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USE OF A CORRELATION CHOPPER FOR TIME OF FLIGHT NEUTRON SCATTERING (*) PART II : DECONVOLUTION IN THE EXPERIMENTAL CASE

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Résumé. — Dans un article précédent [1] nous avons développé un formalisme matriciel permettant de résoudre facilement, dans le cas idéal, le problème de déconvolution lorsqu'on utilise un chopper statistique dans des expériences de temps de vol. Nous considérons maintenant le cas pratique. La fonction signal émise par un chopper mécanique n'est pas rectangulaire : c'est une fonction triangulaire. Nous déconvoluons la fonction observée Z avec une *séquence inverse*, soit rectangulaire (déconvolution rectangle-triangle), soit triangulaire (déconvolution triangle-triangle). Nous montrons que dans ce cas il y a une perte de résolution par rapport au cas idéal. Ensuite nous considérons les perturbations introduites par l'utilisation d'un dispositif mécanique imparfait et nous montrons qu'il apparaîtra, en diffraction élastique, une *image négative* de la fonction de diffraction due à la variation de la transmission du chopper en fonction de la longueur d'onde. Cet effet peut être corrigé *a posteriori*. Les autres perturbations induisent des pertes de résolution, ou une modulation du bruit de fond.

Abstract. — The deconvolution problem for a correlation chopper in time of flight diffraction experiments has been treated in a previous paper [1] by a matrix formalism. A practical case is now considered since the signal function obtained with a mechanical chopper is not rectangular, but triangular. This observed function Z is deconvoluted by means of either a rectangular *inverse* sequence (rectangle-triangle deconvolution) or a triangular one (triangle-triangle deconvolution). It is shown that there is a loss of resolution. Perturbations arising from the use of an imperfect mechanical device in elastic scattering, give rise to a *negative image* of the diffraction function due to variation of the chopper transmission with wavelength. This effect can be corrected *a posteriori*. The other perturbations give rise to loss of resolution or background modulation.

1. Introduction. — In a previous paper [1] a matrix formalism has been developed to solve the deconvolution problem, considering only the ideal case of a rectangular signal function. In practice, using a mechanical chopper, things are not so ideal. The shape of a neutron pulse is not rectangular, but triangular. The deconvolution problem can now be carried out using rectangular and triangular *inverse* sequences.

In spite of all the precautions taken in constructing a correlation chopper, it cannot be perfect. The usefulness of the matrix formalism is that it allows the expression in mathematically simple terms of all perturbations that may occur and which may affect the observed diffraction function.

2. Deconvolution in the practical case. — **2.1 THE SIGNAL FUNCTION OF A MECHANICAL CHOPPER.** — The neutron pulse emitted by a disc chopper is obtained by a slot of width ΔT crossing a neutron beam that is assumed to have the same width as the slot. The resulting pulse shape is the convolution of two identical rectangular functions $S(t)$, representing the slot and the beam respectively.

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$$S_T(t) = \int_{-\infty}^{+\infty} S_R(\tau) S_R(t - \tau) d\tau \quad (1)$$

where subscript T signifies triangular and R rectangular. Both $S_T(t)$ and $S_R(t)$ are unit functions. $S_T(t)$ is a triangle of full width at half maximum (FWHM) ΔT centered on $t = 0$ as represented in figure 1.

FIG. 1. — Resolution functions of the correlation chopper : a) rectangle-triangle function ; b) triangle-triangle function.

The triangular signal function $S_T(t)$ of the correlation chopper is then :

$$S_T(t) = \sum_{i=0}^{N-1} a_i S_T(t + i \Delta T). \quad (2)$$

If one uses mN analysing channels (m integer) of width $\Delta t = \Delta T/m$, an element of the new sequence $\{a'_i\}_T$ is the integral of $S_T(t)$ in an interval of width Δt about $i \Delta t$.

$S_T(t)$ being a continuous linear function, in such an interval, the element a'_{iT} of the new sequence will be :

$$a'_{iT} = \frac{1}{2} [S_T(i \Delta T) + S_T((i + 1) \Delta T)]. \quad (3)$$

The linear system of equations defined in [1] is :

$$Z = A_T F \quad (4)$$

where A_T is the matrix deduced from sequence $\{a'_i\}_T$

2.2 MATRIX A_T OF A TRIANGULAR SIGNAL FUNCTION. The triangular sequence $\{a'_i\}_T$ is obtained after convolution of the rectangular one by a rectangular function $S_R(t)$ and integration over an interval of time Δt . The corresponding matrix A_T can be written as :

$$A_T = A' T \sigma \quad (5)$$

— A' is the matrix defined in [1] ;

— T is a circulant $mN.mN$ matrix and the product $A' T$ represents the convolution of eq. [2]. The first line of T is :

a) for m even

$$\frac{1}{m} \left| \underbrace{1 \ 1 \ \dots \ 1}_{\frac{m}{2} \text{ terms equal to } 1} \ 0 \ \dots \ 0 \ \underbrace{1 \ \dots \ 1}_{\frac{m}{2} \text{ terms equal to } 1} \right|$$

b) for m odd :

$$\frac{1}{m} \left| \underbrace{1 \ 1 \ \dots \ 1}_{\frac{m+1}{2} \text{ terms equal to } 1} \ 0 \ \dots \ 0 \ \underbrace{1 \ \dots \ 1}_{\frac{m-1}{2} \text{ terms equal to } 1} \right|$$

the other lines are deduced by consecutive circular permutation of one element to the right hand side.

σ is also a circulant $mN.mN$ matrix representing the integration of eq. [3]

$$\sigma = \frac{1}{2} \begin{vmatrix} 1 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 1 & 0 & 0 & \dots & 0 \\ 0 & 0 & 1 & 1 & 0 & \dots & 0 \\ \vdots & & & & & & \\ 1 & 0 & 0 & 0 & 0 & \dots & 1 \end{vmatrix} \quad (6)$$

T and σ are singular matrices. The product T is a symmetric circulant.

One may notice that the matrix K defined in [1] eq. (40) can be written :

$$K = T T^* = T^* T \quad (7)$$

T^* being the transposed matrix of T .

2.3 DECONVOLUTION OF Z WITH RECTANGULAR INVERSE SEQUENCE. — The linear system is now :

$$Z = A' T \sigma F. \quad (8)$$

If one uses the matrix B as defined in [1] and calculates the product BZ , the deconvolution of a triangular Z function by a rectangular function (rectangle-triangle deconvolution) is performed and one obtains as a result F'_k :

$$\begin{aligned} F'_R = BZ &= \frac{2}{m(N+1)} (2A^* - E) Z \\ &= T T^* T \sigma F = \varphi_R F \end{aligned} \quad (9)$$

φ_R is a symmetric circulant which represents the so-called resolution function $\varphi_R(t)$ plotted in figure 1a

$$\varphi_R(t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} S_R(t - t_1) S_R(t_1 - t_2) \times S_R(t_2) dt_1 dt_2. \quad (10)$$

Appendix A gives its analytical expression. Integrating on consecutive intervals of width Δt the calculated diffraction function is :

$$F'_{Rk} = \sum_{i=0}^{mN-1} \varphi_R(k-i) F_i. \quad (11)$$

The calculated diffraction function is the convolution of the real one by the resolution function φ_R of 1,268 ΔT FWHM. There is a loss of resolution with respect to a conventional chopper.

2.4 DECONVOLUTION OF Z WITH TRIANGULAR INVERSE SEQUENCE. — As the effective signal function is a triangular one, one may think that it is necessary to deconvolute using a triangular inverse sequence [3]. This is performed using the corresponding matrix :

$$B_T = B(T\sigma) = (T\sigma) B \quad (12)$$

and :

$$F'_T = T\sigma BZ = \frac{2}{m(N+1)} T\sigma(2A^* - E)F \\ = T\sigma T T^* \sigma F = \varphi_T F \quad (13)$$

φ_T is the representation of the resolution function $\varphi_T(t)$ of figure 1b :

$$\varphi_T(t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} S_R(t - t_1) S_R(t_1 - t_2) \times S_R(t_2 - t_3) S_R(t_3) dt_1 dt_2 dt_3 \quad (14)$$

or more simply :

$$\varphi_T(t) = \int_{-\infty}^{+\infty} \varphi_R(\tau) S_R(t - \tau) d\tau. \quad (15)$$

Its analytical expression is given in Appendix A. As $\varphi_T(t)$ FWHM is 1.444 ΔT , the *triangle-triangle* deconvolution introduces a greater loss in resolution than the *rectangle-triangle* case.

2.5 CONCLUSION. — For *triangle-triangle* deconvolution, b_i values are different from 0 and 1 which are very convenient for computer calculations. So one can perform the first type of deconvolution, and at the end of the experiment a simple convolution symbolised by the matrix product $T\sigma$ can allow for the *triangle-triangle* case.

One may notice that the inferred Gaussian shape of the peaks is affected by the resolution function which is not Gaussian. It is not obvious that *triangle-triangle* deconvolution improves the observed diffrac-

tion function, as although the diagram appears smoother there is an important loss of resolution.

3. Perturbations. — **3.1 INTRODUCTION.** — Neutron pulses are generated by means of a mechanical device which cannot be perfect, in spite of all care taken in construction. In general terms, the experiment can be described by :

$$Z = (A' T\sigma + P) F \quad (16)$$

P being a $mN.mN$ matrix taking into account the deviation between the effective signal function and the ideal one.

When deconvoluting, the result is :

$$F' = BZ = \varphi_R F + BPF = \varphi_R F + f. \quad (17)$$

Since most of the perturbations are small, f appears only as a background modulation. However, if BP is a circulant similar to K , perturbations will be *correlated* with $\{a'_i\}$ and will introduce more important phenomena.

The different imperfection sources are now considered to demonstrate their effect on the observed diffraction pattern.

3.2 NEUTRON BEAM WIDER OR NARROWER THAN THE CHOPPER SLOT. — If the beam is wider, matrix T , in the product $A' T\sigma$, becomes :

$$T = \frac{1}{m} \begin{vmatrix} 0 & \dots & 0 & \varepsilon & 1 & \dots & 1 & \varepsilon & 0 & \dots & 0 \end{vmatrix} \\ \underbrace{(m+2) \text{ non zero terms}} \quad (18)$$

The resolution function will be wider resulting in a loss of resolution.

If the beam is narrower, T becomes :

$$T = \frac{1}{m} \begin{vmatrix} 0 & \dots & 0 & 1 - \varepsilon & 1 & \dots & 1 & 1 - \varepsilon & 0 & \dots & 0 \end{vmatrix} \\ \underbrace{m \text{ non zero terms}} \quad (19)$$

The resolution function will be narrower, and in the limiting case of a point beam will give rise to rectangular pulses.

3.3 DISPLACEMENT OF THE ZERO TIME ELECTRONIC SIGNAL. — The chopper gives an electronic signal t_0 at each revolution [2] which starts the counting of the neutrons. This signal must be reproducible, though its position with respect to the slot may not be known precisely because of the gradual increase of the electronic signal as well as machining inaccuracy. These are of little importance in conventional time of flight.

With a correlation chopper, if there is a shift between the theoretical and the effective position of the signal, there will also be a shift between the emitted and the mathematical signal function. This

shift cannot be measured, but can be expressed by multiplying matrix $A' T$ by matrix D :

$$D = \begin{vmatrix} \varepsilon & 1 - \varepsilon & 0 & 0 & \dots & 0 \\ 0 & \varepsilon & 1 - \varepsilon & 0 & \dots & 0 \\ 0 & 0 & \varepsilon & 1 - \varepsilon & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 - \varepsilon & 0 & 0 & 0 & \dots & \varepsilon \end{vmatrix}. \quad (20)$$

This introduces a loss in resolution, and also a shape asymmetry for peaks defined by only a few points.

3.4 VARIATIONS IN VELOCITY. — The variations in velocity may be of long or short duration.

3.4.1 Long variations of duration. — Their periods are considerably longer than those of the disc. The width ΔT and the sequence origin fluctuate, but ΔT can be considered as a constant over one period. At the end of the experiment a mean value will be observed with a slight broadening of the resolution function.

3.4.2 Short variations of duration. — Their periods are of the same order of magnitude as those of the chopper. If they are asynchronous, a mean value will be observed as in the previous case. If they are synchronous, a matrix form P will need to be used for their representation. Since these short duration velocity variations will not be large the elements of the matrix P will be small so that only a background modulation will be observed.

3.5 INACCURACY IN MACHINING. — Inaccuracy in machining the slots of the mechanical chopper will give rise to a background modulation, in the same way as synchronous short duration speed variations. For example if the slot j is missing P is obtained by j consecutive permutations of the lines of the identity matrix and

$$f = BPF = \frac{4}{m(N+1)} A^* F - \frac{2}{m(N+1)} EF \quad (21)$$

which is very similar to $4/m(N+1) Z$. The background modulation will resemble the undeconvoluted Z function.

3.6 CHOPPER TRANSMISSION FUNCTION. — Contrary to what has been assumed so far, the chopper transmission function is not wavelength independent. The absorbing material of the disc cannot be infinitely thin. Let 1 be its thickness. Neutrons will take a time t to pass through the slot :

$$t \text{ (}\mu\text{s)} = 0.252 \cdot 8.1 \text{ (mm)} \cdot \lambda \text{ (}\text{\AA}\text{)} \quad (22)$$

and the pulse width ΔT will change with wavelength :

$$\Delta T(\lambda) = \Delta T(0) \left[1 - \frac{t}{\Delta T(0)} \right] = \Delta T(0) [1 - \varepsilon(\lambda)]. \quad (23)$$

FIG. 2. — a) Neutron pulse given by a chopper ; b) The same pulse after centering by calibration ; c) The function $S_R(t)$ and its derivative.

$\Delta T(0)$ being the pulse width for an infinitely thin absorber. Figure 2a shows a theoretical triangular pulse $S_T(t, 0)$ and the dotted line the pulse $S_T(t, \lambda)$ for wavelength λ . This is displaced by the time $\Delta T(0) \cdot \varepsilon(\lambda)/2$ which is linear with λ .

It will be assumed that the necessary calibration of the experiment [2] takes into account this displacement, and we suppose that the origin remains the same (Fig. 2b).

A first order perturbation exists when the derivative of $S_T(t, 0)$ with respect to the time is non zero. This can be written :

$$s_T(t, \lambda) = S_T(t, 0) - \frac{\varepsilon(\lambda)}{2} \left| \frac{d}{dt} S_T(t, 0) \right| \quad (24)$$

with a similar expression for the signal function :

$$S_T(t, \lambda) = S_T(t, 0) - \frac{\varepsilon(\lambda)}{2} \left| \frac{d}{dt} S_T(t, 0) \right|. \quad (25)$$

It is shown in Appendix B that the absolute value of the derivative of $S_T(t, 0)$, with respect to the time, is the theoretical rectangular signal function $S_R(t, 0)$, displaced in time $(q - \frac{1}{2}) \Delta T$ for shift register sequences where the displacement q is the number of sequence elements between the largest succession of consecutive non-zero elements and the largest one of consecutive zeros. The effective signal function becomes :

$$S_T(t, \lambda) = S_T(t, 0) - \frac{\varepsilon(\lambda)}{2} S_R[t + (q - \frac{1}{2}) \Delta T] \quad (26)$$

and the perturbation matrix P is :

$$P = -\frac{\varepsilon(\lambda)}{2} AR \quad (27)$$

R being a $mNmN$ matrix representing the shift, obtained by q consecutive circular permutations of the rows of the identity matrix.

The deconvolution result is then :

$$F' = BZ = KT\sigma F - \frac{\varepsilon(\lambda)}{2} KRF. \quad (28)$$

The product RF is a displaced F function.

The thickness of the absorber causes a *negative image* of the spectrum to appear. The diffraction peaks are automatically corrected by the chopper transmission, but the resolution function of the negative peaks is K , whereas it is KT for the diffraction peaks.

One can correct *a posteriori* the observed spectrum by calculating a diffraction function F_k'' :

$$F_k'' = F_k' + \frac{\varepsilon(\lambda)}{2} F_{k-m(q-1/2)}'. \quad (29)$$

In the case of a general (N, n, r) sequence,

$$\left| \frac{d}{dt} S_T(t, 0) \right|$$

is no longer $S_R(t, 0)$ and the whole spectrum may be perturbed by a background modulation.

4. Conclusion. — The advantage of the matrix formalism appears when it becomes necessary to allow for the imperfections of a real system. Due to the triangular shape of the neutron pulses, the observed diffraction function is the convolution of the theoretical curve by a resolution function wider than the elementary pulse. This introduces a loss in resolution and also a modification of the peaks' profiles which may be slightly different from Gaussians.

Most perturbations give rise to a loss of resolution, but short duration synchronous speed variations and inaccuracy in machining the slots may introduce background modulation.

The occurrence of *negative image* of the diffraction peaks, when using shift register sequences is the most important feature. These negative peaks can coincide and hence alter true diffraction peaks. As there are several sequences for a given number N of elements, one must select a sequence with q close to $N/2$, which gives negative peaks far from the true ones. If nevertheless overlapping occurs, the intensities can be corrected knowing the chopper transmission function. In no cases is a transmission correction needed for true unperturbed peaks.

The measurement of the signal function by means of a detector as close as possible to the disc does not improve the deconvolution as compared to the use of a theoretical function. In fact, the measured signal function is a mean value for the wavelength distribution in the incident beam, and the neutron pulses are broadened by the necessary distance between disc and detector.

Appendix A. — 1. RESOLUTION FUNCTION FOR *rectangle-triangle* DECONVOLUTION :

$$\varphi_R(\tau) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} S_R(\tau - t_1) S_R(t_1 - t_2) S_R(t_2) dt_1 dt_2 \quad \left(\tau = \frac{t}{\Delta T} \right)$$

$$\frac{1}{2} \leq |\tau| \leq \frac{3}{2} \quad \varphi_R(|\tau|) = \frac{1}{2} |\tau|^2 + \frac{3}{2} |\tau| + \frac{9}{8}$$

$$0 \leq |\tau| \leq \frac{1}{2} \quad \varphi_R(|\tau|) = -|\tau|^2 + \frac{6}{8}$$

$$|\tau| \geq \frac{3}{2} \quad \varphi_R(|\tau|) = 0.$$

2. RESOLUTION FUNCTION FOR *triangle-triangle* DECONVOLUTION :

$$\varphi_T(\tau) = \int_{-\infty}^{+\infty} S_R(\tau - t_1) \varphi_R(t_1) dt_1$$

$$1 \leq |\tau| \leq 2 \quad \varphi_T(|\tau|) = \frac{1}{6} |\tau|^3 + |\tau|^2 + 2|\tau| + \frac{4}{3}$$

$$0 \leq |\tau| \leq 1 \quad \varphi_T(|\tau|) = \frac{1}{2} |\tau|^3 - |\tau|^2 + \frac{2}{3}$$

$$|\tau| \geq 2 \quad \varphi_T(|\tau|) = 0.$$

Appendix B. — Calculation of $\left| \frac{d}{dt} S_T(t, 0) \right|$

$S_T(t, 0)$ is given in eq. (2), then :

$$\left| \frac{d}{dt} S_T(t, 0) \right| = \left| \frac{d}{dt} \left\{ \sum_{i=0}^{N-1} a_i \int_{-\infty}^{+\infty} S_R(\tau) S_R(t + i \Delta T - \tau) d\tau \right\} \right|$$

where $S_R(t)$ is the rectangular function of figure 2c and a_i being positive :

$$\left| \frac{d}{dt} S_T(t, 0) \right| = \sum_{i=0}^{N-1} a_i \int_{-\infty}^{+\infty} S_R(\tau) \left| \frac{d}{dt} S_R(t + i \Delta T - \tau) \right| d\tau$$

$S_R(t)$ having a discontinuity for $t = \pm \frac{\Delta T}{2}$ and being constant elsewhere :

$$\left| \frac{d}{dt} S_R(t) \right| = \left| \delta\left(t + \frac{\Delta T}{2}\right) - \delta\left(t - \frac{\Delta T}{2}\right) \right|$$

$\delta(t)$ is a Dirac function.

Then we find :

$$\left| \frac{d}{dt} S_T(t, 0) \right| = \sum_{i=0}^{N-1} a_i \left| S_R\left(t + i \Delta T + \frac{\Delta T}{2}\right) - S_R\left(t + i \Delta T - \frac{\Delta T}{2}\right) \right|$$

which is equivalent to :

$$\left| \frac{d}{dt} S_T(t, 0) \right| = \sum_{i=0}^{N-1} |a_{i+1} - a_i| S_R\left(t + i \Delta T - \frac{\Delta T}{2}\right)$$

the value of $|a_{i+1} - a_i|$ is 0 or + 1, and can be written as $(a_{i+1} + a_i) \bmod 2$.

A sequence $\{C_j\}$ can be defined in this way. In the case of shift register sequence, considering the way they are constructed [4], it is easy to show that $\{C_j\}$ is identical with $\{a_i\}$ for a shift.

Looking at a shift register sequence, with $N = 2^p - 1$, one can see that the largest succession of consecutive elements + 1 includes p terms, and the largest succession of zeros includes $(p - 1)$ terms. Taking the beginning of the first succession as the origin, one finds :

$$\begin{array}{cccccccc} & & \overbrace{p \text{ consecutive } 1} & & & & & \\ \{a_i\} & = & 1 & 1 & \dots & 1 & 1 & 0 \dots 0 \\ \{a_{i+1}\} & = & 1 & 1 & \dots & 1 & 0 & \dots \dots 1 \\ \{a_{i+1} + a_i\} \bmod 2 & = & 0 & 0 & \dots & 0 & 1 & \dots \dots 1 \\ & & \underbrace{(p-1) \text{ consecutive}}_{\text{zero}} & & & & & \end{array}$$

This gives the shift between sequence $\{C_j\}$ and $\{a_i\}$ as the number of sequence elements between the largest successions of 1 and the largest succession of 0.

In the case of other sequences, this is no longer true and $\{a_{i+1} + a_i\} \bmod 2$ is very different from $\{a_i\}$.

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