Rational approximation to Thomas–Fermi equations

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Abstract

We show that a simple and straightforward rational approximation to the Thomas–Fermi equation provides the slope at origin with unprecedented accuracy and that relatively small Padé approximants are far more accurate than more elaborate approaches proposed recently by other authors. We consider both the Thomas–Fermi equation for isolated atoms and for atoms in strong magnetic fields.

1 Introduction

The Thomas–Fermi (TF) equation has proved useful for the treatment of many physical phenomena that include atoms [1–5], molecules [3,6], atoms in strong magnetic fields [1,4,5], crystals [7] and dense plasmas [8] among others. It is well–known that an accurate solution to that equation is based on the accurate calculation of the slope at origin [9–11]. In particular we mention the rational approximation in terms of Padé approximants [12,13] because it is relevant to

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present discussion. As expected from the great physical significance of the TF equation, its mathematical aspects have been studied in detail [14–17].

In spite of being a quite old problem in theoretical physics, there has recently been a renewed interest in analytical solutions to the TF equation. For example, Liao [18] and later Khan and Xu [19] proposed the application of the so-called homotopy analysis method (HAM). More recently Parand and Shahini [20] showed that a pseudospectral method based on Chebyshev polynomials is more accurate than HAM. Unfortunately, Parand and Shahini [20] were not aware that we had earlier shown that the well-known straightforward Padé approximants are much more accurate than HAM [21]. Therefore, they compared their pseudospectral results with the rather insufficiently accurate HAM ones that do not constitute a suitable benchmark.

The purpose of this paper is twofold: first we compare the results of the simple and straightforward Hankel–Padé method (HPM) [21] with the supposedly accurate Chebyshev pseudospectral ones [20]. Second, we show that the HPM also gives accurate results for the TF equation for atoms in strong magnetic fields that has not been treated before in this way.

In Section 2 we briefly introduce the TF equations for both problems and show how to transform them into more tractable differential equations. In Section 3 we outline the main ideas behind the HPM, apply it to both TF equations, and compare HPM and Chebyshev pseudospectral results for isolated atoms. In Section 4 we summarize the main results and comment on other approaches to nonlinear ordinary differential equations.
The Thomas–Fermi equation

The dimensionless form of the TF equation for atoms [1–5]

\[ u''(x) = \sqrt{\frac{u(x)^3}{x}}, \quad u(0) = 1, \quad u(\infty) = 0 \]  

(1)

is an example of two-point nonlinear boundary-value problem. When solving this ordinary differential equation one faces the calculation of the slope at origin \( u'(0) \) that is consistent with the physical boundary conditions indicated in equation (1).

In order to make this letter self contained we review the main features of the HPM [21]. It is convenient to define the variables \( t = x^2 \) and \( f(t) = u(t^2)^{1/2} \), so that the TF equation becomes

\[ t \left[ f(t)f''(t) + f'(t)^2 \right] - f(t)f'(t) - 2t^2f(t)^3 = 0 \]  

(2)

We expand the solution \( f(t) \) in a Taylor series about \( t = 0 \):

\[ f(t) = \sum_{j=0}^{\infty} f_j t^j \]  

(3)

where the coefficients \( f_j \) depend on the only unknown one \( f_2 = f''(0)/2 = u'(0)/2 \). On substituting the series (3) into equation (2) we easily calculate as many coefficients \( f_j \) as desired; for example, the first ones are

\[ f_0 = 1, \quad f_1 = 0, \quad f_3 = \frac{2}{3}, \quad f_4 = \frac{-f_2^2}{2}, \quad f_5 = \frac{-4f_2}{15}, \ldots \]  

(4)

The TF equation for atoms in strong magnetic fields is somewhat simpler [1,4,5]

\[ u''(x) = \sqrt{xu(x)}, \quad u(0) = 1, \quad u(\infty) = 0 \]  

(5)
By means of the same change of variables we obtain

$$t \left[ f(t)f''(t) + f'(t)^2 \right] - f(t)f'(t) - 2t^4 f(t) = 0$$  \hspace{1cm} (6)

as well as the solution in the form of the Taylor series \(^3\) with coefficients

$$f_0 = 1, \ f_1 = 0, \ f_3 = 0, \ f_4 = -\frac{f_2^2}{2}, \ f_5 = \frac{2}{15}, \ldots$$  \hspace{1cm} (7)

where \(f_2 = u'(0)/2\) as in the preceding case.

3 The Hankel–Padé method

The HPM is based on the transformation of the power series \(^3\) into a rational function or Padé approximant

$$[M/N](t) = \frac{\sum_{j=0}^{M} a_j t^j}{\sum_{j=0}^{N} b_j t^j}$$  \hspace{1cm} (8)

One would expect that \(M < N\) in order to have the correct limit at infinity; however, in order to obtain an accurate value of \(f_2\) it is more convenient to choose \(M = N + d, \ d = 0, 1, \ldots\) as in previous applications of the approach to the Schrödinger equation (in this case it was called Riccati–Padé method (RPM)) \([22–30]\).

The rational function \(^8\) has \(2N + d + 1\) coefficients that we may choose so that \(T([M/N], t) = \mathcal{O}(t^{2N+d+1})\), where \(T(f, t) = 0\) stands for either equation \(^2\) or \(^6\), and in both cases the coefficient \(f_2\) remains undetermined. If we require that \(T([M/N], t) = \mathcal{O}(t^{2N+d+2})\) we have another equation from which we obtain \(f_2\). However, it is simpler and more practical to proceed in a different (and entirely equivalent) way and require that

$$[M/N](t) - \sum_{j=0}^{2N+d+1} f_j t^j = \mathcal{O}(t^{2N+d+2})$$  \hspace{1cm} (9)
In order to satisfy this condition it is necessary that the Hankel determinant vanishes

\[ H_D^d = |f_{i+j+d+1}|_{i,j=0,1,...N} = 0, \quad (10) \]

where \( D = N + 1 \) is the dimension of the Hankel matrix. Each Hankel determinant is a polynomial function of \( f_2 \) and we expect that there is a sequence of roots \( f_2^{[D,d]} \), \( D = 2, 3, \ldots \) that converges towards the actual value of \( u'(0)/2 \) for a given value of \( d \). We compare sequences with different values of \( d \) for inner consistency (all of them should give the same limit).

Present approach is simple and straightforward: we just obtain the Taylor coefficients \( f_j \) from the differential equations (2) or (6) in terms of \( f_2 \), construct the Hankel determinant, and calculate its roots. Since \( f_4 \) is the first nonzero coefficient that depends on \( f_2 \) we choose Hankel sequences with \( d \geq 3 \).

The Hankel determinant \( H_D^d \) exhibits many roots and their number increases with \( D \). If we compare the roots of \( H_D^d \) with those of \( H_{D-1}^d \) we easily identify the sequence \( f_2^{[D,d]} \) that converges towards \( u'(0)/2 \).

Present HPM may be considered to be a systematic generalization of Tu’s approach [12] and is clearly different from the strategy proposed by Epele et al [13]. We stress that we have been using the Hankel condition (10) for quite a long time [22–30].

We first consider the TF equation for atoms. The convergence of the HPM has already been discussed in our earlier paper [21]; therefore, here we simply compare our results with those of Parand and Shahini [20]. Our estimate of \( u'(0) -1.588071022611375313 \) is by far more accurate than the one obtained by Parand and Shahini [20] –1.5880702966, Liao [18] –1.58606 and Khan and Xu [19] –1.586494973. Notice that all those authors kept several inaccurate digits in their results. This practice is misleading because it suggests that the
calculations are more accurate than what they really are.

Table 1 shows our earlier results [21], those of Parand and Shahini [20] and the numerical calculation of Kobayashi et al [9]. Those HPM results obtained from a relatively small \( \frac{5}{8} \) Padé approximant are more accurate than the numerical ones for \( x \leq 1 \). We appreciate that the simple and straightforward Padé approximants are far more accurate than the more elaborated pseudospectral approach [20]. Notice that also in this case Parand and Shahini [20] kept several misleading inaccurate digits.

Fig. 1 shows \( L_{D,d} = \log |2f_2^{[D,d]} - 2f_2^{[D-1,d]}| \) for \( D = 3, 4, \ldots \) that provides a reasonable indication of the convergence of the sequence of roots for the TF equations for atoms in strong magnetic fields. We clearly appreciate the great convergence rate of the sequences with \( d = 4 \) and \( d = 5 \) (the rate of convergence for the case \( d = 3 \) is slightly smaller but still suitable for practical applications). From those sequences we estimate \( u' (0) = -0.93896688764395889306 \) that is exact to the last digit and considerably more accurate than the results published earlier [1, 4, 5].

4 Conclusions

In this letter we have shown that the well–known simple and straightforward Padé approximants provide much more accurate results for the TF equation than the more elaborated Chebyshev pseudospectral method [20], exactly as we did earlier with the rather cumbersome HAM [21]. We also applied the HPM to the TF equation for an atom in a strong magnetic field, analyzed the convergence of the Hankel sequences towards the slope at origin, and obtained its value with unprecedented accuracy.

The TF equation is an example of two–point boundary value problems that
are most important in theoretical physics. We have already applied the HPM to other such problems [31]. There are alternative approaches for the accurate treatment of two–point boundary value problems. Here we mention the work of Boisseau et al [32], Bervillier et al [33, 34], and in particular a recent comprehensive discussion of power–series methods for ordinary differential equations [35].

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Table 1
Values of the Thomas–Fermi function $u(x)$ obtained by present method, the Chebyshev pseudospectral one [20], and numerical integration [9].

| $x$ | HPM   | Chebyshev | Numerical |
|-----|-------|-----------|-----------|
| 1   | 0.424008 | 0.424333179 | 0.42401   |
| 5   | 0.078808 | 0.078277758 | 0.078808  |
| 10  | 0.024315 | 0.025044744 | 0.024314  |
| 20  | 0.005786 | 0.006585633 | 0.0057849 |
| 50  | 0.000633 | 0.000761317 | 0.00063226|
| 100 | 0.0001005 | 0.000023409 | 0.00010024|

Fig. 1. $L_{D,d} = \log |2f_2^{[D,d]} - 2f_2^{[D-1,d]}|$ for $d = 4$ (circles) and $d = 5$ (filled circles)