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REPORT

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Investigation of: ORDER-DISORDER TRANSFORMATIONS IN CRYSTALS

Subject of Report: Harmonic Synthesizer Having 20 Sine and 20 Cosine Terms

Submitted by: P. M. Harris

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HARMONIC SYNTHESIZER
HAVING 20 SINE AND 20 COSINE TERMS

During work on structural transformations in crystals we have had the problem of determining the structures of the phases involved. In this connection, determination of the structure from x-ray diffraction measurements, as is commonly the case, has required summation of Fourier series of the general form:

$$S_{xyz} = \sum_h \sum_k \sum_\ell A_{hk\ell} \exp 2\pi i(hx+ky+\ell z) \tag{1}$$

where the sum is real and the coefficients, A, h, k, ℓ, are, in general, complex. This sum may be written in the form:

$$S_3 = \sum_h \sum_k \sum_\ell |F_{hk\ell}| \cos \left[2\pi(hx+ky+\ell z) + \alpha_{hk\ell}\right]. \tag{2}$$

In order to obtain sufficient resolution in complicated cases, such a sum may require evaluation at each of 60 values of each of the coordinates in the range 0 - π. Such sums are necessarily too laborious unless performed by punched-card methods or by suitable programming on high-speed electronic computers[1,2]. (However, the very elegant XRAC computer of Pepinsky[3] is specially designed to compute 2-dimensional sections for such series.)

In the earlier stages of such structure investigations simpler forms of the series are often useful. These may often be 1- or 2-dimensional and centrosymmetric:

$$S_2 = \sum_h \sum_k A_{hk0} \cos 2\pi\ (hx+ky) \tag{3}$$

and

$$S_1 = \sum_h A_{k00} \cos 2\pi\ hx, \tag{4}$$

and the coefficients are now real. For the purpose of computation (3) may be expanded:

$$S_2 = \sum_k \left[\sum_h A_{hk0} \cos 2\pi\ kx \right] \cos 2\pi\ hy - \sum_k \left[\sum_h A_{hk0} \sin 2\pi\ kx \right] \sin 2\pi\ hy. \tag{5}$$

Evaluations of (4) and (5) are normally carried out using a manually operated calculating machine and Beevers-Lipson[4] (or Patterson-Tunell[5]) strips which carry values $A \begin{Bmatrix} \sin \\ \cos \end{Bmatrix} 2\pi hx$ at intervals of $\frac{2\pi}{60}$ or $\frac{2\pi}{120}$.

It is as an alternative to this procedure that attention was turned to the possibility of devising a simple computer to perform these summations. To be useful, such a computer must have great ease of operation, require little or no maintenance, and furnish results of sufficient accuracy (1% or better).

Numerous approaches have been made to this problem in the past. Huggins[6] designed a series of masks on photographic film with proper distribution of density to permit the summation of (3) directly. Woolfson[7] has replaced the photographic film with masks made from sets of holes drilled in brass sheet. Neither of these methods permits summing over indices h and k greater than about 10. With Huggins' method it is difficult to get very good accuracy.

A novel analog machine for computing a sum of the type (3) has been described by Shimizu, Elsey and McLachlan[8]. This machine has been built with eight terms. It would appear to be cumbersome and quite expensive if extended to many more terms. However, it has the great advantage of inherently rapid operation.

Among the one-dimensional machines designed previously are a number of different types, of which several are noteworthy. The historical prototype and well-known harmonic synthesizer of Michelson[9] is not well adapted to rapid numerical calculation. More recently designed machines involve the use of harmonically tapped potentiometers[10] and mechanical generators based on the principle of the scotch-yoke crosshead[11] which was also incorporated in some models of Lord Kelvin's "Tide Predictors".

These designs all have certain drawbacks. Most of them are quite expensive. Probably the most attractive one from the standpoint of cost and utility is the machine using the harmonic potentiometer but this computer is reported to give a gain in time of only about 4:1 over the use of strip-adding machine methods.

Consideration of the design of a computer for summing series of the type,

$$S_1 = \sum_n \begin{Bmatrix} a_n \cos 2\pi nx \\ b_n \sin 2\pi nx \end{Bmatrix}, \tag{6}$$

requires that a decision be made concerning certain main features. Numerical methods, while well adapted tofinal calculations, do not appear promising from a speed or cost standpoint. Analog computers by nature appear better suited to the problem. It was decided to survey the methods for generating and adding harmonic functions. Formally, such a computer would have the components shown in Fig. 1

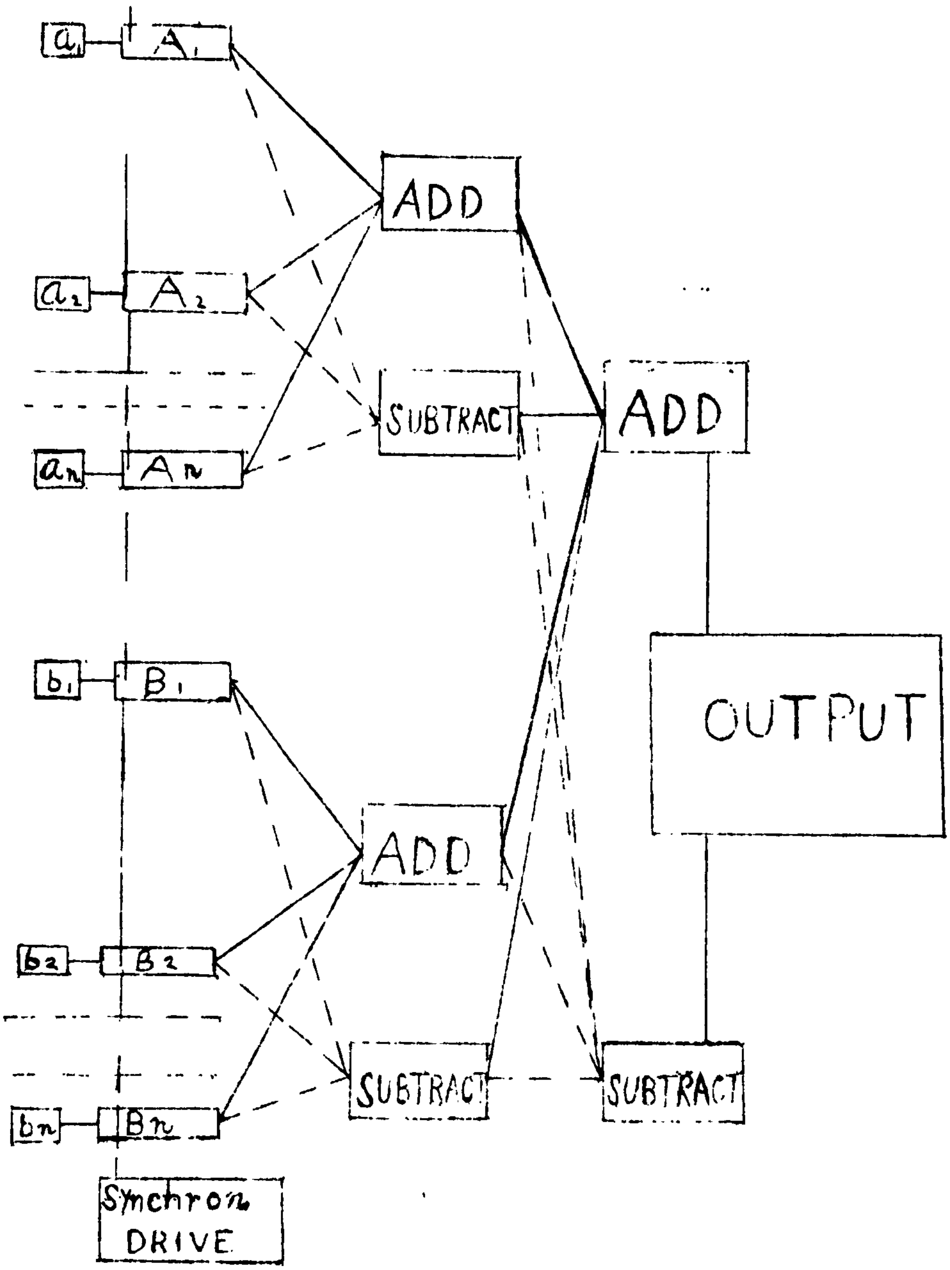

FIGURE 1

A_1 - - - - A_n, Cosine Generators, cos n θ.
B_1 - - - - B_n, Sine Generators, sin n θ.
a_1 - - - - a_n, Cosine Amplitude Controls.
b_1 - - - - b_n, Sine Amplitude Controls.

Briefly, the requirements to be met are as follows:

(1) The cosine and sine sections should have at least 20 terms each.

(2) The generators A_n (B_n) must be free of overtones. (Error less than 1%).

(3) Amplitudes of generators must be readily controlled.

(4) A simple method of addition and subtraction must be available so that the terms can be added or subtracted at will.

(5) The output must be of a type easily and quickly read. It is desirable that automatic recording be achieved simply.

(6) Cost should be low, otherwise punched-card methods compete.

(7) Over-all simplicity and speed of operation must be such that the method is a marked improvement over the strip-calculation methods.

Consideration shows that the generators may be of either of two classes, namely, (1) those for which the amplitude depends on the time or (2) those in which the amplitude is a function of a positional coordinate only. The first class is exemplified by the various oscillators, electronic and otherwise, in which the amplitude is given an expression of the form

$$A_t = A_o \sin \dot{\theta} t \qquad (7)$$

For the purpose in hand, such generators are not best suited since amplitudes must be sampled at properly chosen times. They have marked advantages when elaborated to the extent Pepinsky has gone in the XRAC.

As a result, we have confined our attention to generators of the second class of which the "scotch-yoke" and sine-tapped potentiometers are examples. Such generators develop amplitudes which are functions of a position coordinate

$$A = A_o \begin{Bmatrix} \sin \\ \cos \end{Bmatrix} \theta \tag{8}$$

This makes for marked simplicity in withdrawing a result from the machine.

It seemed that the requirements listed might be met best by making application of the law of Malus for the transmission of light through a pair of polarizers:

$$I_{tr} = I_o \cos^2 \theta/2 = \frac{I_o}{2} (1+\cos \theta) \tag{9}$$

Such a generator would consist of a small incandescent filament light source, a rotatable polarizer, a fixed polarizer and a photocell pick-up. This scheme apparently has not been used previously and is now feasible because of the present low cost of polaroid material and of commercial phototubes. The maximum amplitude of the term is controllable by adjustment of the heating current for the light source. Linearity of response is achieved by use of a vacuum type photocell.

A test with Type "J" Polaroid in conjunction with a 922 (S-1 surface) cell indicated that equation (9) was obeyed within ± 0.1% except for an additive constant attributable to a light leak in the red. On recommendation, Type "H" Polaroid was selected since its predominant light leak is in the blue. Transmission measurements with the polaroids in crossed position and a S-1 cell still showed an appreciable leak in the red. However, use of a 929 (S-4 surface) cell reduced the response to light leak to a negligible value.*

As a result of these tests a design for a complete analog harmonic synthesizer was worked out. Balancing economy against sufficient flexibility and accuracy, the number of sine and cosine terms was set at twenty each. Figure 2 shows the generator design.

The synchronized drive for the two groups of generators is similar to that employed by Michelson and is furnished by a cone of spur gears each having 10n teeth, the cone-shaft being driven by a 60:1 worm reduction gear. Each generator carries a 20-tooth spur gear to engage with the corresponding cone gear. Thus rotation of the cone shaft through an angle of Θ rotates a generator through an angle of $n(\frac{\Theta}{2})$. (Rotation of the worm shaft by one revolution is equivalent to 6° in Θ). Figure 3 shows the assembly.

Figure 4 is a photograph of the assembly. A pair of sine and cosine generators are on opposite sides of the corresponding cone gear, supported by a cross member through the center of which passes the cone shaft. The shaft hole in each case is bushed with a needle bearing. In the lower part of the assembly each succeeding cross member is advanced through an angle of $\pi/4$ to provide clearance for the generators, while in the upper portion the angle of advance is necessarily increased to $\pi/2$.

The wiring circuit is shown in Figure 5. Each gang of light sources is powered from one-half the secondary of a six-volt, center-tapped transformer. In series with each lamp bulb is a 10-ohm wire-wound rheostat permitting selection of (maximum) amplitude.

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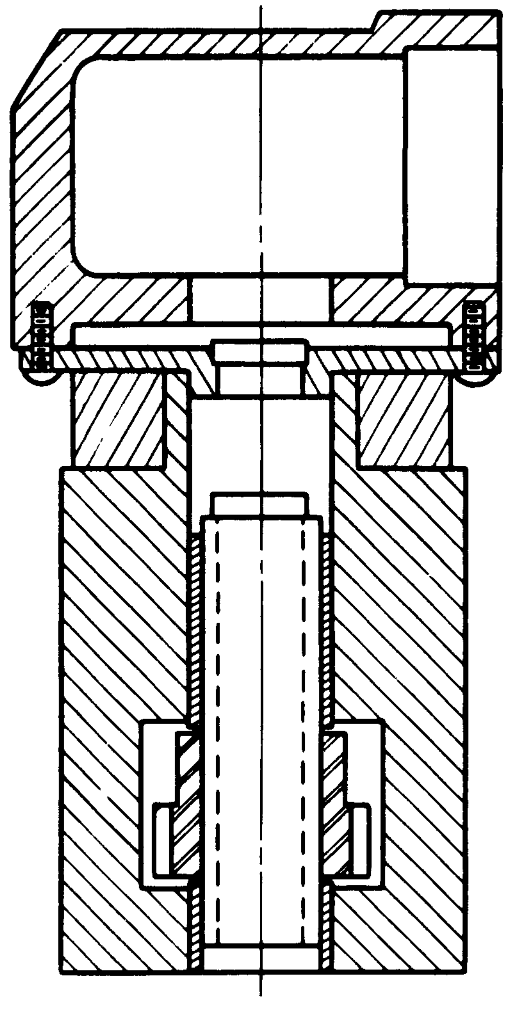
*We are indebted to Dr. Donald Tuomi for making the transmission measurements and suggesting the use of the S-4 surface.



SECTION X–X

Fig. 2.

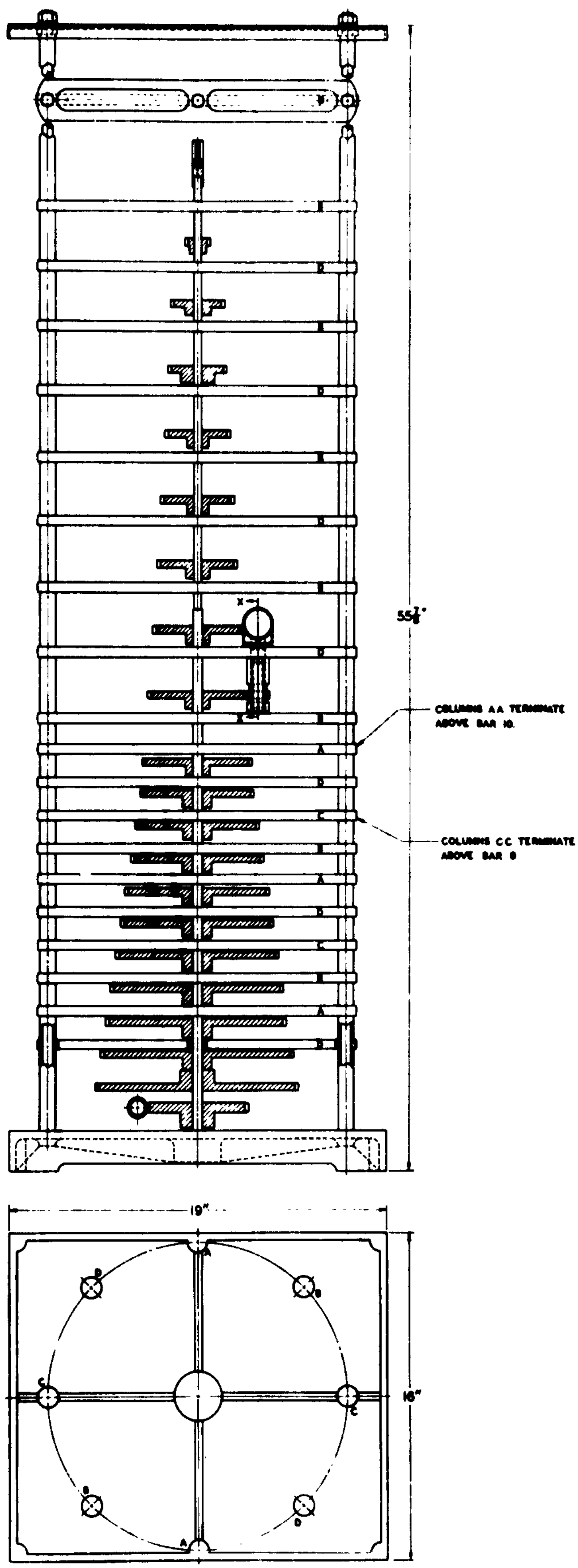

55 7/8"
COLUMNS AA TERMINATE
ABOVE BAR 10.
COLUMNS CC TERMINATE
ABOVE BAR 8
19"
16"

Fig. 3.

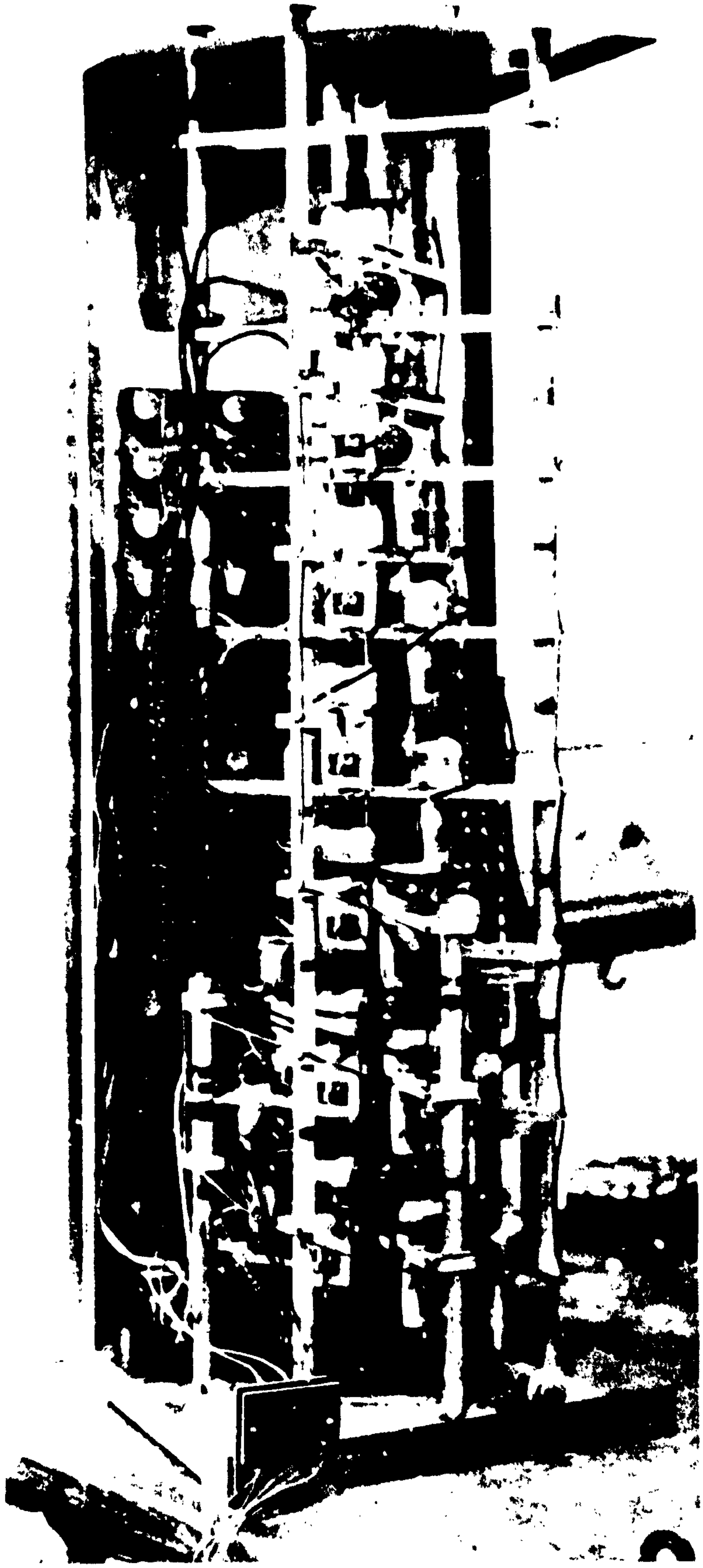


Fig. 4

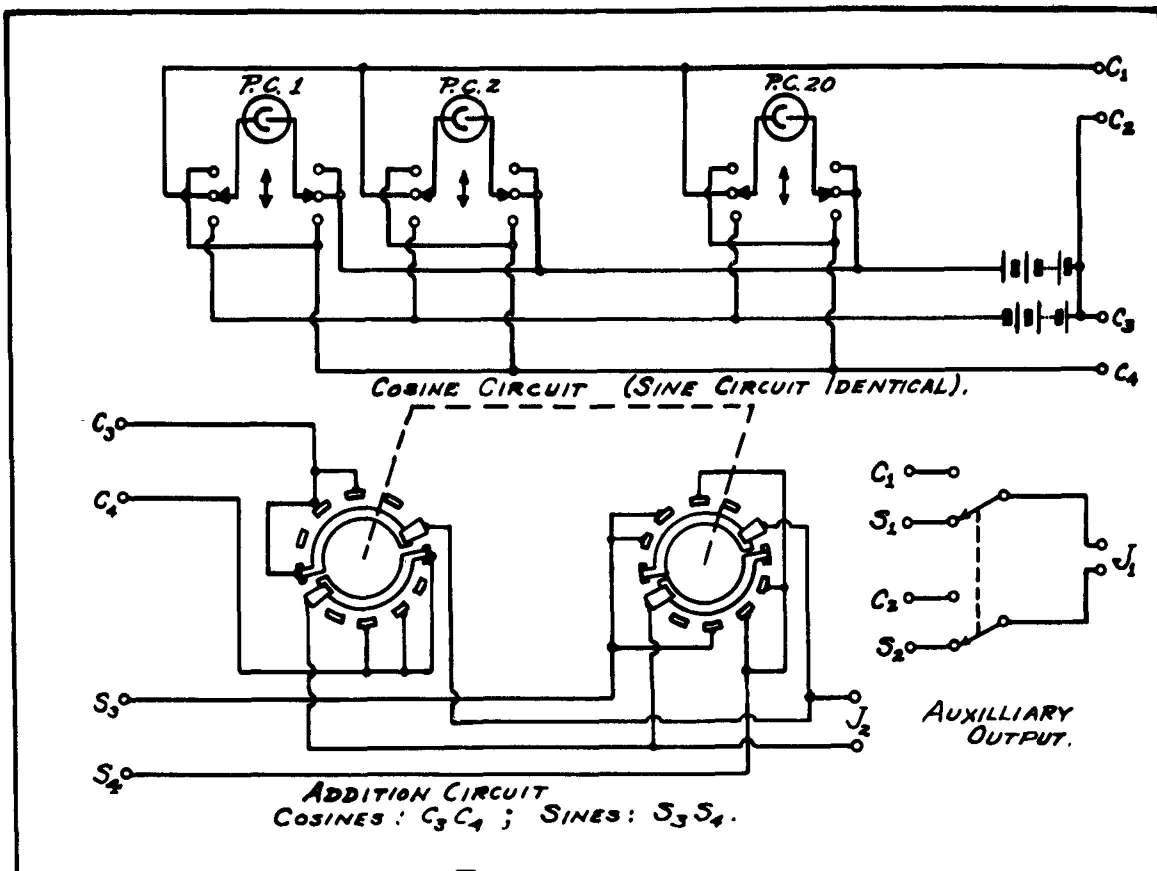


FIGURE 5a.

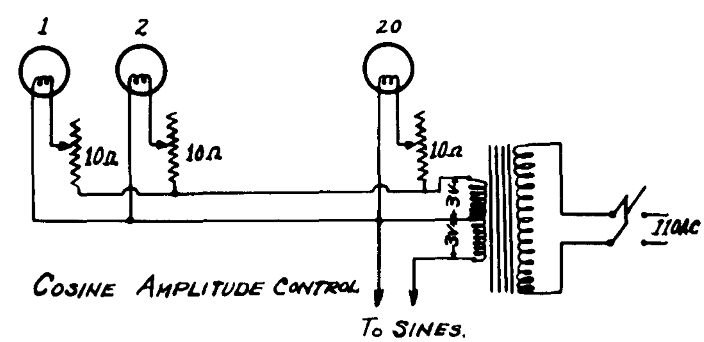


FIGURE 5b.

Addition and subtraction are simply effected by adding the photocurrents in parallel or antiparallel, respectively. For this purpose the cosine cells (and similarly, the sines) have as voltage supply two 135-volt B-batteries, one for addition and the other for subtraction. Each pair of leads from a photocell terminates at a 2-pole, 3-position switch. The three positions correspond to + connection, connection to auxiliary output and - connection.

The sum actually produced is

$$S_1' = \sum_n a_n + \sum_n a_n \cos n\,\theta_C \pm \sum_n b_n \pm \sum_n b_n \sin n\,\theta_S \tag{10}$$

in which the coefficients a_n and b_n may be + or - and for the sine terms $\theta_S = \theta_C + \frac{3\pi}{2n}$. (The phase angle, $\frac{3\pi}{2n}$, is introduced by initial adjustment of the fixed polaroids in the sine generators.) The sum required is

$$S_1 = a_o + \sum_n a_n \cos n\,\theta \pm \sum_n b_n \sin n\,\theta \tag{6'}$$

The sum S_1 is obtained from S_1' thus

$$S_1 = S_1' - (\sum_n a_n \pm \sum_n b_n) + a_o. \tag{11}$$

The removal of the second term of (11) is accomplished by addition (or subtraction) of a parallel current furnished by a 1.5-volt dry cell and controlled by a separate rheostat. In a similar manner a_o is introduced. Arrangement is made for the addition or subtraction of the sine sum and the cosine sum.

A view of the control panel is exhibited in Figure 6. Shown in the upper portion of the panel are the 3-position photocell switches, each

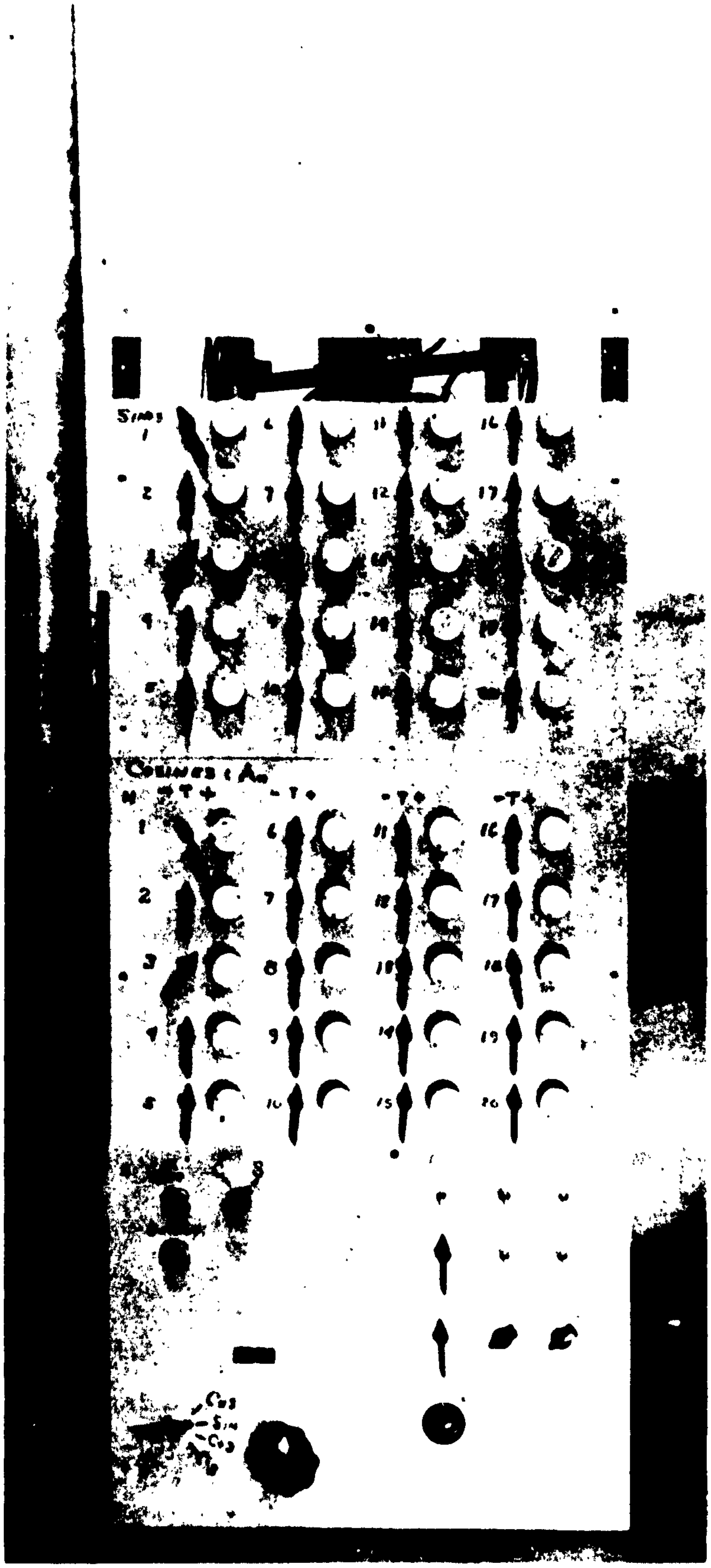


Fig. 6

with its amplitude control knob. The set of 20 cosine terms is immediately below the set of sines. Below on the left are two output jacks. The upper (J_1) is for auxiliary output and the lower (J_2) is a microammeter on which the total sum is read.

Just below the jacks is a 4-position switch which connects to the main output (1) $\sum$ cosines, (2) $\sum$ sines, (3) $\sum$ cosines + $\sum$ sines, (4) $\sum$ cosines - $\sum$ sines. At the right of the lower panel are the power switches, and switches and controls for introducing and removing constant terms.

In practice each photocell is connected in turn to J_1 to which is connected a sensitive microammeter. The control for the term in question is then adjusted to produce the proper amplitude. This is done with the cone-shaft worm wheel set at 0 as shown on the revolution counter. In this position the output is 2 a_n for a cosine term and b_n for a sine term (by equation (10)). As a result twice the coefficient must be introduced for cosine terms while the coefficient itself is used for sine terms.

After adjustment of these coefficients, the terms are connected into the summing circuit + or - depending on the sign of a_n, b_n. Now, with the 4-position switch set in Position 1 the $\sum$ cosines is determined (i.e. $\sum 2\ a_n$) and half of its value is removed by adjustment of the proper rheostat at the right. The sines are treated similarly, using Position 2 of the 4-position switch, except that the output is reduced to zero by the proper rheostat adjustment (at the right).

The total sum can now be read on the main output in Position 3 or 4. Each half-revolution of the worm drive shaft corresponds to change in θ of 3°.

While it has not been so used, a recording microammeter could be connected conveniently to the output. With a synchronous drive applied to the worm shaft, each sum over h at constant k of (5) would then be automatically computed as a continuous function of x. The sums over k at selected x's would then be recorded as continuous functions of y.

We are indebted to the University Committee for Allocation of Research Foundation Grants for aid covering most of the shop work of assembly. We wish to express our appreciation to Mr. Gordon Laverack and Mr. Audrey Stennett for their skillful workmanship.

Numerous additional applications of this machine are possible. One, of interest to the present work, is in connection with the determination of the roots of a polynomial. Since it is possible to take out sine and cosine sums separately and simultaneously by the introduction of an extra output jack on the panel, the machine will serve as an "isograph" (12) by connection of these outputs to an "x,y" recorder.

As is well known from the theory of functions of complex variables, if z_i are the roots of a polynomial, $p(z) = \sum_{n=0}^{m} A_n z^n$, for $p(z) = 0$, then the number of roots whose magnitudes are less than an arbitrarily chosen number, p, can be determined from an x,y plot of

$$x = \sum_{n=1}^{m} p^n A_n \sin n\theta \text{ and } y = \sum_{n=1}^{m} p^n A_n \cos n\theta.$$

The number of times the function wraps itself around the point $x = 0$, $y = -A_0$ is then the number of roots for which $|z_j|$ is not greater than p. Iteration then will lead to values of the roots.

This problem arises in the direct solution of the structure amplitude equation for coordinates of the atoms in the unit cell, for instance as outline by Avrami[13]. For an especially simple (but frequently met) centro-symmetric case, the amplitude equation becomes:

$$\frac{F_{h00}}{f_{atom}} = A_h = \sum_{i=1}^{N} \cos h\, \alpha_i .$$

It is here assumed all atoms have identical scattering power, f, there are N atoms per cell and the parameters $x_i = \frac{\alpha_i}{2\pi}$. The signs as well as experimental magnitudes of the quantities F_{h00} are presumed known for a sequence of N values. These A_h may be readily written as linear functions of $\sum \cos^h \alpha_i, \sum \cos^{h-2} \alpha_i$, etc. and the quantities $\cos \alpha_i$ are roots of the polynomial

$$a_o + a_1 x + a_2 x^2 + a_3 x^3 - \text{---} + a_N x^N = 0.$$

The coefficients a_n are easily obtained from the quantities $S_n = \sum_i \cos^n x_i$ and therefore from the amplitudes, F_{h00}.

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