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# A METHOD FOR THE SUMMATION OF THE FOURIER SERIES USED IN THE X-RAY ANALYSIS OF CRYSTAL STRUCTURES

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ABSTRACT

This paper describes in detail a method that has proved useful in the summation of one-dimensional Fourier series, and a procedure that enables this method to be applied to the summation of two-dimensional series such as those by which the electron density of a crystal is represented as a function of the coordinates in the projection of the unit cell on a particular plane. The method, like those of Robertson and of Lipson and Beevers, utilizes cardboard strips, each carrying a series of values of a certain trigonometric function, but differs from the other two in that the selection of numbers to be added from a series of strips for a given point of the unit cell is accomplished by one of a set of stencils. Experience has shown that this method is well adapted to the range of $F$-values (or of $|F|^2$-values) from 0 to 1000.

## INTRODUCTION

In recent years there has been a very widespread use of the Fourier series in the analysis of the data obtained by the diffraction of $x$-rays in crystals. The electron density in a crystal can be represented by a three-dimensional Fourier series in which the coefficients are the structure factors $F(hkl)$, the intensities of the diffraction lines, corrected for certain known trigonometric factors, being proportional to $|F(hkl)|^2$. The projection of the electron density on a plane perpendicular to a zone axis can be represented by a two-dimensional series using only the $F$'s of the reflections in that zone. Various methods[1] which lead to the successful analysis of $x$-ray data have been devised which depend on the summation of Fourier series. Routine methods for carrying out the summation of such series have therefore become part of the necessary equipment of any laboratory specializing in $x$-ray analysis.

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[1] For a summary article on such methods see Robertson, J. M.: Reports on Progress in Physics, *Physical Society*, London, **4,** 332 (1938).

The usual methods for summing two- and three-dimensional Fourier series involve splitting these summations into a number of summations of one-dimensional series according to a scheme proposed by Beevers and Lipson.[2] Three numerical methods[3,4,5] have been suggested for the rapid handling of the one-dimensional summations, and it is the purpose of the present paper to describe one of these methods[5] in detail.

The paper is divided into two parts. In the first part, the process for the summation of a one-dimensional Fourier series is discussed and a description of the appliances used by the authors is given. In the second part, an account is given of the routine methods used by us in combining the one-dimensional summations into two-dimensional summations.

## Part I. The Summation of One-Dimensional Fourier Series

### *1. Simplification of the summation of series by rearrangement of terms*

The method for the summation of one-dimensional series to be described in the present paper is in essential due to L. Hermann[6] who made use of it in the analysis of voice records. The application of the method to Fourier synthesis[5] was made without knowledge of the earlier work. It will be evident to those who have read the original papers, that we have made considerable use of short-cuts suggested by Beevers and Lipson[2,4] and by Robertson.[3] To avoid interruption of the line of argument, acknowledgment of this indebtedness is made here.

In its most general form, a one-dimensional Fourier series may be written

$$f(x) = \sum_{h=-\infty}^{\infty} A(h) \cos 2\pi hx/a + B(h) \sin 2\pi hx/a \tag{1}$$

in which

$$A(h) = A(\bar{h}) \quad \text{and} \quad B(h) = -B(\bar{h}). \tag{1'}$$

Such a series is of course periodic with a period $a$. We shall usually wish to sum this series at $N$ points which divide the period $a$ into $N$ equal parts. It is thus convenient for our purpose to choose a new coordinate $X$ such that $X = Nx/a$, where $X$ is an integer. We shall call such a coordinate $X$ a coordinate on the base $N$, and shall use coordinates of this type throughout the remainder of the paper. We then have to sum the two different kinds of series, i.e.

$$C(X) = \sum_{h=-\infty}^{\infty} A(h) \cos 2\pi hX/N \tag{2}$$

[2] Beevers, C. A., and Lipson, H.: *Phil. Mag.* (7), **17,** 855 (1934).
[3] Robertson, J. M.: *Phil. Mag.* (7), **21,** 176 (1936).
[4] Lipson, H., and Beevers, C. A.: *Proc. Phys. Soc.*, **48,** 772 (1936).
[5] Patterson, A. L.: *Phil. Mag.* (7), **22,** 753 (1936).
[6] Hermann, L.: *Archiv für die gesammte Physiologie*, **47,** 44 (1890).

and

$$S(X) = \sum_{h=-\infty}^{\infty} B(h) \sin 2\pi hX/N, \tag{3}$$

for $0 \leqq X \leqq N/2$ and to combine the results according to the relations

$$\begin{aligned} f(X) &= C(X) + S(X) \\ f(N - X) &= C(X) - S(X). \end{aligned} \tag{4}$$

We may now reduce the number of terms[7] in the summations (2) and (3) by making use of the two relations

$$\cos 2\pi X(pN \pm h)/N = \cos 2\pi hX/N, \qquad p = 0, \pm 1, \pm 2, \cdots, \tag{5}$$

and

$$\sin 2\pi X(pN \pm h)/N = \pm \sin 2\pi hX/N, \quad p = 0, \pm 1, \pm 2, \cdots.$$

It is thus possible to write (2) and (3) in the forms

$$C(X) = \sum_{h=0}^{N/2} C(h) \cos 2\pi hX/N \tag{6}$$

and

$$S(X) = \sum_{h=0}^{N/2} S(h) \sin 2\pi hX/N \tag{7}$$

respectively, in which

$$\begin{aligned} C(h) &= 2A(h) + 2\sum_{p=1}^{\infty} \{A(pN - h) + A(pN + h)\} \\ S(h) &= 2B(h) - 2\sum_{p=1}^{\infty} \{B(pN - h) - B(pN + h)\} \\ C(0) &= A(0) + 2\sum_{p=1}^{\infty} A(pN) \\ C(N/2) &= 2\sum_{p=0}^{\infty} A(\overline{2p+1} \cdot N/2) \\ S(0) &= S(N/2) = 0.^{8} \end{aligned} \tag{8}$$

If we sum the odd and the even terms of the series (6) and (7) separately, we can still further reduce the number of points over which it will be necessary to compute these series. We note that

$$\begin{aligned} \cos 2\pi h(N/2 - X)/N &= (-1)^h \cos 2\pi hX/N \\ \sin 2\pi h(N/2 - X)/N &= (-1)^{h+1} \sin 2\pi hX/N \end{aligned} \tag{9}$$

[7] If the indices of the planes for which $x$-ray intensities are available are all less than $N/2$, and this is the common case, the full analysis of this paragraph is unnecessary. In this case the coefficients of the series (6) and (7) are given by $C(h) = 2A(h)$; $S(h) = 2B(h)$; $C(0) = A(0)$; and $S(0) = 0$ instead of the more complicated expressions (8).

[8] This last result follows from the fact that

$$\sin 2\pi \left(\frac{pN}{2} \frac{X}{N}\right) = \sin \pi pX = 0$$

so that the terms whose coefficients are $B(pN/2)$ make no contribution to the sum (3 .

and, if $N$ is an even number,

$$\begin{aligned} C(X) &= C_e(X) + {}_o(CX) \\ C(N/2 - X) &= C_e(X) - C_o(X) \\ S(X) &= S_e(X) + S_o(X) \\ S(N/2 - X) &= - S_e(X) + S_o(X) \end{aligned} \qquad (10)$$

provided that $C_e$ and $S_e$ are the partial sums of the even terms and $C_o$ and $S_o$ are the partial sums of the odd terms of the series $C(X)$ and $S(X)$ respectively.

## 2. *A stencil method for the summation of sine and cosine series*

In the last section we have seen that the summation of the Fourier series (1) can be reduced to a number of summations of one of two types, i.e.

$$\sum_{h=0}^{N/2} C(h) \cos 2\pi hX/N \quad (11a) \qquad \text{or} \qquad \sum_{h=1}^{N/2} S(h) \sin 2\pi hX/N. \quad (11b)$$

In these summations we shall be concerned with $X$ values in the range between zero and $N/4$ and either even or odd values of $h$ in the range including zero and $N/2$. If we could have available all possible products of the type $D \cos 2\pi hX/N$ or $D \sin 2\pi hX/N$ in which $D$ were any number which we might meet as a $C$ or an $S$ coefficient, then the summations (11) would be reduced to mere additions. If we notice that

$$\sin 2\pi(N/4 - hX)/N = \cos 2\pi hX/N$$

and that $(N/4-hX)$ and $hX$ are both integers if $N$ is divisible by 4 we, see that all possible *numerical* values of $D \cos 2\pi hX/N$ or $D \sin 2\pi hX/N$ will be listed if we list the values

$$D \cos 2\pi s/N \quad (s = 0, 1, 2, \cdots, N/4)$$

for all values of $D$ which we may meet as coefficients $C(h)$ or $S(h)$, where $s$ is the number of the position in the series reading from left to right. Such listings are conveniently arranged on cardboard strips. Typical strips are shown in Fig. 1. The strips corresponding to positive $D$ values are of white card; those corresponding to negative $D$ values are of card of a different color.

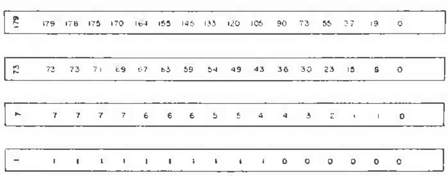


FIG. 1. Typical strips for $N=60$. The numbers shown are $D \cos (s6°)$, where $s$ gives the position of the number on the strip ($s=0, 1, \cdots, 15$). The $D$-values shown are 179, 73, 7, and 1, respectively.

In forming the sums $C_e$ and $C_o$, a strip is selected for each value of $C(h)$. There will be, at the most, $(N/2+1)$ such strips, which are then arranged in order of their $h$ values in a grooved rack (Figs. 2*a* and 2*b*).

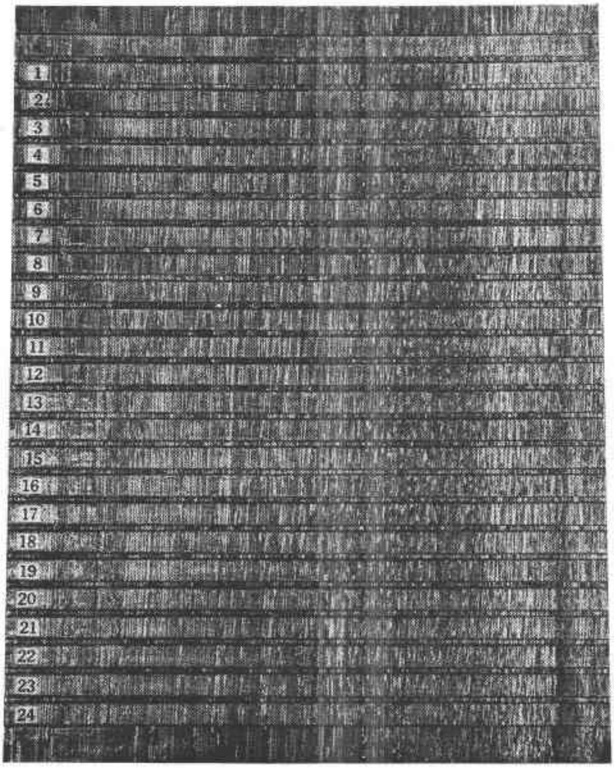


FIG. 2a. Rack for $N=48$ to handle $h$ values 0 to 25.

These strips in their rack (Figs. 3*a* and 3*c*) then form a table which contains all the *numerical* values which will be needed in the computation of the sums $C_e$ and $C_o$, that is in the computation of the series $C(X)$ of equation (2). It only remains to devise some means of selecting the values needed in making the summation for a particular point. This is done by means of a set of stencils. There is a $C_e$ and a $C_o$ stencil for each value of $X$. In these stencils the openings are arranged to select the correct numerical value for a given $h$. One such stencil is shown in place in each of the racks in Fig. 3*b*. The holes which select the positive values are unmarked, while those corresponding to negative values are ringed with appropriate paint. When the number seen through a ringed hole is on a colored card the number is to be taken with a positive sign, the negative property of the ringed hole offsetting the negative property of the colored strip.

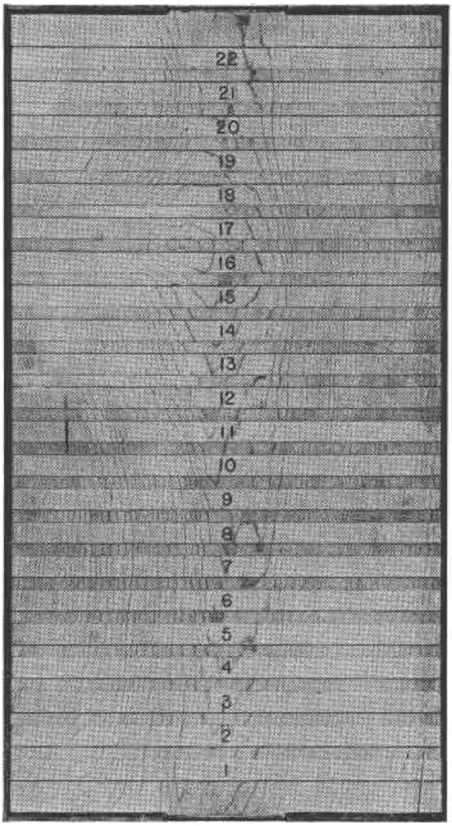


FIG. 2b. Rack for $N=60$ to handle $h$ values 1 to 22. (Note. The rack for $N=60$ would have a greater range of utility if additional slots for $h=23$ to 30 inclusive were present, although no case has yet been encountered where these additional slots were needed. A slot for $h=0$ would add slightly to the convenience of use.)

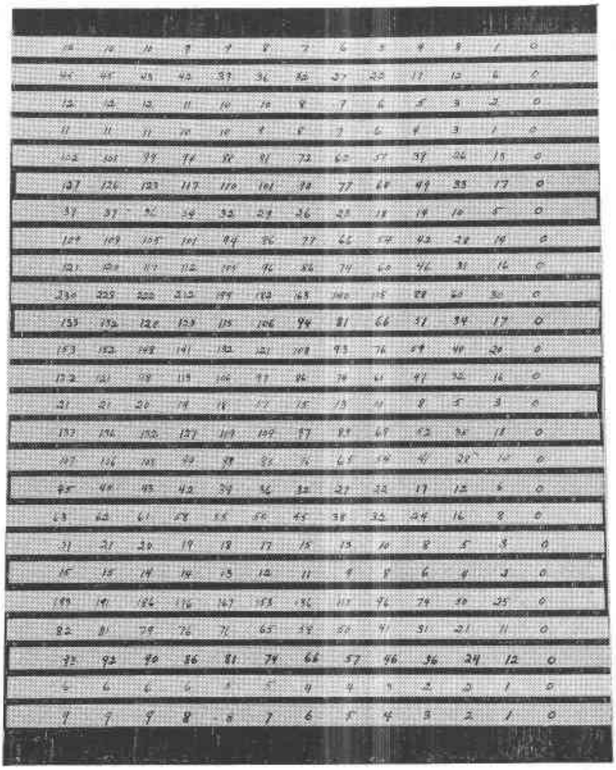

FIG. 3a. Rack for $N=48$ with strips in place.

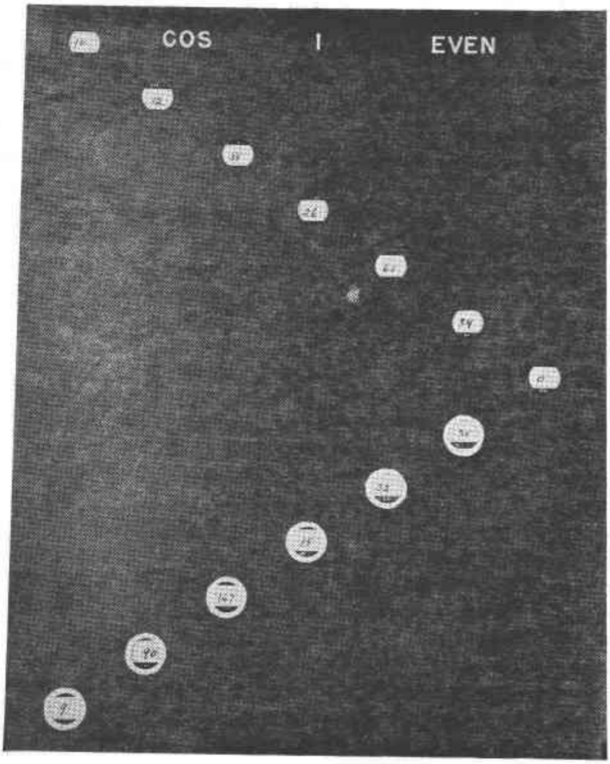


FIG. 3b. Rack for $N=48$ with stencil in place for summation $C(h)\cos 2\pi hX/N$ for $X=1$, even indices.

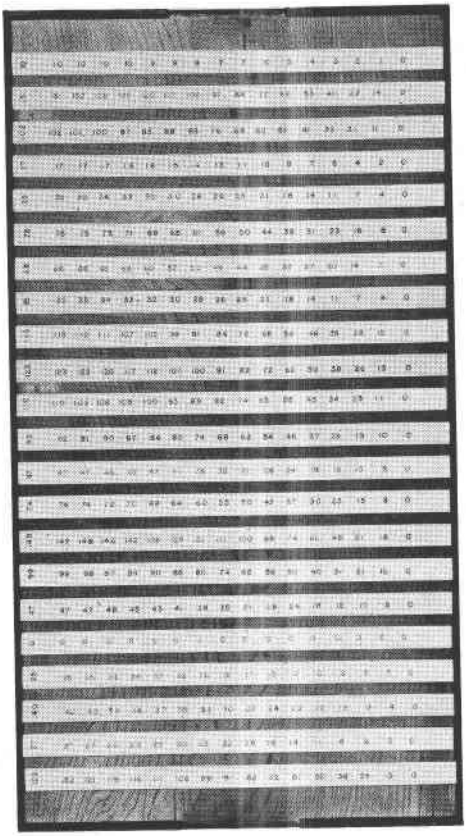

FIG. 3c. Rack for $N=60$ with strips in place.

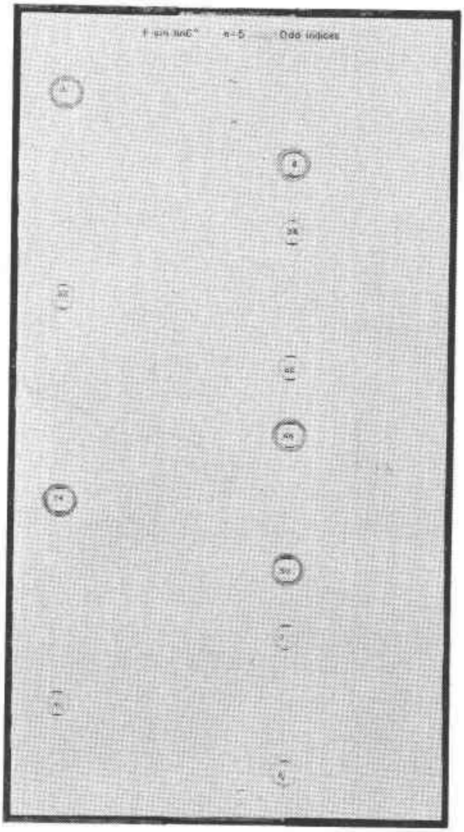


FIG. 3d. Rack for $N=60$ with stencil in place for summation $S(h) \sin 2\pi hX/N$ for $X=5$, odd indices.

In a similar manner strips can be selected and racked so as to build up a table containing all the numerical values which will be needed in the computation of the sums $S_e$ and $S_o$. The same set of strips can be used for sine and cosine summations, but in the case of the sine summations the numbers on the strips are taken as representing $D \sin 2\pi(N/4-s)/N$, $(s=0, 1, \cdots, N/4)$, where $s$ as before is the number of the position on the strip reading from left to right. Another set of stencils can then be arranged to select from this table the values necessary for the summations $S_e$ and $S_o$ for each value of $X$ (Fig. 3*d*).

*3. Layout for stencils*

In describing the layout scheme for a set of stencils, we shall discuss in considerable detail the case of $N=20$. For this small value of $N$ we can illustrate the full set of stencils and describe the process of laying them out. We shall then give the tables that are needed to make the layouts necessary for the more useful values $N=48$ and $N=60$. After study of these tables the reader should be in a position to set up such tables for himself for any other values of $N$ that may be needed.

In making a cosine summation one strip is chosen for each $C(h)$ value and placed in the $h$th position in the rack. For a given $X$ and a given $h$ we shall need to select the value

$$C(h) \cos 2\pi hX/N$$

from among the values

$$C(h) \cos 2\pi s/N$$

carried on the strip in the $h$th position on the rack. A table must therefore be constructed of the $s$ values corresponding to given values of $h$ and $X$ for a specified $N$. Such a table is given below for cosine summations for $N=20$, $X=0, 1, \cdots, 5$ and $h=0, 1, \cdots, 10$. The $s$ values for a given $h$ appear in a vertical column, while those for a given $X$ appear in a horizontal row. The $C_e$ and $C_o$ stencils for $X=0$ thus have all 0 values of $s$ and therefore select values of $C(h) \cos 2\pi s/N$ corresponding to $\cos 2\pi s/N=1$. The correct arrangement of holes for this stencil is shown in Fig. 4 in the stencil labelled[9] "Cos, $X=0$, $h$ even" which selects the values $C(h)$ for all $h$ even. Similarly the stencil "Cos, $X=0$, $h$ odd" selects the values $C(h)$ for all $h$ odd. The "Cos, $X=1$, $h$ even" stencil selects the values $C(0)$, $C(2) \cos 4\pi/20$, $C(4) \cos 8\pi/20$, $-C(6) \cos 8\pi/20$, $-C(8) \cos 4\pi/20$, $-C(10)$. These are then added to give the partial sum $C_e(X)$ obtained by adding the even terms of the series (6). In Figs. 3*b* and

[9] In labelling stencils, one of us (P.) has used the abbreviated notation shown on the stencil of Fig. 3*b* for $N=48$; the other (T.) has used the more detailed label shown on the $N=60$ stencil of Fig. 3*d*.

TABLE 1. TABLE OF VALUES OF $s$ AS FUNCTION OF $h$ AND $X$ FOR COSINE STENCILS ($N=20$). A LINE UNDER THE $s$ VALUE INDICATES A NEGATIVE VALUE FOR $D \cos 2\pi s/N$

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 1 | 2 | 3 | 4 | 5 | $\underline{4}$ | $\underline{3}$ | $\underline{2}$ | $\underline{1}$ | $\underline{0}$ |
| 2 | 0 | 2 | 4 | $\underline{4}$ | $\underline{2}$ | $\underline{0}$ | $\underline{2}$ | $\underline{4}$ | 4 | 2 | 0 |
| 3 | 0 | 3 | $\underline{4}$ | $\underline{1}$ | $\underline{2}$ | 5 | 2 | 1 | 4 | $\underline{3}$ | $\underline{0}$ |
| 4 | 0 | 4 | $\underline{2}$ | $\underline{2}$ | 4 | 0 | 4 | $\underline{2}$ | $\underline{2}$ | 4 | 0 |
| 5 | 0 | 5 | $\underline{0}$ | 5 | 0 | 5 | $\underline{0}$ | 5 | 0 | 5 | $\underline{0}$ |

*3d* stencils are shown in place on the racks for $N=48$ and $N=60$. The reader can easily assure himself that the other cosine stencils will select the appropriate values to form the partial sums of the odd terms and the even terms of the series (6) for various values of $X$.

To sum the series (7) we must place in the rack the strips

$$S(h) \cos 2\pi s/N$$

and plan a set of stencils to select from among them the values which correspond to the quantities

$$S(h) \sin 2\pi hX/N$$

needed in forming the partial sums of the odd and even terms of the series (7). The appropriate $s$ values are shown in Table 2.

TABLE 2. TABLE OF VALUES OF $s$ AS FUNCTION OF $h$ AND $X$ FOR SINE STENCILS ($N=20$)

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 1 | 5 | 4 | 3 | 2 | 1 | 0 | 1 | 2 | 3 | 4 | 5 |
| 2 | 5 | 3 | 1 | 1 | 3 | 5 | $\underline{3}$ | $\underline{1}$ | $\underline{1}$ | $\underline{3}$ | 5 |
| 3 | 5 | 2 | 1 | 4 | $\underline{3}$ | $\underline{0}$ | $\underline{3}$ | 4 | 1 | 2 | 5 |
| 4 | 5 | 1 | 3 | $\underline{3}$ | $\underline{1}$ | 5 | 1 | 3 | $\underline{3}$ | $\underline{1}$ | 5 |
| 5 | 5 | 0 | 5 | $\underline{0}$ | 5 | 0 | 5 | $\underline{0}$ | 5 | 0 | 5 |

The sine stencils constructed on this scheme are also illustrated in Fig. 3. It is easily seen that the backs of the cosine stencils can be used for the sine stencils.

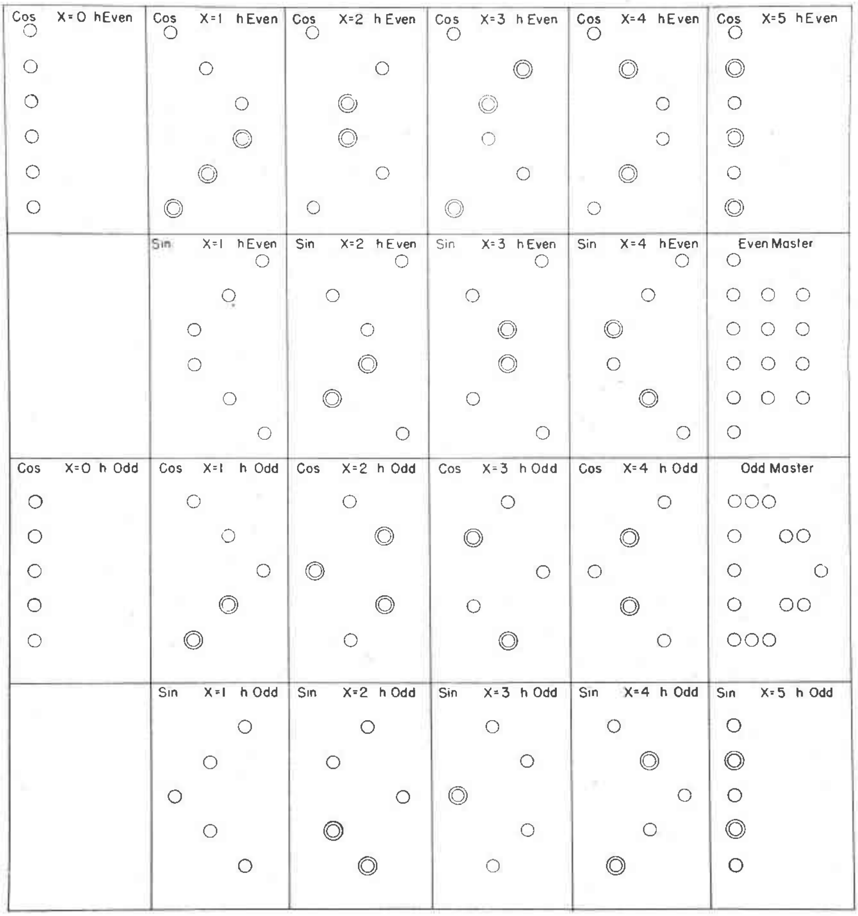


FIG. 4. Layout of stencils for $N=20$. The ringed holes correspond to negative values. The same cards can be used for the sine and the cosine stencils, one side of each card serving for the cosine summation and the other side for the sine summation.

In Tables 3–6 the $s$ values are given for the cosine and sine stencils for $N=48$ and $N=60$. Both these values of $N$ have been found satisfactory in the laboratories of the writers and elsewhere for the summation of the Fourier series that arise in $x$-ray analysis. If the reader wishes to use any other value of $N$, he will find it easy to construct corresponding tables provided that $N$ is divisible by 4.

TABLE 3. TABLE OF VALUES OF $s$ AS FUNCTION OF $h$ AND $X$ FOR COSINE STENCILS ($N=48$)

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | $\underline{11}$ | $\underline{10}$ | $\underline{9}$ | $\underline{8}$ | $\underline{7}$ | $\underline{6}$ | $\underline{5}$ | $\underline{4}$ | $\underline{3}$ | $\underline{2}$ | $\underline{1}$ | $\underline{0}$ |
| 2 | 0 | 2 | 4 | 6 | 8 | 10 | 12 | $\underline{10}$ | $\underline{8}$ | $\underline{6}$ | $\underline{4}$ | $\underline{2}$ | $\underline{0}$ | $\underline{2}$ | $\underline{4}$ | $\underline{6}$ | $\underline{8}$ | $\underline{10}$ | 12 | 10 | 8 | 6 | 4 | 2 | 0 |
| 3 | 0 | 3 | 6 | 9 | 12 | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ | $\underline{3}$ | $\underline{6}$ | $\underline{9}$ | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ |
| 4 | 0 | 4 | 8 | 12 | $\underline{8}$ | $\underline{4}$ | $\underline{0}$ | $\underline{4}$ | $\underline{8}$ | 12 | 8 | 4 | 0 | 4 | 8 | 12 | $\underline{8}$ | $\underline{4}$ | $\underline{0}$ | $\underline{4}$ | $\underline{8}$ | 12 | 8 | 4 | 0 |
| 5 | 0 | 5 | 10 | $\underline{9}$ | $\underline{4}$ | $\underline{1}$ | $\underline{6}$ | $\underline{11}$ | 8 | 3 | 2 | 7 | 12 | $\underline{7}$ | $\underline{2}$ | $\underline{3}$ | $\underline{8}$ | 11 | 6 | 1 | 4 | 9 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ |
| 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 | 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 | 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 | 6 | 0 |
| 7 | 0 | 7 | $\underline{10}$ | $\underline{3}$ | $\underline{4}$ | $\underline{11}$ | 6 | 1 | 8 | $\underline{9}$ | $\underline{2}$ | $\underline{5}$ | 12 | 5 | 2 | 9 | $\underline{8}$ | $\underline{1}$ | $\underline{6}$ | 11 | 4 | 3 | 10 | $\underline{7}$ | $\underline{0}$ |
| 8 | 0 | 8 | $\underline{8}$ | $\underline{0}$ | $\underline{8}$ | 8 | 0 | 8 | $\underline{8}$ | $\underline{0}$ | $\underline{8}$ | 8 | 0 | 8 | $\underline{8}$ | $\underline{0}$ | $\underline{8}$ | 8 | 0 | 8 | $\underline{8}$ | $\underline{0}$ | $\underline{8}$ | 8 | 0 |
| 9 | 0 | 9 | $\underline{6}$ | $\underline{3}$ | 12 | 3 | 6 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 6 | 3 | 12 | $\underline{3}$ | $\underline{6}$ | 9 | 0 | 9 | $\underline{6}$ | $\underline{3}$ | 12 | 3 | 6 | $\underline{9}$ | $\underline{0}$ |
| 10 | 0 | 10 | $\underline{4}$ | $\underline{6}$ | 8 | 2 | 12 | $\underline{2}$ | $\underline{8}$ | 6 | 4 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 4 | 6 | $\underline{8}$ | $\underline{2}$ | 12 | 2 | 8 | $\underline{6}$ | $\underline{4}$ | 10 | 0 |
| 11 | 0 | 11 | $\underline{2}$ | $\underline{9}$ | 4 | 7 | $\underline{6}$ | $\underline{5}$ | 8 | 3 | $\underline{10}$ | $\underline{1}$ | 12 | 1 | 10 | $\underline{3}$ | $\underline{8}$ | 5 | 6 | $\underline{7}$ | $\underline{4}$ | 9 | 2 | $\underline{11}$ | $\underline{0}$ |
| 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 |

TABLE 4. TABLE OF VALUES OF $s$ AS FUNCTION OF $h$ AND $X$ FOR SINE STENCILS ($N=48$)

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 | 12 |
| 1 | 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 2 | 12 | 10 | 8 | 6 | 4 | 2 | 0 | 2 | 4 | 6 | 8 | 10 | 12 | $\underline{10}$ | $\underline{8}$ | $\underline{6}$ | $\underline{4}$ | $\underline{2}$ | $\underline{0}$ | $\underline{2}$ | $\underline{4}$ | $\underline{6}$ | $\underline{8}$ | $\underline{10}$ | 12 |
| 3 | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ | $\underline{3}$ | $\underline{6}$ | $\underline{9}$ | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 |
| 4 | 12 | 8 | 4 | 0 | 4 | 8 | 12 | $\underline{8}$ | $\underline{4}$ | $\underline{0}$ | $\underline{4}$ | $\underline{8}$ | 12 | 8 | 4 | 0 | 4 | 8 | 12 | $\underline{8}$ | $\underline{4}$ | $\underline{0}$ | $\underline{4}$ | $\underline{8}$ | 12 |
| 5 | 12 | 7 | 2 | 3 | 8 | $\underline{11}$ | $\underline{6}$ | $\underline{1}$ | $\underline{4}$ | $\underline{9}$ | 10 | 5 | 0 | 5 | 10 | $\underline{9}$ | $\underline{4}$ | $\underline{1}$ | $\underline{6}$ | $\underline{11}$ | 8 | 3 | 2 | 7 | 12 |
| 6 | 12 | 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 | 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 | 6 | 0 | 6 | 12 | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | 12 |
| 7 | 12 | 5 | 2 | 9 | $\underline{8}$ | $\underline{1}$ | $\underline{6}$ | 11 | 4 | 3 | 10 | $\underline{7}$ | $\underline{0}$ | $\underline{7}$ | 10 | 3 | 4 | 11 | $\underline{6}$ | $\underline{1}$ | $\underline{8}$ | 9 | 2 | 5 | 12 |
| 8 | 12 | 4 | 4 | 12 | $\underline{4}$ | $\underline{4}$ | 12 | 4 | 4 | 12 | $\underline{4}$ | $\underline{4}$ | 12 | 4 | 4 | 12 | $\underline{4}$ | $\underline{4}$ | 12 | 4 | 4 | 12 | $\underline{4}$ | $\underline{4}$ | 12 |
| 9 | 12 | 3 | 6 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 6 | 3 | 12 | $\underline{3}$ | $\underline{6}$ | 9 | 0 | 9 | $\underline{6}$ | $\underline{3}$ | 12 | 3 | 6 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 6 | 3 | 12 |
| 10 | 12 | 2 | 8 | $\underline{6}$ | $\underline{4}$ | 10 | 0 | 10 | $\underline{4}$ | $\underline{6}$ | 8 | 2 | 12 | $\underline{2}$ | $\underline{8}$ | 6 | 4 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 4 | 6 | $\underline{8}$ | $\underline{2}$ | 12 |
| 11 | 12 | 1 | 10 | $\underline{3}$ | $\underline{8}$ | 5 | 6 | $\underline{7}$ | $\underline{4}$ | 9 | 2 | $\underline{11}$ | $\underline{0}$ | $\underline{11}$ | 2 | 9 | $\underline{4}$ | $\underline{7}$ | 6 | 5 | $\underline{8}$ | $\underline{3}$ | 10 | 1 | 12 |
| 12 | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 | 0 | 12 | $\underline{0}$ | 12 |

TABLE 5. TABLE OF VALUES OF $s$ AS FUNCTION OF $h$ AND $X$ FOR COSINE STENCILS ($N=60$)

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | $\underline{14}$ | $\underline{13}$ | $\underline{12}$ | $\underline{11}$ | $\underline{10}$ | $\underline{9}$ | $\underline{8}$ | $\underline{7}$ | $\underline{6}$ | $\underline{5}$ | $\underline{4}$ | $\underline{3}$ | $\underline{2}$ | $\underline{1}$ | $\underline{0}$ |
| 2 | 0 | 2 | 4 | 6 | 8 | 10 | 12 | 14 | $\underline{14}$ | $\underline{12}$ | $\underline{10}$ | $\underline{8}$ | $\underline{6}$ | $\underline{4}$ | $\underline{2}$ | $\underline{0}$ | $\underline{2}$ | $\underline{4}$ | $\underline{6}$ | $\underline{8}$ | $\underline{10}$ | $\underline{12}$ | $\underline{14}$ | 14 | 12 | 10 | 8 | 6 | 4 | 2 | 0 |
| 3 | 0 | 3 | 6 | 9 | 12 | 15 | $\underline{12}$ | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ | $\underline{3}$ | $\underline{6}$ | $\underline{9}$ | $\underline{12}$ | 15 | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 | 15 | $\underline{12}$ | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ |
| 4 | 0 | 4 | 8 | 12 | $\underline{14}$ | $\underline{10}$ | $\underline{6}$ | $\underline{2}$ | $\underline{2}$ | $\underline{6}$ | $\underline{10}$ | $\underline{14}$ | 12 | 8 | 4 | 0 | 4 | 8 | 12 | $\underline{14}$ | $\underline{10}$ | $\underline{6}$ | $\underline{2}$ | $\underline{2}$ | $\underline{6}$ | $\underline{10}$ | $\underline{14}$ | 12 | 8 | 4 | 0 |
| 5 | 0 | 5 | 10 | 15 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ | $\underline{5}$ | $\underline{10}$ | 15 | 10 | 5 | 0 | 5 | 10 | 15 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ | $\underline{5}$ | $\underline{10}$ | 15 | 10 | 5 | 0 | 5 | 10 | 15 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ |
| 6 | 0 | 6 | 12 | $\underline{12}$ | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | $\underline{12}$ | 12 | 6 | 0 | 6 | 12 | $\underline{12}$ | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | $\underline{12}$ | 12 | 6 | 0 | 6 | 12 | $\underline{12}$ | $\underline{6}$ | $\underline{0}$ | $\underline{6}$ | $\underline{12}$ | 12 | 6 | 0 |
| 7 | 0 | 7 | 14 | $\underline{9}$ | $\underline{2}$ | $\underline{5}$ | $\underline{12}$ | 11 | 4 | 3 | 10 | $\underline{13}$ | $\underline{6}$ | $\underline{1}$ | $\underline{8}$ | 15 | 8 | 1 | 6 | 13 | $\underline{10}$ | $\underline{3}$ | $\underline{4}$ | $\underline{11}$ | 12 | 5 | 2 | 9 | $\underline{14}$ | $\underline{7}$ | $\underline{0}$ |
| 8 | 0 | 8 | $\underline{14}$ | $\underline{6}$ | $\underline{2}$ | $\underline{10}$ | 12 | 4 | 4 | 12 | $\underline{10}$ | $\underline{2}$ | $\underline{6}$ | $\underline{14}$ | 8 | 0 | 8 | $\underline{14}$ | $\underline{6}$ | $\underline{2}$ | $\underline{10}$ | 12 | 4 | 4 | 12 | $\underline{10}$ | $\underline{2}$ | $\underline{6}$ | $\underline{14}$ | 8 | 0 |
| 9 | 0 | 9 | $\underline{12}$ | $\underline{3}$ | $\underline{6}$ | 15 | 6 | 3 | 12 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 12 | 3 | 6 | 15 | $\underline{6}$ | $\underline{3}$ | $\underline{12}$ | 9 | 0 | 9 | $\underline{12}$ | $\underline{3}$ | $\underline{6}$ | 15 | 6 | 3 | 12 | $\underline{9}$ | $\underline{0}$ |
| 10 | 0 | 10 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 10 | 0 | 10 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 10 | 0 | 10 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 10 | 0 | 10 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 10 | 0 | 10 | $\underline{10}$ | $\underline{0}$ | $\underline{10}$ | 10 | 0 |
| 11 | 0 | 11 | $\underline{8}$ | $\underline{3}$ | $\underline{14}$ | 5 | 6 | $\underline{13}$ | $\underline{2}$ | $\underline{9}$ | 10 | 1 | 12 | $\underline{7}$ | $\underline{4}$ | 15 | 4 | 7 | $\underline{12}$ | $\underline{1}$ | $\underline{10}$ | 9 | 2 | 13 | $\underline{6}$ | $\underline{5}$ | 14 | 3 | 8 | $\underline{11}$ | $\underline{0}$ |
| 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 | 12 | $\underline{6}$ | $\underline{6}$ | 12 | 0 |
| 13 | 0 | 13 | $\underline{4}$ | $\underline{9}$ | 8 | 5 | $\underline{12}$ | $\underline{1}$ | $\underline{14}$ | 3 | 10 | $\underline{7}$ | $\underline{6}$ | 11 | 2 | 15 | $\underline{2}$ | $\underline{11}$ | 6 | 7 | $\underline{10}$ | $\underline{3}$ | 14 | 1 | 12 | $\underline{5}$ | $\underline{8}$ | 9 | 4 | $\underline{13}$ | $\underline{0}$ |
| 14 | 0 | 14 | $\underline{2}$ | $\underline{12}$ | 4 | 10 | $\underline{6}$ | $\underline{8}$ | 8 | 6 | $\underline{10}$ | $\underline{4}$ | 12 | 2 | $\underline{14}$ | $\underline{0}$ | $\underline{14}$ | 2 | 12 | $\underline{4}$ | $\underline{10}$ | 6 | 8 | $\underline{8}$ | $\underline{6}$ | 10 | 4 | $\underline{12}$ | $\underline{2}$ | 14 | 0 |
| 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ |

TABLE 6. TABLE OF VALUES OF $s$ AS FUNCTIONS OF $h$ AND $X$ FOR SINE STENCILS ($N=60$)

| $X$ \ $h$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 | 15 |
| 1 | 15 | 14 | 13 | 12 | 11 | 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
| 2 | 15 | 13 | 11 | 9 | 7 | 5 | 3 | 1 | 1 | 3 | 5 | 7 | 9 | 11 | 13 | 15 | $\underline{13}$ | $\underline{11}$ | $\underline{9}$ | $\underline{7}$ | $\underline{5}$ | $\underline{3}$ | $\underline{1}$ | $\underline{1}$ | $\underline{3}$ | $\underline{5}$ | $\underline{7}$ | $\underline{9}$ | $\underline{11}$ | $\underline{13}$ | 15 |
| 3 | 15 | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 | 15 | $\underline{12}$ | $\underline{9}$ | $\underline{6}$ | $\underline{3}$ | $\underline{0}$ | $\underline{3}$ | $\underline{6}$ | $\underline{9}$ | $\underline{12}$ | 15 | 12 | 9 | 6 | 3 | 0 | 3 | 6 | 9 | 12 | 15 |
| 4 | 15 | 11 | 7 | 3 | 1 | 5 | 9 | 13 | $\underline{13}$ | $\underline{9}$ | $\underline{5}$ | $\underline{1}$ | $\underline{3}$ | $\underline{7}$ | $\underline{11}$ | 15 | 11 | 7 | 3 | 1 | 5 | 9 | 13 | $\underline{13}$ | $\underline{9}$ | $\underline{5}$ | $\underline{1}$ | $\underline{3}$ | $\underline{7}$ | $\underline{11}$ | 15 |
| 5 | 15 | 10 | 5 | 0 | 5 | 10 | 15 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ | $\underline{5}$ | $\underline{10}$ | 15 | 10 | 5 | 0 | 5 | 10 | 15 | $\underline{10}$ | $\underline{5}$ | $\underline{0}$ | $\underline{5}$ | $\underline{10}$ | 15 | 10 | 5 | 0 | 5 | 10 | 15 |
| 6 | 15 | 9 | 3 | 3 | 9 | 15 | $\underline{9}$ | $\underline{3}$ | $\underline{3}$ | $\underline{9}$ | 15 | 9 | 3 | 3 | 9 | 15 | $\underline{9}$ | $\underline{3}$ | $\underline{3}$ | $\underline{9}$ | 15 | 9 | 3 | 3 | 9 | 15 | $\underline{9}$ | $\underline{3}$ | $\underline{3}$ | $\underline{9}$ | 15 |
| 7 | 15 | 8 | 1 | 6 | 13 | $\underline{10}$ | $\underline{3}$ | $\underline{4}$ | $\underline{11}$ | 12 | 5 | 2 | 9 | $\underline{14}$ | $\underline{7}$ | $\underline{0}$ | $\underline{7}$ | $\underline{14}$ | 9 | 2 | 5 | 12 | $\underline{11}$ | $\underline{4}$ | $\underline{3}$ | $\underline{10}$ | 13 | 6 | 1 | 8 | 15 |
| 8 | 15 | 7 | 1 | 9 | $\underline{13}$ | $\underline{5}$ | $\underline{3}$ | $\underline{11}$ | 11 | 3 | 5 | 13 | $\underline{9}$ | $\underline{1}$ | $\underline{7}$ | 15 | 7 | 1 | 9 | $\underline{13}$ | $\underline{5}$ | $\underline{3}$ | $\underline{11}$ | 11 | 3 | 5 | 13 | $\underline{9}$ | $\underline{1}$ | $\underline{7}$ | 15 |
| 9 | 15 | 6 | 3 | 12 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 12 | 3 | 6 | 15 | $\underline{6}$ | $\underline{3}$ | $\underline{12}$ | 9 | 0 | 9 | $\underline{12}$ | $\underline{3}$ | $\underline{6}$ | 15 | 6 | 3 | 12 | $\underline{9}$ | $\underline{0}$ | $\underline{9}$ | 12 | 3 | 6 | 15 |
| 10 | 15 | 5 | 5 | 15 | $\underline{5}$ | $\underline{5}$ | 15 | 5 | 5 | 15 | $\underline{5}$ | $\underline{5}$ | 15 | 5 | 5 | 15 | $\underline{5}$ | $\underline{5}$ | 15 | 5 | 5 | 15 | $\underline{5}$ | $\underline{5}$ | 15 | 5 | 5 | 15 | $\underline{5}$ | $\underline{5}$ | 15 |
| 11 | 15 | 4 | 7 | $\underline{12}$ | $\underline{1}$ | $\underline{10}$ | 9 | 2 | 13 | $\underline{6}$ | $\underline{5}$ | 14 | 3 | 8 | $\underline{11}$ | $\underline{0}$ | $\underline{11}$ | 8 | 3 | 14 | $\underline{5}$ | $\underline{6}$ | 13 | 2 | 9 | $\underline{10}$ | $\underline{1}$ | $\underline{12}$ | 7 | 4 | 15 |
| 12 | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 | 3 | 9 | $\underline{9}$ | $\underline{3}$ | 15 |
| 13 | 15 | 2 | 11 | $\underline{6}$ | $\underline{7}$ | 10 | 3 | $\underline{14}$ | $\underline{1}$ | $\underline{12}$ | 5 | 8 | $\underline{9}$ | $\underline{4}$ | 13 | 0 | 13 | $\underline{4}$ | $\underline{9}$ | 8 | 5 | $\underline{12}$ | $\underline{1}$ | $\underline{14}$ | 3 | 10 | $\underline{7}$ | $\underline{6}$ | 11 | 2 | 15 |
| 14 | 15 | 1 | 13 | $\underline{3}$ | $\underline{11}$ | 5 | 9 | $\underline{7}$ | $\underline{7}$ | 9 | 5 | $\underline{11}$ | $\underline{3}$ | 13 | 1 | 15 | $\underline{1}$ | $\underline{13}$ | 3 | 11 | $\underline{5}$ | $\underline{9}$ | 7 | 7 | $\underline{9}$ | $\underline{5}$ | 11 | 3 | $\underline{13}$ | $\underline{1}$ | 15 |
| 15 | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 | $\underline{0}$ | 15 | 0 | 15 |

*4. The construction of strips, racks, and stencils*

The strips upon which the values of $D \cos 2\pi s/N$ are tabulated can be prepared in any width suitable for the type of lettering used. One of us (P.) has used strips of width $\frac{5}{16}''$. The numbers were entered freehand, using a guide to insure their correct location with respect to the stencil openings. For $N=48$ a length of $8\frac{1}{2}''$ proved appropriate. In another case (T.) strips of width $\frac{1}{2}''$ were used and a length of $9\frac{1}{2}''$ proved appropriate for $N=60$. A Leroy lettering guide (#3240 120CL) was used in entering the numbers on the strips in this case. In both cases, white card was used for the positive values, while another color (green or blue) was chosen for the negative values. The strips may be cut to appropriate size in a printer's guillotine or on a sheet metal cutter.

The rack for the strips can be cut out of hardwood or aluminum with the aid of a milling cutter whose width is slightly greater than that of the strips. The depth of the grooves should be equal to the thickness of the strips, so that the filled board presents a flat surface on which the stencils may rest. Brass strips around the edge of the board serve to locate the stencils accurately with respect to the rack. The details of the construction of the board can be readily seen in Figs. 2*a* and 2*b*.

The stencils can be cut from pressboard or other similar material. The positions of the holes are laid out on master stencils (cf. Fig. 3) in accordance with the scheme adopted in laying out the rack and the strips. The holes in the stencils may then be cut out with a hand punch using the master stencil as a guide, or a punch press may be used. The writers have made use of a simple punch mounted in a drill press. The male punch was mounted in the chuck of a drill press, while the female punch was located in a flat board clamped to the table of the press. If pressboard is used for the stencils, the identification marks can be lettered on them in Duco white with use of a Leroy lettering pen with the cleaner removed.

The strips must be stored in such a manner as to make them readily available. The container used by one of us (T.) is illustrated in Fig. 5; it has a separate hole for strips of each $D$ value. The positive and negative strips of the same $D$ value are filed in the same hole with the negative strips placed in the rear. The method is only limited in extent of $D$ values by the convenience of filing the strips. The storage container shown has 208 holes for $D$ values from 0 to 207 inclusive. A convenient container could be made on the same design to accommodate strips with $D$ values 0 to 1000 inclusive.

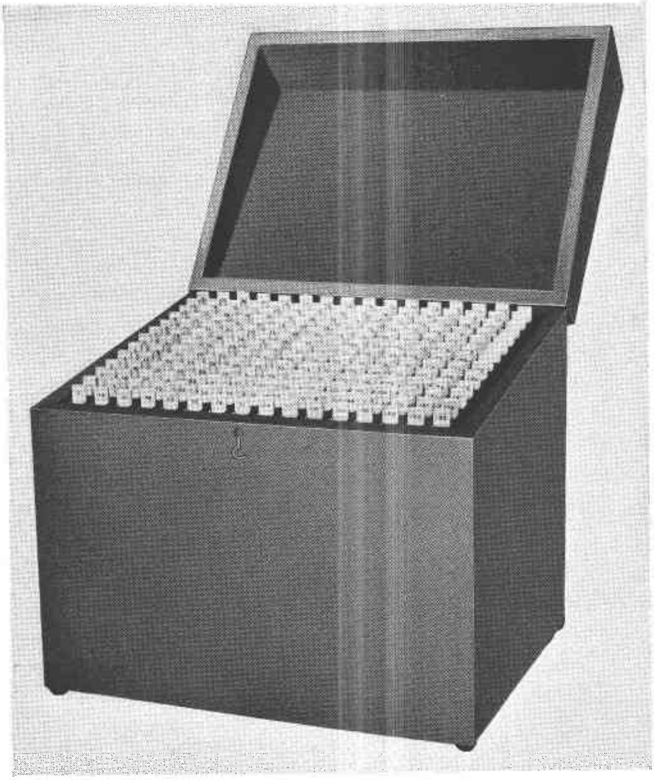

FIG. 5. Container for strips for $N=60$, with places for strips for $D$-values 0 to 207. The positive and negative strips of the same $D$-value are filed in the same hole.

## PART II. METHODS FOR TWO-DIMENSIONAL SUMMATIONS

### 5. *The summation of two-dimensional series*

The two-dimensional series which appear in crystal analysis are of the form[10]

$$f(X'Y') = \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \{A(hk) \cos 2\pi(hX' + kY') + B(hk) \sin 2\pi(hX' + kY')\} \qquad (12)$$

where

$$X' = \frac{X}{N}, \qquad X = 0, \pm 1, \pm 2, \cdots, \pm N,$$

[10] Bragg, W. L.: *Proc. Roy. Soc.*, **A123,** 537 (1929); Robertson, J. M.: *Reports on Progress in Physics*, **4,** 332 (1938).

Cf. especially equation II*a*, p. 3, Lonsdale, K.: Simplified Structure Factor and Electron Density Formulae for the 230 Space Groups of Mathematical Crystallography, Bell & Sons, London (**1936**).

and

$$Y' = \frac{Y}{N}, \qquad Y = 0, \pm 1, \pm 2, \cdots, \pm N,$$

with

$$A(\bar{h}\bar{k}) = A(hk) \qquad B(hk) = -B(\bar{h}\bar{k}).$$

If we write

$$\mathbf{A}(X'Y') = \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} A(hk) \cos 2\pi(hX' + kY') \tag{13}$$

and

$$\mathbf{B}(X'Y') = \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} B(hk) \sin 2\pi(hX' + kY') \tag{14}$$

then we may write (12) in the form

$$f(X'Y') = \mathbf{A}(X'Y') + \mathbf{B}(X'Y'). \tag{15}$$

We note that the function $\mathbf{A}(X'Y')$ possesses a center of symmetry at the origin, and that the operation of a center at the origin reproduces $\mathbf{B}(X'Y')$ with a reversal of sign. We need only compute these two functions for points covering one half of the unit cell. If the function $f(X'Y')$ has a center of symmetry at the origin, we must have $f(X'Y') = f(\overline{X}'\overline{Y}')$ and consequently $\mathbf{B}(X'Y') = 0$ everywhere and $B(hk) = 0$ for all values of $h$ and $k$.

The summations (13) and (14) are now split up into one-dimensional summations following the method suggested by Beevers and Lipson.[2] We shall discuss the expression (13) first. It may be written

$$\begin{aligned} \mathbf{A}(X'Y') &= \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} A(hk) \{\cos 2\pi hX' \cos 2\pi kY' - \sin 2\pi hX' \sin 2\pi kY'\} \\ &= \mathbf{C}(X'Y') - \mathbf{S}(X'Y'), \end{aligned} \tag{16}$$

in which

$$\mathbf{C}(X'Y') = \sum_{h=0}^{\infty} \sum_{k=0}^{\infty} C(hk) \cos 2\pi hX' \cos 2\pi kY' \tag{17}$$

with

$$\begin{aligned} C(00) &= A(00), \qquad C(h0) = 2A(h0), \qquad C(0k) = 2A(0k), \\ C(hk) &= 2A(hk) + 2A(\bar{h}k), \end{aligned} \tag{17'}$$

and

$$\mathbf{S}(X'Y') = \sum_{h=1}^{\infty} \sum_{k=1}^{\infty} S(hk) \sin 2\pi hX' \sin 2\pi kY' \tag{18}$$

with

$$S(hk) = 2A(hk) - 2A(\bar{h}k). \tag{18'}$$

The expression (17) may now be summed completely. We may sum first with respect to $h$, or with respect to $k$ as we wish.[11] Suppose we sum with respect to $k$ first. Thus (17) may be written

[11] It is usual to sum first over the index that has the highest value represented among the values $C(hk)$; in this way, the number of initial summations to be performed is made as small as possible.

$$C(X'Y') = \sum_{h=0}^{\infty} c(hY') \cos 2\pi hX' \tag{19}$$

in which

$$c(hY') = \sum_{k=0}^{\infty} C(hk) \cos 2\pi kY'. \tag{20}$$

We can compute this latter series by the methods described earlier, and use the results of this computation as coefficients in performing the computation (19) by the same methods. This process will be described in detail below.

The summation $S(X'Y')$ may be split up in exactly the same way, i.e.,

$$S(X'Y') = \sum_{h=1}^{\infty} s(hY') \sin 2\pi hX' \tag{21}$$

in which

$$s(hY') = \sum_{k=1}^{\infty} S(hk) \sin 2\pi kY'. \tag{22}$$

The series for $B(X'Y')$ may be written

$$\begin{aligned} B(X'Y') &= \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} B(hk)\{\sin 2\pi hX' \cos 2\pi kY' + \cos 2\pi hX' \sin 2\pi kY'\} \\ &= SC(X'Y') + CS(X'Y') \end{aligned} \tag{23}$$

in which

$$SC(X'Y') = \sum_{h=0}^{\infty} \sum_{k=0}^{\infty} SC(hk) \sin 2\pi hX' \cos 2\pi kY' \tag{24}$$

$$CS(X'Y') = \sum_{h=0}^{\infty} \sum_{k=0}^{\infty} CS(hk) \cos 2\pi hX' \sin 2\pi kY'. \tag{25}$$

In these expressions the coefficients are related to the $B(hk)$ by the relations

$$\begin{aligned} &SC(0k) = SC(00) = CS(h0) = CS(00) = 0, \\ &SC(h0) = 2B(h0), \qquad SC(hk) = 2B(hk) + 2B(h\bar{k}) \\ &CS(0k) = 2B(0k), \qquad CS(hk) = 2B(hk) - 2B(h\bar{k}). \end{aligned} \tag{26}$$

The two sums (24) and (25) can now be split up into one-dimensional series in strict analogy with the process described for the series (17) and (18). We shall give no further discussion of the series $B(X'Y')$ in this paper since most two-dimensional series met with in crystal analysis have a center of symmetry, in which case $B(X'Y')=0$. If the need for it arise, the reader, who has made himself familiar with the summation of series of the type $A(X'Y')$, will have no difficulty in setting up a scheme for $B(X'Y')$.

### 6. *Arrangement of numerical work*

A scheme for the computation of a series of the type $A(X'Y')$ is shown in Fig. 6. The quantities $A(hk)$ are assumed to be known either from ex-

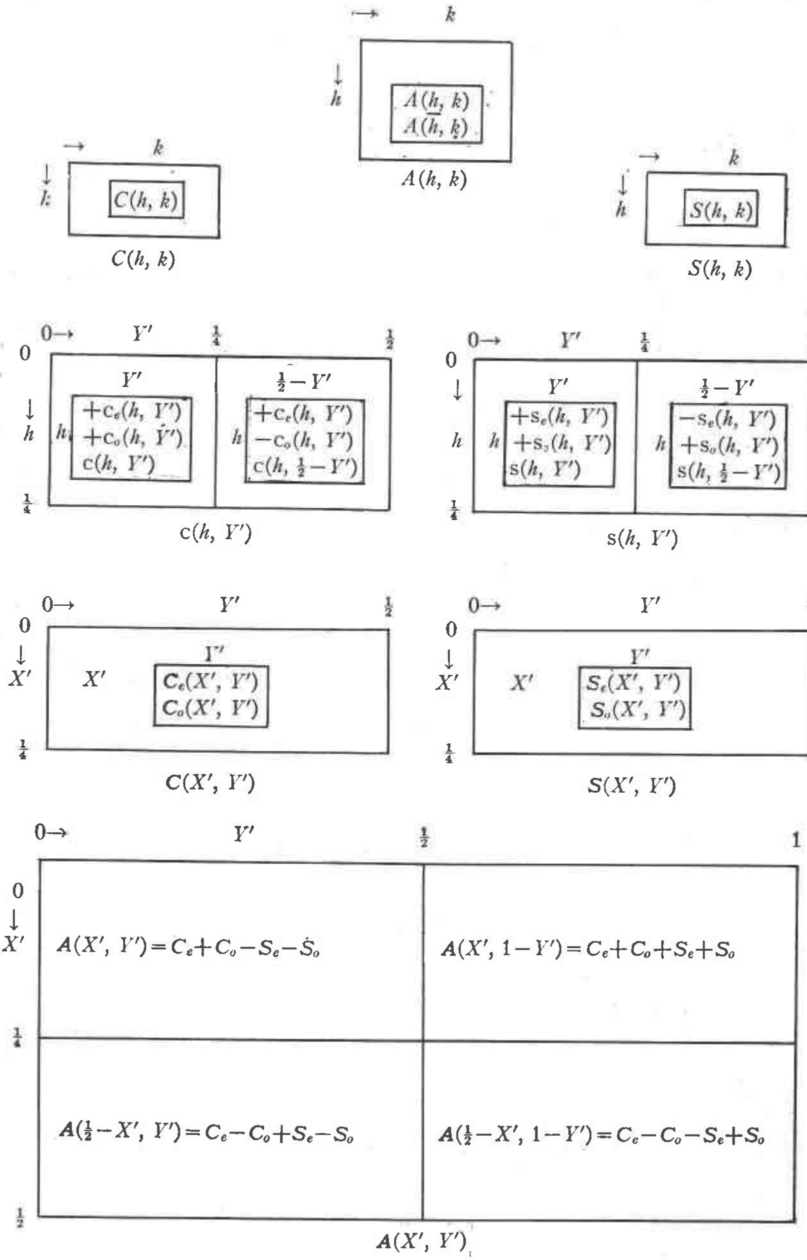


FIG. 6. Arrangement of numerical work for two dimensional cosine series.

periment or as a result of a previous calculation.[12] In general $A(\bar{h}k)$ will be different from $A(hk)$, but $A(\bar{h}\bar{k})$ will be equal to $A(hk)$. The value of $A(hk)$ can thus be entered in a table in which the indices $h$ and $k$ run from 0 to the largest value of $h$ or $k$ for which $A(hk)$ has significance, provided $A(hk)$ and $A(\bar{h}k)$ are written in the same box one above the other. The two tables $C(hk)$ and $S(hk)$ are then constructed from the $A(hk)$ values according to the rules of equations (17′) and (18′) which define these quantities. The table $C(hk)$ provides the material for the summation which leads to $\mathbf{C}(X'Y')$. The first step is a summation over $k$ given by equation. (20). There will be as many such series to sum as there are values of $h$, and each series will be summed for the points 0 to $N/4$. The results of this summation are entered in the $\mathrm{c}(hY')$ table. The summations for the even $k$ values lead to the quantities $\mathrm{c}_e(hY')$ and those for odd $k$ lead to $\mathrm{c}_o(hY')$. Both these sets of quantities are entered in the same box in the table, and their sum gives the values of $\mathrm{c}(hY')$ for $Y'$ values from 0 to $N/4$. This table is now extended to $N/2$ by writing $\mathrm{c}_e(hY')$ and $-\mathrm{c}_o(hY')$ in the $N/2-Y'$ box, the sum of these two quantities being the value of $\mathrm{c}(h, \overline{N/2-Y'})$.

We must now sum $(N/2+1)$ series of the type (19) for the points 0 to $N/4$. The results of these summations, i.e. $\mathbf{C}_e(X'Y')$ and $\mathbf{C}_o(X'Y')$ are entered in the same box in the $\mathbf{C}(X'Y')$ tables and their sum in each case then gives the $\mathbf{C}(X'Y')$ values for the points in question.

A similar procedure now leads to a computation of the table $\mathbf{S}(X'Y')$ from the table $S(hk)$, the only difference being in the use of sine stencils instead of cosine stencils and in the rules for combination of the even and odd parts of the various sums. In the final table, according to equation (16) the function $\mathbf{A}(X'Y')$ is formed by subtracting $\mathbf{S}(X'Y')$ from $\mathbf{C}(X'Y')$ while the values at the points $(X', N-Y')$ are obtained by adding these two quantities.[13]

The reader who finds it necessary to sum a series that does not possess a center of symmetry, and must therefore sum the series $\mathbf{B}(X'Y')$ given by equation (14), will find no difficulty in setting up a scheme entirely

[12] $A(hk)$ may be either the structure factor $F$ or the square of the absolute value of the structure factor. The magnitudes of the structure factors can be determined from measurements of the intensities of the diffracted $x$-ray beams from the crystal planes. The signs of the absolute values of the structure factors are not determinable by measurement, however, and must be obtained from a previous solution, either by trial and error, or by the use of an $|F|^2$ series, or, in some cases, by comparison with those of another member of the same isomorphous series of crystals.

[13] Since the tables of $\mathbf{C}_e(X'Y')$, $\mathbf{C}_o(X'Y')$ and $\mathbf{S}_e(X'Y')$, $\mathbf{S}_o(X'Y')$ are always the same size (for a given number of divisions in the unit cell e.g. 48 or 60) a strip of cardboard with 2 suitable notches can be used to select quickly the four values needed for combination into the final value of $\mathbf{A}(X'Y')$. This device was first used in these summations by Mrs. Selma Blazer Brody and we are indebted to her for the suggestion.

analogous to that of Fig. 6. The difference will lie in a different use of stencils and a different combination procedure. Equations (23) to (26) and the results of equations (5) and (9) provide all the information necessary for the purpose.

The computation outlined in Fig. 6 can conveniently be carried out on squared paper of dimensions 50 cm. × 75 cm. ruled in 1 cm. squares. Since the three numbers required in one entry in the tables $c(hY')$, $s(hY')$, etc. can readily be entered in a 1 cm. square, the whole computation with the exception of the final $A(X'Y')$ table can be entered on one sheet. The $A(X'Y')$ table then occupies a separate sheet.

## 7. *Conclusion*

In this paper, we have described in detail a method for the summation of one dimensional Fourier series[14] and a procedure that enables this method to be applied to the summation of two-dimensional series. In conclusion it is perhaps desirable to make a brief comparison between this method and the two others which have been described previously. The method of Robertson[3] and the present method are the same in principle, but in practice they differ in one important point. In Robertson's method the strips are mounted in slides. Each slide is set for a given $X'$ value by means of an indicator. The advantage of his method is that the numbers to be added appear in a vertical column, and can be added with maximum ease. In the method we have described the selection of numbers is by means of stencils, and the addition is along a slanting or zigzag sequence of holes. Owing to the relatively small number of holes in any one stencil, this adds little or no difficulty to the process of addition. In going from one point to the next, in Robertson's method all the strips must be individually reset, whereas in the method here described it is only necessary to replace one stencil by another.

The method of Lipson and Beevers[4] differs quite radically from the other two[3,5] in that their strips carry the values

$$D \cos 2\pi hX/N \quad \text{and} \quad D \sin 2\pi hX/N$$

for fixed values of $h$ and for varying values of $X$. Strips for sine or cosine are then selected for a given $D$ and its appropriate $h$. After the strips have been selected, they are arranged one above the other and the figures in vertical columns are simply added. If positive and negative values are both present they must be added separately and the results combined.

[14] Those familiar with the processes of Fourier analysis will have no difficulty in recognizing that the method is equally applicable to Fourier analysis by the method of equidistant ordinates. Cf. Whittaker and Robinson: The Calculus of Observations, Blackie, London (**1924**), and Eagle, A.: Fourier's Theorem, Longmans, Green, London (**1925**).

The Lipson and Beevers method thus requires very many more strips than are required by the present method. This disadvantage is, however, somewhat reduced by the fact that strips for the numbers 1 to 100 have been printed and are available. In the method of Lipson and Beevers, the Miller index, the *D*-value with its sign, and the nature of the function (sine or cosine) all must be watched in the selection of the strip; whereas in the method described here, only the *D*-value with its positive or negative sign determines the selection. A comparison of the experience of workers using the Lipson-Beevers method and of those using the one under discussion here, seems to indicate that the time taken for a summation is not greatly different for *D*-values ranging from 0 to 100. For *D*-values ranging from 0 to 1000, or more, the method of Lipson and Beevers would require such an enormous number of strips that it would not be so convenient as the stencil method, which experience has shown to be well adapted to this range.[15]

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[15] Sets of 1800 strips (*F*-values 0 to 300, negative and positive, three strips of each kind) for use with the method described in this paper may be obtained from Prof. J. D. H. Donnay, Institut de Géologie et de Minéralogie, Boulevard de l'Entente, Québec, P. Q., Canada. (Price $9.00 per set.)