THE EXTENSION AND APPLICATION
OF DIFFERENTIAL ANALYZER TECHNIQUE IN THE SOLUTION
OF ORDINARY DIFFERENTIAL EQUATIONS.

by

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For a period of three years, I enjoyed the privilege of almost daily association with Dr. Vannevar Bush in the development, and later the operation of the Differential Analyzer. In these formal words, I cannot fittingly acknowledge my indebtedness to Dr. Bush as a teacher, friend, and helpful critic, but hope that this thesis will show to some extent that his hard work has not been entirely in vain.

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INTRODUCTION

The development of any machine brings with it the necessity of devising methods of using the machine in order to derive full benefit from it. With a machine as comprehensive as the Differential Analyzer1, this necessity is a continuing one, for, except for certain general procedures, the method of using the machine is dependent largely on the requirements of the problem in hand. To a certain extent, then, any successful attack on a new type of problem will almost invariably leave behind it a contribution to that aggregate of basic methods which constitutes a technique.

Until about one year ago, exploratory work on the Differential Analyzer related largely to the field of electrical engineering - a natural consequence of the fact that the machine was developed by electrical engineers. Other fields were receiving some attention, but not to the extent that seemed desirable. This situation has now changed considerably, and a real demand has arisen for the use of the machine in other branches of science and engineering. In particular, the application of the machine in atomic physics has been extended rapidly, and much of the material of this thesis deals with this type of work.

In the field of atomic physics there was, and still is, abundant opportunity for exploring the possibilities of attack by means of the Differential Analyzer. The physicist has an assortment of theoretical methods - as developed by Heisenberg, Schrödinger, Dirac, and others - from which he can set up the equations governing a given atomic configuration, but with the exception of the hydrogen atom and the

1. See bibliography for all numbered references.
hydrogen-like atoms, he can obtain no specific solutions for those
equations. Approximate methods have, of course, been developed, and
give excellent results in a number of cases, especially in those cases
where the answers to similar problems are known. As a last resort, the
method of numerical integration can be applied, usually with reasonable
success, and always with a great deal of labor.

In entering this field of activity, the writer did not first
make a general survey with the idea of picking a likely looking point
for attack. Rather he entered it in a spirit of inquisitiveness,
impelled by the fact that on at least three different occasions he had
told visiting members of the Physics Department staff that the Differ-
ential Analyzer could handle the differential equations of atomic physics
which they brought with them. On the fourth occasion, he not only an-
tered "yes" again but decided that it would be highly appropriate to
prove that that answer was right. In February 1931 the Differential
Analyzer method was tried, and in accordance with the established custom,
it was tried first on the hydrogen atom. The success which followed
merely gave further evidence to support the growing tradition that almost
any method works with hydrogen.

The plan of attack developed in this first operation was fairly
simple. In fact, it was too simple because the desired result was known
analytically, and it was easy enough to make sure the machine was operat-
ing satisfactorily. Nevertheless, the work did show that it was possible
to attack the more difficult cases provided a method could be developed
to insure uniformity of operation of the machine. The principal object
of the work to be described was, therefore, to investigate and enlarge
the range of application, adaptability and reliability of the Differential Analyzer. In the course of the work, the writer, by applying the philosophy of the machine method, was able to make an improvement in the basic method of solving the problem chosen, and has therefore made it a second object of this thesis to present as an illustrative example an extension of Hartree's method for obtaining the wave functions of atomic configurations containing a nucleus and two electrons.

The presentation which follows is divided into four main sections. First, there is given an account of the methods and procedures developed for handling problems in electrical engineering, including a short résumé of the progress made with the product integrator. This is followed by a treatment of certain general problems of broad interest, particularly the classical problems of three bodies and the more modern cosmic ray problem according to the Lemaitre-Vallarta theory. In the next section is presented a general discussion of various problems of atomic physics from the point of view of Differential Analyzer technique; this serves as a background for the final section which describes the writer's work in this field.
Chapter I.

APPLICATIONS OF THE DIFFERENTIAL ANALYZER IN ELECTRICAL ENGINEERING

In examining the work done in connection with the Differential Analyzer in the field of electrical engineering, frequent reference is found to the forerunner of this machine - the product integraph\(^2,3,4\). Although relatively inaccurate and of decidedly limited range in comparison with the present machine, the product integraph was a highly effective instrument in the hands of the many men who worked with it. Some conception of the extent to which it was used may be gained from the fact that, in electrical engineering alone, there were fourteen theses submitted and seven papers (exclusive of papers describing the machine) published describing work in which the product integraph was used. It is appropriate to include this material in the discussion which follows, because the work originally undertaken on the product integraph has been continued and greatly extended on the Differential Analyzer, and also because methods and procedures developed in this earlier work have been to a large extent applied directly to the present machine.

Most of the solutions carried out on the product integraph which will be discussed here, were in the field of machine transients. This program has been continued and enlarged on the Differential Analyzer. Likewise solutions for both steady-state and transient conditions in electric circuits constitute another important group of electrical engineering applications. More recently, the Differential Analyzer has been applied to the solution of acoustics equations and it is expected that an extensive program will be carried out in that field.
a) **Machine transients**

Solutions have been obtained on either the product integraph or the Differential Analyzer for machine transients problems of three types, namely: machine behavior under short-circuit conditions, machine performance under variable or suddenly applied load, and the influence of various factors of design and operation on the pulling-into-step ability of synchronous machines.

The first work on the computation of short-circuit currents was that carried out in 1927-28 by F. G. Kear, using the product integraph\(^5\). Although the results of the immediate study were negative, definite progress was made in two directions. First, during the course of the study the machine as it existed at that time was altered to permit treatment of more general types of equations. Second, the need for a still more general type of machine and a more accurate one was shown. Kear's description is especially vivid in dealing with the various errors encountered in the product integraph and the means employed to eliminate them\(^*\). These errors were, in fact, encountered and corrected during the course of his investigation of short-circuit currents in alternators, to the extent that the integraph became a machine sufficiently flexible and reliable to turn out a steady stream of solutions of the two other types of problems discussed below.

The short circuit problem received no further machine computation treatment until last year when C. Kingsley, Jr. carried out on the Differential Analyzer solutions of three-phase short-circuit currents on a synchronous machine\(^6\). This work involved the solution of

\[^*\] The equation \( \frac{d^2y}{dx^2} = -ky \), which Kear labelled "classic" because of the many attempts made to solve it accurately on the product integraph was also the first equation solved on the Differential Analyzer. The latter machine also failed to handle it accurately until the "frontlash" unit was developed to eliminate the backlash in the gear trains.
two semi-simultaneous equations. The first was a linear equation of the third order, with constant coefficients, and from it the field current transients were obtained. The second equation was used to evaluate the armature current, using the field transients derived from the first equation. Although the first equation could have been solved analytically, a separate Differential Analyzer set-up was made for it, largely because of the time saved in plotting out the field transient over a number of cycles. Since the coefficients were linear, no manual operation was necessary and the solutions proceeded rapidly.

The problem of determining the performance of synchronous machines under conditions of variable or suddenly impressed load was treated rather extensively on the product integraph (see references 7 - 17 inclusive). Up to the present time none of this work has been done on the Differential Analyzer*. Aside from the improvement in the accuracy of the results which would be derived from a repetition of this work, by using the new machine a distinct improvement in technique is possible in at least one respect. The type of equation used in most of the previous studies was

\[
\frac{d^2 \theta}{dt_1^2} + P(\theta) \frac{d\theta}{dt_1} + \sin \theta = P_0 + P f
\]

(1)

It should be noted that the coefficient \(P(\theta)\) is a function of the angle \(\theta\). In order to introduce this variation on the product integraph, the term \(P(\theta) \frac{d\theta}{dt_1}\) was plotted as a function of \(\frac{d\theta}{dt_1}\) for a

* A repetition of some of the work of Edgerton and Lyon\(^3\) is scheduled to be carried out by Levine and Snell. This is for the purpose of getting more accurate solutions.
number of different values of $\theta$. These plots were, of course, simply straight lines. During the course of the solution one operator stationed at the output platen read off the values of $\theta$ from the result plot and called them to the operator following the $P \frac{d\theta}{dt}$ versus $\frac{d\theta}{dt_1}$ plots. The latter followed the line corresponding to the last value of $\theta$ called to him, and shifted from line to line in accordance with the result.

On the Differential Analyzer the step approximation described above is unnecessary. The machine is now sufficiently flexible so that the variable coefficient can be continuously evaluated as a function of its argument and applied to the first derivative as indicated in the equation.

The same approximation was made in the earlier work on pulling-into-step phenomena (see references 18 - 22 inclusive). Recently, however, this work has been largely repeated and extended using the Differential Analyzer (see references 23 - 26 inclusive) and the approximation has been removed. It will be instructive to examine the procedures used in the last series of solutions.

Before taking up this topic, it would be well to consider the method used for classifying the results, this method having been developed originally in connection with the product integraph solutions. It is apparent that the solution of a given problem on a machine like the Differential Analyzer always consists of individual solutions of particular cases. The variations between solutions are caused by adjusting one or more of the parameters of the equation, or by altering the starting conditions.
In formal solutions, on the other hand, it is possible to express a result so that by altering certain terms in the equation of that result any of the desired solutions may be obtained. The utility of machine solutions is enhanced greatly by any process which tends toward such generalization.

The method of generalization used in the pulling-into-step problem (and also in the problem of variable or suddenly applied load) proceeds from the equation*:

$$\frac{d^2 \theta}{dt^2} + \frac{P_d}{P_j} \frac{d \theta}{dt} + \frac{P_M}{P_j} \sin \theta \mathbf{I} = \frac{P_L}{P_j} \tag{2}$$

The coefficients $P_j$ and $P_M$ are constant, but $P_d$ is a function of $\theta$ (see equation (7), p. 10). These coefficients depend only on the machine design and vary widely between different machines. For any particular machine the equation can be solved as given, but the results thus obtained would be of little value in attempting to gauge the performance of another machine of different design. It is out of the question, of course, to obtain solutions for each desired combination of design constants and load.

Fortunately, by a simple change of variable, the entire picture can be simplified and the equation can be thrown into form from which it is feasible to obtain a general set of solutions. Dividing equation (2) by $P_j$, there results

$$\frac{d^2 \theta}{dt^2} + \frac{P_d}{P_j} \frac{d \theta}{dt} + \frac{P_M}{P_j} \sin \theta \mathbf{I} = \frac{P_L}{P_j} \tag{3}$$

* In the equation as given, the term $P_R \sin 2\theta$ for reluctance torque has been omitted; this does not affect the procedure, and the equation with it included will be discussed later.
By this process, the number of coefficients has been reduced by one, and can be reduced still further by a change of independent variable.

Let \( t = a \lambda \), then

\[
\frac{d\theta}{dt} = \frac{d\theta}{d\lambda} \cdot \frac{1}{a} = \frac{d\theta}{d\lambda}
\]

and

\[
\frac{d^2\theta}{dt^2} = \frac{1}{a^2} \frac{d^2\theta}{d\lambda^2}
\]

Substituting these in (3)

\[
\frac{1}{a^2} \frac{d^2\theta}{d\lambda^2} + \frac{1}{a} \frac{P_d}{P_j} \frac{d\theta}{d\lambda} + \frac{P_M}{P_j} \sin \phi \mathcal{I} = \frac{P_L}{P_j} \quad (4)
\]

Multiply through by \( a^2 \), then

\[
\frac{d^2\theta}{d\lambda^2} + a \frac{P_d}{P_j} \frac{d\theta}{d\lambda} + a^2 \frac{P_M}{P_j} \sin \phi \mathcal{I} = a^2 \frac{P_L}{P_j} \quad (5)
\]

Since "a" is arbitrary, the value of any of the coefficients containing it can be arbitrarily adjusted. The coefficient \( a^2 \frac{P_M}{P_j} \) is constant and it is convenient to set it equal to unity. Accordingly,

\[
a = \sqrt{\frac{P_j}{P_M}}
\]

which when substituted in (5) gives the final equation

\[
\frac{d^2\theta}{d\lambda^2} + \frac{P_d}{\sqrt{P_j P_M}} \frac{d\theta}{d\lambda} + \sin \phi \mathcal{I} = \frac{P_L}{P_M} \quad (6)
\]

Thus there is obtained an equation with only two parameters, \( \frac{P_L}{P_M} \) and \( \frac{P_d}{\sqrt{P_j P_M}} \). The first is a function of the load on the machine and of the maximum synchronizing power; the second contains only design parameters. It is a much simpler problem to solve this equa-
tion for various values of the parameters thus combined, than to solve it for various values of the individual constants.

The procedure described can be applied at least in part to many problems and is a primary method of generalizing solutions obtained on the Differential Analyzer.

In discussing the method of solving the pulling-into-step equation, the most recent solution made by Edgerton (see reference 23) will be taken as an illustrative example. He introduces a term due to reluctance torque together with an expression which approximates closely the variation of $P_d$ with $\theta$ and, after indicating two integrations, obtains as his working equation

$$\theta = \int \left[ \int \left( \frac{P_L}{P_M} \sin \theta - \frac{P_R}{P_M} \sin 2\theta \right) d\lambda - \int_{\theta_0}^{\theta} k(1 - b \cos 2\theta) d\phi \right] d\lambda$$

The information desired from solving this equation is the maximum value of load ratio $\frac{P_L}{P_M}$ for which a motor having its field switched on at a given angle will synchronize. From a series of such results taken at different switching angles, the limiting switching angle for any load ratio is obtained. The usual procedure is to run a series of solutions with fixed switching angle and with varying $\frac{P_L}{P_M}$, until two values of this ratio very close together are known, between which the solution changes from the stable to the unstable type. This procedure is repeated for a number of values of switching angle.

Edgerton made a radical change in the method, which eliminated the trial and error feature entirely. He first obtained solutions
at different values of $\frac{P_L}{P_M}$ for the steady-state slip versus steady-state angle, prior to field switching. A series of solutions using the same values of $\frac{P_L}{P_M}$ was then made with the Analyzer running backwards. To start each of these solutions, the angle was set very close to the unstable equilibrium angle and the slip at zero. The intersection of each of these solutions with the steady-state solution for the same load ratio gave the angle at which the field would have to be switched on in order to attain the unstable equilibrium angle. Thus, except for accidents, each pair of solutions gave a useful result, and the wasted effort inherent to the previous method was eliminated.

The Differential Analyzer connections used in this work were quite conventional. Three integrators were employed, and the functions $(\sin \theta + \frac{P_R}{P_M} \sin 2\theta)$ and $k(l - b \cos 2\theta)$ were introduced from plots. The schematic connections are shown in Fig. 1*.

Examination of equation (7) shows that it is possible to carry out this solution without using plotted functions, by the following method. The second integral within the brackets is evaluated formally giving the equation:

$$\theta = \int \left[ \int \left( \frac{P_L}{P_M} - \sin \theta \lambda - \frac{P_R}{P_M} \sin 2\theta \right) d\lambda \right. \left. - k(\theta - \theta_0 - \frac{b}{2} \sin 2\theta + \frac{b}{2} \sin 2\theta_0) \right] d\lambda$$

(8)

* See Appendix E for the list of symbols used in these diagrams, and their meaning.
Then substituting \((2 \sin \theta \cos \theta)\) for \(\sin 2\theta\),

\[
\theta = \int \left[ \left( \int \frac{P_L}{F_M} \ - \sin \theta \ 1 \ - \ 2 \frac{P_R}{P_M} \ \sin \theta \ \cos \theta \right) d\lambda \right] d\lambda \\
- k(\theta - b \sin \theta \ \cos \theta - \theta_o + \frac{b}{2} \sin 2\theta_o) \right] d\lambda
\]

(9)

The equation now contains the functions \(\sin \theta\) and \(\cos \theta\) and these can be obtained as the solution of the auxiliary equation

\[
\frac{dy}{d\theta^2} = -cy,
\]

for which \(y = c \sin \theta\) and \(\frac{dy}{d\theta} = c \cos \theta\) (or vice versa).

In order to carry out all the necessary operations with the six integrators available at present, the terms of the equation must be somewhat rearranged. Also, the term \(\frac{P_L}{P_M}\), which is a constant for any particular solution, must be integrated once formally in order to save an integrator. The transformed equation becomes

\[
\theta = \int \left[ \frac{P_L}{P_M} \lambda - \sin \theta \ 1 \ d\lambda - 2 \frac{P_R}{P_M} \int \sin \theta \ \cos \theta \ d\lambda \right] d\lambda \\
- k \int (\theta - \theta_o + \frac{b}{2} \sin 2\theta_o) d\lambda + k \ b \ \int \sin \theta \ \cos \theta \ d\lambda
\]

(10)

The parameters \(\frac{P_L}{P_M}\), \(\frac{P_R}{P_M}\) and \(k\) must be introduced by gear ratios, but this presents no serious obstacle since a series of values for plotting is usually desired. If particular values are desired, they can be supplied either exactly or very closely by proper choice of scales or manipulation of gears. In Fig. 2 is shown schematically an entirely mechanical connection which will handle equation (10).
Fig. 2.
b) Electric circuits

The ordinary differential equations of linear circuits are not troublesome and in general the Differential Analyzer is not required for their solution. Used merely as a means of plotting desired solutions of higher order equations, it is to some extent valuable as a time saver, but usually the analytic result is of more value. In cases where circuits contain non-linear elements, however, the situation is quite different, and the Differential Analyzer has a real part to play.

It is immediately apparent upon examination of the problem, that the same difficulty exists as was found in the study of machine transients. The solution for a particular case is readily obtainable, but in order to permit any variation of the parameters of the circuit, many separate solutions must be obtained. To a large extent, therefore, the utility of the machine is limited to the study of cases of immediate interest. This limitation appears not because of failure of the machine, but because of the failure of the mathematical language used to set up the equations. Furthermore, this limitation is present more or less in every problem handled on the Differential Analyzer. It is particularly troublesome in dealing with non-linear circuit elements because of the wide variations of parameters which are possible and physically important; in other problems, such as those of atomic physics, it gives little trouble because only certain solutions have physical significance, and continuous variation of the parameters is in many cases not required.

Some generality can be attained by extending the method of changing variables described on page 8. The following example has been carried through to illustrate the procedure and also to show the
amount of repetition necessary to obtain solutions applicable over a wide range of parameters in even a simple case.

Consider the circuit consisting of a constant resistance $R$ in series with an iron core inductance. If $R$ includes the resistance of the coil, and the inductance* is represented by $L(i)$, then the equation holding when a steady voltage $E$ is suddenly impressed is

$$Ri + L(i) \frac{di}{dt} = E \quad (11)$$

or

$$i = \int \frac{E}{L(i)} \, dt - \int \frac{R}{L(i)} \, i \, dt \quad (12)$$

Now introduce the change of variable

$$\tau = \frac{R}{L(o)} \, t, \quad dt = \frac{L(o)}{R} \, d\tau$$

where $L(o)$ is the value of $L(i)$ at $i = 0$, and equation (12) becomes

$$i = \int \frac{E}{R} \cdot \frac{L(o)}{L(i)} \, d\tau - \int \frac{L(o)}{L(i)} \, i \, d\tau \quad (13)$$

The factor $\frac{E}{R}$ is the steady-state current and must be treated as a parameter. Representing it by $i_s$, and dividing both sides** of (13) by $i_s$

$$\frac{i}{i_s} = I = \int \frac{L(o)}{L(i)} \, d\tau - \int \frac{L(o)}{L(i)} \, I \, d\tau \quad (14)$$

or

$$I = \int \frac{L(o)}{L(i)} \, (1 - I) d\tau \quad (15)$$

* Hysteresis is neglected. $L(i)$ is defined as $N \frac{\phi}{di} \times 10^{-8}$, where $\phi$ is in maxwells and $i$ is in amperes.

** This is permissible because $\frac{E}{R} = i_s$ is constant for any particular solution.
The interpretation of the quantity \( \frac{L(0)}{L(1)} \) in terms of measurable characteristics leads to an interesting result. Starting with the B-H curve of the iron, Fig. 3(a), the slope as a function of \( H \) is evaluated, giving the \( \frac{dB}{dH} \) versus \( H \) curve of Fig. 3(b). The inductance \( L(1) \) as used in this treatment is proportional to \( \frac{dB}{dH} \) and to the dimensions of the coil. For a particular coil, therefore, the ratio \( \frac{d(B/\mu)}{dH} \) is the same as the ratio \( \frac{L(0)}{L(1)} \) for the same values of \( H \), provided the effect of leakage inductance is neglected, or is included in the B-H curve and considered to have a negligible effect in varying the inductance ratios of different coils and cores. Hence in Fig. 3(c) the ratio plotted is that of inductance as a function of \( H \).

The plots thus far are all drawn with \( H \) as the variable, while the variable derived from equation (15) is \( I = \frac{i}{i_s} \). The latter variable is, of course, merely a ratio and represents the fraction of steady-state current reached at any value of the independent variable \( T \). In order to make a chart of solutions valid for any coil on an iron core having the B-H characteristic of Fig. 3(a), it is necessary to have solutions for a number of values of \( i_s \), or rather, for a number of values of \( B_{\text{max}} \). The points of maximum density chosen on the B-H curve are projected on the \( \frac{L(0)}{L(1)} \) versus \( H \) curve as shown in Fig. 3(c). The part of the curve between \( H = 0 \) and \( H = \text{maximum value} \), for each value of \( B_{\text{max}} \), is now replotted on an expanded scale of \( I \) so that the point \( H = 0 \) corresponds to \( I = 0 \) and the point \( H = \text{maximum value} \) is at \( I = 1.0 \) (that is, \( i = i_s \), or since \( H \) is proportional to \( i \), \( H = H_s \)). These partial curves are plotted in Fig. 3(d), where each curve
Fig. 3

Graph (a) shows the relationship between $B$ and $H$.

Graph (b) illustrates the derivative $dB/dH$.

Graph (c) represents the derivative $dB/dH$.

Graph (d) depicts the ratio $L(c)/L(I)$.
corresponds to a different value of maximum (steady state) flux density.

Using this last set of curves in equation (15), the equation can be written more properly in the form

\[ I = \int \frac{L_0}{L} (I) \left[ 1 - I \right] d \tau, \]  

(16)

thus indicating that the inductance ratio is used as a function of \( I \) rather than \( i \). The solutions of this equation are obtained for each of the curves of Fig. 3(d), using the Analyzer connections of Fig. 4.

If a sufficient number of steady-state flux densities are considered, then a chart of curves of \( I \) versus \( \tau \) can be prepared for each kind of iron. By interpolation in such a chart, the current-time curve due to constant \( E \) impressed in any \( R, L \) circuit using this iron can be determined, within the limits of the assumptions set forth.

Up to the present time, very little work on the application of the Differential Analyzer to general non-linear circuits (exclusive of those containing vacuum tubes) has been undertaken. Bachli and Chibas \(^{27}\) have studied a series-parallel circuit containing an iron core inductance, and T. R. Smith \(^{28}\) studied an \( R, L(i), C \) series circuit. In both of these studies, the object was to ascertain the response to sinusoidal voltages. In view of the engineering importance of \( d-c. \) operated non-linear circuits (e.g. exciters, relays), further study of the \( d-c. \) cases would seem appropriate.
Fig. 4
The vacuum tube as a circuit element has had increasing importance during recent years. Its development and application has proceeded largely on an experimental basis, with relatively little analysis of an exact nature. The Differential Analyzer is of direct aid in exact computation of the performance of vacuum tubes as circuit elements.

One of the principal difficulties in the machine treatment of the vacuum tube problem is in the nature of the characteristic curves which describe the tube. These curves form a surface* along which the operating point shifts. On the Analyzer, this calls for a three-dimensional input table if the representation is to be exact. This is a possibility which cannot be overlooked; the table can be constructed, but so far no procedure for constructing surfaces to scale and with reasonable economy of time has been devised.

In order to avoid the difficulty, a closely spaced family of curves is used, and the operator following the curves shifts from one to another as the value of the third variable changes**. (This procedure is the same as that applied in some of the machine transients work on the product integrator (see page 6). While it must be recognized that the method involves more or less abrupt changes, depending on the skill of the operators, and that some degree of approximation is thereby introduced, actual duplicate runs show such close repetition of results that the procedure can be regarded as substantially exact.

* For the dynatron oscillator (Gager and McGraw99), only two dimensional characteristics are required.
** Radford50 set up a telephone system between the operator and an observer who could read off the value of the third variable directly from a scale.
In the matter of generalizing the process, little can be said at present. In the studies already completed (references 29, 30), circuit constants were used directly with no attempt to combine parameters. Further work in this field is under way at the present writing (references 31 - 33) in which ratios of parameters are used to some extent. The problem is inherently non-general because of the wide variety of tubes and circuits. This, together with the fact that unexplained discrepancies exist between experimentally observed results and those calculated by the machine, makes it necessary for the present to apply the Differential Analyzer to the solution of particular problems. In other words, the principal functions of the Analyzer at the present time is to aid in coordinating theory and experiment.

The machinery of the Differential Analyzer can be of use in the evaluation of integrals of the form \( \int_{0}^{t} A(t - \lambda)E(\lambda) d \lambda \), encountered in the study of linear networks with applied forces variable with time. It is a straightforward integrating process which is carried out for a sufficient number of values of \( t \) to give an adequate description of the variation. Although the process can be performed in more elegant manner by machines of the type developed by Gould\(^34\) and Gray\(^35\), and now under further development as the Cinema Integraph, the Differential Analyzer is useful as an alternative in important cases. This problem has also a special interest because it was for the purpose of carrying out such computations that Dr. V. Bush and Messrs. Gage, Craig and Stewart built the watt-hour meter integrating unit which formed the nucleus of the product integraph\(^36\). Another example of work of this
type (performed on the product integraph) may be found in the analysis of three-phase transmission line transients carried out by Finley and Williams.

c) Acoustics

A study of the "Distribution of intensity in a sound field bounded by a rigid hyperbola of revolution" was carried out on the Differential Analyzer last year*. This is the first solution thus far obtained of an acoustic field with boundaries which are surfaces of revolution generated by curves other than straight lines; it is a fine example of the power of the machine in handling problems which are completely unmanageable analytically. In addition to providing a qualitative check of some recent experimental results obtained by Hall, the study furnished verification of the existence of standing waves without external reflection - a condition previously suspected from experimental evidence in this particular type of field.

In setting up the problem, Professor Fay was able to separate the variables of the original partial differential equations by making a particular selection of the shapes of both source and boundaries.

The ordinary differential equations resulting were

\[
\frac{d^2y}{d \beta^2} = -y \left[ B^2 \cos^2 \beta + \frac{1}{4} \cot^2 \beta + \frac{1}{2} - A \right] \tag{17}
\]

and

\[
\frac{d^2z}{d \alpha^2} = \frac{1}{2^3} - z \left[ B^2 \sinh^2 \alpha - \frac{1}{4} \tanh^2 \alpha - \frac{1}{2} + A \right] \tag{18}
\]

* This problem was formulated and proposed by Professor R. D. Fay, to whom the writer is indebted for interpretative material which has not yet been published.
In equation (17), which was the first treated, B is the frequency parameter while A is an unknown parameter to be obtained from the solution*.

The means of determining A is contained in the boundary conditions to be satisfied by the solution. For equation (17) these are:

at \( \beta = 0, y = 0 \), and at \( \beta = \beta_1 \) (at the boundary), \( \frac{d\beta}{d\beta} = \frac{Y}{\cot \beta} \).

Only the first of these conditions can be established when the machine is started, so for a given starting condition it is necessary to vary A until the required end condition is established. Once A is found for a particular value of B, both parameters can be inserted directly in (18) and that equation is then ready for direct solution.

It will be recalled that in the solution of the pulling-into-step problem of synchronous motors, much the same process was carried through. For a given set of conditions the \( P_L/P_M \) ratio was varied over a range in order to find the critical value, that is, the maximum value for which the machine would synchronize. The requirement that the machine should synchronize meant that the slip had to reach zero, or in other words, a boundary condition was applied to the end of the run just as in the case described above.

As will be brought out later, the same type of requirement must be met in the solution of the equations of atomic configuration in the steady state. In spite of the widely different characteristics of the three physical problems, much the same mathematical idiom is used in their description, and for solution on the Differential Analyzer, the techniques have many features in common.

* The process for determining unknown parameters of this type was used previously by the writer in studying the radial wave equation for the hydrogen atom.
Chapter II.

GENERAL APPLICATIONS

The many applications of the Differential Analyzer to problems of electrical engineering have been natural consequences of its development by electrical engineers. But the electrical engineer must express himself mathematically by language used in common with many other sciences, and the machine he builds to carry out his computations is directly applicable to other problems which are formulated by the same mathematical processes.

In the discussion below, the work on atomic physics is omitted, since it will be treated in detail in the following chapters. The problems taken up have in some cases already been treated on the Analyzer; the others are important in the literature and can be handled by the Differential Analyzer method to advantage.

a) Dynamics

The problem par excellence of dynamics is that known as the "Problem of Three Bodies". It may be stated*: "Three particles attract each other according to the Newtonian law, so that between each pair of particles there is an attractive force which is proportional to the product of the masses of the particles and the inverse square of their distance apart; they are free to move in space, and are initially supposed to be moving in any given manner; to determine their subsequent motion."

This problem has been a subject of research for some of the greatest mathematicians and on it over eight hundred books and papers have been

published within the last two hundred years. In the general form as stated above, it cannot be solved in terms of any of the functions known at present. It cannot be solved on the present Differential Analyzer either, because the machine does not contain a large enough number of the required units. But a consideration of this classic problem from the standpoint of machine technique is instructive, and affords in a preliminary way a picture of what a more general Differential Analyzer must accomplish and how large a machine it must be.

The equations of motion of three bodies with respect to fixed rectangular axes form an 18th order system, that is, there are nine differential equations each of second order. Using dots over the coordinates to indicate differentiation with respect to time, and changing the time scale so that the gravitation constant becomes unity, the equations of motion with respect to fixed axes are:

\[
\begin{align*}
\dot{x}_1 &= m_2 \frac{x_2 - x_1}{r_{12}^3} + m_3 \frac{x_3 - x_1}{r_{13}^3} \\
\dot{y}_1 &= m_2 \frac{y_2 - y_1}{r_{12}^3} + m_3 \frac{y_3 - y_1}{r_{13}^3} \\
\dot{z}_1 &= m_2 \frac{z_2 - z_1}{r_{12}^3} + m_3 \frac{z_3 - z_1}{r_{13}^3} \\
\dot{x}_2 &= m_3 \frac{x_3 - x_2}{r_{23}^3} + m_1 \frac{x_1 - x_2}{r_{21}^3} \\
\dot{y}_2 &= m_3 \frac{y_3 - y_2}{r_{23}^3} + m_1 \frac{y_1 - y_2}{r_{21}^3} \\
\dot{z}_2 &= m_3 \frac{z_3 - z_2}{r_{23}^3} + m_1 \frac{z_1 - z_2}{r_{21}^3} \\
\end{align*}
\]
\[ x_3 = m_1 \frac{x_1 - x_3}{r_{31}^3} + m_2 \frac{x_2 - x_3}{r_{32}^3} \]  \hspace{1cm} (1) \text{ cont'd.}

\[ y_3 = m_1 \frac{y_1 - y_3}{r_{31}^3} + m_2 \frac{y_2 - y_3}{r_{32}^3} \]

\[ z_3 = m_1 \frac{z_1 - z_3}{r_{31}^3} + m_2 \frac{z_2 - z_3}{r_{32}^3} \]

Equations (1) may be reduced to a 12th order system by changing to a new set of axes with one of the bodies at the origin, and expressing the relative motion of the other two with respect to it. No loss of generality is involved in this procedure; the forces acting preclude the possibility of there being any acceleration of the center of gravity of the system as a whole, so that only the relative motion is significant.

Let body 3 be located at the new origin; the coordinates of the moving origin with respect to the fixed axes are \((\alpha, \beta, \gamma)\). The new axes are allowed to move by translation only; that is, \(O'X'\) remains parallel to \(OX\), \(O'Y'\) remains parallel to \(OY\), and \(O'Z'\) remains parallel to \(OZ\), where the primes refer to the new system of coordinates. The coordinates of any body with respect to the new system are then given by:

\[ x_n = x_n' + \alpha \]
\[ y_n = y_n' + \beta \]
\[ z_n = z_n' + \gamma \]  \hspace{1cm} (2)

and by differentiation

\[ \dot{x}_n = \dot{x}_n' + \dot{\alpha} \]
\[ \dot{y}_n = \dot{y}_n' + \dot{\beta} \]
\[ \dot{z}_n = \dot{z}_n' + \dot{\gamma} \]  \hspace{1cm} (3)
Substituting (2) and (3) in (1), and dropping the accents

\begin{align*}
x_1 + \alpha &= m_2 \frac{x_2 - x_1}{r_{12}^3} + m_3 \frac{x_3 - x_1}{r_{13}^3} \\
y_1 + \beta &= m_2 \frac{y_2 - y_1}{r_{12}^3} + m_3 \frac{y_3 - y_1}{r_{13}^3} \\
z_1 + \gamma &= m_2 \frac{z_2 - z_1}{r_{12}^3} + m_3 \frac{z_3 - z_1}{r_{13}^3} \\
x_2 + \alpha &= m_3 \frac{x_3 - x_2}{r_{23}^3} + m_1 \frac{x_1 - x_2}{r_{21}^3} \\
y_2 + \beta &= m_3 \frac{y_3 - y_2}{r_{23}^3} + m_1 \frac{y_1 - y_2}{r_{21}^3} \\
z_2 + \gamma &= m_3 \frac{z_3 - z_2}{r_{23}^3} + m_1 \frac{z_1 - z_2}{r_{21}^3} \\
x_3 + \alpha &= m_1 \frac{x_1 - x_3}{r_{31}^3} + m_2 \frac{x_2 - x_3}{r_{32}^3} \\
y_3 + \beta &= m_1 \frac{y_1 - y_3}{r_{31}^3} + m_2 \frac{y_2 - y_3}{r_{32}^3} \\
z_3 + \gamma &= m_1 \frac{z_1 - z_3}{r_{31}^3} + m_2 \frac{z_2 - z_3}{r_{32}^3} \\
\end{align*}

Since in the new system, body 3 is fixed at the origin of coordinates,

\[ x_3 = y_3 = z_3 = 0, \]

and also

\[ x_3 = y_3 = z_3 = 0. \]

Making these substitutions in the last three equations of (4),
\[ a = m_1 \frac{x_1}{r_1} + m_2 \frac{x_2}{r_2} \]
\[ \beta = m_1 \frac{y_1}{r_1} + m_2 \frac{y_2}{r_2} \]
\[ \gamma = m_1 \frac{z_1}{r_1} + m_2 \frac{z_2}{r_2} \] (5)

In (5), \( r_1 \) and \( r_2 \) are now the distances of body 1 and body 2, respectively, from the origin. Placing the values of \( a, \beta, \) and \( \gamma \) from (5) in the first six equations of (4), the reduced equations are finally given by the 12th order system:

\[ x_1 = m_2 \frac{x_2-x_1}{r_{12}^3} - (m_1 + m_3) \frac{x_1}{r_1} - m_2 \frac{x_2}{r_2} \]
\[ y_1 = m_2 \frac{y_2-y_1}{r_{12}^3} - (m_1 + m_3) \frac{y_1}{r_1} - m_2 \frac{y_2}{r_2} \]
\[ z_1 = m_2 \frac{z_2-z_1}{r_{12}^3} - (m_1 + m_3) \frac{z_1}{r_1} - m_2 \frac{z_2}{r_2} \]
\[ x_2 = m_1 \frac{x_2-x_1}{r_{12}^3} - (m_2 + m_3) \frac{x_2}{r_2} - m_1 \frac{x_1}{r_1} \]
\[ y_2 = m_1 \frac{y_2-y_1}{r_{12}^3} - (m_2 + m_3) \frac{y_2}{r_2} - m_1 \frac{y_1}{r_1} \]
\[ z_2 = m_1 \frac{z_2-z_1}{r_{12}^3} - (m_2 + m_3) \frac{z_2}{r_2} - m_1 \frac{z_1}{r_1} \] (6)

where

\[ r_{12} = \sqrt{(x_2-x_1)^2 + (y_2-y_1)^2 + (z_2-z_1)^2} \]
\[ r_1 = \sqrt{x_1^2 + y_1^2 + z_1^2} \]
\[ r_2 = \sqrt{x_2^2 + y_2^2 + z_2^2} \]
The system of equations (6), although not of the lowest possible order, is the best for attack by means of a Differential Analyzer, to the best present knowledge of the writer. The equations can be reduced to a system as low as the sixth order*. Analytically such reduction is of value, but the complexity of the functions which must be evaluated in solving the lower order system by machine methods is a decidedly unfavorable factor. The eighth order system is somewhat better in this respect, but still not as simple as that of the twelfth which has been given. It did not seem necessary for the purposes of this treatment to derive and analyze the intermediate orders. Possibly a ninth or an eleventh order system is superior to the twelfth, and this possibility should be thoroughly investigated before attempting an actual solution. The principles and methods used here will be equally applicable to a different set of equations.

Equations (6) can be somewhat simplified by again changing the time scale so as to divide through by either \( m_1 \) or \( m_2 \). Using the latter, and recalling that the gravitational constant \( G \) has already been eliminated in this manner, the new time scale is such that

\[
t = \frac{T}{\sqrt{m_2 G}} \text{ seconds,}
\]

(7)

By this change of variable, the final equations become

\[
\begin{align*}
\dot{x}_1 &= \frac{x_2 - x_1}{r_1 r_2^3} - (A + B) \frac{x_1}{r_1^3} - \frac{x_2}{r_2^3} \\
\dot{x}_2 &= A \frac{x_2 - x_1}{r_1 r_2^3} - (1 + B) \frac{x_2}{r_2^3} - A \frac{x_1}{r_1^3}
\end{align*}
\]

(8)

* cf. Whittaker, loc. cit.
(with similar equations for the y's and z's),

where

\[ A = \frac{m_1}{m_2} \quad \text{and} \quad B = \frac{m_3}{m_2}. \]

It should be noted that only two parameters appear, and these are both ratios of masses so that the equations may be applied without change to systems of either celestial or atomic dimensions.

Fig. 5 shows schematically the machine connections suggested for the solution of this problem. Gears in general are not indicated but those necessary in order to introduce the various parameters of the problem are shown. It will be observed that three input tables are indicated as producing the necessary \(-3/2\) powers. These functions could be produced by integrators as follows:

Let \( p = q^{-3/2} \)

\[ \frac{dp}{dq} = -\frac{3}{2} q^{-5/2} \]

\[ \frac{1}{p} \frac{dp}{dq} = -\frac{3}{2} q^{-1} \]

\[ p = -\frac{3}{2} \int p \frac{dq}{q} \] \hspace{1cm} (a)

Now let, \( t = \frac{1}{q} \)

\[ \frac{dt}{dq} = -\frac{1}{q^2} \]

or \[ \frac{1}{q} = -\int \left( \frac{1}{q} \right)^2 dq \] \hspace{1cm} (b)
The mechanical connections in which the relations in (a) and (b) are applied to produce the desired function are shown in Fig. 6.

Four integrators are required to produce only one of the \(-3/2\) power functions, and since three such functions appear in equations (8) a total of twelve integrators would be required for this purpose. This large number of integrators required, together with the fact that reciprocal functions can be produced to better advantage from plots makes it advisable to use input tables as shown in Fig. 5. This is not a weakness in the method; a machine sufficiently comprehensive to solve the three-body problem will certainly have automatic input tables to introduce some functions.

The squares of distances which must be evaluated in this solution are produced using a single integrator for each square to be obtained, by the simple and frequently useful method of integrating the quantity to be squared with respect to itself*. It will be observed

* This method was first used on the Differential Analyzer in connection with a trial study of a problem in ballistics. Later, in a memorandum of June 1, 1931, Dr. V. Bush generalized the procedure by showing that a number of functions, among them the reciprocal \(1/x\), could be produced by regarding them as solutions of auxiliary differential equations. These equations were to be set up as in the example on page 14, so that only integrators and adders would be needed for solution. Guerrieri (ref. 39) carried out an S.M. thesis under the writer's supervision, in which he derived the desired equations for some forty functions. He also suggested the use of two integrators and an adder for multiplication by use of the rule, \(uv = \int udv + \int wdu\).

In this same memorandum, Dr. Bush made another generalization of great theoretical importance. He says, "Any differential equation with variable coefficients (perhaps subject to rather broad conditions) may be regarded as a more complicated differential equation with constant coefficients." This statement contemplates the production of any finite, continuous, single-valued function by the use of integrators and adders; various series expansions may be used for experimental curves. The idea is one which has every prospect of being developed into a powerful method in connection with a more elaborate machine (see footnote, p.36).
\[ p = q^{-3/2} \]

**Fig. 6**
that in all twenty-seven integrators are required for this solution,-four-and-one-half times as many as are available on the present Differential Analyzer.

Various difficulties may occur in the course of a machine solution of this problem. While a few of these difficulties may be anticipated, a complete discussion is impossible because of the lack of knowledge of three-body motion in the general case.

Consider, for example, the case of a sun and two planets, or possibly a sun, planet and moon. For a given set of initial conditions, the solution by machine would probably be quite straightforward. But examining the initial conditions required, it is found that they consist of the initial position and initial velocity of each body (except the one fixed at the origin). These twelve numerical values plus the values of the parameters A and B in equations (8) are necessary to start each solution. Furthermore each of the fourteen quantities can have an infinite number of values over an infinite range.

The immediate problem would be to restrict these ranges either from practical or theoretical considerations. It is obvious also that certain combinations become identical with others when coordinates are interchanged and can be eliminated from the standpoint of symmetry.

A further difficulty arises in those cases in which two of the bodies come very close together, or even collide. The distances \( r_1 \), \( r_2 \), and \( r_{12} \) appear in the denominators of fractions, and if any of these become zero, the corresponding terms in the equations become infinite.
This type of difficulty has been encountered on the present machine. Two procedures can be suggested for overcoming it. Usually, in the vicinity of such singularities it is possible to obtain accurate series solutions which are reliable. In other cases, smaller terms may become negligible, thus allowing simplification of the problem.

Although the Differential Analyzer cannot provide a general solution of the problem, its individual numerical solutions are worth while, if only because of the novelty of getting a result, rather than speculating about it. More can be expected, however, from systematic charting of results, and it is not unreasonable to set out on a definite program to determine, at least over a limited range, the variations in solutions due to systematic variation of parameters and initial conditions. This is particularly true if a machine recently projected can be used*. By using automatic methods for making connections, introducing initial conditions, and changing gears, it would be possible to make real progress in carrying out exhaustive investigations of the type discussed above.

Further information might also be obtainable regarding peculiarities of certain solutions of the three-body problem. If instabilities were possible, they could well be examined. Although it is not probable that general criteria for instability could be established, the fact that there are unstable systems could be demonstrated, if true, and something of their nature could be learned.

* * * * *

* Memoranda of Dr. V. Bush: Dec. 1, 1932; "Differential Analyzer; Specifications for an Improved Model"; Feb. 12, 1933, "Appendix to Specifications".
Considering the electron as a particle, the study of its motion under the action of electric and magnetic fields is of importance in many problems. Using the product integraph Sears found the orbits of an electron oscillating in the space between the filament and the plate of a three-electrode vacuum tube, as part of his investigation of the theory of the Barkhausen-Kurz effect.

More recently, Lemaître and Vallarta have studied the equations of motion of charged particles moving in the magnetic field of a dipole. By this means, they find analytically a variation of cosmic ray intensity with latitude which is in agreement with recent measurements. Their results were obtained by numerical integration of a rather complex equation, and in order to extend the work recourse was had to the Differential Analyzer. An analysis and discussion of the steps taken in the attempt to solve this problem on the machine is of interest, not only because of the importance of the cosmic ray problem, but also because of the splendid example offered of the methods used to extend the range of the Differential Analyzer in difficult cases.

The equation to be solved, as given by Lemaître and Vallarta is

\[ x^2 \left( \frac{d\lambda}{dx} \right)^2 = \frac{-4y^2}{\cos^2\lambda} + C + \int \frac{\sin 2\lambda d\lambda}{x^2} \frac{\cos^2\lambda}{x^2} \]

or dividing through by \( x^2 \) and taking the square root,
Various combinations of apparatus can be used to solve this equation as it stands, but none of them are within the capacity of the present machine. One change which will simplify the mechanical connections and reduce the apparatus requirements, is immediately apparent. Since

\[
\sin 2 \Lambda = 2 \sin \Lambda \cos \Lambda = - \frac{d}{d\Lambda} (\cos^2 \Lambda),
\]

equation (10) can be written:

\[
\frac{d\Lambda}{dx} = \pm \sqrt{\frac{- \frac{4}{\cos^2 \Lambda} + C + \int \frac{\sin 2 \Lambda \, d\Lambda}{x^2}}{x^4 - 4x_1x - Cx^2 - x^2 \int \frac{\sin 2 \Lambda \, d\Lambda}{x^2} - \cos^2 \Lambda}}
\]

This change is possible because the mathematical integrators used will evaluate integrals with respect to any variable present. Further reduction is possible as follows*. Consider the last two terms in the denominator and denote them by \(Q\).

\[
Q = \left[ x^2 \int \frac{d(\cos^2 \Lambda)}{x^2} - \cos^2 \Lambda \right]
\]

\[
\frac{dQ}{d(\cos^2 \Lambda)} = 1 + \frac{d(x^2)}{d(\cos^2 \Lambda)} \int \frac{d(\cos^2 \Lambda)}{x^2} - 1
\]

or

\[
Q = \int d(x^2) \int \frac{d(\cos^2 \Lambda)}{x^2}
\]

\[
= \int \left[ \frac{d(\cos^2 \Lambda)}{x^2} \right] d(x^2)
\]

* This method of simplification was first investigated and applied to machine analysis by the writer in connection with the work on atomic physics. See p. 35/3.
Also, since

\[ x^4 = 2 \int x^2 d(x^2) \]

and

\[ c x^2 = c \int d(x^2), \]

the denominator of (11) can be written

\[ -4 \delta \int x + \int \left[ 2x^2 - c + \int \frac{d(\cos^2 \lambda)}{x^2} \right] d(x^2) \]

and the complete equation now takes as its final form

\[
\frac{d\Lambda}{dx} = \frac{-4 \delta \frac{\cos^2 \lambda}{x^2} + c + \int \frac{d(\cos^2 \lambda)}{x^2}}{\sqrt{\left( -4 \delta \int x + \int (2x^2 - c + \int \frac{d(\cos^2 \lambda)}{x^2}) d(x^2) \right)}}
\]

(12)

Fig. 7 shows schematically the connections of the machine necessary to solve (12). As far as is known to the writer, it represents the form requiring the least amount of apparatus. For purposes of comparison, it is interesting to note the connections shown in Fig. 8, by means of which the same equation can be handled using integrators, adders and gears for all operations. A machine capable of handling the three-body problem would, of course, contain the required number of units.

The results obtained in working with this equation on the Differential Analyzer were most disappointing. Considerable time was spent investigating peculiarities in the machine's behavior, and this resulted in the discovery of two difficulties. First, the terms in \( x \) appearing in the denominator combined so as to produce small differences of large quantities. In order to correct this difficulty, it was necessary
\[ x^2 \]
\[ 2x^2 \]
\[ 4y_1 x \]
\[ \sqrt{x^2} \]
\[ \frac{1}{x^2} \]
\[ N = \text{numerator} \]
\[ D = \text{denominator} \]
\[ \sqrt{N/D} = \lambda \]
\[ \sin 2\lambda \]

**Fig. 7**
to adapt the output table so as to serve as an input table on which was plotted the term \( (x^4 - Cx^2 - 4\sqrt[4]{3}x) \) as a function of \( x \). Although this removed the immediate trouble, much of the elegance of the method was lost, and further trouble still remained.

It was now found that having started the machine, the solution proceeded satisfactorily until the point was reached where the slope \( \frac{dA}{dx} \) passed through zero. From this point on, if no special procedure was adopted, the machine stopped drawing a curve and simply described a straight line parallel to the X-axis; that is, once it reached zero slope, it continued with the same slope. The source of this peculiarity was soon found, - not in the machine, but in the equation.

In equation (12) it may be observed that the slope is equal to a fraction composed of functions of \( x \) and \( \lambda \) in both numerator and denominator. Hence the slope may become zero either if the numerator becomes zero, or if the denominator becomes infinite. It so happens that in this case the numerator becomes zero. Examining the numerator, which is

\[
\frac{4\lambda^2}{\cos^2 \lambda} + C - \int \frac{d(\cos^2 \lambda)}{x^2},
\]

the first term varies only with \( \lambda \), the second is constant, and the third term varies only if \( \lambda \) varies. Hence the numerator will change its value only if \( \lambda \) varies. But when the point of zero slope is reached, not only does the numerator become zero, but it must stay there, since \( \lambda \) does not change. The machine goes on "dead center" and draws only a straight line of zero slope as an answer. This solu-
tion satisfies the differential equation, but has no significance*.

An attempt was made to avoid the difficulty by arbitrarily carrying the slope through zero in as continuous fashion as possible. No consistency could be obtained, however, and the work on the problem was discontinued to await further study. This study was to proceed along three lines: first, to attempt to introduce a second derivative into the equation in accordance with which the slope would be properly varied; second, to study similar equations having known analytic solutions (in particular, the Clairault equation); third, to seek a reformulation of the problem. The first method, although theoretically possible, leads to no useful result because the final equation becomes too complicated for the machine to handle it. The second method was somewhat of a last resort and has not been tried. Recently, however, the writer has had some success in reformulating the problem for the machine. Although, it has not yet been tested on the machine, the method proposed is not subject to the difficulty described above, because acceleration terms are explicitly contained.

* The charged particle is moving in a magnetic field, and the solution found indicated it as moving in a direction at right angles to the axis of the field-producing dipole. This cannot be true physically; the force produced by the motion must alter the path.

Mathematically, the difficulty is that the singular solution \( \lambda = \text{const.} \) exists, and at any point where \( \frac{d\lambda}{dx} = 0 \), this solution is tangent to the desired particular solution. No information is supplied the machine to enable it to continue on the particular solution, and since no further guidance is required for it to follow the singular solution, it proceeds to do so. Lemaitre and Vallarta do not mention this difficulty in their paper; they encountered it in their numerical integration, but the true nature of the difficulty was completely recognized only after the machine study was attempted.
It seemed logical in attempting a reformulation of the problem to go back to the unreduced equations of motion. They express the real physical problem, and since they contain the force terms explicitly any solution of them must represent the motion of the particle under the action of the forces present. The question is, can they be handled on the present Differential Analyzer?

Lemaitre and Vallarta gave the equations of motion in polar coordinates. Reducing these equations to the form in which they were most easily handled by machine left them still far too complicated for the present equipment. Following this, the work of Carl Störmer\textsuperscript{42} was consulted for details of the methods he had used on the same problem in studying the phenomena of aurora borealis.

Briefly, Störmer sets up the equations of motion in rectangular coordinates. Since the force acting on a charged particle in a magnetic field is always perpendicular to its motion, the velocity is constant. Störmer therefore changes to the independent variable defined by $ds = v \, dt$. He then transforms to equations in cylindrical coordinates defined by:

\begin{align*}
x &= R \cos \varphi \\
y &= R \sin \varphi \quad Z = Z
\end{align*}

The motion is separated into two components, the first, motion in the meridian plane, and the second, rotation of the meridian plane about the magnetic axis. Since the rotation of the meridian plane can be determined after the motion of the particle in the plane is known, only the equations dealing with the latter motion need be considered immediately.

* Lemaitre and Vallarta referred to Störmer's work both in their paper and in conversations with the writer. At the time of the first study, however, his equations had not been reduced to a form suitable for the machine. This step was taken by the writer in the present investigation.
Neither the rectangular coordinates nor the cylindrical coordinates are quite suitable for reducing the problem to permit an immediate machine study. Fortunately, Størmer had made another change of variables in order to simplify his own computation problem, and his final equations are susceptible to machine attack.

Using a transformation due to Goursat, the cylindrical coordinates are replaced by two new dependent variables \( u \) and \( v \), and a new independent variable \( \sigma \), defined by the equations

\[
\begin{align*}
R &= \frac{1}{2} \frac{1}{\gamma_1} \varepsilon \cos v \\
z &= \frac{1}{2} \frac{1}{\gamma_1} \varepsilon \sin v \\
ds &= \frac{1}{8} \frac{1}{\gamma_1} \varepsilon \ 2u \\
\end{align*}
\]

(13)

Using these variables, Størmer gives the equations for motion in the meridian plane in the form

\[
\frac{d^2 u}{d\sigma^2} = \frac{1}{2} \frac{\partial P}{\partial u} \\
\frac{d^2 v}{d\sigma^2} = \frac{1}{2} \frac{\partial P}{\partial v} \\
\]

(14)

\[
\left( \frac{du}{d\sigma} \right)^2 + \left( \frac{dv}{d\sigma} \right)^2 = P
\]

\[
P = \frac{1}{16} \varepsilon^2 + 2\varepsilon \frac{2u}{\cos^2 v} - \frac{1}{\cos^2 v} - \varepsilon^2 \cos^2 v
\]
Evaluating the partial derivatives, and indicating derivatives with respect to $G$ by dots, the required equations become

$$
\ddot{u} = a - u + \varepsilon \cos^2 v
$$

$$
\ddot{v} = \varepsilon^{-2u} \sin v \cos v - \frac{\sin v}{\cos^2 v}
$$

where $a = \frac{1}{16^{1/4}}$

The third equation in (14) is not independent but can be derived from the two given in (15) as will be shown later. It must be satisfied, however, by the initial conditions. Hence only three of the quantities, $u, v, \dot{u}$ and $\dot{v}$ can be specified arbitrarily in starting a solution.

To put equations (15) into forms which can be handled on the present machine, two simple changes are necessary. Factoring out $\varepsilon^{-2u}$ in the first equation and $(\sin v \cos v)$ in the second, and then indicating an integration of each, they may be written

$$
\dot{u} = \int \frac{4u}{a - u + \cos v} d\sigma
$$

$$
\dot{v} = \int \frac{\sin v \cos v}{\varepsilon^{-2u} - \frac{1}{\cos^4 v}} d\sigma
$$

These equations can be solved with six integrators and five input tables, which is just the limit of present equipment; Fig. 9 shows the connections required. At the present writing a new attack on the problem, using these equations is being planned.
The method of demonstrating the relation given in (14) that

\[ \dot{u}^2 + \dot{v}^2 = P \]

brings out equations which throw some further light on the difficulty encountered with the Lemaitre and Vallarta equation. In equations (15) multiply the first equation by \( \dot{u} \) and the second by \( \dot{v} \), and then integrate both with respect to \( \sigma \). Since \( \frac{du}{d\sigma} \cdot d\sigma = du \), and \( \frac{dv}{d\sigma} \cdot d\sigma = dv \), some of the integrations can be completed. When carried through, the final results are

\[
\begin{align*}
\dot{u}^2 & = a \epsilon^{2u} + 2 \epsilon^{-u} - \int \cos^2 v \, d(\epsilon^{-2u}) \\
\dot{v}^2 & = -\int \epsilon^{-2u} \, d(\cos^2 v) - \frac{1}{\cos^2 v}
\end{align*}
\]

(17)

Adding these it is apparent that the correct value of \( P \) is obtained.

The equations are of further interest, however, because in the form

\[
\begin{align*}
\dot{u} & = \sqrt{a \epsilon^{2u} + 2 \epsilon^{-u} - \int \cos^2 v \, d(\epsilon^{-2u})} \\
\dot{v} & = \sqrt{-\int \epsilon^{-2u} \, d(\cos^2 v) - \frac{1}{\cos^2 v}}
\end{align*}
\]

(18)

they can be set up on the present machine. But the old difficulty again crops up, this time in a two-fold way, for if either \( \dot{u} \) or \( \dot{v} \) reaches zero, it stays there. This time, fortunately, the source of the difficulty is apparent. In deriving (18) the equations of (15) were multiplied by \( \dot{u} \) and \( \dot{v} \) respectively. Hence the terms on both sides of the equations all go to zero together, and the whole expression
vanishes. Although the writer has not carried through in detail the steps indicated by Lamaitre and Vallarta in their derivation*, a similar process seems to have been carried out there.

The machine method indicated in Fig. 9 is by no means the best obtainable; its only real advantage is that the present machine can handle it. Unfortunately, all the integrating units are required for strictly integrating purposes and none are available to generate functions. With additional integrators available, the situation would be:

<table>
<thead>
<tr>
<th>Number of additional integrators</th>
<th>Manual operators required</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>7</td>
<td>0</td>
</tr>
</tbody>
</table>

b) Astrophysics

In the general field of astrophysics, both the three-body problem and the problem of the motion of a charged particle in a dipole magnetic field (the earth's) must be included. These were discussed under the heading of "dynamics" for the sake of generality.

It is to be hoped that investigations using the Differential Analyzer will be undertaken in the near future along other lines. In particular, the theory of stellar structure finds mathematical expression to a large degree in the Emdem** equation (and others)

\[ \frac{1}{\xi^2} \frac{d}{d\xi} \left( \xi^2 \frac{d\phi}{d\xi} \right) + \theta^n = 0 \]  

(19)

* The derivation given in their paper (40) is very brief and contains none of the detail steps which would furnish information on this point.
** R. Emden, Gaskugeln (Leipzig, 1907).
Much has been written on this equation and the nature of its solutions, with but few actual solutions to write about. In one volume of a single publication (Monthly Notices of the Royal Astronomical Society, Vol. 91, 1930-31) about ten papers appear dealing with this single equation or its variations. The technique of its solution by the Differential Analyzer has been explored by Bush and Caldwell in a study of the Thomas-Fermi equation, which is the same as the Emden equation except for a change of sign.

c) Miscellaneous

The ordinary differential equations of chemistry are familiar to every student of differential equations. These deal principally with reaction rates and are usually solved analytically. In some cases, however, problems of this type cannot be solved analytically and are well suited for Differential Analyzer treatment.

Various equations, such as the Mathieu equation, are of interest as mathematical problems as well as from the practical point of view. The Mathieu equation

\[ \frac{d^2y}{dx^2} + (a - 2\theta \cos 2x)y = 0 \quad (20) \]

has been extensively treated by mathematicians and it is widely applicable to problems of engineering interest. Tables of solutions are partially available and these could readily be enlarged.

*     *     *     *     *     *     *
In these introductory chapters, besides reviewing much of the important work carried out on the Differential Analyzer and its predecessor, the Product Integraph, the writer has attempted to show by various examples how the machine method may be adapted and extended to meet new problems. In some cases the objective is reached if the problem can be handled at all. The next step is to simplify the method, both with regard to the number of solutions required and the complexity of the machine connections. Finally, there comes the ultimate step of making the machine do all the work, or as so aptly expressed by Dean Bush, "... relegating to the machine those parts of the processes of thought which are inherently mechanical and repetitive."

In the problem to be taken up in detail in the following chapters, the first two steps have already been taken and the methods are known for taking the final step.
Chapter III.

APPLICATIONS IN ATOMIC PHYSICS

a) Atomic structure in the stationary state

In the three decades which have passed since Planck introduced his revolutionary idea of discrete, quantized energy states, the science of atomic physics has developed to the extent that its theoretical concepts are of practical interest to engineers in many fields. Within relatively few years, the electron has come to play an important role in everyday life; from it have come new industries and others have been revolutionized as a result of the engineer's deeper understanding of electronic phenomena.

The general historical development of this and other aspects of atomic physics is treated in many books and papers on the subject. Briefly, the commonly accepted model of the atom is, or was, that proposed by Rutherford, in which there is a relatively heavy central core or proton about which revolves one or more lighter particles called electrons. These bodies are electrically charged, with each electron carrying the same amount of negative charge and the proton carrying a positive charge equal to the sum of the electronic charges. Most of the theoretical analysis prior to 1925 was based on this simple model, and it is still used to a considerable extent, at least for qualitative purposes, at the present time. Much explanatory material in connection with various phenomena of electronics, gaseous conduction, ionization processes and photoelectric effects, etc., still deals with this simple model.
For some time prior to the more recent developments in atomic theory, the shortcomings of this model were becoming apparent. The quantum theory based on it had become more and more a patchwork composed principally of classical mechanics and numerous arbitrary rules which had been introduced in order to bring theoretical results in accord with experiment. Furthermore, a number of cases had appeared in which definite failure of the theory occurred*. Of these, among the most serious was the inability to predict the spectral frequencies for atoms containing more than one electron. Even for neutral helium, which contained only one additional electron, the theoretical results were definitely not in accord with experiment.

An additional and rather fundamental shortcoming of quantum theory had been known for some time, namely, that even though the theory might be patched up so that it would give reasonably accurate predictions of the frequencies of emitted radiation, there was still no way of calculating the intensity of the radiation. This situation was inherent to quantum theory. No difficulty was encountered in computing the amplitude of radiation from a simple oscillator, but quantum theory postulated that radiation occurred only when an electron changed from one orbit (or state of oscillation) to another. No laws governing the intensity of the radiation produced by such a change had been formulated, and in this respect at least it was quite evident that a radical change in procedure was necessary.

The first step to correct the latter difficulty was taken in 1925 when Heisenberg undertook to develop a method of using the

* Reference 44, Chap. VIII.
classical laws of radiation, and introduced a double subscript notation so as to make the intensity dependent on both the beginning and end states of the electron. This method was studied and extended by Heisenberg and others and has developed to the present-day matrix mechanics. It has since been shown to give results equivalent to those obtained by the later wave mechanics. Not only did later theories make radiation intensity calculations possible, but they have also been shown to give results much more nearly or exactly in accord with experiment in many cases where the older quantum theory failed.

In 1924 L. de Broglie, in working out a new method for computing energy levels, introduced the idea of a wave motion associated with electrons in motion. This idea was later amplified and extended by Schrödinger in his original papers on wave mechanics. As has been mentioned above, the results given by Schrödinger's theory are identical with those given by Heisenberg's. In fact, the two methods are exactly equivalent in content although entirely dissimilar in form.

* * * * *

The general problem of wave mechanics is to solve for any particular case the Schrödinger wave equation*

\[ \nabla^2 \psi + \frac{\hbar^2 m}{\epsilon^2} (W - V) \psi = 0, \]  

(1)

* Valid for stationary state problems in which the variation with time is assumed to be simple harmonic.
where $\psi$ is the wave function, $\mu$ is the mass of the particle considered, $\hbar$ is Planck's constant, $W$ is the total energy, and $V$ is the potential energy. This is, of course, a partial differential equation and is not susceptible to direct attack by present machines. Before any solution can be obtained, it is necessary to find coordinates in which the variables will separate.

In this discussion it will be assumed that the variables have been separated properly, and that the equation for the radial component of the wave function is given. This equation is an ordinary differential equation, and in the case of hydrogen is written

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dS}{dr} \right) - \frac{1}{r^2} \left( 1 + \frac{1}{r} \right) S + \frac{8\pi^2 \mu}{\hbar^2} \left( W + \frac{e^2}{r} \right) S = 0,$$

(2)

where $S$ is the radial component of $\psi'$. It is customary to study this equation after two changes are made. The first is to change to the variable $R = Sr$. The second is to introduce new units such that distance is measured in terms of the radius of the first Bohr orbit ($= 0.529 \times 10^{-8}$ cm.), and energy in terms of the ionization potential of normal hydrogen ($= 13.54$ electron volts). These changes simplify the form of the equation and the coefficients. For hydrogen, the resulting expression is

$$\frac{d^2R}{dx^2} + \left( \varepsilon - \frac{1}{x^2} \left( 1 + \frac{1}{x} \right) + \frac{2}{x} \right) R = 0$$

(3)

Only certain particular solutions of equation (3) are significant, and these are found by satisfying certain conditions.
inherent to the physical problem. In the first place, the wave function \( \Psi \) of equation (1) is presumably a quantity of some physical significance, and it is conceivably a measurable quantity. If so, it must be finite throughout the entire range of variables. Since \( S \) is a component of \( \Psi \), it must obey the same restriction, and hence \( R \) must have the value zero at \( r = 0 \) (or \( x = 0 \)) because \( R = Sr \). Now as \( r \) approaches \( \infty \), if only the criterion of finiteness of \( S \) is applied, the function \( R \) can become infinite, and under this condition it is impossible to select a significant solution.

Other reasoning, based upon the physical interpretation of the \( \Psi \) function, furnishes a definite condition to be satisfied. Not only must \( \psi \) be finite over all space, but it must satisfy the relation

\[
\int_V \psi \bar{\psi} \, dV = 1, \tag{4}
\]

where \( \bar{\psi} \) is the complex conjugate of \( \psi \) and \( dV \) is the volume element of the particular coordinates in which \( \psi \) is expressed. If \( \psi \) is a real quantity, the condition of (4) becomes simply

\[
\int_V \psi^2 \, dv = 1. \tag{5}
\]

In order that this be true, both \( \psi \) and its component \( S \) must become zero as \( r \) approaches infinity. The related function \( R \) in equation (3) must also approach zero as \( x \) approaches infinity; in fact, \( R \) itself must satisfy the equation

\[
\int_0^\infty R^2 \, dx = 1. \tag{6}
\]
Since equation (3) is linear, it is apparent that the absolute magnitude of \( R \) is indeterminate. The actual scale of \( R \) is known only after it has been made to satisfy equation (6), a process called normalization.

The physical interpretation of the \( \Psi' \)-function from which the normalization integral (4) is set up is given in various forms. It is commonly accepted that the expression \( \Psi'^2 \, dv \) represents the probability that an electron is located in the element \( dv \). Since the wave equation is set up for a single electron moving in the potential field \( V \), if this probability is integrated over all space, the integral must equal unity because there is the certainty of one electron being present. Thus equation (4) is written directly. In similar manner, \( R^2 \) represents the probability that the electron is in the volume element between \( x \) and \( x + dx \), and as written in equation (6), the integral over all values of the variable \( x \) must equal unity.

Summarizing, the conditions which a solution of equation (3) must satisfy are: first, \( R \) must be zero at \( x = 0 \) and at \( x = \infty \); second, the function must be normalized. The Differential Analyzer technique must be such as to produce solutions which meet these conditions.

The second of these conditions is readily met in a large number of cases, of which the hydrogen atom is an example. When the equation is linear, there is no need to consider the question of normalization until after the solution is obtained. The scale of the wave function can be anything and satisfy the differential equation.
It is the normalization condition which is then used to fix the scale.

It will be shown later that valid wave equations which are non-linear can be written. In general the criterion is that if the potential terms (in equation (3) the terms \(-\frac{1}{x^2} + \frac{1}{x}\)) are known functions of the independent variable, or functions which are assumed to be known, the wave equation is linear. If, on the other hand, the potential energy is not known as a function of the independent variable and must be expressed in terms of the wave function itself, the equation becomes non-linear. In these latter cases, the normalization condition must be satisfied by the immediate solution because the scale factor of the wave function is no longer arbitrary.

There still remains the first condition, namely, \(R(0) = 0\) and \(R(\infty) = 0\); this must be satisfied in any event. How is the machine to be operated in order to satisfy this condition? Consider the equation written in a slightly different form, namely:

\[
\frac{d^2 R}{dx^2} + \left[ \varepsilon + f(x) \right] R = 0, \tag{7}
\]

where \(f(x)\) is any known potential function and \(\varepsilon\) is the term associated with the total energy. Fig. 10 indicates the machine connections required if the equation is rewritten

\[
\frac{dR}{dx} = - \int_{0}^{x} \left[ \varepsilon + f(x) \right] R \, dx. \tag{8}
\]

Now suppose a solution is to be obtained satisfying the condition stated above. Starting at \(x = 0\), the abscissa displacement of the
Fig. 10.
input table will be set at this point, and the pointer will be cranked to the initial ordinate. Next the integrator displacements must be set to their initial values. Integrators II and III are, of course, set at the initial values of \( R \) and \( \frac{dR}{dx} \) respectively. \( R \) is initially zero as required and \( \frac{dR}{dx} \) can have any value (within the limitation that the maximum available displacement on the lead screw must not be exceeded) since its scale is arbitrary.

Integrator I as yet has no definite starting displacement. It must be displaced in proportion to the term \( \epsilon + f(x) \), but only \( f(x) \) is known initially. The total energy constant \( \epsilon \) is unknown and must be guessed. Thus, one more condition \( (R(\infty) = 0) \) is to be fulfilled and there is the one parameter \( \epsilon \) which can be varied as required. For a given \( f(x) \) there are only certain values of \( \epsilon \) which will make \( R \) go to zero as \( x \) becomes infinite. These values of \( \epsilon \) are known as the "characteristic values" or the "eigenwerte"; the corresponding \( R(x)'s \) are called the eigen-functions.

Mathematical proof of the uniqueness of eigenwerte and eigenfunctions is given in standard texts on wave mechanics. Considered as a Differential Analyzer problem the role of the eigenwert as a necessary adjustable parameter is quite apparent.

Certain difficulties appear when these solutions are tried. Inaccuracies of machine operation are particularly troublesome. If, for example, equation (3) were to be solved for a constant potential, it could be written

\[
\frac{d^2R}{dx^2} = KR \tag{9}
\]
The solutions of this equation are exponential if \( K \) is positive and sinusoidal if \( K \) is negative. In stationary state atomic problems, the coefficient of \( R \) is negative near the nucleus and becomes positive for larger values of radius.

Now suppose some slight error has appeared momentarily, sufficient to change \( R \) from its true value by an amount \( \Delta \). The machine is still connected to solve the equation, but the variable has been changed and the equation can be written

\[
\frac{d^2(R + \Delta)}{dx^2} = K(R + \Delta) \tag{10}
\]

Subtracting equation (9) from (10) there results the equation due to the momentary error.

\[
\frac{d^2\Delta}{dx^2} = K\Delta \tag{11}
\]

The error term as thus given is of exactly the same form as the desired function. In the range of \( x \) where \( K \) is negative any errors which are introduced are sinusoidal and do not tend to cumulate rapidly. In this region the operation of the machine is quite stable and results can be repeated without difficulty. When \( K \) becomes positive, however, the errors introduced accumulate exponentially and the situation is critical. It is complicated by the fact that if the total energy is not exactly an eigenwert, the \( R \)-function itself diverges toward either plus or minus infinity exponentially. The problem of distinguishing between an exponential error term and an exponential result is one of
the principal difficulties encountered; the method used to separate them and to eliminate the error term will be described in the next chapter.

In the discussion given above, nothing was said about the form of the potential function \( f(x) \). The method outlined is straightforward and workable provided \( f(x) \) is finite throughout the entire working range. It is characteristic of the atomic problem, however, that the potential function becomes infinite at the nucleus where \( x = 0 \). Hence, in general, solutions cannot be obtained in the simple manner described above.

This limitation does not invalidate the argument which shows that \( \mathcal{E} \) must have a particular value in order to make \( R(\infty) = 0 \). It simply means that the starting conditions at some small positive value of \( x \) must be specified, instead of those at \( x = 0 \). A small value of \( x \) is necessary because over a small enough range, the solution can be written in series form, and from this series the ratio of function (\( R \)) to slope (\( dR/dx \)) can readily be obtained. With this exception, the procedure is as outlined above.

b) Non-stationary state atomic problems

In addition to the stationary state problems there is a group of wave problems in which the principal interest is in collision processes; these may be classified as problems of the non-stationary atomic state.

The equations governing the phenomena have been studied extensively on the Differential Analyzer, particularly by Prof. P. M. Morse
and Dr. W. P. Allis*. It would be impossible within the scope of this thesis to discuss the collision problem adequately. It is interesting, however, to note the form in which the equation most recently studied was presented.

\[
\frac{d^2 R}{dr^2} + \left(k^2 + V(r) - \frac{\lambda(\lambda + 1)}{r^2}\right) R =
\]

\[
- \frac{2}{2\lambda + 1} \int_{r}^{\infty} 2 \varepsilon \left[ \int_{r}^{\infty} 2 r \epsilon^{-1} r \frac{\lambda + 1}{2} R dr + \int_{r}^{\infty} 2 r \epsilon^{-1} R dr \right].
\]

(12)

The rather formidable problem of handling this equation on the present machine was solved by taking advantage of certain symmetries which exist. If two new functions of \( r \) are defined by the equations

\[
\alpha = \int_{r}^{\infty} 2 \varepsilon^{-1} r \frac{\lambda + 1}{2} dr
\]

\[
\beta = \int_{r}^{\infty} 2 \varepsilon^{-1} r \frac{-\lambda}{2} dr,
\]

and the limits of integration are made uniform, this equation reduces to

\[
\frac{d^2 R}{dr^2} + \left(k^2 + V(r) - \frac{\lambda(\lambda + 1)}{r^2}\right) R =
\]

\[
- \frac{2}{2\lambda + 1} \left[ \int d\alpha \int R d\beta - \int d\beta \int R d\alpha \right].
\]

(13)

* A paper by these men describing the most recent work is to be published soon in the Physical Review. Also see "Quantum Mechanics of Collision Processes", by Philip M. Morse, Rev. of Modern Physics, 4, 577 (1932).
The final step necessary is to transform the integral on the left, writing for it

\[ \int (k^2 + V(r) + \frac{\ell(\ell+1)}{r^2}) \, R \, dr = k^2 r + \int R \, dV_1(r) \quad (14) \]

where \[ V_1(r) = \int \left( V(r) - \frac{\ell(\ell+1)}{r^2} \right) \, dr \quad (15) \]

This step is necessary so that the available number of integrating units will be sufficient. It means simply that the integral in equation (15) must be evaluated prior to machine operation.

Since the results of this work and the procedure followed are soon to be published by Morse and Allis, no further discussion will be given here.

c) Potential field problems

As indicated in section (a) of this chapter, the potential field plays an important part in the solution of the wave equation. In fact, in many cases, the problem is almost solved if the form of the potential function is definitely known.

The potential field problem is really one of determining charge distribution. It is usually assumed then that the macroscopic law

\[ V = \int \rho \frac{d\tau}{r} \]

holds in atomic dimensions, and the potential is computed from it.
The justification for this assumption is that potential fields thus calculated give results in accord with experiment.

In many of the problems of interest the potential field can be written immediately. Thus, in the case of the hydrogen atom - that "proving-ground" of all atomic theories - or the hydrogen-like atoms, it can be written directly as

\[ V(r) = - \frac{Z e^2}{r} \]

where \( Z \) is the atomic number, and \( e \) is the charge on an electron.

This function when used in the wave equation leads to solutions which check spectroscopic results.

Unfortunately, in the majority of cases, the form of the potential function is not known. Approximate methods are available, however, and these would be made more useful if, for example, wave functions were obtained for a wide assortment of empirical potential fields. The Differential Analyzer is well adapted to supply such aids to analysis.

The atoms with more than one electron are of particular interest, and their potential field problems are difficult. If there are very many electrons, the problem can be considered as a statistical one in the manner of Thomas and Fermi. The Thomas-Fermi equation has already been solved on the Differential Analyzer by Dr. V. Bush and the writer, and the results are in the literature. Another method of treating the many-electron atom is due to Hartree. This method is applicable where the fields are spherically
symmetrical - the so-called central field - or where they can be assumed as central without introducing too much doubt. Consider the case of the helium-like atoms in which there is a nucleus and two electrons. Besides the assumption of a central field, Hartree assumes that both electrons are identical and therefore have identical wave functions. The wave function is obtained by solving the wave equation for one of the electrons moving in the field of the nucleus and the other electron. In order to find the component of potential due to the second electron, its wave function must be known, and hence the solution of the whole problem must be known. This, of course, is a situation in which successive approximation methods are used, and Hartree follows that procedure. His steps are

Initial field

Initial field corrected for electron contributions

Solutions of Wave Equation

Distribution of charge

Final field

The desired solution is found when the successive cycles of calculations repeat, that is, when the final field is the same as the initial field. The final wave function is the one which is characteristic of the self-consistent field.

In the next chapter, a new method is described for obtaining the self-consistent field solutions. It has been successfully applied in eight cases and the method has been developed to the point where a solution for a single helium-like atom can be found in a reasonable length of time.
Chapter IV

THE PROBLEM OF THE SELF-CONSISTENT FIELD

a) The Hartree method

Two principal computation processes are required to solve an atomic problem by Hartree's method. First, a normalized wave function is given and from it and whatever known charge distribution is present, a potential field is computed. Second, given this or another potential field, the corresponding wave equation is solved for a wave function which satisfies the boundary conditions of the physical problem. It is assumed in referring to these processes that the functions dealt with cannot conveniently be represented analytically.

Considering the first process as a machine problem, there is given a normalized function \( S(r) \) which is a real function of \( r \) only. This function is to be interpreted so that the charge density is given by its square; that is, in the potential integral \( V = \int \frac{\gamma}{r} \), the value \( S^2 \) is to be substituted for \( \gamma \).

The expression for the potential due to \( S^2 \) contains two terms, derived as follows. It is apparent that since the charge density \( S^2 \) is spherically symmetrical, the equipotential surfaces are concentric spheres. Consider a spherical surface of radius \( r \); the charge of the electron is partly within and the remainder outside of this surface. Due to the charge entirely within the surface, the potential on the surface is given by the integral

\[
V_1 = \frac{1}{r} \int_0^r S^2 \cdot 4\pi r^2 \, dr, \quad \text{(inner potential)}
\]
The second term, due to that portion of the charge which is outside the surface is

\[ V_0 = \int_{r}^{\infty} \frac{S^2 \cdot 4\pi r^2 dr}{r}, \quad \text{(outer potential)} \quad (2) \]

The total potential due to the charge density \( S^2 \) is the sum of (1) and (2).

In the case to be studied, it is convenient to change the variables of the original equation; the variable \( S \) is replaced by \( \Psi \) and the scale of the independent variable is altered so that the \( 4\pi \) factors of (1) and (2) are removed. Therefore, the working integrals from which the potential is derived are given by:

\[ V(x) = \frac{1}{x} \int_{0}^{x} \Psi^2 dx + \int_{x}^{\infty} \frac{\Psi^2 dx}{x} \quad (3) \]

The evaluation of such integrals on the Differential Analyzer is a simple matter. The connections required are shown in Fig. 11. (See also Figs. 12, 13, 14).

Having found the potential energy expression, the second principal part of the Hartree procedure, which is to solve the corresponding wave equation, can be carried out as described in Chapter III, part (a). The result is a new \( \Psi \) which is used to compute a new potential in order to repeat the process. With enough repetitions, the condition will eventually be reached in which the \( \Psi \) used to compute the potential energy is the same as that found by solving the wave equation containing this potential energy expression. The name
"self-consistent field" is applied to the potential field which satisfies this condition, and it is the immediate object of the Hartree method to find the self-consistent field for each problem studied. From this, the desired wave function (eigen-function) and total energy (eigenwert) are determined.

The above described process is readily carried out on the Differential Analyzer. Two distinct sets of connections are required, but there is sufficient equipment to permit both to be set up at the same time. For the solution of the wave equation, the basic connections are those shown in Fig. 10, and to evaluate the potential integrals, there must be added the connections of Fig. 11 as an entirely independent set-up.

Hartree's procedure translated into terms of machine operation on this basis now takes the following form:

1. Assume an initial field (for the helium-like atoms that due to the nucleus and one electron).
2. Solve the wave equation for this field, using the connections of Fig. 10.
3. Normalize the wave function; that is, satisfy the condition
   \[ \int_{-\infty}^{\infty} \psi^2 \, dx = 1 \]
4. Put the normalized \( \psi \) into the set-up of Fig. 11 and from it find the potential terms due to the electronic charge distribution. Adding this potential algebraically to that of the nucleus gives the final field.
5. Compare the final field with the field first used. If they are identical, the $\psi$ obtained in step 2 is the solution desired. If not, replace the field used in step 1 by that found in step 4 or by some interpolated field and repeat until correspondence is attained.

Although this method offered no insurmountable difficulties of execution, it was not a particularly attractive one. The idea of having to carry out the calculations a piece at a time was bothersome, probably because it seemed entirely out of line with the philosophy of the machine method. The question kept arising, - why not connect the two parts of the machine together so that the part in Fig. 10 fed its $\psi$ into the part in Fig. 11, and the part in Fig. 11 fed its potential right back into the part in Fig. 10 where it belonged? True, it was then no longer the Hartree method, but it was evident that if the potential function used in the wave equation was continuously generated from the solution of the wave equation, then every solution obtained was a self-consistent one. Hence, if the machine could be controlled so that a normalized, finite solution was obtainable, that solution would be the same as would be obtained from the original Hartree method.

There remained two questions. Could the problem be formulated in its entirety, including the steps which in the first method would be done on paper, and still be within the capacity of the Differential Analyzer? If so, then could a solution satisfying all conditions be obtained within a reasonable time?
b) An extension of Hartree's method for the helium-like atoms

For a single particle, in the field of a nucleus of charge $Z$, the wave equation for the radial component may be written (using atomic units, see page 55).

$$\frac{d^2\psi}{dr^2} + \left(\frac{2Z}{r} - \epsilon\right)\psi = 0 \quad (4)$$

In the helium-like* atoms, however, the electron under consideration moves in the resultant field of the nucleus and the other electron. It is assumed that the resultant field is central and that the wave functions of both electrons are identical. The latter assumption is necessary so that the wave function of the electron studied can be used to find the component of potential due to the other electron. In equation (4), this change is conveniently made by replacing $Z$ by the so-called "effective charge for potential", $Z^e$, which is defined by

$$Z^e = Z - r v(r) \quad (5)$$

In equation (5), $v(r)$ is the component of potential due to the distributed electronic charge and is multiplied by the radius so that it will have the dimensions of a charge located at the nucleus (in a central field). $Z$ is the ordinary nuclear charge. Replacing $v(r)$ by the potential integrals previously derived,

$$Z^e = Z - \int_0^r \psi^2 dr - r \int_r^\infty \psi^2 \frac{dr}{r} \quad (6)$$

* These include not only helium itself, but also the "stripped" atoms containing a nucleus and two electrons.
It is more convenient in using the Differential Analyzer to use the same limits of integration in both the integral terms of (6), so the equation is expanded to

\[ Z^0 = Z - \int_0^r \psi^2 \, dr - r \int_0^\infty \frac{\psi^2 \, dr}{r} + r \int_0^r \frac{\psi^2 \, dr}{r} \]  

(7)

Now the integral \( \int_0^r \frac{\psi^2 \, dr}{r} \) is a definite integral and for any solution which is of physical interest it may be replaced by an unknown, but finite, constant \( C \). Since only these significant solutions are to be retained, the substitution may be made immediately, and \( Z^0 \) hence becomes

\[ Z^0 = Z - Cr - \int_0^r \psi^2 \, dr + r \int_0^r \frac{\psi^2 \, dr}{r} \]  

(8)

Replacing the \( Z \) of equation (4) by the \( Z^0 \) thus computed, and also introducing the changes of variable

\[ x = Zr \]  

(9)

\[ \beta = \frac{\psi}{Z^2} \]  

(10)

the equation to be solved becomes

\[ \frac{d^2 \psi}{dx^2} + \left[ \frac{2}{x} - \frac{2C}{Z} + \frac{2}{Z} \int_0^x \frac{\psi^2 \, dx}{x} - \frac{2}{Z^2} \int_0^x \frac{\psi^2 \, dx}{x} \right] \psi = 0 \]  

(11)

(The change of variable in (9) was introduced in order that the maximum of \( \psi \) would be reached in all cases near \( x = 1 \) instead of...
getting closer to the origin as \( Z \) increased. Since \( \varepsilon \) varies approximately as \( Z^2 \) for this problem, the substitution of (10) was made in order to introduce a parameter which varied only slightly in the neighborhood of \( \beta = 1 \). These changes were suggested by Dr. L. A. Young of the Physics Department.)

Examining equation (11), it is apparent that the constant \( C \) introduced adds no complication. The method of solving the wave equation requires that the value of \( \beta \) be found by trial, and it is no more difficult to do this for the value of \( (\beta + \frac{2C}{Z}) \). These values can later be separated as will be shown. Of more immediate concern is the fact that the equation is not linear, and hence the scale of \( \psi \) and its derivatives is no longer arbitrary. Moreover, since the potential is derived directly from \( \psi' \), the wave function must be normalized as it leaves the machine - it cannot be normalized in a separate operation. Hence, the technique used in operating the machine must be such that the resulting wave function is a normalized function which is zero at \( x = 0 \) and at \( x = \infty \).

As has been shown before, the condition that \( \psi(0) = 0 \) is satisfied by starting with a zero value of \( \psi \). Also, the parameter \( (\beta + \frac{2C}{Z}) \) is available and this can be adjusted so that \( \psi'(\infty) = 0 \). The condition that \( \int_0^\infty \psi^2 \, dx = 1 \) can be attained by varying the starting slope, since now the size of \( \frac{d\psi}{dx} \) at \( x = 0 \) has a direct effect on the shape of \( \psi \). Multiplying the initial slope by an arbitrary constant no longer has the effect of merely multiplying all values of \( \psi \) by the same constant.
Summarizing, there are two conditions to be satisfied (aside from the condition $\psi(0) = 0$

$$\psi(\infty) = 0$$

$$\int_0^\infty \psi^2 \, dx = 1$$

and to satisfy these conditions there are two adjustable quantities, $(\beta + \frac{2C}{Z})$ and $\frac{d\psi}{dx}$ at $x = 0$. Actually, of course, the latter condition and the starting value $\psi'(0) = 0$ cannot be used directly because the term $\frac{2}{x}$ in equation (11) becomes infinite at $x = 0$. A series solution is used in order to find the ratio $(\frac{d\psi}{dx})/\psi$ at a very small value of $x$.

This is now recognized as a problem requiring two-way interpolation among solutions of a differential equation. The double variation must be carried out systematically in order to reach a result in a reasonable time. Furthermore, it has been shown that a serious type of error can enter into these solutions. Hence it is vitally necessary if any interpolation is to be reliable, that the amount of error be reduced to a negligible amount.

c) Procedure on the Differential Analyzer

Several different machine connections were used in the first attempt to solve equation (11) on the Differential Analyzer. Although the net results of these trials were meagre, the experience gained in dealing with the problem was of direct benefit in the later work. The changes made as the study progressed may best be traced in Figs. 12, 13 and 14, corresponding to equations (12), (13), and (14), respectively.
$$F_1 = \beta + \frac{2e}{Z} - \frac{2}{Z} \int \psi^2 \frac{dx}{x} - \left( \frac{1}{Z} \right) \left( z - \frac{3}{Z} \int \psi^2 dx \right)$$
\[ F_3 = \beta + \frac{2C}{x} - \frac{2}{x} \int \psi^2 \frac{dx}{x} + \frac{2}{x^2} \int \psi^2 dx \]
These equations show the different ways in which the terms of equation (11) were arranged in the search for the most desirable machine method.

\[
\frac{d\psi}{dx} = \left[ \beta + \frac{2c}{Z} - \frac{8}{Z} \int \psi^2 d(ln x) - \frac{1}{x} (2 - \frac{2}{Z}) \int \psi^2 dx \right] \psi dx \\
(12)
\]

\[
\frac{d\psi}{dx} = \left[ \beta + \frac{2c}{Z} - \frac{2}{Z} \int \psi^2 d(ln x) - \frac{2}{Z} \int \int \psi^2 dx \psi dx \right] \psi dx \\
(13)
\]

\[
\frac{d\psi}{dx} = \left[ \beta + \frac{2c}{Z} - \frac{2}{Z} \int \psi^2 d(ln x) + \frac{2}{Z} \int \psi^2 dx \psi dx - \int \int \psi d(ln x) \right] \psi dx \\
(14)
\]

The change made in going from equation (12) to (13) was to introduce the \( \frac{2}{x} \) term separately rather than to try to put it in by means of the multiplier*. This was necessary because of the difficulty of evaluating \( \frac{2}{x} \) precisely with the scale factor required for the \( x \). Later it was noticed that by again rearranging as in (14), the number of men required to turn cranks was reduced from four to three – always a worthwhile step.

Using the connections shown in Fig. 14 a series of runs were made for the case \( Z = 2 \) (helium). The final result was very encouraging; a comparison of the \( \psi \) thus obtained with that obtained by Hartree showed a remarkably close check (Table I).

* It should be understood that the multiplier unit on the Differential Analyzer can also be used for division by an interchange of output shaft.
At this stage, the machine method still left much to be desired. In particular, the necessity of having three operators for the input tables made it difficult to maintain a steady pace. Furthermore, the multiplier was not working under favorable conditions because of small initial displacements with consequent lack of accuracy. The difficulty of making rapid headway made it desirable to stop and reconsider the problem on paper with the view of simplifying the machine requirements and systematizing the procedure.

Numerous changes of variable were tried in the attempt to get a simpler equation or an equation which had more tractable solutions. The substitution $\psi = \phi e^{-bx}$ looked good enough to warrant a trial on the machine. In this case $\phi$ would be a function behaving approximately as a positive exponential, and therefore of a relatively simple form. The difficulty found with it was that the result was very

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sensitive to changes in the initial slope and this could not be controlled with sufficient accuracy. As a result of making this attempt, however, a method of reducing the equation in Θ was found to be applicable to equation (11) in $\psi'$. The simplification effected was sufficient to permit the development of a workable method.

Consider in equation (11) the terms represented by $Q$

$$Q = \int_0^X \psi^2 \frac{dx}{x} - \frac{1}{x} \int_0^X \psi^2 \, dx$$  \hspace{1cm} (15)

Differentiating with respect to $x$,

$$\frac{dQ}{dx} = \frac{\psi^2}{x} - \frac{\psi^2}{x} + \frac{1}{x^2} \int_0^X \psi^2 \, dx$$

$$= \frac{1}{x^2} \int_0^X \psi^2 \, dx$$  \hspace{1cm} (16)

Integrating with respect to $x$,

$$Q = \int_0^X \frac{dx}{x^2} \int_0^X \psi^2 \, dx$$

$$= - \int_{\infty}^{X} \left( \frac{1}{x} \psi^2 \right) dx = \int_{0}^{X} \psi^2 \, dx, \, d \frac{1}{x}$$  \hspace{1cm} (17)

where the comma is used to indicate that the order of integration is not in general reversible. Replacing the potential integrals in (11) by the double integral* of (17), equation (11) may be rewritten

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* This method of reduction will be recognized as that which was later applied by the writer to the Lemaître-Vallarta cosmic ray equation (see page 38).
\[
\frac{d^2\Psi}{dx^2} + \left[ \frac{2}{x} - (\beta + \frac{2\xi}{Z}) - \frac{2}{Z} \int\int \psi^2 \, dx, \, d(\frac{1}{x}) \right] \psi = 0 \quad (18)
\]

This equation, although little better in appearance, can be set up on the Differential Analyzer in much simpler fashion, as shown in Fig. 15.

(See also Figs. 30 and 31 in Appendix D for details of the connections.)

Two important gains are made at once; only one operator is required instead of three, and no multiplier is used at all. Profiting from previous experience, the term containing \( \frac{2}{x} \) due to the nuclear charge is evaluated separately. For convenience in designing the connections, equation (18) is rearranged in the form

\[
\frac{d\psi}{dx} = \left[ \beta + \frac{2\xi}{Z} + \frac{2}{Z} \int\int \psi^2 \, dx, \, d(\frac{1}{x}) \right] \psi \, dx - 2 \int \psi \, dx
\]

It is interesting to observe that with two additional integrators equation (19) could be solved by an entirely mechanical interconnection. An operator is required to introduce the function \( \frac{1}{x} \), and this can be done with two integrators by setting them up to solve the auxiliary equation \( \frac{dy}{dx} = -y^2 \). This is the ultimate aim of the machine method in all cases — to reduce the human effort required to the point where only design and supervision are required, and to simplify the procedures so that even this effort is a minimum.

The connections of Fig. 15 were found to be suitable and using them the consistency of operation of the machine was much

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*These integrators would probably require special design because for values of \( x \ll 1 \), the output shaft representing \( \frac{1}{x} \) must rotate much more rapidly than the \( x \)-shaft. If the scale factors are altered to compensate for this difference, the time required for solution with present integrators is excessive. A set of change gear boxes designed for quick shifts would also be applicable in eliminating the difficulty.
\[ F = \beta + \frac{2\mathcal{C}}{\mathcal{Z}} + \frac{2}{\mathcal{Z}} \int \psi^2 dx, \, d\left( \frac{1}{x} \right) \]
improved over what it had been before. There was still the problem of eliminating the errors and particularly the positive exponential error which appeared when x became large.

In Fig. 16, the solid curve shows the form of a \( \psi \) curve, of the type studied, which satisfies the boundary conditions. Its nature, and the difficulties encountered in dealing with it, either mechanically or by numerical integration, may best be understood by considering three regions of the curve. Between the origin and a point \( x = a \) the curve is

\[ \begin{align*}
\psi \\
\end{align*} \]

\[ \begin{align*}
\alpha \\
\beta \\
\delta \\
\end{align*} \]

\[ \begin{align*}
x \\
a \\
b \\
\end{align*} \]

**Fig. 16**
essentially sinusoidal and is very stable. In this region the small errors of machine operation have a negligible influence, on the average, and consistency of operation is readily obtainable. In the region from \( x = a \) to \( x = b \), the solution changes from one which is essentially sinusoidal to one which is essentially exponential, and this region may be described as a transition region. It is characterized by the tendency of the solution to become unstable, to a degree determined by the values of "a" and "b" which are assumed as the boundaries of the region. Here the errors begin to accumulate exponentially and must be accounted for. The region from \( x = b \) to \( x = \infty \) is critical; the solutions are of exponential form, as are also the errors. If the initial settings are not quite right to produce an eigen-function, the solutions will turn off exponentially toward either \( +\infty \) or \( -\infty \) as illustrated by the dotted curves \( \infty, \beta, \gamma, \delta \) in Fig. 15. Moreover, this same thing will happen in any case if the error is allowed to accumulate from the start. It is apparent, therefore, that the inherent error must be controlled in order that the behavior of the solution itself may be discerned.

It is useful in order to visualize the workings of the method more clearly to consider what procedure would be necessary if an absolutely perfect machine were used so that no errors of operation could appear. The solution cannot be started at \( x = 0 \) because of the singularity in the potential at that point. In order to start at some small value of \( x \) an analytic solution over a small range near the origin must be known. The solution used was

\[
\psi \approx 2(1 - \frac{5}{16Z})^{3/2} \quad x \in -(1 - \frac{5}{16Z})^x
\]  

(20)
(The use of this expression for \( q \) was suggested by Dr. L. A. Young.) It was used only to obtain the ratio \( \frac{\psi'}{\psi} \) at \( x = 0.02 \). Differentiating (20) and dividing this result by (20), the ratio is

\[
\frac{\psi'}{\psi} = \frac{1}{x} - \left(1 - \frac{5}{16z}\right)
\]

(21)

and for \( x = 0.02 \),

\[
\frac{\psi'}{\psi} = 49 + \frac{5}{16z}
\]

(22)

All solutions for the same \( z \) were started at \( x = 0.02 \) with the same value of \( \frac{\psi'}{\psi} \), as given by equation (22). This satisfied the condition that \( \psi(0) = 0 \).

Working with a perfect machine, it would now be necessary to choose a value of \((\beta + \frac{2c}{z})\) and run a series of solutions with different starting slopes until one was found which did not run off to either \(+\infty\) or \(-\infty\), but followed a course similar to the one shown in Fig. 16 by the solid line. Even with a perfect machine which introduced no error, this would be impossible, because for a given value of \((\beta + \frac{2c}{z})\) the initial slope (and hence the initial function) must have a value equal to some particular number, with no tolerance allowed. For any finite range of adjustment, the number of possible settings of an index is infinite, and the probability of setting an index at one particular point out of an infinite number is zero. Hence the statement that even with a perfect machine, the desired result cannot be obtained exactly.
In spite of this difficulty, the solution satisfying the boundary condition $\psi(\infty) = 0$ can be found with sufficient accuracy. As the critical value of slope is approached, the solutions proceed to larger and larger values of $x$ before they begin to diverge. Now if two solutions are obtained, corresponding to two slightly different starting slopes, such that at some large value of $x$ (in practice $x > 8$) one diverged toward $+\infty$ and the other toward $-\infty$, the true solution would be known within very close limits since it would lie between them. As a matter of fact when the critical value of slope is known to lie between two values which lie very close together, it is found that over a large range of $x$ the corresponding solutions are almost identical, and for all practical purposes the true solution over this range can be obtained by averaging. After the trial solutions begin to diverge, however, the location of the true solution becomes doubtful.

The method of obtaining the true $\psi$ at large values of $x$ depends upon representing the two trial solutions by empirical functions for values of $x > 5$. Since most of the charge of the electron is in the region between $x = 0$ and $x = 5$, an approximate expression for $\psi$ beyond $x = 5$ is satisfactory provided it fits the observed points within a few per cent.*

From the form of the equation, it has previously been shown that the solution for large $x$ is exponential. The desired solution must contain only negative exponential terms since it must approach zero as $x$ approaches infinity. A trial solution very near the true solution must

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* A one per cent error in fit, if always in the same direction, would throw the entire solution off about $1/20$ of one per cent.
contain also either additive or subtractive positive exponential terms to account for the divergence toward $+\infty$ or $-\infty$.

From these considerations, the form of the empirical function was chosen to be*

$$\mathcal{V} = \Lambda e^{Bx} + C e^{Dx} \quad (x > 5) \quad (23)$$

Accordingly, this expression was applied to the trial solutions by using a sufficient number of observed values to determine the values of $A$, $B$, $C$, and $D$. (See Appendix C for the method employed.)

The results of these calculations were as follows:

1. In all cases one of the exponentials turned out to be negative, and the other positive.
2. For trial solutions diverging toward $+\infty$, the positive exponential was additive; for those diverging toward $-\infty$ the positive exponential was subtractive.
3. Comparison of the expression for two trial solutions going toward $+\infty$ and $-\infty$ respectively, showed that both had negative exponential terms of the same order of magnitude.

From each pair of oppositely diverging trial solutions a pair of negative exponentials would be obtained by discarding the positive exponential terms. An average of these negative exponentials provided a satisfactory end region of the solution, satisfying the condition $\mathcal{V}(\infty) = 0$. As a matter of fact, it was found that if the solution could be pushed beyond the value $x = 8$ before either $\mathcal{V}$ became zero (solution diverging to $-\infty$) or before $\mathcal{V}$ became zero (solution

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* A better form would have been $\mathcal{V} = \Lambda e^{Bx} - C e^{Dx}$, but this possibility was overlooked at the time of carrying out the calculations.
diverging to \( +\infty \) that either type of solution could be used in establishing the true solution without finding the oppositely diverging type. In the latter case, the positive exponential term was removed as described*.

Thus far a single solution satisfying the requirements at \( x = 0 \) and \( x = \infty \) has been obtained, using a perfect machine. Now the solution must be examined to see if it is normalized. It would be a rare accident to get a normalized solution on the first attempt so some provision must be made so that this condition can be controlled. It will be noted in Fig. 15, that the output of one of the integrators is \( \int_0^x \psi^2 \, dx \), and this output displaces the disc of another integrator. During the last part of the solution, this integral hardly changes, particularly if the solution is of the type which goes to \(-\infty\). Hence this integrator displacement serves during machine operation as a fairly reliable guide as to whether the solution is above or below the required normalization. (Later, during computations, the final evaluation of the normalization integral is obtained by Simpson's rule from \( x = 0 \) to \( x = 5 \), and by integrating the negative exponential squared from \( x = 5 \) to \( x = \infty \)). Having found one solution which is above or below normal, the value of \( (\beta + \frac{2c}{2}) \) is decreased or increased, and the entire procedure repeated. A little experience soon shows how much the eigenwert should be changed in order to produce another solution which is slightly on the other side of the normal solution. The object is to get two finite solutions very close together with the normal solution between them.

* It should be remembered in this treatment assuming a perfect machine, that in the actual case the positive exponential term may be partly due to error of operation. The entire term is discarded in any case.
The final step is to evaluate \( \int_0^\infty \psi^2 \, dx \) for each solution and then to interpolate between the two so that for the final curve this integral has the value unity.

d) Control and reduction of errors

Before starting any important work on the Differential Analyzer certain precautions against systematic and gross error must be taken. Unless they are subjected to severe overloads or damaged, the integrators give little trouble. Plotted functions must be carefully drawn and checked and all scale factors must be verified after the machine connections are designed. Similarly, after the machine has been connected, all connections and gearing must be checked against the drawing. Bearings must be oiled to reduce friction and all drives should be tested to make sure there are no slipping set screws. Frontlash units must be inserted in every drive in which the direction of rotation reverses; these are adjusted to compensate the backlash present before any runs are made. These routine precautions are adequate protection in most cases against errors arising within the machine. Although no such protection is available against gross human errors in using the machine, these errors usually have no serious consequences because it does not require much variation to make the solutions of different equations behave very unreasonably, and the machine frequently shows signs of distress.

The accidental errors encountered are due principally to small errors in initial displacements and to irregularities in following curves manually. These can be somewhat reduced by care and skill, but in general this is not sufficient. Irregularities of curve follow-
ing tend to average out if the operator tries diligently to keep on the curve. This is particularly true where the plotted function appears under an integral sign in the equation. By choosing large enough scale factors the errors of initial settings can usually be made negligible.

In the problem under consideration these precautions are not sufficient to prevent serious error in the solutions. As has been indicated previously, after a certain point in the solution is reached, any error then present or appearing later, begins to increase exponentially. Although there is undoubtedly some averaging out of error, it is a matter of experimental fact that no consistency of operation can be obtained over the desired range unless corrections are applied against the accumulated error. The method of correction described below is the best which has been devised thus far, both because of its effectiveness and because it adds the least complication to the main procedure.

Consider a series of solutions of equation (19) in the region from \( x = 0 \) to \( x = a \) (see Fig. 16), where each solution is started with a different slope. These partial solutions are shown in Fig. 17 drawn to a larger scale. They should show certain regularities; in particular, a plot of \( \psi \) at \( x = a \) against the starting slope should be a smooth curve. Systematic errors will not alter this result, but accidental errors will. It is assumed, therefore, that the usual precautions against systematic errors have been taken and in the remainder of this discussion the word "error" will connote the accidental type only.

The effect of error in the solutions of Fig. 17 will be observable in a plot of \( \Psi(a) \) against \( \Psi(0) \) because the plotted points
will not lie exactly on a smooth curve. In order to remove the errors, it is necessary to locate the true smooth curve with respect to the plotted points. Since, however, the shape and location of this curve is unknown, some reasonable approximation must be adopted. In general, the true curve can be represented by a power series, and if the original solutions are drawn close enough together this series can in most cases be limited to the first two or three terms. It is essential in carrying
out this method that the initial variations be of limited range so that the end results always have a linear or parabolic variation.

Now although the exact position of this curve cannot be determined, it is possible to locate it in its most probable position. This is accomplished by finding the equation of the curve (straight line or parabola) by the method of least squares. The equation thus obtained is used to calculate the corrected values of the variable - in this case the $\psi(a)$ of Fig. 17, but in general any of the variables of the problem. These corrected values of the variables are now used as starting points for the next region, at the end of which the process is repeated.

Translated into the language of machine operation, the final procedure may now be given.

1. For a given fixed value of $(\beta + \frac{2c}{Z})$, chosen to give a normalized solution as nearly as possible, compute initial settings for five runs, varying the initial slope by equal small intervals. These solutions are all to start at $x = 0.02$ and the ratio $\dot{\psi}/\psi$ is to be kept constant at its computed value.

2. Without recording any results, run the five solutions out to the point $x = 0.5$ and stop the machine. At this point read and record all integrator displacements.

3. Using the schedule method derived in Appendix A, compute by least squares, the most probable values of the integrator displacements.
4. Using the values computed in step 3, continue the solutions through the second region, stopping the machine at \( x = 2.2 \). Again read and record all integrator displacements.

5. Repeat the computations of step 3 on this last set of readings.

6. Continue the solutions using the corrected displacements just found. If the range of initial variation has been properly selected, one or more of these five solutions will diverge toward \( +\infty \) and the other toward \( -\infty \).

7. Interpolate between two adjacent but oppositely diverging solutions until a solution is obtained for which neither \( \psi \) nor \( \psi' \) reach zero before \( x = 8 \). Record this solution from \( x = 2.2 \) to \( x = 8 \).

8. Make the same interpolation at \( x = 0.02 \) and record the solution from there to \( x = 0.5 \).

9. Repeat at \( x = 0.5 \) and record to \( x = 2.2 \) (Note that the starting conditions at \( x = 0.5 \) are interpolated from the data obtained in step 5.)

10. From the result of step 7, read the magnitude of \( \int_{\phi}^{\psi} 2 \, dx \) and determine whether the solution is above or below normal. If this reading is very near unity the final value is uncertain, and the estimate may be wrong. This does not matter because the recorded solution will then be very near the desired result and extrapolation can be used, if necessary, with safety.
Repeat steps 1 - 10 with a new value of $\beta + \frac{2C}{Z}$ to correct or slightly over-correct the normalization.

Thus two sets of data are obtained, bracketing the normalized wave function, and in both sets the solutions are run out far enough that the remaining positive exponentials, due either to accumulated error or incorrect eigenvalues, can be eliminated by computation.

e) Computations

The results obtained from the machine consist, for each value of $Z$, of two sets of partial curves; both satisfy the condition $\psi(0) = 0$, neither show marked tendency to diverge until after the point $x = 8$ is reached, and the normal solution lies somewhere between them. Fig. 18 shows the form of the curves; in order to indicate how the curve is started fresh at the beginning of each region, the accumulated error has been exaggerated. The solid lines show the curves as they are obtained from the machine and the dotted line shows the position of the desired curve; regions are designated by the roman numerals. The steps taken to compute the final results from these data are the following:

1. Fit the curve in region IV to the expression
   \[ \psi = A e^{Bx} + C e^{Dx} \]
   and discard the positive exponential part of the result. The remaining negative exponential is the true curve for region IV. (See Appendix B.)

2. Use the curve found in step 1 to determine the value of $\psi(5)$, which is the end value for the curve of region III. The corrected initial value for region III is known and
is (2.2). At the point \( x = 5 \), the difference between the end value of curve III and the starting value of the corrected curve IV is the error accumulated in region III. Since the error has not been allowed to accumulate over a large distance, it is assumed that over a single region the increase of error is essentially linear, and a proportionate amount of the total error is subtracted at each point. This brings the two curves together at \( x = 5 \), but does not change the value of \( x \) at \( x = 2.2 \). In effect, the section of the curve in region III is rotated about its initial point until the difference at \( x = 5 \) is removed.
3. By similar computations make the curve of region II continuous with that of region III, and likewise finally make the curve of region I continuous with that of region II.

4. Repeat steps 1 - 3 for the other set of curves obtained for the same value of \( Z \).

5. Determine for each curve the value of the integral
\[
\int_0^\infty \psi^2 \, dx.
\]
From \( x = 0 \) to \( x = 5 \), use Simpson's rule (50 ordinates were used by the writer). From \( x = 5 \) to \( x = \infty \), integrate the exponential obtained in step 1.

6. Interpolate between the two curves using the results of step 5 so that for the final curve \( \int_0^\infty \psi^2 \, dx = 1 \).

7. From the curve obtained in step 6 find the value of the integral \( \int_0^\infty \psi^2 \frac{dx}{x} \). This is the constant \( C \) in the term \( \beta + \frac{2C}{Z} \). The value of this term is known from the initial conditions used; subtracting \( \frac{2C}{Z} \) from it gives the value of the energy parameter \( \beta \).

As a final check on the work, the values of \( \psi \) are plotted against \( Z \) for various values of \( x \). These curves are shown in Fig. 19. They are particularly valuable as a check, because the entire procedure is carried out independently for each value of \( Z \), and the smooth curves obtained indicate clearly that the procedure is effective in eliminating accidental error. The only irregularities are in the points for \( Z = 6 \); the wave function for \( Z = 6 \) can, as a matter of fact, be read off more correctly from the curves of Fig. 19 than from the original data.
Variation of Wave Functions with Atomic Number (Z).

Fig. 19.
Additional computations were made in order to fit the empirical equation $\psi = ax^b + cx^d$ to the final wave functions*. Using the method of Appendix B, the values of $a$, $b$, $c$ and $d$ were found. The constants were such that one of the terms, say $ax^b$, was larger than the other in each case, and became relatively still larger as either $x$ or $Z$ increased. When "$a"$ and "$b"$ were plotted against $Z$, fairly smooth curves were obtained, but "$c"$ and "$d"$, which determined the size of the smaller term, were irregular. In order to get a consistent set of equations, the "smoothed" values of "$a"$ and "$b"$ were taken directly from their plots as functions of $Z$. Then "$c"$ and "$d"$ were adjusted so that the final equation gave the correct initial slope and also satisfied the condition $\int_0^\infty \psi^2 dx = 1$; the values of "$c"$ and "$d"$ thus obtained were regular with respect to $Z$. The details of these calculations are omitted, but the final equations are given.

Finally, these empirical expressions for $\psi$ were used to compute values of $\beta$ to compare with the direct machine results. The method of computation is given in Appendix C, and the results are included in the next section.

f) Results

Calculations of $\psi$ were carried out for $Z = 2, 3, 4, 5, 6, 7, 8, \text{and } 32$. The collected results of these calculations are presented in Tables 2 - 9 inclusive and in Figs. 20 to 27.

* This type of equation for $\psi$ is one which is frequently used in analytic studies.
For each value of \( Z \) there are tabulated the numerical values of \( \psi \) as a function of \( x \), the empirical equation for \( \psi \), the value of \( \beta \) derived directly from the machine results, and the value of \( \beta \) computed from the empirical equation. The curve accompanying each table shows the comparison between the values of \( \psi \) given directly by the machine and the values computed from the empirical equation.

In Table 10 are grouped for comparison values of \( \beta \) as determined by various computational methods, together with the experimental values. Fig. 28 shows the variation of \( \beta \) with \( Z \) (\( Z = 2 \) to \( Z = 8 \) only).

g) Discussion of method and results

It is interesting to compare the method just described for obtaining self-consistent solutions, with that which would be required if the machine were used simply as a means of carrying out the original Hartree steps. The essential steps for the latter case are listed on page 70. Having assumed an initial potential field, it is necessary to solve a linear wave equation and obtain a finite wave function. In order to control the errors and to adjust the eigenwert, a series of solutions with varying eigenwert are required, divided into regions as in the writer's method. From one series of solutions, a single, finite, continuous wave function is obtained by the method of computation described in part (e).

Thus far both methods involve the same amount of work. In the next step of the writer's method, the same process is repeated, and from these two results, the final wave function can be computed readily.
The following equation fits the above points better than the first equation listed, but the coefficients do not form part of a smooth curve when plotted against $Z$.

\[ \psi = 1.010 \times e^{0.715x} + 0.711 \times e^{-1.499x} \]
Wave Function of Normal Helium $Z = 2$

Fig. 20.

Direct machine points

Computed from empirical equation.
Table 3

Z = 3 (Lithium⁺)

<table>
<thead>
<tr>
<th>x</th>
<th>ψ</th>
<th>x</th>
<th>ψ</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.6</td>
<td>0.6323</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1822</td>
<td>1.7</td>
<td>0.6147</td>
</tr>
<tr>
<td>0.2</td>
<td>0.2942</td>
<td>1.8</td>
<td>0.5958</td>
</tr>
<tr>
<td>0.3</td>
<td>0.4000</td>
<td>1.9</td>
<td>0.5761</td>
</tr>
<tr>
<td>0.4</td>
<td>0.4853</td>
<td>2.0</td>
<td>0.5559</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5483</td>
<td>2.2</td>
<td>0.5144</td>
</tr>
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<td>0.6</td>
<td>0.5972</td>
<td>2.4</td>
<td>0.4732</td>
</tr>
<tr>
<td>0.7</td>
<td>0.6352</td>
<td>2.6</td>
<td>0.4435</td>
</tr>
<tr>
<td>0.8</td>
<td>0.6581</td>
<td>2.8</td>
<td>0.3931</td>
</tr>
<tr>
<td>0.9</td>
<td>0.6756</td>
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<td>0.3558</td>
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<td>0.2731</td>
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<td>0.6836</td>
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<td>0.2056</td>
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<td>4.5</td>
<td>0.1532</td>
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<td>5.0</td>
<td>0.1132</td>
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<tr>
<td>1.4</td>
<td>0.6619</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.6481</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The following equation fits the above points better than the first equation listed, but the coefficients do not form part of a smooth curve when plotted against Z.

\[
\psi = 1.265x \in ^{-0.807x} + 0.550x \in ^{-1.533x}
\]

\[
\beta = 0.632 \quad \text{(machine result)}
\]

\[
\beta = 0.579 \quad \text{(computed)}
\]
Wave Function of Lithium$^+$
$Z = 3$

+ Direct machine points

○ Computed from empirical equation.

Fig. 21.
Table 4

Z = 4 (Beryllium++)

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\psi$</th>
<th>$x$</th>
<th>$\psi$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.6</td>
<td>0.6376</td>
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<tr>
<td>0.1</td>
<td>0.1657</td>
<td>1.7</td>
<td>0.6185</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3004</td>
<td>1.8</td>
<td>0.5983</td>
</tr>
<tr>
<td>0.3</td>
<td>0.4084</td>
<td>1.9</td>
<td>0.5772</td>
</tr>
<tr>
<td>0.4</td>
<td>0.4933</td>
<td>2.0</td>
<td>0.5594</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5594</td>
<td>2.2</td>
<td>0.5115</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6094</td>
<td>2.4</td>
<td>0.4874</td>
</tr>
<tr>
<td>0.7</td>
<td>0.6457</td>
<td>2.6</td>
<td>0.4243</td>
</tr>
<tr>
<td>0.8</td>
<td>0.6710</td>
<td>2.8</td>
<td>0.3851</td>
</tr>
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<td>0.9</td>
<td>0.6864</td>
<td>3.0</td>
<td>0.3445</td>
</tr>
<tr>
<td>1.0</td>
<td>0.6945</td>
<td>3.5</td>
<td>0.2594</td>
</tr>
<tr>
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<td>0.6954</td>
<td>4.0</td>
<td>0.1916</td>
</tr>
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<td>4.5</td>
<td>0.1395</td>
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<td>1.3</td>
<td>0.6823</td>
<td>5.0</td>
<td>0.1007</td>
</tr>
<tr>
<td>1.4</td>
<td>0.6701</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.6548</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\psi = 1.482 \times \varepsilon - 0.861x - 1.495x + 0.295 \times \varepsilon
\]

$\beta = 0.715$ (machine result)

$\beta = 0.688$ (computed)
Wave Function of Beryllium$^{++}$
$Z = 4$

Fig. 22.
### Table 5

\(Z = 5 \quad \text{Boron} \ + \ III\)

<table>
<thead>
<tr>
<th>x</th>
<th>(\psi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1609</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3064</td>
</tr>
<tr>
<td>0.3</td>
<td>0.4161</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5025</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5691</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6195</td>
</tr>
<tr>
<td>0.7</td>
<td>0.6559</td>
</tr>
<tr>
<td>0.8</td>
<td>0.6507</td>
</tr>
<tr>
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<td>0.6957</td>
</tr>
<tr>
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</tr>
<tr>
<td>1.1</td>
<td>0.7030</td>
</tr>
<tr>
<td>1.2</td>
<td>0.6976</td>
</tr>
<tr>
<td>1.3</td>
<td>0.6879</td>
</tr>
<tr>
<td>1.4</td>
<td>0.6745</td>
</tr>
<tr>
<td>1.5</td>
<td>0.6580</td>
</tr>
</tbody>
</table>

\(x = 1.6 \quad 1.7 \quad 1.8 \quad 1.9 \quad 2.0 \quad 2.2 \quad 2.4 \quad 2.6 \quad 2.8 \quad 3.0 \quad 3.5 \quad 4.0 \quad 4.5 \quad 5.0\)

\[
\psi = 1.586 x - 0.888 x + 0.235 x - 1.58 x
\]

\(\beta = 0.771 \quad \text{(machine result)}\)

\(\beta = 0.744 \quad \text{(computed)}\)
Wave Function of Boron$^+$ III

$Z = 5$

Direct machine points

Computed from empirical equation.
Table 6

$Z = 6$ (Carbon IV)

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\psi$</th>
<th>$x$</th>
<th>$\psi$</th>
</tr>
</thead>
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<td>0.1</td>
<td>0.1687</td>
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<td>0.6202</td>
</tr>
<tr>
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<td>0.3059</td>
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<td>0.5983</td>
</tr>
<tr>
<td>0.3</td>
<td>0.4162</td>
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<td>0.5757</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5026</td>
<td>2.0</td>
<td>0.5528</td>
</tr>
<tr>
<td>0.5</td>
<td>0.5702</td>
<td>2.1</td>
<td>0.5502</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6207</td>
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<td>0.5602</td>
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<tr>
<td>0.7</td>
<td>0.6574</td>
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<td>0.4602</td>
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<td>0.8</td>
<td>0.6827</td>
<td>2.4</td>
<td>0.4155</td>
</tr>
<tr>
<td>0.9</td>
<td>0.6990</td>
<td>2.5</td>
<td>0.4155</td>
</tr>
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<td>1.0</td>
<td>0.7044</td>
<td>3.0</td>
<td>0.3355</td>
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<td>1.1</td>
<td>0.7052</td>
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<td>0.2478</td>
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<td>1.4</td>
<td>0.6758</td>
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</tbody>
</table>

$\psi = 1.650x - 0.904x - 1.65x$

$\beta = 0.810$ (machine result)

$\beta = 0.788$ (computed)
Wave Function of Carbon\(^+\) IV

\(Z = 6\)

+ Direct machine points

- Computed from empirical equation.

Fig. 24.
Table 7

\[ Z = 7 \ (\text{Nitrogen} ) \]

<table>
<thead>
<tr>
<th>( x )</th>
<th>( \psi )</th>
<th>( x )</th>
<th>( \psi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.5</td>
<td>0.6424</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1710</td>
<td>1.6</td>
<td>0.6211</td>
</tr>
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<td>0.3101</td>
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<td>0.5997</td>
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<td>0.4213</td>
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<td>0.5756</td>
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<td>0.5531</td>
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<td>0.7045</td>
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</tr>
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</table>

\[ \psi = 1.695 x - 0.916 x + 0.172 x \]

\[ \beta = 0.832 \quad \text{(machine result)} \]

\[ \beta = 0.818 \quad \text{(computed)} \]
Wave Function of Nitrogen + V

$Z = 7$

+ Direct machine points

○ Computed from empirical equation.

Fig. 25
Table 8

\[ Z = 8 \quad \text{(Oxygen + VI)} \]

<table>
<thead>
<tr>
<th>( z )</th>
<th>( \psi )</th>
<th>( x )</th>
<th>( \psi )</th>
</tr>
</thead>
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<td>0.3</td>
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<td>1.9</td>
<td>0.5758</td>
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<td>0.5783</td>
<td>2.0</td>
<td>0.5518</td>
</tr>
<tr>
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<td>0.6295</td>
<td>2.2</td>
<td>0.5037</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6666</td>
<td>2.4</td>
<td>0.4560</td>
</tr>
<tr>
<td>0.7</td>
<td>0.6915</td>
<td>2.6</td>
<td>0.4098</td>
</tr>
<tr>
<td>0.8</td>
<td>0.7065</td>
<td>2.8</td>
<td>0.3658</td>
</tr>
<tr>
<td>0.9</td>
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<td>3.0</td>
<td>0.3253</td>
</tr>
<tr>
<td>1.0</td>
<td>0.7124</td>
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<td>0.2377</td>
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<tr>
<td>1.1</td>
<td>0.7060</td>
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<td>0.1699</td>
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<td>0.6953</td>
<td>4.5</td>
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</tr>
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<td>0.6804</td>
<td>5.0</td>
<td>0.0831</td>
</tr>
<tr>
<td>1.4</td>
<td>0.6651</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ \psi = 1.730 \, x - 0.926x + 0.155 \, x - 1.75x \]

\[ \beta = 0.850 \quad \text{(machine result)} \]

\[ \beta = 0.841 \quad \text{(computed)} \]
Wave Function of Oxygen+ VI
Z = 8

Fig. 26.

Direct machine points

Computed from empirical equation.
Table 9

$Z = 32 \ (\text{Germanium})$

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\psi$</th>
<th>$x$</th>
<th>$\psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.6</td>
<td>0.6442</td>
</tr>
<tr>
<td>0.1</td>
<td>0.1789</td>
<td>1.7</td>
<td>0.6202</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3243</td>
<td>1.8</td>
<td>0.5950</td>
</tr>
<tr>
<td>0.3</td>
<td>0.4397</td>
<td>1.9</td>
<td>0.5694</td>
</tr>
<tr>
<td>0.4</td>
<td>0.5304</td>
<td>2.0</td>
<td>0.5455</td>
</tr>
<tr>
<td>0.5</td>
<td>0.6002</td>
<td>2.2</td>
<td>0.4919</td>
</tr>
<tr>
<td>0.6</td>
<td>0.6519</td>
<td>2.4</td>
<td>0.4415</td>
</tr>
<tr>
<td>0.7</td>
<td>0.6882</td>
<td>2.6</td>
<td>0.3933</td>
</tr>
<tr>
<td>0.8</td>
<td>0.7118</td>
<td>2.8</td>
<td>0.3482</td>
</tr>
<tr>
<td>0.9</td>
<td>0.7253</td>
<td>3.0</td>
<td>0.3066</td>
</tr>
<tr>
<td>1.0</td>
<td>0.7294</td>
<td>3.5</td>
<td>0.2192</td>
</tr>
<tr>
<td>1.1</td>
<td>0.7286</td>
<td>4.0</td>
<td>0.1536</td>
</tr>
<tr>
<td>1.2</td>
<td>0.7178</td>
<td>4.5</td>
<td>0.1059</td>
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<td>1.3</td>
<td>0.7059</td>
<td>5.0</td>
<td>0.0725</td>
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<td>1.4</td>
<td>0.6869</td>
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<td></td>
</tr>
<tr>
<td>1.5</td>
<td>0.6666</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\psi = 1.926 \times e^{-0.980x} + 0.045 \times e^{-1.89x}$

$\beta = 0.965 \quad \text{(machine result)}$

$\beta = 0.961 \quad \text{(computed)}$
Wave Function of Germanium

$Z = 32$

Direct machine points

Computed from empirical equation.

Fig. 27
### Table 10

<table>
<thead>
<tr>
<th>Z</th>
<th>$\beta$ (direct machine value)</th>
<th>$\beta$ (computed from wave function)</th>
<th>$\beta$ See note</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.465</td>
<td>0.408</td>
<td>0.4517</td>
</tr>
<tr>
<td>3</td>
<td>0.632</td>
<td>0.579</td>
<td>0.6178</td>
</tr>
<tr>
<td>4</td>
<td>0.715</td>
<td>0.688</td>
<td>0.7087</td>
</tr>
<tr>
<td>5</td>
<td>0.771</td>
<td>0.744</td>
<td>0.7825 ± 0.0006</td>
</tr>
<tr>
<td>6</td>
<td>0.810</td>
<td>0.788</td>
<td>0.7999 ± 0.0008</td>
</tr>
<tr>
<td>7</td>
<td>0.832</td>
<td>0.818</td>
<td>—</td>
</tr>
<tr>
<td>8</td>
<td>0.850</td>
<td>0.841</td>
<td>—</td>
</tr>
<tr>
<td>*</td>
<td>*</td>
<td>*</td>
<td>*</td>
</tr>
<tr>
<td>32</td>
<td>0.965</td>
<td>0.961</td>
<td>—</td>
</tr>
</tbody>
</table>


$\beta \sim \text{Ionization potential (in electron volts)}$  
$\frac{13.54}{Z^2}$
Variation of Eigenwerte ($\beta$) with Atomic Number ($Z$)

- Direct machine values
- Computed from empirical wave functions
- Experimental ionization potentials.

Fig. 28.
To continue with the Hartree procedure, the wave function just obtained is normalized, and from it a new potential field is computed by means of the machine connections of Fig. 11. If this potential curve is the same as that originally assumed, the calculations are complete. If not, they must be repeated, as many times as are necessary to obtain correspondence.

In view of the fact that in the writer's method, the extra step of computing potentials is eliminated, it is apparent that more operations are required using the Hartree steps if the cycle need only be gone through twice. Actually, the possibility of assuming an initial field so nearly correct is rather remote, and in general the machine operations for the Hartree method will require more time than is needed for the method described.

From inspection of the wave function curves of Figs. 20 to 27, it is apparent that the points calculated from the empirical equations derived check the machine points very closely except for $Z = 2$ and $Z = 3$. These discrepancies appeared after the numerical coefficients of all the equations were adjusted as described in the preceding section. As $Z$ decreases, the relative contributions of the two exponential terms in the equation for $\psi$ become more nearly of the same magnitude. The method of adjusting the coefficients, however, depends for accuracy on having one term considerably larger than the other. If the curve of each coefficient against $Z$ could be extended below $Z = 2$, the results would be improved because the position of the curve could then be determined more accurately at $Z = 2$ and $Z = 3$. To do this, it would be necessary to obtain the data by solving
the wave equation for, say, \( Z = 1.5 \) - a strange atomic configuration, but merely another gear ratio on the Differential Analyzer.

In both Tables 2 and 3, it will be noted that another empirical equation for the wave function is given; these equations are normalized and fit their respective machine curves, but the coefficients do not lie on smooth curves when plotted with those of the higher atomic numbers.

Fig. 28, which gives the variation of the eigenwert \( \beta \) with respect to the atomic number \( Z \) shows clearly that consistent results are obtainable by the method used. The values of \( \beta \) obtained directly from the machine check approximate values computed from experimental results to within about three per cent at \( Z = 2 \) and within nearly one per cent at \( Z = 6 \). (No experimental data are available for higher values of \( Z \).) These discrepancies between \( \beta \) as obtained directly from the machine and as computed from known ionization potentials are not indications of error. It so happens that the two results are almost equal numerically, but the true ionization potential should be computed from the energy parameter \( \beta \) as follows:

The total energy of electron 1 with respect to the nucleus and electron 2 is equal to \( \beta Z^2 \). Likewise the total energy of electron 2 with respect to the nucleus and electron 1 is given by the same value \( \beta Z^2 \). If these are added, the total energy of the atom thus obtained is too large because the mutual energy of the two electrons has been taken into account twice. It is necessary, therefore, to subtract a term equal to this mutual energy*.

* This is obtained as an integral over all space of the form

\[ \int \psi^2 v(x) \, dx \]

where \( v(x) \) is that given by equation (3) of this chapter. It can be computed from the data presented in Tables 2 - 9.
atom which is left after one electron is removed by ionization is
given by $Z^2$. The difference between the total energy of the original
helium-like atom and that of the final hydrogen-like atom is the re-
quired ionization potential (in atomic units). This is given by the
expression

$$W = 2 \beta Z^2 - Z^2 - (\text{mutual energy of the two}
\text{electrons}).$$

This computation is not carried out here because it is not strictly
part of the machine problem of this thesis. All the data required for
the computation are in the tabulated results.

The overall accuracy of machine operation on this problem is
difficult to estimate. In applying the least-square correction to
eliminate the error accumulated in a single region, the maximum correc-
tion of wave function required was about 0.6 per cent while the aver-
age was less than 0.2 per cent. These figures indicate the extent to
which the machine results can be repeated in the presence of cumulative
error. With allowance for systematic error, the wave functions are
probably accurate to within 0.3 per cent from $x = 0$ to $x = 5$. Beyond
this point, the results are less certain. But it should be remembered
that only about 5 per cent of the total charge of the electron is
located in the region beyond $x = 5$ and hence a 10 per cent error in
ordinates although large on an absolute basis is small in its effect
on the overall distribution.
a) **Range of application of the present machine**

From the computational methods described and proposed in the preceding chapters, it is clearly evident that the range of application of the present Differential Analyzer cannot be defined in terms of the specific types of ordinary differential equations which it will solve. The machine is a structure consisting of a limited number of basic units, usable in whatever sequences and combinations are required. Any statement of its scope must take this important characteristic into account.

Among the various mechanisms contained in the Analyzer, the integrator is, of course, the most important single unit. At least one integrator is needed to solve any differential equation, and the limited number of these units is the principal limitation of the present machine. It is in terms of integrators that the range of application of the machine must at present be defined.

Now the integrator is a rather versatile mechanism, in a mathematical sense, especially in combination with others of its kind, and it is therefore necessary to distinguish in some way between the operations it performs. It is suggested that two types of integrators be defined, an *essential integrator* and a *functional integrator*. Essential integrators are those which are used only to lower the order of derivatives; this includes carrying out integrations explicitly indicated in differential equations, because such equations can be written without explicit integrals, but in terms of higher order
derivatives. The functional integrator, used either singly or in combination with others, performs principally those auxiliary integrating processes which are not inherent to the problem in hand, but which are deliberately introduced to gain advantages resulting from automatic operation.

From the definitions given it can be seen that for any problem the number of essential integrators required is equal to the order of the equation. This follows from the fact that an $n^{th}$ order derivative must be put through $n$ integrations in order to obtain the dependent variable as a function of the independent variable, and further, that the order of a differential equation is by definition equal to that of the highest order derivative appearing in it. Since the dependent variable must be produced explicitly, it follows that the minimum number of integrators required is equal to the order of the equation. Hence the upper limit of the range of application of the present Differential Analyzer is the solution of sixth order differential equations.

For any particular equation which is to be placed on the present machine, the number of integrating units available as functional integrators is equal to six minus the order of the equation. It would be an undue restriction to set up rules in general for the use of these available functional integrators. As a matter of experience, however, it has been found that for certain processes, integrators should be used rather than input tables or multipliers, and in considering the disposition of available functional integrators, they should be assigned first to such processes. As an example,
consider the differential equation
\[
\frac{d^2y}{dx^2} = xy.
\]
This is a second order equation, and at least two integrators are required to solve it. There are three basic ways in which it can be put on the machine, as illustrated in Fig. 29. The first method, Fig. 29(a), uses the minimum number of integrators, because a multiplier produces the term \(xy\). In this connection, both integrators are clearly of the essential type. The direct replacement of the multiplier by two functional integrators is shown in Fig. 29(b). This connection is better than that of Fig. 29(a) because manual control is eliminated. A still better connection is shown in Fig. 29(c); it follows from the equation rewritten in the form
\[
\frac{dy}{dx} = \int x\, y\, dx.
\]
This method of evaluating products under the integral sign is an important basic procedure*. In most problems where such integrals occur, available functional integrators should be assigned first to the evaluation of these integrals.

An interesting question arises from consideration of Fig. 29(c) - two of the three integrators are essential integrators, but which two? Integrator III is clearly of the essential type, but it is not at all clear which of the others meets the definition. According to the definition suggested, an essential integrator is one which is used only

* Note: In Fig. 29(c) the term \(\int xy\, dx\) can also be obtained by first getting \(\int x\, dx\) and then \(\int xy\, dx\) instead of the method shown. This is simply a variation of the same basic method.
to lower the order of a derivative. Neither integrator I nor integrator II do this explicitly, but integrator II produces the $\frac{dy}{dx}$ term finally, and by liberal interpretation may be designated as an essential integrator. Still further trouble is encountered, however, in certain cases which arise where a derivative is ultimately produced as a sum of other terms. If the derivative thus produced is of the same order as the equation, then it will be reduced by a series of essential integrators. But it frequently happens that it is more convenient to produce a lower order derivative as a sum of other terms, and in such cases it is impossible to distinguish all of the essential integrators. The point to be made is that although theoretically a problem can be set up on the Analyzer so that the essential integrators can be clearly designated, the principal object of classification of this sort is to aid in defining minimum requirements and maximum range.

Without going further into the details of how to design machine connections, the following list shows in order of importance and utility the uses to which available functional integrators should be put.

1. Evaluation of products under the integral sign.
2. Production of simple functions such as squares and exponentials where one integrator replaces one manual operator.
3. Multiplication by use of the rule $uv = \int u \, dv + \int v \, du$
4. Production of general functions. In choosing which functions to produce by integrators, the first object should be to replace a manual operation by as few integrators as possible. If the choice on this basis is immaterial, then design for optimum mechanical performance. For example,
if two integrators are available to produce either a sine function or a reciprocal, use them to produce the sine.

5. Integrators may be used instead of change gears for fine control of adjustable parameters.

The order given above need not, of course, be followed rigorously if any advantage is obtainable by departing from it. In certain cases, for example, the order of items 3 and 4 might well be reversed to advantage; this depends on the requirements of the specific problem.

As illustrated by the very simple example of Fig. 29, there is great flexibility in the use of integrators for functional purposes. The maximum range of the machine from the standpoint of essential integrating processes has been stated, but it is doubtful whether a categorical statement of the allowable complexity of an equation can be given.

b) Desirable additions to present equipment

As was mentioned in the preceding section, the principal limitation on the use of the present Differential Analyzer is in the restricted number of integrators available. When this machine was first built, six integrators were considered adequate to handle practically all the demands which would be made on the machine for some time to come. Within two months of the time the machine was put into service, problems arose in which additional integrators could have been used to advantage.

Besides the specific uses of functional integrators which have been mentioned, certain general advantages accrue from having a
more adequate supply of these units. The introduction of functional
relations automatically is not only more convenient, but also greater
speed and improved accuracy are thereby obtainable. A machine contain-
ing sufficient integrators can, if desired, be divided and used for two
problems simultaneously, and still be available as a whole. Furthermore,
the necessity for repair of the units is obvious, and with present operat-
ing schedules it is very difficult to maintain the units properly; even
a single spare integrator would take care of this situation nicely.

The number of additional integrating units which can be in-
stalled to advantage on the present machine is to some extent controlled
by the physical difficulties of getting them in without rebuilding too
much of the machine. By adding one more bay of special design at the
end of the machine now occupied by the recording counter, four addi-
tional integrators can be installed. In addition, the output table can
be shifted to one of the input table positions and the space it now uses
can hold two more integrators. The output table would, of course, be
modified so that it would serve as either an input or an output table
in its new location. The six integrators which could thus be added
would double the present capacity of the machine in this respect and
would greatly increase its utility, speed and accuracy.

At the present time, an investigation is going forward on
methods of following plotted curves automatically*. The results ob-
tained at the present writing are encouraging, and it appears that it
will be feasible in the near future to introduce this refinement on
the machine. There are several reasons why this is a desirable step.

* This investigation is being carried on by Mr. H. A. Traver as an
S.M. thesis.
In the first place, no matter how many integrators within reason there are available, it is almost certain that problems will arise for which the number of integrators is inadequate, and input plots will have to be used. For some types of experimental curves, the integrator connections required to produce them are entirely too complicated. There are also certain analytic functions which are more satisfactorily introduced from plots than from integrators. In all these cases, it is usually advantageous to be able to follow the plots automatically, because of the higher speed and improved accuracy which are available. The hand control must be retained, of course, for use with certain types of plots where automatic following is not feasible (e.g. vacuum tube characteristics).

c) Significance of the Differential Analyzer method

The Differential Analyzer method must be regarded in the last analysis as simply another method of computing certain results. It is unique, however, in that it combines the power of numerical integration to handle analytically unmanageable terms and combinations, with the exactness of analytic solution, which is unattainable numerically except at the expense of unreasonable labor. Although it is in itself a powerful method, it must be supplemented by skill and thorough understanding on the parts of the men who use it. The human brain must plan the attack in every problem, using such mathematical devices as are necessary and available to produce a workable procedure. In the preceding chapters a number of examples have been given which show both the general application of the method and the extent to which the basic method
can be modified in order to overcome limitations of equipment.

There is more to the Differential Analyzer than merely setting up a machine and operating it so as to obtain solutions of a differential equation. No achievement can be claimed for using muscles instead of nerve tissue to solve mathematical problems. The true aim of the method is to let the machine do all the work and to reduce even supervision to a minimum. This has a direct bearing on the one serious limitation of the method. It has been pointed out that the machine can only produce individual solutions of a given equation. In many cases it is possible by applying methods of generalization to make one of these single solutions mean more than the answer to a single part of the problem. Even then, a great many solutions are required in order to complete an adequate study of the equation over the range of variables which is of interest. Anything which speeds up the process of obtaining a solution is a step toward the removal of the limitation expressed above. Much can be accomplished in this respect by the complete mechanization of all operations, and there is every hope that this objective will be realized in the not-too-distant future (see footnote page 96).

In addition to its primary role as a computing method, there is some indication that the machine method may be of aid to analysis. As an example, the consolidation of the Hartree steps made by the writer was effected because of previous knowledge of the possibilities of the machine method. The question was not how to solve a given problem on the machine, but how to express certain physical and mathematical conditions so that the given machine could be used more effectively. In
other problems, certain generalizations have been suggested by peculiarities in the behavior of the machine. Further developments of this type will undoubtedly appear as the work on the machine proceeds.

d) Utility and significance of the work in atomic physics

It has been demonstrated that the machine method is directly applicable to problems of atomic structure in the stationary state. The method finally developed is straightforward and with care and systematic operation will produce the desired results in a reasonable length of time. Working with one assistant, the writer was finally able to carry out in less than twelve hours all machine operations and associated least-square computations necessary to solve for a single wave function (one atom). This time was possible, of course, only after the machine had been set up and after the necessary procedures had been established. If a series of wave functions is to be obtained (which is usually the case) it can be maintained as a steady pace. A unique feature of the procedure is the method used to control the cumulative error due to accidental inaccuracies of operation.

Eight wave functions are presented both numerically and with corresponding empirical formulas. These results have already been applied in further work and are applicable to other studies in atomic physics. As brought out in Chapter IV, the energy values given are first approximations to the ionization potentials. Further integrations are necessary in order to compute the corrections applicable to these values.
The theory of atomic structure, as expressed in quantum mechanics, has undergone revolutionary change and phenomenal development in very recent years. It has attained a unity of construction which permits direct application of basic principles in the writing of the wave equations for given states, and in the interpretation of the solutions of these equations in physical and chemical terms. But the gap between the wave equation and its solutions is still large, even in relatively simple cases. The success which has thus far attended the effort to close this gap by means of the Differential Analyzer is encouraging; this machine and its projected improvements offer to atomic physics unique procedures for further advance, by removing computation barriers which now stand in the way.
Appendix A

Derivation of Schedule Used in Applying the Method of Least Squares for the Control of Accidental Error.

Given a series of observed points \((x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\), through which the most probable straight line or parabola is to be drawn. The coefficients of the equation of either curve are to be determined by the method of least squares. By working with five values of \(y\) with respect to equidistant values of the argument designated as \(x\), the necessary computations are organized into a simple schedule, which can be carried out rapidly on a computing machine. The argument \(x\) in the calculations of Chapter IV was the initial slope \(\frac{d\psi}{dx}\).

Since \(x\) is varied in equidistant steps, it can be given arbitrary equidistant values; the values 0, 1, 2, 3, 4 are most convenient for the present purposes.

Straight Line

The equation to which the data are to be fitted is

\[
y = a + bx
\]  

(1)

By the method of least squares, the criterion of fit is that the sum of the squares of the deviations of the data from the curve be a minimum. Therefore, the data must satisfy the equations

\[
\frac{d}{da}\sum (y - a - bx)^2 = 0
\]  

(2)

\[
\frac{d}{db}\sum (y - a - bx)^2 = 0
\]  

(3)
Carrying out the operations indicated

\[ \sum 2(y - a - bx)(-1) = 0 \]  \hspace{1cm} (4)

\[ \sum 2(y - a - bx)(-x) = 0 \]  \hspace{1cm} (5)

\[ \sum y = \sum a + \sum bx = na + b \sum x \]  \hspace{1cm} (6)

\[ \sum xy = \sum ax + \sum bx^2 = a \sum x + b \sum x^2 \]  \hspace{1cm} (7)

where \( n \) represents the number of observed points. By substituting the observed data in equations (6) and (7), two simultaneous equations are obtained from which the coefficients \( a \) and \( b \) are calculated.

As stated above, five points are used, corresponding to the values of \( x = 0, 1, 2, 3, 4 \). Hence, \( n = 5, \sum x = 10, \sum x^2 = 30 \).

Substituting in (6) and (7),

\[ \sum y = 5a + 10b \]  \hspace{1cm} (8)

\[ \sum xy = 10a + 30b \]  \hspace{1cm} (9)

\[ a = \frac{3 \sum y - \sum xy}{5} \]  \hspace{1cm} (10)

\[ b = \frac{\sum xy - 2 \sum y}{10} \]  \hspace{1cm} (11)

Let

\[ \sum y = y_1 + y_2 + y_3 + y_4 + y_5 \]  \hspace{1cm} (12)

\[ \sum xy = 0 + y_2 + 2y_3 + 3y_4 + 4y_5 \]  \hspace{1cm} (13)
Substituting (12) and (13) in (10) and (11),

\[
a = \frac{3y_1 + 2y_2 + y_3 - y_5}{5}
\]

(14)

\[
b = \frac{-3y_1 - y_2 + y_4 + 2y_5}{10}
\]

(15)

The substitution of the observed \(y\)'s in (14) and (15) is rapidly accomplished on a computing machine by the use of the schedule below

| \(y_1\) x 3 | \(y_5\) x 2 |
| \(y_2\) x 2 | \(y_4\) x 1 |
| \(y_3\) x 1 | \(y_2\) x-1 |
| \(y_5\) x-1 | \(y_1\) x-2 |

Sum = 5) \(a=\) 

Sum = 10) \(b=\)

Parabola

The equation to be fitted to the five points is

\[y = a + bx + cx^2.\]

(16)

By least squares this requires that

\[
\frac{\partial}{\partial a} \sum (y - a - bx - cx^2)^2 = 0
\]

(17)

\[
\frac{\partial}{\partial b} \sum (y - a - bx - cx^2)^2 = 0
\]

(18)

\[
\frac{\partial}{\partial c} \sum (y - a - bx - cx^2)^2 = 0
\]

(19)
Reducing these equations by steps similar to those taken for the straight line,

\[ \sum y = na + b \sum x + c \sum x^2 \]  
\[ \sum xy = a \sum x + b \sum x^2 + c \sum x^3 \]  
\[ \sum x^2y = a \sum x^2 + b \sum x^3 + c \sum x^4 \]

(20) \hspace{2cm} (21) \hspace{2cm} (22)

\[ \sum y = 5a + 10b + 30c \]  
\[ \sum xy = 10a + 30b + 100c \]  
\[ \sum x^2y = 30a + 100b + 354c \]

(23) \hspace{2cm} (24) \hspace{2cm} (25)

The explicit equations for a and b are rather inconvenient for rapid, schedule computation. It is convenient, however, to evaluate the coefficient c, which turns out to be

\[ c = \frac{2y_1 - y_2 - 2y_3 - y_4 + 2y_5}{14} \]

(26)

This calculation is made on a computing machine, using the schedule:

\[ y_1 \times 2 = \]
\[ y_2 \times 1 = \]
\[ y_3 \times 2 = \]
\[ y_4 \times 1 = \]
\[ y_5 \times 2 = \]
\[ \text{Sum} = \]
\[ \frac{14}{c} = \]
Knowing c, the value of $cx^2$ at each point can be determined, and when subtracted from the original parabolic data, the result is a series of points which can be represented by a straight line. Thus

\[ y_1' = y_1 \]
\[ y_2' = y_2 - c \]
\[ y_3' = y_3 - 4c \]
\[ y_4' = y_4 - 9c \]
\[ y_5' = y_5 - 16c \]

The equation of the straight line through the $y'$ data is obtained using the schedule on page 35.
Method of Fitting Empirical Wave Functions to the Machine Data

The equation to which the data is fitted is

\[ \psi = ax^b e^{bx} + cx^e dx \]  

This is conveniently handled in the form

\[ y = \frac{\psi}{x} = a e^{bx} + c e^{dx} \]  

The constants of equation (2) are found by the following method*.

Consider three successive y-values, \( y_1, y_2, y_3 \), corresponding to the equidistant x-values \( x_1, x_1 + h, x_1 + 2h \). For these the equations are written

\[ y_1 = a e^{bx_1} + c e^{dx_1} \]  

\[ y_2 = a e^{b(x_1+h)} + c e^{d(x_1+h)} = a e^{bx_1} b h + c e^{dx_1} d h \]  

\[ y_3 = a e^{b(x_1+2h)} + c e^{d(x_1+2h)} = a e^{bx_1} 2 b h + c e^{dx_1} 2 d h \]  

Multiplying equation (3) by \( e^{(b+d)h} \) and equation (4) by \( -e^{bh} - e^{dh} \), and adding these products to equation (5),

\[ y_3 - (e^{bh} + e^{dh})y_2 + e^{(b+d)h} y_1 = 0 \]  

---

* Lipka, "Graphical and Mechanical Computation", p. 156.
or \( \frac{y_3}{y_1} = (\varepsilon^{bh} + \varepsilon^{dh}) \frac{y_2}{y_1} = \varepsilon^{(b+d)h} \) \( (7) \)

Substituting \( A = (\varepsilon^{bh} + \varepsilon^{dh}) \), and \( B = \varepsilon^{(b+d)h} \), the equation for any set of successive values of \( y \) is written

\[
\frac{y_{n+2}}{y_n} = A \frac{y_{n+1}}{y_n} - B
\]

This is the equation of a straight line in \( \frac{y_{n+2}}{y_n} \) and \( \frac{y_{n+1}}{y_n} \), and from it the exponential coefficients \( b \) and \( d \) are determined.

Knowing \( b \) and \( d \), the original equation \( (2) \) is rewritten

\[
y \varepsilon^{-dx} = a \varepsilon^{(b-d)x} + c
\]

This equation is linear in \( y \varepsilon^{-dx} \) and \( \varepsilon^{(b-d)x} \), and from it the coefficients \( a \) and \( c \) are determined.

Although the coefficients of the original equation could be determined directly by least squares, the process is very complicated and requires entirely too much time. The same results are achieved by using the method described above, and fitting straight lines to equations \( (8) \) and \( (9) \) by the method of least squares. This method was used in the present work and was found to be very satisfactory.
APPENDIX C

Calculation of Energy Parameter from the Equation of the Wave Function

The wave equation which was solved is

\[
\frac{d^2\psi}{dx^2} = \left( \beta + \frac{2C}{x} - \frac{2}{x} + \frac{2}{x^2} \int \psi^2 \, dx - \frac{2}{x} \int \psi^2 \, \frac{dx}{x} \right) \psi \tag{1}
\]

where \( C = \int \psi^2 \, \frac{dx}{x} \). If the terms of equation (1) are rearranged so as to solve for \( C \), and the expression

\[
\psi = ax \epsilon + bx \epsilon
\]

is substituted, it can be shown that \( \beta \) varies from an infinite value at \( x = 0 \) to a zero value at \( x = \infty \). The desired value of \( \beta \) is the most probable value, and this found by using the wave function as a weighting function and integrating over all space. Accordingly, the expression to be evaluated is

\[
\int_{-\infty}^{\infty} \psi^2 \beta \, dx.
\]

The reduction of this integral in terms of the coefficients of the wave function (2) is rather involved, and will be omitted since it consists merely of algebraic substitution and integration. The final expression for \( \beta \) as thus calculated, is given below.
\[
\beta = \left( \frac{a^2}{4b} + \frac{4abcd}{(b+d)^3} + \frac{c^2}{4d} \right) + \left( 1 - \frac{1}{Z} \right) \left( \frac{a^2}{2b^2} + \frac{4ac}{(b+d)^2} + \frac{c^2}{2d^2} \right)
\]

\[- \frac{3}{64Z} \left( \frac{a^4}{b^3} + \frac{4c^4}{d^5} \right) - \frac{a^2c^2}{Z} \left( \frac{1 + b}{2b^3} + \frac{5}{(b+d)^5} + \frac{1 + d}{2d^5} \right)\]

\[- \frac{8ac}{Z(b+d)^2} \left[ \frac{a^2(1 + 3b + d)}{(3b + d)^3} + \frac{c^2(1 + b + 3d)}{(b + 3d)^3} \right] \]

\[- \frac{ac}{Z} \left[ \frac{a^2}{(3b+d)^3} \cdot \frac{5b + d}{b^3} + \frac{c^2}{(b+3d)^3} \cdot \frac{b + 5d}{4d^3} \right] \]

This expression is not particularly simple to use numerically, but the calculated value of \( \beta \) thus obtained is useful as a check against gross error in the wave function.
APPENDIX D

Calculation of Scale Factors

For the problem of the self-consistent field using the equation

\[
\frac{d\Psi}{dx} = \left[ \beta + \frac{eC}{Z} + \frac{2}{Z} \int (\psi^2 dx, \int \psi dx, \int \frac{1}{x} \psi dx, \int \frac{2}{x} \psi dx \right]
\]

the machine connections with gear ratios indicated are shown in Fig. 30.

It will be observed that unknown gear ratios are indicated at all points where the driven shaft is connected directly to a shaft of limited displacement. Furthermore, gear ratios are inserted in drives to differential gears (adders) in order to permit equalization of scale factors at these points.

In assigning the scale factors to the various shafts, it is customary to start with the shaft representing the independent variable. This shaft is labelled \( Ax \) in this case, meaning that the shaft rotates \( A \) turns for every unit of \( x \), and its displacement at any instant is hence the product \( Ax \). Since this shaft drives the abscissa lead screw of the input table, which has a maximum allowable displacement of 480 turns, it is stepped down by the gear ratio \( n_1 \). The ordinate scale of the plot is unknown, hence the scale factor \( B \) is assigned to the \( \frac{1}{x} \) shaft; the maximum allowable displacement of the ordinate lead screw is 360 turns. For the \( \psi \)-shaft, another unknown scale factor \( C \) is assigned as shown. All remaining scale factors can be computed from those now assigned, making use of the fact that the scale factor of the
\[
\begin{align*}
\frac{1}{32} n_3 n_4 n_5 n_6 A^2 BC & = \frac{1}{4} \cdot \frac{1}{32} n_3 n_5 n_7 A^2 BC \\
C & = \frac{1}{2} \cdot \frac{1}{32} n_3 n_5 n_7 A^2 BC
\end{align*}
\]
output of an integrator is $1/32$ times the product of the scale factors of the displacing and disc-rotating drive shafts.

At the bottom of Fig. 30, two "closing equations" are given. The first of these is obtained by equating the scale factors of the shafts driving the adder. The second is obtained by equating the scale factor of the last integrator output to $1/32$ times the product of the scale factors of the $x$ and $\frac{dy}{dx}$ shafts which feed this integrator. This is necessary as a closing step because "C" was originally chosen arbitrarily. In the calculation of numerical scale factors, these two equations must be satisfied.

**Numerical computations**

The lead screws of the input tables and the displacements of integrators can have only limited displacements, as follows.

**Input table:**
- Abscissae - 480 turns (machine driven)
- Ordinates - 360 turns (hand cranked)

**Integrator:**
- Maximum displacement 40 turns,
  preferably not much over 38 turns.

Maximum values of equation variables appearing on these shafts:

- $x_m = 10 \quad (x = 0.02 \text{ minimum})$
- $\frac{1}{x_m} = 50$
- $\psi_m = 0.8$
- $\int \psi^2 \, dx_{\text{max}} = 1$
- $f_m = 1.35$
- $\frac{dy}{dx}_{m} = 2$
The closing equations reduce to

\[
\frac{2}{32^2} \frac{n_3^2 n_4 n_5 n_6 A C^2}{n_2 n_7} = 1
\]

\[
\frac{1}{2} \cdot \frac{1}{32^2} n_2 n_3 n_7 A^2 B = 1
\]

and because of limited displacements, the following inequalities must hold:

\[
n_1 A \times 10 \ll 480
\]

\[
50 B \ll 360
\]

\[
50 n_2 B < 40
\]

\[
\frac{1}{32^2} n_3^2 n_4 A C^2 < 40
\]

\[
n_3 C \times 0.8 < 40
\]

\[
\frac{1}{32^2} n_3^2 n_4 n_5 A B C^2 \times 1.35 \ll 40
\]

\[
\frac{1}{32^2} n_2 n_3 n_7 A B C < 40
\]

Previous trials showed that in order to obtain the desired accuracy, the time of a single run should be about 16 minutes. At 480 r.p.m. (nominal speed), the x-shaft should make a total of 16 x 480 revolutions.

Since x has the maximum value of 10 in this time.

\[
A \times 10 = 16 \times 480
\]

\[
A = 768
\]
Using the entire range on the abscissa scale,

\[ n_1 \times 768 \times 10 = 480 \]

\[ n_1 = \frac{1}{16} \]

50 \( B \) < 360; \( n_2 \) 50 \( B \) < 40

\[ n_2 = \frac{1}{6} \]

\[ n_3 \times C < 50; \quad n_3 \times C^2 < 2500 \]

\[ n_3^2 \times C^2 \cdot \frac{n_4 \times n_5 \times n_6}{n_7} = \frac{32^3}{2} \times \frac{1}{9} \times \frac{1}{768} = \frac{64}{27} \]

Let

\[ n_3^2 \times C^2 = \frac{1024 \times 64}{27}; \quad n_3 \times C = \frac{256}{323} \]

\[ \frac{n_4 \times n_5 \times n_6}{n_7} = \frac{1}{1024} \]

Note: Gears available are 1:1, 2:1, 2:3, and 4:1.

\[ n_7 \times B < \frac{40 \times 32^2 \times 9 \times 3/3}{256 \times 768} \approx 9.8 \]

\[ B < 7.2 \quad n_7 < 1 \]

\[ n_7 = 1 \]

\[ n_3 \times B = \frac{2 \times 32^3 \times 9}{768^2} = 1 \]

\[ n_3 = \frac{1}{6} \]

\[ n_4 \times n_5 \times n_6 = \frac{1}{1024} \]

\[ C = \frac{512}{\sqrt{3}} \]

\[ n_4 \times \frac{40 \times 32^2 \times 27}{1024 \times 64 \times 768} \]

\[ n_4 = \frac{1}{48} \]
\[ n_5 \cdot n_6 = \frac{3}{64} \]

\[ n_5 < \frac{40 \cdot 3^2 \cdot 27 \cdot 48}{1.35 \cdot 1024 \cdot 64 \cdot 768} \quad \frac{n_5 = 1}{n_6 = \frac{3}{64}} \]

**Summary**

\[ A = 768 \quad n_1 = \frac{1}{16} \quad n_4 = \frac{1}{48} \]

\[ B = 6 \quad n_2 = \frac{1}{9} \quad n_5 = 1 \]

\[ C = \frac{512}{\sqrt{3}} \quad n_3 = \frac{1}{6} \quad n_6 = \frac{3}{64} \]

\[ n_7 = 1 \]

Using these scale factors, the physical set-up of the machine is designed as shown in Fig. 31. On this sheet, the complete set of shaft constants is also recorded. The necessary gear changes are indicated also; these must be such that the closing equations are still satisfied and no displacements are too large.
APPENDIX E

Symbols

It is convenient to have standard symbols to represent the machine units. These symbols have been employed throughout this thesis in illustrating methods of dealing with various problems on the machine. In Fig. 32, the symbols of the most common units are shown.

Of the symbols shown, those of the integrator, multiplier-divider, input table, and adder appear most frequently; the others are used only in the physical connection diagram of Fig. 31.
Input Table
\( P = f(Q) \)

Multiplier - Divider
\( s = krt \)

Spiral Gear Boxes
(right hand)  (left hand)

Adder
\( c = a + b \)

Spur Gear Set
(ratio shown by figures)

Frontlash Unit

Fig. 32.
BIBLIOGRAPHY


BIOGRAPHICAL SKETCH

The writer completed his secondary school work at the Frankford High School, Philadelphia, Pa., in February, 1921, and entered the Massachusetts Institute of Technology, in October, 1921. He registered in Course VI-A at the Institute and took his co-operative work with the General Electric Co. principally at the Lynn, Mass. plant, starting in March 1923. Assignments at the General Electric Co. included tests on constant-current transformers, small motors and generators, and rectifiers at Lynn, and large induction motors at Schenectady. His thesis research for the Master's degree was carried out in the Tungar laboratory at Lynn on "Characteristics and Theory of Operation of a Dry Electrolytic Rectifier". In June 1926, he was awarded by the Institute the degrees of S.B. (as of 1925), and S.M.

In February 1926, he was appointed as an Assistant in the Electrical Engineering Department and assigned to carry on work in the cable research sponsored by the National Electric Light Association. This work was completed in the spring of 1928, and in February 1928, the writer was appointed Instructor in Electrical Engineering, which rank he now holds.

The summer of 1928 was spent with the American Telephone and Telegraph Co. at Houlton, Maine, working on the transatlantic radio-telephone receiving system. In 1929, the writer worked during the summer in the engineering department of the Samson Electric Co. Since October 1929, he has been in charge of the Electrical Engineering Research Laboratory at the Institute, and summers have been spent in the work of that laboratory.
A list of the writer's publications follows:

Miniature Power Systems. How Vast Electrical Transmission Networks are Duplicated and Studied in a Laboratory.


Thomas-Fermi Equation Solution by the Differential Analyzer.


An Improved Form of Electrocardiograph.


Research in Electrocardiography.