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Intensities of X-ray Scattering from a One-Dimensionally Disordered Crystal Having the Multilayer Averaged Structure. Reduction of the Number of Parameters Denoting the Degree of Disorder

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In the actual interpretation of diffuse scattering of X-rays from a one-dimensionally disordered crystal by the method of Takaki & Sakurai [*Acta Cryst.* (1976), A**32**, 657–663], one of the problems is how to reduce the number of independent parameters denoting the degree of disorder. For this purpose it is assumed that J_m is real for any value of m, where J_m is the mean value of the product $F_n^*F_{n+m}$ of the structure factors of two layers separated by m interlayer spaces. Several conditions for J_m to be real are presented.

Introduction

Takaki & Sakurai (1976, hereinafter TS) have given a formula for the intensities of X-rays diffracted by a one-dimensionally disordered crystal having the 'multilayer averaged structure'; its period is p times the thickness of one layer and each layer site of the p layers is occupied by one of t layers with different structure factors.

In their treatment, the stacking mode of layers is represented in terms of probabilities of finding a particular layer after the preceding one, and hence the number of independent parameters (probabilities) increases rapidly with increasing p and/or t. Therefore, reduction of the number of independent parameters may be one important problem in applying their treatment to the analysis of diffuse scattering. The purpose of the present paper is thus to propose a procedure by which the number of independent parameters may be considerably reduced in certain cases, especially when a symmetric distribution of the diffuse intensities is observed. In this paper the same notation as in TS is used.

Preliminary ideas

The intensity formula given by TS is as follows:

$$I(\varphi)=I_L(\varphi)+I_D(\varphi) \tag{1}$$

where the first term gives the intensity of a Bragg reflexion from the 'averaged structure' with equal thickness of layers and the second term that of diffuse scattering. They are given by

$$I_L(\varphi)=NK_0+\sum_{m=1}^{N-1}(N-m)K_m\exp(-im\varphi)+\text{conj}\,. \tag{2}$$

with

$$\left.\begin{aligned}K_m&=\mathrm{Tr}\,\mathbf{VWK}^m\\ K_0&=\frac{1}{p}\sum_{j=1}^{p}|\bar F^{(j)}|^2 \text{ with } \bar F^{(j)}=\sum_{k=1}^{t}w_k^{(j)}F_k^{(j)}\end{aligned}\right\}$$

and

$$I_D(\varphi)=NR_0+\sum_{m=1}^{N-1}(N-m)R_m\exp(-im\varphi)+\text{conj}\,. \tag{3}$$

with

$$\left.\begin{aligned}R_m&=\mathrm{Tr}\,\mathbf{VWR}^m\\ R_0&=\frac{1}{p}\sum_{j=1}^{p}\sum_{k<l}^{t-1}\sum^{t}w_k^{(j)}w_l^{(j)}|F_k^{(j)}-F_l^{(j)}|^2\end{aligned}\right\}$$

where $\varphi=2\pi\xi$, ξ being a continuous variable along $\mathbf{a}^*$ (say), $F_k^{(j)}$ is the structure factor of the layer $F_k^{(j)}$ ($k=1,\ldots,t$) and $w_k^{(j)}$ the probability of finding the layer $F_k^{(j)}$ in the jth-layer site. Combining (2) and (3) we have

$$I(\varphi)=NJ_0+\sum_{m=1}^{N-1}(N-m)J_m\exp(-im\varphi)+\text{conj}\,. \tag{4}$$

with

$$\left.\begin{aligned}J_m&=K_m+R_m=\mathrm{Tr}\,\mathbf{VWP}^m\\ J_0&=\mathrm{Tr}\,\mathbf{VW}\,.\end{aligned}\right\}$$

This has already been given by Kakinoki & Komura (1965).

From the relation $\mathbf{HP}=\mathbf{PH}=\mathbf{H}$ given in the previous paper, the number of independent parameters $\alpha_{kl}^{(j)}$ is given by $p(t-1)^2$ which increases with increasing p and/or t. The proposed way of reducing the number of the parameters is as follows. On many photographs obtained from disordered crystals, one may often find that the distributions of the diffuse intensities are symmetric about $0KL$ (suppose that the diffuse streaks lie along the rows parallel to $\mathbf{a}^*$), for example, in *o*-chlorobenzamide (Takaki, Kato & Sakurai, 1975), 2-*p*-bromophenylindane-1,3-dione (Bechtel, Bravic, Gaultier & Hauw, 1974) and μ-oxo-bis[bis-(*N*-*p*-chlorophenylsalicylaldiminato)iron(III)] (Davies & Gatehouse, 1973). These distributions may be obtained, in the calculation of diffuse intensities, by introducing the condition that R_m is real for any value of m ($m=1,2,\ldots$), if the resultant $R_m(\varphi)$ is symmetric about $0KL$ (say). The independent parameters may then be reduced in general. Our next proposal is to apply tentatively the above condition to the case where an asymmetric distribution of the diffuse intensities is observed. Of course, the validity of the assumption should be examined by comparing observed and calculated intensities.

Note that, if diffuse scattering is due to displacive disorder such as seen in close-packed disordered structures, the number of independent parameters may be strongly reduced by using such an assumption that the probability of finding a layer A after B is equal to that of finding C after B and A after C when *Reichweite* = 1. In this paper we shall give several conditions for R_m to be real and show that these conditions, except for a special case, also satisfy the conditions for J_m to be real.

Conditions for R_m, K_m and J_m to be real

Let $\tilde{\mathbf{V}}$ be the complex conjugate of the matrix $\mathbf{V}$. Then R_m can be rewritten in the form

$$R_m=\tfrac{1}{2}\mathrm{Tr}(\mathbf{V}+\tilde{\mathbf{V}})\mathbf{W}\mathbf{R}^m+\tfrac{1}{2}\mathrm{Tr}(\mathbf{V}-\tilde{\mathbf{V}})\mathbf{W}\mathbf{R}^m \quad (5)$$

where the first term is the real part of R_m and the second the imaginary part. From the definition of the matrix $\mathbf{V}$ the following relation may be obtained:

$$\tilde{\mathbf{V}}=\mathbf{V}^T \quad (6)$$

where $\mathbf{V}^T$ is the transpose of $\mathbf{V}$. Using this relation we have

$$R_m=\tfrac{1}{2}\mathrm{Tr}\,\mathbf{V}[\mathbf{W}\mathbf{R}^m+(\mathbf{W}\mathbf{R}^m)^T]+\tfrac{1}{2}\mathrm{Tr}\,\mathbf{V}[\mathbf{W}\mathbf{R}^m-(\mathbf{W}\mathbf{R}^m)^T]. \quad (7)$$

The general condition for R_m to be real is then given by

$$\mathrm{Tr}\,\mathbf{V}\mathbf{W}\mathbf{R}^m=\mathrm{Tr}\,\mathbf{V}(\mathbf{W}\mathbf{R}^m)^T. \quad (8)$$

The same procedure gives the conditions for K_m and J_m to be real. They are as follows:

$$\mathrm{Tr}\,\mathbf{V}\mathbf{W}\mathbf{K}^m=\mathrm{Tr}\,\mathbf{V}(\mathbf{W}\mathbf{K}^m)^T \quad (9)$$

and

$$\mathrm{Tr}\,\mathbf{V}\mathbf{W}\mathbf{P}^m=\mathrm{Tr}\,\mathbf{V}(\mathbf{W}\mathbf{P}^m)^T. \quad (10)$$

Conditions for $p=1$

The elements of the matrices $\mathbf{V}$, $\mathbf{W}$, $\mathbf{K}$, $\mathbf{P}$ and $\mathbf{R}$ (order τ) for $p=1$ are given by $(\mathbf{V})_{kl}=F_k^*F_l$, $(\mathbf{W})_{kl}=w_l\delta_{kl}$, $(\mathbf{K})_{kl}=w_l$, $(\mathbf{P})_{kl}=\alpha_{kl}$ and $(\mathbf{R})_{kl}=\beta_{kl}$, where δ_{kl} is Kronecker's delta and $\beta_{kl}=\alpha_{kl}-w_l$. Referring to (23) and (25) of TS we have

$$K_m=|\bar{F}|^2$$

where $\bar{F}=\sum_{k=1}^{\tau} w_kF_k$. Then, from the relation $J_m=K_m+R_m$, it is evident that the conditions for R_m to be real are equivalent to those for J_m to be real. Therefore, we consider only the conditions for J_m to be real in this section.

Condition (10) may be satisfied if a relation

$$\mathbf{W}\mathbf{P}^m=(\mathbf{W}\mathbf{P}^m)^T$$

holds for any value of m. This relation is further reduced by mathematical induction to

$$\mathbf{W}\mathbf{P}=(\mathbf{W}\mathbf{P})^T \ \text{(condition } A\text{)}. \quad (11)$$

Thus, J_m is real if we choose the parameters α_{kl} so that the matrix $\mathbf{WP}$ is symmetric.

Let us show another condition for J_m to be real. Let the matrices $\mathbf{V}$, $\mathbf{W}$ and $\mathbf{P}$ be

$$\mathbf{V}=\begin{bmatrix}\mathbf{v}_{11}\cdots\mathbf{v}_{1q}\\ \vdots \quad\quad \vdots\\ \vdots \quad\quad \vdots\\ \mathbf{v}_{q1}\cdots\mathbf{v}_{qq}\end{bmatrix},\quad \mathbf{W}=\begin{bmatrix}\mathbf{w}_1 & & \\ & \ddots & \\ & & \mathbf{w}_q\end{bmatrix}\ \text{and}\ \mathbf{P}=\begin{bmatrix}\mathbf{p}_{11}\cdots\mathbf{p}_{1q}\\ \vdots \quad\quad \vdots\\ \vdots \quad\quad \vdots\\ \mathbf{p}_{q1}\cdots\mathbf{p}_{qq}\end{bmatrix} \quad (12)$$

where $\mathbf{v}_{ij}$, $\mathbf{w}_j$ and $\mathbf{p}_{ij}$ are the minor matrices of order τ. Then, introducing a matrix

$$\mathbf{n}=\begin{bmatrix} & & 1\\ & ⋰ & \\ 1 & & \end{bmatrix}_{(\tau)}, \quad (13)$$

we have the condition for J_m to be real as follows:

$$\mathbf{n}\mathbf{v}_{ij}\mathbf{n}=\tilde{\mathbf{v}}_{ij},\ \mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j\ \text{and}\ \mathbf{n}\mathbf{p}_{ij}\mathbf{n}=\mathbf{p}_{ij}\ \text{(condition } B\text{)}. \quad (14)$$

This means that $\tilde{\mathbf{v}}_{ij}$ is generated from $\mathbf{v}_{ij}$ by inversion with respect to the centre of the matrix, while $\mathbf{w}_j$ and $\mathbf{p}_{ij}$ remain unchanged under the same symmetry operation. The verification of this condition is given in Appendix I.

In a special case where the disordered structure consists of two kinds of layers A and B, the condition for R_m to be real is given by

$$\mathbf{v}_{ij}=\begin{bmatrix}A^*A\mathbf{m} & A^*B\mathbf{m}\\ B^*A\mathbf{m} & B^*B\mathbf{m}\end{bmatrix},\ \mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j\ \text{and}\ \mathbf{n}\mathbf{p}_{ij}\mathbf{n}=\mathbf{p}_{ij} \ \text{(condition } C\text{)}, \quad (15)$$

where

$$\mathbf{m}=\begin{bmatrix}1\cdots 1\\ \vdots \quad \vdots\\ 1\cdots 1\end{bmatrix}_{(\tau/2)}.$$

Condition B may be applicable to the case of a disordered close-packed structure (displacive disorder). For example, the matrices $\mathbf{V}$, $\mathbf{W}$ and $\mathbf{P}$ for both Wilson and Jagodzinski cases (see Kakinoki, 1967) satisfy condition B (for $q=1$).

Note that, if the matrix $\mathbf{P}$ in (12) is replaced by

$$\mathbf{P}=\begin{bmatrix} & \mathbf{p}_2 & & \\ & & \mathbf{p}_3 & \\ & & & \ddots\ \mathbf{p}_q\\ \mathbf{p}_1 & & & \end{bmatrix},$$

conditions B and C may be rewritten:

$$\mathbf{n}\mathbf{v}_{ij}\mathbf{n}=\tilde{\mathbf{v}}_{ij},\ \mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j \text{ and } \mathbf{n}\mathbf{p}_j\mathbf{n}=\mathbf{p}_j \quad (\text{condition } D) \quad (16)$$

and

$$\mathbf{v}_{ij}=\begin{bmatrix} A^*A\mathbf{m} & A^*B\mathbf{m} \\ B^*A\mathbf{m} & B^*B\mathbf{m}\end{bmatrix},\ \mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j \text{ and } \mathbf{n}\mathbf{p}_j\mathbf{n}=\mathbf{p}_j \quad (\text{condition } E) \quad (17)$$

respectively. These conditions correspond to those for J_m to be real for $p\geq 2$.

Conditions for $p\geq 2$

TS have given R_m in the form

$$R_m=\mathrm{Tr}\ \mathbf{VWR}^m = \frac{1}{p}\sum_{j=1}^{p}\mathrm{Tr}\ \mathbf{v}_{j+m,j}\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m} \quad (18)$$

where $\mathbf{v}_{ij}$, $\mathbf{w}_j$ and $\mathbf{r}_j$ are minor matrices of order t and have elements $(\mathbf{v}_{ij})_{kl}=F_k^{*(i)}F_l^{(j)}$, $(\mathbf{w}_j)_{kl}=w_l^{(j)}$ and $(\mathbf{r}_j)_{kl}=\beta_{kl}^{(j)}$ respectively. From the definition of $\mathbf{v}_{ij}$ we obtain

$$\tilde{\mathbf{v}}_{ij}=\mathbf{v}_{ji}^T. \quad (19)$$

Using this relation and remembering the relation $\tilde{\mathbf{V}}=\mathbf{V}^T$ we have

$$\mathrm{Tr}\ \mathbf{V}(\mathbf{WR}^m)^T=\mathrm{Tr}\ \tilde{\mathbf{V}}\mathbf{WR}^m = \frac{1}{p}\sum_{j=1}^{p}\mathrm{Tr}\ \mathbf{v}_{j,j+m}(\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m})^T. \quad (20)$$

Comparing (20) with (18) we find that condition (8) can be reduced to

$$\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m}=(\mathbf{w}\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m})^T, \quad (21)$$

if a relation

$$\mathbf{v}_{ij}=\mathbf{v}_{ji} \quad (22)$$

exists.

Referring to the above relations we found, after some trials, that the following conditions satisfy the requirement for R_m to be real:

condition F:

$$t\geq 3;\ \mathbf{v}_{ij}=\mathbf{v}_{ji},\ \mathbf{w}_j=\mathbf{w},\ \mathbf{w}\mathbf{r}_j=(\mathbf{w}\mathbf{r}_j)^T \text{ and } \mathbf{r}_i\mathbf{r}_j=\mathbf{r}_j\mathbf{r}_i. \quad (23a)$$

$$t=2;\quad \mathbf{v}_{ij}=\mathbf{v}_{ji}; \quad (23b)$$

condition G:

$$\mathbf{v}_{ij}=\mathbf{v}_{g+1-i,g+1-j},\ \mathbf{w}_j=\mathbf{w}_{g+1-j}$$

and

$$\mathbf{w}_j\mathbf{r}_{j+1}=(\mathbf{w}_{g-j}\mathbf{r}_{g+1-j})^T \quad (24)$$

where g is an integer ($p\geq g\geq 1$), and $\mathbf{v}_{i+p,j+p}=\mathbf{v}_{ij}$, $\mathbf{w}_{j+p}=\mathbf{w}_j$ and $\mathbf{r}_{j+p}=\mathbf{r}_j$. The verifications of conditions F and G are given in Appendix II.

Similarly, we examined the conditions for K_m to be real and found that these were contained in conditions (23*a*) and (24); regarding (23*b*) K_m is real only in a special case as shown below. Other conditions for K_m to be real are as follows:

condition H:

$$t\geq 2;\quad \mathbf{v}_{ij}=\mathbf{v}_{ji} \text{ and } \mathbf{w}_j=\mathbf{w}; \quad (25a)$$

$$t=2;\quad \mathbf{v}_{ij}=(-1)^{n(i+j)}\mathbf{v}\quad (n=0 \text{ or } 1); \quad (25b)$$

condition I:

$$\mathbf{v}_{ij}=\mathbf{v}_{g+1-i,g+1-j} \text{ and } \mathbf{w}_j=\mathbf{w}_{g+1-j}. \quad (26)$$

The verification of condition (25*b*) is given in Appendix II.

Comparing the conditions for R_m and K_m to be real given above and remembering $J_m=K_m+R_m$, we have the following conditions for J_m to be real:

condition J:

$$t\geq 2;\ \mathbf{v}_{ij}=\mathbf{v}_{ji},\ \mathbf{w}_j=\mathbf{w},\ \mathbf{w}\mathbf{p}_j=(\mathbf{w}\mathbf{p}_j)^T \text{ and } \mathbf{p}_i\mathbf{p}_j=\mathbf{p}_j\mathbf{p}_i. \quad (27a)$$

$$t=2;\quad \mathbf{v}_{ij}=(-1)^{n(i+j)}\mathbf{v}\quad (n=0 \text{ or } 1); \quad (27b)$$

condition K:

$$\mathbf{v}_{ij}=\mathbf{v}_{g+1-i,g+1-j},\ \mathbf{w}_j=\mathbf{w}_{g+1-j}$$

and

$$\mathbf{w}_j\mathbf{p}_{j+1}=(\mathbf{w}_{g-j}\mathbf{p}_{g+1-j})^T \quad (28)$$

where $(\mathbf{p}_j)_{kl}=\alpha_{kl}^{(j)}$.

Concluding remarks

From the above results we propose the following procedures. [It is of course necessary that the parameters w_k ($p=1$) or $w_k^{(j)}$ ($p\geq 2$) are known.]

(1) *For* $p=1$. Choose the parameters α_{kl} so that the matrix $\mathbf{WP}$ is symmetric (condition A). Particularly, if the conditions $\mathbf{n}\mathbf{v}_{ij}\mathbf{n}=\tilde{\mathbf{v}}_{ij}$ $\left(\text{or } \mathbf{v}_{ij}=\begin{bmatrix} A^*A\mathbf{m} & A^*B\mathbf{m} \\ B^*A\mathbf{m} & B^*B\mathbf{m}\end{bmatrix}\right)$ and $\mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j$ are satisfied, choose the parameters so as to satisfy the condition $\mathbf{n}\mathbf{p}_{ij}\mathbf{n}=\mathbf{p}_{ij}$ (conditions B and C).

For $p\geq 2$. If the conditions $\mathbf{n}\mathbf{v}_{ij}\mathbf{n}=\tilde{\mathbf{v}}_{ij}$ $\left(\text{or } \mathbf{v}_{ij}=\begin{bmatrix} A^*A\mathbf{m} & A^*B\mathbf{m} \\ B^*B\mathbf{m} & B^*B\mathbf{m}\end{bmatrix}\right)$ and $\mathbf{n}\mathbf{w}_j\mathbf{n}=\mathbf{w}_j$ are satisfied, choose the parameters $\alpha_{kl}^{(j)}$ so as to satisfy the condition $\mathbf{n}\mathbf{p}_j\mathbf{n}=\mathbf{p}_j$ (conditions D and E). If any of the conditions for K_m to be real (conditions H and I) is satisfied, choose the parameters so as to satisfy the corresponding conditions for J_m to be real (conditions J and K). Note that when only (25*b*) is satisfied, the number of independent parameters cannot be reduced because there is no condition concerning $\alpha_{kl}^{(j)}$ in (27*b*).

(2) Examine the validity of the assumption that J_m is real by comparing observed and calculated intensities.

A typical example is seen in the disordered structures, γ and δ forms, of *o*-chlorobenzamide (Takaki, Kato & Sakurai, 1975) which have been solved by the method given by TS; the number of independent parameters is two in the γ form ($p=2$ and $t=2$) and four in the δ form ($p=4$ and $t=2$). It is very interesting that the resultant parameters of the γ form satisfy condition K with $g=1$, and similarly those of the δ form satisfy condition K with $g=3$. These results show that the number of independent parameters would be reduced to one for the γ form and to two for the δ form if the above procedure was applied.

Another example is seen in the disordered structure of CdI_2 (Minagawa, 1977) which has also been solved by the procedure given by TS with two independent parameters ($p=2$ and $t=2$). It is seen that in this case also condition K with $g=1$ is almost satisfied.

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APPENDIX I

Verification of condition B

Let us introduce a matrix

$$\mathbf{N}=\begin{bmatrix} \mathbf{n} & & \\ & \ddots & \\ & & \mathbf{n} \end{bmatrix}_{(q)} \qquad (29)$$

with the minor matrix $\mathbf{n}$ defined by (13). Since $\mathbf{nn}=1$ (unit matrix of order τ) and accordingly $\mathbf{NN}=\mathbf{E}$ (unit matrix of order $q\tau$), J_m can be rewritten as

$$J_m=\mathrm{Tr}\ \mathbf{NVNNWN}(\mathbf{NPN})^m .$$

From condition B we have

$$\mathbf{NVN}=\tilde{\mathbf{V}},\ \mathbf{NWN}=\mathbf{W}\ \text{ and }\ \mathbf{NPN}=\mathbf{P} .$$

Therefore

$$J_m=\mathrm{Tr}\ \tilde{\mathbf{V}}\mathbf{WP}^m=J_m^* .$$

Hence J_m is real if condition B is satisfied.

APPENDIX II

Verification of condition F

For $t\geq 3$

Using the relation in (23*b*) we have

$$\begin{aligned}\mathbf{wr}_{j+1}\ldots\mathbf{r}_{j+m}&=(\mathbf{r}_{j+1})^T\mathbf{wr}_{j+2}\ldots\mathbf{r}_{j+m}\\&=(\mathbf{r}_{j+1}\mathbf{r}_{j+2})^T\mathbf{wr}_{j+3}\ldots\mathbf{r}_{j+m}\\&\ldots\ldots\ldots\ldots\ldots\\&=(\mathbf{wr}_{j+1}\ldots\mathbf{r}_{j+m})^T .\end{aligned}$$

Hence condition (21) is satisfied, *i.e.* R_m is real.

For $t=2$

Using (36) of TS we have

$$\begin{aligned}\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m}&=w_1^{(j)}w_2^{(j)}\begin{bmatrix}1 & -1\\ -1 & 1\end{bmatrix}\prod_{v=1}^{m}(\alpha_{11}^{(j+v)}-\alpha_{21}^{(j+v)})\\&=(\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m})^T .\end{aligned}$$

Hence condition (21) is satisfied, *i.e.* R_m is real.

Verification of condition G

Using the relations in (24) we have

$$\begin{aligned}\mathbf{w}_j\mathbf{r}_{j+1}\ldots\mathbf{r}_{j+m}&=(\mathbf{r}_{g+1-j})^T\mathbf{w}_{j+1}\mathbf{r}_{j+2}\ldots\mathbf{r}_{j+m}\\&=(\mathbf{r}_{g+1-j-1}\mathbf{r}_{g+1-j})^T\mathbf{w}_{j+2}\mathbf{r}_{j+3}\ldots\mathbf{r}_{j+m}\\&\ldots\ldots\ldots\ldots\ldots\\&=(\mathbf{w}_{g+1-j-m}\mathbf{r}_{g+1-j-m+1}\ldots\mathbf{r}_{g+1-j})^T . \quad (30)\end{aligned}$$

Substitution into (20) gives

$$\mathrm{Tr}\ \mathbf{V}(\mathbf{WR}^m)^T =\frac{1}{p}\sum_{j=1}^{p}\mathrm{Tr}\ \mathbf{v}_{j,\,j+m}\mathbf{w}_{g+1-j-m}\mathbf{r}_{g+1-j-m+1}\ldots\mathbf{r}_{g+1-j} .$$

Putting $\varrho=g+1-j-m$ or $j=g+1-m-\varrho$ and using the relations in (24) we have

$$\begin{aligned}\mathrm{Tr}\ \mathbf{V}(\mathbf{WR}^m)^T &=\frac{1}{p}\sum_{\varrho=g-m}^{g-m+1-p}\mathrm{Tr}\ \mathbf{v}_{g+1-m-\varrho,\,g+1-\varrho}\mathbf{w}_\varrho\mathbf{r}_{\varrho+1}\ldots\mathbf{r}_{\varrho+m}\\&=\frac{1}{p}\sum_{\varrho=1}^{p}\mathrm{Tr}\ \mathbf{v}_{\varrho+m,\,\varrho}\mathbf{w}_\varrho\mathbf{r}_{\varrho+1}\ldots\mathbf{r}_{\varrho+m}\\&=\mathrm{Tr}\ \mathbf{VWR}^m .\end{aligned}$$

Hence condition (8) is satisfied.

Verification of condition (25*b*)

K_m can be written in the form (TS)

$$K_m=\frac{1}{p}\sum_{j=1}^{p}\mathrm{Tr}\ \mathbf{v}_{j+m,\,j}\mathbf{w}_j\mathbf{h}_{j+m}$$

where $(\mathbf{h}_{j+m})_{kl}=w_l^{(j+m)}$. Using relations in (25*b*) we have

$$K_m=\frac{1}{p}(-1)^{nm}\mathrm{Tr}\ \mathbf{v}\sum_{j=1}^{p}\mathbf{w}_j\mathbf{h}_{j+m}$$

where $(\mathbf{v})_{kl}=F_k^*F_l$. Subtracting K_m^* we have

$$\begin{aligned}K_m-K_m^*&=\frac{1}{p}(-1)^{nm}\mathrm{Tr}(\mathbf{v}-\tilde{\mathbf{v}})\sum_{j=1}^{p}\mathbf{w}_j\mathbf{h}_{j+m}\\&=\frac{1}{p}(-1)^{nm}(F_1^*F_2-F_2^*F_1)\sum_{j=1}^{p}[w_1^{(j+m)}-w_1^{(j)}]\\&=0 .\end{aligned}$$

Hence K_m is real.

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