



An explicit analytic solution to the Thomas–Fermi equation

Shijun Liao

*School of Naval Architecture and Ocean Engineering, Shanghai Jiao Tong University,
Shanghai 200030, China*

Abstract

A new kind of analytic technique, namely the homotopy analysis method, is employed to give an *explicit* analytic solution of the Thomas–Fermi equation and the related recurrence formulae of constant coefficients. This solution can be regarded as the definition of the exact solution of the Thomas–Fermi equation.

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Keywords: Explicit analytic solution; Thomas–Fermi equation; Nonlinear ODE

1. Introduction

Consider a differential equation used to calculate the electrostatic potential in the Thomas–Fermi atom model [1,2], called the Thomas–Fermi equation

$$u''(x) = \sqrt{\frac{u^3(x)}{x}} \quad (1)$$

with boundary conditions

$$u(0) = 1, \quad u(+\infty) = 0 \quad (2)$$

in the common case. Thomas–Fermi atom model views the electrons in an atom as a gas and derives atomic structure in terms of the electrostatic potential and

E-mail address: sjliao@mail.sjtu.edu.cn (S. Liao).

the electron density in the ground state. The above equation describes the spherically symmetric charge distribution about a many electron atom.

The analytic approximations of the Thomas–Fermi equations were proposed by some different techniques such as the variational approach [3,4], the δ -expansion method [5–7], the decomposition method [8–11] and so on [12–17]. However, to the best of our knowledge, there does not exist an elegant, simple and *explicit* analytic solution to the Thomas–Fermi equation.

In this paper the analytic approximate technique for nonlinear problems, namely the homotopy analysis method [18–26], is employed to give an *explicit* analytic solution of the Thomas–Fermi equation. Unlike perturbation techniques [27,28], the artificial small parameter method [29], the δ -expansion method [30] and the decomposition method [31], the homotopy analysis method *itself* provides us with a convenient way to *control* the convergence of approximation series and *adjust* convergence regions when necessary. Briefly speaking, the homotopy analysis method has the following advantages:

1. it is valid even if a given nonlinear problem does *not* contain any small/large parameters *at all*;
2. it itself can provide us with a convenient way to control the convergence of approximation series and adjust convergence regions when necessary;
3. it can be employed to *efficiently* approximate a nonlinear problem by *choosing* different sets of base functions.

In this paper an explicit analytic solution of the Thomas–Fermi equation and the related recurrence formulae of constant coefficients are given.

2. Mathematical formulations

Rewrite the original equation (1) as

$$x[u''(x)]^2 - u^3(x) = 0. \quad (3)$$

Note that Eq. (3) contains neither linear terms nor small or large parameters.

The essence to approximate a problem is to represent its solution by means of a complete set of base functions. Considering the boundary conditions (2) and the physical meaning of $u(x)$, it is straightforward that $u(x)$ should decrease from 1 to 0 as x increase from 0 to ∞ . Thus, it is reasonable to *choose* the set of base functions

$$\{(1+x)^{-m} | m \geq 1\} \quad (4)$$

to represent $u(x)$, i.e.

$$u(x) = \sum_{m=1}^{+\infty} c_m (1+x)^{-m}, \quad (5)$$

where c_m is coefficient. This provides us with the *Rule of Solution Expression*.

Under the Rule of Solution Expression described by (5) and due to the boundary conditions (2), it is straightforward to choose

$$u_0(x) = (1+x)^{-1} \quad (6)$$

as the initial guess of $u(x)$. Note that the original equation (1) is a nonlinear second-order differential equation. So, under the Rule of Solution Expression, one can choose the auxiliary linear operator

$$\mathcal{L}[\phi(x;p)] = \frac{(1+x)}{2} \frac{\partial^2 \phi(x;p)}{\partial x^2} + \frac{\partial \phi(x;p)}{\partial x} \quad (7)$$

such that

$$\mathcal{L}[C_1(1+x)^{-1} + C_2] = 0 \quad (8)$$

holds for any constant coefficients C_1 and C_2 .

Based on Eq. (3), the following nonlinear operator can be defined

$$\mathcal{N}[\phi(x;p)] = x \left[\frac{\partial^2 \phi(x;p)}{\partial x^2} \right]^2 - \phi^3(x;p). \quad (9)$$

Then, one can construct several homotopies as follows:

$$\mathcal{H}[\phi(x;p); \hbar, p] = (1-p)\mathcal{L}[\phi(x;p) - u_0(x)] - \hbar p \mathcal{N}[\phi(x;p)], \quad (10)$$

$$\mathcal{H}_0^b[\phi(0;p); p] = \phi(0;p) - 1, \quad (11)$$

$$\mathcal{H}_\infty^b[\phi(+\infty;p); p] = \phi(+\infty;p), \quad (12)$$

where \hbar is a non-zero auxiliary parameter. Setting

$$\mathcal{H}[\phi(x;p); \hbar, p] = 0, \quad \mathcal{H}_0^b[\phi(0;p); p] = 0, \quad \mathcal{H}_\infty^b[\phi(+\infty;p); p],$$

one has a family of equations

$$(1-p)\mathcal{L}[\phi(x;p) - u_0(x)] = \hbar p \mathcal{N}[\phi(x;p)], \quad x \geq 0, \quad p \in [0, 1], \quad (13)$$

with boundary conditions

$$\phi(0;p) = 1, \quad \phi(+\infty;p) = 0. \quad (14)$$

Note that the homotopy $\mathcal{H}[\phi(x;p); \hbar, p]$ contains the auxiliary parameter \hbar and besides one has great freedom to choose a proper value for it. Note also that when $\hbar = -1$ the homotopy (10) is constructed in the traditional way. So, the homotopy (10) is more general than traditional ones.

Due to (13), (14) and the definition (6) of $u_0(x)$, it holds when $p = 0$ that

$$\phi(x; 0) = u_0(x). \tag{15}$$

When $p = 1$, Eqs. (13) and (14) are the same as the original ones (3) and (2), provided

$$\phi(x; 1) = u(x). \tag{16}$$

Thus, as p increases from 0 to 1, $\phi(x; p)$ varies from the initial guess $u_0(x)$ to the exact solution $u(x)$ of Eqs. (3) and (2). This kind of variation is called deformation in topology. So, Eqs. (13) and (14) are called *the zero-order deformation equations*.

Due to (15), $\phi(x; p)$ can be expressed in the Maclaurin series

$$\phi(x; p) \sim u_0(x) + \sum_{k=1}^{+\infty} u_k(x)p^k, \tag{17}$$

where

$$u_k(x) = \frac{1}{k!} \left. \frac{\partial^k \phi(x; p)}{\partial p^k} \right|_{p=0}. \tag{18}$$

Note that $\phi(x; p)$ contains the auxiliary parameter \hbar . Assuming that \hbar is properly chosen such that the Maclaurin series (17) converges when $p = 1$, one has due to (16) that

$$u(x) = u_0(x) + \sum_{k=1}^{+\infty} u_k(x). \tag{19}$$

So, it is the auxiliary parameter \hbar that provides us with a convenient way to control the convergence of approximation series and adjust convergence regions when necessary.

The governing equation and boundary conditions of $u_k(x)$ ($k = 1, 2, 3, \dots$) are derived as follows. Differentiating k times the zero-order deformation Eqs. (13) and (14) with respect to p and then setting $p = 0$ and finally dividing them by $k!$, one has the so-called *kth-order deformation equations*

$$\mathcal{L}[u_k(x) - \chi_k u_{k-1}(x)] = \hbar R_k(x), \tag{20}$$

with boundary conditions

$$u_k(0) = 0, \quad u_k(+\infty) = 0, \tag{21}$$

where

$$R_k(x) = \sum_{j=0}^{k-1} \left[x u_j''(x) u_{k-1-j}''(x) - u_{k-1-j}(x) \sum_{i=0}^j u_i(x) u_{j-i}(x) \right] \tag{22}$$

and

$$\chi_k = \begin{cases} 0, & k \leq 1, \\ 1, & k > 1. \end{cases} \tag{23}$$

It should be emphasized that $u_k(x)$ ($k \geq 1$) is governed by the *linear* equation (20) with the linear boundary conditions (21), which can be easily solved by symbolic computation software such as Maple and Mathematica. Thus, through (19), the homotopy analysis method transfers the original nonlinear problem, governed by the fully nonlinear equation (3), to an infinite number of linear sub-problems, governed by (20) and (21). Note that such a kind of transformation needs not any small or large parameters at all.

Let $u_k^*(x)$ denote a special solution of equation

$$\mathcal{L}[u_k^*(x)] = \hbar R_k(x).$$

Then, due to the property (8), the general solution of Eq. (20) is

$$u_k(x) = \chi_k u_{k-1}(x) + u_k^*(x) + C_1(1+x)^{-1} + C_2, \tag{24}$$

where the coefficients C_1 and C_2 are determined by the boundary conditions (21).

In this way one can successively solve the k th-order deformation equations (20) and (21). It is found that $u_k(x)$ can be expressed by

$$u_k(x) = \sum_{n=1}^{4k+1} \alpha_{k,n} (1+x)^{-n}, \tag{25}$$

where $\alpha_{k,n}(\hbar)$ are coefficients. Substituting the above expression into the k th-order deformation equations (20) and (21), one has the following recurrence formulae:

$$\begin{aligned} \alpha_{k,n} &= \chi_k (1 - \chi_{n-4k+4}) \alpha_{k-1,n} \\ &+ \frac{2\hbar (\chi_{n-2} \beta_{k-1,n-2} - \chi_{n-3} \beta_{k-1,n-3} - \gamma_{k-1,n+1})}{n(n-1)}, \end{aligned} \tag{26}$$

where $k \geq 1$, $2 \leq n \leq 4k + 1$, the coefficient χ_k is defined by (23) and

$$\beta_{m,j} = \sum_{k=0}^m \sum_{n=\max\{1, j+4k-4m-1\}}^{\min\{j-1, 4k+1\}} n(n+1)(j-n)(j-n+1) \alpha_{k,n} \alpha_{m-k, j-n}, \tag{27}$$

$$\gamma_{m,j} = \sum_{k=0}^m \sum_{n=\max\{2, j+4k-4m-1\}}^{\min\{j-1, 4k+2\}} \delta_{k,n} \alpha_{m-k, j-n}, \tag{28}$$

$$\delta_{m,j} = \sum_{k=0}^m \sum_{n=\max\{1, j+4k-4m-1\}}^{\min\{j-1, 4k+1\}} \alpha_{k,n} \alpha_{m-k, j-n}, \tag{29}$$

respectively. Besides, the coefficient $\alpha_{k,1}$ is given by

$$\alpha_{k,1} = - \sum_{n=2}^{4k+1} \alpha_{k,n}. \quad (30)$$

Due to the definition (6) of $u_0(x)$, one has the first coefficient

$$\alpha_{0,1} = 1.$$

Thus, using the foregoing recurrence formulas and the known first coefficient $\alpha_{0,1} = 1$, all other coefficients $\alpha_{k,n}$ can be calculated successively. This provides us with an explicit analytic solution of the Thomas–Fermi equation

$$u(x) = \sum_{k=0}^{+\infty} \sum_{n=1}^{4k+1} \alpha_{k,n} (1+x)^{-n}. \quad (31)$$

The corresponding m th-order approximation is

$$u(x) \approx \sum_{k=0}^m \sum_{n=1}^{4k+1} \alpha_{k,n} (1+x)^{-n}. \quad (32)$$

Note that this analytic solution contains the auxiliary parameter \hbar , which can be employed to control the convergence of approximations and adjust convergence regions when necessary. Note that $\hbar = -1$ corresponds to the traditional way to construct a homotopy. However, it is found that when $\hbar = -1$ the series (31) diverges in the whole region $0 < x < +\infty$. Thus, if one constructs the homotopy (10) in the traditional way one cannot get a convergent analytical result. Fortunately, it is found that when $-1/2 \leq \hbar < 0$ the series (31) converges in the *whole* region $0 \leq x < +\infty$. When $\hbar = -1/2$ the analytic results at the 40th and 60th-order approximations agree quite well, as shown in Fig. 1. This illustrates that the auxiliary parameter \hbar can indeed control the convergence of approximations and adjust convergence regions when necessary. It should be emphasized that the proposed approach fails if \hbar were not introduced. That is the essential reason why the auxiliary parameter \hbar is introduced in the homotopy (10) and in the zero-order deformation equation (13). So, the auxiliary parameter \hbar plays a very important role in the homotopy analysis method.

Theorem 1 (Convergence theorem). *If the series*

$$u_0(x) + \sum_0^{+\infty} u_k(x)$$

is convergent, where $u_k(x)$ is governed by Eqs. (20) and (21) under the definitions (7), (22) and (23), it must be an exact solution of the Thomas–Fermi equation.

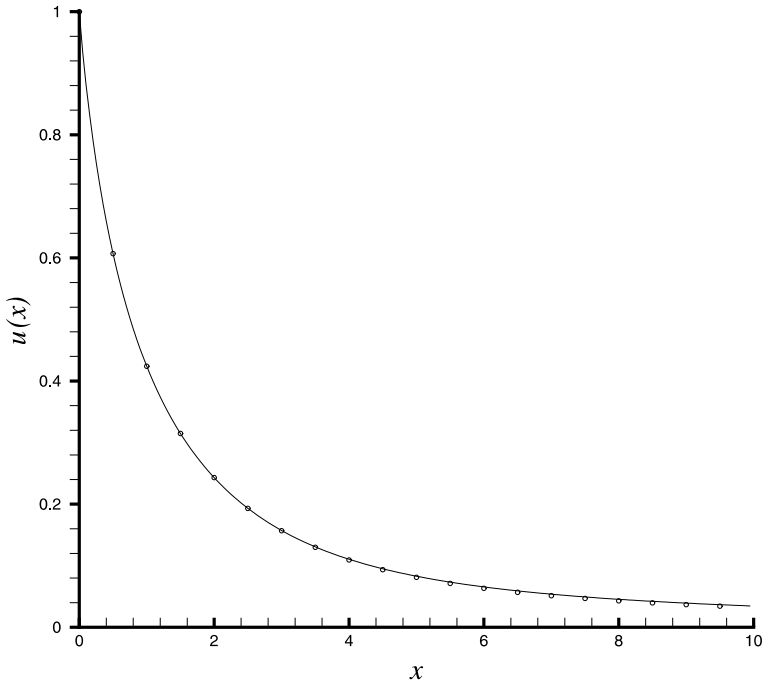


Fig. 1. The analytic result of the Thomas–Fermi equation when $\hbar = -1/2$. Solid line: 60th-order approximation; symbols: 40th-order approximation.

Proof. Write

$$s(x) = u_0(x) + \sum_{k=1}^{+\infty} u_k(x).$$

Owing to the convergence of the above series, it is necessary that

$$\lim_{m \rightarrow +\infty} u_m(x) = 0.$$

Due to (20), the definitions (7) and (23) and above expression, one has

$$\begin{aligned} \hbar \sum_{k=1}^{+\infty} R_k(x) &= \lim_{m \rightarrow +\infty} \sum_{k=1}^m \mathcal{L}[u_k(x) - \chi_k u_{k-1}(x)] \\ &= \mathcal{L} \left\{ \lim_{m \rightarrow +\infty} \sum_{k=1}^m [u_k(x) - \chi_k u_{k-1}(x)] \right\} \\ &= \mathcal{L} \left[\lim_{m \rightarrow +\infty} u_m(x) \right] \\ &= 0, \end{aligned}$$

which gives due to $\hbar \neq 0$ that

$$\sum_{k=1}^{+\infty} R_k(x) = 0.$$

Then, due to the definition (22) and above expression, one has

$$\begin{aligned} \sum_{k=1}^{+\infty} R_k(x) &= \sum_{k=1}^{+\infty} \sum_{j=0}^{k-1} \left[x u_j''(x) u_{k-1-j}''(x) - u_{k-1-j}(x) \sum_{i=0}^j u_i(x) u_{j-i}(x) \right] \\ &= x \left[\sum_{k=0}^{+\infty} u_k''(x) \right]^2 - \left[\sum_{k=0}^{+\infty} u_k(x) \right]^3 \\ &= x \left[\frac{d^2 s(x)}{dx^2} \right]^2 - s^3(x) \\ &= 0. \end{aligned}$$

Besides, due to (21) and definition (6) of $u_0(x)$, one has

$$s(0) = 1, \quad s(+\infty) = 0.$$

So, $s(x)$ satisfies the Thomas–Fermi equation (3) and the corresponding boundary conditions (2) and therefore is its exact solution. This ends the proof. \square

When $\hbar = -1/2$, the analytic result at the 40th-order of approximation agrees well with that at the 60th-order of approximation, as shown in Fig. 1. So, it is obvious that the series (31) converges when $\hbar = -1/2$. Then, due to above convergence theorem, it *must* be the exact solution of the Thomas–Fermi equation. This is indeed true. The analytic approximation at the 60th-order of approximation agrees well with the numerical result, as shown in Fig. 2.

The energy of a neutral atom in the Thomas–Fermi model is determined by

$$E = \frac{6}{7} \left(\frac{4\pi}{3} \right)^{2/3} Z^{7/3} u'(0),$$

where Z is the unclear charge. The initial slope $u'(0)$ of the Thomas–Fermi equation is provided by Kobayashi [32] as

$$u'(0) = -1.588071. \quad (33)$$

The approximations of the initial slope $u'(0)$ given by (32) are listed in the Table 1. Obviously, the error decreases as the order of approximation increases.

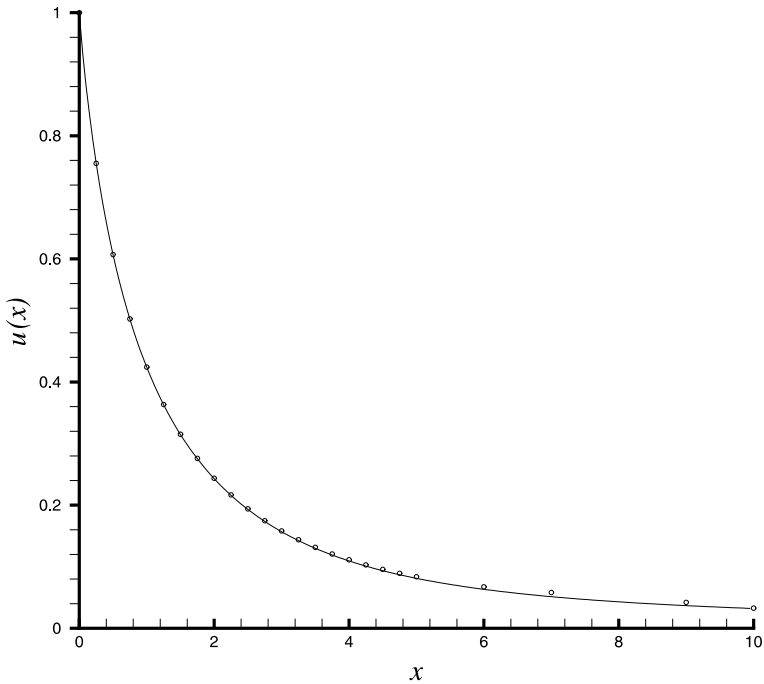


Fig. 2. Comparison of the analytic result of the Thomas–Fermi equation with the numerical result. Solid line: analytic result at the 60th-order approximation when $\hbar = -1/2$; symbols: numerical result.

Table 1
Approximations of the initial slope $u'(0)$ given by (31) when $\hbar = -1/2$ and the corresponding errors to Kobayashi’s result

Order of approximation	$u'(0)$	Error (%)
10	-1.50014	5.54
20	-1.54093	2.97
30	-1.55595	2.02
40	-1.56373	1.53
50	-1.56848	1.23
60	-1.57168	1.03
70	-1.57399	1.01
80	-1.57572	0.78
90	-1.57708	0.69
100	-1.57816	0.62

Due to (16) it holds

$$u'(0) = \left. \frac{\partial \phi(x; p)}{\partial x} \right|_{p=1, x=0}.$$

Table 2

Approximations of the initial slope $u'(0)$ given by diagonal Padé approximants of (31) when $\hbar = -1/2$ and the corresponding errors to Kobayashi's result

Padé approximants	$u'(0)$	Error (%)
[10/10]	-1.51508	4.6
[20/20]	-1.58281	3.3×10^{-1}
[30/30]	-1.58606	1.3×10^{-1}
[40/40]	-1.58668	8.8×10^{-2}
[45/45]	-1.58702	6.6×10^{-2}
[50/50]	-1.58712	6.0×10^{-2}

Table 3

Approximations of $u''(0)$ given by (32) when $\hbar = -1/2$

Order of approximation	$u''(0)$
10	13.0003
20	23.0819
30	33.1119
40	43.1275
50	53.1370
60	63.1434
70	73.1480
80	83.1514
90	93.1542
100	103.1560

Due to (17), one has

$$\left. \frac{\partial \phi(x; p)}{\partial x} \right|_{x=0} = u'_0(0) + \sum_{k=1}^{+\infty} u'_k(0) p^k. \quad (34)$$

Employing the $[m/m]$ diagonal Padé approximants [33,34] to the above power series of p and then setting $p = 1$, one gains more accurate approximations of the initial slope $u'(0)$, as shown in Table 2. Note that the error decreases with the increase of the degree of the Padé approximants.

Due to Eq. (1), it holds $u''(0) \rightarrow +\infty$ as $x \rightarrow 0$. The approximations of $u''(0)$ given by (32) when $\hbar = -1/2$ are listed in the Table 3. Obviously, $u''(0)$ of the analytic solution (31) indeed tends to infinity.

3. Conclusion and discussions

The homotopy analysis method has some advantages over other analytic approaches such as perturbation methods, artificial parameter method, the δ -expansion method, the decomposition method and so on. First, the homotopy analysis method does not depend upon any small parameters so that one can

employ it to the fully nonlinear equation (3). Besides, the homotopy analysis method provides us with freedom to choose the initial guess (6) and the auxiliary linear operator (7) so that one can represent the solution of the Thomas–Fermi equation by the set of base functions (5). Finally but most importantly, the homotopy analysis method provides us with a convenient way to control the convergence of approximation series and adjust convergence regions when necessary, which is a fundamental qualitative difference in analysis between the homotopy analysis method and *all* other reported analytic techniques.

Note that $\hbar = -1$ corresponds to the traditional way to construct a homotopy. It should be emphasized that the series (31) is divergent when $\hbar = -1$ but convergent when $-1/2 \leq \hbar < 0$. So, the auxiliary parameter \hbar plays a very important role in the homotopy analysis method.

To the best of our knowledge it is the first time such an elegant and explicit analytic solution of the Thomas–Fermi equation is given. By means of the recurrence formulas (26)–(30), it is quite easy to gain high-order approximations of the Thomas–Fermi equations. Note that a lot of fundamental functions are defined by such kind of recurrence formulas. So, the series (31) (when $-1/2 \leq \hbar < 0$) can be regarded as one *definition* of the exact solution of the Thomas–Fermi equations. This illustrates the validity and potential of the homotopy analysis method for nonlinear problems in the science and engineering.

Acknowledgement

This work is supported by National Science Fund for Distinguished Young Scholars of China (approval no. 50125923).

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