On the Majorana solution to the Thomas-Fermi equation

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Abstract

We analyse the solution to the Thomas-Fermi equation discovered by Majorana. We show that the series for the slope at origin enables one to obtain results of accuracy far beyond those provided by available methods. We also estimate the radius of convergence of this series and conjecture that the singularity closest to origin is a square-root branch point.

1 Introduction

There has been great interest in the accurate calculation of the solution to the nonlinear differential equation that comes from the Thomas-Fermi model for neutral atoms [1–13]. Several approaches have been applied for this purpose; for example: Padé Hankel method [13], fractional order of rational Euler functions [6], fractional order of rational Bessel functions collocation method [7], fractional order of rational Jacobi functions [8], rational Chebyshev functions [4], fractional order of rational Chebyshev functions of the second kind [10], a hybrid approach based on the collocation and Newton-Kantorovich methods plus fractional order of rational Legendre functions [11], Newton iteration with spectral

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algorithms based on fractional order of rational Gegenbauer functions \[12\] and rational Chebyshev series accelerated through coordinate transformations \[13\]. We have just mentioned the most accurate results. Other authors have already obtained less accurate ones and more often than not reported many wrong digits as shown in the tables of some of the papers just mentioned \[6–11\].

The purpose of this paper is the discussion of a semi-analytical solution to the Thomas-Fermi equation discovered by Majorana in 1928 that remained unpublished for a long time as revealed in an enlightening pedagogical article by Esposito \[14\]. Although the Majorana solution was mentioned in some of the papers just quoted \[4–8,8–10\] none of those authors used it for testing their calculations. They did not realize that this approach enables one to obtain the slope at origin with any desired accuracy and in fact 100 significant digits have been reported in Wikipedia (https://en.wikipedia.org/wiki/Thomas%E2%80%93Fermi_equation#cite_note-11). As far as we know, this is the most accurate value of the slope at origin available nowadays.

One may reasonably argue that theoretical results of such an accuracy have no physical meaning. However, the Thomas-Fermi equation is commonly chosen as a benchmark for testing algorithms for solving nonlinear differential equations numerically and, for this reason, accurate results may be useful. The purpose of this paper is the analysis of the remarkable accuracy of the Majorana approach to the Thomas-Fermi equation. In section \[2\] we summarize the main equations shown by Esposito \[14\], in section \[3\] we analyze the convergence properties of the Majorana series numerically and in section \[4\] we summarize the main results and draw conclusions.

## 2 The Majorana transformation

The Thomas-Fermi equation for neutral atoms can be easily reduced to the dimensionless nonlinear second-order differential equation

$$\varphi''(x) = x^{-1/2} \varphi(x)^{3/2}, \quad \varphi(0) = 1, \quad \varphi(\infty) = 0. \quad (1)$$
In order to solve this equation one has to determine the unknown slope at origin 
\( \varphi'_{0} = \varphi'(0) \) that is consistent with the boundary conditions. By means of the 
change of independent and dependent variables

\[
t = 144^{-1/6} x^{1/2} \varphi^{1/6}, \quad u = - \left( \frac{16}{3} \right)^{1/3} \varphi^{-4/3} \varphi',
\]

Majorana derived the nonlinear first-order differential equation \[14\]

\[
\frac{du(t)}{dt} = 8 \frac{tu(t)^2 - 1}{1 - t^2 u(t)} \quad u(1) = 1.
\]

It can be proved that the slope at origin is given by

\[
\varphi'_{0} = - \left( \frac{3}{16} \right)^{1/3} u(0).
\]

The solution \( u(t) \) can be expanded as

\[
u(t) = \sum_{j=0}^{\infty} a_{j} \tau^{j}, \quad a_{0} = 1, \quad \tau = 1 - t,
\]

where the coefficients \( a_{n} \) satisfy the recurrence relation \[14\].

\[
a_{m} = \frac{1}{2(m+8) - (m+1)a_{1}} \left\{ m^{-2} \sum_{n=1}^{m-2} a_{m-n} \left[ \begin{array}{c} (n+1)a_{n+1} - 2(n+4)a_{n} \\ + (n+7)a_{n-1} \end{array} \right] + \left[ m + 7 - 2(m+3)a_{1} \right] a_{m-1} + (m+6)a_{1}a_{m-2} \right\}
\]

and \( a_{1} \) is a root of \( a_{1}^2 - 18a_{1} + 8 = 0 \). If \( a_{1} = 9 - \sqrt{73} \) then the coefficients \( a_{m} \) 
are all positive and Esposito \[14\] estimated \( a_{n}/a_{n-1} \sim 4/5 \) for \( n \to \infty \). On the 
other hand, when \( a_{1} = 9 + \sqrt{73} \) the magnitude of the coefficients \( |a_{n}| \) appears to 
increase unboundedly and the ratio \( |a_{n}/a_{n-1}| \) oscillates. Therefore, one expects 
to obtain reasonable results only for the first choice that we consider from now 
on.

It follows from equations \[4\] and \[5\] that one can obtain approximate solutions to the slope at origin from the sequence of partial sums

\[
\varphi'_{0,N} = - \left( \frac{3}{16} \right)^{1/3} S_{N}, \quad S_{N} = \sum_{j=0}^{N} a_{j}, \quad N = 1, 2, \ldots
\]

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Esposito \[14\] estimated $\varphi'_0 = -1.588$ (notice that there is a misprint in his paper) and this result has been cited by several authors \[6\]–\[10\]. However, none of them tried to obtain accurate results from equations (6) and (7), except for the accurate value of the slope at origin in Wikipedia mentioned above.

This approach exhibits two great advantages: first, the expansion coefficients $a_n$ are positive so that $S_N < S_{N+1}$ and the sequence converges from below. Second, the expansion coefficients decrease exponentially as shown in Figure 1 and, consequently, the rate of convergence is remarkable. From the first $N \leq 5000$ partial sums we estimate

$$\varphi'_{0,5000} = -1.588071022612700450945274662167482$$

that is supposed to be accurate to the last digit as we carried out the calculation numerically with sufficient accuracy (a simple Python program for this purpose is available at https://zenodo.org/record/4681779#.YH2Zorh1Yqg). It is unlikely that any of the approaches applied to this problem \[1\]–\[7\], \[9\]–\[11\], \[13\] (and references therein) can provide a result of such an accuracy. Notice that the error of a calculation based on $S_N$ is roughly of the order of $a_{N+1}$.

3 Analysis of the series

In this section we will try to determine some features of the Majorana series \[15\] numerically. To this end we resort to a method discussed by Hunter and Guerrieri \[15\] some time ago that we develop in what follows in a less general
and a simpler way, more suitable for present needs.

The function

$$f(x) = A \left(1 - \frac{x}{x_0}\right)^\nu,$$  \hspace{1cm} (8)

exhibits a singular point at \( x = x_0 \) for any real exponent \( \nu \), except when it is a positive integer. It is sufficient for present purposes to consider \( x \) real. This function can be expanded in a Taylor series

$$f(x) = \sum_{j=0}^{\infty} f_j x^j,$$  \hspace{1cm} (9)

that converges for all \( |x| < |x_0| \). It follows from the differential equation

$$\left(1 - \frac{x}{x_0}\right) f' = -\frac{\nu}{x_0} f,$$  \hspace{1cm} (10)

that the expansion coefficients satisfy the recurrence relation

$$(n+1)f_{n+1} = \frac{n}{x_0} f_n - \frac{\nu}{x_0} f_n, \hspace{0.5cm} n = 0, 1, \ldots$$  \hspace{1cm} (11)

We appreciate that the ratio \( f_{n+1}/f_n \) is a linear function of \( 1/(n+1) \)

$$\frac{f_{n+1}}{f_n} = \frac{1}{x_0} - \frac{\nu + 1}{x_0(n+1)}.$$  \hspace{1cm} (12)

From equation (11) we can derive two linear equations

$$x_0(n+1)f_{n+1} + \nu f_n = nf_n,$$

$$x_0 nf_n + \nu f_{n-1} = (n-1)f_{n-1},$$  \hspace{1cm} (13)

from which we obtain

$$x_0 = \frac{f_n f_{n-1}}{(n+1) f_{n+1} f_{n-1} - nf_n^2},$$

$$\nu = \frac{(n^2 - 1) f_{n+1} f_{n-1} - n^2 f_n^2}{(n+1) f_{n+1} f_{n-1} - nf_n^2}.$$  \hspace{1cm} (14)

As stated in section 2, the coefficients \( a_n \) are all positive and decrease exponentially which suggests that \( u(t) \) may exhibit a singular point as shown in equation (8). We can therefore obtain both the location \( \tau_0 \) and the exponent \( \nu \) of the singular point closest to the origin from the approximate straight line

$$\frac{a_{n+1}}{a_n} \approx \frac{1}{\tau_0} - \frac{\nu + 1}{\tau_0(n+1)}, \hspace{0.5cm} n \gg 1.$$  \hspace{1cm} (15)
as suggested by equation (12). Alternatively, we may resort to equation (14) and estimate these parameters from

\[
\tau_{0,n} = \frac{a_n a_{n-1}}{(n+1) a_{n+1} a_{n-1} - n a_n^2}, \quad \tau_0 = \lim_{n \to \infty} \tau_{0,n},
\]

\[
\nu_n = \frac{(n^2 - 1) a_{n+1} a_{n-1} - n^2 a_n^2}{(n+1) a_{n+1} a_{n-1} - n a_n^2}, \quad \nu = \lim_{n \to \infty} \nu_n.
\]

(16)

The second and third columns of Table 1 show values of \(\tau_{0,n}\) and \(\nu_n\), respectively, obtained from equation (16) for sufficiently large values of \(n\). The convergence is rather slow but it seems that \(\nu_n\) converges towards \(\nu = 1/2\) from below when \(n \to \infty\). The convergence of these sequences can be improved by means of Aitken extrapolation [16] and results obtained from the last 15 entries in the third column of table 1 confirms this conjecture. The fourth column shows results for

\[
\tau_{0,n} (\nu = 1/2) = \frac{n - 1/2}{n + 1} \frac{a_n}{a_{n+1}}.
\]

(17)

It seems that \(\tau_{0,n} (\nu_n)\) and \(\tau_{0,n} (\nu = 1/2)\) appear to be monotonously decreasing and increasing, respectively. On assuming that this behaviour already applies to all \(n\) we conjecture that \(1.20168605688 < \tau_0 < 1.2016860577\). Straightforward application of Aitken extrapolation to the last 15 entries in both columns enables us to sharpen those bounds to \(1.2016860571 < \tau_0 < 1.2016860575\). The same analysis on the third column yields \(\nu = 0.4998\).

On the other hand, from a numerical fit of the ratio \(a_{n+1}/a_n\) to a straight line we estimate \(\tau_0 = 1.2016860577\) and \(\nu = 0.4997\) in agreement with the results above.

### 4 Conclusions

In this paper we have shown that the Majorana transformation brought to light by Esposito [14] in a pedagogical paper enables one to obtain the slope at origin of the solution to the Thomas-Fermi equation with an accuracy that has not been achieved with any of the methods proposed so far. The slope at origin is necessary for the application of any approach because it is the relevant
unknown in the nonlinear differential equation just mentioned. In addition to it, we estimated the parameters that determine the singular point closest to the origin of the function $u(t)$ appearing in the Majorana transformation of the dimensionless Thomas-Fermi equation. We conjectured that the singularity is a square-root branch point and estimated its location with reasonable precision by means of lower and upper bounds.

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| $n$ | $\tau_{0,n}$ | $\nu_n$ | $\tau_{0,n}$ ($\nu = 1/2$) |
|-----|-------------|---------|-----------------|
| 40000 | 0.49970543274176466970358977642 | 0.49970543274176466970358977642 | 1.20168605792402935360388 |
| 40100 | 0.499706138316160983219059053 | 0.499706138316160983219059053 | 1.201686059145949790600257 |
| 40200 | 0.499706854236214125630603936 | 0.499706854236214125630603936 | 1.20168606195934317123844 |
| 40300 | 0.499707507924710852958505934 | 0.499707507924710852958505934 | 1.201686064714597523083248 |
| 40400 | 0.49970819423146182098280176 | 0.49970819423146182098280176 | 1.20168606746779411227932 |
| 40500 | 0.49970904453757616318062888 | 0.49970904453757616318062888 | 1.20168607064643209422634 |
| 40600 | 0.49970975620917629540549793 | 0.49970975620917629540549793 | 1.20168607358475637046764 |
| 40700 | 0.49971046391666275852417201 | 0.49971046391666275852417201 | 1.20168607655634931776676 |
| 40800 | 0.49971117843264684309560012 | 0.49971117843264684309560012 | 1.20168607957125288461176 |
| 40900 | 0.49971189371089414205210738 | 0.49971189371089414205210738 | 1.20168608259792949958203 |

Table 1: Parameters for the singular point
Figure 1: Logarithm of the expansion coefficients