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The improved homotopy analysis method for the Thomas–Fermi equation

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ABSTRACT

The homotopy analysis method (HAM) is sharpened to solve the Thomas–Fermi equation. Some techniques are employed, including the use of asymptotic analysis to introduce proper transformation, and the use of optimal initial guess and optimal auxiliary linear operator to accelerate the convergence of homotopy approximations. The optimal convergence-control parameters are determined by the minimum of the squared residual error. As a result, the initial slop is provided with more-than-10-digit accuracy, which is far more accurate than the results obtained by other authors using the same method. It demonstrates the flexibility and power of the HAM equipped with these techniques.

1. Introduction

One of the most important nonlinear ordinary differential equations that occurs in mathematical physics is the Thomas–Fermi (TF) equation [1,2]

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

with the boundary conditions

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

in common case. The above equation is defined in a semi-infinite interval which has a singularity at $x = 0$ since $u''(x) \to \infty$ as $x \to 0$. Because of the importance of this problem in physics, it has been solved by different methods during the past century, such as the differential analyzer [2], the δ-expansion method [3,4], the variational approach [5], Adomian's decomposition method [6], the Chebyshev pseudospectral method [7], and the Hankel–Padé method [8,9]. All of these solutions give the value of the initial slope $u'(0)$, which plays an important role in determining the energy for a neutral atom. The best-known result is given by Kobayashi [10], who employed the inward numerical integration and gave the initial slope $u'(0) = -1.5880710$. So far, the most accurate value of $u'(0)$ is -1.588071022611375313, given by Fernández [9] using Hankel–Padé method.

As an analytic tool to solve nonlinear differential equations, the homotopy analysis method (HAM) [11] has been successfully used to investigate a variety of nonlinear problems in science and engineering. The HAM enjoys great freedom in choosing auxiliary linear operator and initial guess. In particular, it provides a convenient way to guarantee the convergence of solution series. In most cases, the solution series given by the HAM converge quickly. However, when the HAM is applied to the TF equation [11–15], which has a singularity at $x = 0$, the approximations of the initial slope $u'(0)$ converge rather slowly, as pointed out by Fernández [8,9]. We analyzed the reason of the slow convergence and found that the singular

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property at $x = 0$ is not automatically satisfied in the homotopy series solutions given by the previous HAM-based approaches. This finding inspires us to make proper transformations so that the singular property is satisfied automatically in the series solution. We introduce the transformation through the analysis of asymptotic property about the singularity. Furthermore, since the HAM provides us freedom to choose initial guess and auxiliary linear operator, we choose optimal ones so as to improve the convergence rate of the solution series. Our current approximations converge much faster than those given by the previous HAM approach [12], and especially we gain a very accurate value of the initial slope $u'(0)$ with only $6.6 \times 10^{-12}\%$ relative error.

This paper is arranged as follows: In Section 2 we analyze the asymptotic property of the TF equation. Using this information, the original equation is transformed into a new but more tractable one. In Section 3 the HAM is applied to gain quickly convergent solution series. Section 4 gives the results in details, which show that the current approximations are much better than the results given by the previous HAM-based approach. Some conclusions and discussions are made in the final section.

2. Asymptotic property

Although the exact solution $u(x)$ of the TF equation is unknown, we can get some valuable information by analyzing its asymptotic properties as $x \to 0$ and $x \to +\infty$. Many authors have discussed the asymptotic properties of the solution of TF equation [16,17]. However, we recalculate some of these asymptotic properties to make the derivation of the transformations (4) and the extra boundary condition (8) easy to understand.

As $x \to 0$, it holds from Eq. (1) that $u''(x) \sim 1/\sqrt{x}$, which gives

$$u'(x) \sim 2\sqrt{x} + \mu, \quad \text{as } x \to 0,$$

where $\mu = u'(0)$ is an unknown constant. Then, we have the asymptotic property

$$u(x) \sim 1 + \mu x + \frac{4}{3}x^{3/2} + \cdots, \quad \text{as } x \to 0. \tag{3}$$

So, from the asymptotic property $u''(x) \sim 1/\sqrt{x}$ as $x \to 0$, it is natural to introduce a new independent variable $\xi = \sqrt{x}$. Besides, considering the right-hand side term $u^{3/2}(x)$ of Eq. (1), it is natural to define such a new dependent variable $w = \sqrt{u(x)}$. Thus, under the transformation

$$w(\xi) = \sqrt{u(x)}, \quad \xi = \sqrt{x}, \tag{4}$$

the original Eq. (1) becomes

$$\xi[w(\xi)w''(\xi) + w'2(\xi)] - w(\xi)w'(\xi) - 2\xi^2 w^3(\xi) = 0, \tag{5}$$

subject to the boundary conditions

$$w(0) = 1, \quad w(+\infty) = 0. \tag{6}$$

Accordingly, the asymptotic property (3) becomes

$$w(\xi) \sim 1 + \frac{1}{2}\mu\xi^2 + \frac{2}{3}\xi^3 + \cdots, \quad \text{as } \xi \to 0. \tag{7}$$

In case of $\xi \to 0$, according to the asymptotic property (7), $w(\xi)$ does not contain the linear term ξ. Thus, we have one additional boundary condition

$$w'(0) = 0. \tag{8}$$

Note that there exist three boundary conditions now, but the governing Eq. (5) is only second-order. Differentiating both sides of Eq. (5) with respect to ξ, we have

$$w(\xi)w'''(\xi) + 3w'(\xi)w''(\xi) - 6\xi w^2(\xi)w'(\xi) - 4w^3(\xi) = 0, \tag{9}$$

subject to the three boundary conditions

$$w(0) = 1, \quad w'(0) = 0, \quad w(+\infty) = 0. \tag{10}$$

Note that the above third-order differential equation is equivalent to Eq. (1), but the singularity at origin is removed, as can be seen from property (7). Hence, trying to find a proper transformation like (4) from asymptotic analysis is what we advised to apply the HAM to nonlinear problems with singularity. If such transformation is found, then the series solution obtained by the HAM would converge quickly. Otherwise, the series would converge slowly.

Now let us analyze the asymptotic property of solution at infinity. To change the domain from $[0, +\infty]$ to $[1, +\infty]$, we make the transformation [11]

$$t = 1 + \lambda\xi, \quad g(t) = w(\xi), \tag{11}$$

where $\lambda > 0$ is a parameter to be chosen. Then, Eq. (9) becomes

$$\lambda^3 g(t)g'''(t) + 3\lambda^3 g'(t)g''(t) - 6(t-1)g^2(t)g'(t) - 4g^3(t) = 0, \tag{12}$$

subject to the boundary conditions

$$g(1) = 1, \quad \left.\frac{dg(t)}{dt}\right|_{t=1} = 0, \quad g(+\infty) = 0. \tag{13}$$

Assume that $g(t) \to 0$ algebraically so that $g(t)$ has the asymptotic property

$$g(t) \sim t^k \quad \text{as } at \to +\infty, \tag{14}$$

where $k < 0$ is an unknown constant. Substituting it into Eq. (12) and balancing the main terms, we have

$$k = -3. \tag{15}$$

Assume that $g(t)$ can be expressed by the set of base functions

$$\{t^{-m} | m \geqslant 3\} \tag{16}$$

in the form

$$g(t) = \sum_{m=3}^{+\infty} c_m t^{-m}, \tag{17}$$

where c_m is a coefficient. This provides us with the so-called solution expression, which plays an important role in the frame of the HAM. The solution of the original Eq. (1) reads

$$u(x) = g^2(1 + \lambda\sqrt{x}). \tag{18}$$

3. Mathematical formulation

To obey the solution expression (17), we choose the initial guess

$$g_0(t) = \frac{4+\epsilon}{t^3} + \frac{-3-2\epsilon}{t^4} + \frac{\epsilon}{t^5}, \tag{19}$$

where ϵ is an unknown parameter to be determined later. Note that the initial guess $g_0(t)$ satisfies the boundary conditions (13). For different values of ϵ, Eq. (19) corresponds to different initial guesses, and thus there should exist an optimal one among them. To obey the solution expression (17), we choose the auxiliary linear operator

$$\mathcal{L}_p[\Phi(t;q)] = t^3 \frac{\partial^3 \Phi}{\partial t^3} + k_1 t^2 \frac{\partial^2 \Phi}{\partial t^2} + k_2 t \frac{\partial \Phi}{\partial t} + k_3 \Phi \tag{20}$$

with the property

$$\mathcal{L}_p(t^j) = 0, \quad j = p, -3, -4, \tag{21}$$

where p is an integer more than -2, and the coefficients k_1, k_2 and k_3 are determined by means of the property (21). Its inverse operator $\mathcal{L}_p^{-1}$ has the property

$$\mathcal{L}_p^{-1}(t^n) = \frac{t^n}{(n+3)(n+4)(n-p)}, \quad n \leqslant -5. \tag{22}$$

Note that (20) implies a family of linear operators. For different values of p, it corresponds to different auxiliary linear operators, and there should exist an optimal one among them in the frame of the HAM.

Based on Eq. (12), we define the nonlinear operator

$$\mathcal{N}[\Phi(t;q)] = \lambda^3 \Phi \frac{\partial^3 \Phi}{\partial t^3} + 3\lambda^3 \frac{\partial \Phi}{\partial t} \frac{\partial^2 \Phi}{\partial t^2} - 6(t-1)\Phi^2 \frac{\partial \Phi}{\partial t} - 4\Phi^3. \tag{23}$$

Let c_0 denote a nonzero auxiliary parameter, $H(t)$ the auxiliary function, respectively. We construct the zeroth-order deformation equation

$$(1-q)\mathcal{L}_p[\Phi(t;q) - g_0(t)] = qc_0 H(t)\mathcal{N}[\Phi(t;q)], \tag{24}$$

subject to the boundary conditions

$$\Phi(1;q) = 1, \quad \left.\frac{d\Phi(t;q)}{dt}\right|_{t=1} = 0, \quad \Phi(+\infty;q) = 0, \tag{25}$$

where

$$\Phi(t;q) = \sum_{m=0}^{+\infty} g_m(t) q^m \tag{26}$$

is the Maclaurin series, $q \in [0,1]$ is an embedding parameter, and $g_m(t)$ is an unknown function to be determined.

Applying the derivative operator

$$D_m(\square) = \frac{1}{m!} \frac{\partial^m \square}{\partial q^m}\bigg|_{q=0} \tag{27}$$

to both sides of Eq. (24) and using its properties [18], we quickly gain the corresponding mth-order deformation equation

$$\mathcal{L}_p[g_k(t) - \chi_k g_{k-1}(t)] = c_0 H(t) \delta_{k-1}(t), \tag{28}$$

subject to the boundary conditions

$$g_k(1) = g_k'(1) = g_k(+\infty) = 0, \quad k \geqslant 1, \tag{29}$$

where

$$\delta_{k-1}(t) = \sum_{j=0}^{k-1}\left[\lambda^3 (g_j(t) g_{k-1-j}'''(t) + 3 g_j'(t) g_{k-1-j}''(t)) - 6(t-1) g_{k-1-j}'(t) \sum_{i=0}^{j} g_{j-i}(t) g_i(t) - 4 g_{k-1-j}(t) \sum_{i=0}^{j} g_{j-i}(t) g_i(t)\right] \tag{30}$$

and

$$\chi_m = \begin{cases} 0, & m \leqslant 1, \\ 1, & m > 1. \end{cases} \tag{31}$$

The solution of Eqs. (28) and (29) reads

$$g_k(t) = \chi_k g_{k-1}(t) + g_k^*(t) + C_1 t^p + C_2 t^{-3} + C_3 t^{-4}, \tag{32}$$

where

$$g_k^*(t) = \mathcal{L}_p^{-1}[c_0 H(t) \delta_{k-1}(t)] \tag{33}$$

is a particular solution of Eq. (28), and

$$C_1 = 0, \quad C_2 = -4 g_k^*(1) - \frac{d g_k^*}{dt}\bigg|_{t=1}, \quad C_3 = -C_2 - g_k^*(1) \tag{34}$$

are determined by the boundary conditions (29).

Let $H(t)$ be of the simplest form $H(t) = c t^{\sigma}$, which might obey the solution expression (17). It is found that when $\sigma > 4$ the solution $g_k^*(t)$ contains the term $t \ln t$ that disobeys the rule of solution expression (17). When $\sigma < 4$ the coefficient of some term in the approximation cannot be improved even if the order of approximation tends to infinity. Hence, we choose [11]

$$H(t) = \frac{t^4}{\lambda^3} \tag{35}$$

to obey the solution expression (17). The denominator λ^3 in (35) comes from the coefficient of $\Phi \frac{\partial^3 \Phi}{\partial t^3}$ in the nonlinear operator (23).

Remark 1

(i) Using (21) and (22) we can directly write out the solution of Eqs. (28) and (29).
(ii) $g_1, g_2, \ldots$ can be gained one after the other.
(iii) The mth-order approximation of $g(t)$ is given by

$$G_m(t) = \sum_{k=0}^{m} g_k(t). \tag{36}$$

(iv) To measure the accuracy of G_m, the squared residual error of Eq. (12) is defined by

$$E_m = \int_1^{+\infty} [\mathcal{N}(G_m(t))]^2 dt. \tag{37}$$

The smaller E_m, the more accurate the mth-order approximation $G_m(t)$.

(v) The corresponding mth-order approximation of $u(x)$ is given by

$$U_m(x) = G_m^2(1 + \lambda\sqrt{x}), \tag{38}$$

which automatically satisfies the asymptotic property of $u(x)$ as $x \to 0$ and $x \to +\infty$.

4. Results and analysis

As mentioned above, the squared residual error E_m defined by (37) is a kind of measurement of the accuracy of the mth-order approximation. However, the exact squared residual error E_m is expensive to calculate when m is large. In practice, we approximate E_m by

$$E_m \approx \sum_{i=0}^{M} [\mathcal{N}(G_m(t))]^2|_{t=1+i\Delta t}, \tag{39}$$

or

$$E_m \approx \sum_{i=0}^{M} \left(\sum_{k=0}^{m-1} \delta_k(t) \right)^2 \Bigg|_{t=1+i\Delta t}. \tag{40}$$

In this paper, E_m is approximated by (40), $M = 200$ and $\Delta t = 0.1$ are used.

Note that we have four unknown auxiliary parameters, namely p, ϵ, λ and c_0, whose optimal values are determined by the minimum of E_m, as suggested by Liao [19]. However, it is difficult to gain the exact optimal values because of expensive computation. Hence, we determine these parameters as follows: first, setting $c_0 = -1$, we obtain $p = 15$ by minimizing E_2 which is a function of p, ϵ and λ; secondly, setting $p = 15$, we obtain $\lambda \approx 0.318 \approx 5/16$ and $\epsilon \approx -5.057 \approx -86/17$ by minimizing E_6 which is a function of λ, ϵ and c_0; finally, setting $p = 15, \lambda = 5/16$ and $\epsilon = -86/17$, we obtain $c_0 \approx -1.382 \approx -11/8$ by minimizing E_{12} which is a function of c_0. In this way, we have the "optimal" auxiliary parameters

$$p = 15, \quad \lambda = 5/16, \quad \epsilon = -86/17, \quad c_0 = -11/8, \tag{41}$$

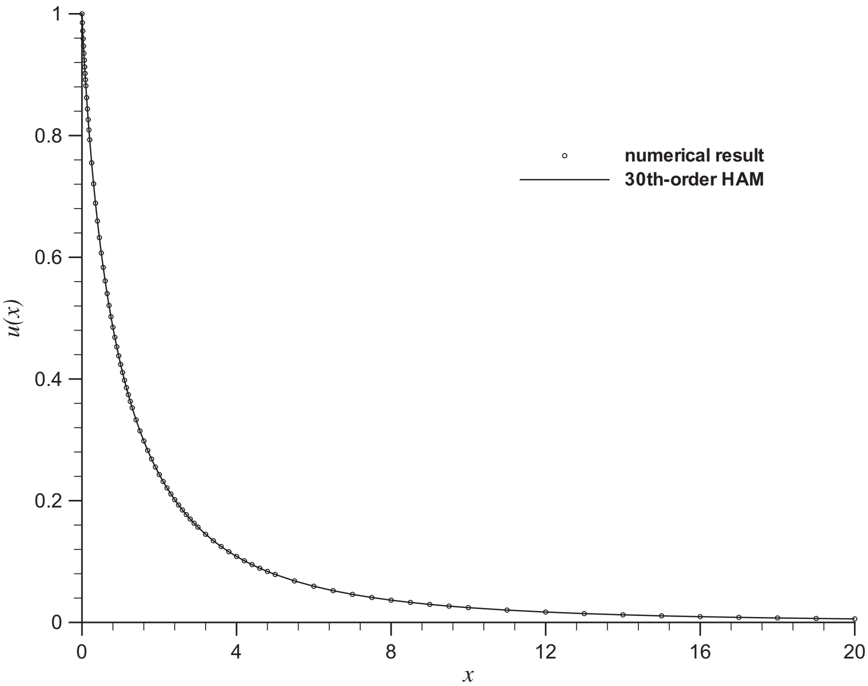

Fig. 1. Comparison of the 30th-order HAM approximations with Kobayashi's numerical result. Circles: numerical result; solid line: 30th-order homotopy approximation.

and the corresponding auxiliary linear operator reads

$$\mathcal{L}_{15}[\Phi(t;q)] = t^3\frac{\partial^3\Phi}{\partial t^3} - 5t^2\frac{\partial^2\Phi}{\partial t^2} - 100t\frac{\partial\Phi}{\partial t} - 180\Phi. \tag{42}$$

Note that $\mathcal{L}_{15}$ can be regarded as an optimal auxiliary linear operator, so does (19) as an optimal initial guess.

It should be emphasized that the four auxiliary parameters p, ϵ, λ and c_0 have no physical meanings, but they play an important role in the convergence of the solution series. Thus, all of them can be regarded as convergence-control parameters. Using these optimal convergence-control parameters, the corresponding series converge quickly. The 30th-order approximation agrees well with the numerical values given by Kobayashi [10], as shown in Fig. 1. As shown in Table 1, the approximations given by the current optimal HAM approach converge much faster than those given by Liao's early approach [12]: the 60th-order approximation of $u'(0)$ has 1.0% relative error for Liao's early approach, but only 3.0×10^{-9} relative error for the current approach. Furthermore, the Padé technique [20–21] is applied to accelerate the convergence of $u'(0)$, as shown in Table 2: the [30,30] Padé approximation of $u'(0)$ given by the current optimal HAM approach has only 6.6×10^{-12} relative error. The [30,30] Padé approximations of $u(x)$ and $u'(x)$ are compared with the numerical results [10] in Table 3, where 0.0^246029 means 0.0046029. Note that the singular property $u''(0) = \infty$ is automatically satisfied in the current approach, since $u''(x) \sim cx^{-1/2}$ as x tends to 0. However, this singular property is not automatically satisfied in Liao's early HAM-based approach [12]. This is the reason why the approximations of $u'(0)$ by Liao's early approach converge slowly.

As the computational efficiency is concerned, the current approach takes less than 70 seconds to gain the 20th-order approximation on a PC with an Intel Core 2 Quad 2.66GHz CPU. However, the CPU time increases quickly for higher-order approximations. We have handled this problem by a kind of truncation technique, which projects the right hand side of the deformation equation to its first few terms so as to reduce the number of terms in the series solution. We will describe this technique in details somewhere else.

Table 1
The comparison of $u'(0)$.

Order m	Liao [12]		Present work	
	$u'(0)$	Relative error (%)	$u'(0)$	Relative error (%)
10	−1.50014	5.5	−1.5880699210	9.6×10^{-5}
20	−1.54093	3.0	−1.5880710127	5.9×10^{-7}
30	−1.55595	2.0	−1.5880710212	8.1×10^{-8}
40	−1.56373	1.5	−1.5880710222	2.1×10^{-8}
50	−1.56848	1.2	−1.5880710225	7.2×10^{-9}
60	−1.57168	1.0	−1.5880710226	3.0×10^{-9}
Fernández's result [9]: −1.588071022611375313				

Table 2
The $[m, m]$ Padé approximations comparison of $u'(0)$.

$[m,m]$	Liao [12]		Present work	
	$u'(0)$	Relative error (%)	$u'(0)$	Relative error (%)
[10,10]	−1.51508	4.6	−1.5880710217246	5.6×10^{-8}
[20,20]	−1.58281	3.3×10^{-1}	−1.5880710226081	2.0×10^{-10}
[30,30]	−1.58606	1.3×10^{-1}	−1.5880710226113	6.6×10^{-12}
Fernández's result [9]: −1.588071022611375313				

Table 3
The [30, 30] Padé approximations of $u(x)$ and $u'(x)$.

x	$u(x)$		$u'(x)$	
	Present	Numerical [10]	Present	Numerical [10]
0.1	0.88170	0.88170	0.99535	0.99535
0.5	0.60699	0.60699	0.48941	0.48941
1	0.42401	0.42401	0.27399	0.27399
10	0.024314	0.024314	0.0^246029	0.0^246029
20	0.0^257849	0.0^257849	0.0^364725	0.0^364725
50	0.0^363226	0.0^363226	0.0^432499	0.0^432499
100	0.0^310042	0.0^310024	0.0^527089	0.0^527393

5. Conclusions

In this paper the HAM is sharpened to solve the famous TF equation and gives rather good approximation of the initial slope. Using the asymptotic property of the TF equation, the original differential equation is transformed into an equivalent but more tractable one so that the singular property is automatically satisfied in the solution series. Moreover, we choose the optimal initial value and optimal auxiliary linear operator to accelerate the convergence of the solution series. As a result, the initial slop of the TF function is obtained with more-than-10-digit accuracy, which is far more accurate than the approximations given by the early HAM approach. We believe that the techniques of the HAM presented in this work can be used in general to handle other similar nonlinear problems with singularity so as to obtain much better approximations.

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