Fourier transforms that respect crystallographic symmetries

by L. Auslander
M. Shenefelt

In crystallography one has to compute finite Fourier transforms that are often very large and often respect crystallographic symmetries. In this paper we discuss efficient finite Fourier transform algorithms on 5 × 5 × 5 points that respect a collection of crystallographic symmetries. Although the size is too small for any practical problems, the methods indicated in this paper can be extended to problems of meaningful size.

1. Introduction

Although crystallographic groups were classified about 1890 and a problem related to them occurred in the celebrated Hilbert problems at the turn of the 20th century, many mathematicians do not know these groups or why they are important. But what is probably more of a mystery to a mathematician is the title of this paper. What does it mean for a Fourier transform to respect crystallographic group symmetries, and why is it important to understand such transforms? We take a little time in this introduction to answer these questions.

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Let $R(3)$ denote the group of rigid motions of Euclidean 3-space. Then $R(3)$ contains the normal subgroup T of translations, and $R(3)$ is the semidirect product of the orthogonal group $O(3)$ and T, which we denote by $O(3) \ltimes T$. Now let **C** be a collection of labeled atoms that we think of as forming the atomic arrangements of a crystal C. We think of a crystal as being regularly repeating so that we can imagine an idealized crystal as filling 3-space. Let the subgroup **R** of $R(3)$ be the group of symmetries of **C** or the collection of rigid motions that provides a 1 to 1 correspondence between the labeled atoms of C. **R** is called the group of the crystal C, or a crystallographic group.

Let us now examine some properties of **R**. Since atoms are at a finite distance from each other, there cannot exist a subset of **R** that forms a Cauchy sequence and so **R** is a discrete subgroup of $R(3)$. Next, we come back to the concept of "regularly repeating." By this we mean that if we have a piece of a crystal, we can in our mind create a crystal to fill all of 3-space. This can be formulated by the precise hypothesis that the quotient space $R(3)/\mathbf{R}$ is compact.

We formalize this in the following definition: A crystallographic group **R** is

1. A subgroup of $R(3)$.
2. A discrete subset of $R(3)$.
3. Such that $R(3)/\mathbf{R}$ is compact.

L. Bieberbach [1] about 1910 showed that if **R** is a crystallographic group, then $\mathbf{R} \cap T = L$ is a lattice, where T is the group of translations. In other words, every crystallographic group contains 3 linearly independent translations t_1, t_2, t_3 such that

$$\mathbf{R} \cap T = \left\{ \sum_{i=1}^{3} a_i t_i \mid a_i \in Z \right\} = L.$$

Now although crystallographic groups were classified in 1891 and studied by Bieberbach, they were not used until 1919 by crystallographers. It was not until after the advent of X-ray diffraction techniques in the study of crystallography that the crystallographic groups became important. Indeed, until X-ray diffraction techniques were available, given a crystal, there was no way of determining its crystallographic group. Let us now very briefly indicate the type of information about a crystal that X-ray diffraction yields.

Consider $D(x)$, the electron density in the crystal. $D(x)$ is invariant under the crystallographic group, i.e.,

$$D(rx) = D(x), \qquad r \in \mathbf{R}.$$

Now let $L \subset \mathbf{R}$ be its lattice subgroup. Then D is L-invariant and so may be considered as either triply periodic or living on the torus T/L. As such, it has a Fourier expansion

$$D(x) = \sum_{l \in L} A_l e^{2\pi i l \cdot x},$$

where the dot denotes the dot product. Stated in its briefest form, the result of an X-ray diffraction of a crystal is the determination of the absolute value of A_l, $|A_l|$. Phase information is lost in X-ray diffraction. But what we are interested in is $D(x)$. Thus we see that the basic problem of X-ray diffraction in its simplest form is the following: Given $|A_l|$, $l \in L$, determine D. The reason this can even be solved is that not all triply periodic functions $D(x)$ can actually occur because of physical and chemical constraints.

This explains why we are concentrating our attention on computing Fourier transforms of functions that are invariant under crystallographic groups.

Now let us assume we know the crystallographic group $\mathbf{R}$ of our crystal. Then we have

$$D(rx) = D(x), \qquad r \in \mathbf{R}.$$

This implies relations among the A_l that can greatly simplify computations involved in crystallographic studies.

In order to explain the relations among the A_l, we have to look further at the structure of crystallographic groups $\mathbf{R}$. We have already seen that $\mathbf{R} \supset L$, a lattice of pure translations. Clearly, L is a normal subgroup of $\mathbf{R}$ and so we may consider the quotient group $\mathbf{R}/L = G$ or the exact sequence of groups

$$1 \rightarrow L \rightarrow \mathbf{R} \rightarrow G \rightarrow 1.$$

We call G the point group of the crystallographic group $\mathbf{R}$. It follows from the fact that $R(3)/\mathbf{R}$ is compact that G is finite. This gives us the following intrinsic characterization of crystallographic groups.

Let Z^3 denote the direct sum of 3 copies of the integers. A crystallographic group $\mathbf{R}$ is any group that satisfies the exact sequence

$$1 \rightarrow Z^3 \rightarrow \mathbf{R} \rightarrow G \rightarrow 1,$$

where G is a finite group and Z^3 is a maximal Abelian normal subgroup of $\mathbf{R}$. There is another intrinsic formulation of a crystallographic group that is also useful. Let us now look at a bit of structure that will enable us to formulate this alternative definition.

Consider the exact sequence of groups

$$1 \rightarrow \mathrm{A} \xrightarrow{i} \mathrm{B} \xrightarrow{j} \mathrm{C} \rightarrow 1,$$

where we assume A to be Abelian as well as normal. Let $\mathrm{Aut}(A)$ be the group of automorphisms of the group A. Then the above exact sequence determines a homomorphism or representation τ of C into $\mathrm{Aut}(A)$,

$$\tau : C \rightarrow \mathrm{Aut}(A),$$

as follows: For $c \in C$, let $j^{-1}(c)$ be any element b such that $j(j^{-1}(c)) = c$. Consider $j(c)A(j^{-1}(c))^{-1}$. This is an automorphism of A which will be denoted by $\tau(c)$. Since A is commutative, $\tau(c)$ is well defined.

Let $\mathbf{R}$ satisfy

$$1 \rightarrow Z^3 \rightarrow \mathbf{R} \rightarrow G \rightarrow 1,$$

with G finite and $\tau(G)$ an isomorphism. Then $\mathbf{R}$ is a crystallographic group. Since $\mathrm{Aut}(Z^3)$ can be identified with 3×3 matrices with integer entries and determinant ± 1, $GL(3, Z)$, τ provides a faithful representation of G by such matrices.

For the rest of this paper, we make some simplifying assumptions in order to expose in a reasonable amount of space the most important features of our results.

Henceforth we make the following assumptions:

1. $\mathbf{R} = G \ltimes Z^3$.
2. $\det(\tau(g)) = 1, \qquad g \in G.$

It follows that we are dealing with a very small class of crystallographic groups. Indeed, out of the possible 230 crystallographic groups, we treat only 65 explicitly. However, the general crystallographic group can be dealt with by a slight modification of the method presented here.

For this class of crystallographic groups, it is very simple to write down the relations between the Fourier coefficients. This is because of the following well-known result. Let L be a lattice in 3-space and let $D(x + l) = D(x)$, $l \in L$. Let g be a linear transformation of 3-space such that $g(L) = L$. Then, if $D(gx) = D(x)$,

$$A_l = A_{((g^{-1})^t)l}, \qquad \text{for} \quad l \in L,$$

where $(\ )^t$ denotes the transpose.

Hence we should be able to reduce the input and output of the computation of the Fourier transform by a factor that is about the order of the group G.

We are now faced with the problem of actually carrying out the computation. We do it by sampling and computing the finite Fourier transform. For sampling size $N \times N \times N$, this requires time proportional to $3N^3 \log N$. Now the above discussion shows that if r is of the order of G, then we can reduce the computation to evaluating an $(N^3/r) \times (N^3/r)$ matrix acting on N^3/r vectors. A brute force computation would require N^6/r^2 arithmetic operations compared to $3N^3 \log N$, and since N is large compared to r, the symmetry would not help. *The essential problem is to show that we can take advantage of crystallographic symmetry and still arrive at a computation for which a fast algorithm exists.*

In this paper we show how this can be done for certain toy-size problems. Recently the method has been carried out for certain realistic problems, and it is clear that it can always be done. Our basic strategy is to produce skew-circulant blocks to which Winograd's fast convolution algorithms can be applied.

2. G-invariant finite Fourier transforms

Let f be a continuous function on R^3 that is $G \ltimes L$-invariant. Then certainly f is L-invariant, and so we may view f as a continuous function on R^3/L, a three-dimensional torus. As such, it has a Fourier expansion which may be made explicit as follows: Let l_1, l_2, l_3 be a basis of L so that

$$L = \{n_1 l_1 + n_2 l_2 + n_3 l_3 \mid n_a \in Z,\ a = 1, 2, 3\},$$

and let $x = x_1 l_1 + x_2 l_2 + x_3 l_3$. As usual, we suppress the basis l_1, l_2, l_3 and write elements of L as (n_1, n_2, n_3) and elements of R^3 as (x_1, x_2, x_3). Then

$$f(x) = \sum_{l \in L} A_l \exp(2\pi i l \cdot x).$$

Let $g \in G$. Then $gL = L$. Let h be a function in $L^2(R^3/L)$ with Fourier expansion

$$h(x) = \sum_{l \in L} B_l \exp(2\pi i l \cdot x).$$

Consider the function $h(gx)$:

$$h(gx) = \sum_{l \in L} B_l \exp(2\pi i l \cdot gx)$$
$$= \sum_{l \in L} B_l \exp(2\pi i g^t l \cdot x).$$

Let $l' = g^t l$. Then $l = (g^t)^{-1} l'$, and if $g^* = (g^t)^{-1}$, then

$$h(gx) = \sum_{l' \in L} B_{g^* l} \exp(2\pi i l' \cdot x).$$

But $h(gx)$ has a Fourier series,

$$h(gx) = \sum_{l \in L} C_l \exp(2\pi i l \cdot x).$$

Hence $C_l = B_{g^* l}$, $l \in L$.

Finally, if $h(gx) = h(x)$, we have $B_l = B_{g^* l}$, for all $l \in L$ and $g^* \in G^*$. Notice that the set of elements of G^* really constitutes a group, because

$$(g_1 g_2)^* = ((g_1 g_2)^t) = (g_2^t g_1^t)^{-1} = (g_1^t)^{-1} (g_2^t)^{-1} = g_1^* g_2^*.$$

Now we replace a continuous function by a function on a finite set, so that we can use digital computers to make the computation. This is called the sampling process and introduces an error called the aliasing error. We now show how to do this while introducing a group of symmetries analogous to the crystallographic group symmetries on the finite set.

Let N be a fixed positive integer and consider the lattice $(1/N)L$,

$$(1/N)L = \{(1/N)l \mid l \in L\}.$$

Then $(1/N)L/L \approx Z/N \oplus Z/N \oplus Z/N = A \subset R^3/L$. Clearly, since G maps L onto itself and is linear, G maps $(1/N)L$ onto itself also. Thus we have a representation τ of G, G_A, by automorphisms of the group A. Our first task is to compute the kernel of τ. Let I denote the identity mapping of R^3. We claim that $g \in G$ is the kernel of τ if and only if $(g - I)$:$(1/N)L \to L$. To see this, notice that if g is in the kernel of τ, then for every $l' \in (1/N)L$, $g(l') = l' + l$, where $l \in L$. Hence $g - I$ maps $(1/N)L$ onto L. The converse is obvious.

Remark If we represent g as an integer matrix, M_g, relative to the above coordinate system, we have that g is in the kernel of τ if and only if reduction of the entries of M_g to mod N is the identity matrix.

Now let f be a continuous function that is $G \ltimes L$-invariant. Then $f\,|_A = f_S$ is well defined and f_S is easily seen to be G_A-invariant. But f_S as a function on the Abelian group A has a Fourier transform of $f\hat{}_S$. Our first task is to relate $f\hat{}_S$ to $f\hat{}$, the Fourier transform of f. Since

$$f(x) = \sum_{l \in L} A_l \exp(2\pi i l \cdot x),$$

$$f_S(a) = f(a) = \sum_{l \in L} A_l \exp(2\pi i l \cdot l'/N), \qquad a = l'/N,$$

$$= \sum_{k \in A} \left(\sum_{l \in L} A_{k+Nl} \right) \exp(2\pi i k \cdot l'/N).$$

Now let $C_k = \sum A_{k+Nl}$, $k \in A$, and view a as an element of L/NL. Then we have

$$f(a) = \sum_{k \in A} C_k \exp(2\pi i k \cdot a/N)$$

and

$$f\hat{}_S(k) = C_k = \sum_{k \in A} f(a) \exp(-2\pi i k \cdot a/N).$$

We now see the relation between the Fourier transform of f and $f\hat{}_S$. If $\sum_{l \in L} A_{k+Nl}$ approximates A_k, we may use the finite

Fourier transform to approximate the continuous Fourier transform. The error in this process is the aliasing error.

Since G_A acts on A, A is the disjoint union of G_A orbits and f is constant on each orbit. Similarly, since G_{A^*} acts on A, A is the disjoint union of G_{A^*} orbits and $f\hat{}$ is constant on G_{A^*} orbits. We now see how to use this to reduce the $N^3 \times N^3$ matrix representing the linear transformation of the Fourier transform to a smaller matrix.

From each G_A orbit choose a point a and denote the orbit containing a by $O(a)$. Denote the space of G_A orbits by X_G and view $a \in X_G$. Make a similar construction for G_{A^*} acting on A. Denote the elements of X_{G^*} by b and the orbits by $O(b)$. Then

$$f\hat{}(b) = \sum_{a \in X_G} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/N) f(a) \right), \qquad b \in X_{G^*}.$$

This linear transformation from G_A-invariant functions to G_{A^*}-invariant functions will be called the G-invariant Fourier transform on A.

3. Point groups

Although the point groups were classified a long time ago, we now list them by their intrinsic group structure. This is not done just to be elegant; we need them in this presentation to construct G_A and G_{A^*} orbits.

Let us first see that every element of G has order 2, 3, 4, or 6. Since $\tau(G)$ is faithful, $\tau(G) \in SL(3, Z)$ and $\tau(g)$ has determinant 1, the characteristic polynomial of $\tau(g)$ has integer coefficients, and (because G is finite) every element of $\tau(G)$ has at least one eigenvalue 1. Hence we know that the characteristic polynomial of $\tau(g)$ has the form

$$(x - 1)(x^2 + ax + b).$$

Because the determinant is 1, we have that $b = 1$ and

$$x^2 + ax + 1 = (x - \theta)(x + \bar{\theta}),$$

where $|\theta| = 1$. Hence $a = 2\cos\alpha$ or $a = 0, \pm 1, \pm 2$. This corresponds to rotations of $2\pi/n$, $n = 1, 2, 3, 4, 6$, or groups of order 1, 2, 3, 4, or 6.

It follows from the classification of the point groups that they are all solvable. We use this fact to organize the list of the point groups with positive determinant.

Abelian groups $Z/2$, $Z/3$, $Z/4$, $Z/6$, $Z/2 \oplus Z/2$

Let β_n, $n = 3, 4, 6$, be the automorphism of period two that takes a into $-a$ in an Abelian group. Then we form *2-step solvable groups* $\{\beta_n\} \ltimes Z/n$ and $Z/3 \ltimes (Z/2 \oplus Z/2)$, where $Z/3$ is a cyclic shift on the 3 nonzero elements of $Z/2 \oplus Z/2$.

3-Step solvable group

$$1 \rightarrow Z/2 \oplus Z/2 \rightarrow G \rightarrow P(3) \rightarrow 1,$$

where $P(3)$ is the permutation group on 3 elements. $P(3)$ satisfies

$$1 \rightarrow Z/3 \rightarrow P(3) \rightarrow Z/2 \rightarrow 1.$$

Our next task is to write out all presentations of these groups in $SL(3, Z)$ up to integer unimodular equivalence.

For Z/n, we only need to specify a matrix for a generator:

$Z/2$

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

$Z/3$

$$\begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

$Z/4$

$$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

$Z/6$

$$\begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

To represent $\{\beta_n\} \ltimes Z/n$, $n = 3, 4, 6$, we only need to represent a generator of Z/n and a matrix B_n of β_n such that

$$B_n M_n B_n^{-1} = M_n^{-1},$$

where M_n generates Z/n, $n = 3, 4, 6$. Following is the respective list of B_n for the above list of Z/n:

B_3

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}; \quad \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

B_4

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

B_6

$$\begin{pmatrix} -1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

To represent $Z/3 \ltimes (Z/2 \oplus Z/2)$, we need a representation τ for $(Z/2 \oplus Z/2)$ and a matrix B such that

$$B\tau(a)B^{-1} = \tau(b),$$

$$B\tau(b)B^{-1} = \tau(c),$$

$$B\tau(c)B^{-1} = \tau(a),$$

where 1, a, b, and c are the elements of $Z/2 \oplus Z/2$:

$$B = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}.$$

To represent the 3-step solvable group, we need representation τ of $Z/3 \ltimes (Z/2 \oplus Z/2)$ and the matrix $P(3)$ such that

$$P(3)\tau(a)P(3)^{-1} = b,$$

$$P(3)\tau(b)P(3)^{-1} = a,$$

where a and b are the elements of order 3:

$$P(3) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

When we finitize the problem to G_A, where $A = Z/N \oplus Z/N \oplus Z/N$ and N is relatively prime to 2 or 3, we have for each G only one matrix representation up to conjugation in $GL(3, Z/N)$. We always use the representation listed first in the above table. These groups are denoted as follows (we use the notation of crystallographers):

P_2; $Z/2$.

P_3; $Z/3$.

P_4; $Z/4$.

P_6; $Z/6$.

P_{222}; $Z/2 \oplus Z/2$.

P_{321}; $B_3 \ltimes Z/3$.

P_{422}; $B_4 \ltimes Z/4$.

P_{622}; $B_6 \ltimes Z/6$.

P_{322}; $B \ltimes (Z/2 \oplus Z/2)$.

P_{432}; the 3-step solvable group.

4. Examples of a G-invariant finite Fourier transform

We choose $N = 5$ and consider $A = Z/5 \oplus Z/5 \oplus Z/5$ with the automorphism group P_3 generated by

$$g = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix};$$

g is of order 3 with entries in $Z/5$ and acting on $(x, y, z) \in A$ by

$$\begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}.$$

Notice that since $Z/5$ is a field, the nonzero elements of $Z/5$ form a multiplicative cyclic group $(Z/5)^x$ of order 4. If we represent $a \in (Z/5)^x$ by

$$d{:}a \rightarrow \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix},$$

we have that $d(a)$ and g commute. [Although in practice one could use the group $(Z/5)^x \times (Z/5)^x$ to obtain a bigger group which commutes with g, we have chosen to use $(Z/5)^x$ to simplify the discussion.] Let O be a P_3 orbit. Then $d(a)O$ is a P_3 orbit, because

$$d(a)gb = gd(a)b, \qquad b \in A,$$

and so if O is the P_3 orbit determined by b, $d(a)O$ is the P_3 orbit determined by $d(a)b$. If $a \neq 1$, then $d(a)O \cap O = \varnothing$ because

$$\begin{pmatrix} ax \\ ay \\ az \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

implies that $(x, y, z)^t$ is an eigenvector of the matrix g or g^2. But the characteristic equation of g or g^2 is $x^2 + x + 1$, which has no roots modulo 5, and so neither g nor g^2 can have an eigenvector.

Hence, once we know a $(Z/5)^x$ orbit decomposition, we can use it to determine a P_3 orbit picture. See **Tables 1** and **2.**

Now, to compute

$$f^{\wedge}(b) = \sum_{a \in X_{P_3}} \left(\sum_{c \in \mathcal{O}(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \quad b \in X_{P_{3*}},$$

we can read off the elements $a \in X_{P_3}$ and $c \in O(a)$ from Table 2 of P_3 orbits and the elements $b \in X_{P_{3*}}$ from **Table 3** of P_{3*} orbits.

Consider now $\{\beta_3\} \ltimes Z/3$. Then, since B_3 normalizes $Z/3$, we have

$$B_3(gx) = g^2 B_3(x).$$

Thus B_3 of the P_3 orbit is a P_3 orbit and we have the orbit picture for $P_{321} = B_3 \ltimes P_3$ presented in **Table 4.**

Table 1 $(Z/5)^x$ orbits in $A^x = A - \{0, 0, 0\}$ (orbits are listed vertically).

001	010	011	012	013	014	100	101	102	103
003	030	033	031	034	032	300	303	301	304
004	040	044	043	042	041	400	404	403	402
002	020	022	024	021	023	200	202	204	201
104	110	111	112	113	114	120	121	122	123
302	330	333	331	334	332	310	313	311	314
401	440	444	443	442	441	430	434	433	432
203	220	222	224	221	223	240	242	244	241
124	130	131	132	133	134	140	141	142	143
312	340	343	341	344	342	320	323	321	324
431	420	424	423	422	421	410	414	413	412
243	210	212	214	211	213	230	232	234	231
144									
322									
411									
233									

Table 2 P_3 orbits in $A^\times$.

	$a \in X_{P_3}$	$O(a)$			$a \in X_{P_3}$	$O(a)$			$a \in X_{P_3}$	$O(a)$		
a	001	001			010	010	100	440	011	011	101	441
$3a$	003	003			030	030	300	220	033	033	303	221
$4a$	004	004			040	040	400	110	044	044	404	114
$2a$	002	002			020	020	200	330	022	022	202	332
a	012	012	102	442	013	013	103	443	014	014	104	444
$3a$	031	031	301	221	034	034	304	224	032	032	302	222
$4a$	043	043	403	113	042	042	402	112	041	041	401	111
$2a$	024	024	204	334	021	021	201	331	023	023	203	333
a	120	120	140	340	121	121	141	341	122	122	142	342
$3a$	310	310	320	420	313	313	323	423	311	311	321	421
$4a$	430	430	410	210	434	434	414	214	433	433	413	213
$2a$	240	240	230	130	242	242	232	132	244	244	234	134
a	123	123	143	343	124	124	144	344				
$3a$	314	314	324	424	312	312	322	422				
$4a$	432	432	412	212	431	431	411	211				
$2a$	241	241	231	131	243	243	233	133				

Table 3 P_{3^*} orbits in $A^\times$.

	$a \in X_{P_{3^*}}$	$O(a)$			$a \in X_{P_{3^*}}$	$O(a)$			$a \in X_{P_{3^*}}$	$O(a)$		
a	001	001			010	010	400	140	011	011	401	141
$3a$	003	003			030	030	200	320	033	033	203	323
$4a$	004	004			040	040	100	410	044	044	104	414
$2a$	002	002			020	020	300	230	022	022	302	232
a	012	012	402	142	013	013	403	143	014	014	404	444
$3a$	031	031	201	321	034	034	204	324	032	032	202	322
$4a$	043	043	103	413	042	042	102	412	041	041	101	411
$2a$	024	024	304	234	021	021	301	231	023	023	303	233
a	120	120	220	210	121	121	221	211	122	122	222	212
$3a$	310	310	110	130	313	313	113	133	311	311	111	131
$4a$	430	430	330	340	434	434	334	344	433	433	333	343
$2a$	240	240	440	420	242	242	442	422	244	244	444	424
a	123	123	223	213	124	124	224	214				
$3a$	314	314	114	134	312	312	112	132				
$4a$	432	432	332	342	431	431	331	341				
$2a$	241	241	441	421	243	243	443	423				

The P_{321}-invariant Fourier transform is then

$$f^\wedge(b) = \sum_{a \in X_{P_{321}}} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \quad b \in X_{P_{321^*}}.$$

As before, the elements $a \in X_{P_{321}}$ and $c \in O(a)$ are read off from Table 4 of the P_{321} orbits and $b \in X_{P_{321^*}}$ from the P_{321^*} orbits presented in **Table 5**.

Consider now the group $P_6 = Z/6$. Then, since P_3 is normal in P_6, P_6 of a P_3 orbit is again a P_3 orbit, and we have the orbit picture of P_6 presented in **Tables 6** and **7**.

The P_6-invariant Fourier transform is

$$f^\wedge(b) = \sum_{a \in X_{P_6}} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \quad b \in X_{P_{6^*}}.$$

With the orbit picture for P_6, we now consider the group $P_{622} = B_6 \ltimes P_6$. B_6 normalizes P_6, and B_6 of a P_6 orbit is again a P_6 orbit. We have the P_{622} orbit picture given in **Tables 8** and **9**.

The P_{622}-invariant Fourier transform is

$$f^\wedge(b) = \sum_{a \in X_{P_{622}}} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \quad b \in X_{P_{622^*}}.$$

5. An algorithm

Once we order X_G and X_{G^*}, we can represent the G-invariant Fourier transform as a matrix. We use the ordering or indexing suggested by the $(Z/5)^\times$ orbits in X_G and X_{G^*}: We view every $(Z/5)^\times$ orbit as ordered by a generator 3. Then by

Table 4 P_{321} orbits in A^x.

	$a \in X_{P_{321}}$	$O(a)$					
a	010	010	100	440			
$3a$	030	030	300	220			
$4a$	040	040	400	110			
$2a$	020	020	200	330			
a	011	011	101	441	104	014	444
$3a$	033	033	303	223	302	032	222
$4a$	044	044	404	114	401	041	111
$2a$	022	022	202	332	203	023	333
a	012	012	102	442	103	013	443
$3a$	031	031	301	221	304	034	224
$4a$	043	043	403	113	402	042	112
$2a$	024	024	204	334	201	021	331
a	001	001	004				
$3a$	003	003	002				
a	120	120	140	340	210	410	430
$3a$	310	310	320	420	130	230	240
a	121	121	141	341	214	414	434
$3a$	313	313	323	423	132	232	242
a	122	122	142	342	213	413	433
$3a$	311	311	321	421	134	234	244
a	123	123	143	343	212	412	432
$3a$	314	314	324	424	131	231	241
a	124	124	144	344	211	411	431
$3a$	312	312	322	422	133	233	243

Table 5 $P_{321\bullet}$ orbits in A^x.

	$a \in X_{P_{321\bullet}}$	$O(a)$					
a	120	120	220	210			
$3a$	310	310	110	130			
$4a$	430	430	330	340			
$2a$	240	240	440	420			
a	121	121	221	211	214	224	124
$3a$	313	313	113	133	132	112	312
$4a$	434	434	334	344	341	331	431
$2a$	242	242	442	422	423	443	243
a	122	122	222	212	213	223	123
$3a$	311	311	111	131	134	114	314
$4a$	433	433	333	343	342	332	432
$2a$	244	244	444	424	421	441	241
a	001	001	004				
$3a$	003	003	002				
a	010	010	400	140	100	040	410
$3a$	030	030	200	320	300	020	230
a	011	011	401	141	104	044	414
$3a$	033	033	203	323	302	022	232
a	012	012	402	142	103	043	413
$3a$	031	031	201	321	304	024	234
a	013	013	403	143	102	042	412
$3a$	034	034	204	324	301	021	231
a	014	014	404	144	101	041	411
$3a$	032	032	202	322	303	023	233

Table 6 P_6 orbits in A^x.

	$a \in X_{P_6}$	$O(a)$					
a	001	001					
$3a$	003	003					
$4a$	004	004					
$2a$	002	002					
a	011	011	101	441	401	111	041
$3a$	033	033	303	223	203	333	023
$4a$	044	044	404	114	104	444	014
$2a$	022	022	202	332	302	222	032
a	012	012	102	442	402	112	042
$3a$	031	031	301	221	201	331	021
$4a$	043	043	403	113	103	443	013
$2a$	024	024	204	334	304	224	034
a	121	121	141	341	411	211	431
$3a$	313	313	323	423	233	133	243
$4a$	434	434	414	214	144	344	124
$2a$	242	242	232	132	322	422	312
a	122	122	142	342	412	212	432
$3a$	311	311	321	421	231	131	241
$4a$	433	433	413	213	143	343	123
$2a$	244	244	234	134	324	424	314
a	010	010	100	440	400	110	040
$3a$	030	030	300	220	200	330	020
a	120	120	140	340	410	210	430
$3a$	310	310	320	420	230	130	240

Table 7 $P_{6\bullet}$ orbits in A^x.

	$a \in X_{P_{6\bullet}}$	$O(a)$					
a	001	001					
$3a$	003	003					
$4a$	004	004					
$2a$	002	002					
a	011	011	401	141	101	411	041
$3a$	033	033	203	323	303	233	023
$4a$	044	044	104	414	404	144	014
$2a$	022	022	302	232	202	322	032
a	012	012	402	142	102	412	042
$3a$	031	031	201	321	301	231	021
$4a$	043	043	103	413	403	143	013
$2a$	024	024	304	234	204	324	034
a	121	121	221	211	341	431	331
$3a$	313	313	113	133	423	243	443
$4a$	434	434	334	344	214	124	224
$2a$	242	242	442	422	132	312	112
a	122	122	222	212	342	432	332
$3a$	311	311	111	131	421	241	441
$4a$	433	433	333	343	213	123	223
$2a$	244	244	444	424	134	314	114
a	010	010	400	140	100	410	040
$3a$	030	030	200	320	300	230	020
a	120	120	220	210	340	430	330
$3a$	310	310	110	130	420	240	440

Table 8 P_{622} orbits in A^x.

	$a \in X_{P_{622}}$	$O(a)$											
a	001	001	004										
$3a$	003	003	002										
a	010	010	100	440	400	110	040						
$3a$	030	030	300	220	200	330	020						
a	011	011	101	441	401	111	041	114	404	044	104	014	444
$3a$	033	033	303	233	203	333	023	332	202	022	302	032	222
a	012	012	102	442	402	112	042	113	403	043	103	013	443
$3a$	031	031	301	221	201	331	021	334	204	024	304	034	224
a	120	120	140	340	410	210	430						
$3a$	310	310	320	420	230	130	240						
a	121	121	141	341	411	211	431	124	344	144	214	414	434
$3a$	313	313	323	423	233	133	243	412	422	322	132	232	242
a	122	122	142	342	412	212	432	123	343	143	213	413	433
$3a$	311	311	312	421	231	131	241	314	424	324	134	234	244

Table 9 P_{622^*} orbits in A^x.

	$a \in X_{P_{622^*}}$	$O(a)$											
a	001	001	004										
$3a$	003	003	002										
a	010	010	400	140	100	410	040						
$3a$	030	030	200	320	300	230	020						
a	011	011	401	141	101	411	041	014	144	404	414	104	044
$3a$	033	033	203	323	303	233	023	032	322	202	232	302	022
a	012	012	402	142	102	412	042	013	143	403	413	103	043
$3a$	031	031	201	321	301	231	021	034	324	204	234	304	024
a	120	120	220	210	340	430	330						
$3a$	310	310	110	130	420	240	440						
a	121	121	221	211	341	431	331	434	344	334	224	124	214
$3a$	313	313	113	133	423	243	443	242	422	442	112	312	132
a	122	122	222	212	342	432	332	433	343	333	223	123	213
$3a$	311	311	111	131	421	241	441	244	424	444	114	314	134

placing tails to heads of the $(Z/5)^x$ orbits, we have the indexing of X_G and X_{G^*}. The matrix we obtain this way consists of blocks corresponding to $(Z/5)^x$ orbits. Let F_G denote the matrix representation of a G-invariant Fourier transform. Then the indexed output vector $[f^\wedge(b)]$, $b \in X_{G^*}$ is obtained by the matrix multiplication

$$[F_G][f(a)]_{a \in X_G},$$

where $[f(a)]$ is the indexed input vector. Since the $(Z/5)^x$ orbits are ordered by a (multiplicative) generator, the square blocks constituting F_G are skew-circulant. Hence the square blocks can be diagonalized by multiplication by the one-dimensional finite Fourier transform on both sides. Let $S(O^*, O_i)$ be a square block corresponding to $(Z/5)^x$ orbits O^* and O_i in X_{G^*} and X_G, respectively. Then we may replace $S(O^*, O_i)$ by the diagonal matrix $D(O^*, O_i) = F(n)S(O^*, O_i)F(n)$, where $F(n)$ is the one-dimensional finite Fourier transform matrix, to compute

$$[f^\wedge(O^*)]_i = F^{-1}(n)D(O^*, O_i)(F^{-1}(n)[f(O_i)]),$$

where $[f^\wedge(O^*)]_i = S(O^*, O_i)[f(O_i)]$, and $[f(O_i)]$ is the subvector of $[f(a)]$ corresponding to the orbit O_i.

The matrix representation of the P_3-invariant Fourier transform is 44×44 and consists of 121 4×4 skew-circulant submatrices. The matrix representation of the P_{321}-invariant Fourier transform is 24×24, consisting of four 4×4 and 36 2×2 skew-circulant submatrices, 12 2×4 and 12 4×2 submatrices. The P_6-invariant Fourier transform matrix is 24 × 24, consisting of 25 4 × 4 and four 2 × 2 skew-circulant matrices, 10 2 × 4 and 10 4 × 2 matrices. The P_{622}-invariant Fourier transform matrix is 14 × 14, consisting of 49 2 × 2 skew-circulant matrices.

Now there exist Winograd fast algorithms for evaluating skew-circulant matrices. Thus, the above calculations can be done efficiently with fast algorithms.

6. Summary

In this paper we have shown that for the subset of crystallographic symmetries with no screw motions and that preserve orientation, we can, for 5 × 5 × 5 sample points, reduce the size of the problem to take advantage of the crystal symmetries and arrive at a calculation that can be done by a fast algorithm. It is clear that these or similar procedures will enable one to carry out this program for all crystallographic groups and problems of realistic sizes.

Appendix

In this appendix, we briefly discuss G-invariant finite Fourier transforms for the series of groups P_2, P_{222}, P_{23}, P_{432}, P_4, and P_{422}.

Before we give the orbit pictures of the above groups, let us observe a fact that will greatly simplify the orbit pictures. If a group G_2 contains G_1 as a normal subgroup, then we can find X_{G_2} in X_{G_1}. Hence, we only need to find the G_2 orbits in X_{G_1}.

We use the $(Z/5)^x$ orbit decomposition presented in Table 1 to write the orbit pictures. (Because $G = G^*$ for the groups G listed above, the orbit pictures for G and G^* are the same.)

Using the information in **Table 10** to order the elements in X_{P_2} by the $(Z/5)^x$ orbits, we have the matrix of the P_2-invariant Fourier transform matrix. This matrix is of size 64 × 64, consisting of 169 4 × 4 and 36 2 × 2 skew-circulant submatrices, 78 4 × 2 and 78 2 × 4 matrices.

P_{222} contains P_2 as a normal subgroup. This enables us to construct **Table 11**, the P_{222} orbits in X_{P_2}. Ordering the elements of $X_{P_{222}}$, we have the matrix of the P_{222}-invariant Fourier transform of size 34 × 34, consisting of 16 4 × 4 and 81 2 × 2 skew-circulant matrices, 36 2 × 4 and 36 4 × 2 matrices.

Let us pause for a moment to compare the matrices of the P_2-invariant Fourier transform and the P_{222}-invariant Fourier transform. The P_2-invariant Fourier transform is

$$f^{\wedge}(b) = \sum_{a \in X_{P_2}} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \qquad b \in X_{P_2},$$

where $O(a)$ denotes the P_2 orbit of a. The P_{222}-invariant

Table 10 P_2 orbits.

	$a \in X_{P_2}$	$O(a)$		$a \in X_{P_2}$	$O(a)$		$a \in X_{P_2}$	$O(a)$	
a	001	001		010	010	040	011	011	041
$3a$	003	003		030	030	020	033	033	023
$4a$	004	004					044	044	014
$2a$	002	002					022	022	032
a	012	012	042	100	100	400	101	101	401
$3a$	031	031	021	300	300	200	303	303	203
$4a$	043	043	013				404	404	104
$2a$	024	024	034				202	202	302
a	102	102	402	110	110	440	111	111	441
$3a$	301	301	201	330	330	220	333	333	223
$4a$	403	403	103				444	444	114
$2a$	204	204	304				222	222	332
a	112	112	442	120	120	430	121	121	431
$3a$	331	331	221	310	310	240	313	313	243
$4a$	443	443	113				434	434	124
$2a$	224	224	334				242	242	312
a	122	122	432	130	130	420	131	131	421
$3a$	311	311	241	340	340	210	343	343	213
$4a$	433	433	123				424	424	134
$2a$	244	244	314				212	212	342
a	132	132	422	140	140	410	141	141	411
$3a$	341	341	211	320	320	230	323	323	233
$4a$	423	423	133				414	414	144
$2a$	214	214	344				232	232	322
a	142	142	412						
$3a$	321	321	231						
$4a$	413	413	143						
$2a$	234	234	324						

Table 11 P_{222} orbits in X_{P_2}.

	$a \in X_{P_{222}}$	$O(a) \subset X_{P_2}$		$a \in X_{P_{222}}$	$O(a) \subset X_{P_2}$	
a	111	111	414	112	112	413
$3a$	333	333	232	331	331	234
$4a$	444	444	141	443	443	142
$2a$	222	222	323	224	224	321
a	121	121	424	122	122	423
$3a$	313	313	212	311	311	214
$4a$	434	434	131	433	433	132
$2a$	242	242	343	244	244	341
a	001	001	004	010	010	
$3a$	003	003	002	030	030	
a	011	011	014	012	012	013
$3a$	033	033	032	031	031	034
a	100	100		101	101	
$3a$	300	300		303	303	
a	102	403		110	110	410
$3a$	301	204		330	330	230
a	120	120	420			
$3a$	310	310	210			

Table 12 P_{322} orbits in $X_{P_{222}}$.

	$a \in X_{P_{322}}$	$O(a) \subset X_{P_{222}}$			$a \in X_{P_{322}}$	$O(a) \subset X_{P_{222}}$		
a	111	111			112	112	121	211
$3a$	333	333			331	331	313	133
$4a$	444	444			433	433	334	343
$2a$	222	222			244	244	442	242
a	001	001	010	100	011	011	110	101
$3a$	003	003	030	300	033	033	330	303
a	012	012	120	201				
$3a$	031	031	310	103				

Table 13 P_{432} orbits in $X_{P_{322}}$.

	$a \in X_{P_{432}}$	$O(a) \subset X_{P_{322}}$		$a \in X_{P_{432}}$	$O(a) \subset X_{P_{322}}$	
a	111	111	141	112	112	142
$3a$	333	333	323	331	331	321
a	001	001		011	011	101
$3a$	003	003		033	033	303
a	012	012	120			

Fourier transform is

$$f^{\wedge}(b) = \sum_{a \in X_{P_{222}}} \left(\sum_{c \in O(a)} \exp(2\pi i b \cdot c/5) f(a) \right), \qquad b \in X_{P_{222}},$$

where $O(a)$ here denotes the P_{222} orbit of a.

But the P_{222} orbit of a contains the P_2 orbit of a; i.e., part of the inner sum in (2) has been computed in (1).

Table 14 P_4 orbits in X_{P_2}.

	$a \in X_{P_4}$	$O(a) \subset X_{P_2}$		$a \in X_{P_4}$	$O(a) \subset X_{P_2}$	
a	001	001		011	011	101
$3a$	003	003		033	033	303
$4a$	004	004		044	044	404
$2a$	002	002		022	022	202
a	012	012	102	111	111	141
$3a$	031	031	301	333	333	323
$4a$	043	043	403	444	444	414
$2a$	024	024	204	222	222	232
a	112	112	142	121	121	241
$3a$	331	331	321	313	313	123
$4a$	443	443	413	434	434	314
$2a$	224	224	234	242	242	432
a	131	131	341			
$3a$	343	343	423			
$4a$	424	424	214			
$2a$	212	212	132			
a	010	010	100	330	330	320
$3a$	030	030	300	110	110	140
a	120	120	240	130	130	340

Table 15 P_{422} orbits in X_{P_4}.

	$a \in X_{P_{422}}$	$O(a) \subset X_{P_4}$		$a \in X_{P_{422}}$	$O(a) \subset X_{P_4}$	
a	121	121	134			
$3a$	313	313	342			
$4a$	434	434	421			
$2a$	242	242	213			
a	001	001	004	010	010	040
$3a$	003	003	002	030	030	020
a	011	011	044	012	012	043
$3a$	033	033	022	031	031	024
a	110	110	140	111	111	114
$3a$	330	330	320	333	333	322
a	112	112	143			
$3a$	331	331	324			
a	120	120	130			

Furthermore, $X_{P_{222}}$ is contained in X_{P_2}. This implies, in the matrix representation, that the matrix of the P_{222}-invariant Fourier transform is obtained from that of the P_2-invariant Fourier transform by crossing out the blocks of rows indexed by elements $b \notin X_{P_{222}}$, then adding the blocks of columns indexed by the elements $a \in X_{P_2}$ belonging to the same P_{222} orbits in X_{P_2}.

P_{322} contains P_{222} as a normal subgroup, and we have the P_{322} orbit picture in $X_{P_{222}}$ given in **Table 12.**

Ordering the elements by $(Z/5)^X$ orbits in $X_{P_{322}}$, we have the matrix representation of the P_{322}-invariant Fourier transform of size 14×14, consisting of four 4×4 and nine

2×2 skew-circulant matrices, six 2×4 and six 4×2 matrices. This matrix can be obtained from the matrix of the P_{222}-invariant Fourier transform.

P_{432} contains P_{322} as a normal subgroup and **Table 13** gives the P_{432} orbit picture. By this orbit picture, we have that the matrix of the P_{432}-invariant Fourier transform is 9×9, consisting of 16 2×2 skew-circulant matrices, four 1×2 and four 2×1 matrices.

P_4 contains P_2 as a normal subgroup, and we have the orbit picture of P_4 in **Table 14.** The P_4-invariant Fourier transform matrix is then 34×34, consisting of 49 4×4 and four 2×2 skew-circulant matrices, 14 2×4 and 14 4×2 matrices, 14 1×4, 14 4×1, four 1×2, four 2×1, and four 1×1 matrices.

Let us now consider $P_{422} = B_4 \ltimes P_4$. Since B_4 normalizes P_4, we have the orbit picture of P_{422} as presented in **Table 15.** The matrix of the P_{422}-invariant Fourier transform is 19×19, consisting of one 4×4 and 49 2×2 skew-circulant matrices, seven 2×4, seven 4×2, seven 1×2, seven 1×2, and one 1×1 matrix.

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Louis Auslander *City University of New York, Center for Large Scale Computation, New York, New York 10036.* Dr. Auslander is currently Distinguished Professor of Mathematics and Computer Science and Director of the Center for Large Scale Computation at the Graduate School and University Center of the City University of New York. He received his Ph.D. from the University of Chicago, Illinois, in 1954 and held academic positions at Yale University, New Haven, Connecticut, Indiana University, Bloomington, Purdue University, West Lafayette, Indiana, and the University of California, Berkeley. In addition he received a National Science Foundation postdoctoral fellowship and a Guggenheim Fellowship, both of which he spent at the Institute for Advanced Study in Princeton, New Jersey. His nonacademic experience includes periods of consultation with the Naval Research Laboratory and the IBM Thomas J. Watson Research Center, Yorktown Heights, New York.

Myoung Shenefelt *City University of New York, Graduate Center, 33 West 42nd Street, New York, New York 10036.* Ms. Shenefelt is a student at the City University of New York working on her doctoral dissertation in mathematics. She received her B.S. in mathematics in 1981 from the Polytechnic Institute of New York, Brooklyn, where she was a Teaching Fellow in mathematics. In 1982 she was an instructor in mathematics at Touro College, New York, New York. From 1983 to 1985, she taught mathematics and computer science at H. H. Lehman College, Bronx, New York. Her research interests are in finite Fourier transforms in X-ray crystallography at the Large Scale Computing Center, New York, and in the implementation of an algorithm on finite Fourier transforms with crystallographic symmetry.