and they contain the unique half of the Hermitian-symmetric transform **F**.

(*c*) *Calculation of electron densities*

The computation may be summarized as follows:

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

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

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

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

$$\begin{pmatrix} \mathscr{Re}\, Z \\ \mathscr{Im}\, Z \end{pmatrix} = \begin{pmatrix} c' & s'' \\ -s' & c'' \end{pmatrix} \begin{pmatrix} R' \\ R'' \end{pmatrix}.$$

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

$$\begin{pmatrix} R' \\ R'' \end{pmatrix} = \frac{1}{c'c'' + s's''} \begin{pmatrix} c'' & -s'' \\ s' & c' \end{pmatrix} \begin{pmatrix} \mathscr{Re}\, Z \\ \mathscr{Im}\, Z \end{pmatrix}$$

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:

$$\rho(\mathbf{m}'_1 + 2\mathbf{m}_2) = \mathscr{Re}\, Y(\mathbf{m}_2),$$
$$\rho(\mathbf{m}''_1 + 2\mathbf{m}_2) = \mathscr{Im}\, Y(\mathbf{m}_2).$$

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 **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.

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

The symmetry or antisymmetry properties of **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

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

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 **M** diagonal can be computed using only 2^{n-1} partial transforms $F(\mathbf{M})$ instead of 2^n.

references