1.3. FOURIER TRANSFORMS IN CRYSTALLOGRAPHY

$p - 1 = nq$. If g is a generator of the cyclic symmetry, the generator γ of $U(p)$ may be chosen in such a way that $g = \gamma^q$. The action of g is then to increment the j index in D_1 and D_2 by q, and the (j_1, j_2) index in U by (q, q). Since the data items whose indices are related in this way have identical values, the DFTs used to diagonalize the Rader cyclic convolutions will operate on *periodized data*, hence yield *decimated results*; and the non-zero results will be obtained from the unique data by DFTs n times smaller than their counterparts in the absence of symmetry.

A more thorough analysis is needed to obtain a Winograd factorization into the normal from **CBA** in the presence of symmetry (see Bricogne & Tolimieri, 1990).

Non-primitive translations and dihedral symmetry may also be accommodated within this framework, as in case 1.

This reindexing by means of algebraic integers yields larger orbits, hence more efficient algorithms, than that of Auslander *et al.* (1988) which only uses ordinary integers acting by scalar dilation.

1.3.4.3.5. *Treatment of conjugate and parity-related symmetry properties*

Most crystallographic Fourier syntheses are real-valued and originate from Hermitian-symmetric collections of Fourier coefficients. Hermitian symmetry is closely related to the action of a centre of inversion in reciprocal space, and thus interacts strongly with all other genuinely crystallographic symmetry elements of order 2. All these symmetry properties are best treated by factoring by 2 and reducing the computation of the initial transform to that of a collection of smaller transforms with less symmetry or none at all.

1.3.4.3.5.1. *Hermitian-symmetric or real-valued transforms*

The computation of a DFT with Hermitian-symmetric or real-valued data can be carried out at a cost of half that of an ordinary transform, essentially by 'multiplexing' pairs of special partial transforms into general complex transforms, and then 'demultiplexing' the results on the basis of their symmetry properties. The treatment given below is for general dimension n; a subset of cases for $n = 1$ was treated by Ten Eyck (1973).

(a) Underlying group action

Hermitian symmetry is not a geometric symmetry, but it is defined in terms of the action in reciprocal space of point group $G = \bar{1}$, *i.e.* $G = \{e, -e\}$, where e acts as $\mathbf{I}$ (the $n \times n$ identity matrix) and $-e$ acts as $-\mathbf{I}$.

This group action on $\mathbb{Z}^n / \mathbf{N}\mathbb{Z}^n$ with $\mathbf{N} = \mathbf{N}_1 \mathbf{N}_2$ will now be characterized by the calculation of the cocycle $\boldsymbol{\eta}_1$ (Section 1.3.4.3.4.1) under the assumption that $\mathbf{N}_1$ and $\mathbf{N}_2$ are both *diagonal*. For this purpose it is convenient to associate to any integer vector

$$\mathbf{v} = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \text{ in } \mathbb{Z}^n \text{ the vector } \boldsymbol{\zeta}(\mathbf{v}) \text{ whose } j\text{th component is}$$

$$\begin{cases} 0 \text{ if } & v_j = 0 \\ 1 \text{ if } & v_j \neq 0. \end{cases}$$

Let $\mathbf{m} = \mathbf{m}_1 + \mathbf{N}_1 \mathbf{m}_2$, and hence $\mathbf{h} = \mathbf{h}_2 + \mathbf{N}_2 \mathbf{h}_1$. Then

$$-\mathbf{h}_2 \bmod \mathbf{N}\mathbb{Z}^n = \mathbf{N}\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2,$$
$$-\mathbf{h}_2 \bmod \mathbf{N}_2\mathbb{Z}^n = \mathbf{N}_2\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2,$$

hence

$$\boldsymbol{\eta}_1(-e, \mathbf{h}_2) = \mathbf{N}_2^{-1}\{[\mathbf{N}\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2] - [\mathbf{N}_2\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2]\} \bmod \mathbf{N}_1\mathbb{Z}^n$$
$$= -\boldsymbol{\zeta}(\mathbf{h}_2) \bmod \mathbf{N}_1\mathbb{Z}^n.$$

Therefore $-e$ acts by

$$(\mathbf{h}_2, \mathbf{h}_1) \longmapsto [\mathbf{N}_2\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2, \mathbf{N}_1\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1 - \boldsymbol{\zeta}(\mathbf{h}_2)].$$

Hermitian symmetry is traditionally dealt with by factoring by 2, *i.e.* by assuming $\mathbf{N} = 2\mathbf{M}$. If $\mathbf{N}_2 = 2\mathbf{I}$, then each $\mathbf{h}_2$ is invariant under G, so that each partial vector $\mathbf{Z}^*_{\mathbf{h}_2}$ (Section 1.3.4.3.4.1) inherits the symmetry internally, with a 'modulation' by $\boldsymbol{\eta}_1(g, \mathbf{h}_2)$. The 'multiplexing–demultiplexing' technique provides an efficient treatment of this singular case.

(b) Calculation of structure factors

The computation may be summarized as follows:

$$\rho \overset{\mathbf{dec}(\mathbf{N}_1)}{\longmapsto} \mathbf{Y} \overset{\bar{F}(\mathbf{N}_2)}{\longmapsto} \mathbf{Y}^* \overset{\text{TW}}{\longmapsto} \mathbf{Z} \overset{\bar{F}(\mathbf{N}_1)}{\longmapsto} \mathbf{Z}^* \overset{\mathbf{rev}(\mathbf{N}_2)}{\longmapsto} \mathbf{F}$$

where $\mathbf{dec}(\mathbf{N}_1)$ is the initial decimation given by $Y_{\mathbf{m}_1}(\mathbf{m}_2) = \rho(\mathbf{m}_1 + \mathbf{N}_1\mathbf{m}_2)$, TW is the transposition and twiddle-factor stage, and $\mathbf{rev}(\mathbf{N}_2)$ is the final unscrambling by coset reversal given by $F(\mathbf{h}_2 + \mathbf{N}_2\mathbf{h}_1) = \mathbf{Z}^*_{\mathbf{h}_2}(\mathbf{h}_1)$.

(i) *Decimation in time* $(\mathbf{N}_1 = 2\mathbf{I}, \mathbf{N}_2 = \mathbf{M})$

The decimated vectors $\mathbf{Y}_{\mathbf{m}_1}$ are real and hence have Hermitian transforms $\mathbf{Y}^*_{\mathbf{m}_1}$. The 2^n values of $\mathbf{m}_1$ may be grouped into 2^{n-1} pairs $(\mathbf{m}'_1, \mathbf{m}''_1)$ and the vectors corresponding to each pair may be multiplexed into a general complex vector

$$\mathbf{Y} = \mathbf{Y}_{\mathbf{m}'_1} + i\mathbf{Y}_{\mathbf{m}''_1}.$$

The transform $\mathbf{Y}^* = \bar{F}(\mathbf{M})[\mathbf{Y}]$ can then be resolved into the separate transforms $\mathbf{Y}^*_{\mathbf{m}'_1}$ and $\mathbf{Y}^*_{\mathbf{m}''_1}$ by using the Hermitian symmetry of the latter, which yields the demultiplexing formulae

$$Y^*_{\mathbf{m}'_1}(\mathbf{h}_2) + iY^*_{\mathbf{m}''_1}(\mathbf{h}_2) = Y^*(\mathbf{h}_2)$$

$$\overline{Y^*_{\mathbf{m}'_1}(\mathbf{h}_2)} + i\overline{Y^*_{\mathbf{m}''_1}(\mathbf{h}_2)} = Y^*[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2].$$

The number of partial transforms $\bar{F}(\mathbf{M})$ is thus reduced from 2^n to 2^{n-1}. Once this separation has been achieved, the remaining steps need only be carried out for a unique half of the values of $\mathbf{h}_2$.

(ii) *Decimation in frequency* $(\mathbf{N}_1 = \mathbf{M}, \mathbf{N}_2 = 2\mathbf{I})$

Since $\mathbf{h}_2 \in \mathbb{Z}^n / 2\mathbb{Z}^n$ we have $-\mathbf{h}_2 = \mathbf{h}_2$ and $\boldsymbol{\zeta}(\mathbf{h}_2) = \mathbf{h}_2 \bmod 2\mathbb{Z}^n$. The vectors of decimated and scrambled results $\mathbf{Z}^*_{\mathbf{h}_2}$ then obey the symmetry relations

$$Z^*_{\mathbf{h}_2}(\mathbf{h}_1 - \mathbf{h}_2) = \overline{Z^*_{\mathbf{h}_2}[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1]}$$

which can be used to halve the number of $\bar{F}(\mathbf{M})$ necessary to compute them, as follows.

Having formed the vectors $\mathbf{Z}_{\mathbf{h}_2}$ given by

$$Z_{\mathbf{h}_2}(\mathbf{m}_1) = \left[\sum_{\mathbf{m}_2 \in \mathbb{Z}^n/2\mathbb{Z}^n} \frac{(-1)^{\mathbf{h}_2 \cdot \mathbf{m}_2}}{2^n} \rho(\mathbf{m}_1 + \mathbf{M}\mathbf{m}_2) \right] e[\mathbf{h}_2 \cdot (\mathbf{N}^{-1}\mathbf{m}_1)],$$

we may group the 2^n values of $\mathbf{h}_2$ into 2^{n-1} pairs $(\mathbf{h}'_2, \mathbf{h}''_2)$ and for each pair form the multiplexed vector:

$$\mathbf{Z} = \mathbf{Z}_{\mathbf{h}'_2} + i\mathbf{Z}_{\mathbf{h}''_2}.$$

After calculating the 2^{n-1} transforms $\mathbf{Z}^* = \bar{F}(\mathbf{M})[\mathbf{Z}]$, the 2^n individual transforms $\mathbf{Z}^*_{\mathbf{h}'_2}$ and $\mathbf{Z}^*_{\mathbf{h}''_2}$ can be separated by using for each pair the demultiplexing formulae

$$Z^*_{\mathbf{h}'_2}(\mathbf{h}_1) + iZ^*_{\mathbf{h}''_2}(\mathbf{h}_1) = Z^*(\mathbf{h}_1)$$

$$Z^*_{\mathbf{h}'_2}(\mathbf{h}_1 - \mathbf{h}'_2) + iZ^*_{\mathbf{h}''_2}(\mathbf{h}_1 - \mathbf{h}''_2) = \overline{Z^*[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1]}$$

which can be solved recursively. If all pairs are chosen so that they differ only in the jth coordinate $(\mathbf{h}_2)_j$, the recursion is along $(\mathbf{h}_1)_j$ and can be initiated by introducing the (real) values of $Z^*_{\mathbf{h}'_2}$ and $Z^*_{\mathbf{h}''_2}$ at $(\mathbf{h}_1)_j = 0$ and $(\mathbf{h}_1)_j = M_j$, accumulated *e.g.* while forming $\mathbf{Z}$ for that pair. Only points with $(\mathbf{h}_1)_j$ going from 0 to $\frac{1}{2}M_j$ need be resolved,

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and they contain the unique half of the Hermitian-symmetric transform $\mathbf{F}$.

(c) *Calculation of electron densities*

The computation may be summarized as follows:

$$\mathbf{F} \overset{\mathbf{scr}(\mathbf{N}_2)}{\longmapsto} \mathbf{Z}^* \overset{F(\mathbf{N}_1)}{\longmapsto} \mathbf{Z} \overset{\mathrm{TW}}{\longmapsto} \mathbf{Y}^* \overset{F(\mathbf{N}_2)}{\longmapsto} \mathbf{Y} \overset{\mathbf{nat}(\mathbf{N}_1)}{\longmapsto} \rho$$

where $\mathbf{scr}(\mathbf{N}_2)$ is the decimation with coset reversal given by $\mathbf{Z}^*_{\mathbf{h}_2}(\mathbf{h}_1) = F(\mathbf{h}_2 + \mathbf{N}_2\mathbf{h}_1)$, TW is the transposition and twiddle-factor stage, and $\mathbf{nat}(\mathbf{N}_1)$ is the recovery in natural order given by $\rho(\mathbf{m}_1 + \mathbf{N}_1\mathbf{m}_2) = Y_{\mathbf{m}_1}(\mathbf{m}_2)$.

(i) *Decimation in time* $(\mathbf{N}_1 = \mathbf{M}, \mathbf{N}_2 = 2\mathbf{I})$

The last transformation $F(2\mathbf{I})$ has a real-valued matrix, and the final result ρ is real-valued. It follows that the vectors $\mathbf{Y}^*_{\mathbf{m}_1}$ of intermediate results after the twiddle-factor stage are real-valued, hence lend themselves to multiplexing along the real and imaginary components of half as many general complex vectors.

Let the 2^n initial vectors $\mathbf{Z}^*_{\mathbf{h}_2}$ be multiplexed into 2^{n-1} vectors

$$\mathbf{Z}^* = \mathbf{Z}^*_{\mathbf{h}'_2} + i\mathbf{Z}^*_{\mathbf{h}''_2}$$

[one for each pair $(\mathbf{h}'_2, \mathbf{h}''_2)$], each of which yields by $F(\mathbf{M})$ a vector

$$\mathbf{Z} = \mathbf{Z}_{\mathbf{h}'_2} + i\mathbf{Z}_{\mathbf{h}''_2}.$$

The real-valuedness of the $\mathbf{Y}^*_{\mathbf{m}_1}$ may be used to recover the separate result vectors for $\mathbf{h}'_2$ and $\mathbf{h}''_2$. For this purpose, introduce the abbreviated notation

$$e[-\mathbf{h}'_2 \cdot (\mathbf{N}^{-1}\mathbf{m}_1)] = (c' + is')(\mathbf{m}_1)$$
$$e[-\mathbf{h}''_2 \cdot (\mathbf{N}^{-1}\mathbf{m}_1)] = (c'' + is'')(\mathbf{m}_1)$$
$$R_{\mathbf{h}_2}(\mathbf{m}_1) = Y^*_{\mathbf{m}_1}(\mathbf{h}_2)$$
$$\mathbf{R}' = \mathbf{R}_{\mathbf{h}'_2}, \quad \mathbf{R}'' = \mathbf{R}_{\mathbf{h}''_2}.$$

Then we may write

$$\mathbf{Z} = (c' + is')\mathbf{R}' + i(c'' + is'')\mathbf{R}''$$
$$= (c'\mathbf{R}' + s''\mathbf{R}'') + i(-s'\mathbf{R}' + c''\mathbf{R}'')$$

or, equivalently, for each $\mathbf{m}_1$,

$$\begin{pmatrix} \mathscr{R}e\ Z \\ \mathscr{I}m\ Z \end{pmatrix} = \begin{pmatrix} c' & s'' \\ -s' & c'' \end{pmatrix} \begin{pmatrix} R' \\ R'' \end{pmatrix}.$$

Therefore $\mathbf{R}'$ and $\mathbf{R}''$ may be retrieved from $\mathbf{Z}$ by the 'demultiplexing' formula:

$$\begin{pmatrix} R' \\ R'' \end{pmatrix} = \frac{1}{c'c'' + s's''} \begin{pmatrix} c'' & -s'' \\ s' & c' \end{pmatrix} \begin{pmatrix} \mathscr{R}e\ Z \\ \mathscr{I}m\ Z \end{pmatrix}$$

which is valid at all points $\mathbf{m}_1$ where $c'c'' + s's'' \neq 0$, *i.e.* where

$$\cos[2\pi(\mathbf{h}'_2 - \mathbf{h}''_2) \cdot (\mathbf{N}^{-1}\mathbf{m}_1)] \neq 0.$$

Demultiplexing fails when

$$(\mathbf{h}'_2 - \mathbf{h}''_2) \cdot (\mathbf{N}^{-1}\mathbf{m}_1) = \tfrac{1}{2} \text{ mod } 1.$$

If the pairs $(\mathbf{h}'_2, \mathbf{h}''_2)$ are chosen so that their members differ only in one coordinate (the jth, say), then the exceptional points are at $(\mathbf{m}_1)_j = \frac{1}{2}M_j$ and the missing transform values are easily obtained *e.g.* by accumulation while forming $\mathbf{Z}^*$.

The final stage of the calculation is then

$$\rho(\mathbf{m}_1 + \mathbf{M}\mathbf{m}_2) = \sum_{\mathbf{h}_2 \in \mathbf{Z}^n/2\mathbf{Z}^n} (-1)^{\mathbf{h}_2 \cdot \mathbf{m}_2} R_{\mathbf{h}_2}(\mathbf{m}_1).$$

(ii) *Decimation in frequency* $(\mathbf{N}_1 = 2\mathbf{I}, \mathbf{N}_2 = \mathbf{M})$

The last transformation $F(\mathbf{M})$ gives the real-valued results ρ, therefore the vectors $\mathbf{Y}^*_{\mathbf{m}_1}$ after the twiddle-factor stage each have Hermitian symmetry.

A first consequence is that the intermediate vectors $\mathbf{Z}_{\mathbf{h}_2}$ need only be computed for the unique half of the values of $\mathbf{h}_2$, the other half being related by the Hermitian symmetry of $\mathbf{Y}^*_{\mathbf{m}_1}$.

A second consequence is that the 2^n vectors $\mathbf{Y}^*_{\mathbf{m}_1}$ may be condensed into 2^{n-1} general complex vectors

$$\mathbf{Y}^* = \mathbf{Y}^*_{\mathbf{m}'_1} + i\mathbf{Y}^*_{\mathbf{m}''_1}$$

[one for each pair $(\mathbf{m}'_1, \mathbf{m}''_1)$] to which a general complex $F(\mathbf{M})$ may be applied to yield

$$\mathbf{Y} = \mathbf{Y}_{\mathbf{m}'_1} + i\mathbf{Y}_{\mathbf{m}''_1}$$

with $\mathbf{Y}_{\mathbf{m}'_1}$ and $\mathbf{Y}_{\mathbf{m}''_1}$ *real-valued.* The final results can therefore be retrieved by the particularly simple demultiplexing formulae:

$$\rho(\mathbf{m}'_1 + 2\mathbf{m}_2) = \mathscr{R}e\ Y(\mathbf{m}_2),$$
$$\rho(\mathbf{m}''_1 + 2\mathbf{m}_2) = \mathscr{I}m\ Y(\mathbf{m}_2).$$

1.3.4.3.5.2. *Hermitian-antisymmetric or pure imaginary transforms*

A vector $\mathbf{X} = \{X(\mathbf{k})|\mathbf{k} \in \mathbb{Z}^n/\mathbf{N}\mathbb{Z}^n\}$ is said to be Hermitian-antisymmetric if

$$X(\mathbf{k}) = -\overline{X(-\mathbf{k})} \text{ for all } \mathbf{k}.$$

Its transform $\mathbf{X}^*$ then satisfies

$$X^*(\mathbf{k}^*) = -\overline{X^*(\mathbf{k}^*)} \text{ for all } \mathbf{k}^*,$$

i.e. is purely imaginary.

If $\mathbf{X}$ is Hermitian-antisymmetric, then $\mathbf{F} = \pm i\mathbf{X}$ is Hermitian-symmetric, with $\rho = \pm i\mathbf{X}^*$ real-valued. The treatment of Section 1.3.4.3.5.1 may therefore be adapted, with trivial factors of i or -1, or used as such in conjunction with changes of variable by multiplication by $\pm i$.

1.3.4.3.5.3. *Complex symmetric and antisymmetric transforms*

The matrix $-\mathbf{I}$ is its own contragredient, and hence (Section 1.3.2.4.2.2) the transform of a symmetric (respectively antisymmetric) function is symmetric (respectively antisymmetric). In this case the group $G = \{e, -e\}$ acts in both real and reciprocal space as $\{\mathbf{I}, -\mathbf{I}\}$. If $\mathbf{N} = \mathbf{N}_1\mathbf{N}_2$ with both factors diagonal, then $-e$ acts by

$$(\mathbf{m}_1, \mathbf{m}_2) \longmapsto [\mathbf{N}_1\boldsymbol{\zeta}(\mathbf{m}_1) - \mathbf{m}_1, \mathbf{N}_2\boldsymbol{\zeta}(\mathbf{m}_2) - \mathbf{m}_2 - \boldsymbol{\zeta}(\mathbf{m}_1)],$$
$$(\mathbf{h}_2, \mathbf{h}_1) \longmapsto [\mathbf{N}_2\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2, \mathbf{N}_1\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1 - \boldsymbol{\zeta}(\mathbf{h}_2)],$$

i.e.

$$\boldsymbol{\mu}_2(-e, \mathbf{m}_1) = -\boldsymbol{\zeta}(\mathbf{m}_1) \text{ mod } \mathbf{N}_2\mathbb{Z}^n,$$
$$\boldsymbol{\eta}_1(-e, \mathbf{h}_2) = -\boldsymbol{\zeta}(\mathbf{h}_2) \text{ mod } \mathbf{N}_1\mathbb{Z}^n.$$

The symmetry or antisymmetry properties of $\mathbf{X}$ may be written

$$X(-\mathbf{m}) = -\varepsilon X(\mathbf{m}) \text{ for all } \mathbf{m},$$

with $\varepsilon = +1$ for symmetry and $\varepsilon = -1$ for antisymmetry.

The computation will be summarized as

$$\mathbf{X} \overset{\mathbf{dec}(\mathbf{N}_1)}{\longmapsto} \mathbf{Y} \overset{\bar{F}(\mathbf{N}_2)}{\longmapsto} \mathbf{Y}^* \overset{\mathrm{TW}}{\longmapsto} \mathbf{Z} \overset{\bar{F}(\mathbf{N}_1)}{\longmapsto} \mathbf{Z}^* \overset{\mathbf{rev}(\mathbf{N}_2)}{\longmapsto} \mathbf{X}^*$$

with the same indexing as that used for structure-factor calculation. In both cases it will be shown that a transform $F(\mathbf{N})$ with $\mathbf{N} = 2\mathbf{M}$ and $\mathbf{M}$ diagonal can be computed using only 2^{n-1} partial transforms $F(\mathbf{M})$ instead of 2^n.

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