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A Punched Card Method for Radial Distribution Calculations in X-Ray and Electron Diffraction Studies

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The numerical calculations in structure investigations by X-ray or electron diffraction procedures may conveniently be facilitated by punched card methods. Different systems have been developed for this purpose in connection with X-ray investigations of crystals [1–3] and electron diffraction studies of gases [4]. The present paper deals with the numerical calculations involved in the sector method of electron diffraction, and in X-ray investigations of liquids and amorphous solids.

In the methods used in our laboratories [5,6], the structure investigations are carried out using the following functions:

$$M(r) = \int Y(s)\sin sr\, ds \quad \text{and} \quad N(r) = \int Y(s)\cos sr\, ds \tag{1}$$

$Y(s)$ is obtained experimentally, $M(r)$ gives information about the interatomic distances to be obtained, and $N(r)$ may be used for the final structure interpretation and the estimation of accuracy [7].

For the numerical calculation equations (1) are put in the form

$$M(r_m) = \sum_n Y(s_n) \sin s_n r_m \text{ and } N(r_m) = \sum_n Y(s_n) \cos s_n r_m \tag{2}$$

If the values of $Y(s_n)$ are measured at equidistant s values, $s_1, s_2, \ldots\ldots s_n$, the values of $M(r_m)$ and $N(r_m)$ can be obtained for equidistant r values, $r_1, r_2, \ldots\ldots r_m$. The value most frequently used here is $s_n = \frac{1}{4}\, n$ (Å^{-1}), n being equal to 1, 2, 3, ... 90, and $r_m = {}^{8\pi}/_{360}\, m$ (Å), m being equal to 1, 2, 3, ... 90. Then all the angles $s_n r_m$ will be given in whole degrees, expressed by ${}^{2\pi}/_{360}\, nm$.

EQUIPMENT AND FILE

For the evaluation of equation (2) by punched-card machines, the following two or three standard I. B. M. units are used — a "collator" (type 077) and a "numerical accounting machine with progressive totals" (type 416). The latter may be replaced by an "alphabetical accounting machine" (type 405) with a "summary punch" for making progressive totals. Eleven usual selectors, two digit selectors, and sixteen counters are used in the tabulator. For the units (416) and (405) one semi-fixed plugboard can be used for the different operations mentioned below.

For calculating $M(r)$ we use a sine-file consisting of 9 000 cards which will be described below. The calculation of $N(r)$ is carried out using a corresponding file where the sin sr values are replaced by cos sr values.

The 9 000 cards of the sine-file are split up in 10 R groups, called R_1, R_2, ... R_{10}. The 900 cards of each R group are divided in 90 s groups, corresponding to s_1, s_2, s_3, ... s_{90}. Each s group contains 10 cards called α_0, α_1, α_2 ..... α_9. The first two of these, α_0 and α_1 are sign-cards; the rest, α_2 to α_9 are sine-cards. Each of these corresponds to different Y (s_n) sin $s_n r_m$ values. Each α number represents a constant Y value according to the binary system (Table 1).

Table 1.

α:	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9
Y	1	2	4	8	16	32	64	128

A given, arbitrary Y value is expressed by a certain selection of α cards. For example, $Y = -69$ is expressed by α_1 and the sum of the cards α_8, α_4 and α_2.

Table

Columns:	1—2	3—4	5	6—8	9—10	11—12
Information punched in the sign-cards:	R	s	α		+ or − for $Y(s)$ $(0<r<2\pi)$	+ or − for $Y(s)$ $(2\pi<r<4\pi)$
Information punched in the sine-cards:	R	s	α	$Y(s)$		

Each of the 9 00 cards belonging to a certain R group is characterized by a certain s value having 90 possible values, and by a certain α-value (10 possibilities). In each sine-card the values of $Y(s_n)$ sin $s_n r_m$ for 9 different r values are punched. The group R_1 corresponds to $r_1, r_2, \ldots\ldots r_9$, the group R_2 to $r_{10}, r_{11}, \ldots\ldots r_{18}$ and so on, the last group R_9 corresponding to $r_{82}, r_{83}, \ldots\ldots r_{90}$.

The 80 columns of a sine-card are used in the following way. Columns 18 to 71 contain the numerical values of the nine Y sin sr values, and the columns 72—80 the corresponding signs. Columns 1 and 2 give the R value, and columns 3 and 4 the s values column 5 gives the α-number, and 6—8 the Y value. In the sine-cards, columns 9 to 17 are not used.

In the sign-cards columns 1 to 5 are used for indication of the R, s, and α values as in the sine-cards. Columns 9 and 10 give the sign for the Y function and columns 11 to 13 are used for special purposes discussed below. A scheme of the information punched in the cards is given in Table 2.

THE WORKING SCHEME

The evaluation of equations (1) on the basis of given Y (s_n) values, is performed as a simple addition of numbers punched in a certain selection of cards from the main file. The addition is first carried out for the 9 r values of the R_1 cards, then for the R_2 cards and so on. The working scheme for a complete calculation will therefore be:

1) Cards corresponding to R_1 are selected by hand from the main file. For each s value one has to pick out a certain number of α cards corresponding to the Y (s) value in question. The hand-sorting is simplified by the α-values which are punched in column 5.
2) Corresponding selections for $R_2, R_3, \ldots\ldots R_{10}$ are performed by use of the collator. The machine picks out the cards by comparing s and α values of the main file with those of the R_1 cards.

2.

13	18—23	24—29	.....	66—71	72—80
termination					
	Y sin sr_i	Y sin $sr_i + 1$	.....	Y sin $sr_i + 8$	sign for sin sr_i—sin $sr_i + 8$

3) The selected cards are run through the accounting machine and the results are tabulated or punched in new cards by the summary punch. In the tabulator the signs for Y (s) and sin sr are combined in the right way by selectors.
4) All the cards are rearranged by the collator, and the card file is ready for the next calculation.

The mean time of a calculation 1) to 4) has been found to be about 1 ½ hours. Using an electrical desk machine the same calculation usually requires more than 25 hours, or 3—4 working days.

ADDITIONAL ARRANGEMENTS

Besides the requirements strictly necessary for the evaluation of equation (2), our system includes some additional features which make the application more effective. These extra features include facilities 1) for checking purposes, 2) for intermediate terminations of the series, and 3) for extension to higher s and r values.

1. Checking

To make sure that the right cards have passed through the machine, a direct summation of the Y (s) values are carried out parallel to the 9 ordinary summations of a given R series. As the same Y (s) values repeat for every new R value, this verification is easily performed by comparison with the corresponding Y (s) summations directly based on the experimental data. To detect failures in the individual counters, a special check-summation is carried out in the tabulator before and after the calculation.

2. Intermediate terminations

Very often smaller parts of the series are wanted, say from s_1 to s_i, i being some arbitrary number. These values are obtained by a special use of column 13 of the sign cards. A certain number, say 1, is punched in the cards following those s values at which the terminations are wanted, and the tabulator (416) is adjusted to print the corresponding progressive totals. The same thing can be achieved with a tabulator (405) and summary punch. The twelve places of column 11 give twelve possibilities for successive series of terminations and combinations of these twelve sequences give still more possibilities.

3. Extension of the s and r values

The card system has been extended to cover s values higher than s_{90} ($= 22.5$ Å^{-1}). This is easily done because of the symmetry of all $\sin s_n r_m$ values with respect to s_{90}. The same symmetry makes it possible to perform a cosine-summation directly from the sine-cards, for all even values of m.

The card system is symmetrical also with respect to r_{90} ($= 2\pi$ Å). One may therefore use the same cards for calculations beyond r_{90} by a change of sign for odd values of n. Columns 11 and 12 of the sign cards are used for these alternative signs of the $Y(s)$ functions.

One may of course use an arbitrary equidistant sequence of s, given by $s_n = kn$. Then the system described will correspond to the r values, $r_m = \frac{2\pi m}{360\, k}$.

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