JOURNAL OF COMPUTATIONAL PHYSICS 47, 308–312 (1982)

Note

Numerical Integration of the Thomas–Fermi Equation from Zero to Infinity

The Thomas–Fermi equation is expanded in a series at both $x = 0$ and $x = \infty$. Forward numerical integration from $x = 0$ determines an initial slope of -1.5880710226. Backward integration from $x = \infty$ depends on one parameter. By fitting the backward and forward integrations near $x = 30$, the parameter is determined and the numerical solution is obtained from zero to infinity with a high degree of accuracy.

The solution of the Thomas–Fermi equation has been of interest for half a century. The nonlinear equation

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

has the boundary conditions $\phi = 1$ at $x = 0$ and $\phi = 0$ at $x = \infty$. Sommerfeld [1] derived a closed approximation to ϕ, namely,

$$\phi_S = 144\ (1 + 12^{2n/3}/x^n)^{-\lambda}/x^3 \tag{2}$$

where $n\lambda = 3$, $n = (-7 + \sqrt{73})/2 = 0.77200187266$, and $12^{2n/3} = 3.5927$. This solution is reasonably good for large values of x, but rather poor for small values of x since ϕ_S' is equal to $-\infty$ at $x = 0$.

Bush and Caldwell [2] utilized an expansion at $x = 0$ given by Baker [3], and solved for ϕ utilizing the M.I.T. differential analyzer and obtained $-B = -1.589$ for the initial slope at $x = 0$. The misprint (or error) in the Baker expansion is repeated by Davis [4] and presented correctly by Feynmann [5]. Utilizing a Marchand hand calculator Slater and Krutter [6] obtained a value of $B = 1.58808$. Miranda [7], utilizing a novel technique, obtained a value of $B = 1.588046$ with a stated error of less than 10^{-6}. A table of values from $x = 0$ to $x = \infty$ is also presented. Filohakov [8] presents a table of values of ϕ to $x = 70$ for $B = 1.5880710220$ and $B = 1.5880710221$ with corresponding values $\phi(70) = 0.000190$ and $\phi(70) = 0.000137$.

The procedure presented herein embodies several ideas derived from some of the references, leading to a numerical solution of estimated high accuracy.

The series expansion of ϕ near $x = 0$ in terms of $x^{1/2}$ is given by

$$\begin{aligned}\phi = {} & 1 - Bx + 4x^{3/2}/3 - 2Bx^{5/2}/5 + x^3/3 + 3B^2x^{1/2}/70 - 2Bx^4/15 \\ & + (14/3 + B^3/4)\,x^{9/2}/63 + B^2x^5/175 + (B^4/1056 - 31B/1485)\,x^{11/2} \\ & + (4/405 - 4B^3/1575)\,x^6 + (557B^2/100,100 + 3B^5/9152)\,x^{13/2} \\ & - (20B + 29B^4/7)\,x^7/3465 + 0.011276x^{15/2} + \cdots .\end{aligned} \tag{3}$$

0021-9991/82/080308–05$02.00/0

Since ϕ is a monotonic function starting at one at $x = 0$ and diminishing to 0 at $x = \infty$, the numerical integration was started at $x = 0.02$ utilizing a CDC 6600 with single precision. The last term in the expansion is approximately 3×10^{-15}, so that the initial accuracy is at least 10^{-14}. The Runge–Kutta method [9] for the second-order equation was used for the numerical integration of ϕ and the Runge–Kutta method for a first order equation was used for the numerical integration of ϕ'. The initial value of $h = 0.00020$ to $x = 0.08$, then $h = 0.0005$ to $x = 0.22$, was changed to larger intervals as determined by keeping the fifth order term $h^5/5!\, d^{\mathrm{V}}\phi/dx^{\mathrm{V}} \leqslant 5 \times 10^{-15}$. The numerical integration was stopped when ϕ became negative or $d\phi/dx$ became positive. The program was started with $B = 1.588$ and by iteration the final solution occurred at

$$B = 1.5880710226 \tag{4}$$

in excellent agreement with Filohakov. The numerical values of ϕ are in very good agreement as far as $x = 40$, after which deviations became more pronounced. At $x = 60$ this method gives $\phi = 0.00039388$ and the Filohakov values are 0.000395 and 0.000379.

The Thomas–Fermi equation was examined at $x = \infty$, by setting $u = 1/x$ and $\phi(x) = \phi(u)$ so that

$$\phi(u) = 144u^3 y(u) \tag{5}$$

or

$$u^2 y'' + 8uy' + 12y = 12y^{3/2} \tag{6}$$

Now let

$$y = 1 + au^n + a_2 u^{2n} + a_3 u^{3n} + \cdots . \tag{7}$$

Substituting Eq. (7) into Eq. (6), squaring both sides, and equating like powers of u^n, the first result obtained is $n = (-7 + \sqrt{73})/2$, exactly the same result given by Sommerfeld (the other solution $(-7 - \sqrt{73})/2$ is discarded for improper behavior at $u = 0$). The next terms were $a_2 = 9a^2/(36 - 28n)$ and $a_3 = (18 + 7n)\,a^3/8(9 - 7n)(8 - 7n)$. Finally, y is expressed in terms of au^n.

$$\begin{aligned} y = 1 + au^n &+ 0.6256975(au^n)^2 + 0.3133861(au^n)^3 + 0.137391\,(au^n)^4 \\ &+ 0.055083\,(au^n)^5 + 0.020707(au^n)^6 + 0.007415(au^n)^7 + \cdots \end{aligned} \tag{8}$$

From Sommerfeld's equation, $a = -13.96$. A rough estimate of $a \cong -13.3$ was obtained by matching $\phi(50)$ to $144(0.02)^3 y(0.02)$. Equation (6) was numerically integrated starting at $u = 0.002$ with $a = -13.25$ utilizing the Runge–Kutta method. The calculations were repeated with a decreasing in steps of 0.0025 as far as $a = -13.35$.

Interpolating so that $\phi(u)$ and $-u^2 d\phi/du$ were the same as $\phi(x)$ and $d\phi/dx$ for the forward calculations at $x = 20$, 25, 30, and 40, the best average fit occurred for $a = -13.2710 \pm 0.0010$.

The degree of fit is indicated in Table I.

TABLE I

	ϕ Forward	ϕ Back	ϕ' Forward	ϕ' Back
$x = 20$	0.00578494	0.00578492	−0.000647254	−0.000647252
$x = 25$	0.00347375	0.00347375	−0.000324043	−0.000324042
$x = 30$	0.00225583	0.00225583	−0.000180670	−0.000180671
$x = 40$	0.00111363	0.00111363	−0.000069669	−0.000069668

TABLE II

ϕ and ϕ' Versus x

x	ϕ	$-\phi'$
0.00	1.000000000	1.588071023
0.02	0.971976639	1.309304963
0.04	0.946962774	1.199103451
0.06	0.923826768	1.117740319
0.08	0.902153033	1.051608480
0.10	0.881697077	0.995354646
0.12	0.862291781	0.946194872
0.14	0.843813275	0.902454221
0.16	0.826164915	0.863028591
0.18	0.809268576	0.827142829
0.20	0.793059432	0.794227009
0.30	0.720639476	0.661799780
0.40	0.659541161	0.564642444
0.50	0.606986383	0.489411613
0.60	0.561162024	0.429171872
0.70	0.520791457	0.379794745
0.80	0.484930988	0.338607156
0.90	0.452858715	0.303775756
1.00	0.424008052	0.273989052
1.20	0.374241230	0.225908594
1.40	0.332901370	0.189041426
1.60	0.298097707	0.160115008
1.80	0.268469510	0.136998438
2.00	0.243008507	0.118243192
2.20	0.220949979	0.102830976
2.40	0.201702701	0.090026276
2.60	0.184802149	0.079285763
2.80	0.169878264	0.070200388

Table continued

TABLE II (*Continued*)

x	ϕ	$-\phi'$
3.00	0.156632673	0.062457131
3.50	0.129369597	0.047501047
4.00	0.108404257	0.036943758
4.50	0.091948134	0.029271448
5.00	0.078807779	0.023560075
5.50	0.068160362	0.019221348
6.00	0.059422949	0.015867549
7.00	0.046097819	0.011142532
8.00	0.036587255	0.008088603
9.00	0.029590936	0.006033075
10.00	0.024314293	0.004602882
12.00	0.017063922	0.002830536
14.00	0.012478407	0.001844501
16.00	0.009424081	0.001257435
18.00	0.007304845	0.000888831
20.00	0.005784941	0.000647254
25.00	0.003473753	0.000324043
30.00	0.002255835	0.000180670
35.00	0.00155093	0.00010891
40.00	0.00111363	0.00006967
45.00	0.00082755	0.00004669
50.00	0.00063225	0.00003250
60.00	0.00039392	0.00001720
70.00	0.00026227	0.00000915
80.00	0.00018355	0.00000617
90.00	0.00013355	0.000004025
100.00	0.000100242	0.000002739
150.00	0.000032634	0.000000609
200.00	0.000014502	0.000000206

In summary, forward numerical integration utilizing Eq. (3) with $B = 1.5880710226$ will lead to values of ϕ with an estimated accuracy of eight decimal places at $x = 30$. Backward integration utilizing Eq. (8) with $a = -13.2710$ will lead to values of ϕ from ∞ to $x = 30$ with five significant figures. Not surprisingly, if Sommerfeld's equation is slightly modified to

$$\phi_{\mathrm{S,mod.}} = 144\ (1 + 3.422/x^n)^{-\lambda}/x^3, \tag{9}$$

then it can be utilized for calculations of ϕ for $x \geqslant 30$ with four to five significant figure accuracy. Table II presents some values of ϕ versus x. Values of ϕ for x larger than 40 were obtained from the backward integration.

REFERENCES

1. A. SOMMERFELD, *Z. Phys.* **78** (1932).
2. V. BUSH AND S. H. CALDWELL, *Phys. Rev.* **38** (1931), 1898.
3. E. B. BAKER, *Phys. Rev.* **36** (1930), 630.
4. T. DAVIS, "Introduction to Nonlinear Differential and Integral Equations," Dover, New York, 1962.
5. R. P. FEYNMAN, N. METROPOLIS, AND E. TELLER, *Phys. Rev.* **75** (1949), 1561.
6. J. C. SLATER AND H. KRUTTER, *Phys. Rev.* **47** (1935), 559.
7. C. MIRANDA, *Accademico Francesco Severl* (Nov. 1933).
8. P. F. FILOHAKOV, "Numerical and Graphical Methods of Applied Mathematics," Navkova Dunka, Kiev, 1970.
9. J. B. SCARBOROUGH, "Numerical Mathematical Analysis," Johns Hopkins, Baltimore, 1962.

RECEIVED: October 28, 1981; REVISED March 19, 1982

HARRY KRUTTER

Naval Air Development Center
Warminster, Pa. 18974