$$\eta_{1,2n+1}-\eta_{2,2n+1}=-\frac{\gamma_0}{\gamma_g}\frac{\gamma_g''}{\gamma_0''}\left(\frac{\gamma_0'}{\gamma_g'}\frac{\gamma_g''}{\gamma_0''}\right)^n x_{0,2n+1}\,. \quad (B9d)$$

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The One-Dimensional Anti-phase Domain Structures. II. Refinement of Fujiwara's Method of the Analysis of the Structure with a Non-integral Value for the Half Period, $\tilde{M}$

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One-dimensional anti-phase domain structures with an out-of-step vector $\mathbf{u}=(\mathbf{a}+\mathbf{b})/2$ sometimes have half periods of non-integral value. Fujiwara interpreted this structure as a disordered structure (a *statistical assembly*) deviating from a *standard structure* which he defined by a step function. In the present paper, it is pointed out that the unitary intensity of a superlattice reflexion for the standard structure is obtained in a much simpler form than that given by Fujiwara. By the use of this intensity formula we verify the fact that a pair of intensities with special l-indices, ν and $-\nu$, is very strong while the others are extremely weak, so that we apparently obtain a non-integral value for the half period from the strongest pair. The statistical assembly, *i.e.* the disordered structure presented by Fujiwara, is interpreted using an easily understandable model, and a simple form of the corresponding intensity formula is obtained, which indicates that the intensities other than the pair, $\bar{I}_\nu$ and $\bar{I}_{\bar{\nu}}$, practically vanish. This fact implies that the non-integral half period, $\tilde{M}$, may be obtained experimentally from a pair of satellites corresponding to $\bar{I}_\nu$ and $\bar{I}_{\bar{\nu}}$. Some important remarks are made in the Appendix concerning the Fourier expansion of the step function.

1. Introduction

In part I of this series (Kakinoki & Minagawa, 1971) the one-dimensional anti-phase domain structures, with an out-of-step vector $\mathbf{u}=(\mathbf{a}+\mathbf{b})/2$ and the corresponding phase factor $\varepsilon=(-1)^{h+k}$, were classified into three kinds, and they were denoted by the layer sequence symbols which are similar to the Zhdanov symbol for the close-packed structures, as follows:

(1) the complex out-of-step structure, denoted by

$$(a_1\bar{b}_1a_2\bar{b}_2\ldots a_t\bar{b}_t) \text{ with } P=\sum_{i=1}^{t}(a_i+b_i)\,,$$

(2) the complex *APD* (anti-phase domain) structure, denoted by

$$([M]|[\bar{M}]) \text{ with } [M]=(a_1\bar{b}_1a_2\bar{b}_2\ldots a_s\bar{b}_sa_{s+1})$$

and

$$P/2=M=\sum_{i=1}^{s+1}a_i+\sum_{i=1}^{s}b_i\,,$$

(3) the simple *APD* structure, denoted by

$$(M|\bar{M}) \text{ with } P=2M,$$

where P is the period and a_i and b_i are the numbers of successive positive and negative layers respectively, where the positive and negative layers indicate the layers without and with the out-of-step vector, as shown in Fig. 1. The vertical and horizontal short lines in the symbols $([M]|[\bar{M}])$ and $(M|\bar{M})$ mean that the last M layers are obtained by changing all the signs of the corresponding layers of the first M layers.

The unitary intensities of superlattice reflexions in the case of simple APD structure are given by†

$$\left.\begin{array}{l}\left\{\begin{array}{ll}I_l=0 & \text{for } l\text{: even}\\ I_l=4I_l^* & \text{for } l\text{: odd}\end{array}\right.\\ \text{with}\quad I_l^*=\dfrac{1}{\sin^2\dfrac{\pi l}{P}}\ .\end{array}\right\} \quad (1)$$

† Refer to equations (I.16), (I.18) and (I.19). In order to avoid confusion, the equation number in part I of this series is written as (I.1), (I.2) *etc.*, and that in Fujiwara's (1957) paper as (F1), (F2) *etc.*

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For example, I_l's for $M=6$ are as schematically shown in Fig. 2. In this case, the half period, M, is given by

$$M=\frac{AB}{CD} \tag{2}$$

where CD is the separation between $l=-1$ and 1 corresponding to a pair of the strongest intensities, and AB is that between $l=0$ and $l=P$.

In many peculiar cases, however, it happens that the values of M obtained from equation (2) are not integers, as found in some examples listed in Table 1. Such a non-integral value of the half period is here denoted by $\tilde{M}$ in order to distinguish it from integral M.

Table 1. *Examples of the alloys with non-integral values for the half period,* $\tilde{M}$

	$\tilde{M}$	Reference
Ag_3Mg	$1{\cdot}77\sim 2{\cdot}0$	(*a*), (*b*)
Cu_3AuII	$8\sim 10$	(*c*), (*d*), (*e*)
Cu_3Pt	$6\sim 8$	(*a*)
$Cu_{3+}Pd$	$7\sim 11$	(*a*), (*f*), (*g*)
CuAuII	$5\sim 6$	(*h*), (*i*)

(*a*) : Schubert, Kiefer, Wilkens & Haufler (1955).
(*b*) : Fujiwara, Hirabayashi, Watanabe & Ogawa (1958).
(*c*) : Scott (1960).
(*d*) : Yakel (1962).
(*e*) : Yamaguchi, Watanabe & Ogawa (1962).
(*f*) : Watanabe & Ogawa (1956).
(*g*) : Hirabayashi & Ogawa (1957).
(*h*) : Jehanno & Pério (1962).
(*i*) : Toth & Sato (1962).

Fujiwara (1957) interpreted the non-integral structure as a disordered structure which he called the *statistical assembly of irregular arrangements.* This disordered structure is a structure deviating from a regular structure which he called the *regular arrangements with uniform mixing*. For brevity, in the present paper the former is called the *statistical assembly* and the latter the *standard structure*. Discussion of the statistical assembly is given in §§ 6 and 7.

2. The standard structure

Fujiwara defined the standard structure by the use of the step function*

$$S(\xi)=\begin{cases} 1 \text{ for } & 2k\tilde{M}\le\xi<(2k+1)\tilde{M} \\ -1 \text{ for } & (2k+1)\tilde{M}\le\xi<2(k+1)\tilde{M} \end{cases} \qquad k\colon 0, \pm 1, \pm 2, \ldots \tag{3}$$

(F3)† as follows: The sign of the nth layer is positive or negative according as $S(n)=1$ or -1. In this case, the period P of the standard structure is subject to the relation

$$P=2\nu\tilde{M} \tag{4}$$

where ν is the minimum positive integer in this relation [refer to (F4)]. The standard structure thus obtained from the step function is, for example,

the complex out-of-step structure $(2\bar{2}2\bar{1}2\bar{2}12\bar{2}\bar{1})$ for $\tilde{M}=1{\cdot}7$,

the complex *APD* structure $((2\bar{2}2\bar{2}1)|(\bar{2}2\bar{2}2\bar{1}))$ for $\tilde{M}=1{\cdot}8$,

and so on as shown in Fig. 3, where the upper row indicates the positive layer and the lower one the negative layer.

$S(\xi)$ can be expanded in Fourier series as

$$S_0(\xi)=\frac{4}{\pi}\sum_{m=0}^{\infty}\frac{1}{2m+1}\sin\frac{\pi}{\tilde{M}}(2m+1)\xi \tag{5}$$

where the suffix 0 in S_0 is added in order to distinguish $S_0(\xi)$ from $S(\xi)$ with respect to their properties at singular points such as $\xi=0$, where $S(0)=1$ while $S_0(0)=0$. He suggested that the strongest peak is found at

$$\zeta=\frac{l}{P}=\frac{1}{2\tilde{M}} \quad \text{with} \quad l=\nu \tag{6}$$

using an intensity formula for the standard structure as follows

$$\begin{aligned} FF^* &= \left|\sum_{n=0}^{N-1} S_0(n)\exp(2\pi i n\zeta)\right|^2 \\ &= \frac{4}{\pi^2}\left|\sum_{m=0}^{\infty}\frac{1}{2m+1}\left[\exp\left\{i\pi\left(\zeta+\frac{2m+1}{2\tilde{M}}\right)(N-1)\right\}\right.\right. \\ &\quad \times\frac{\sin N\pi\{\zeta+(2m+1)/2\tilde{M}\}}{\sin\pi\{\zeta+(2m+1)/2\tilde{M}\}} \\ &\quad -\exp\left\{i\pi\left(\zeta-\frac{2m+1}{2\tilde{M}}\right)(N-1)\right\} \\ &\quad \left.\left.\times\frac{\sin N\pi\{\zeta-(2m\tilde{+}1)/2M\}}{\sin\pi\{\zeta-(2m+1)/2\tilde{M}\}}\right]\right|^2 \end{aligned} \tag{7}$$

where N is the total number of layers and ζ is a continuous parameter along **c***, **c*** being the vector reciprocal to **c** corresponding to one layer thickness. Equation (7) is the same as equation (F6) with slight modifications in notation‡. Fujiwara also suggested that other peaks are extremely weak. As a result, CD in equation (2) turns out to be not the separation between $l=-1$ and 1 but that between $l=-\nu$ and ν, and hence we apparently get the relation

$$\frac{AB}{CD}=\frac{P}{2\nu}=\tilde{M} \tag{8}$$

which is not an integer.

Usually, the intensity formula is expressed as the product of a Laue function and the square of the

* Fujiwara called $S(\xi)$ the anti-phase function for the standard structure.

† Refer to the footnote † on page 120.

‡ l in Fujiwara's paper is a continuous parameter along **c*** and is the same as ζ in the present paper.

absolute value of the structure factor. On the other hand, because equation (7) is not of this form, the numerical evaluation of equation (7) cannot be made unless the total number of layers, N, is given. In the present paper, equation (7) is rewritten in the form usual for intensity formula, and on this basis Fujiwara's suggestion is verified. Also, some important remarks are given relating to the application of the step function of the form in equation (5) (Appendix F).

3. The intensity formula for the standard structure

Since the standard structure has a period P subject to equation (4), equation (7) is rewritten as

$$FF^* = I_l G^2(\zeta) \quad (9)$$

with

$$G^2(\zeta) = \frac{\sin^2 \pi N_0 P \zeta}{\sin^2 \pi P \zeta} \text{ with } PN_0 = N$$

$$I_l = \psi_l \psi_l^* \quad \text{with} \quad \psi_l = \sum_{n=0}^{P-1} S_0(n) \exp(inl\theta) \quad (10)$$

$$\text{and } \theta = \frac{2\pi}{P}$$

where the suffix l is determined by the location of each peak of the Laue function $G^2(\zeta)$ at

$$\zeta = \frac{l}{P} \qquad l: 0, \pm 1, \pm 2, \pm 3, \ldots .$$

I_l in equation (10) is the same as that in equation (I.7) with ε_n replaced by $S_0(n)$.

It should be noted that if we take a square of $|\psi_l|$ after calculating ψ_l by the use of equation (5), as was done by Fujiwara with equation (7), an incorrect result is obtained in calculation of I_l (see Appendix F). The correct result is obtained by the use of the equation

$$I_l = \sum_{m=0}^{P-1} D_m \cos ml\theta \quad \theta = \frac{2\pi}{P} \quad (11)$$

given by equation (I.22), where D_m is the self-convolution of $S_0(n)$, *i.e.*

$$D_m = \sum_{p=0}^{P-1} S_0(p) S_0(p+m) \quad (12)$$

(see Appendix F). The calculation of I_l in terms of D_m is complicated so that the details are left to Appendices B and C. The result is given by

$$I_l = \frac{(1,4)}{\sin^2 \pi x} \quad (13)$$

with

$$\begin{cases} x = \dfrac{2n^*+1}{2H} = \dfrac{QP+l}{\nu^* P}, \; n^*: 0,1,2, \ldots H-1 \quad (14) \\ (1,4) \text{ or generally } (a,b) = \end{cases}$$

$$\begin{cases} a \text{ for } \nu^*: \text{ even, } i.e. \text{ Case I} \\ b \text{ for } \nu^*: \text{ odd, } i.e. \text{ Case II} \end{cases} \quad (15)$$

where ν^* is the minimum positive integer satisfying the relation

$$\begin{cases} \nu^* \tilde{M} = H & H: \text{positive integer} \\ P = (1,2)H & \text{(see Appendix } A) \end{cases} \quad (16)$$

and n^* is a minimum positive integer including 0 satisfying the relations

$$1 \le 2n^* + 1 = (QP + l)/\nu \le 2H - 1, \quad i.e. \; l = \nu(2n^*+1) - QP \quad (17)$$

Q being a positive or negative integer including 0.

In Case II, *i.e.* the case of the complex APD structure (see Appendix A), since P is even and $\nu = \nu^*$ is odd, we have no solution of equation (17) if l is even. Thus we have

$$\left.\begin{array}{l} I_l = \begin{cases} 0 & \text{when } l \text{ is even} \\ 4I_l^* & \text{when } l \text{ is odd} \end{cases} \\ I_l^* = \dfrac{1}{\sin^2 \pi x} \end{array}\right\} \quad (18)$$

which gives a selection rule for the complex APD structure.

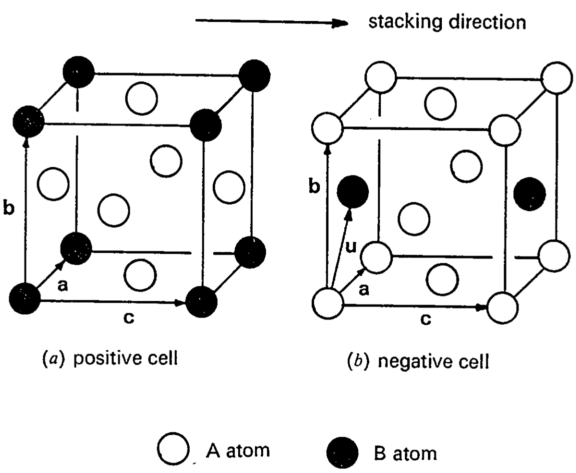

Fig. 1. Two kinds of unit cells in the one-dimensional anti-phase domain structure of A_3B-type with an out-of-step vector $\mathbf{u} = (\mathbf{a} + \mathbf{b})/2$.

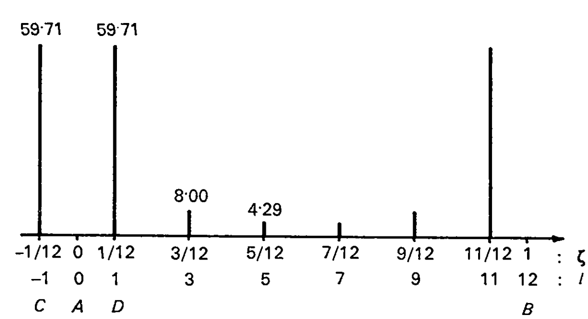

Fig. 2. The unitary intensities of the superlattice reflexions for the simple APD structure, $(6 \mid \overline{6})$, with $P = 12$.

Equations (13) and (18) are much simpler intensity expressions for the standard structure than equation (7). These equations give the square of the structure factor, and they may be calculated only if n^* in equation (14) is given so as to satisfy equation (17).

Appendix F should be referred to for some important remarks on the Fourier expansion of the step function $S(\xi)$.

4. Some remarks on I_l

We list here some general relations and special results which are derived in Appendix D. Since from equation (18) we have $I_l=0$ for Case II with l:even, we may consider odd l only. Then, l is conveniently expressed as

$$l=2r+1 \quad \text{for Case II.} \tag{19}$$

(i) There is one to one correspondence between (l,r) and n^* if (l,r) and n^* are in the ranges

$$0 \le (l,r) \le H-1 \quad \text{and} \quad 0 \le n^* \le H-1. \tag{20}$$

(ii) If the obtained n^* is larger than p^* which is given by

$$p^* = \tfrac{1}{2}[H-1;H-1,H-2], \tag{21}$$

we may replace n^* by $n^{*\prime}$ given by

$$n^{*\prime}=H-1-n^*. \tag{22}$$

Here the expression $[a;b,c]$ means

$$[a;b,c]=\begin{cases} a \text{ for Case I} \\ b \text{ for Case II-odd } (H=M\text{:odd}) \\ c \text{ for Case II-even } (H=M\text{:even}). \end{cases} \tag{23}$$

By the replacement of n^* by $n^{*\prime}$, the range of n^* may be further limited as

$$0 \le n^* \le p^*. \tag{24}$$

The use of $n^{*\prime}$ corresponds to the use of the relation $I_{P-l}=I_l$ given by equation (I.27).

(iii) Any $(l,2r+1)$ can be expressed in the form

$$(l,2r+1)+qP=(2l_0+1)v \tag{25}$$

where q and l_0 are integers and in this case n^* is given by

$$0 \le n^* = l_0 - mH \le H-1\,. \tag{26}$$

Here m is an integer and is chosen so as to satisfy the above inequalities.

(iv) We can derive the following special results:

$$(a) \quad I_0=1 \;\therefore \sum_{m=0}^{P-1} D_m = 1 \quad \text{for Case I.} \tag{27}$$

$$(b) \quad I_M=4 \;\therefore \sum_{m=0}^{P-1} (-1)^m D_m = 4 \quad \text{for Case II-odd}\,. \tag{28}$$

(c) When $\tilde{M}$ is a half odd integer, we have

$$I_l=\begin{cases} \dfrac{1}{\cos^2 \dfrac{\pi l}{2P}} \text{ for } l\text{: even} \\ \dfrac{1}{\sin^2 \dfrac{\pi l}{2P}} \text{ for } l\text{: odd} \end{cases} \tag{29}$$

which is the same as equation (I.15) for $(M\;\overline{M+1})$.

(v) Let ΔM be the fractional part of $\tilde{M}$, and if l is expressed in the form

$$l=2vl_0+l' \quad \text{with} \quad l_0\text{: integer and } 0 \le l' \le 2v-1, \tag{30}$$

then values of Q in equation (17) are listed in Table 2 for Case I with $\Delta M=0{\cdot}1$, $0{\cdot}3$, $0{\cdot}7$, $0{\cdot}9$ and for Case II with $\Delta M=0{\cdot}2$, $0{\cdot}4$, $0{\cdot}6$, $0{\cdot}8$ (refer to Table 6).

5. The strongest intensity of I_l

One of the solutions of equations (25) and (26) is given by

$$(l,2r+1)=v \quad \therefore q=l_0=n^*=m=0$$

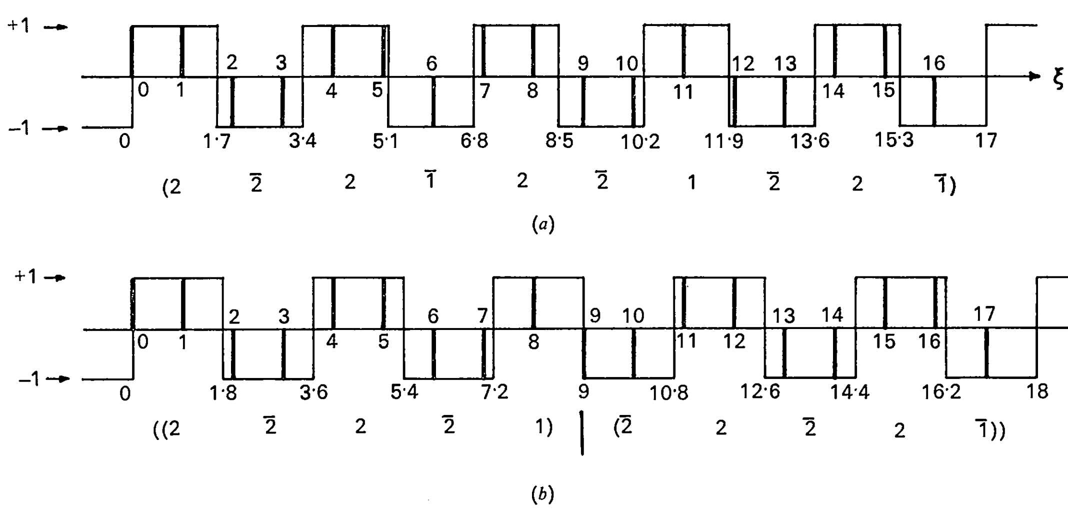

Fig. 3. The standard structures obtained from the step function $S(\xi)$. (a): $\tilde{M}=1{\cdot}7$, (b): $\tilde{M}=1{\cdot}8$.

Table 2. *Values of Q*

$$Q=\frac{(2g+1)\nu-l'}{(1,2)\Delta H}\ \text{[Equation (A 49)]}$$

Case I

ΔM	0·1	0·3	0·7	0·9
ΔH \ l'	1	3	7	9
0	5	5	5	5
1	4	8	2	6
2	3	1	9	7
3	2	4	6	8
4	1	7	3	9
5	0	0	0	0
6	9	3	7	1
7	8	6	4	2
8	7	9	1	3
9	6	2	8	4

$\Delta H=\nu^*\Delta M=10\Delta M$

Case II

ΔM	0·2	0·4	0·6	0·8
$2\Delta H$ \ l'	2	4	6	8
1	2	1	4	3
3	1	3	2	4
5	0	0	0	0
7	4	2	3	1
9	3	4	1	2

$2\Delta H=2\nu^*\Delta M=10\Delta M$

which, with equations (13) and (14), gives

$$I_\nu=\frac{(1,4)}{\sin^2\dfrac{\pi}{(2,1)P}}=\frac{4P^2}{\pi^2}\,\frac{1}{\left(\dfrac{\sin\pi x}{\pi x}\right)^2}\ \text{with}\ x=\frac{1}{(2,1)P}\,. \tag{31}$$

Since $I_{P-l}=I_l$ from equation (I.27), we get the relation

$$0{\cdot}81=\frac{8}{\pi^2}<R_\nu\equiv\frac{2I_\nu}{P^2}\le\tfrac{8}{9}=0{\cdot}89 \tag{32}$$

where $\frac{8}{9}$ comes from the fact that the minimum P is 3 for $\tilde{M}=1{\cdot}5$ and hence $x\le\frac{1}{6}$. Since we have the relation

$$\sum_{l=0}^{P-1} I_l=P^2$$

from equation (I.27), equation (32) means that the sum of the remaining intensities except $l=\nu$ and $l=P-\nu$ is less than $0{\cdot}2P^2$, *i.e.* I_ν is the strongest and the others are weak. Thus Fujiwara's suggestion is verified, namely the strongest peak is found at the position given by equation (6).

The second strongest intensity is given for

$$n^*=1\quad\text{and}\quad(l,2r+1)=3\nu\quad\text{with}\quad l_0=1\quad\text{and}\quad q=m=0\,,$$

and its ratio to I_ν is given by

$$\frac{I_{3\nu}}{I_\nu}=\frac{1}{\left(3\text{–}4\sin^2\dfrac{\pi}{2H}\right)^2}>\tfrac{1}{9}\,. \tag{33}$$

6. The intensity formula for the statistical assembly

According to equation (33), the ratio of the second strongest intensity, $I_{3\nu}$, to the strongest one, I_ν, is larger than $\frac{1}{9}$ for any standard structure. An example is shown in Table 3 where the unitary intensities for the standard structure with $\tilde{M}=1{\cdot}8$, *i.e.* $([M]\|[\tilde{M}])$ with $[M]=(2\bar{2}2\bar{2}1)$ and $P=18$, are listed. In this case the ratio, $I_3^*\ (=I_{15}^*):I_5^*$, is about 0·12. Therefore, with such a standard structure I_3^* and I_{15}^* may be clearly observed on diffraction photographs. In practice, however, they were observed only very faintly. In order to elucidate this circumstance, Fujiwara considered the *statistical assembly*, *i.e.* a disordered structure which deviates from the standard structure in the following way. Similar to the standard structure which has been defined by the use of the step function given by equation (3), the disordered structure, *i.e.* the statistical assembly, is defined by the use of an *assembly function**

$$f(\xi)=\frac{4}{\tilde{M}}\sum_{m=0}^{\infty} b_{2m+1}\sin\frac{\pi}{\tilde{M}}(2m+1)\xi \tag{34}$$

with

$$b_{2m+1}=\int_0^{\tilde{M}/2}\operatorname{erf}(\eta)\sin\frac{\pi}{\tilde{M}}(2m+1)\eta\,d\eta \tag{35}$$

Table 3. *The unitary intensities, I_l^*, of the superlattice reflexions for $([M]\|[\tilde{M}])$ with $[M]=(2\bar{2}2\bar{2}1)$ and $P=18$*

l	$\zeta=l/18$	I_l^*
1, 17	0·056, 0·944	1·1
3, 15	0·167, 0·833	4·0
5, 13	0·278, 0·722	33·2
7, 11	0·389, 0·611	1·7
9	0·5	1·0
		$\Sigma I_l^*=9^2=81$

[refer to (F14)]. In the standard structure the nth layer has a value $+1$ or -1 according as $S(n)=1$ or -1, while in the statistical assembly the effective value of the nth layer is put equal to $f(n)$. The assembly function $f(\xi)$ is a weighted mean function of modified step functions which are defined as follows: for a modified step function, the boundaries at $\xi=2k\tilde{M}$ and $(2k+1)\tilde{M}$ in the original step function, $S(\xi)$, are allowed to shift by δ as shown in Fig. 4 and each shift occurs at each boundary independently of other boundaries, with a probability

$$N(\delta,\sigma)=\frac{1}{\sqrt{2\pi}\sigma}\exp\left(-\frac{\delta^2}{2\sigma^2}\right) \tag{36}$$

which is a normalized Gauss function with a standard deviation σ. If the absolute value of the separation be-

* Fujiwara called $f(\xi)$ the anti-phase function for the statistical assembly.

tween a point at $\xi=n$ and its nearest boundary is denoted by x_n, as shown in Fig. 5 where the case of the boundary at $2k\tilde{M}$ is shown, then the probability, w_n^+, that the nth layer is positive is given by

$$w_n^+=\int_{-\infty}^{\pm x_n} N(\delta,\sigma)\mathrm{d}\delta=\tfrac{1}{2}\{1\pm\mathrm{erf}\,(x_n)\}$$

where the upper or the lower sign in the double sign is taken according as the nth layer in the standard structure is positive [Fig. 5(a)] or negative [Fig. 5(b)], and erf(x) is the error function defined as

$$\mathrm{erf}(x)=2\int_0^x N(\delta,\sigma)\mathrm{d}\delta \quad \text{with} \quad \mathrm{erf}\,(\infty)=1\,. \tag{37}$$

Similarly, the probability, w_n^-, that the nth layer is negative is given by

$$w_n^-=\int_{\pm x_n}^{\infty} N(\delta,\sigma)\mathrm{d}\delta=\tfrac{1}{2}\{1\mp\mathrm{erf}\,(x_n)\}\,.$$

Since these results hold even in the case where the boundary is at $(2k+1)\tilde{M}$, they are generally rewritten as

$$\begin{cases} w_n^+=\tfrac{1}{2}\{1+\varepsilon_n^{(0)}\mathrm{erf}\,(x_n)\} \\ w_n^-=\tfrac{1}{2}\{1-\varepsilon_n^{(0)}\mathrm{erf}\,(x_n)\} \end{cases} \tag{38}$$

where

$$\varepsilon_n^{(0)}=\begin{cases} 1 & \text{when the } n\text{th layer in the standard structure is positive} \\ -1 & \text{when the } n\text{th layer in the standard structure is negative.} \end{cases} \tag{39}$$

Thus, the effective value, $f(n)$, of the nth layer is given by

$$f(n)=w_n^+-w_n^-=\varepsilon_n^{(0)}\mathrm{erf}\,(x_n)\,. \tag{40}$$

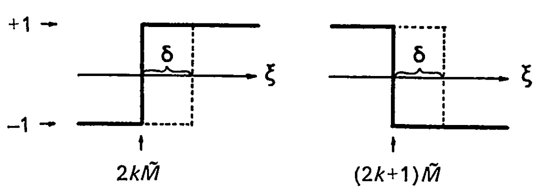

Fig. 4. The shift, δ, of the boundaries at $\xi=2k\tilde{M}$ and $(2k+1)\tilde{M}$ in the original step function $S(\xi)$ shown by the thick lines.

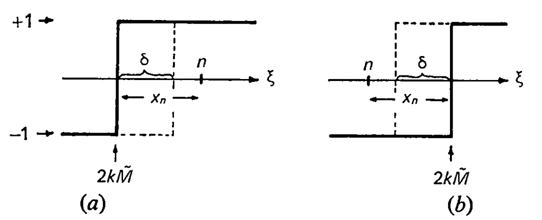

Fig. 5. The separation, x_n, between a point at $\xi=n$ and its nearest boundary at $2k\tilde{M}$. (a): when the nth layer in the standard structure is positive, (b): when it is negative.

This $f(n)$ can be generalized to the functions of continuous ξ, as

$$\begin{cases} f(\xi)=\mathrm{erf}\,(\xi) & \text{for} \quad 0\le\xi<\dfrac{\tilde{M}}{2} \\ f(\xi)=\mathrm{erf}\,(\tilde{M}-\xi) & \text{for} \quad \dfrac{\tilde{M}}{2}\le\xi<\tilde{M} \\ f(\xi)=-\mathrm{erf}\,(\xi-\tilde{M}) & \text{for} \quad \tilde{M}\le\xi<\dfrac{3\tilde{M}}{2} \\ f(\xi)=-\mathrm{erf}\,(2\tilde{M}-\xi) & \text{for} \quad \dfrac{3\tilde{M}}{2}\le\xi<2\tilde{M}\,. \end{cases} \tag{41}$$

These functions are shown by the thick curve in Fig. 6 where the thin line shows $S(\xi)$.

Since $f(\xi)$ has a periodicity of $2\tilde{M}$, $f(\xi)$ can be expanded, as was done by Fujiwara, in Fourier series, and we obtain equations (34) and (35). Thus, the intensity formula for the statistical assembly is given by

$$\Psi\Psi^*=\left|\sum_{n=0}^{N-1} f(n)\exp\,(inl\theta)\right|^2 \quad \text{with} \quad \theta=\frac{2\pi}{P}\,. \tag{42}$$

Equation (42), with substitution of equations (34) and (35), is the same as the first term of equation (F14). As in the case of equation (7), equation (42) is not of the form of the usual intensity formula. By noticing that $f(n)$ has a periodicity of P given by equation (4), however, equation (42) can be rewritten as

$$\Psi\Psi^*=\overline{I_l}G^2(\zeta) \tag{43}$$

with

$$\overline{I_l}=\left|\sum_{n=0}^{P-1} f(n)\exp\,(inl\theta)\right|^2. \tag{44}$$

Thus, the structure of the statistical assembly can be considered as a hypothetical structure in which the nth layer has the effective value equal to the height of the vertical thick line at $\xi=n$ as shown in Fig. 7.

On substitution of equations (34) and (35) in (44), $\overline{I_l}$ becomes

$$\overline{I_l}=16\nu^2\left(\sum_{m=-\infty}^{\infty} b_{2n^*+1+2mH}\right)^2 \tag{45}$$

$$=(1,4)\left[2\sum_{p=1}^{p^*}\mathrm{erf}\left(\frac{P}{\nu^*}\right)\sin 2\pi px+[0;0,1] \times(-1)^{n^*}\,\mathrm{erf}\left(\frac{\tilde{M}}{2}\right)\right]^2 \tag{46}$$

(see Appendix E), where n^*, p^*, x and the notation $[a;b,c]$ are given by equations (17), (21), (14) and (23) respectively. Equation (46) is an intensity expression for the statistical assembly which is much simpler than equation (42) combined with equations (34) and (35). For $\overline{I_l}$ corresponds to the square of the structure factor in the usual intensity formula while equation (42) is not expressed in the form of the product of a Laue function and the square of the structure factor.

The strongest intensity in the statistical assembly is found at $l=\pm\nu$ as in the case of the standard structure. The ratio of the second strongest intensity, $\overline{I_{3\nu}}$, to the strongest one, $\overline{I_\nu}$, varies with σ in equation (36). From equation (46) with $\tilde{M}=1{\cdot}8$, the ratio is calculated as shown in Table 4, in which it can be seen that the intensities of the reflexions other than $l=\pm\nu$ may practically vanish for suitably selected values of σ. In such a case, only a pair of satellites corresponding to $\overline{I_\nu}$ and $\overline{I_{\bar\nu}}$ may be experimentally observed. As a result, a non-integral value for the half period, $\tilde{M}$, will be observed from these satellites.

Table 4. *The ratio of the second strongest to the strongest intensity in the statistical assembly with* $\tilde{M}=1{\cdot}8$, $\nu^*=\nu=5$, $H=9$ *and* $P=18$

The ratio decreases with increasing σ, the standard deviation.

σ	Ratios
0	0·0933
0·05	0·0933
0·10	0·0859
0·16	0·0595
0·20	0·0419
0·25	0·0242
0·32	0·0090
0·40	0·0018
0·50	0·00000

7. The interpretation of the statistical assembly

The statistical assembly discussed in §6 is interpreted as follows: For the example shown in Fig. 7, x_n and w_n^+ and w_n^- given by equation (38) are obtained as shown in Table 5. If we distribute $+1$ and -1 at 18 positions from $n=0$ to $n=17$, then we have $C=2^{18}$ configurations in total. Corresponding to each configuration, the structure factor is denoted by F_s with $s=1,2,3,\ldots,C$. If, for example, configuration $s=1$ is $(11111\ldots11)$ (all 1), then, from Table 5 its existence probability, $w^{(1)}$, is given by

$$w^{(1)}=w_0^+w_1^+w_2^+w_3^+W$$
$$=\tfrac{1}{16}\{1+\mathrm{erf}\,(0{\cdot}8)\}\,\{1-\mathrm{erf}\,(0{\cdot}2)\}\,\{1-\mathrm{erf}\,(0{\cdot}6)\}W$$

with

$$W=\prod_{n=4}^{17} w_n^+$$

because the shifts of boundaries of the original step function, $S(\xi)$, occur independently of each other. If configuration $s=2$ is $(11\bar{1}11\ldots11)$, $w^{(2)}$ is given by

$$w^{(2)}=w_0^+w_1^+w_2^-w_3^+W$$
$$=\tfrac{1}{16}\{1+\mathrm{erf}(0{\cdot}8)\}\,\{1+\mathrm{erf}\,(0{\cdot}2)\}\,\{1-\mathrm{erf}\,(0{\cdot}6)\}W.$$

If configuration $s=3$ is $(\bar{1}\bar{1}111\ldots11)$, $w^{(3)}$ is given by

$$w^{(3)}=w_0^-w_1^-w_2^+w_3^+W$$
$$=\tfrac{1}{16}\{1-\mathrm{erf}\,(0{\cdot}8)\}\,\{1-\mathrm{erf}\,(0{\cdot}2)\}\,\{1-\mathrm{erf}\,(0{\cdot}6)\}W$$

and so on.

If the continuing probability, P_{st}, of finding F_t after F_s is equal to $w^{(t)}$, *i.e.* the existence probability of F_t, then the case concerned is that called the case of no-correlation (Kakinoki & Komura, 1952), and the intensity is given by

$$I(\zeta)=\overline{I'_l}\,\frac{\sin^2 \pi N_0 P\zeta}{\sin^2 \pi P\zeta}+N_0\{\overline{F^2}-(\bar{F})^2\},\; PN_0=N \qquad (47)$$

with

$$\overline{I'_l}=\left|\sum_{s=1}^{C} w^{(s)}F_s(l)\right|^2 \qquad (48)$$

and

$$\left.\begin{aligned}(\bar{F})^2&=\left|\sum_{s=1}^{C} w^{(s)}F_s(\zeta)\right|^2\\ \overline{F^2}&=\sum_{s=1}^{C} w^{(s)}F_s(\zeta)F_s^*(\zeta)\,.\end{aligned}\right\} \qquad (49)$$

The first term with Laue function in equation (47) is the Laue term which gives sharp maxima at $\zeta=l/P$ with l: integers, and the last one with N_0 is the diffuse term. The structure factor for the configuration s, F_s, is generally expressed as

$$F_s(\zeta)=\sum_{n=0}^{P-1}\varepsilon_n^{(s)}\exp\,(2\pi in\zeta) \qquad (50)$$

where

$$\varepsilon_n^{(s)}=\begin{cases}1 & \text{when the } n\text{th layer in configuration } s \text{ is positive}\\ -1 & \text{when the } n\text{th layer in configuration } s \text{ is negative,}\end{cases} \qquad (51)$$

and from the definition we get the relations

$$\left.\begin{aligned}&\sum_{s=1}^{C} w^{(s)}\varepsilon_n^{(s)}=w_n^+-w_n^-=f(n)\\ \text{and}\quad&\sum_{s=1}^{C} w^{(s)}\varepsilon_n^{(s)}\varepsilon_{n+m}^{(s)}=f(n)f(n+m)\,.\end{aligned}\right\} \qquad (52)$$

Thus, $\overline{I'_l}$ and the diffuse term can be calculated as follows (see equations (A51), (A52) and (A58) in Appendix *E*):

$$\overline{I'_l}=\overline{I_l} \qquad (53)$$

$$\overline{F^2}-(\bar{F})^2=P-\sum_{n=0}^{P-1}f^2(n)=P$$
$$-\left\{(2,4)\sum_{p=1}^{p^*}\mathrm{erf}^2\left(\frac{p}{\nu^*}\right)+[0;0,2]\mathrm{erf}^2\left(\frac{\tilde{M}}{2}\right)\right\} \qquad (54)$$

where n^*, p^* and the notation $[a;b,c]$ are given by equations (17), (21) and (23) respectively.

In this way, the model of the statistical assembly presented by Fujiwara can be interpreted as a disordered structure which consists of all possible configurations with existence probabilities, $w^{(s)}$, corresponding to the case of no-correlation. Equation (54) multiplied by N_0 is the same as the second and the third terms of equation (F14).

8. Discussion

If the standard deviation σ in equation (36) tends to 0, erf(x) tends to 1 except at $x=0$. At the limit $\sigma \to 0$, equations (46) and (54) tend to

$$\overline{I_l}=(1,4)\left(\sum_{p=0}^{H-1} \sin 2\pi p x\right)^2=(1,4)\cot^2 \pi x \qquad (55)$$

and

$$\overline{F^2}-(\overline{F})^2=(1,2) \qquad (56)$$

respectively. However, equation (55) is different from (13) but equal to equation (A65) in Appendix *F*. In addition, the quantity in the left hand side of equation (56) is what should vanish for the standard structure. These inconsistencies are due to the fact that $f(\xi)$ in equation (34) does not tend to $S(\xi)$ but to $S_0(\xi)$ in equation (5) at the limit $\sigma \to 0$, because b_{2m+1} in equation (35) tends to $M/\{(2m+1)\pi\}$. We must be careful in using equations (46) and (54) as they do not give the relations appropriate to the standard structure at the limit $\sigma \to 0$.

In both the models of the standard structure and of the statistical assembly, we have considered the period which is subject to $P=2\nu\tilde{M}=(1,2)\nu^*\tilde{M}$ given by equations (4) and (16). Therefore, if $\tilde{M}$ is 1·8, we have $P=18$ and if $\tilde{M}$ is 1·81, it becomes 181 and so on. However, such long periods seem to be not realistic. In part III of this series, we shall propose a new model for non-integral values of the half period, $\tilde{M}$. In this model, $\tilde{M}$ is naturally obtained from the peak shift due to a disordered structure between the M and $M+1$ layers, where $\tilde{M}$ lies between M and $M+1$.

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APPENDIX *A*
The minimum integer, ν^*, making $\nu^*\tilde{M}$ an integer

It is convenient to define the minimum positive integer, ν^*, in the relation

$$\nu^*\tilde{M}=H \qquad (A1)$$

where H is a positive integer. According as ν^* is even or odd, the standard structure defined by the step function $S(\xi)$ is found to be the complex out-of-step structure or the complex *APD* one, as mentioned below.

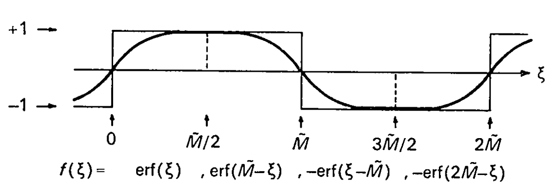

Fig. 6. The definition of $f(\xi)$ and its schematic representation. The thick curve indicates the assembly function $f(\xi)$ and the thin line the original step function $S(\xi)$.

If ν^* is even, we may put $\nu^*=2\nu_0$. In this case H should be odd, for, if H is even, *i.e.* $H=2H_0$, we get

$$\nu_0\tilde{M}=H_0$$

which contradicts the definition of ν^*. Therefore, we have

$$H=P\text{:odd} \quad \text{and} \quad \nu^*=2\nu_0=2\nu$$

from equation (4). The standard structure in this case should be a complex out-of-step structure, because the period $P=H$ is odd.

If ν^* is odd, the step next to the ν^*th step belongs to the region where $S(\xi)=-1$ according to equation (3). Therefore, another ν^* steps are necessary for getting a period P and hence we have

$$P=2H=2\nu^*\tilde{M},\ \nu^*=\nu \quad \text{and} \quad H=\nu^*\tilde{M}=M=P/2.$$

In this case the standard structure should be a complex *APD* structure including the simple *APD* structure.

Thus we have two cases:

$$\left\{\begin{array}{ll} \text{Case I} & (\nu^*\text{:even}) \\ & \nu^*=2\nu,\ H=\nu^*\tilde{M}=P\text{:odd and the standard structure is a complex out-of-step structure} \\ \text{Case II} & (\nu^*\text{:odd}) \\ & \nu^*=\nu,\ H=\nu^*\tilde{M}=M=P/2 \text{ and the standard structure is a complex } APD \text{ structure including the simple } APD \text{ structure.} \end{array}\right. \qquad (A2)$$

This situation is conveniently expressed by the notations

$$\nu^*=(2,1)\nu \text{ or } 2\nu=(1,2)\nu^*,$$

and

$$H=\nu^*M=(P,\tilde{M}) \text{ or } P=(1,2)H \qquad (A3)$$

where the notation of the form (a,b) implies that

$$(a,b)=\left\{\begin{array}{l} a \text{ for Case I} \\ b \text{ for Case II}. \end{array}\right. \qquad (A4)$$

APPENDIX *B*
Derivation of equation (13)

Substitution of $S_0(\xi)$ in equation (5) into D_m in equation (12) gives

$$D_m=\frac{8P}{\pi^2}\left\{\sum_{n=0}^{\infty}{}^{*}\sum_{n'=0}^{\infty}{}^{*}\frac{1}{(2n+1)(2n'+1)} \times \cos\frac{\pi}{\tilde{M}}(2n'+1)m - \sum_{n=0}^{\infty}{}^{**}\sum_{n'=0}^{\infty}{}^{**}\frac{1}{(2n+1)(2n'+1)} \times \cos\frac{\pi}{\tilde{M}}(2n'+1)m\right\} \qquad (A5)$$

where the symbols * and ** mean that the summations with respect to n and n' are carried out over the values satisfying the relations

$$\begin{cases} * & n-n'=q_1H \\ ** & n+n'+1=q_2H \end{cases} \quad \text{(A6)}$$

where q_1 and q_2 are integers. In this calculation, the following relations are used:

$$\begin{cases} \sum_{p=0}^{P-1} \cos\frac{2\pi}{\tilde{M}}np = \sum_{p=0}^{P-1}\cos\frac{2\pi}{P}2vnp \\ \qquad = P\delta_{2vn,rP}=P\delta_{n,qH} \\ \sum_{p=0}^{P-1}\sin\frac{2\pi}{\tilde{M}}np=0 \end{cases} \quad \text{(A7)}$$

where $\delta_{2vn,rP}$ and $\delta_{n,qH}$ are Kronecker's delta functions with r and q: integers. Putting

$$0\le n_1=n-n',\ 1\le n_2=n'-n \text{ and } 1\le n_3=n+n'+1$$

and rearranging the similar terms, we obtain from equation (A5)

$$D_m=\frac{8P}{\pi^2}\left\{\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\cos\frac{\pi}{\tilde{M}}(2n+1)m \right.$$
$$+2\sum_{n''=1}^{\infty}{}^{*}\left[\sum_{n=0}^{\infty}\frac{1}{(2n+1)\{2(n''+n)+1\}}\times\cos\frac{\pi}{\tilde{M}}(2n+1)m\right.$$
$$\left.\left.-\sum_{n=0}^{n''-1}\frac{1}{2n''(2n+1)}\cos\frac{\pi}{\tilde{M}}(2n+1)m\right]\right\}$$

where the symbol * means that the summation with respect to n'' is carried out over the values satisfying the relation

$$n''=qH.$$

Since the two terms in the square brackets in the above equation are found to cancel each other, D_m becomes

$$D_m=\frac{8P}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\cos\frac{\pi}{\tilde{M}}(2n+1)m \quad \text{(A8)}$$
$$=\frac{8P}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{(2n-1)^2}\cos\pi(2n-1)z$$
$$=P-2Pz_0 \quad \text{(A9)}$$

where

$$z=\frac{m}{\tilde{M}}=\frac{mv^*}{H}=\frac{2vm}{P} \quad \text{(A10)}$$

and z_0 is the principal value of z and is in the range

$$0\le z_0\le 1. \quad \text{(A11)}$$

Putting $m=0$, we have

$$z=z_0=0 \quad \therefore D_0=P$$

which gives, by definition, the correct value of D_0.

Substitution of equation (A8) into the expression for I_l in equation (11) gives

$$I_l=\frac{4P^2}{\pi^2}\left\{\sum_{n_1=0}^{\infty}{}^{*}\frac{1}{(2n_1+1)^2}+\sum_{n_2=0}^{\infty}{}^{**}\frac{1}{(2n_2+1)^2}\right\} \quad \text{(A12)}$$

where the symbols * and ** mean that the summations with respect to n_1 and n_2 are carried out over the values satisfying the following relations:

$$\begin{cases} * & v(2n_1+1)=q_1P+l \quad 0\le n_1 \\ ** & v(2n_2+1)=q_2P-l \quad 0\le n_2\,. \end{cases} \quad \text{(A13)}$$

From equation (A13) we obtain (see Appendix C)

$$\begin{cases} 2n_1+1=2n^*+1+2m_1H \quad \text{with} \quad m_1=0,1,2,\ldots \\ 2n_2+1=-(2n^*+1+2m_2H) \\ \qquad\qquad \text{with} \quad m_2=-1,-2,-3,\ldots \end{cases} \quad \text{(A14)}$$

where n^* is the minimum positive integer including 0 satisfying the relations

$$1\le 2n^*+1=(QP+l)/v\le 2H-1$$
$$\text{and} \quad 0\le n^*\le H-1\,, \quad \text{(A15)}$$

Q being a positive or negative integer including 0. Thus, equation (A12) becomes

Table 5. *Some values of* x_n, w_n^+ *and* w_n^- *in the statistical assembly shown in Fig.* 7

n	0	1	2	3	...
x_n	0	0·8	0·2	0·6	...
w_n^+	$\frac{1}{2}$	$\frac{1}{2}\{1+\text{erf}\ (0{\cdot}8)\}$	$\frac{1}{2}\{1-\text{erf}\ (0{\cdot}2)\}$	$\frac{1}{2}\{1-\text{erf}\ (0{\cdot}6)\}$	...
w_n^-	$\frac{1}{2}$	$\frac{1}{2}\{1-\text{erf}\ (0{\cdot}8)\}$	$\frac{1}{2}\{1+\text{erf}\ (0{\cdot}2)\}$	$\frac{1}{2}\{1+\text{erf}\ (0{\cdot}6)\}$	...

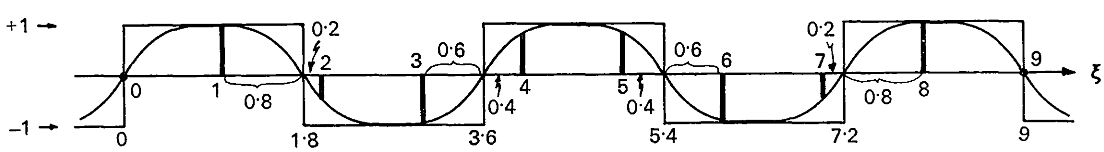

Fig. 7. The effective value (the vertical thick line) of the nth layer in the statistical assembly deviated from the standard structure, $([M]\,|\,[\tilde{M}])$ with $[M]=(2\bar{2}2\bar{2}1)$, $P=18$ and $\tilde{M}=1{\cdot}8$.

$$I_l = \frac{4P^2}{\pi^2} \sum_{m=-\infty}^{\infty} \frac{1}{(2mH+2n^*+1)^2}$$
$$= (1,4)\frac{1}{\pi^2} \sum_{m=-\infty}^{\infty} \frac{1}{(m+x)^2}$$
$$= \frac{(1,4)}{\sin^2 \pi x} \quad \text{(A16)}$$

with

$$x = \frac{2n^*+1}{2H} = \frac{QP+l}{\nu^* P}. \quad \text{(A17)}$$

Equations (A16), (A17) and (A15) give equations (13), (14) and (17) respectively.

APPENDIX *C*
Derivation of equation (A14)

Equation (A14) in Appendix *B* is derived from equation (A13), *i.e.*

$$\begin{cases} {}^{*} \ \nu(2n_1+1) = q_1P + l \quad 0 \le n_1 \\ {}^{**} \ \nu(2n_2+1) = q_2P - l \quad 0 \le n_2 \end{cases} \quad \text{(A18)}$$

as follows: let $\{n_1, q_1\}$ and $\{n_1+\Delta n_1, q_1+\Delta q_1\}$ be two suc-cessive sets which satisfy the former relation in equation (A18). Taking the difference between the corres-ponding two equations, we obtain

$$2\nu\Delta n_1 = P\Delta q_1, \quad i.e. \quad \nu^*\Delta n_1 = H\Delta q_1$$

from which we get

$$\Delta q_1 = \nu^* \quad \text{and} \quad \Delta n_1 = H$$

because ν^* and H have no common divisor from the definition of H, *i.e.* equation (A1). The same result can be obtained from the latter relation in equation (A18). As a result, the intervals, Δn of n_1 and n_2 and Δq of q_1 and q_2, which satisfy equation (A18) are given by

$$\Delta n = H \quad \text{and} \quad \Delta q = \nu^*. \quad \text{(A19)}$$

Let n_1^* and n_2^* be the minimum values of n_1 and n_2 respectively, and let Q_1 and Q_2 be the corresponding values of q_1 and q_2 respectively. Then we have, from equation (A18),

$$\begin{cases} 2\nu n_1^* = Q_1P + l - \nu \\ 2\nu n_2^* = Q_2P - l - \nu \end{cases} \quad \text{(A20)}$$

with

$$0 \le n_1^* \le H-1 \quad \text{and} \quad 0 \le n_2^* \le H-1. \quad \text{(A21)}$$

Taking the sum of the two equations in equation (A20), we get

$$2\nu(n_1^*+n_2^*) = (Q_1+Q_2)P - 2\nu$$

from which, with equations (4) and (A21), we have the relation

$$0 \le n_1^*+n_2^* = (Q_1+Q_2)\tilde{M} - 1 \le 2H-2.$$

Since $(Q_1+Q_2)\tilde{M}$ should be an integer which satisfies the above equation, we get at once the results

$$Q_1+Q_2 = \nu^* \quad \text{and} \quad n_1^*+n_2^* = H-1. \quad \text{(A22)}$$

Thus we can calculate n_2 as

$$\begin{aligned} n_2 &= n_2^* + m_2''H & m_2''&: 0,1,2,\ldots \\ &= H-1-n_1^*+m_2''H & & \\ &= m_2'H - n_1^* - 1 & m_2'&: 1,2,3,\ldots. \end{aligned}$$

At the same time, we can put

$$n_1 = n_1^* + m_1H \qquad m_1: 0,1,2,\ldots.$$

Finally we have the relations

$$\begin{cases} 2n_1+1 = 2n^*+1+2m_1H \quad \text{with} \quad m_1: 0,1,2,\ldots \\ 2n_2+1 = -(2n^*+1+2m_2H) \\ \qquad\qquad \text{with} \quad m_2: -1,-2,-3,\ldots \end{cases} \quad \text{(A23)}$$

with

$$1 \le 2n^*+1 = (QP+l)/\nu \le 2H-1 \quad \text{and} \quad 0 \le n^* \le H-1, \quad \text{(A24)}$$

equations (A23) and (A24) giving equations (A14) and (A15) in Appendix *B*.

APPENDIX *D*
Derivation of the relations (i) to (v) in §4

Since we have $I_l = 0$ for Case II with l: even from equation (18), l may be restricted to an odd integer and is put as equation (19), *i.e.*

$$l = 2r+1 \quad \text{for Case II.} \quad \text{(A25)}$$

(i) Since we have the relation $I_{l+P} = I_l$, we can limit l as $0 \le l \le P-1$ which is, with equation (A24), the same as equation (20), *i.e.*

$$0 \le (l,r) \le H-1 \quad \text{and} \quad 0 \le n^* \le H-1. \quad \text{(A26)}$$

Thus the total numbers of different values of (l,r) and n^* are both equal to H.

On the other hand, equation (A24) can be rewritten as

$$2\nu n^* - QP = (l, 2r+1) - \nu$$
$$\therefore n^*\nu^* - QH = (l,r) - \tfrac{1}{2}(\nu^*, \nu^*-1) \quad \text{(A27)}$$

by equation (A3). Since the right hand side of equation (A27) is an integer [$\because \nu^*$: (even, odd)] and ν^* and H have no common divisor, there should be an infinite number of sets of solutions of equation (A27), of the form $\{n^*-mH, Q-m\nu^*\}$ with m: integer. Thus we can find n^* within the region given by equation (A26) for a given (l,r).

If there were different sets, $\{(l,r), Q\}$ and $\{(l',r'), Q'\}$, for a given n^*, we would have the relation

$$(Q'-Q)H = (l-l', r-r') \quad \text{(A28)}$$

from equation (A27). Considering equation (A26), we can find no solution for equation (A28) except for $(l,r) = (l',r')$ and $Q = Q'$.

As a result, there should be one to one correspondence between (l,r) and n^* so long as they are limited by equation (A26).

(ii) Since we have the relation $I_{P-l}=I_l$ from equation (I.27), $I_{l'}$ calculated from equation (13) must be equal to I_l, if l' is given by

$$l'=P-l, \text{ i.e. } (l',r')=(H-l,H-1-r). \quad (A29)$$

The equation for (l',r') corresponding to equation (A27) is

$$n^{*\prime}v^*-Q'H=(H-l,H-1-r)-\tfrac{1}{2}(v^*,v^*-1). \quad (A30)$$

Taking the sum of equations (A27) and A(30), we get

$$(n^*+n^{*\prime}+1)v^*=(Q+Q'+1)H$$

from which we can derive the relations

$$n^{*\prime}=H-1-n^* \quad \text{and} \quad Q'=v^*-1-Q \quad (A31)$$

for the reason that v^* and H have no common divisor and n^* and $n^{*\prime}$ are limited by equation (A26). Substitution of $n^{*\prime}$ from equation (A31) into equation (13) with equation (14) gives $I_{l'}=I_{P-l}=I_l$, *i.e.* both n^* and $n^{*\prime}$ given by equation (A31) give the same intensity. Thus, if n^* is replaced by $n^{*\prime}$ for larger n^* than p^*, n^* may be further limited as

$$0\le n^*\le p^* \quad \text{with} \quad p^*=\tfrac{1}{2}[H-1;H-1,H-2] \quad (A32)$$

where p^* is given by equation (21) with equation (23).

(iii) The fact that we have solutions, for a given (l,r), of equation (A27) which is equivalent to equation (A24), means that any $(l,2r+1)$ can be expressed in the form

$$(l,2r+1)+qP=(2l_0+1)v \quad (A33)$$

where q and l_0 are integers. Substitution of the right hand side of the above equation in the expression for l in equation (A24) gives

$$2n^*+1=2l_0+1+2Q\tilde{M}.$$

Putting $Q=-mv^*$, we get the relation

$$0\le n^*=l_0-mH\le H-1 \quad (A34)$$

where m is an integer and is chosen so as to satisfy the above inequalities.

(iv) Substitution of $l=(0,M)$ with M:odd and $Q=(\tfrac{1}{2})(v^*,v^*-1)$ into equation (A24) gives $2n^*+1=H$ from which, by equation (13) with equation (14), we obtain the results

$$I_{(0,M)}=(1,4). \quad (A35)$$

As a result, from equation (11), we get

$$\sum_{m=0}^{P-1} D_m=1 \quad \text{for Case I} \quad (A36)$$

$$\sum_{m=0}^{P-1} (-1)^m D_m=4 \quad \text{for Case II-odd.} \quad (A37)$$

When $\tilde{M}$ is a half odd integer, we have $v^*=2$, $v=1$ and $P=H$:odd by which equation (A24) becomes

$$1\le 2n^*+1=\begin{Bmatrix} H+l & \text{for} & l\text{:even} \\ l & \text{for} & l\text{:odd} \end{Bmatrix}\le 2H-1 \quad (A38)$$

so long as l is limited by equation (A26). Substitution of equation (A38) into equation (13) with equation (14) gives

$$I_l=\begin{cases} \dfrac{1}{\cos^2\dfrac{\pi l}{2P}} & \text{for } l\text{:even} \\ \dfrac{1}{\sin^2\dfrac{\pi l}{2P}} & \text{for } l\text{:odd.} \end{cases} \quad (A39)$$

(v) The determination of Q is as follows: $\tilde{M}$, H and $(l,2r+1)$ are conveniently expressed as

$$\begin{cases} \tilde{M}=M_0+\Delta M \quad M_0\text{: integer and } 0<\Delta M<1 & (A40) \\ H=H_0+\Delta H \quad H_0=v^*M_0 \text{ and } 1\le \Delta H=v^*\Delta M\le v^*-1 & (A41) \\ l=2vl_0+l' \quad l_0\text{: integer and } 0\le l'\le 2v-1. & (A42) \end{cases}$$

Substitution of these equations into equation (A24) gives

$$2vn^*+v=Q(1,2)\,(v^*M_0+\Delta H)+2vl_0+l'$$

Table 6. *Values of* $(2g+1)v-l'$ [*equation*(A49)]

Case I ΔM: 0·1, 0·3, 0·7, 0·9 ($v=5$)

g	0	1	2	3	4	5	6	7	8
$(2g+1)v-l'=10g+5-l'$	$5-l'$	$15-l'$	$25-l'$	$35-l'$	$45-l'$	$55-l'$	$65-l'$	$75-l'$	$85-l'$
l'									
0	5	15	25	35	45	55	65	75	85
1	4	14	24	34	44	54	64	74	84
2	3	13	23	33	43	53	63	73	83
3	2	12	22	32	42	52	62	72	82
4	1	11	21	31	41	51	61	71	81
5	0	10	20	30	40	50	60	70	80
6		9	19	29	39	49	59	69	79
7		8	18	28	38	48	58	68	78
8		7	17	27	37	47	57	67	77
9		6	16	26	36	46	56	66	76

Table 6 (*cont.*)

Case II ΔM: 0·2, 0·4, 0·6, 0·8 ($v=5$)

g	0	1	2	3
$(2g+1)v-l'=10g+5-l'$	$5-l'$	$15-l'$	$25-l'$	$35-l'$
l'				
1	4	14	24	34
3	2	12	22	32
5	0	10	20	30
7		8	18	28
9		6	16	26

which is rewritten as

$$l'-v+(1,2)Q\Delta H=2v\{n^*-(QM_0+l_0)\}\equiv 2vg(\text{put})$$

where g is an integer. Finally we get the two relations

$$\begin{cases} l'-v=(1,2)\,(gv^*-Q\Delta H) & \text{(A43)} \\ 0\le n^*=QM_0+l_0+g\le H-1. & \text{(A44)} \end{cases}$$

Since v^* and $\Delta H=v^*\Delta M$ have no common divisor, any integer G can be expressed in the form

$$G=g'v^*-Q'\Delta H \quad =(g'-m\Delta H)v^*-(Q'-mv^*)\Delta H$$

where g′ and Q' are any integers which satisfy the above equation and m is an undetermined integer. Thus we can find infinite numbers of sets for Q and g which satisfy equation (A43) for a given l'. Let Q' and g' be any set of them and putting

$$Q=Q'-mv^* \quad \text{and} \quad g=g'-m\Delta H\,, \qquad \text{(A45)}$$

we can rewrite equation (A44) as

$$0\le n^*=Q'M_0+l_0+g'-mH\le H-1 \qquad \text{(A46)}$$

by which m can be determined.

In practice, it is convenient to limit l as in equation (A26). In this case, from equation (A27), we can limit Q as

$$0\le Q\le v^*-1\,. \qquad \text{(A47)}$$

From equation (A43) with equations (A41), (A42) and (A47), we obtain the relation

$$0\le l'+(1,2)Q\Delta H=(2g+1)v\le 2v(v^*-1)+(0,1)$$

from which we get the two relations

$$\begin{cases} 0\le g\le v^*-2 & \text{(A48)} \\ Q=\dfrac{(2g+1)v-l'}{(1,2)\Delta H}\,. & \text{(A49)} \end{cases}$$

Examples for

Case I ΔM: 0·1, 0·3, 0·7, 0·9 with $v^*=10$, $v=5$, $0\le g\le 8$ and $(2g+1)v=10g+5$

Case II ΔM: 0·2, 0·4, 0·6, 0·8 with $v^*=v=5$, $0\le g\le 3$ and $(2g+1)v=10g+5$

are shown in Tables 6 and 2 where the values of $(2g+1)v-l'$ are listed in Table 6 and the obtained Q's are listed in Table 2.

APPENDIX *E*
Calculation of equations (45), (46) and (54)

Substitution of equation (50) with equation (52) into equation (49) gives

$$\begin{aligned}(\bar{F})^2&=\left|\sum_{s=1}^{C} w^{(s)}F_s(\zeta)\right|^2\\ &=\left|\sum_{n=0}^{P-1}\left\{\sum_{s=1}^{C} w^{(s)}\varepsilon_n^{(s)}\right\}\exp\,(i2\pi n\zeta)\right|^2\\ &=\left|\sum_{n=0}^{P-1} f(n)\exp\,(i2\pi n\zeta)\right|^2 \end{aligned} \qquad \text{(A50)}$$

and

$$\begin{aligned}\overline{F^2}&=\sum_{s=1}^{C} w^{(s)}F_s(\zeta)F_s^*(\zeta)\\ &=\sum_{s=1}^{C} w^{(s)}\left|\sum_{n=0}^{P-1}\varepsilon_n^{(s)}\exp\,(i2\pi n\zeta)\right|^2\\ &=\sum_{s=1}^{C} w^{(s)}\left[P+\sum_{m=1}^{P-1}\left\{\sum_{n=0}^{P-1-m}\varepsilon_n^{(s)}\varepsilon_{n+m}^{(s)}\right\}\right.\\ &\qquad\left.\times\exp\,(-i2\pi m\zeta)+\text{conj.}\right]\\ &=P-\sum_{n=0}^{P-1}f^2(n)+\left[\sum_{n=1}^{P-1}f^2(n)\right.\\ &\quad+\sum_{m=1}^{P-1}\left\{\sum_{n=0}^{P-1-m}f(n)f(n+m)\right\}\\ &\quad\left.\times\exp\,(-i2\pi\, m\zeta)+\text{conj.}\right]=P-\sum_{n=0}^{P-1}f^2(n)+(\bar{F})^2\end{aligned}$$

from which we have

$$\overline{I_l'}=\left|\sum_{n=0}^{P-1}f(n)\exp\,(inl\theta)\right|^2=\overline{I}_l\,,\ \theta=\frac{2\pi}{P} \qquad \text{(A51)}$$

$$\overline{F^2}-(\bar{F})^2=P-\sum_{n=0}^{P-1}f^2(n)\,. \qquad \text{(A52)}$$

Equations (A51) and (A52) give equations (53) and (54) respectively.

Substitution of equation (34) with equation (35) into equation (A51) gives, by the use of equation (A7),

$$\overline{I}_l=16v^2\left(\sum_{m_1=0}^{\infty}{}^{*}\,b_{2m_1+1}-\sum_{m_2=0}^{\infty}{}^{**}\,b_{2m_2+1}\right)^2$$

where the symbols * and ** indicate the same meaning as in equation (A13). Thus we can use equation (A14) with equation (A15) and hence $\overline{I}_l$ turns to

$$\overline{I}_l=16v^2\left(\sum_{m=-\infty}^{\infty}b_{2n+1+2mH}^*\right)^2 \qquad \text{(A53)}$$

$$= 16v^2 \left[\int_0^{\tilde{M}/2} \text{erf}(\eta) \times \sum_{m=-\infty}^{\infty} \sin \frac{2\pi}{P} v(2n^*+1+2mH)\eta d\eta \right]^2$$

$$= 16v^2 \left[\int_0^{\tilde{M}/2} \text{erf}(\eta) \sin \frac{2\pi}{P} v(2n^*+1)\eta \times \sum_p \delta(v^*\eta - p) d\eta \right]^2$$

from which we obtain finally the relation

$$\bar{I}_l = (1,4) \left\{ 2 \sum_{p=1}^{p^*} \text{erf}\left(\frac{p}{v^*}\right) \sin 2\pi px + [0;0,1](-1)^{n^*} \text{erf}\left(\frac{\tilde{M}}{2}\right) \right\}^2 \quad \text{(A54)}$$

where n^*, p^*, x and the notation $[a;b,c]$ are given by equations (17), (21), (14) and (23) respectively. Equations (A53) and (A54) give equations (45) and (46) respectively.

From the definition of $f(\xi)$ given by equation (41), $f^2(\xi)$ is newly defined as having a periodicity, $\tilde{M}$, and

$$f^2(\xi) = \text{erf}^2(|\xi|) \quad \text{for} \quad -\frac{\tilde{M}}{2} \le \xi < \frac{\tilde{M}}{2} \quad \text{(A55)}$$

which can be expanded in Fourier series as

$$f^2(\xi) = a_0 + \sum_{m=1}^{\infty} a_m \cos \frac{2\pi}{\tilde{M}} m\xi \quad \text{(A56)}$$

with

$$a_0 = \frac{2}{\tilde{M}} \int_0^{\tilde{M}/2} \text{erf}^2(\eta) d\eta, \quad a_m = \frac{4}{\tilde{M}} \int_0^{\tilde{M}/2} \times \text{erf}^2(\eta) \cos \frac{2\pi}{\tilde{M}} m\eta d\eta . \quad \text{(A57)}$$

Substitution of equation (A56) with equation (A57) into equation (A52) gives

$$\overline{F^2} - (\bar{F})^2 = P - \left(Pa_0 + \sum_{m=1}^{\infty} a_m \sum_{n=0}^{P-1} \cos \frac{2\pi}{P} 2vmn \right)$$

$$= P - \left(Pa_0 + P \sum_{m=1}^{\infty} a_m \delta_{m,qH} \right)$$

$$= P - P \left\{ a_0 + \frac{4}{\tilde{M}} \int_0^{\tilde{M}/2} \text{erf}^2(\eta) \times \sum_{q=1}^{\infty} \cos 2\pi q v^* \eta d\eta \right\}$$

$$= P - P \left[a_0 + \frac{2}{\tilde{M}} \int_0^{\tilde{M}/2} \text{erf}^2(\eta) \times \left\{ \sum_p \delta(v^*\eta - p) - 1 \right\} d\eta \right]$$

$$= P - \left\{ (2,4) \sum_{p=1}^{p^*} \text{erf}^2\left(\frac{p}{v^*}\right) + [0;0,2] \text{erf}^2\left(\frac{\tilde{M}}{2}\right) \right\} . \quad \text{(A58)}$$

Equation (A58) gives the right hand side of equation (54). In deriving both the equations (A54) and (A58) we used the general relation

$$\int_0^a g(x)\delta(x-a)dx = \tfrac{1}{2}g(a) . \quad \text{(A59)}$$

APPENDIX *F*
Remarks on the use of the step function, $S_0(\xi)$

From the definition of $S(\xi)$ in equation (3), we have

$$\begin{cases} S(pP) = 1 \quad p: 0, \pm 1, \pm 2, \ldots \\ S[(2p+1)M] = -1 \quad \text{for complex } APD \text{ structure} \end{cases} \quad \text{(A60)}$$

while, from $S_0(\xi)$ given by equation (5), we have

$$\begin{cases} S_0(pP) = 0 \\ S_0[(2p+1)M] = 0 \quad \text{for complex } APD \text{ structure.} \end{cases} \quad \text{(A61)}$$

Therefore, it is convenient to relate $S_0(\xi)$ to $S(\xi)$ by a conventional expression

$$S(\xi) = S_0(\xi) + S'(\xi) \quad \text{(A62)}$$

where

$$S'(\xi) = \sum_{p=-\infty}^{\infty} \{\delta_{\xi,pP} - (0,1)\delta_{\xi,(2p+1)M}\} . \quad \text{(A63)}$$

In § 3 and Appendix *B*, I_l was calculated not from equation (10) but from equation (11) combined with equation (12). If I_l is calculated by taking a square of $|\psi_l|$ after ψ_l is calculated by using the form of equation (10), we get an incorrect result as shown below.

Let $\psi_l^{(0)}$ be the function which is obtained by substituting $S_0(\xi)$ given by equation (5) into ψ_l in equation (10). Then, using equations (A7), (A13) and (A14), we have

$$\psi_l^{(0)} = \frac{4}{\pi} \sum_{m=0}^{\infty} \frac{1}{2m+1} \sum_{n=0}^{P-1} \sin \frac{2\pi}{P} v(2m+1)n \times \exp\left(i \frac{2\pi}{P} nl\right)$$

$$= i \frac{2P}{\pi} \left(\sum_{n_1=0}^{\infty}{}^{*} \frac{1}{2n_1+1} - \sum_{n_2=0}^{\infty}{}^{**} \frac{1}{2n_2+1} \right)$$

$$= i \frac{2P}{\pi} \sum_{m=-\infty}^{\infty} \frac{1}{2mH+2n^*+1}$$

$$= i(1,2) \cot \pi x \quad \text{(A64)}$$

and hence

$$\psi_l^{(0)} \psi_l^{(0)*} = (1,4) \cot^2 \pi x \quad \text{(A65)}$$

which is different from equation (13).

On the other hand, let ψ_l' be the function which is obtained by substituting $S'(\xi)$ given by equation (A63) into ψ_l in equation (10), then we have

$$\psi'_l = \sum_{n=0}^{P-1} \left[\sum_{p=-\infty}^{\infty} \{\delta_{n,pP} - (0,1)\delta_{n,(2p+1)M}\} \right] \times \exp\left(i\frac{2\pi}{P}nl\right) = 1-(0,1)(-1)^l. \quad \text{(A66)}$$

Therefore, if we put

$$\psi_l = \psi_l^{(0)} + \psi'_l = 1-(0,1)(-1)^l + i(1,2)\cot \pi x,$$

then we obtain

$$I_l = \psi_l \psi_l^* = \begin{cases} 1+\cot^2 \pi x = \dfrac{1}{\sin^2 \pi x} \text{ for Case I} \\ 0 \text{ for Case II with } l\text{:even} \\ 4I_l^* \text{ for Case II with } l\text{:odd} \\ \quad \text{with } I_l^* = 1+\cot^2 \pi x = \dfrac{1}{\sin^2 \pi x}. \end{cases}$$

These results agree with those in equations (13) and (18), and also imply that the expression in equation (F6), *i.e.* equation (7) or equation (10) is incorrect.

In § 3 and Appendix *B*, I_l was calculated by the use of D_m given by equation (12), where we used not $S(\xi)$ but $S_0(\xi)$, and yet we obtained the correct result. If we use $S(\xi)$ defined by equation (A62) in the calculation of D_m and denote it by D_m^* in distinction from D_m in equation (12), then we have

$$\begin{aligned} D_m^* &= \sum_{p=0}^{P-1} S(p)S(p+m) \\ &= \sum_{p=0}^{P-1} \{S_0(p)+S'(p)\}\{S_0(p+m)+S'(p+m)\} \\ &= D_m + D'_m \end{aligned} \quad \text{(A67)}$$

where D'_m represents the remaining three terms not in D_m and is calculated as

$$D'_m = \delta_{m,0} + (0,1)(\delta_{m,0} - 2\delta_{m,M}). \quad \text{(A68)}$$

As a result, the difference between D_m and D_m^* exists only in the cases of $m=0$ and M.

On the other hand, when $m=0$, D_0 is expressed and calculated as

$$D_0 = \sum_{p=0}^{P-1} S^2(p) = P \quad \text{(A69)}$$

because we can calculate $S_0^2(\xi)$, by the similar transformations to those from equation (A5) to equation (A8), as follows:

$$\begin{aligned} S_0^2(\xi) &= \frac{16}{\pi^2} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{1}{(2n+1)(2n'+1)} \\ &\quad \times \sin\frac{2\pi}{P} v(2n+1)\xi \sin\frac{2\pi}{P} v(2n'+1)\xi \\ &= \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = 1. \end{aligned} \quad \text{(A70)}$$

We can see from this result that the singularity existing in the Fourier series given by equation (5) has disappeared by taking a square of $S_0(\xi)$, as is also so for $S(\xi)$.

When $m=M$ for Case II, we can see generally, from equation (5),

$$S_0(\xi+M) = -S_0(\xi)$$

and hence

$$D_M = \sum_{p=0}^{P-1} S_0(p)S_0(p+M) = -\sum_{p=0}^{P-1} S_0^2(p) = -P$$

which gives the correct value of D_M. As a result, D_m defined only by $S_0(\xi)$ as in equation (12) has given the correct result.

But even when we calculate I_l with the form of equation (11) by the use of equation (12), if we change the order of summation as

$$\begin{aligned} I_l &= \sum_{m=0}^{P-1} D_m \cos ml\theta \\ &= \sum_{m=0}^{P-1} \left\{ \sum_{p=0}^{P-1} S_0(p)S_0(p+m) \right\} \cos ml\theta \\ &= \sum_{p=0}^{P-1} S_0(p) \left\{ \sum_{m=0}^{P-1} S_0(p+m) \cos ml\theta \right\}, \end{aligned}$$

then we again obtain an incorrect result like equation (A65).

Thus, when we use Fourier expansion, $S_0(\xi)$, of a step function, $S(\xi)$, we should proceed as follows:

(i) Calculate a given function of $S(\xi)$ by the use of equation (A62) which connects $S_0(\xi)$ with $S(\xi)$ by the correction term, $S'(\xi)$.

(ii) Find the special conditions such that the correction term, $S'(\xi)$, has an influence upon the result. [For example, $m=0$ and M in equation (A68)].

(iii) Examine whether the difference between $S(\xi)$ and $S_0(\xi)$ still exists in the function at the special conditions, or not.

(iv) If the difference $\left\{\begin{matrix}\text{still exists} \\ \text{disappears}\end{matrix}\right\}$ in the function, the correction term is $\left\{\begin{matrix}\text{necessary} \\ \text{unnecessary}\end{matrix}\right\}$.

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