THOMAS-FERMI EQUATION SOLUTION BY THE DIFFERENTIAL ANALYZER

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Abstract

A numerical solution of the Thomas-Fermi equation $d^2\phi/dx^2=\phi^{3/2}/x^{1/2}$, with the boundary conditions $\phi(0)=1$ and $\phi(\infty)=0$, is presented, as obtained mechanically by means of the Differential Analyzer. This device for solving ordinary differential equations is described in a separate paper in the Journal of the Franklin Institute. The results are given for larger values of argument than have previously been reported, and at high values of argument precision has been improved. Over a part of the range, previously published results are checked, and the entire range is checked by an independent integration.

A MACHINE recently developed at the Massachusetts Institute of Technology is capable of the solution of many forms of ordinary differential equations.[1] This paper presents the results obtained by its use in the solution of the Thomas-Fermi[2,3] equation, which was picked as one of the first problems for attack largely because it brought out certain interesting points in connection with the operation of the machine.

The equation with dimensionless variables introduced is

$$\frac{d^2\phi}{dx^2}=\frac{\phi^{3/2}}{x^{1/2}} \tag{1}$$

and the boundary conditions are

$$\phi(0) = 1 \tag{2.0}$$

$$\phi(\infty) = 0. \tag{2.1}$$

An equation of this type, with boundary conditions as given, is inherently difficult to solve by any method. It is nonlinear and involves a singularity at $x=0$. Moreover, the boundary conditions are such that they cannot be satisfied directly; one must be satisfied at the point of singularity at $x=0$, and the other at infinity. It is also characteristic of this equation that small errors introduced when solving with x increasing have a cumulative effect as the solution proceeds.

The second derivative in Eq. (1) becomes infinite for $x=0$, so the solution for the region from $x=0$ to $x=0.2$ was taken from an expansion given by Baker.[4] The remainder of the problem was divided for solution into two parts,

[1] V. Bush, Jour. Franklin Inst. **212**, 447 (1931).
[2] L. H. Thomas, Proc. Camb. Phil. Soc. **23**, 542 (1927).
[3] E. Fermi, Zeits. f. Physik **48**, 73 (1928).
[4] E. B. Baker, Phys. Rev. **36**, 630 (1930).

corresponding to the regions from $x=0.2$ to $x=10$ and from $x=10$ to $x=\infty$.

In the region from $x=0.2$ to $x=10$, in order to keep the ordinates in the result large and hence maintain precision, there was introduced in Eq. (1) a new variable

$$\psi = \phi\epsilon^{x/2} \tag{3}$$

which gave the equation

$$\frac{d^2\psi}{dx^2} = \frac{d\psi}{dx} - \frac{\psi}{4} + \frac{\psi^{3/2}}{x^{1/2}\epsilon^{x/4}} \tag{4}$$

Moreover, it was found advisable to operate the machine with x decreasing in order to minimize the effect of casual errors, which in this region produced a cumulative effect with increasing x. The required starting conditions at $x=10$ were obtained by running a family of solutions in the region from $x=10$ to $x=\infty$, using a range of values for $\phi(10)$ within which the correct value was known to lie. Each of these solutions satisfied Eqs. (1) and (2.1), and was extended back by means of Eq. (4) to $x=0.2$. At that point the values of ϕ and ϕ' were read and plotted, together with points computed from Baker's expansion for different values of $\phi'(0)$. The intersection of the two curves established by interpolation the values of $\phi(10)$ and $\phi'(10)$ for which the solution satisfied the original equation and both boundary conditions.

In the region from $x=10$ to $x=\infty$, a change of variables was made, introducing

$$u = \frac{1}{x}, \quad q = \phi u \tag{5}$$

after which Eqs. (1) and (2.1) became

$$\frac{d^2q}{du^2} = \frac{q^{3/2}}{u^4} \tag{6}$$

and

$$q(0) = 0. \tag{7}$$

The procedure here was to assume a value of q at $u=0.1$ and to adjust by trial the corresponding values of q' so that Eq. (7) was satisfied when the machine was run with q decreasing. This was repeated for a number of values of q covering the desired range. This procedure, while exceedingly laborious when using formal methods, is not unduly time consuming on the analyzer, for a single solution can be run in a few minutes when once the machine is set up.

For the solution of Eqs. (4) and (6), the differential analyzer was connected as shown in Figs. 1 and 2 respectively.[5] In these diagrams scales, signs

[5] For explanation of symbols used, see reference 1.

and gear ratios are disregarded. The revolutions of each shaft are proportional to the quantities indicated.

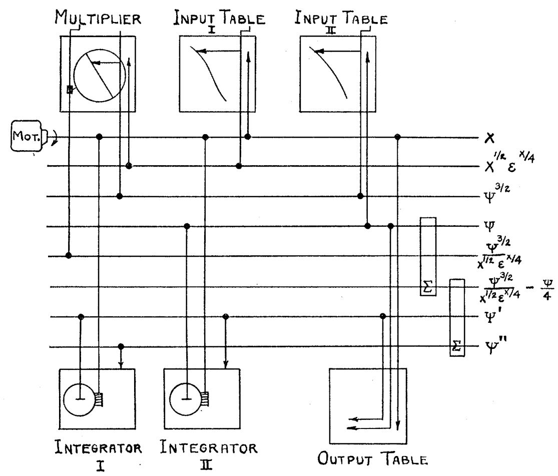

Fig. 1. Connections of the Differential Analyzer to solve the equation

$$\frac{d^2\psi}{dx^2}=\frac{d\psi}{dx}-\frac{\psi}{4}+\frac{\psi^{3/2}}{x^{1/2}\epsilon^{x/4}}\,.$$

Table I shows the numerical solution obtained for the region from $x=0.2$ to $x=36.92$. These values agree to within less than one percent with those reported by Baker,[4] whose table covers the range up to $x=14.88$. In the region from $x=15$ to $x=20$, Fermi[3] gives values of one significant figure; the present

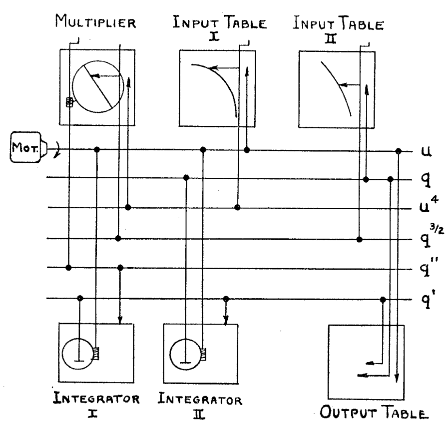

Fig. 2. Connections of the Differential Analyzer to solve the equation

$$\frac{d^2q}{du^2}=\frac{q^{3/2}}{u^4}\,.$$

table gives two significant figures for all values beyond $x=16$. The initial slope was found to be -1.589 and thus agrees with Baker's value.

TABLE I.

x	ϕ	x	ϕ	x	ϕ
0	1.000*	2.500	0.193	10.44	0.0225
0.010	0.985*	2.708	0.176	10.67	0.0216
0.030	0.959*	2.918	0.162	10.92	0.0206
0.060	0.924*	3.125	0.150	11.16	0.0198
0.080	0.902*	3.333	0.138	11.43	0.0189
0.100	0.882*	3.542	0.127	11.72	0.0180
0.150	0.835*	3.750	0.118	12.01	0.0171
0.200	0.793	3.960	0.110	12.31	0.0163
0.250	0.755	4.167	0.102	12.63	0.0155
0.292	0.727	4.375	0.0956	12.97	0.0147
0.333	0.700	4.583	0.0895	13.33	0.0139
0.375	0.675	4.792	0.0837	13.72	0.0131
0.417	0.651	5.000	0.0788	14.12	0.0123
0.458	0.627	5.209	0.0739	14.55	0.0116
0.500	0.607	5.418	0.0695	15.01	0.0109
0.542	0.582	5.625	0.0656	15.48	0.0102
0.584	0.569	5.834	0.0619	16.00	0.0094
0.625	0.552	6.042	0.0587	16.56	0.0088
0.667	0.535	6.250	0.0554	17.14	0.0081
0.709	0.518	6.458	0.0526	17.78	0.0075
0.750	0.502	6.667	0.0500	18.46	0.0069
0.792	0.488	6.875	0.0473	19.20	0.0064
0.833	0.475	7.083	0.0450	20.00	0.0058
0.875	0.461	7.292	0.0430	20.87	0.0053
0.917	0.449	7.500	0.0408	21.82	0.0048
0.958	0.436	7.708	0.0389	22.85	0.0043
1.000	0.425	7.917	0.0371	24.00	0.0038
1.042	0.414	8.125	0.0355	25.26	0.0034
1.083	0.406	8.333	0.0340	26.67	0.0030
1.125	0.393	8.542	0.0321	28.24	0.0026
1.167	0.382	8.750	0.0310	30.00	0.0022
1.208	0.374	8.958	0.0298	32.00	0.0019
1.250	0.364	9.167	0.0287	34.29	0.0016
1.458	0.322	9.375	0.0275	36.92	0.0011
1.667	0.287	9.583	0.0265		
1.875	0.259	9.792	0.0255		
2.083	0.234	10.000	0.0244		
2.292	0.212	10.22	0.0235		

* Computed points.

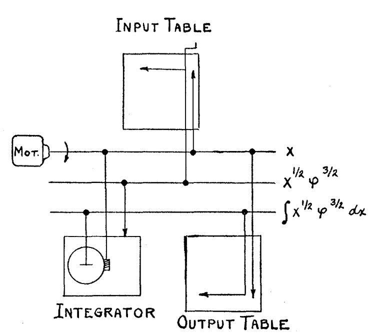

Fig. 3. Connections of the Differential Analyzer to perform the integration

$$\int x^{1/2}\phi^{3/2}dx.$$

A condition which ϕ must satisfy and which was not used in making the solution is given by

$$\int_0^\infty \phi^{3/2} x^{1/2} dx = 1. \tag{7}$$

This was used as a final check on the work, with the machine connected as in Fig. 3. The integral between the limits $x=0$ to $x=30$ had the value 0.994.

This problem was suggested by Professor R. M. Langer of the Department of Physics, and we are greatly indebted to him for his many suggestions and the active interest he took in the solution. Messrs. S. E. Caldwell, G. B. Hoadley, and J. R. Outt assisted in the operation of the machine and the measurement of final results.