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Another Rational Analytical Approximation to the Thomas-Fermi Equation

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Abstract

A new rational analytic approximation to the solution of the Thomas-Fermi boundary value problem is presented. The approximation is a development of the original conception of J.C. Mason [5] and has been developed to reproduce the numerical work of Parand et al [11], as far as proved feasible. The fit to the numerical data, by a basic collocation process applied to the rational approximation, proved excellent.

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Introduction

In recent years great interest has again arisen in the Thomas-Fermi equation. We mention, in particular, the work of Amore et al [1], Boyd [4] and Parand et al [8, 9, 10 and 11]. (The literature on the Thomas-Fermi equation is vast and we make no attempt at a literature review here. However, the above quoted reference contain a considerable number and should be referred to if guidance on the literature is required.) In this paper we propose a new compact analytical approximation to the Thomas-Fermi equation based on the original analytical approximation of Mason [5] and the numerical studies of Parand et al [11]. The approximation (equation (11) below) is a rational function and is a natural variant of Mason's original rational analytic approximate solution to the Thomas-Fermi boundary value problem. Also, equation (11) below, when differentiated, produces an excellent approximation to the derivative of the solution of the Thomas-Fermi equation

Background and Proposed Form of Approximate Solution

The Thomas-Fermi equation is the nonlinear ordinary differential equation (ODE) [1]

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

and its solution is subject to the boundary conditions

$$y(0)=1, \quad y(\infty)=0 \tag{2}$$

There is no exact solution to the boundary value problem (BVP) represented by (1) and (2), however there are two exact asymptotic solutions to (1).

First, there is the series solution to (1) for 'small' x [4]

$$y(x)=1+\beta x+\tfrac{4}{3}x^{3/2}+\tfrac{3}{10}\beta^2 x^{7/2}+\tfrac{1}{3}x^3+\cdots \tag{3}$$

where β, the Baker number [3], that is, the 'missing' initial condition

$$y'(0)=\beta \tag{4}$$

which has to be (in some way) determined. Secondly, we have the series for 'large' x [4]

$$y(x)=\tfrac{144}{x^3}\left(1-\tfrac{A}{x^\lambda}+0.62569\left(\tfrac{A}{x^\lambda}\right)^2+0.31383\left(\tfrac{A}{x^\lambda}\right)^3+\cdots\right) \tag{5}$$

where $A\approx 13.27094$ and $\lambda\approx 0.772001872$ Actually, the leading term in (5) is an exact particular solution of (1) and satisfies the second of the boundary conditions in (2).

In fact, in addition to the above facts and constraints, there are additional restrictions or
conditions that the solution of the Thomas-Fermi equation must satisfy and these are presented below as part of the 'goodness-of-fit' criteria that any approximate analytical solution of (1) is expected to satisfy.

Finally, the Thomas-Fermi equation, (1), can be obtained as the solution of the variational problem of minimizing the integral [2]

$$I = \int_0^\infty \left(\frac{1}{2} y'(x)^2 + \frac{2}{5} \frac{y(x)^{5/2}}{x^{1/2}} \right) dx \tag{6}$$

subject to the BC (2); indeed, equation (1) follows from the Euler equation for the minimization of the integral (8).

While there is no exact solution to the BVP represented by (1) and (2), there are many approximate analytical solutions to this problem. One of the best is that of Mason [5]. Mason's [5] analytical approximation to (1) is

$$y(x) = \left(\frac{1 + 1.81061\sqrt{x} + 0.60112x}{1 + 1.81061\sqrt{x} + 1.39515x + 0.77112x^{3/2} + 0.21465x^2 + 0.04792x^{5/2}} \right)^2 \tag{7}$$

An examination of Mason's function (7) determines that it is a rational function in terms of $\sqrt{x}$. The dependence of (7) on $\sqrt{x}$ is not surprising, as the series solution of (1) given by (3) is an expansion in terms of $\sqrt{x}$ also. The expression (7) is known to be an excellent 'fit' to the boundary value problem, with the initial condition (4) being approximated to five places of decimals (when evaluated via (7), but with the asymptotic coefficient given as 157 instead of 144. Below, we consider means of overcoming this asymptotic problem and put forward a related type of rational analytical approximation to that of (7).

As Mason makes clear in his original paper [5], (7) is part of a family of approximate analytical solution to (1) and here we consider natural variants of Mason's formula (7) that incorporate the initial condition (4) and the leading term of the asymptotic series (5) explicitly. As a first example of these natural variants of (7), we could consider

$$y_1(x) = \left(\frac{1 + a\sqrt{x} + \sqrt{144}bx}{1 + a\sqrt{x} + (12b - \beta/2)x + cx^{3/2} + dx^2 + bx^{5/2}} \right)^2 \tag{8}$$

Expression (8) satisfies all of the conditions as well as having the correct asymptotic form. However, (8) has only five coefficients available to form a fit to the problem. In this case, we may use a more general form of our variation of Mason's formula and consider, instead of (8), an alternative given as

$$y_2(x) = \left(\frac{1 + a\sqrt{x} + bx + \sqrt{144}cx^{3/2}}{1 + a\sqrt{x} + (b - \beta/2)x + dx^{3/2} + ex^2 + fx^{5/2} + cx^3} \right)^2 \tag{9}$$

Expression (9) satisfies all of the conditions as well as having the correct asymptotic form again. Now, though, (9) has seven coefficients available to produce a fit to the problem. The problem, then, is how to determine the unknown coefficients in (9).

There are various ways to determine the coefficients in the trial solution (9). In this paper we will consider only the method of collocation, whereby we will fit the trial solutions against a known solution to equation (1) for six points on the solution curve of (1), the value of β being taken as a *given* to obtain the best fit possible. While we note that are various standard ways of picking the collocation points see Amore et al [1], for an example, in this case the collocation points were chosen through numerical experience (trial and error!). Even so, the resulting analytical approximation proved remarkably good over the entire range of values examined.

Analysis, Results and Conclusions

Using data from Table 5 of Parand et al [11], the values of *a* to *f* in (9) were evaluated by collocation, while the value of β was taken from Table 3 of the same reference. The six points of collocation and the accompanying values of the Thomas-Fermi function ($y(x)$) used are given in Table 1 below.

x	$y(x)$
0.25	0.75520146531333312760
1	0.42400805208070560002
1.5	0.31477746370045817290
5	7.880777925136990042e-2
10	2.431429298868086418e-2
25	3.473754416765632470e-3

Table 1. Collocation Points and Given Values of the Thomas-Fermi Function.

The value of β used was $\beta = -1.588071022611375312718684509423950109$. In fact, the values used in the collocation process were rounded, as shown in Table 2 below.

Collocation Parameter	Parameter Value
a	1.977880202
b	0.880361414
c	0.00578866639
d	0.9735905328
e	0.324021964
f	0.07619038231

Table 2. Values of the Collocation Parameters

There are various ways of checking the goodness of fit of the model (9) with the parameter values as given in Table 2. Obviously a comparison with the other values in Table 5 of Parand et al [11] can be made, along with a comparison of the values of the derivative $y'_2(x)$ versus those presented in Table 6 of Parand et al [11]. (A comparison of the fit of (9) and its derivative can be made with Table 3 and Table 4 of the arXiv version of [1], but these results are, for our purpose, effectively the same as those of [11]) Further, we can examine the values of the following integral relations, which are the constraints that any solution to (1) is expected to conform to, as mentioned above. Indeed, when this is done we get the following results [12]

$$I_C = \int_0^\infty x^{1/2} y_2(\mathrm{x})^{3/2} dx = 1 \approx 0.9999991551 \quad (10a)$$

and

$$I_P = \int_0^\infty x^{-1/2} y_2(\mathrm{x})^{3/2} dx = 1.58807098 \approx 1.587859476 \quad (10b)$$

and

$$I_K = \int_0^\infty x^{-1/2} y_2(x)^{5/2} dx = 1.134336414 \approx 1.134124621 \quad (10c)$$

and the fit is apparently very close.

This close fit to the data is confirmed by the direct comparison of the calculated values of $y_2(x)$ and $y'_2(x)$ with the tabulate values of $y(x)$ and $y'(x)$ in Tables 5 and 6 of Parand et al [11], with agreement in the first 5 or 6 decimal places between the fit and the 'raw data'. Further, when we evaluate the integral in (6), we find that

$$I_2 = \int_0^\infty \left(\frac{1}{2} y_2(x)^2 + \frac{2}{5} \frac{y_2(x)^{5/2}}{x^{1/2}} \right) dx \approx 0.6805173749 \quad (11)$$

in good agreement, again, with published figures [2]. This close fit to the data continues when comparison is made with numerical data quoted in Oulne's work [6, 7] for small values of x.

It is instructive to make a comparison of the 'fit' of (9) to the data with that of Mason's original conception given by (7). The Mason function (7) is still a very good approximation to the numerical solution of Parand et al [11], agreeing to within four decimal places with the Parand et al data up to $x = 100$, after which it gradually tails-off. The fit obtained by (9) tails-off slightly from the numerical data also, but even at the end $(x = 5{,}000)$ is still within 0.33% of the numerical solution whereas by this point Mason's function (9) is more than 6.4% out from the numerical data. Further the Mason approximation (7) is a poorer fit to the constraints (10a), (10c) and (11), though (7) is a good fit to (10b). Similar results hold for the derivatives of (7) and (9).

In conclusion, we have presented a natural variant of Mason's [5] rational approximate analytical solution to the Thomas-Fermi equation that incorporates an explicit representation of the Baker number and the correct asymptotic format of the known particular solution. The final fit to the numerical data of our variant (9) agrees with the data [11] to within 0.33% across the entire range of value quoted in [11], as well as giving close agreement with the known constraints represented by (10) and (11). Indeed, the fit (11) gives a closer fit to the data and constraints across the entire range of value quoted in [11] than (7), as would be hoped, if not expected.

References

[1] P. Amore, J. Boyd, F. Fernández, Accurate calculation of the solutions to the Thomas-Fermi equations, *Applied Mathematics and Computation*, **232** (2014), 929–943. https://doi.org/10.1016/j.amc.2014.01.137

[2] N. Anderson, A.M. Arthurs and P.D. Robinson, Variational Solutions of the Thomas-fermi Equation, *Il Nuovo Cimento B Series 10*, **57** (1968) 523–526. https://doi.org/10.1007/bf02710218

[3] E.B. Baker, The application of the Fermi-Thomas statistical model to the calculation of potential distribution in positive ions, *Physical Review*, **36** (1930), 630–647. https://doi.org/10.1103/physrev.36.630

[4] J.P. Boyd, Rational Chebyshev series for the Thomas–Fermi function: Endpoint singularities and spectral methods, *Journal of Computational and Applied Mathematics*, **244** (2013), 90–101. https://doi.org/10.1016/j.cam.2012.11.015

[5] J.C. Mason, Rational Approximations to the Ordinary Thomas-Fermi Function and its Derivative, *Proceedings of the Physical Society*, **84** (1964), 357–359. https://doi.org/10.1088/0370-1328/84/3/304

[6] M. Oulne, Analytical solution of the Thomas-Fermi equations for atoms, 2005. arXiv:physics/0511017v2 [physics.atom-ph].

[7] M. Oulne, Variation and series approach to the Thomas-Fermi equation, *Applied Mathematics and Computation*, **218** (2011), 303–307. https://doi.org/10.1016/j.amc.2011.05.064

[8] K. Parand, M. Dehghan and A. Pirkhedri, The Sinc-collocation method for solving the Thomas–Fermi equation, *Journal of Computational and Applied Mathematics*, **237** (2013), 244–252. https://doi.org/10.1016/j.cam.2012.08.001

[9] K. Parand, H. Yousefi and M. Delkhosh, Numerical Study on the Thomas-Fermi Differential Equation Using Fractional Order of the Euler Functions, *The 8th National Conference on Mathematics of Payame Noor University*, (2016), Lorestan, Iran, 339-343.

[10] K. Parand, A. Ghaderi, H. Yousefi and M. Delkhosh, A New Approach for Solving Nonlinear Thomas-Fermi equation Based on Fractional Order of Rational Bessel Functions, *Electronic Journal of Differential Equations*, **2016** (2016), no. 331, 1–18.

[11] K. Parand, P. Mazaheri, H. Yousefi and M. Delkhosh, Fractional order of rational Jacobi functions for solving the non-linear singular Thomas-Fermi equation, *European Physical Journal Plus*, **132** (2017), 77. https://doi.org/10.1140/epjp/i2017-11351-x

[12] G.J. Pert, *Approximations for the rapid evaluation of the Thomas-Fermi equation*, *Journal of Physics B: Atomic, Molecular and Optical Physics*, **32** (1999), 249–266. https://doi.org/10.1088/0953-4075/32/2/009

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