpha^* F\left(\begin{bmatrix}h\\k\end{bmatrix}\right) &= e_{\mathbf{A}}\left(\begin{bmatrix}h\\k\end{bmatrix}, \begin{bmatrix}0\\-1\end{bmatrix}\right) F\left(\begin{bmatrix}0 & -1\\1 & 0\end{bmatrix}\begin{bmatrix}h\\k\end{bmatrix}\right) \\ &= \exp\left(-2\pi i\begin{bmatrix}h & k\end{bmatrix}\begin{bmatrix}1/2N & 0\\0 & 1/2N\end{bmatrix}\begin{bmatrix}0\\-1\end{bmatrix}\right) F\left(\begin{bmatrix}-k\\h\end{bmatrix}\right) \\ &= \exp\left(\frac{\pi i k}{N}\right) F\left(\begin{bmatrix}-k\\h\end{bmatrix}\right). \end{aligned}$$

Finally,

$$S_\alpha^* F(h,k) = \exp(\pi i k/N) F(-k,h). \tag{17}$$

By analogy,

$$\begin{aligned} S_\alpha^{2*} F(h,k) &= \exp[\pi i(h+k)/N] F(-h,-k) \\ S_\alpha^{3*} F(h,k) &= \exp(\pi i h/N) F(k,-h). \end{aligned}$$

The phase shifts are due to the change of the origin of the coordinate system (16). Since $S_g^* F(\mathbf{h}) = F(\mathbf{h})$ for every $g \in G$, it follows from (17) that

$$F(N,N) = -F(-N,N) = -F(N,N),$$

so

$$F(N,N) = 0.$$

Analogously, using the symmetry operator $S_{\alpha^2}^*$, one can prove that

$$F(N,0) = 0 \quad \text{and} \quad F(0,N) = 0.$$

By the Shannon interpolation formula (Shannon, 1949), values of the Fourier transform at points with modulus of $\mathbf{h}$ above a maximum resolution are not linearly independent. This phenomenon occurs for any grid choice. For our choice, it causes zeros in the points (N,N), $(N,0)$ and $(0,N)$.

A minimal set of points at which the Fourier transform must be evaluated in order to retrieve the Fourier transform in the whole unit cell will be called a *FFT-asymmetric unit* in the reciprocal space. It might seem at first glance that a good choice of a FFT-asymmetric unit in reciprocal space is X_1^*, which is dual to Γ_0, the asymmetric unit in the real space. However, from (17), it follows that

$$S_\alpha^* F(h,0) = F(0,h).$$

Therefore, since we want to have only independent data in the FFT-asymmetric unit in the reciprocal space, the good choice of such a unit will be similar to X_1^*, with points

$$\left[\begin{bmatrix}0\\1\end{bmatrix}\right]_{\mathbf{A}_1}, \left[\begin{bmatrix}0\\2\end{bmatrix}\right]_{\mathbf{A}_1}, \ldots, \left[\begin{bmatrix}0\\N-1\end{bmatrix}\right]_{\mathbf{A}_1}$$

replaced by

$$\left[\begin{bmatrix}N\\1\end{bmatrix}\right]_{\mathbf{A}_1}, \left[\begin{bmatrix}N\\2\end{bmatrix}\right]_{\mathbf{A}_1}, \ldots, \left[\begin{bmatrix}N\\N-1\end{bmatrix}\right]_{\mathbf{A}_1}.$$

The FFT-asymmetric unit in the reciprocal space is depicted in Fig. 5.

In practice, it is easier to compute Y in X_1^*, and additionally in the N above points. At the end, one can reconstruct the Fourier transform of the whole unit cell using formula (15):

$$\begin{aligned} F(\mathbf{h}_1) &= Z(\mathbf{h}_1,\mathbf{t}_e) + Z(\mathbf{h}_1,\mathbf{t}_\alpha) + Z(\mathbf{h}_1,\mathbf{t}_{\alpha^2}) + Z(\mathbf{h}_1,\mathbf{t}_{\alpha^3}), \\ F(\mathbf{h}_1 + N\mathbf{e}_1) &= Z(\mathbf{h}_1,\mathbf{t}_e) + Z(\mathbf{h}_1,\mathbf{t}_\alpha) - Z(\mathbf{h}_1,\mathbf{t}_{\alpha^2}) - Z(\mathbf{h}_1,\mathbf{t}_{\alpha^3}), \\ F(\mathbf{h}_1 + N\mathbf{e}_2) &= Z(\mathbf{h}_1,\mathbf{t}_e) - Z(\mathbf{h}_1,\mathbf{t}_\alpha) - Z(\mathbf{h}_1,\mathbf{t}_{\alpha^2}) + Z(\mathbf{h}_1,\mathbf{t}_{\alpha^3}), \\ F(\mathbf{h}_1 + N\mathbf{e}_1 + N\mathbf{e}_2) &= Z(\mathbf{h}_1,\mathbf{t}_e) - Z(\mathbf{h}_1,\mathbf{t}_\alpha) + Z(\mathbf{h}_1,\mathbf{t}_{\alpha^2}) - Z(\mathbf{h}_1,\mathbf{t}_{\alpha^3}). \end{aligned}$$

Hints and tips regarding implementation are discussed in Rowicka *et al.* (2002), where the $p3$ symmetry group is used as the example. The same decomposition as for the $p4$ group works also for all other primitive orthorhombic groups with four elements and also for some primitive four-element tetragonal groups (for details see Appendix *A*). In particular, the symmetry operators for the space group $P4$ are the same as for the plane group $p4$, if one neglects their trivial action along the z axis. Therefore, the symmetry-reduction algorithm for the $P4$ symmetry group is exactly the same as for the $p4$ symmetry and is described by

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
$P4$	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y$	2x2y

4.2. Primitive orthorhombic or tetragonal groups

All primitive orthorhombic groups with eight elements and some eight-element primitive tetragonal groups can be solved by the algorithm described below. These algorithms will be denoted by 2x2y2z in Appendix *A*

The transition to the grid coordinate system is described by

$$\mathbf{A} \quad \text{and} \quad \mathbf{b} = -\tfrac{1}{2}(\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3).$$

The matrix $\mathbf{A}$ in this case is given by

$$\mathbf{A}_{\text{orth}} = \begin{bmatrix}2N & 0 & 0\\0 & 2M & 0\\0 & 0 & 2P\end{bmatrix} \quad \text{or} \quad \mathbf{A}_{\text{tetr}} = \begin{bmatrix}2N & 0 & 0\\0 & 2N & 0\\0 & 0 & 2M\end{bmatrix},$$

where N, M and P are positive integers. The matrix $\mathbf{A}_{\text{orth}}$ is used in the case of the orthorhombic space groups and the matrix $\mathbf{A}_{\text{tetr}}$ for tetragonal ones. The asymmetric unit in both cases is described by the same matrix $\mathbf{A}_0$:

$$\mathbf{A}_0 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

The grid decomposition and the asymmetric unit is depicted in Fig. 6.

A generalization from the 2x2y algorithm to the 2x2y2z algorithm is straightforward. Basically, there is no fundamental difference between x, y and z directions in this case.

Examples of the the 2x2y2z algorithm are the *Pmmm* group, which is orthorhombic, and the $P4/m$ group, which is tetragonal:

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
Pmmm	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
$P4/m$	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y.2\|z$	2x2y2z

Since it is very similar to the 2x2y case, we can skip the detailed explanation and proceed to the $p3$ symmetry case, where new difficulties arise.

4.3. The $p3$ symmetry

This algorithm will be denoted by 3(x+y) in Appendix *A*.

In the $p3$ symmetry case, the affine transformation from the crystallographic coordinate system to the grid coordinate system is given by

$$\mathbf{A} = 3N\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = -\tfrac{1}{3}\begin{bmatrix} 2 \\ 1 \end{bmatrix},$$

where N is a positive integer. Moreover,

$$\mathbf{A}_0 = \begin{bmatrix} 0 & 1 \\ 3 & -1 \end{bmatrix} \quad \text{and} \quad \mathbf{A}_1 = \begin{bmatrix} N & N \\ 3N & 0 \end{bmatrix}.$$

The equivalence classes are defined as

$$\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0} = \left\{\mathbf{x} \in \Gamma : \mathbf{x} = \begin{bmatrix} 0 & 1 \\ 3 & -1 \end{bmatrix}\begin{bmatrix} n \\ m \end{bmatrix} = \begin{bmatrix} m \\ 3n-m \end{bmatrix},\ n, m \in \mathbb{Z}\right\}.$$

In this equivalence class are all elements from the original grid Γ, whose sum of x and y coordinates is divisible by 3. By analogy,

$$\left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0} = \left\{\mathbf{x} \in \Gamma : \mathbf{x} = \begin{bmatrix} 0 & 1 \\ 3 & -1 \end{bmatrix}\begin{bmatrix} n \\ m \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} m+1 \\ 3n-m \end{bmatrix},\ n, m \in \mathbb{Z}\right\}.$$

In this equivalence class are all elements from Γ, whose sum of x and y coordinates equals 1 modulo 3. The third equivalence class contains points whose sum of x and y coordinates equals 2 modulo 3.

In this case,

$$X_0 = \mathbb{Z}^2/\mathbf{A}_0\mathbb{Z}^2 = \left\{\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}, \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}, \left[\begin{bmatrix} 2 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}\right\}.$$

On the other hand,

$$X_1 = \mathbb{Z}^2/\mathbf{A}_1\mathbb{Z}^2 = \left\{\left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right], \left[\begin{bmatrix} 0 \\ 1 \end{bmatrix}\right], \ldots, \left[\begin{bmatrix} N-1 \\ 3N-2 \end{bmatrix}\right], \left[\begin{bmatrix} N-1 \\ 3N-1 \end{bmatrix}\right]\right\}.$$

Moreover,

$$\Gamma_0 = \mathbf{A}_0 X_1 = \left\{\begin{bmatrix} 0 & 1 \\ 3 & -1 \end{bmatrix}\begin{bmatrix} \xi \\ \eta \end{bmatrix} : \begin{bmatrix} \xi \\ \eta \end{bmatrix} \in \mathbb{Z}^2/\mathbf{A}_1\mathbb{Z}^2\right\} = \left[\begin{bmatrix} 0 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}.$$

Let the counterclockwise rotation by 120° around the origin of the crystallographic coordinate system be denoted α. Then $G = \{e, \alpha, \alpha^2\}$. The symmetry operators are given in the grid coordinates by

$$\mathbf{R}_\alpha = \begin{bmatrix} 0 & -1 \\ 1 & -1 \end{bmatrix} \quad \text{and} \quad \mathbf{t}_\alpha = \begin{bmatrix} -1 \\ 0 \end{bmatrix} \in \left[\begin{bmatrix} 2 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0} \tag{18}$$

$$\mathbf{R}_{\alpha^2} = \begin{bmatrix} -1 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{t}_{\alpha^2} = \begin{bmatrix} -1 \\ -1 \end{bmatrix} \in \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}. \tag{19}$$

Similarly, as in the case of $p4$ symmetry, one can check that

$$S_\alpha(\Gamma_0) = \left[\begin{bmatrix} 2 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0} \quad \text{and} \quad S_{\alpha^2}(\Gamma_0) = \left[\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right]_{\mathbf{A}_0}.$$

The subgrid Γ_0 (asymmetric unit) is depicted in Fig. 7 by the blue rhombi. The green rhombi symbolize elements of $S_{\alpha^2}(\Gamma_0)$, while yellow ones belong to $S_\alpha(\Gamma_0)$. The symmetry operators in

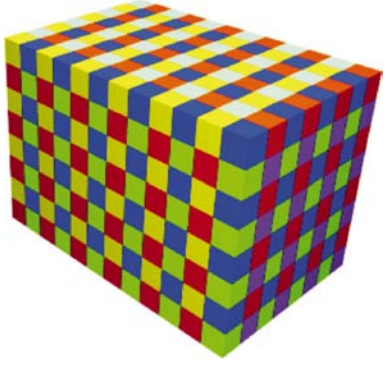

Figure 6
Example of 2x2y2z subgrid decomposition. The grid points are in the centres of the coloured cubes. A set of coloured cubes of any colour is a valid choice of an asymmetric unit.

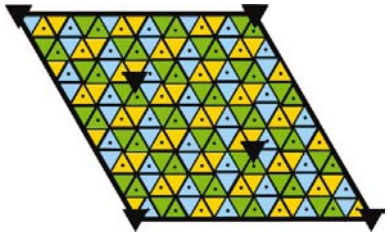

Figure 7
Subgrid decomposition for $p3$ group, for $N = 3$. The data point locations are symbolized by black dots. The asymmetric unit Γ_0 consists of data points located in blue rhombi.

Table 1
Algorithms for crystallographic FFT with one-step symmetry reduction; columns 1 and 2: crystallographic group number and symbol; column 3: number of elements; column 4: origin shift; column 5: minimal divisibility conditions for unit-cell sides; column 6: algorithm type (see §4).

ITC No.	Name	$\|G\|$	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm.
2	$P\bar{1}$	2	$(\frac{1}{2},0,0)$	$2\|x$	2x
3	$P121$	2	$(\frac{1}{2},0,0)$	$2\|x$	2x
3 alt	$P112$	2	$(\frac{1}{2},0,0)$	$2\|x$	2x
4	$P12_11$	2	$(\frac{1}{2},0,0)$	$2\|x, 2\|y$	2x
4 alt	$P112_1$	2	$(\frac{1}{2},0,0)$	$2\|x, 2\|z$	2x
6	$P1m1$	2	$(0,\frac{1}{2},0)$	$2\|y$	2y
7	$P1c1$	2	$(0,\frac{1}{2},0)$	$2\|y, 2\|z$	2y
10	$P12/m1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
11	$P12_1/m1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 4\|y$	2x2y
13	$P12/c1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
14	$P12_1/c1$	4	$(0,\frac{1}{2},\frac{1}{2})$	$4\|y, 4\|z$	2y2z
16	$P222$	4	$(0,\frac{1}{2},\frac{1}{2})$	$2\|y, 2\|z$	2y2z
17	$P222_1$	4	$(\frac{1}{2},0,\frac{1}{2})$	$2\|x, 2\|z$	2x2z
18	$P2_12_12$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 4\|y$	2x2y
18 alt	$P2_12_12a$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 2\|y$	2x2y
19	$P2_12_12_1$	4	$(\frac{1}{2},0,\frac{1}{2})$	$4\|x, 2\|y, 2\|z$	2x2z
25	$Pmm2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y$	2x2y
26	$Pmc2_1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
27	$Pcc2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
28	$Pma2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 2\|y$	2x2y
29	$Pca2_1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 2\|y, 2\|z$	2x2y
30	$Pnc2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 4\|y, 2\|z$	2x2y
31	$Pmn2_1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
32	$Pba2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 4\|y$	2x2y
33	$Pna2_1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 4\|y, 2\|z$	2x2y
34	$Pnn2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$4\|x, 4\|y, 2\|z$	2x2y
47	$Pmmm$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
48	$Pnnn$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z
49	$Pccm$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
50	$Pban$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z
51	$Pmma$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 2\|y, 2\|z$	2x2y2z
52	$Pnna$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z
53	$Pmna$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 2\|y, 4\|z$	2x2y2z
54	$Pcca$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 2\|y, 4\|z$	2x2y2z
55	$Pbam$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z
56	$Pccn$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z
57	$Pbcm$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 4\|y, 4\|z$	2x2y2z
58	$Pnnm$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z
59	$Pmmn$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
59 alt	$Pmmn2$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 2\|z$	2x2y2z
60	$Pbcn$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 2\|y, 4\|z$	2x2y2z
61	$Pbca$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z
62	$Pnma$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z
75	$P4$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y$	2x2y
76	$P4_1$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 4\|z$	2x2y
77	$P4_2$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 2\|z$	2x2y
78	$P4_3$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y, 4\|z$	2x2y
81	$P\bar{4}$	4	$(\frac{1}{2},\frac{1}{2},0)$	$2\|x, 2\|y$	2x2y
83	$P4/m$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
84	$P4_2/m$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
85	$P4/n$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
86	$P4_2/n$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
89	$P422$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
90	$P42_12$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
91	$P4_122$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 8\|z$	2x2y2z
92	$P4_12_12$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
93	$P4_222$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
94	$P4_22_12$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
94 alt	$P4_22_12a$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$4\|x, 4\|y, 4\|z$	2x2y2z
95	$P4_322$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 8\|z$	2x2y2z
96	$P4_32_12$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
115	$P\bar{4}m2$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
116	$P\bar{4}c2$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
117	$P\bar{4}b2$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 2\|z$	2x2y2z
118	$P\bar{4}n2$	8	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$2\|x, 2\|y, 4\|z$	2x2y2z
143	$P3$	3	$(\frac{2}{3},\frac{1}{3},0)$	$3\|x, 3\|y$	3(x+y)
144	$P3_1$	3	$(\frac{2}{3},\frac{1}{3},0)$	$3\|x, 3\|y, 3\|z$	3(x+y)
145	$P3_2$	3	$(\frac{2}{3},\frac{1}{3},0)$	$3\|x, 3\|y, 3\|z$	3(x+y)
149	$P312$	6	$(\frac{2}{3},\frac{1}{3},\frac{1}{2})$	$3\|x, 3\|y, 2\|z$	3(x+y) 2z
151	$P3_112$	6	$(\frac{2}{3},\frac{1}{3},\frac{1}{2})$	$3\|x, 3\|y, 6\|z$	3(x+y) 2z
153	$P3_212$	6	$(\frac{2}{3},\frac{1}{3},\frac{1}{2})$	$3\|x, 3\|y, 6\|z$	3(x+y) 2z
174	$P\bar{6}$	6	$(\frac{2}{3},\frac{1}{3},\frac{1}{2})$	$3\|x, 3\|y, 2\|z$	3(x+y) 2z

the reciprocal space are given by (9). The final symmetry-reduction formulae are the following:

$$F(\mathbf{h}_1) = Z_0(\mathbf{h}_1) + Z_1(\mathbf{h}_1) + Z_2(\mathbf{h}_1)$$
$$F(\mathbf{h}_1 + N(\mathbf{e}_1^* + \mathbf{e}_2^*)) = Z_0(\mathbf{h}_1) - \exp(\pi i/3)Z_1(\mathbf{h}_1) + \exp(2\pi i/3)Z_2(\mathbf{h}_1)$$
$$F(\mathbf{h}_1 + 2N(\mathbf{e}_1^* + \mathbf{e}_2^*)) = Z_0(\mathbf{h}_1) + \exp(2\pi i/3)Z_1(\mathbf{h}_1) - \exp(\pi i/3)Z_2(\mathbf{h}_1).$$

This algorithm is depicted in Appendix *A* as

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
$P3$	$(\frac{2}{3},\frac{1}{3},0)$	$3\|x, 3\|y$	3(x+y)

The case of the $p3$ symmetry with points in special positions will be addressed in Rowicka *et al.* (2003*b*).

4.4. The $P\bar{6}$ group

This kind of decomposition is represented in Appendix *A* as

Name	Vector $-\mathbf{b}$	Matrix $\mathbf{A}$	Algorithm
$P\bar{6}$	$(\frac{2}{3},\frac{1}{3},\frac{1}{2})$	$3\|x, 3\|y, 2\|z$	3(x+y) 2z

This may seem to be a two-step algorithm, but actually 3(x+y) 2z denotes a one-step symmetry reduction, with matrix $\mathbf{A}_0$ being the product of matrices describing 3(x+y) and 2z decompositions:

$$\mathbf{A}_0 = \begin{bmatrix} 0 & 1 & 0 \\ 3 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

We will not go into details, since they can be easily deduced from the previously described cases.

5. Discussion

We have shown how to reduce, for 67 space groups, the evaluation of the unit-cell FFT to calculating $P1$ FFT in the asymmetric unit. Thus, one can profit from a substantial effort made in developing very efficient $P1$ FFT routines (*e.g.* Frigo & Johnson, 1998; Intel, 2001).

All crystallographic groups discussed in this paper share the use of a non-standard asymmetric unit. Our asymmetric unit retains the periodicity of the unit cell, so it is automatically non-contiguous. This is not a problem as long as one performs point operations (for example multiplying electron density by a function) or convolutions (which are point operations in the reciprocal space). However, in some applications, a contiguous asymmetric unit is needed. A single permutation is then necessary to change our asymmetric unit into any contiguous

one. At the end of the Fourier transform, a reordering of data ('bit reversal'), which is also a permutation, is needed anyway. Since composition of two permutations is also a permutation, the change of the asymmetric unit may easily be incorporated into the bit reversal procedure causing no loss of efficiency.

Another possible source of problems is that the coordinate system we used has its origin shifted with respect to the traditional one. This shift is of no consequence to the application of the FFT, except for the obvious requirement that other modules use the same coordinate system. This may cause incompatibilities with some existing programs. However, conventions used in these programs have no fundamental justification and adjusting them should require only minimal changes. Moreover, in paper IV (Rowicka *et al.*, 2003*b*), we will present conceptually more complex algorithms that allow for a conventional choice of coordinate system (*i.e.* with symmetry axes going through the origin).

The symmetry-reduction formula does not provide full symmetry reduction for all space groups. Those that cannot be solved by this method fall into one of three following cases. First, the most obvious obstacle for application of this formula is non-existence of a computational grid without points in special positions. This applies, among others, to all cubic groups. The algorithms for such cases will be presented in paper IV. Second, the symmetry-reduction formula cannot be also applied to centred lattices – the asymmetric unit in such a case cannot be described by a matrix $\mathbf{A}_0$, as in (10). These cases, in which the symmetry-reduction formula leads to only partial symmetry reduction, will be completely solved in paper III (Rowicka *et al.*, 2003*a*). The third class in which we cannot apply our symmetry-reduction formula are groups containing the symmetry operators like $y, x, z + \frac{1}{2}$. Because of the translation along the z axis, they may have no points in special positions, however, this does not make dealing with the diagonal mirror operator y, x in the XY plane any easier. Cases similar to this one will be covered also in paper IV.

APPENDIX *A*
Table of algorithms

Table 1 describes the algorithms for specific crystallographic space groups. Each row starts with the ITC number and name of the group (alternative description of the same group are marked by alt). Following is the number of symmetry operators, denoted by $|G|$. It is approximately equal to the increase in speed and reduction of memory usage achieved by using our algorithms. Then we list the vectors $-\mathbf{b}$ and the matrix $\mathbf{A}$ that define the grid coordinate system by (16). For example, the symbols $2|x, 2|y, 4|z$ given as a description of matrix $\mathbf{A}$ should be understood as follows:

$$\mathbf{A} = \begin{bmatrix} 2N & 0 & 0 \\ 0 & 2M & 0 \\ 0 & 0 & 4Q \end{bmatrix},$$

where N, M and Q are arbitrary positive integers (this is for example the case of the *Pccm* group), and $N = M$ for tetragonal (for example for the $P4_222$ group) or trigonal groups.

There are various origins of requirements imposed on the entries of matrix $\mathbf{A}$. First, if our algorithm is to take every second point along x, y and z axes, we want to make sure first that the number of points along these axes is even. This requirement would lead to condition $2|x, 2|y, 2|z$. Another reason we impose additional conditions is that we want the computational grid to be invariant under the action of symmetry operators.

The last column contains a list of basic algorithms used.

Symbol explanation: 2x: regular subgrid consisting of every second point along the x axis (a very similar 2z is mentioned in §4.4). 2x2y: regular subgrid consisting of every second point along x and y axes (discussed in §4.1, depicted in Fig. 4). 2x2y2z: regular subgrid consisting of every second point along x, y and z axes (see §4.2 and Fig. 6). 3(x+y): subgrid of $x + y$ divisible by 3 (see §4.3 and Fig. 7).

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