(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

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

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

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

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 $\mathcal{G}$ 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),

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

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

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

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