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TECHNICAL REPORT 1

A ONE-DIMENSIONAL FOURIER ANALOGUE COMPUTER

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A One-Dimensional Fourier Analogue Computer

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Abstract

A computer has been constructed to sum Fourier series having up to 30 terms. Although this is a one-dimensional computer it can be used for double and triple summations by using standard trigonometric expansions. Secondly, it can be used for computing trial structure factors.

O.D.F.A.C. sums $\sum_n F_n \frac{\sin 2\pi n x}{\cos 2\pi n x}$ electrically. The trigonometric function is produced by a variable-angle transformer known as a resolver. Each amplitude is set by a variac which regulates the input to a particular resolver. The frequencies $2\pi n x$ for 31 values of n are arranged by gearing the rotors of the resolvers in ratios 0, 1, 2, . . . 30. The resultant individual currents are added in parallel and the value at point x (in intervals of $\frac{1}{60}$, $\frac{1}{120}$, or $\frac{1}{240}$ of a cell edge) is read on a voltmeter and the phase is read on an oscilloscope.

The relative speed of a computation is five to ten times faster than the standard strip methods. The average

error in a computation compares favorably with the rounding-off error in conventional two-place strips.

Introduction

Earlier computers. Fourier series are important in many branches of science. One-dimensional, two-dimensional, and three-dimensional Fourier series are especially important in x-ray crystallography. Since the computation of these functions is tedious, a number of devices have been developed to perform the computation, only a few of which have come into common use. Among these are the electrical digital devices of Beevers^{1,2}, the electrical analogue machines of Hägg and Laurent³, Ramsay, et al⁴, the mechanical analogue devices of McLachlan and Champayne⁵, Rose⁶, Vand⁷ and Beevers and Robertson⁸. All these devices sum one-dimensional series. Robertson⁹, Pepinsky^{10,11}, and McLachlan et al¹² have devised electrical analogue machines for two-dimensional Fourier summations.

Basis for design. When the number of Fourier syntheses to be computed in the Crystallographic Laboratory of M.I.T. became large enough to warrant using a special computing device, several of these machines were closely investigated. Some were found to have obvious defects, such as contact trouble when multiple telephone switches were used. Most of them were found to handle too limited

a number of Fourier terms. Guided by this survey, a decision was reached to build a one-dimensional electrical analogue computer which would sum a comparatively large number of Fourier terms. This was specifically set at 30, since this is about as high as ever required in the analysis of ordinary non-protein crystal structures. McLachlan's computer¹² served as a guide and as a point of departure. His machine compounds phases electrically by using selsyns. It performs a two-dimensional synthesis but is limited to 8 x 8 terms.

The transformation of an angle, ϕ , into a trigonometric function can be performed electrically in many different ways. The two devices considered in the early stages of designing ODFAC were sine potentiometers and resolvers. A sine potentiometer consists of a continuous resistor winding tapped to produce a voltage which varies as the sine of the angle of rotation of the main shaft. A resolver is a transformer using as its primary the rotor member and as its secondary two separate stator windings placed 90 degrees apart. When a voltage is applied to the primary winding the voltages of the two secondary windings vary respectively as the sine and cosine of the angle of rotation. Resolvers were chosen for the construction of ODFAC because the isolating property of a transformer makes the adding circuit independent of variations in the input stages.

Principle of operation. Fig. 1 shows, in outline form, the operation of ODTAC. The input to each resolver, R , is fed from a variac, V . The variac thus controls the amplitude or Fourier coefficient, A , of the Fourier component of a particular resolver. The two outlet leads of the resolver then deliver voltages proportional to $A \cos \varphi$ and $A \sin \varphi$. The shafts of 30 such resolvers are geared so that the shaft displacement of a particular resolver, n , is an integral multiple, n , of the shaft displacement of a fundamental shaft. The outputs of the individual resolvers are therefore a set of voltages proportional to

$$\begin{array}{ll}
 A_0 & \\
 A_1 \cos \varphi_1 & A_1 \sin \varphi_1 \\
 A_2 \cos \varphi_2 & A_2 \sin \varphi_2 \\
 \cdot & \cdot \\
 \cdot & \cdot \\
 A_{30} \cos \varphi_{30} & A_{30} \sin \varphi_{30}
 \end{array}$$

If the outputs are appropriately coupled, the machine produces voltages proportional to

$$\sum_{n=0}^{30} A_n \cos \varphi_n \quad \text{and} \quad \sum_{n=0}^{30} A_n \sin \varphi_n$$

which can be read on a voltmeter, VM . In crystallographic problems $\varphi_n = 2\pi n x$ where n is the number of the harmonic and x is the sampling interval expressed as a fraction of one complete period.

Design and construction

~~Mechanical Features.~~ The production of thirty harmonics in the Fourier series requires that one complete rotation of the rotor in the first resolver corresponds to two complete rotations of the rotor in the second resolver, etc., up to thirty complete rotations of the rotor in the thirtieth resolver. This is accomplished in ODFAC by means of a gear train represented by Fig. 2.

The main shaft leading from the motor is geared by worms and worm gears to three horizontal shafts whose relative angles of rotation are given by the ratios of the worms and gears. Each horizontal shaft carries a series of spur gears which engage with the spur gears mounted on the rotors of the individual resolvers. The angle of rotation of each rotor shaft is, therefore, a function of the ratio of its spur gears modified by the angular rotation of the horizontal shafts. The actual gear train is shown in Fig. 3. This particular gear train has several advantages. One is that most gears used are commercially available, stock sizes. Only 10 of the 82 gears are non-standard size and had to be obtained by special order. Another advantage is that high gear ratios are avoided, the largest step-down ratio being 5:4. This decreases inaccuracies in the positioning of the resolver shafts. Because of low frictional losses, all 30 resolvers can be driven at the desired speed by a small, $\frac{1}{1500}$ h.p. motor.

Electrical circuit. The wiring diagram of the electrical components of ODFAC is shown in Fig. 4. The input voltage is fed from the variacs, V, through a DPDT phase-selector switch, S, to the rotors of the resolvers, R, which are linked by the gear train illustrated in Fig. 3. Each output line of the stator winding of the resolvers contains a series resistance, r, of 500,000 ohms whose purpose is to make any stray losses in the secondary circuit negligible. All the cosine (and sine) windings of even harmonics are connected in parallel. Similarly the cosine (and sine) windings of the odd harmonics are connected in parallel. These lines lead to a gang switch which permits various combinations of the lines to be made.

The use of a parallel, rather than a series adding circuit is preferred for the following reasons: In a series circuit all the stator windings would be directly connected causing a cumulation of errors due to mutual inductance between the individual primary and secondary windings and the secondary windings of adjacent resolvers. The addition of voltages in a series circuit would also have the disadvantage of building up very high voltages and currents with possible damage to the windings. All of these disadvantages are overcome by a parallel circuit in which the isolation of the individual resolvers limits the current in each secondary winding to that induced by the primary. This isolation permits the insertion of a large resistance to minimize losses in the line. The maximum output voltage

obtained from such a circuit can never exceed the input line voltage because the individual voltages are averaged over all 31 branches.

The output voltage lines pass through a 4-gang switch which selects combinations of odd and even harmonics of the sine or cosine lines for transmission to the voltmeter and oscilloscope. The separation of the odd and even harmonics into separate lines permits the utilization of the symmetry inherent in sine and cosine functions. This is standard practice in crystallographic applications¹³. The meter has a $50/\mu$ a movement and three ranges which correspond to the voltages expected from the number of variacs supplying input voltages. A fourth range, actuated by a push-button, permits a clear reading of low voltages.

The cathode-ray tube is part of a standard oscilloscope circuit not having a sweep generator. The output voltage is placed across two deflecting plates and a reference voltage across the other two. Since both sets of plates have the same frequency applied to them, the resulting Lissajous figure on the tube face is a straight line whose angular inclination depends on the magnitude and relative phase of the output voltage.

Constructional details. The rear view of the assembled machine is shown in Fig. 5. The resolvers are held in place by aluminum clamps (see also Fig. 3) which, in turn, are fastened to two aluminum angles forming a

track-like shelf. Each shelf holds five resolvers and supports its horizontal drive shaft mounted in ball-bearing supports. The clamps have built-in means for adjusting the angular position of the resolvers. The horizontal drive shafts are driven by the main drive shaft which runs vertically, in the center of Fig. 5, from the motor (hidden by the bottom shelf) to the control mechanism.

The control mechanism is connected directly to the drive shaft by a set of change gears. It consists of a shaft which carries a change gear and a cam. The cam actuates a micro-switch which controls the number of revolutions made by the motor for the sampling interval. The motor is a dynamic-braking motor which can be stopped instantaneously by applying a reverse field to its rotor. A horizontal shaft, permanently geared to the main drive shaft, rotates a dial on the front panel indicating the angular position of the main shaft. The change gears in the control mechanism permit the selection of intervals of $\frac{1}{60}$, $\frac{1}{120}$, or $\frac{1}{240}$ of one complete period.

The motor-generator set at the bottom of Fig. 5 provides the input voltage (120 v., 400 ~) to the variacs only. The driving mechanism and service components operate on the regular line voltage. The purpose of the motor-generator set is to provide a constant current source with an undistorted wave shape, making the adding circuits in ODFAC independent of line fluctuations.

Performance

Operation. A front view of CDFAC in operation is shown in Fig. 6. The variacs are numbered and arranged on removable panels in sets of five. The amplitudes are set by means of a friction-drive dial permitting an accurate, rapid setting from 0-100. The phases are set by means of a plus-minus toggle switch placed directly above each dial. Each bank of five resolvers can be switched in or out of the input circuit by means of an additional toggle switch on the left of each panel. The numbering and location of the dials is such that the operator sits facing the first sixteen dials, the next fifteen dials being within arm's-length to his right. The dials need be set only once for each one-dimensional summation.

A panel to the left of the operator contains the meter on which the value of the Fourier series is read, the CRO tube on which the positive and negative quadrants are marked, the sine-cosine selector switch, and a push-button that advances the computer mechanism to the next sample setting. A pilot light indicates that the motor has advanced the computer to the next sample setting and the meter may be read. Once the amplitudes (variac dials) and the phases (plus-minus switches) have been set, and the type series (sine or cosine) has been selected, all the operator does is read the meter, note the phase, and

push the button to advance to the next reading. A drop-leaf table is attached to the front of ODFAC to provide a convenient surface for recording readings.

The speed of a computation on ODFAC depends primarily on the type of series desired, i.e., one-dimensional, two-dimensional, etc., and only secondarily on the number of terms or frequency of interval of sampling desired. The machine time for a complete cycle from 0 to 2π has been selected to take 7 minutes. If the time for setting the variacs and recording the values obtained is added to this, the total computing time amounts to approximately 10-15 minutes, depending on the sampling interval selected. The relative time of computing an average two-dimensional series on ODFAC ranges from $\frac{1}{5}$ to $\frac{1}{10}$ of the time consumed using standard strip methods^{14,15}. The more terms there are in the series and the finer the interval of sampling desired, the more efficient ODFAC becomes when compared with strip methods.

Accuracy. The accuracy of the components used in ODFAC is the highest attainable at a reasonable cost. The resolvers are accurate to within $1\frac{1}{2}$ mechanical degrees. The variacs and resistors are accurate to within 1% of maximum ratings. The meter is accurate to better than 1% of full scale deflection. The backlash in the gears is almost non-existent and the angular accuracy of the gear settings is within a fraction of one degree.

Table 1 shows an actual comparison of the meter

readings of ODFAC with those computed using three-place trigonometric tables. The amplitudes for this one-dimensional series were supplied by Professor M.J. Buerger from a Harker line synthesis for realgar. In the same table are listed corresponding values as computed with the aid of Patterson-Tunell strips¹⁴ and Beevers-Lipson strips¹⁵. If the deviations from the true values are examined it is evident that the errors in the values given by ODFAC are, on the average, as small as, if not smaller than, those due to the rounding-off errors inherent in the strip methods.

Finally, by making all operations other than recording the numerical values automatic, ODFAC eliminates the ever-present source of error - the human error.

Conclusions. The chief advantages of ODFAC are its ability to handle up to 31 coefficients in a Fourier series and to perform the summation rapidly with an accuracy adequate for most purposes. The simplicity of the design of the machine virtually eliminates almost all possibilities of electrical or mechanical failure. In the event such failure should occur, all components are readily accessible and removable for repair.

The slowest part of the operation of ODFAC lies in recording the results. It is proposed to add an automatic recorder for this purpose.

Extension to two dimensions

Use of two units. One ODFAC unit performs a two-dimensional synthesis by means of a Deevens-Lipson expansion. A combination of two such units performs this summation more rapidly. If these units are equipped with chart-type recorders, the most complicated two-dimensional series having 30 x 30 Fourier coefficients can be performed in an afternoon. The utilization of two such units follows the plan indicated below.

The series to be summed has a general expression:

$$\begin{aligned} \rho(xy) &= \sum_h \sum_k F_{hk} \cos 2\pi(hx+ky) \\ &= \sum_h \left[\sum_k F_{hk} \cos 2\pi ky \right] \cos 2\pi hx - \sum_h \left[\sum_k F_{hk} \sin 2\pi ky \right] \sin 2\pi hx \end{aligned}$$

The summations over k are first performed at the same time by the two units working independently. The results of these first summations are then used as coefficients for the second summation over h . In the second operation the two units are connected in parallel to only one recorder, which thus records the results of the final two-dimensional summation.

Two-dimensional computer. A more elaborate extension to two-dimensions can be built by combining two resolvers for every term in the series. The construction entails building k ODFAC units and one "master" ODFAC

having $\underline{h}$ resolvers (without variacs) for each harmonic $\underline{k}$. Such a plan is illustrated in Fig. 7 for $\underline{k} = \underline{h} = 4$.

The ODFAC units, whose resolvers have angular speed ratios proportional to their particular $\underline{h}$, are shown in solid lines. The rectangles in the dotted lines represent the resolvers of the "master" unit. All of these latter resolvers have the same angular settings proportional to $\underline{k}$.

The coupling between all units is electrical only. The resolvers of one ODFAC unit produce voltages proportional to:

$$\begin{aligned} F_{h_1 k_1} \cos 2\pi h_1 x \\ F_{h_2 k_1} \cos 2\pi h_2 x \\ F_{h_3 k_1} \cos 2\pi h_3 x \\ \vdots \\ \vdots \\ \vdots \end{aligned}$$

which are fed to the resolvers, $\underline{R}_{\underline{k}}$, of the master unit. The outputs of these resolvers are thus proportional to:

$$\begin{aligned} (F_{h_1 k_1} \cos 2\pi h_1 x) \cos 2\pi k_1 y \\ (F_{h_2 k_1} \cos 2\pi h_2 x) \cos 2\pi k_1 y \quad \text{etc.} \end{aligned}$$

Appropriate electrical coupling of the resolvers in the master unit then produces a voltage proportional to

$$\sum_h \sum_k F_{hk} \cos 2\pi(hx + ky)$$

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Table 1

One-Dimensional Fourier Synthesis

Computed value	ODFAC	Deviation	Patterson- Tunell	Deviation	Boovers- Lipson	Deviation
30.0	31.4	+1.4	30	0	30	0
33.3	33.3	0	34	+0.7	35	+1.7
32.4	31.8	-0.6	32	-0.4	30	-2.4
17.2	15.5	-1.7	16	-1.2	16	-1.2
-0.3	0	-0.3	0	-0.3	0	-0.3
-4.0	-3.6	-0.4	-4	0	-2	-2.0
0.9	0	-0.9	-1	-1.9	-1	-1.9
2.5	1.5	-1.0	3	+0.5	4	+1.5
6.5	5.6	-0.9	7	+0.5	7	+0.5
24.1	23.6	-0.5	24	-0.1	24	-0.1
49.0	47.8	-1.2	50	+1.0	48	-1.0
70.5	70.0	-0.5	71	+0.5	72	+1.5
89.4	88.3	-1.1	89	-0.4	89	-0.4
110.9	111.0	+0.1	112	+1.1	113	+2.1
119.2	118.0	-1.2	120	+0.8	118	-1.2
98.0	98.5	+0.5	98	0	98	0
59.0	59.0	0	60	+1.0	60	+1.0
29.5	29.2	-0.3	28	-1.5	29	-0.5
17.6	16.0	-1.6	17	-0.6	17	-0.6
10.1	9.3	-0.8	9	-1.1	10	-0.1
3.0	1.0	-2.0	2	-1.0	4	+1.0
-0.7	-1.5	+0.8	-2	+1.3	-2	+1.3
-2.3	-3.1	+0.8	-3	+0.7	-5	+2.7
-9.9	-11.8	+1.9	-11	+1.1	-10	+0.1

-16.9	-17.9	+1.0	-17	+0.1	-17	+0.1
-4.0	-2.6	-1.4	-4	0	-2	-2.0
31.7	32.5	+0.8	32	+0.3	30	-1.7
66.6	66.7	+0.1	66	-0.6	66	-0.6
76.8	77.5	+0.7	76	-0.3	76	-0.8
66.1	68.5	+2.4	66	-0.1	67	+0.9
58.0	56.5	-1.5	58	0	58	0

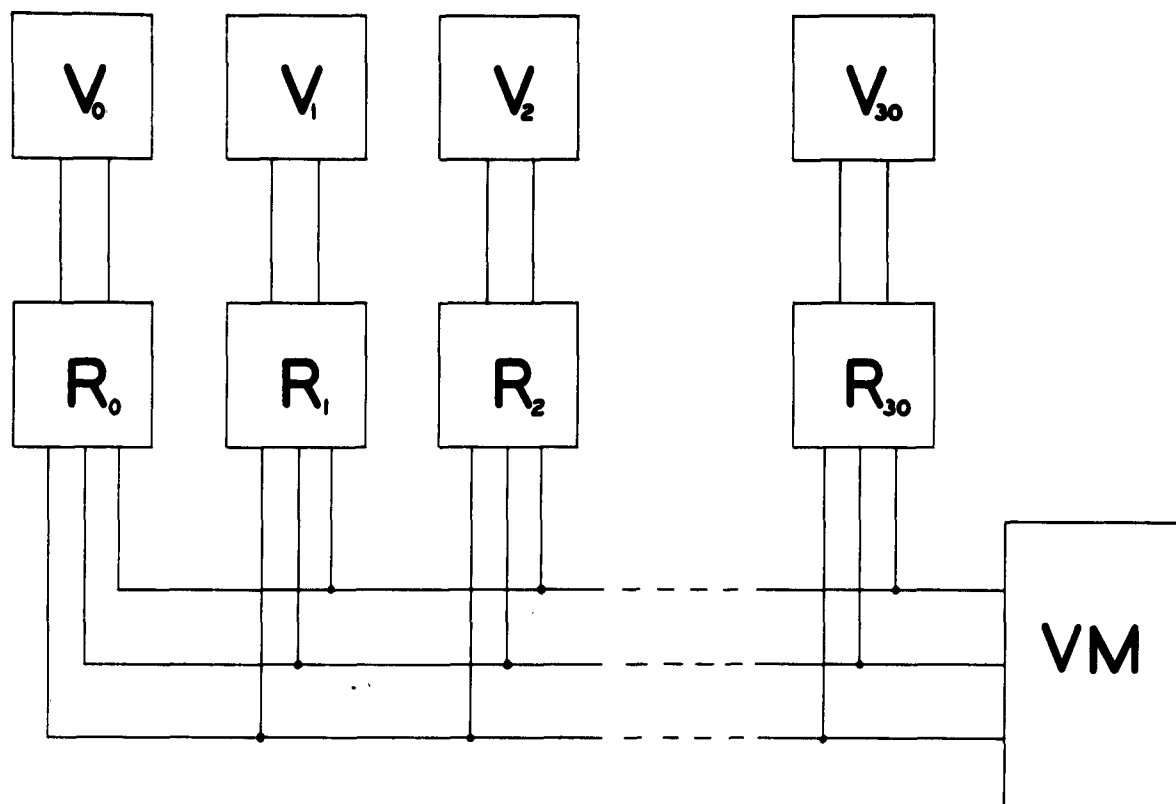


Fig. 1 ODFAC Outline

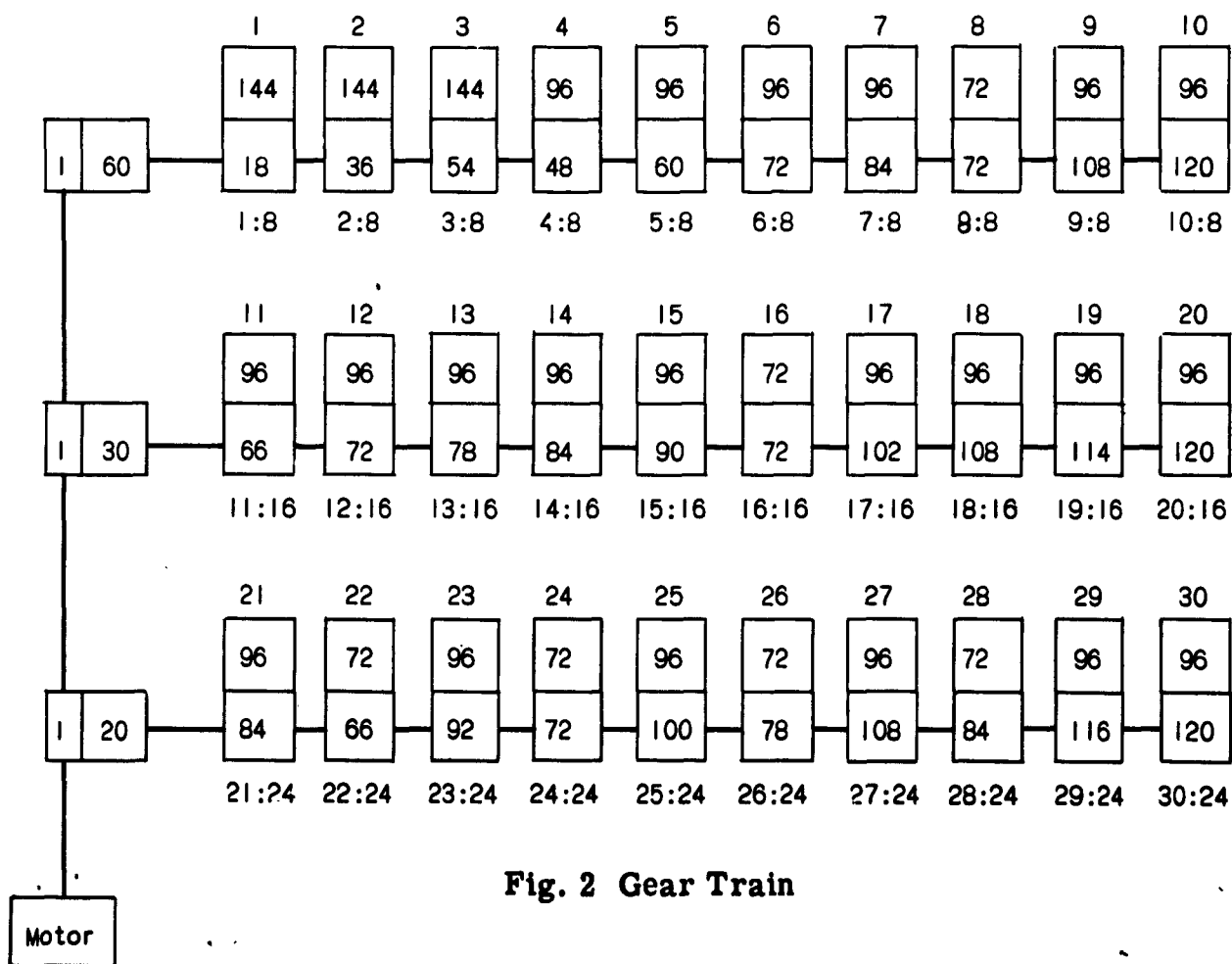


Fig. 2 Gear Train



Fig. 3 Gear Train

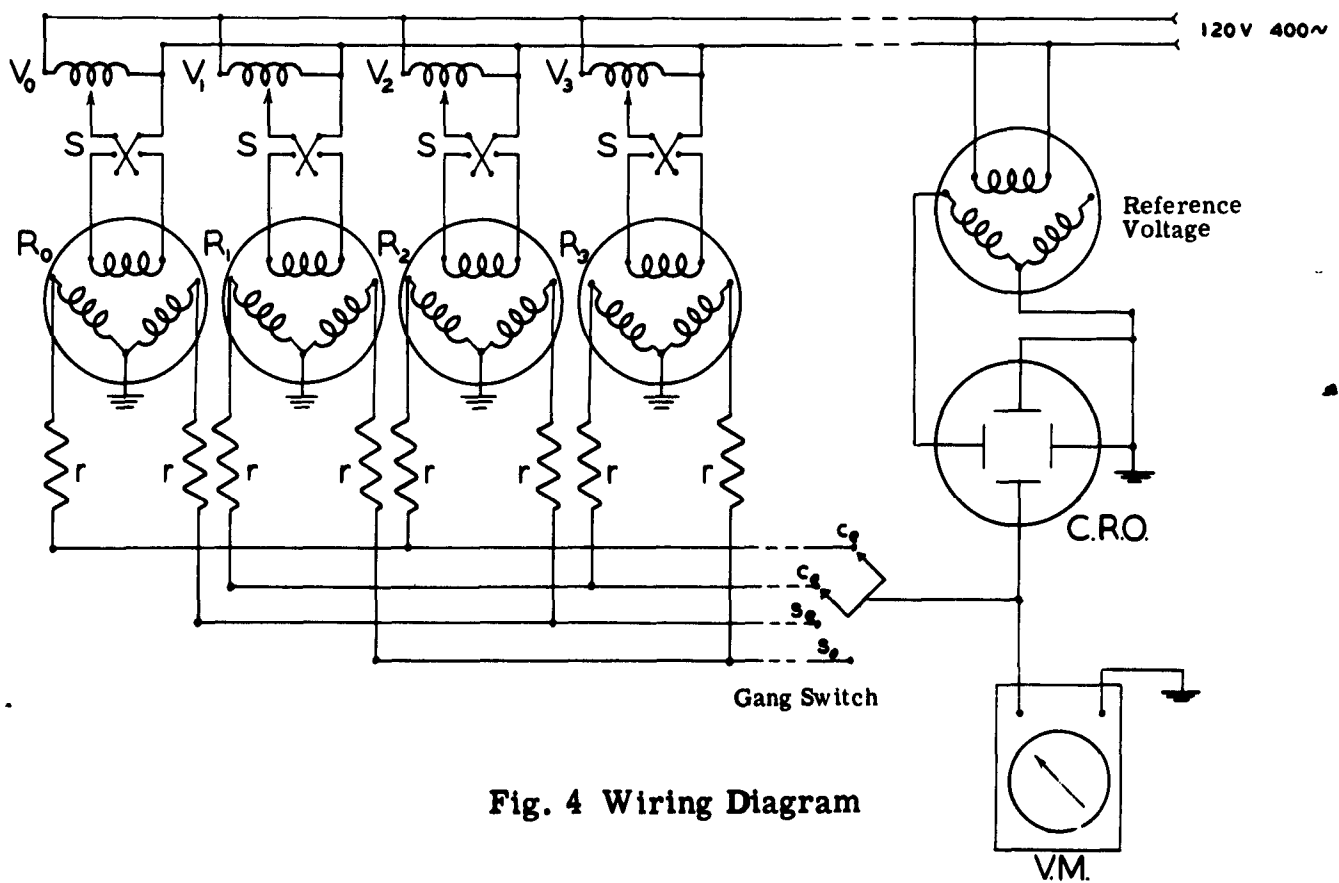


Fig. 4 Wiring Diagram

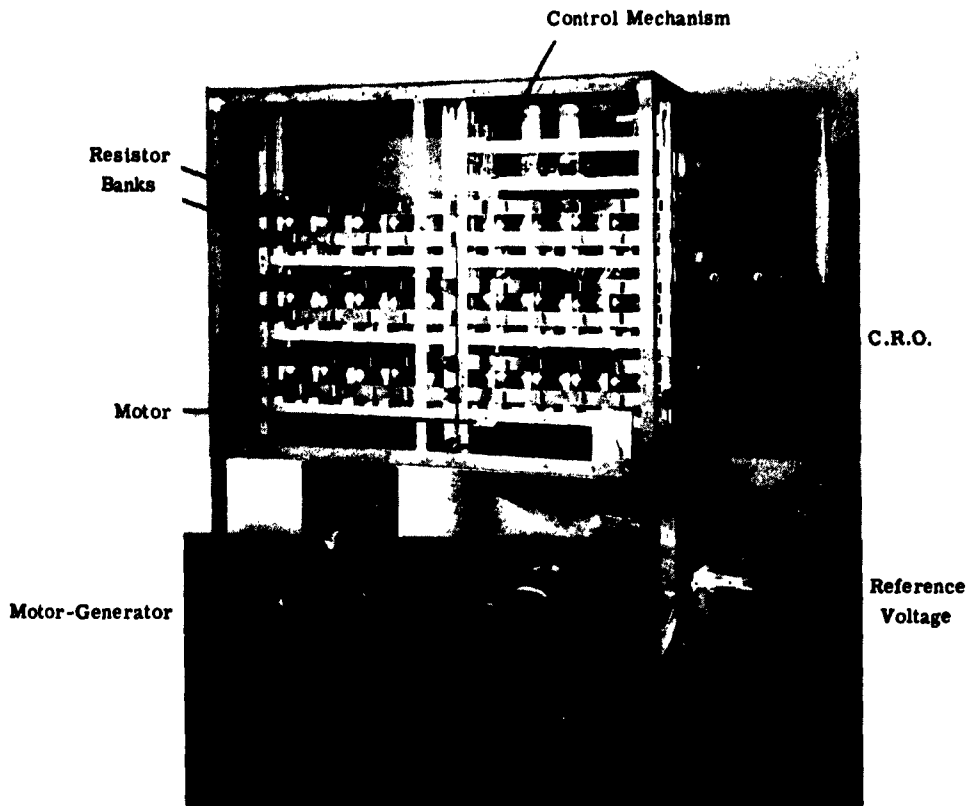


Fig. 5 ODFAC, Rear View



Fig. 6 ODFAC, Front View

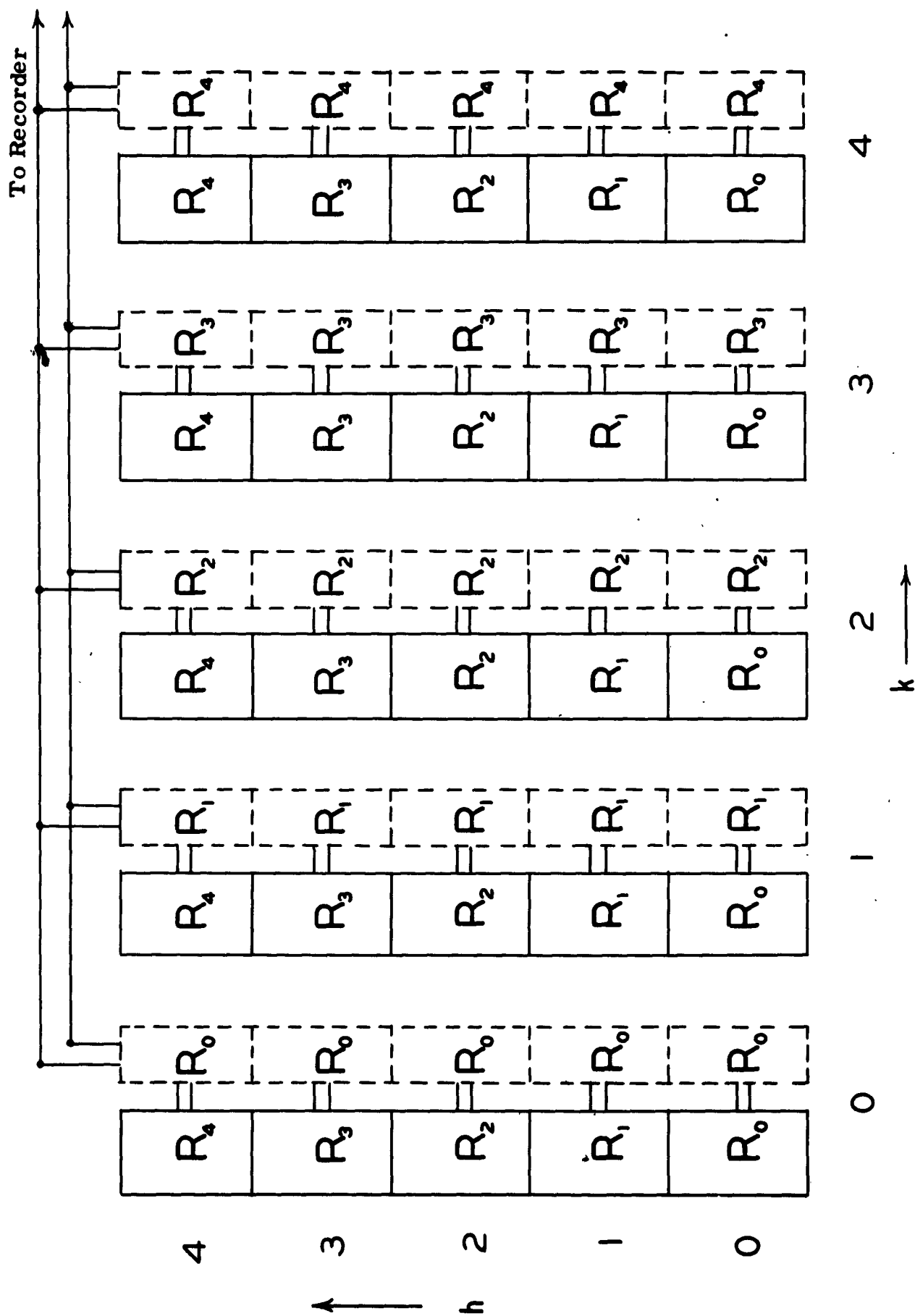


Fig. 7 Two-Dimensional Computer

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