Literatur

EWALD, P. P. (1940). *Proc. Phys. Soc.* **52**, 167.
HOSEMANN, R. & BAGCHI, S. N. (1952). *Acta Cryst.* **5**, 749.
LAUE, M. VON (1948). *Röntgenstrahl-Interferenzen*. Leipzig: Akademische Verlagsgesellschaft.
PATTERSON, A. L. (1939). *Nature, Lond.* **143**, 939.
PATTERSON, A. L. (1944). *Phys. Rev.* **65**, 195.
STOKES, A. R. & WILSON, A. J. C. (1942). *Proc. Camb. Phil. Soc.* **38**, 313.

Acta Cryst. (1953). **6**, 325

A Method of Fourier Synthesis Using a Standard Hollerith Senior Rolling Total Tabulator

BY N. KITZ* AND B. MARCHINGTON†

Birkbeck College Physics Research Department, 21 Torrington Square, London W.C. 1, England

(*Received 4 November 1952 and in revised form 1 December 1952*)

This paper describes a method of setting up a Hollerith Senior Rolling Total Tabulator for the calculation of Fourier synthesis in which the tabulator runs at its maximum tabulating speed and with which no auxiliary Hollerith machinery is required.

During the last few years Hollerith accounting machines have been used increasingly for the computation of Fourier synthesis and several papers, describing various methods of operation, have appeared (Hodgson, Clews & Cochran, 1949; Cox & Jeffrey, 1949; Cox, Gross & Jeffrey, 1949; Greenhalgh & Jeffrey, 1950). At Birkbeck College a technique has been devised for using a standard Hollerith Senior Rolling Total Tabulator having no special adaptations. In this scheme the machine has been made to operate throughout at its maximum tabulating speed and it has also been found possible to perform the entire calculation with one fixed set of plugboards. The method requires a minimum number of card passages and, since only one pack of cards is used, it is essentially inexpensive to run. The mode of operation is so simple that a trained operator is not required.

The pack of cards in use has been kindly supplied by Mr T. B. Boss of the National Physical Laboratory. Each card is double-punched (Greenhalgh, 1950) with sixteen values of the function $A \begin{matrix}\cos\\ \sin\end{matrix}(fx)$ to one decimal place, a negative number $(-y)$ being punched as $(10{,}000-y)$; values of the argument (x) range from 0° to 90° at 6° intervals. The present pack contains amplitudes (A) from 1–5, 10–50, and 100–400, i.e. fourteen cards in all for each frequency (f), which has values in the range 0–59. An extension of the pack to much higher values of (f) is contemplated.

The method of computation is the same as that used with Beevers–Lipson strips. Cards of the required amplitude and frequency are picked out from the main pack and the sums of the sixteen fields are obtained in separate counters. Since there are only six counters and six numerical print banks in a standard Senior Rolling Total Tabulator, not more than six fields can be summed at any one time and three passages of the cards through the machine are necessary.

To avoid changing plugboards, the four multipoint relays (known as selectors) are used to determine the group of fields being summed. These selectors, which are switchable, have eleven positions on both the 'on' and 'off' sides. If they are paired and connected to form a 'tree', it becomes possible to select any group of 22 columns on the card out of a total of 66 input columns.

The first field on the card (i.e. the amplitude) is always summed and printed to check that no cards have been lost between successive insertions of the pack. Hence this particular field need not be selected and the card columns corresponding to it are connected directly into a counter. A group of 25 columns out of the remaining 75 is still to be selected; this exceeds the capacity of the selector 'tree' and therefore a modified method has been adopted.

The most significant digit in each field is always '0' if the field is positive and '9' if it is negative; the next most significant digit has a maximum value of '4' if the field is positive and a minimum value of '5' if it is negative. This distinction is used to determine the signs of the fields, without having to transmit their most significant digit, in the following way.

A normal Senior Rolling Total Tabulator has sixteen inner control relays, connected in series. This chain is broken into groups of four relays by supplying an

* Now at: Istituto Nazionale per le Applicazioni del Calcolo, Piazzale delle Scienze 7, Rome, Italy.
† Now at: Royal Naval Scientific Service, Queen Anne's Mansions, London S.W. 1, England.

impulse at the beginning of every card feed (this impulse therefore occurs at 'nine' time) to every fourth relay. The number of negative values accumulated in a given counter is counted by means of the card count impulse which is sent to the least significant end of the relevant counter via a relay A, whose contacts are found open if the value of the field is positive and closed if it is negative.

To obtain this discrimination the 'hundreds' columns of the field under examination is plugged directly to one of the coils of the following relay B whilst a 'four' impulse is sent to its contacts. If the impulses derived from the card columns occur at 'four', 'three', 'two', 'one' or 'zero' time, the 'four' impulse applied to the contacts of relay B can get through and is then applied to one of the coils of relay A, thus suppressing the card count which arrives much later. If the impulse sent to relay B occurs at any other time, the 'four' impulse finds the contacts of B open and is lost, relay A remains closed and the counter records the fact that a negative field value has been accumulated.

Of the six fields which can be handled by the counters of the machine, one (the amplitude field) is always sent direct to a counter, two are transmitted through the selector 'tree' in their entirety, whilst the remaining three are transmitted without their most significant digit. By simply manipulating the switches which control whether or not a given selector can be put on during card feed, it is possible to select and sum all the sixteen fields in only three card passages.

In the case of fields which are selected in their entirety the counters are used in the conventional way, the most significant column in each field being plugged to several wheels simultaneously to provide the requisite number of 'nines' necessary for complementary subtraction. When the fields are selected without sign indication, some of the spare counter wheels are used to count 'one' impulses which they receive every time a negative field is encountered; the sum thus obtained, suitably corrected for the fact that the tabulator 'rolls' with nines complements, is subtracted, at the end of the card run, from the wheels immediately to the left of those used to accumulate the card columns. The counters then contain correct totals which can be printed.

For the purpose of checking it is advisable to print some indication of the position of the selector switches on the tabulator, i.e. of the group of fields being summed. This is done in conjunction with the rounding off of numbers in the counters. Two cards are fed in at the beginning of each pack; the first contains '1', '2' and '3' punched respectively in the least significant position of the first field of each group of five; the second contains a '5' punched in the least significant position of all fields, except those mentioned above in which '4', '3' and '2', respectively, are punched. The least significant digit of the counter containing the second field is connected to the 'α' list bank and the tabulator group indication switches are put on. A '1', '2' or '3' is printed according to the group of fields being selected.

The technique described above has been very satisfactorily used, during the last four months, by those engaged in the enormous amount of computation involved in the structure determination of ribonuclease now being carried out at Birkbeck College Research Laboratory. It has without doubt reduced the time spent on Fourier computations and the system has been found to be less tedious and more efficient than those methods previously used.

The authors would like to express their thanks to Messrs R. Milne and A. Hook of the B.T.M. Company for their help in the work described above.

References

Cox, E. G., Gross, L. & Jeffrey, G. A. (1949). *Acta Cryst.* **2**, 251.

Cox, E. G. & Jeffrey, G. A. (1949). *Acta Cryst.* **2**, 341.

Greenhalgh, D. M. S. (1950). *Proc. Leeds Phil. Lit. Soc.* **5**, 301.

Greenhalgh, D. M. S. & Jeffrey, G. A. (1950). *Acta Cryst.* **3**, 311.

Hodgson, M. L., Clews, C. J. B. & Cochran, W. (1949). *Acta Cryst.* **2**, 113.