International Tables for Crystallography (2006). Vol. B, Section 1.3.4.3.5.3, pp. 80–81.

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

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

Then we may write

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

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

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

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

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

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

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

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

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

(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:

$$\begin{aligned} \rho(\mathbf{m}'_1 + 2\mathbf{m}_2) &= \mathcal{R}e\, Y(\mathbf{m}_2), \\ \rho(\mathbf{m}''_1 + 2\mathbf{m}_2) &= \mathcal{I}m\, Y(\mathbf{m}_2). \end{aligned}$$

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

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

i.e.

$$\begin{aligned} \boldsymbol{\mu}_2(-e, \mathbf{m}_1) &= -\boldsymbol{\zeta}(\mathbf{m}_1) \bmod \mathbf{N}_2\mathbb{Z}^n, \\ \boldsymbol{\eta}_1(-e, \mathbf{h}_2) &= -\boldsymbol{\zeta}(\mathbf{h}_2) \bmod \mathbf{N}_1\mathbb{Z}^n. \end{aligned}$$

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

Since $\mathbf{m}_1 \in \mathbb{Z}^n/2\mathbb{Z}^n$ we have $-\mathbf{m}_1 = \mathbf{m}_1$ and $\boldsymbol{\zeta}(\mathbf{m}_1) = \mathbf{m}_1 \bmod 2\mathbb{Z}^n$, so that the symmetry relations for each parity class of data $\mathbf{Y}_{\mathbf{m}_1}$ read

$$Y_{\mathbf{m}_1}[\mathbf{M}\boldsymbol{\zeta}(\mathbf{m}_2) - \mathbf{m}_2 - \mathbf{m}_1] = \varepsilon Y_{\mathbf{m}_1}(\mathbf{m}_2)$$

or equivalently

$$\tau_{\mathbf{m}_1}\mathbf{Y}_{\mathbf{m}_1} = \varepsilon\breve{\mathbf{Y}}_{\mathbf{m}_1}.$$

Transforming by $F(\mathbf{M})$, this relation becomes

$$e[-\mathbf{h}_2 \cdot (\mathbf{M}^{-1}\mathbf{m}_1)]\mathbf{Y}^*_{\mathbf{m}_1} = \varepsilon\mathbf{Y}^*_{\mathbf{m}_1}.$$

Each parity class thus obeys a different symmetry relation, so that we may multiplex them in pairs by forming for each pair $(\mathbf{m}'_1, \mathbf{m}''_1)$ the vector

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

Putting

$$\begin{aligned} e[-\mathbf{h}_2 \cdot (\mathbf{M}^{-1}\mathbf{m}'_1)] &= (c' + is')(\mathbf{h}_2) \\ e[-\mathbf{h}_2 \cdot (\mathbf{M}^{-1}\mathbf{m}''_1)] &= (c'' + is'')(\mathbf{h}_2) \end{aligned}$$

we then have the demultiplexing relations for each $\mathbf{h}_2$:

$$\begin{aligned} &Y^*_{\mathbf{m}'_1}(\mathbf{h}_2) + Y^*_{\mathbf{m}''_1}(\mathbf{h}_2) = Y^*(\mathbf{h}_2) \\ &(c' + is')(\mathbf{h}_2)Y^*_{\mathbf{m}'_1}(\mathbf{h}_2) + (c'' + is'')(\mathbf{h}_2)Y^*_{\mathbf{m}''_1}(\mathbf{h}_2) \\ &\quad = \varepsilon Y^*[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_2) - \mathbf{h}_2] \end{aligned}$$

which can be solved recursively. Transform values at the exceptional points $\mathbf{h}_2$ where demultiplexing fails (*i.e.* where $c' + is' = c'' + is''$) can be accumulated while forming $\mathbf{Y}$.

Only the unique half of the values of $\mathbf{h}_2$ need to be considered at the demultiplexing stage and at the subsequent TW and $F(2\mathbf{I})$ stages.

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

The vectors of final results $\mathbf{Z}^*_{\mathbf{h}_2}$ for each parity class $\mathbf{h}_2$ obey the symmetry relations

$$\tau_{\mathbf{h}_2}\mathbf{Z}^*_{\mathbf{h}_2} = \varepsilon\breve{\mathbf{Z}}^*_{\mathbf{h}_2},$$

which are different for each $\mathbf{h}_2$. The vectors $\mathbf{Z}_{\mathbf{h}_2}$ of intermediate results after the twiddle-factor stage may then be multiplexed in pairs as

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

After transforming by $F(\mathbf{M})$, the results $\mathbf{Z}^*$ may be demultiplexed by using the relations

$$\begin{aligned} Z^*_{\mathbf{h}'_2}(\mathbf{h}_1) + Z^*_{\mathbf{h}''_2}(\mathbf{h}_1) &= Z^*(\mathbf{h}_1) \\ Z^*_{\mathbf{h}'_2}(\mathbf{h}_1 - \mathbf{h}'_2) + Z^*_{\mathbf{h}''_2}(\mathbf{h}_1 - \mathbf{h}''_2) &= \varepsilon Z^*[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1] \end{aligned}$$

which can be solved recursively as in Section 1.3.4.3.5.1(*b*)(ii).

1.3.4.3.5.4. *Real symmetric transforms*

Conjugate symmetric (Section 1.3.2.4.2.3) implies that if the data $\mathbf{X}$ are real and symmetric [*i.e.* $X(\mathbf{k}) = \overline{X(\mathbf{k})}$ and $X(-\mathbf{k}) = X(\mathbf{k})$], then so are the results $\mathbf{X}^*$. Thus if $\mathcal{p}$ contains a centre of symmetry, $\mathbf{F}$ is real symmetric. There is no distinction (other than notation) between structure-factor and electron-density calculation; the algorithms will be described in terms of the former. It will be shown that if $\mathbf{N} = 2\mathbf{M}$, a real symmetric transform can be computed with only 2^{n-2} partial transforms $F(\mathbf{M})$ instead of 2^n.

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

Since $\mathbf{m}_1 \in \mathbb{Z}^n/2\mathbb{Z}^n$ we have $-\mathbf{m}_1 = \mathbf{m}_1$ and $\boldsymbol{\zeta}(\mathbf{m}_1) = \mathbf{m}_1 \bmod 2\mathbb{Z}^n$. The decimated vectors $\mathbf{Y}_{\mathbf{m}_1}$ are not only real, but have an internal symmetry expressed by

$$\mathbf{Y}_{\mathbf{m}_1}[\mathbf{M}\boldsymbol{\zeta}(\mathbf{m}_2) - \mathbf{m}_2 - \mathbf{m}_1] = \varepsilon\mathbf{Y}_{\mathbf{m}_1}(\mathbf{m}_2).$$

This symmetry, however, is different for each $\mathbf{m}_1$ so that we may multiplex two such vectors $\mathbf{Y}_{\mathbf{m}'_1}$ and $\mathbf{Y}_{\mathbf{m}''_1}$ into a general *real* vector

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

for each of the 2^{n-1} pairs $(\mathbf{m}'_1, \mathbf{m}''_1)$. The 2^{n-1} Hermitian-symmetric transform vectors

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

can then be evaluated by the methods of Section 1.3.4.3.5.1(*b*) at the cost of only 2^{n-2} general complex $F(\mathbf{M})$.

The demultiplexing relations by which the separate vectors $\mathbf{Y}^*_{\mathbf{m}'_1}$ and $\mathbf{Y}^*_{\mathbf{m}''_1}$ may be recovered are most simply obtained by observing that the vectors $\mathbf{Z}$ after the twiddle-factor stage are real-valued since $F(2\mathbf{I})$ has a real matrix. Thus, as in Section 1.3.4.3.5.1(*c*)(i),

$$\begin{aligned} \mathbf{Y}^*_{\mathbf{m}'_1} &= (c' - is')\mathbf{R}' \\ \mathbf{Y}^*_{\mathbf{m}''_1} &= (c'' - is'')\mathbf{R}'', \end{aligned}$$

where $\mathbf{R}'$ and $\mathbf{R}''$ are real vectors and where the multipliers $(c' - is')$ and $(c'' - is'')$ are the inverse twiddle factors. Therefore,

$$\begin{aligned} \mathbf{Y}^* &= (c' - is')\mathbf{R}' + (c'' - is'')\mathbf{R}'' \\ &= (c'\mathbf{R}' + c''\mathbf{R}'') - i(s'\mathbf{R}' + s''\mathbf{R}'') \end{aligned}$$

and hence the demultiplexing relation for each $\mathbf{h}_2$:

$$\begin{pmatrix} R' \\ R'' \end{pmatrix} = \frac{1}{c's'' - s'c''}\begin{pmatrix} s'' & -c'' \\ -s' & c' \end{pmatrix}\begin{pmatrix} \mathcal{R}e\, Y^* \\ -\mathcal{I}m\, Y^* \end{pmatrix}.$$

The values of $R'_{\mathbf{h}_2}$ and $R''_{\mathbf{h}_2}$ at those points $\mathbf{h}_2$ where $c's'' - s'c'' = 0$ can be evaluated directly while forming $\mathbf{Y}$. This demultiplexing and the final stage of the calculation, namely

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

need only be carried out for the unique half of the range of $\mathbf{h}_2$.

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

Similarly, the vectors $\mathbf{Z}^*_{\mathbf{h}_2}$ of decimated and scrambled results are real and obey internal symmetries

$$\tau_{\mathbf{h}_2}\mathbf{Z}^*_{\mathbf{h}_2} = \varepsilon\breve{\mathbf{Z}}^*_{\mathbf{h}_2}$$

which are different for each $\mathbf{h}_2$. For each of the 2^{n-1} pairs $(\mathbf{h}'_2, \mathbf{h}''_2)$ the multiplexed vector

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

is a Hermitian-symmetric vector without internal symmetry, and the 2^{n-1} real vectors

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

may be evaluated at the cost of only 2^{n-2} general complex $F(\mathbf{M})$ by the methods of Section 1.3.4.3.5.1(*c*). The individual transforms $\mathbf{Z}_{\mathbf{h}'_2}$ and $\mathbf{Z}_{\mathbf{h}''_2}$ may then be retrieved *via* the demultiplexing relations

$$\begin{aligned} Z^*_{\mathbf{h}'_2}(\mathbf{h}_1) + Z^*_{\mathbf{h}''_2}(\mathbf{h}_1) &= Z^*(\mathbf{h}_1) \\ Z^*_{\mathbf{h}'_2}(\mathbf{h}_1 - \mathbf{h}'_2) + Z^*_{\mathbf{h}''_2}(\mathbf{h}_1 - \mathbf{h}''_2) &= Z^*[\mathbf{M}\boldsymbol{\zeta}(\mathbf{h}_1) - \mathbf{h}_1] \end{aligned}$$

which can be solved recursively as described in Section 1.3.4.3.5.1(*b*)(ii). This yields the unique half of the real symmetric results $\mathbf{F}$.

references