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Datenverarbeitungszentrale

Investigations on the Correlation Method in Time-of-Flight Experiments

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Neutron Inelastic Scattering Research

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Abstract

The attempt to increase the time utilization of the reactor beam in time-of-flight experiments has resulted in the construction of pseudostatistical chopping devices in some laboratories. So far choppers with an average transmission of about one half have been used. In this paper the problem of choosing an optimal chopping mechanism is attacked by minimizing a suitable defined statistical error of the time-of-flight distribution. This condition leads to a whole class of choppers with different time utilization of the reactor beam. An extensive error analysis for these choppers is given.

Frequently the analysis of scattering experiments requires integration over a certain part of the time-of-flight distribution. It is shown that the gaussian law of error propagation is not strictly valid when the spectrum is obtained by a correlation method. However, in most practical cases the deviations are small.

Some consideration is given to the feasibility of a pseudostatistical double chopper for slow neutrons, which allows to use all energies in the incident beam and measure all scattered energies simultaneously. The statistical accuracy for such an experiment is discussed. Some experiments were simulated on a computer in order to back up the theoretical investigations.

Zusammenfassung

Der Versuch, die Zeitausnutzung des Reaktorstrahls für Flugzeitexperimente zu verbessern, führte an einigen Reaktoren zur Aufstellung von pseudostatistischen Neutronenmodulatoren. Die Durchlässigkeit dieser Neutronenchopper betrug bisher 50 %. In diesem Report wird die Frage nach einem optimalen pseudostatistischen Chopper untersucht, in dem ein geeignet definierter statistischer Fehler der Flugzeitverteilung zum Minimum gemacht wird. Diese Fragestellung führt zu einer natürlichen Erweiterung der bisher bekannten Systeme, insbesondere zu solchen mit einer Durchlässigkeit, die von 50 % verschieden ist. Eine ausführliche Fehlerdiskussion dieser Chopper wird durchgeführt.

Des öfteren muß bei der Auswertung von Streuexperimenten über einen bestimmten Bereich der Flugzeitverteilung integriert werden. Es wird gezeigt, daß das Gauß'sche Fehlerfortpflanzungsgesetz für Spektren, die über die Korrelationsmethode erhalten wurden, nicht mehr gilt. Für die meisten praktischen Fälle sind die Abweichungen jedoch klein.

Weiterhin wird ein pseudostatistischer Doppelchopper für langsame Neutronen untersucht, der es ermöglicht, alle Energien des einfallenden Reaktorstrahls zu benutzen und gleichzeitig sämtliche gestreuten Energien zu messen. Mit Hilfe eines Computers wurden einige Experimente simuliert, die die theoretischen Untersuchungen bestätigen.

1. Introduction

Pseudorandom pulsing of the reactor beam has proved to be a powerful method in slow neutron scattering experiments, especially when the signal to background ratio is small and the time-of-flight spectrum consists of a small number of peaks. Mechanical and magnetic choppers with a time utilisation of about one have been built at some laboratories [1] [2] [3]. The mechanical chopper at the FR 2 was put into operation about 1 1/2 years ago and has since been applied successfully to powder diffraction and phonon measurements [4] [5].

In this paper we want to present various recent investigations about the application of the correlation method to slow neutron time-of-flight experiments.

In the first part (section 2) the extension of the present systems to a wider class of choppers with different time utilization of the reactor beam is dealt with. In section 3 an error analysis is given for integral intensities when the spectrum is obtained by a correlation method. Finally we shall investigate the possibility to apply the correlation technique to a double chopper system (section 4).

As this report comprises quite different subjects we shall treat the corresponding sections largely independent from each other.

2. Pseudo-Statistical Neutron Beam Modulation with different Time Utilization*

2.1 Formulation of the problem

A sequence of pulses can be generated from a neutron beam by a rotating disc of constant angular frequency made from neutron absorbing material and having a pattern of slits and bridges**. The width of both slits and bridges is assumed to be an integral multiple of the width of a unit slit. Moreover we assume in our idealized model an infinitely small neutron beam which is periodically chopped by the rotating disc into a sequence of rectangular pulses. If the period of the measurement is T, the following relation holds for the counting rate Z(t) at the detector and the background U(t)

$$Z(t) = \int_0^T F(s)\, S(t-s)\, ds + U(t) \quad . \qquad (2.1)$$

In this equation F(t) is the product of the scattering propability and the intensity of the beam which we will call time-of-flight distribution for short. The function S(t) is periodical with the period T and describes the modulation of the intensity of the neutron beam taking only the values 1 and 0. In practical application Z(t) is counted in a multichannel analyzer, whose width $\Delta t = T/N$ has been selected according to the width of a unit slit of the chopper. Thus (2.1) results in the following system of linear equations

$$Z_j - U_j = \sum_{i=1}^{N} S_{j-i}\, F_i = \sum_{i=1}^{N} S_{ij}\, F_i \qquad (j = 1,2,\ldots\ldots,N) \quad . \qquad (2.2)$$

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* A more detailed discussion on this subject is given in Ref. [6].

** In the following we shall use the example of a mechanical chopper. Of course, these considerations are valid for any kind of chopping device.

The matrix

$$S = (S_{ji}) = (S_{j-i}) = \begin{pmatrix} S_N & S_{N-1} & S_{N-2} & \cdots\cdots & S_1 \\ S_1 & S_N & S_{N-1} & \cdots\cdots & S_2 \\ \cdot & & & & \\ \cdot & & & & \\ \cdot & & & & \\ S_{N-1} & S_{N-2} & S_{N-3} & \cdots\cdots & S_N \end{pmatrix}$$

is a circulant. In equation (2.2) the counting rates Z_j and U_j are directly measured physical quantities and we assume that they are poisson distributed with a standard deviation of $\sqrt{Z_j}$ and $\sqrt{U_j}$. When (2.2) has been solved for the F_i, the standard deviation of Z_j and U_j will generate a standard deviation ΔF_i of the time-of-flight distribution F_i. It seems logical to ask for a function S(t) which minimizes the sum $\Sigma \Delta F_i^2$.

We call a chopper a binary chopper, if S_i takes only the values 0 (bridge) and 1 (slit). If there are exactly N unit slits and unit bridges and K unit slits, the time utilization will be $x = K/N$. For a (N,K)-chopper the total counting rate $Z_{tot} = \Sigma Z_j$ is

$$Z_{tot} = N \cdot F_{tot}(x + \alpha) \quad , \tag{2.3}$$

with $\alpha = U_j/F_{tot}$ and $F_{tot} = \Sigma F_i$ is the total time-of-flight distribution of a conventional chopper with the length N.

2.2 Error Minimization for Binary Choppers

The system (2.2) has a unique solution for F_i if the inverse of the matrix $S = (S_{j-i})$ exists. In [6] we have indicated necessary and sufficient conditions for the existence of the inverse $S^{-1} = (\sigma_{lj})$ of the circulant S and prove that the inverse is a circulant too. In the following we shall assume that the inverse $S^{-1} = (\sigma_{lj}) = (\sigma_{l-j})$ exists. In this case we get the solution of (2.2)

$$F_l = \sum_{j=1}^{N} \sigma_{l-j} (Z_j - U_j) \quad . \tag{2.4}$$

As F_l is a linear combination of the Z_j and U_j, it is poisson distributed with a standard deviation

$$\Delta F_l = (\sum_{j=1}^{N} \sigma_{l-j}^{2} (Z_j + U_j))^{1/2} \quad . \tag{2.5}$$

We now define

$$\Delta = (\sum_{i=1}^{N} \Delta F_i^{2})^{1/2} \tag{2.6}$$

which can easily be calculated

$$\Delta = (K \cdot \sum_{i=1}^{N} \sigma_i^{2})^{1/2} \cdot (\frac{F_{tot}(x + 2\alpha)}{x})^{1/2} \quad . \tag{2.7}$$

We now ask for binary choppers which can minimize Δ . This leads to the following problem: Given the integers N,K with $K < N$,

which sequence $\{S_i\}$, $i = 1,2,\ldots,N$ consisting of N-K zeros and K ones will minimize $\Sigma\, \sigma_i^2$.
As derived in [6] it can be shown that $\Sigma\, \sigma_i^2$ is a minimum if

$$\sigma_i = \begin{cases} 1/K & \text{for } S_{N-i} = 1 \\ \frac{1-K}{K(N-K)} & \text{for } S_{N-i} = 0 \end{cases} \quad . \tag{2.8}$$

For the minimum we obtain

$$\text{Min} \sum_{i=1}^{N} \sigma_i^2 = \frac{1}{K}\left(1 + \frac{(K-1)^2}{K(N-K)}\right) \quad . \tag{2.9}$$

For certain combinations of the parameters (N,K) the solution of this minimum problem is given by [7, Chapter 9] in form of difference sets.

2.3 Pseudo-Statistical Binary Sequences for different Duty Cycles

In 1956 Marshall Hall, Jr. [8] presented a survey of difference sets for $0 < K < 50$. For $N < 1000$ there are 127 different parameters for which difference sets are known today. Out of these, 94 have a time utilization $x < \frac{1}{2}$, 4 have $x < \frac{1}{3}$, 10 have $x < \frac{1}{4}$, 3 have $x < \frac{1}{5}$ etc.. The pseudostatistical choppers used to this day correspond to one type of difference sets called Hadamard difference sets. They play a special role in the error analysis of pseudo-statistical choppers, as we will see in section 2.4. As an example the difference set (40,13) is used for a chopper shown in Fig. 1. In [6] we gave a survey of all known difference sets for $N < 1000$.

2.4 Error Analysis of Pseudo-Statistical Choppers

After a rather lengthy calculation that will be omitted here we arrive at the following relation for the absolute error ΔF_l for the general class of statistical choppers

$$\Delta F_l^{\,2} = \frac{K-1}{K(N-K)} \left[\frac{N-2K+1}{K-1} F_l + F_{tot}\left(1 + 2\alpha \frac{KN-2K+1}{K(K-1)}\right)\right] \qquad (2.10)$$

or approximately

$$\Delta F_l^{\,2} \approx \frac{1}{N(1-x)} \left[\frac{1-2x}{x} F_l + F_{tot}\left(1 + \frac{2\alpha}{x}\right)\right] \quad . \qquad (2.11)$$

It is easily seen from (2.10) that for $K = \frac{N+1}{2}$ the error ΔF_l is independent of F_l.
However in cases where $F_l \ll F_{tot}$ and x is not too small ΔF_l varies only slightly over the spectrum and therefore can be approximated rather well by

$$\Delta F_l^{\,2} \approx \frac{1}{1-x} \cdot \overline{F} \cdot \left(1 + \frac{2\alpha}{x}\right) \qquad (2.12)$$

where $\overline{F} = \frac{1}{N} \cdot F_{tot}$ is the average of the F_i.
From Eq. (2.12) we obtain the following table of α-intervals and corresponding optimum time utilizations of pseudo-statistical choppers.

α-Interval	Optimum x
$1/2 < \alpha$	1/2
$2/10 < \alpha < 1/2$	1/3
$1/22 < \alpha < 1/10$	1/4
$1/46 < \alpha < 1/22$	1/5
$1/82 < \alpha < 1/46$	1/7
⋮	⋮

If slits and bridges are interchanged a class of chopper with $x > \frac{1}{2}$ can be constructed. However it does not seem to be meaningful to use such choppers, since it can be shown, that the error ΔF_1 is always smaller for $x < \frac{1}{2}$ than for the complementary chopper with $x > \frac{1}{2}$.

The error ΔF_j for a conventional chopper experiment is given by

$$\Delta F_{j_{conv}} = [F_j + 2\alpha\, F_{tot}]^{1/2} \tag{2.13}$$

Pseudo-statistical pulsing will be superior to the conventional method if

$$\frac{F_{j_{stat}}}{F_{j_{conv}}} = \left[\frac{1}{1-x} \cdot \frac{F(1+\frac{2\alpha}{x})}{F_j + 2\alpha\, F_{tot}}\right]^{1/2} < 1 \tag{2.14}$$

or

$$\frac{F_j}{F} + 2\,\frac{U_j}{F} > \frac{1}{1-x}\left(1 + \frac{2U_j}{K \cdot F}\right). \tag{2.15}$$

Eq. (2.15) is illustrated in Fig. 2. The different straight lines separate the regions, where a conventional chopper (inside) or a pseudostatistical (N,K) chopper (outside) will be better.

The reciprocal square of Eq. (2.14) is just the gain factor γ, which indicates the reduction in measuring time of a correlation experiment compared with the conventional method. Fig. 3 shows this gain factor for N = 100 as a function of α for same values of K. A number of gain factors for α = 0.1 and N = 100 is given below.

x	1/2	1/3	1/4	1/5	1/10
γ	7.14	8.33	8.33	8.0	6.00

In this example the chopper with $x = 1/3$ or $x = 1/4$ is about 17 % better than the one with $x = 1/2$.

In the limit of extremely high background we obtain

x	1/2	1/3	1/4	1/5	1/10
γ	25	22.22	18.75	16	9

This tells us that the optimum is to choose a chopper with a time utilization 1/2 if the background is high.

3. Error analysis for Integrated Intensities

In certain applications of the time-of-flight method it is necessary to determine the integrated intensities of different parts of the measured spectrum. We shall call the total intensity of α_o adjacent channels beginning at channel number k

$$F_k^{\alpha_o} = \sum_{\alpha=0}^{\alpha_o - 1} F_{k+\alpha} \tag{3.1}$$

and the corresponding absolute statistical error is $\Delta F_k^{\alpha_o}$.
In an experiment with a conventional chopper the spectrum of interest is directly given by the channel contents of the time analyzer. As the counting rates in different channels are

indepent, $\Delta F_k^{\alpha_o}$ is given by

$$F_k^{\alpha_o} = \left[\sum_{\alpha=0}^{\alpha_o - 1} (\Delta F_{k+\alpha})^2 \right]^{1/2} \tag{3.2}$$

If the same experiment is performed with the correlation technique the F_k are obtained by a complicated evaluation procedure from the measured spectrum Z_i. Therefore we cannot assume a priori that they can be treated as independent quantities.
This rises the question how $\Delta F_k^{\alpha_o}$ can be calculated for a pseudo-statistical chopper experiment.

As in the previous section we shall assume a rectangular signal sequence S_i. However we will consider only the special case of zero background and a time utilization of $\frac{N+1}{2}$. Then the counting rate in the time analyzer is given by

$$Z_i = \frac{1}{2} \left[\sum_{l=1}^{N} F_l + \sum_{l=1}^{N} S_{i-l} F_l \right] \tag{3.3}$$

where S_i satisfies the conditions*

$$\sum_{i=1}^{N} S_i = 1 \tag{3.4}$$

and

$$\sum_{i=1}^{N} S_i S_{i+k} = \begin{cases} N & k = 0 \\ -1 & k \neq 0 \end{cases} \quad . \tag{3.5}$$

The time-of-flight distribution F_k is obtained as

$$F_k = \frac{2}{N+1} \sum_{i=1}^{N} S_i Z_{i+k} \tag{3.6}$$

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*Contrary to the previous section S_i assumes the values $\pm$ 1.

with an absolute statistical error of

$$\Delta F_k = \sqrt{2\,\frac{N}{N+1}\,\bar{F}} \quad . \tag{3.7}$$

Inserting Eqs. (3.6) into (3.1) yields

$$F_k^{\alpha_o} = \frac{2}{N+1} \sum_{i=1}^{N} \sum_{\alpha=0}^{\alpha_o} S_i\, Z_{i+k+\alpha} = \frac{2}{N+1} \sum_{i=1}^{N} \sum_{\alpha=0}^{\alpha_o} S_{i-\alpha}\, Z_{i+k} \quad . \tag{3.8}$$

Hence

$$\begin{aligned} F_k^{\alpha_o} &= \frac{2}{N+1}\left[\sum_{i=1}^{N} Z_{i+k} \left(\sum_{\alpha=0}^{\alpha_o-1} S_{i-\alpha}\right)^2\right]^{1/2} \\ &= \frac{\sqrt{2}}{N+1}\left[N\bar{F} \sum_{i=1}^{N} \left(\sum_{\alpha=0}^{\alpha_o-1} S_{i-\alpha}\right)^2 + \sum_{l=1}^{N} \sum_{i=1}^{N} S_{i-l+k}\, F_l \left(\sum_{\alpha=0}^{\alpha-1} S_{i-\alpha}\right)^2\right]^{1/2} . \end{aligned} \tag{3.9}$$

In the second line of (3.9) expression (3.3) was inserted.

Using the relations

$$\sum_{l=1}^{N} \sum_{i=1}^{N} S_{i-l-k}\, F_l = N\bar{F} \tag{3.10}$$

and

$$\sum_{i=1}^{N} \left(\sum_{\alpha=0}^{\alpha_o-1} S_{i-\alpha}\right)^2 = \alpha_o \cdot (N+1-\alpha_o) \tag{3.11}$$

we obtain

$$\Delta F_k^{\alpha_o} = \frac{\sqrt{2}}{N+1} \left[N\bar{F}\alpha_o(N-\alpha_o+2)+2G \right]^{1/2} , \tag{3.12}$$

where

$$G = \sum_{l=1}^{N} F_l \sum_{i=1}^{N} S_{i-l+k} \sum_{\substack{\alpha=0 \\ \alpha < \alpha'}}^{\alpha_o-2} \sum_{\alpha'=1}^{\alpha_o-1} S_{i-\alpha} S_{i-\alpha'} . \tag{3.13}$$

For further simplification of expression 3.13 we make use of the relation

$$S_{i-\alpha} S_{i-\alpha'} = -S_{i-\beta(\alpha'-\alpha)} \quad \alpha \neq \alpha' \neq \beta(\alpha'-\alpha) . \tag{3.14}$$

This relation is valid at least for those sequences we are considering in this section [9]. An example for Eq. (3.14) is given in Fig. 4 for N=15 elements. One recognizes that when $\alpha'-\alpha$ runs through all possible values, so does β, however in a quasirandom way. Applying (3.14) to (3.13) and using (3.5) yields

$$G = -\sum_{l=1}^{N} F_l \sum_{i=1}^{N} S_{i-l+k} \sum_{\alpha=0}^{\alpha_o-2} \sum_{\alpha'=1}^{\alpha_o-1} S_{i-\beta(\alpha'-\alpha)}$$

$$= \sum_{l=1}^{N} \sum_{\alpha=0}^{\alpha_o-2} \sum_{\alpha'=1}^{\alpha_o-1} F_l - (N+1) \sum_{\substack{l=1 \\ l=k+\beta(\alpha'-\alpha)}}^{N} \sum_{\alpha=0}^{\alpha_o-2} \sum_{\alpha'=1}^{\alpha_o-1} F_l . \tag{3.15}$$

The double sum over α and α' contains $\frac{1}{2}\alpha_o(\alpha_o-1)$ terms. When we introduce a new index $m(\beta)$ to label those $\frac{1}{2}\alpha_o(\alpha_o-1)$ values of F for which $l=k+\beta(\alpha'-\alpha)$ is fullfilled we finally get

$$G = \frac{1}{2}\alpha_o(\alpha_o-1)\cdot N\bar{F} - (N+1) \sum_{m=1}^{\frac{1}{2}\alpha_o(\alpha_o-1)} F_{k+m(\beta)} \tag{3.16}$$

or

$$\Delta F_k^{\alpha_o} = \sqrt{2 \frac{N}{N+1} \bar{F}} \left[\alpha_o - \frac{2}{N\bar{F}} \sum_{m=1}^{\frac{1}{2}\alpha_o(\alpha_o-1)} F_{k+m(\beta)} \right]^{1/2} . \qquad (3.17)$$

The term before the brackets is just the error for one channel. If we neglect the sum inside the brackets we get the usual law of error propagation for independent F_k. In general $\Delta F_k^{\alpha_o}$ depends on the shape of the spectrum and has to be worked out for each measurement. However, two special cases can be derived easily from Eq. (3.17)

α) F_k = const = F :

$$\Delta F_k^{\alpha_o} = \sqrt{2 \frac{N}{N+1} \bar{F}} \left[\alpha_o \left(1 - \frac{\alpha_o - 1}{N}\right) \right]^{1/2} . \qquad (3.18)$$

ß) $\alpha_o = N$, which means integration over the total spectrum. As in the sum over m each value F_k appears $\frac{1}{2}(N-1)$ times we obtain

$$\Delta F_k^N = \sqrt{2 \frac{N}{N+1} \bar{F}} \left[N-(N-1) \right]^{1/2} = \sqrt{2 \frac{N}{N+1} \bar{F}} . \qquad (3.19)$$

Of course, this result could have been obtained in a much simpler way: If one is only interested in the total intensity it is not necessary to do a time-of-flight analysis at all. The use of a conventional or pseudostatistical chopper just reduces the intensity of the reactor beam by a factor $\frac{1}{N}$ or $\frac{1}{2}\frac{N+1}{N}$ respectively, which means that the ratio of the statistical errors must be

$$\frac{\Delta F^N_{stat.}}{\Delta F^N_{conv.}} = \sqrt{\frac{2}{N+1}}, \qquad \text{or} \quad \Delta F^N_{stat.} = \sqrt{\frac{2}{N+1}} \cdot \sqrt{N\bar{F}} = \sqrt{2 \frac{N}{N+1} \bar{F}}$$

This is identical to Eq. (3.19).

Fig. 5 shows the absolute error of the integrated intensity as a function of the interval width for an experiment with N=15 and F_k=const. according to Eq. (3.18). The dashed line would have been obtained under the assumption that the F_k are independent. The circles and crosses were calculated for spectra consisting of one single peak and two peaks respectively. It is seen that Eq. (3.18) will be a rather good approximation for most practical cases.

4. Investigations on a Pseudorandom Double Chopper

4.1 Principle of the Measurement

The successful application of the pseudorandom beam modulation technique to slow neutron time-of-flight experiments suggests the idea to use this principle twice in order to determine the energies of incident and scattered neutron simultaneously. Fig. 6 shows the scheme of such an experimental setup where two mechanical choppers with pseudorandom absorption patterns are used. The counting rate in the detector recorded as a function of time and relative phase between the two rotors, is then given by

$$Z(t,\varphi) = \frac{1}{4} \int_0^{T_1} d\tau_1 \int_0^{T_2} d\tau_2 \, \tilde{F}(\tau_1,\tau_2) \, \tilde{S}_1(t-\tau_2-\alpha\tau_1+\varphi) \, \tilde{S}_2(t-\tau_2(\alpha+1)\tau_1)+U \qquad (4.1)$$

where

$$\tilde{F}(\tau_1,\tau_2) = \frac{1}{\Delta t_1 \Delta t_2} I_o(\tau_1) \, F(\tau_1,\tau_2) \; . \qquad (4.2)$$

$I_o(\tau_1)$ is the intensity of the reactor beam and Δt_1 and Δt_2 are the smallest slid-widths of the first and second rotor. $F(\tau_1,\tau_2)$ is proportional to the double differential cross-section $\sigma(E_1 \rightarrow E_2,\vartheta)$.

With definition (4.2) the transfer function $I_o(\tau_1)\ F(\tau_1,\tau_2)$ is identical to the counting rate obtained with a conventional double chopper, where each of the two rotors has a single slid of width Δt_1 and Δt_2 respectively. The transmissionsfunctions

$$\frac{1}{2}\tilde{S}_{1,2}(t) = \frac{1}{2}(1 + S_{1,2}(t))$$

are characterised by the periods $T_{1,2}$ which are integral multiples $N_{1,2}$ of $\Delta t_{1,2}$. α measures the distance of the sample from the second rotor in units of the distance L_1 between the two rotors, and U is a time-independent background. L_1, L_2, T_1, T_2, N_1, N_2 have to be chosen suitably that overlap is avoided and the required time resolution is obtained.

In principle $F(\tau_1,\tau_2)$ can be obtained from the two dimensional field $Z(t,\varphi)$ by an inversion of Eq. (4.1).

For the following considerations we restrict ourselves to the case of two identical rotors spinning at the same angular velocity. The phase is changed either continuously or in small steps, however, one has to ensure, that all possible phase differences occur equally frequent during the course of the experiment. In this case it is possible to reconstruct $I_o(\tau_1)\ F(\tau_1,\tau_2)$ from $Z(t,\varphi)$ by the cross correlation technique.

4.2 Reconstruction of the Transferfunction

For simplicity we shall assume that the absorption pattern on the individual rotor has an average transmission of $\frac{1}{2}\,\frac{N+1}{N}$ and that the reactor beam is infinitely small e.g. the signalfunction S(t) is rectangular. Furthermore we neglect at the moment the small distance between the sample and the second rotor (α=0).

Then $Z(t,\varphi)$ is given by

$$Z(t,\varphi) = \frac{1}{4} \int_0^T d\tau_1 \int_0^T d\tau_2 \, \tilde{F}(\tau_1,\tau_2) \, S(t-\tau_2+\varphi) \, S(t-\tau_2-\tau_1) + U \tag{4.3}$$

with

$$\tilde{F}(\tau_1,\tau_2) = \frac{1}{\Delta t^2} \, I_o(\tau_1) \, F(\tau_1,\tau_2) \, . \tag{4.4}$$

We shall need the following relations:

$$\int_0^T S(t) \, dt = \Delta t \tag{4.5}$$

$$\emptyset(t) = \frac{1}{T} \int_0^T \tilde{S}(t+\tau) \, S(\tau) \, d\tau \tag{4.6}$$

$$\int_0^T \emptyset(t) \, dt = \frac{N+1}{N} \Delta t \tag{4.7}$$

$\emptyset(t)$ is the resolution function of a single pseudostatistical chopper [2].

In order to obtain $\tilde{F}(\tau_1,\tau_2)$ the cross correlation procedure is applied twice:

$$\Psi_1(t,\varphi_1) = \frac{1}{T} \int_0^T Z(t,\varphi) \, S(\varphi+\varphi_1) \, d\varphi \quad , \tag{4.8}$$

$$\Psi_2(t,\varphi_2) = \frac{1}{T} \int_0^T \Psi_1(t+\varphi_1,\varphi_1) \, S(\varphi_1-\varphi_2) \, d\varphi_1 \quad . \tag{4.9}$$

Inserting (4.3) into (4.8) yields

$$\psi_1(t,\varphi_1) = \frac{1}{4}\int_0^T d\tau_1 \int_0^T d\tau_2\ \tilde{F}(\tau_1,\tau_2)\ \emptyset(t-\tau_2-\varphi_1)\ S(t-\tau_2-\tau_1)+\frac{U}{N} \qquad (4.10)$$

and from (4.9) and (4.10) we get

$$\psi_2(t,\varphi_2) = \frac{1}{4}\int_0^T d\tau_1 \int_0^T d\tau_2\ \tilde{F}(\tau_1,\tau_2)\ \emptyset(t-\tau_2)\ \emptyset(t+\varphi_2-\tau_2-\tau_1)+\frac{U}{N^2}\ . \qquad (4.11)$$

The second cross correlation is essentially the time-of-flight distribution $\tilde{F}(\tau_1,\tau_2)$ folded with the resolution functions of the two rotors.

If $\tilde{F}(\varphi_1,\varphi_2)$ is variing only slightly within a time interval Δt, it can be taken out of the integrals and we obtain

$$\psi_2(t,\varphi_2) = \frac{1}{4}\left(\frac{N+1}{N}\right)^2 \Delta t^2\ \tilde{F}(\varphi_2,t) + \frac{U}{N^2} \quad ,$$

whence

$$I_o(\varphi_2)\ F(\varphi_2,t) = 4\left(\frac{N}{N+1}\right)^2 \psi_2(t,\varphi_2) - \frac{4\ U}{(N+1)^2} \quad . \qquad (4.12)$$

Performing the same calculations without the neglection of α yields

$$I_o(\varphi_2)\ F(\varphi_2,\ t-\alpha\varphi_2) = 4\left(\frac{N}{N+1}\right)^2 \psi_2(t,\varphi_2) - \frac{4\ U}{(N+1)^2} \quad . \qquad (4.13)$$

It is seen from Eq. (4.12) that the influence of a time independent background is reduced by a factor $\left(\frac{2}{N+1}\right)^2$ compared with a conventional double chopper experiment. This is simply caused by the much better time utilization of the reactor beam, which is increased by a factor $\frac{N+1}{2}$ for each rotor.

If we insert Eqs. (4.8) and (4.9) into (4.12) we obtain the final relation between the transfer function $F(\tau_1,\tau_2)$ and the counting rate at the detector:

$$I_o(\varphi_2)\ F(\varphi_2,t) = 4\left(\frac{N}{N+1}\right)^2 \frac{1}{T^2} \int_0^T d\varphi_1 \int_0^T d\varphi\, Z(t+\varphi_1,\varphi)\ S(\varphi+\varphi_1)\ S(\varphi_1-\varphi_2) - \frac{4\ U}{(N+1)^2} \qquad (4.14)$$

In practical applications the recording of the counting events is done by a two dimensional time analyser with a finite channel width, which we shall assume to be Δt. Therefore $Z(t,\varphi)$ will consist of N·N discrete values and all integrals in the calculations above have to be replaced by sums.
Eq. (4.14) has then to be rewritten as

$$I_o(i)\ F(i,j) = 4\ \frac{1}{(N+1)^2} \sum_{p1} \sum_{p} Z(i+p_1,p)\ S(p+p_1)\ S(p_1-i) - \frac{4\ U}{(N+1)^2} \qquad (4.15)$$

4.3 Error Analysis

From Eq. (4.15) the absolute statistical error is obtained as

$$\Delta(I_o(i)\ F(i,j)) = \frac{4}{(N+1)^2}\left[\sum_{p_1}\sum_{p} (Z(i+p_1,p)+U)\right]^{1/2}$$

$$= \frac{4}{(N+1)^2}\left[Z_{tot} + N^2\ U\right]^{1/2} \qquad (4.16)$$

The total counting rate Z_{tot} can be determined from Eq. (4.3), which yields

$$Z_{tot} = \frac{1}{4} N^2 (N+1)^2 \cdot \overline{I_o F} + N U^2 \quad , \tag{4.17}$$

where

$$\overline{I_o F} = \frac{1}{N^2} \sum_i \sum_j I_o(i) F(i,j) \tag{4.18}$$

is the average of $I_o(i) F(i,j)$ over the total range of the incident and scattered energies.

Hence

$$\Delta(I_o(i) F(i,j)) = 2 \frac{N}{N+1} \left[\overline{I_o F} + \frac{8 U}{(N+1)^2} \right]^{1/2} . \tag{4.19}$$

If the same experiment is carried out with a conventional double chopper the statistical error is given by

$$\Delta(I_o(i), F(i,j)) = \left[I_o(i) F(i,j) + 2 U \right]^{1/2} . \tag{4.20}$$

Therefore we obtain for the ratio of statistical errors of both types of experiments

$$\frac{\Delta \text{pseudostat.}}{\Delta \text{conv.}} = 2 \frac{N}{N+1} \left[\frac{\overline{I_o F} + \frac{8 U}{(N+1)^2}}{I_o(i) F(i,j) + 2U} \right]^{1/2} \tag{4.21}$$

An experiment with pseudorandom pulsing will therefore be superior to the conventional method if

$$I_o(i) F(i,j) > 4 \overline{I_o F} - 2 U \quad , \tag{4.22}$$

valid for $N \gg 1$.

The same experiment can also be performed with a single pseudo-statistical chopper for the energy analysis of the scattered neutrons, whereas the energies of the stationary incident neutron beam are selected by a monochromator. If $\gamma(i) < 1$ characterizes the intensity loss due to the monochromatisation process, the error for this case is given by

$$\Delta (I_o(i, F(i,j)) = \sqrt{\frac{2}{\gamma} \frac{N}{N+1}} \left[\frac{1}{N} \sum_{j=1}^{N} I_o(i) F(i,j) + \frac{4 \cdot U}{N+1} \right]^{1/2} . \qquad (4.23)$$

Comparison of (4.23) and (4.19) shows that for extremely high background the pseudostatistical double chopper is clearly preferable. For moderate to high background the choice will depend on the shape of the distribution and which parts of the spectrum are of main interest.

The advantage of the strong background reduction by a pseudo-statistical double chopper device with an average transmission of about one half for each rotor is somewhat opposed by its limitations for small background. The system may become more flexible if rotors with a smaller time utilization (say 1/4 or 1/5) are used. We have not yet performed an error analysis for this case, however, extrapolation of the above results and those of section 2.4 suggest an approximate relation

$$(I_o(i) F(i,j))_{(N,K)\text{-system}} \approx \frac{N}{N-K} \left[\overline{I_o F} + \frac{2U}{k^2} \right]^{1/2} , \qquad (4.24)$$

which should be valid for $K \gg 1$ and $N/K \lesssim 5$. This yields for $N/K = 4$

$$(I_o(i) F(i,j))_{N/K=4} \approx \frac{4}{3} \left[I_o F + \frac{32}{N^2} U \right]^{1/2} .$$

For negligible background this system will be superior to the conventional double chopper as soon as

$$I_o(i)\ F(i,j) > \frac{16}{9}\ \overline{I_o F} \quad .$$

In order to check the above theoretical investigations experiments with a pseudostatistical chopper were simulated on a computer. Fig. 7 shows the results of a calculation assuming quasielastic scattering from the sample. The solid line is the calculated cross-section whereas the points are the results of the "measurement". Due to the small counting rate the points scatter widely. The dashed lines indicate the standard deviation of the statistical error given by Eq. (4.19).

5. Conclusions

It was shown that all sequences out of the class of difference sets can be used to modulated the reactor beam in time-of-flight experiments. This leads to chopping systems with different time utilization. The choppers used so far with an average transmission of about one half are especially useful if the background is very high. As choppers with a smaller time utilization reduce the statistical errors in the low parts of the spectrum they may be advantageous in cases of moderate background. Thus a chopper with a time utilization of 1/3 should be a reasonable compromise for low and high background situations.

If in addition monochromatization of the pulsed beam is required magnetic systems are more flexible than mechanical choppers. However the spin flip system suffers from a very low efficiency of about 1 %. Pulsing the beam with a ferrite crystal [10] seems to be the most promissing method to fully exploit the advantage of the correlation technique, as it allows to choose the best suited chopping pattern for each application.

An expression was derived for the statistical error of integrals over parts of the time-of-flight spectrum when a chopper with time utilization of 1/2 is used. Whereas the statistical error in the individual channels is constant over the whole spectrum, the error of integrated intensities depends on the shape of the distribution. It is generally smaller than the error obtained for independent quantities. If the integration has to be performed over narrow peaks as it is required for structur analysis, the deviations are negligible.

The principle features of a correlation double chopper were discussed for a system consisting of two rotors with identical absorption patterns running at the same speed. If the average transmission of each rotor is one half an extremely good background reduction is obtained, however, in cases of low background the applications are limited to spectra consisting of a number of narrow peaks. It is therefore proposed to use rotors with an average transmission of about 1/4. This system has a wider range of applications if the background is small and still reduces strongly the influence of a large background. It is intended to perform a more thorough analysis of double choppers with different time utilization.

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List of Captions

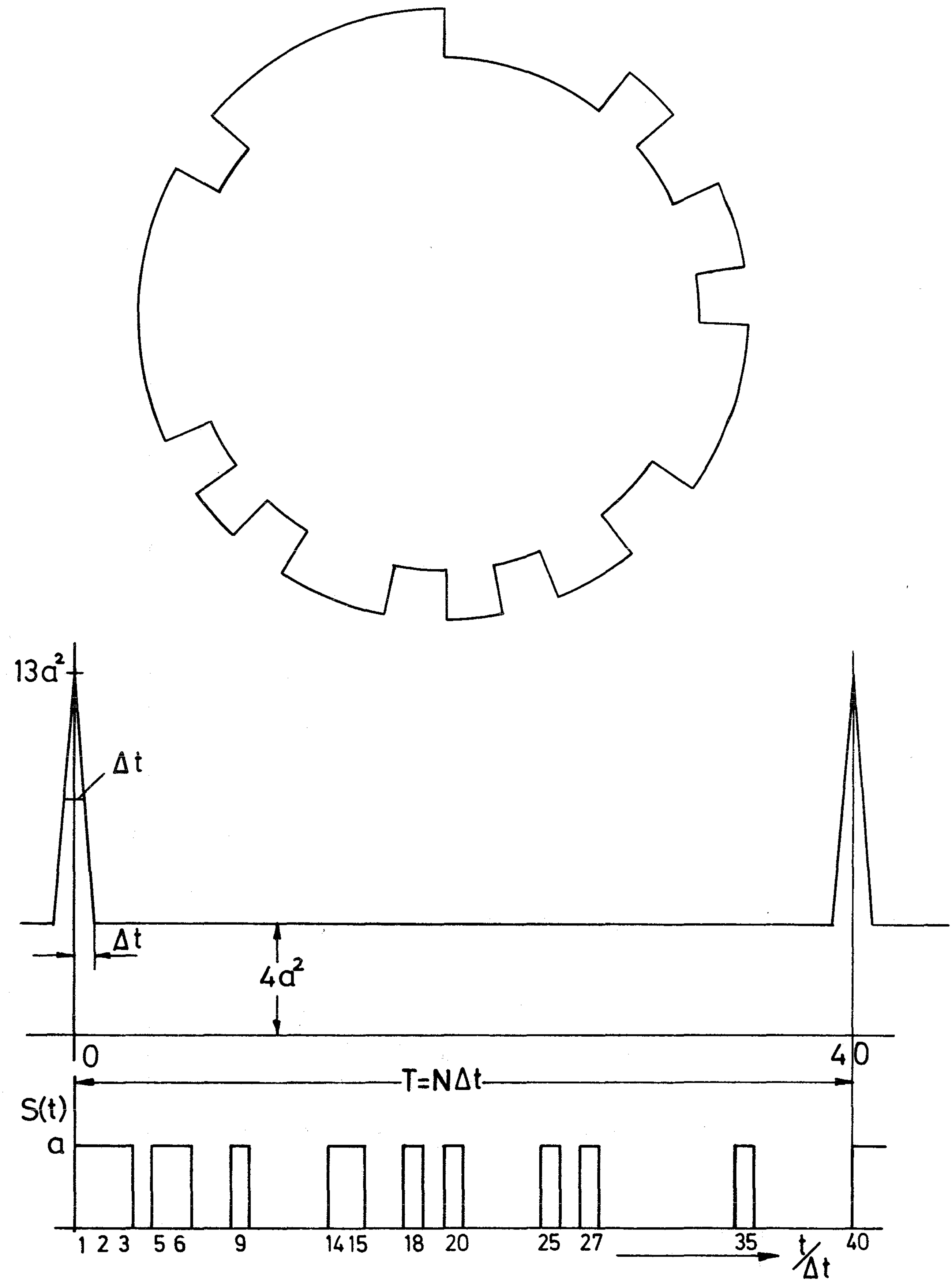

Fig. 1 Example for a binary chopper with average transmission 1/3. Below the binary sequence S(t) and the autocorrelation function is indicated

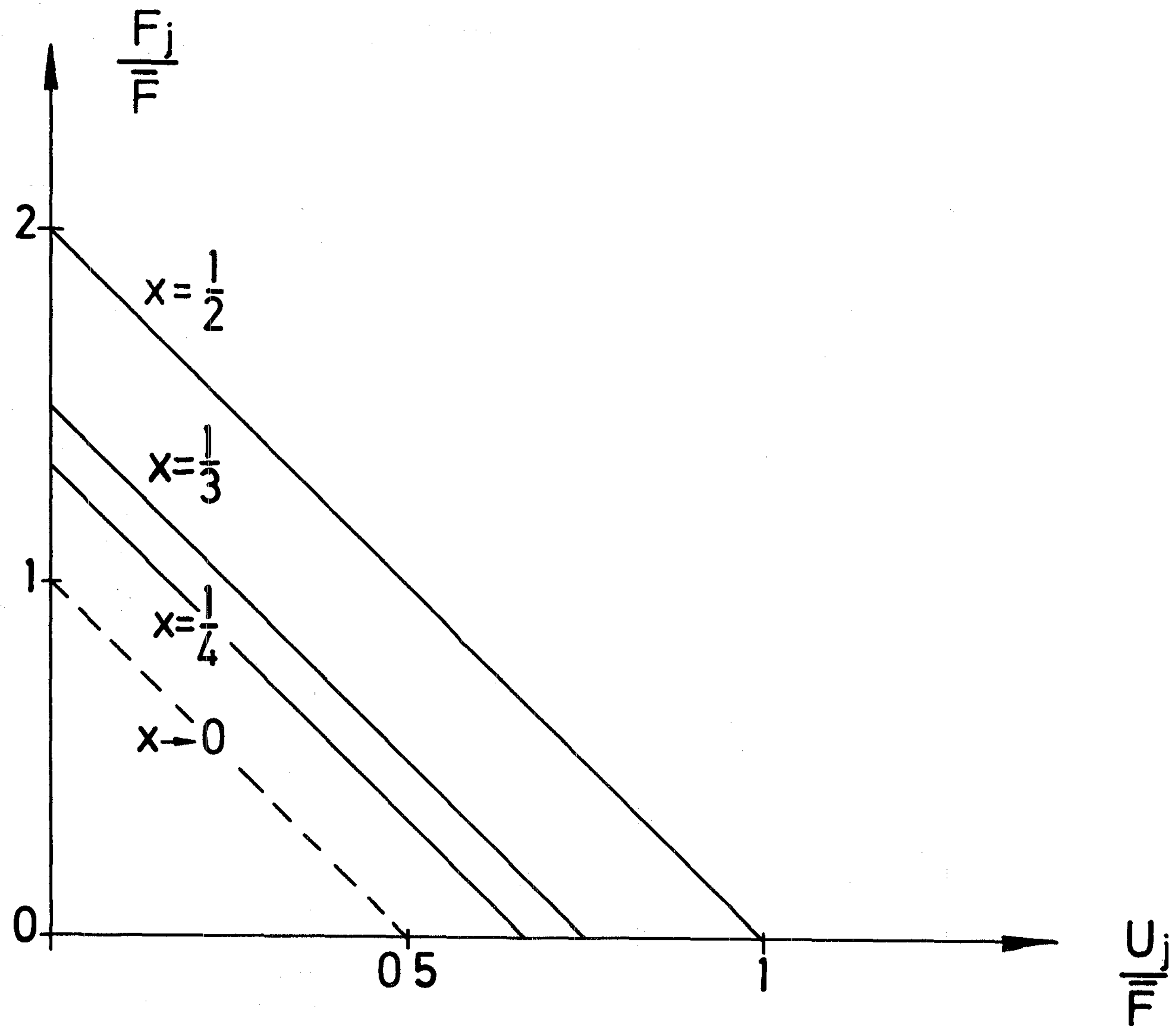

Fig. 2 Comparison of different (N,K)-choppers

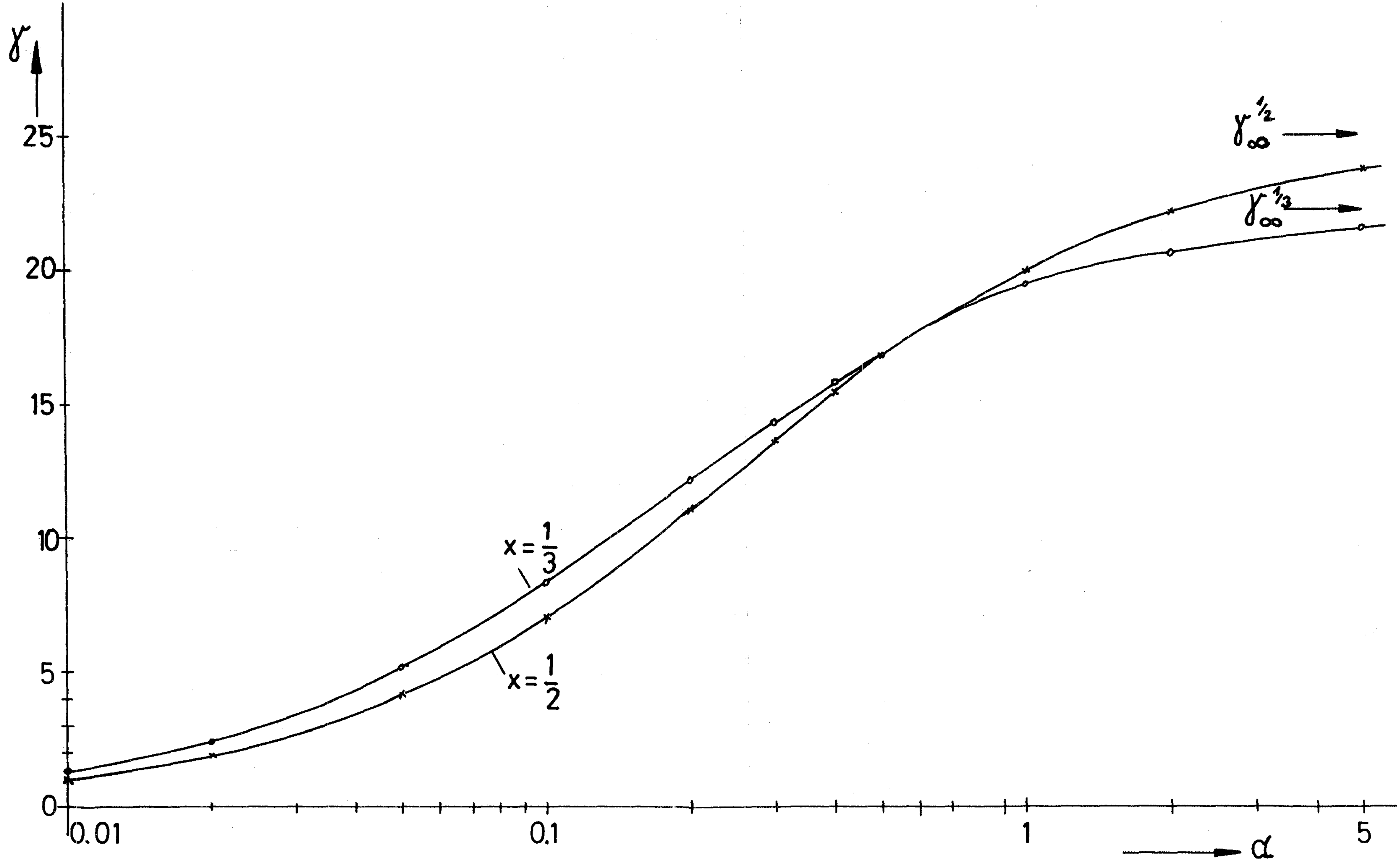

Fig. 3 Gainfactor for choppers of average transmission 1/2 and 1/3 (N=100)

$$S_i^N \, S_{i-j}^N = - S_{i-k(j)}^N \qquad (N = 15)$$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
−	+	+	+	+	−	−	−	+	−	−	+	+	−	+	S_{i-1}
−	+	+	+	−	+	+	−	−	+	−	+	−	−	−	$-S_{i-12}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
+	−	+	+	+	+	−	−	−	+	−	−	+	+	−	S_{i-2}
+	−	+	+	−	−	+	−	+	−	−	−	−	+	+	$-S_{i-9}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
−	+	−	+	+	+	+	−	−	−	+	−	−	+	+	S_{i-3}
−	+	−	+	−	−	−	−	+	+	+	−	+	+	−	$-S_{i-4}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
+	+	−	+	−	+	+	+	+	−	−	−	+	−	−	S_{i-5}
+	+	−	+	+	−	−	+	−	+	−	−	−	−	+	$-S_{i-10}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
−	+	+	−	+	−	+	+	+	+	−	−	−	+	−	S_{i-6}
−	+	+	−	−	+	−	+	−	−	−	−	+	+	+	$-S_{i-8}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
−	−	+	+	−	+	−	+	+	+	+	−	−	−	+	S_{i-7}
−	−	+	+	+	−	+	+	−	−	+	−	+	−	−	$-S_{i-13}$

+	+	+	+	−	−	−	+	−	−	+	+	−	+	−	S_i
−	−	−	+	−	−	+	+	−	+	−	+	+	+	+	S_{i-11}
−	−	−	+	+	+	−	+	+	−	−	+	−	+	−	$-S_{i-14}$

j	k(j)
1	12
2	9
3	4
4	3
5	10
6	8
7	13
8	6
9	2
10	5
11	14
12	1
13	7
14	11

Fig. 4 Demonstration of the relation $S_{i-\alpha} \cdot S_{i-\alpha'} = -S_{i-\beta(\alpha'-\alpha)}$ for N=15

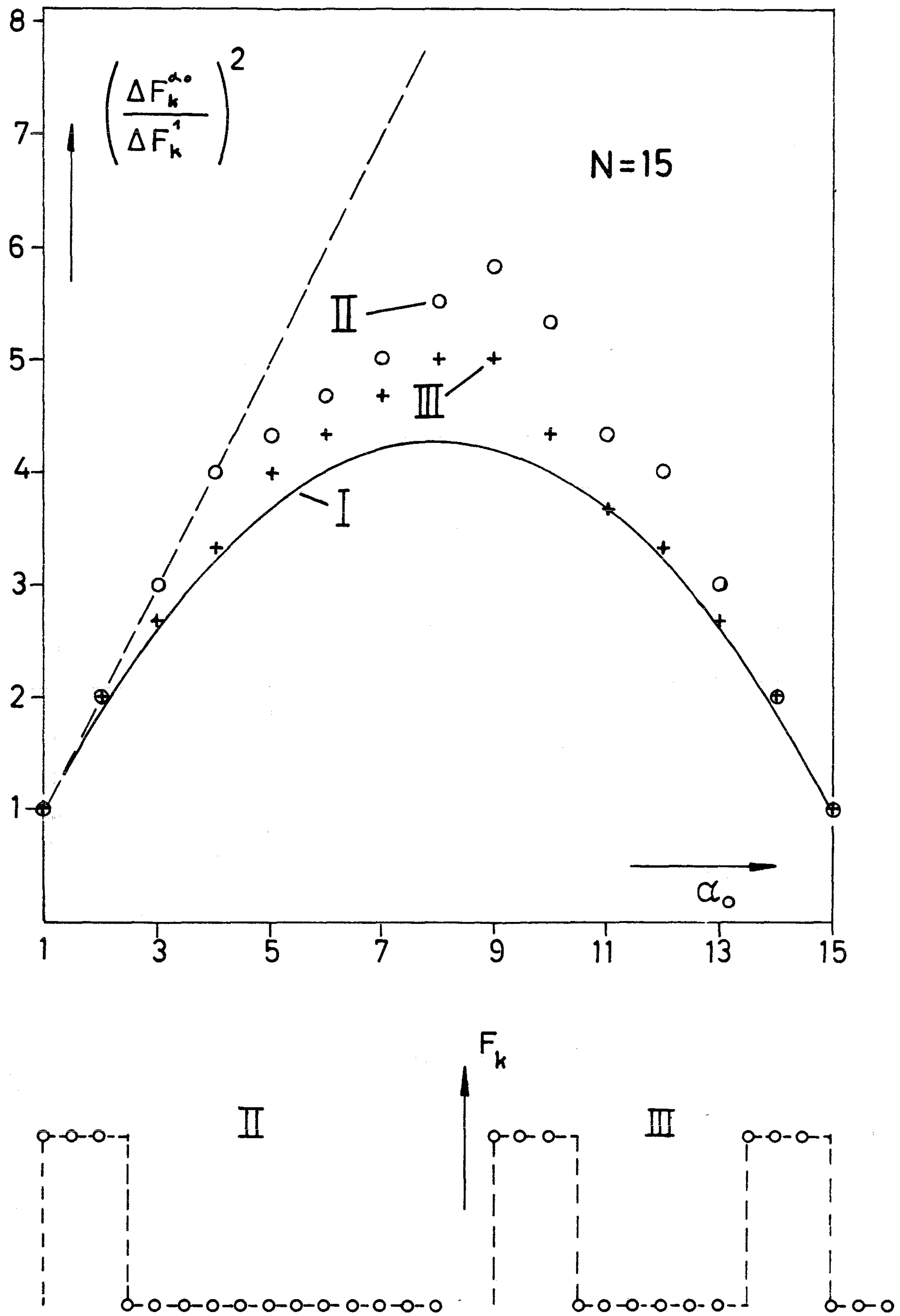

Fig. 5 Statistical error of the integrated intensity as a function of interval width

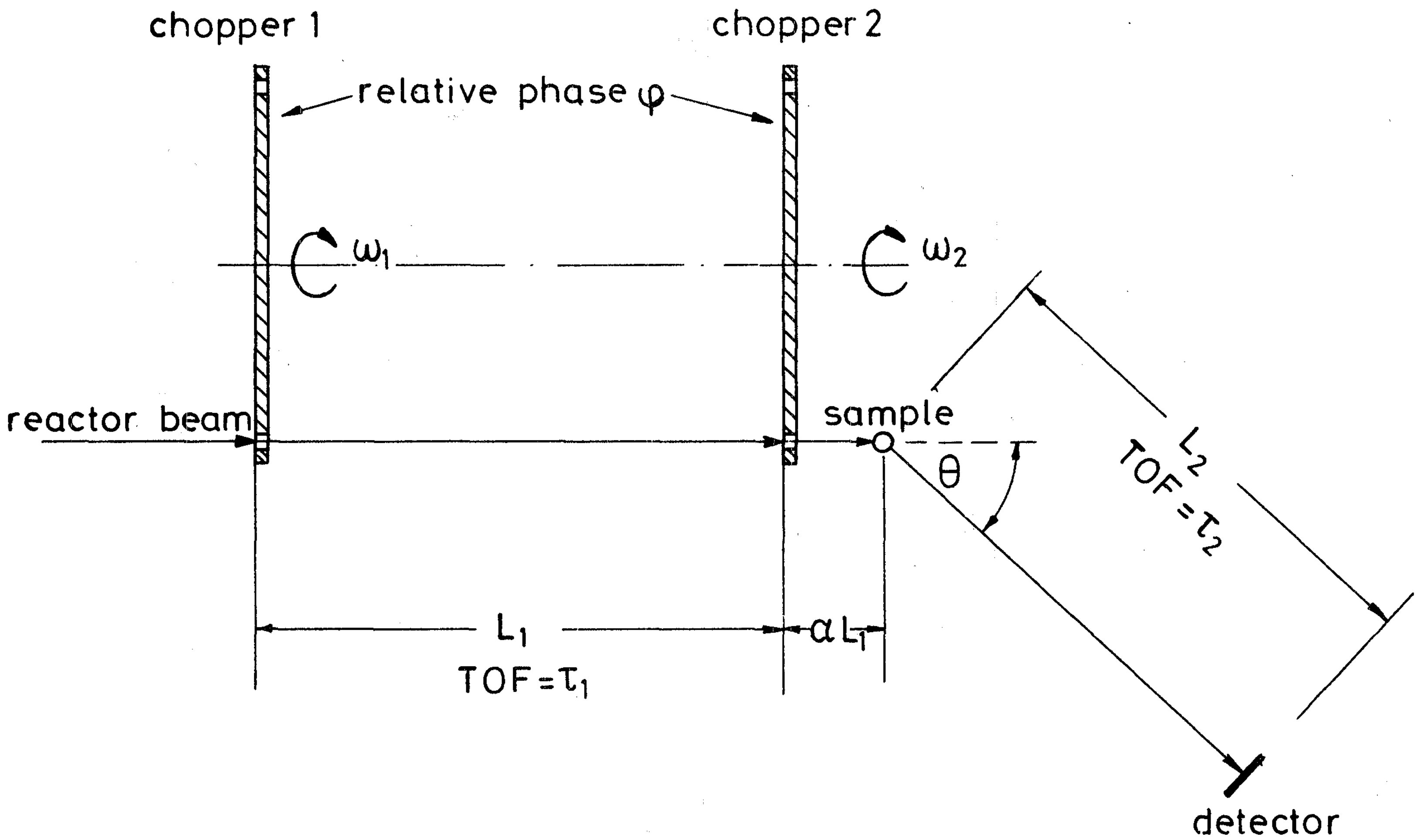

Fig. 6 Scheme of an experiment with a correlation double chopper

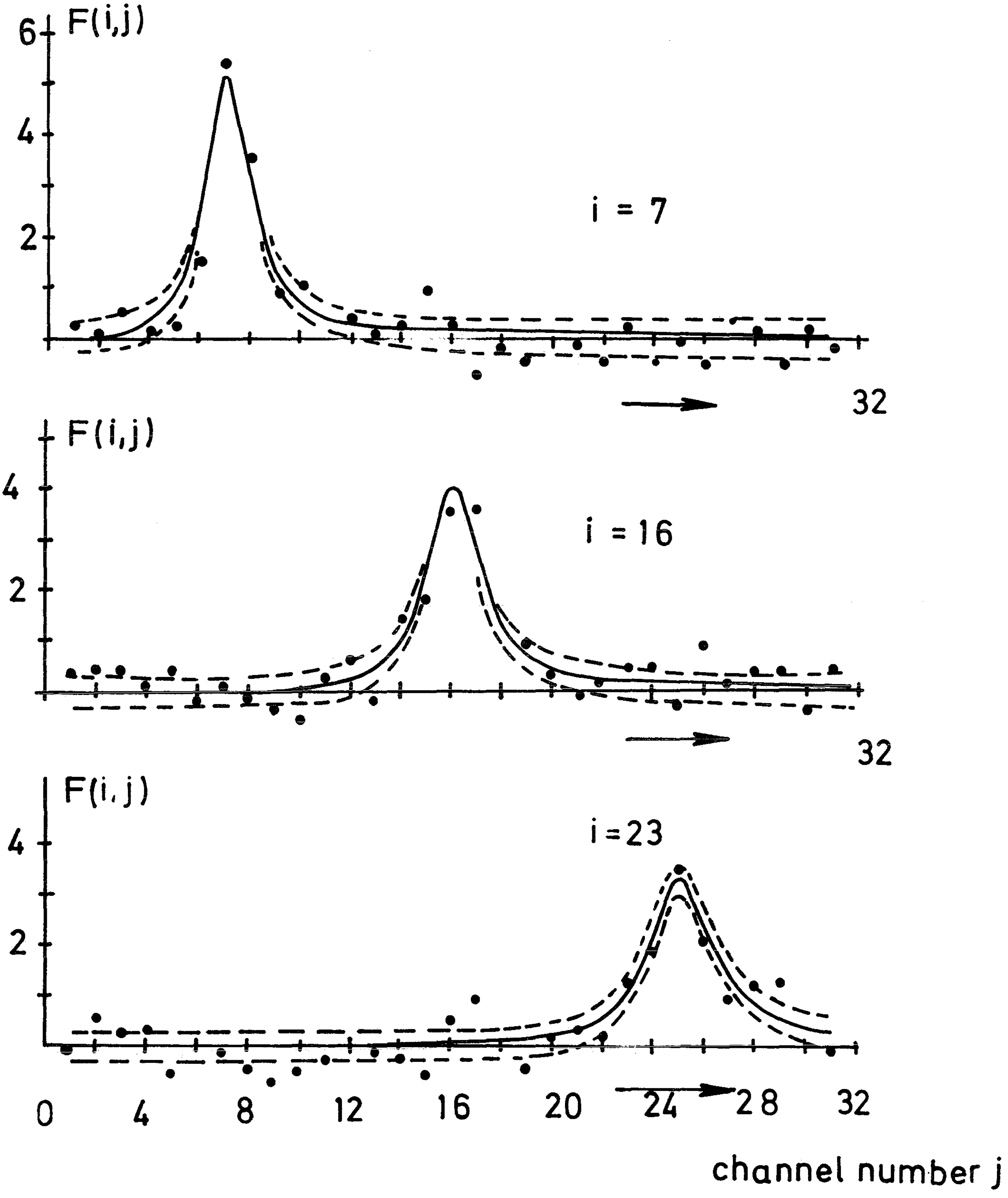

Fig. 7 Results of an experiment with a correlation double chopper simulated on a computer