1. GENERAL RELATIONSHIPS AND TECHNIQUES

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

$$Z_{\mathbf{h}_2'}^*(\mathbf{h}_1) \quad + Z_{\mathbf{h}_2''}^*(\mathbf{h}_1) \qquad = Z^*(\mathbf{h}_1)$$
$$Z_{\mathbf{h}_2'}^*(\mathbf{h}_1 - \mathbf{h}_2') + Z_{\mathbf{h}_2''}^*(\mathbf{h}_1 - \mathbf{h}_2'') = \varepsilon Z^*[\mathbf{M}\zeta(\mathbf{h}_1) - \mathbf{h}_1]$$

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

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

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,

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

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

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

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

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

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

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

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

$$Z_{\mathbf{h}_2'}^*(\mathbf{h}_1) \qquad + Z_{\mathbf{h}_2''}^*(\mathbf{h}_1) \qquad = Z^*(\mathbf{h}_1)$$
$$Z_{\mathbf{h}_2'}^*(\mathbf{h}_1 - \mathbf{h}_2') + Z_{\mathbf{h}_2''}^*(\mathbf{h}_1 - \mathbf{h}_2'') = Z^*[\mathbf{M}\zeta(\mathbf{h}_1) - \mathbf{h}_1]$$

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 $\mathbf{F}$.

1.3.4.3.5.5. Real antisymmetric transforms

If $\mathbf{X}$ is real antisymmetric, then its transform $\mathbf{X}^*$ is purely imaginary and antisymmetric. The double-multiplexing techniques used for real symmetric transforms may therefore be adapted with only minor changes involving signs and factors of i.

1.3.4.3.5.6. Generalized multiplexing

So far the multiplexing technique has been applied to pairs of vectors with similar types of parity-related and/or conjugate symmetry properties, in particular the same value of ε.

It can be generalized so as to accommodate mixtures of vectors with different symmetry characteristics. For example if $\mathbf{X}_1$ is Hermitian-symmetric and $\mathbf{X}_2$ is Hermitian-antisymmetric, so that $\mathbf{X}_1^*$ is real-valued while $\mathbf{X}_2^*$ has purely imaginary values, the multiplexing process should obviously form $\mathbf{X} = \mathbf{X}_1 + \mathbf{X}_2$ (instead of $\mathbf{X} = \mathbf{X}_1 + i\mathbf{X}_2$ if both had the same type of symmetry), and demultiplexing consists in separating

$$\mathbf{X}_1^* = \mathscr{R}e\, \mathbf{X}^*$$
$$\mathbf{X}_2^* = i\mathscr{I}m\, \mathbf{X}^*.$$

references