A Fast Digital Computer for Fourier Operations

BY J. MONTEATH ROBERTSON

Chemistry Department, The University, Glasgow, Scotland

(Received 27 August 1954)

A digital computer designed for Fourier synthesis is described, which is the mechanical analogue of the usual strip methods. Suitable gear ratios are employed to generate the sine and cosine functions and the outputs are recorded by means of printing revolution counters. The machine is built for high-speed working and two-figure and three-figure coefficients (F values) can be set in a few seconds. It does not demand any skill or training on the part of the operator. As only complete revolutions of the output shafts are counted, backlash errors are unimportant. The gear ratios are selected to produce a maximum error of less than 5 parts per million with an average error of about 1 per million, so that five-figure accuracy is possible.

Introduction

Many computers, both analogue and digital, have been designed for Fourier operations. Analogue machines are generally of rather low accuracy, unless made with extreme precision and at great cost. Digital machines of the punched-card type are also costly, require a great deal of space, and demand skill and training on the part of the operator. Modern electronic computers have similar disadvantages for the crystallographer and usually lack storage space for Fourier operations. There is, therefore, need for a more compact device.

The digital computer now designed is non-electrical, apart from the initial drive, and works by simple direct gearing, from the input feed to the output printing counters. It is the mechanical analogue of the usual strip methods, F values being fed in either singly or simultaneously, while the summation totals are printed out automatically. The machine has not yet been completely built, but enough has been constructed to show that the plan is a feasible one and that it possesses certain advantages in accuracy, speed and simplicity over other possible designs. An outline of some of the main features is given in the present paper.

The Fourier operations most commonly encountered in crystal analysis are the evaluation of double or triple series for electron density and other functions, at large numbers of points in the unit cell. Such multidimensional series can generally be expanded and the numerical work put in the form of a large number of summations of single Fourier series. For example, the common double series

$$\varrho(x, y) = \sum_{-\infty}^{\infty} F_{hk} \cos 2\pi (hx/a + ky/b)$$

may be expanded and put in the form

$$\varrho(x, y) = \sum_{-\infty}^{\infty} {}_{k}A \cos 2\pi k y/b - \sum_{-\infty}^{\infty} {}_{k}B \sin 2\pi k y/b ,$$

the coefficients A and B being themselves derived from the sums

$$\sum_{-\infty}^{\infty} {}_{h}F_{hk} \cos 2\pi hx/a$$
 and $\sum_{-\infty}^{\infty} {}_{h}F_{hk} \sin 2\pi hx/a$.

The present machine is designed to deal with such summations. As in the familiar strip methods for numerical calculation (Beevers & Lipson, 1934, 1936; Beevers, 1952; Patterson, 1936; Robertson, 1936, 1948) we now choose some convenient interval of the axial length (a, b or c), in this case sixtieths, or intervals of 6°, and generate sine and cosine functions at these points. To cover the period from 0° to 90°, 15 separate generators are required. (The symmetry of the function can be utilized to cover the other quadrants.) In this machine the results are recorded by counting the revolutions of 15 shafts emerging from the generators. These outputs are fed into a series of revolution counters, from which the final summation totals can then be printed out.

If we confine ourselves to the basic set of 15 generators, then for the second and all higher-order terms in the series (h = 2, 3, 4, ...) a complicated arrangement of switching is necessary in order to convey the output from a given generator to the correct counter. It is a fundamental feature of the present machine that all such switching is avoided. This is achieved by devising a very simple type of generator which can easily be repeated and built into its correct place for each term in the series. We thus have a row of 15 generators for each term (h = 0, 1, 2, ...). These rows correspond exactly to a set of Beevers-Lipson strips arranged for summation. The necessary coefficient, F_h , for each row is then applied by imparting F_{h} revolutions to the input shaft for each row. The machine and counters are capable of operating at high speeds (up to about 6000 revolutions per minute) so that two-figure and three-figure coefficients can be set in a matter of seconds. As soon as all the coefficients have been set, the desired summation totals are recorded by the output counters.

The same basic set of 15 generators, which are described below, could, of course, be used in other

arrangements. If it were desired to employ a switching mechanism to convey the output from a given generator to the correct counter, then a system of synchronous motors might be used (magslip or selsyn mechanisms). Alternatively, the generators might be used to supply electrical impulses which could be conveyed to impulse counters, as in the machine described by Mac-Ewan & Beevers (1942). However, the present purely mechanical arrangement appears to possess some advantages.

Sine and cosine generators

It is first of all necessary to generate the sine and cosine functions accurately and quickly at the chosen intervals of 6° . It has been found that all the required ratios can be obtained with very ample accuracy by employing a simple train of four gear wheels (Fig. 1).

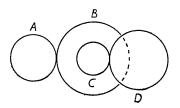


Fig. 1. Gear train.

If A, B, C and D are integers representing the numbers of teeth on these wheels, then $A/B \times C/D$ gives the ratio of the speed, or the number of revolutions, of the shaft of D (output) to that of A (input). The problem is to find sets of integers which give good approximations to the desired sine or cosine factors. For mechanical convenience we have adopted a wheel range lying between 21 and 70 teeth, with a tooth sum range between 165 and 200. With these limitations the 15 factors required can be reproduced with a maximum error of less than 5 parts per million, and an average error of about 1 per million. This ensures a comfortable five-figure accuracy, which is much more than ample for the present purpose.

Details of these ratios are shown in Table 1. The maximum error of 44×10^{-7} occurs for sin 60°, and this cannot be reduced unless the tooth sum is increased to more than 250, with at least one wheel of more than 70 teeth. There is, for example, $29/50 \times 109/73$, with an error of 20×10^{-7} , and nothing else with a highest prime factor of less than 181 until a denominator of 5000 is exceeded. A much better approximation to the sine of 6° than the one shown in Table 1 can be made by using one wheel of 82 teeth, viz. $20/49 \times 21/82$, with an error of 12×10^{-7} , but there is little point in making such an improvement while the error for sin 60° remains at 44×10^{-7} .

The limitations on wheel range and tooth sum range (ΣN) stated in Table 1 ensure reasonably small and compact generating units of fairly uniform size, and avoid the use of any large and expensive wheels. A further mechanical point worth noting is that the desired ratios can be secured as indicated, without having a common factor in the tooth numbers of any mating pair. This is certainly advantageous if the gears used are not of the highest quality, the provision of such 'hunting teeth' ensuring uniform wear over the whole wheel.

The writer obtained most of the ratios shown in the table by a simple arithmetical procedure, with the help of a fast electric calculating machine. But to prove that these are the best possible ratios is a matter of considerable difficulty. A systematic examination of the problem, however, has now been carried out by Mr T. H. O'Beirne, to whom the writer is indebted for

		Wheel range 21–70 teeth, 4	0 d.p.										
		Tooth sum (ΣN) range, 165	-200.										
$\Delta_{\rm av.} = 13 \times 10^{-7}, \Delta_{\rm max.} = 44 \times 10^{-7}.$													
Sin	Cos	$\frac{A}{B} \times \frac{C}{D}$	True value	$\Delta imes 10^7$	ΣN								
6°	84°	$\frac{22}{65} \times \frac{21}{68} = \frac{462}{4420} = 0.1045249$	0.1045285	36	176								
12°	78°	$\frac{92}{65} \times \frac{43}{70} = \frac{946}{4550} = 0.2079121$	0.2079117	+ 4	200								
18°	72°	$\frac{39}{60} \times \frac{39}{61} = \frac{113}{3660} = 0.3090164$	0.3090170	- 6	189								
24°	66°	$\frac{31}{47} \times \frac{37}{60} = \frac{1147}{2820} = 0.4067376$	0.4067366	+ 9	175								
30°	60°	$\frac{30}{43} \times \frac{43}{60} = \frac{1}{2} = 0.5000000$	0.5000000	0	176								
36°	54°	$\frac{36}{33} \times \frac{47}{63} = \frac{12273}{2079} = 0.5877826$	0.5877853	-27	169								
42°	48°	$\frac{27}{46} \times \frac{57}{50} = \frac{1539}{2300} = 0.6691304$	0.6691306	- 2	180								
4 8°	4 2°	$\frac{41}{39} \times \frac{41}{58} = \frac{1681}{2262} = 0.7431477$	0.7431448	+28	179								
54°	36°	$\frac{47}{40} \times \frac{49}{61} = \frac{1974}{2440} = 0.8090164$	0.8090170	- 6	190								
60°	3 0°	$\frac{37}{42} \times \frac{58}{59} = \frac{2146}{2478} = 0.8660210$	0.8660254	-44	196								
66°	24°	$\frac{41}{44} \times \frac{50}{51} = \frac{9050}{2244} = 0.9135472$	0.9135455	+18	186								
72°	18°	$\frac{38}{31} \times \frac{45}{58} = \frac{1710}{1798} = 0.9510567$	0.9510565	+ 2	172								
78°	12°	$\frac{40}{31} \times \frac{47}{62} = \frac{1880}{1922} = 0.9781478$	0.9781476	+ 2	180								
84°	6 °	$\frac{38}{31} \times \frac{48}{53} = \frac{1684}{1648} = 0.9945222$	0.9945219	+ 3	165								

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J. MONTEATH ROBERTSON

Table 2. Arrangement of sine and cosine generators

						Eve	en cosir	nes (p)								
θ (°) = 0	6	12	18	24	30	36	42	48	54	60	66	72	78	84	90
	R	R	R	R	R	R	R	R	R	\boldsymbol{R}	\boldsymbol{R}	R	R	R	R	R
h = 0	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90	90
h = 2	90	78	66	54	4 2	3 0	18	6	$\overline{6}$	$\overline{18}$	$\overline{30}$	$\overline{42}$	$\overline{5}\overline{4}$	$\overline{6}\overline{6}$	$\overline{78}$	$\overline{90}$
h = 4	90	66	42	18	$\overline{6}$	$\overline{30}$	$\overline{5}\overline{4}$	$\overline{78}$	$\overline{78}$	$\overline{5}\overline{4}$	$\overline{30}$	$\overline{6}$	18	42	66	90
h = 6	90	54	18	18	$\overline{5}\overline{4}$	$\overline{90}$	$\overline{5}\overline{4}$	$\overline{18}$	18	54	90	54	18	18	$\overline{54}$	$\overline{90}$
h = 8	90	42	6	$\overline{5}\overline{4}$	78	$\overline{30}$	18	66	<u>66</u>	18	30	78	$\overline{54}$	6	$\frac{42}{2}$	$\frac{90}{10}$
h = 10	90	30	30	$\overline{90}$	30	30	90	30	$\overline{30}$	<u>90</u>	$\overline{30}$	30	90 77	$\frac{30}{37}$	30	$\overline{90}$
h = 12	90	18	$\overline{54}$	$\overline{54}$	18	90	18	54	$\overline{54}$	18	90 70	18	$\overline{5}\overline{4}$	$\overline{54}$	18	$\frac{90}{90}$
h = 14	90	6	$\overline{78}$	18	66	30	$\overline{54}$	$\overline{42}$	42	54	$\overline{30}$	$\overline{66}$	18	78	6	90
Odd cosines (q)																
θ. (*	°) = 0	6	12	18	24	30	36	42	4 8	54	60	66	72	78	84	90
	R	R	R	R	R	R	R	R	R	R	R	R	R	R	R	
h = 1	90	84	78	72	66	60	54	48	42	36	3 0	24	18	12	6	•
h = 3	90	72	54	36	18	•	$\overline{18}$	$\overline{36}$	$\overline{5}\overline{4}$	$\overline{72}$	$\overline{90}$	$\overline{7}\overline{2}$	$\overline{5}\overline{4}$	$\overline{3}\overline{6}$	18	•
h = 5	90	60	30	<u>.</u>	30	60	<u>90</u>	$\overline{60}$	$\overline{30}$	•	3 0	60	90	60	30	•
h = 7	90	48	6	36	78	$\overline{60}$	18	24	66	$\frac{72}{}$	30	12	$5\overline{4}$	$\overline{84}$	$\overline{42}$	·
h = 9	90	36	18	$\overline{72}$	$\overline{5}\overline{4}$	•	54	$\frac{72}{72}$	$\frac{18}{18}$	$\overline{36}$	<u>90</u>	36	18	$\frac{72}{12}$	$\frac{54}{\overline{a}\overline{a}}$	•
h = 11	90	24	42	$\overline{72}$	6	60	$\frac{54}{-1}$	12	78	36	30	84	18	4 8	66	•
h = 13	90	12	$\overline{66}$	$\overline{36}$	42	60	$\overline{18}$	$\overline{84}$	6	72	$\frac{30}{\overline{00}}$	$\overline{48}$	$\overline{5}\overline{4}$	24	78	•
h = 15	90	•	$\overline{90}$	•	90	·	$\overline{90}$	•	90	•	$\overline{90}$	•	90	•	$\overline{90}$	•
						. 0	dd sine	es (r)								
θ(°) = 0	6	12	18	24	3 0	36	42	4 8	54	60	66	72	78	84	90
		R	R	R	R	R	R	R	R	R	R	R	R	R	R	R
h = 1		6	12	18	24	30	36	42	48	54	60	66	72	78	84	90
h = 3	•	18	36	54	72	90	72	54	36	18		18	$\overline{36}$	$\overline{5}\overline{4}$	$\overline{7}\overline{2}$	$\overline{9}\overline{0}$
h = 5	•	30	60	90	60	30		$\overline{30}$	$\overline{60}$	$\overline{90}$	$\overline{60}$	$\overline{30}$		30	60	90
h = 7	•	42	84	54	12	$\overline{30}$	$\overline{72}$	$\overline{66}$	$\overline{2}\overline{4}$	18	60	78	36	6	$\overline{48}$	$\overline{90}$
h = 9	•	54	72	18	$\overline{36}$	90	$\overline{36}$	18	72	54	<u>·</u>	$\overline{5}\overline{4}$	$\overline{72}$	18	36	90
h = 11	•	66	48	18	84	$\overline{3}\overline{0}$	36	78	12	$\overline{54}$	$\overline{60}$	6	$\overline{72}$	42	$\overline{2}\overline{4}$	$\overline{90}$
h = 13	•	78	24	54	$\overline{48}$	30	72	$\overline{6}$	$\overline{8}\overline{4}$	18	60	$\frac{42}{10}$	$\overline{36}$	66	12	90 77
h = 15	•	90	•	$\overline{90}$	•	90	•	$\overline{90}$	٠	90	•	$\overline{90}$	•	90	•	$\overline{9}\overline{0}$
						Ε	ven sir	ies (<i>s</i>)								
θ ($(^{\circ}) = 0$	6	12	18	24	30	36	4 2	48	54	60	66	72	78	84	90
		R	R	R	R	R	R	R	\boldsymbol{R}	\boldsymbol{R}	R	R	R	R	R	
h = 0	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•
h = 2	•	12	24	36	48	60	72	84	84	$\frac{72}{72}$	$\frac{60}{30}$	$\frac{48}{37}$	$\frac{36}{52}$	$\frac{24}{12}$	$\frac{12}{27}$	•
h = 4	•	24	48	72	84	60	$\frac{36}{36}$	$\frac{12}{-7}$	$\overline{12}$	$\overline{36}$	$\overline{6}\overline{0}$	84	$\overline{72}$	48	$\overline{2}\overline{4}$. •
h = 6	•	36	72	72	36		36	$\overline{72}$	$\overline{72}$	36	•	36	72	72 57	$\frac{36}{48}$	•
h = 8	•	48	84	36	$\overline{12}$	60 70	$\overline{72}$	$\overline{2}\overline{4}$	24 60	72	$\frac{60}{80}$	$\frac{12}{\overline{a}\overline{0}}$	$\overline{3}\overline{6}$	84	48 60	•
h = 10	•	60	60 9 <i>0</i>		$\overline{60}$	$\overline{60}$		60 26	$\frac{60}{26}$		$\overline{60}$	$\overline{6}\overline{0}$ 72	36	$\frac{60}{\overline{36}}$	$\frac{60}{7\overline{2}}$	·
h = 12 $h = 14$	٠	72	36	$\overline{36}$	$\overline{72}$ $\overline{24}$	60	72 26	$\frac{36}{\overline{48}}$	$\overline{36} \over \overline{48}$	$\overline{72}$ 36	60	$\frac{72}{\overline{2}\overline{4}}$	$\frac{36}{72}$	36 12	72 84	•
		84	12	$\overline{7}\overline{2}$	24	60	36	40	40	30	00	24 C	14	14	04	•

much helpful advice in this and other connexions. On his authority it is possible to state that better approximations than those shown in the table cannot be obtained without doing one or more of the following: (i) exceeding 200 for the tooth sum, (ii) reducing the smallest wheel from 21 teeth to below 16 teeth, (iii) increasing the largest wheel from 70 to above 81 teeth.

General arrangement of the computer

The general lay-out of a Fourier synthesizer employing these sine and cosine generators will now be briefly described. Representing the basic generators by the angles for which they develop the sines, the required arrangement of the sine and cosine banks of generators is shown in Table 2, where R indicates a revolution counter. For reasons mentioned later, it is desirable at this stage to separate the odd and even terms (h odd and h even). The generators are coupled hori-

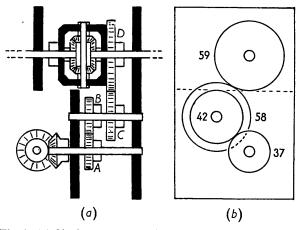


Fig. 2. (a) Single generator unit. (b) End view of generator for sin 60°, showing gear train.

zontally in rows by means of the input shafts, these shafts being driven, at the end of each row, by small reversing electric motors. At the other end of each row there is a small, non-printing revolution counter (not shown in Table 2) to record the input. The desired coefficients can be rapidly run up on the motors to near the correct values, the last few revolutions being effected more slowly, or by hand if desired. For negative coefficients, the motors are run in reverse. The input shafts are coupled to the generators through bevel gears, shown on the lower left-hand side of Fig. 2(a). If a generator is required to deliver a negative rotation, as indicated by a bar over the angle number in Table 2, then the bevel on the output shaft is merely set to engage with the opposite face of the bevel emerging from the generator (Fig. 2(a)).

On the output side the generators are coupled in columns (vertically in Table 2), the final output going into the printing revolution counters marked R. These record the summation totals at the axial intervals (θ) of 0° , 6° , 12° , ..., 90° . While the horizontal input shafts are permanently coupled through the bevel gears to all the generators in any one row, it is not possible to have the same type of fixed coupling of the output shafts to all the generators in any one column. This is because the successive generator output shafts will be revolving with different speeds and these outputs must be added; or, more usually, if the coefficients are being fed in one at a time, one generator in each column will be delivering an output, while the other generators in the same column are stationary. The ideal form of coupling between the generators in each column is a simple differential gear, as shown in the upper part of Fig. 2(a). This permits any rotation of

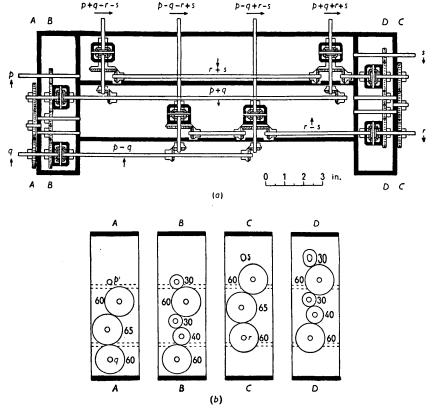
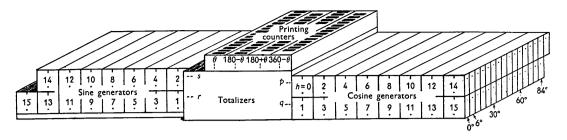


Fig. 3. (a) Totalizer unit for combining sub-totals. (b) End view of gearing in totalizer unit.



6 6 in. Fig. 4. Diagrammatic view of computer.

the output shaft to be transmitted through the gear, which at the same time adds on any additional rotation derived from the generator itself. With this arrangement any one coefficient may be fed in independently of the others, or any number of coefficients may be fed in simultaneously.

There are, however, some practical difficulties in this arrangement. If a number of differentials are coupled together in the manner indicated, the backlash of the gears is considerable. This is not really a serious matter, because as we are only concerned with counting complete revolutions it will at most lead to an uncertainty in the last unit of the summation total. A more serious matter is that in order to ensure smooth running without undue load, the differentials must be made with some precision, with accurate alignment and good bearings for the half-shafts. Accuracy of this order is not an essential requirement in any other part of the mechanism, and it tends to add unduly to the cost.

Another arrangement, which we are now adopting in the latest version of the machine, is to engage successive rows of generators (Table 2) with the output shafts one row at a time, the remaining rows being meanwhile disengaged. This involves a clutch mechanism, which is most easily achieved by mounting the idle shaft of the generator (Fig. 2(a)), which carries the wheels *B* and *C*, epicyclic with the driven shaft carrying wheel *A*. In this way wheel *C* can be engaged or disengaged from *D* by a simple movement, coupled with a self-locking device. The output shafts are then continuous all the way to the counters, and the wheels *D* are permanently fixed to them.

This arrangement abolishes the need for differentials between the generators, and it involves no particular difficulty in construction. It means that one simple movement of a lever is necessary before feeding in each coefficient, and that the coefficients in each bank must be introduced one set at a time. This is not a serious disadvantage, especially as the method of combining the summation sub-totals (described below) ensures that each of the four banks of generators can be operated simultaneously or independently. It follows that single coefficients in each of the four sets can be fed into the machine independently. This is ample for any practical need, and enables up to four operators to work on the machine at the same time, each operator entering successive coefficients in one of the four sets.

Combination of sub-totals

The final value for the electron density or other function at each point in the unit cell is, of course, obtained by combining the summation sub-totals obtained from the four banks of generators shown in Table 2. If we are summing a single Fourier series in the general form

$\Sigma A \cos h\theta + \Sigma B \sin h\theta$

and represent the sums involving even cosines, odd cosines, odd sines and even sines by p, q, r and s respectively, then by the symmetry of the functions we have the well-known relations:

```
sum at \theta = p+q+r+s,
sum at 180^{\circ}-\theta = p-q+r-s,
sum at 180^{\circ}+\theta = p-q-r+s,
sum at 360^{\circ}-\theta = p+q-r-s.
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If we are dealing with an expanded double Fourier series the final form will generally be

$$\Sigma A \cos h\theta - \Sigma B \sin h\theta$$
,

and provision must be made for the change of sign, either by entering coefficients with reversed signs or in some other manner.

If the four banks of generators are operated as independent units, as shown in Table 2, it will then be necessary to combine the p, q, r and s totals in accordance with the above relations in order to evaluate the function at every point over the complete period. This involves a fairly large amount of tedious arithmetical work. In the present machine this combination of sub-totals is carried out automatically, and only the final results are printed out.

This is achieved by placing between the banks of generators a set of totalizing units, one of which is illustrated in Fig. 3. It consists essentially of four sets of coupled differentials. The coupled pairs at each end of the unit produce the following sums and differences:

$$(p+q), (p-q), (r+s), (r-s)$$
.

The two coupled pairs in the interior of the unit then act on these rotations to produce the further sums and differences:

$$[(p+q)+(r+s)], [(p+q)-(r+s)], [(p-q)+(r-s)], [(p-q)-(r-s)].$$

These are the combinations required to effect the sums at the points θ , $360^{\circ}-\theta$, $180^{\circ}-\theta$, and $180^{\circ}+\theta$. The output shafts carrying these rotations then go directly to the printing counters.

In the second case mentioned above, where we are dealing with an expanded double Fourier series, we may neglect the negative sign of B and enter the signs positively, provided that the signs of r and s are in effect reversed in the mechanism. This is carried out by merely reversing the directions of rotations of all the sine generators, and is the mode of operation which would usually be employed in crystal-analysis work.

In assembling the complete machine (Fig. 4) it is convenient to arrange the banks of generators for odd and even terms vertically over each other, and the sine and cosine generators on either side of the central totalizing units. The printing counters for the final outputs are then located above the totalizing units. in a central position. These counters can each be supplied with an independent paper feed, because this is the most convenient arrangement when dealing with a lengthy double synthesis. If, for example, the machine has to produce an array of 1800 summation totals over a certain projection area containing a centre of symmetry, then one axis may be subdivided into 60 parts, which are dealt with simultaneously by the 60 counters. If the other axis is divided into 30 parts, this requires 30 cycles of operation by the machine, and the final results are conveniently produced on 60 strips of paper, each carrying 30 totals in correct order.

As shown in Table 2 and Fig. 4, the machine has generators designed to handle terms up to the fifteenth order (h = 15). Terms of higher order (h = 16 to h = 30) can be handled by using the same generators with the directions of rotation in every second column (Table 2) reversed. Thus, for h = 16 the cosine generators required are

$90\ \overline{6}\ \overline{78}\ 18\ 66\ \overline{30}\ \overline{54}\ 42\ 42\ \overline{54}\ \overline{30}\ 66\ 18\ \overline{78}\ \overline{6}\ 90.$

These are the same as for h = 14 with reversed sign at every second generator. This feature has not yet been fully developed, but a simple method would be to arrange for the clutch mechanism previously described to operate first on the 1st, 3rd, 5th, ... generators in a given row, then on the 2nd, 4th, 6th, ... generators. The coefficient would be fed in positively for the first position, and negatively for the second position. Although more fully automatic and speedy methods for dealing with high-order terms can be devised, this slightly more lengthy procedure would not cause much inconvenience because terms of higher order than 15 occur rather infrequently.

In conclusion, I have pleasure in acknowledging the many helpful and stimulating discussions I have had with Mr T. H. O'Beirne, of Messrs Barr and Stroud, Ltd, in connexion with this project.

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