Cent. Eur. J. Phys. • 9(3) • 2011 • 891-895
DOI: 10.2478/s11534-010-0059-z

VERSITA

Central European Journal of **Physics**

# An optimal iteration method with application to the Thomas-Fermi equation

**Short Communication**

Vasile Marinca*, Nicolae Herişanu†

1 *Politehnica University of Timişoara, Bd. M.Viteazu, nr. 1, 300222 Timişoara, Romania*

2 *Center for Advanced and Fundamental Technical Research, Romanian Academy, Timişoara Branch, Bd. M.Viteazu, nr. 24, 300223 Timişoara, Romania*

**Received 24 May 2010; accepted 17 June 2010**

**Abstract:** The aim of this paper is to introduce a new approximate method, namely the Optimal Parametric Iteration Method (OPIM) to provide an analytical approximate solution to Thomas-Fermi equation. This new iteration approach provides us with a convenient way to optimally control the convergence of the approximate solution. A good agreement between the obtained solution and some well-known results has been demonstrated. The proposed technique can be easily applied to handle other strongly nonlinear problems.

**PACS (2008):** 02.70.-c; 02.60.-x

**Keywords:** Optimal Parametric Iteration Method (OPIM) • Thomas-Fermi equation



## 1. Introduction

We consider the nonlinear differential equation called the Thomas-Fermi equation for the electron density around the nucleus of an atom which may be written as

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

with the boundary conditions

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

This equation is also frequently used for calculating form factors and for obtaining effective potentials which can be used as initial trial potentials in self-consistent field calculations.

Because of the singularity at $x = 0$, it is known that the solution of the Thomas-Fermi equation is very sensitive to the value of the first derivative at $x = 0$, which ensures a smooth and monotonic decay of the solution from 1 at $x = 0$ to 0 at $x = \infty$.

Approximate solutions of the Thomas-Fermi equation were proposed using different techniques such as the numerical solution given by Kobayashi [1], some variational approaches [2–4], a numerical integration technique [5], a monotone discretization technique [6], $\delta$-expansion method [7], a modified decomposition method and Pade approximants [8], the homotopy analysis method [9–12], the Green's function method [13] and some quasi-linearization

*E-mail: vmarinca@mec.upt.ro
†E-mail: herisanu@mec.upt.ro

techniques [14]. The main concern of all these works was to derive an approximate analytical solution to Eq. (1) and to determine a high accurate value for the initial slope of the potential $y'(0)$. The importance of the initial slope $y'(0)$ is that it plays a major role in determining the energy of neutral atom in the Thomas-Fermi approximation.

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

where $Z$ is the nuclear charge.
In recent years, a growing interest toward the application of iterative techniques in nonlinear problems has appeared in science and engineering. J.H. He proposed the variational iteration method via a Lagrange multiplier [15] and some modifications of this method were also reported [16]. Mickens [17] proposed an iteration scheme for a nonlinear problem described as

$$\ddot{x} + f(x) = 0, \quad x(0) = A, \quad \dot{x}(0) = 0, \tag{4}$$

where $f(x)$ is an odd function. The original Mickens procedure is given as

$$x_k'' + \omega^2 x_k = g(\omega, x_{k-1}), \quad k = 1, 2, \ldots, \tag{5}$$

where $g(\omega, x) = \omega^2 x - f(x)$, $\omega$ is the a priori unknown frequency and $x_0(t) = A\cos\omega t$ is the input of the starting function. Lim et al. [18] proposed a modified iteration scheme

$$\ddot{x}_{k+1} + \omega^2 x_{k+1} = g(\omega, x_{k-1}) + g_x(\omega, x_{k-1})(x_k - x_{k-1}), \quad k = 0, 1, 2, \ldots \tag{6}$$

with the inputs of starting functions as $x_{-1}(t) = x_0(t) = A\cos\omega t$, where $g_x = \frac{\partial g}{\partial x}$. Later, Marinca and Herişanu [19, 20] proposed a new iteration method by combining Mickens' and He's iteration methods.
In this paper we propose a new iteration procedure, namely the Optimal Parametric Iteration Method (OPIM), to find analytical approximate solutions to Thomas-Fermi equation (1) with the initial conditions (2). This new iterative approach containing a new iteration scheme involves the presence of a finite number of initially unknown parameters, which are optimally determined later. In the construction of the iteration scheme, the nonlinear function appearing in the nonlinear equation describing the problem under study is replaced by the corresponding truncated Taylor series along with some auxiliary functions which contains the unknown parameters. These unknown parameters are determined in a rigorous way through a computational procedure based on a least square technology and therefore the approximate result rapidly converges to an accurate solution. Alternatively, other methods could be employed in order to obtain the optimal values of these parameters, such as the collocation method or the Galerkin method. The efficiency of our procedure is proved since an accurate periodic solution is explicitly and analytically obtained in this case after only one iteration. The approximate solution obtained through this new approach rapidly converges to an accurate solution.
The paper is organized as follows: section 2 briefly presents the proposed method, section 3 is an application of the proposed method which consists in numerical examples, and the paper ends with section 4 presenting some conclusions.

## 2. Formulation and solution approach

Eq. (1) can be written in the form

$$xy''^2 - y^3 = 0, \tag{7}$$

which can be rewritten in the more general form

$$y'' - \lambda^2 y = f(x, y, y''), \tag{8}$$

where

$$f(x, y, y'') = xy''^2 + y'' - \lambda^2 y - y^3 \tag{9}$$

is a nonlinear function.
Applying the well-known Taylor's theorem for any real values $y_0, y_0'', \alpha$ and $\beta$, we have

$$\begin{aligned} f(x, y_0 + \alpha, y_0'' + \beta) =& f(x, y_0, y_0'') + \frac{\alpha}{1!} f_y(x, y_0, y_0'') \\ &+ \frac{\beta}{1!} f_{y''}(x, y_0, y_0'') + \ldots, \end{aligned} \tag{10}$$

where $F_y = \frac{\partial F}{\partial y}$.
In our procedure, we consider the following functions:

$$\begin{aligned} y_0 &= \sum_{i=1}^{m} C_i e^{-i\lambda x}, \\ y_0'' &= \lambda^2 \sum_{i=1}^{m} C_i i^2 e^{-i\lambda x}, \\ \alpha(x) &= \sum_{j=m+1}^{n} C_j e^{-(j-m)\lambda x}, \\ \beta(x) &= \sum_{k=n+1}^{p} C_k e^{-(k-n)\lambda x}, \end{aligned} \tag{11}$$

where $\lambda$ and $C_1, C_2, \ldots, C_p$ are unknown constants at this moment and $m, n$ and $p$ are positive integers.
We therefore can construct the following iteration formula

$$\begin{aligned} y''_{n+1} - \lambda^2 y_{n+1} =& f(x, y_n, y''_n) + \alpha(x) f_y(x, y_n, y''_n) \\ &+ \beta(x) f_{y''}(x, y_n, y''_n), \\ y_{n+1}(0) =& 1, \\ y_{n+1}(\infty) =& 0, \end{aligned} \tag{12}$$

where the initial approximation $y_0$ and the functions $\alpha(x)$ and $\beta(x)$ are given by Eq. (11) and $n$ takes on the positive integers $0, 1, 2, \ldots$.
If we consider $m = 1, n = 3, p = 6$ and the functions:

$$y_0 = C_1 e^{-\lambda x}, \quad y''_0 = \lambda^2 C_1 e^{-\lambda x}, \tag{13}$$

$$\alpha(x) = C_2 e^{-\lambda x} + C_3 e^{-2\lambda x}, \tag{14}$$

$$\beta(x) = C_4 e^{-\lambda t} + C_5 e^{-2\lambda x} + C_6 e^{-3\lambda x}, \tag{15}$$

then for $n = 0$ into Eq. (2), we obtain

$$\begin{aligned} y''_1 - \lambda^2 y_1 =& f(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}) \\ &+ (C_2 e^{-\lambda x} + C_3 e^{-2\lambda x}) f_y(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}) \\ &+ (C_4 e^{-\lambda x} + C_5 e^{-2\lambda x} + C_6 e^{-3\lambda x}) \\ & f_{y''}(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}), \\ y_1(0) =& 1, \quad y_1(\infty) = 0. \end{aligned} \tag{16}$$

From Eqs. (9) and (13) we obtain

$$f(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}) = \lambda^4 C_1^2 x e^{-2\lambda x} - C_1^3 e^{-3\lambda x}, \tag{17}$$

$$f_y(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}) = -\lambda^2 - 3C_1^2 e^{-2\lambda x}, \tag{18}$$

$$f_{y''}(x, C_1 e^{-\lambda x}, \lambda^2 C_1 e^{-\lambda x}) = 1 + 2\lambda^2 C_1 x e^{-\lambda x}. \tag{19}$$

Substituting Eqs. (17), (18) and (19) into Eq. (16) we obtain

$$\begin{aligned} y''_1 - \lambda^2 y_1 =& \left[C_4 - \lambda^2 C_2\right] e^{-\lambda x} \\ &+ \left[C_5 - \lambda^2 C_3 + (\lambda^4 C_1^2 + 2\lambda^2 C_1 C_4) x\right] e^{-2\lambda x} \\ &+ \left[2\lambda^2 C_1 C_5 x - C_1^3 - 3C_1^2 C_2 + C_6\right] e^{-3\lambda x} \\ &+ \left[2\lambda^2 C_1 C_6 x - 3C_1^2 C_3\right] e^{-4\lambda x}, \\ y_1(0) =& 1, \quad y_1(\infty) = 0. \end{aligned} \tag{20}$$

From Eq. (20) we obtain the first-order approximate solution of Thomas-Fermi equation

$$\begin{aligned} y_1(x) =& (Ax + B) e^{-\lambda x} + (Cx + D) e^{-2\lambda x} \\ &+ (Ex + F) e^{-3\lambda x} + (Gx + H) e^{-4\lambda x}, \end{aligned} \tag{21}$$

where

$$\begin{aligned} A =& \frac{\lambda}{2} C_2 - \frac{1}{2\lambda} C_4, \\ B =& 1 - \frac{4\lambda}{9} C_1^2 - \frac{8}{9\lambda} C_1 C_4 + \frac{1}{3} C_3 - \frac{1}{3\lambda^2} C_5 \\ &- \frac{3}{16\lambda} C_1 C_5 + \frac{3}{8\lambda^2} C_1^2 C_2 + \frac{1}{8\lambda^2} C_1^3 \\ &+ \frac{1}{5\lambda^2} C_1^2 C_3 - \frac{16}{225\lambda} C_1 C_6 - \frac{1}{8\lambda^2} C_6, \\ C =& \frac{\lambda^2}{3} C_1^2 + \frac{2}{3} C_1 C_4, \\ D =& \frac{4\lambda}{9} C_1^2 + \frac{8}{9\lambda} C_1 C_4 - \frac{1}{3} C_3 + \frac{1}{3\lambda^2} C_5, \\ E =& \frac{1}{4} C_1 C_5, \\ F =& \frac{3}{16\lambda} C_1 C_5 - \frac{3}{8\lambda^2} C_1^2 C_2 - \frac{1}{8\lambda^2} C_1^3 + \frac{1}{8\lambda^2} C_6, \\ G =& \frac{2}{15} C_1 C_6, \\ H =& \frac{16}{225\lambda} C_1 C_6 - \frac{1}{5\lambda^2} C_1^2 C_3. \end{aligned} \tag{22}$$

The parameters $\lambda$ and $C_1, C_2, C_3, C_4, C_5, C_6$ can be determined optimally, which means the residual functional J given by

$$J = \int_0^\infty \left[x y''^2_1 - y_1^3\right]^2 dx \tag{23}$$

can be minimized:

$$\frac{\partial J}{\partial \lambda} = \frac{\partial J}{\partial C_1} = \frac{\partial J}{\partial C_2} = \ldots = \frac{\partial J}{\partial C_6} = 0. \tag{24}$$

In this way the solution (21) in the first approximation is well determined.

### Remark 2.1.

The parameters $\lambda$ and $C_i$, can also be identified using various methods, for example the collocation method, the least squares method, the Galerkin method and so on.

### Remark 2.2.

The initial approximation $u_0$ and the functions $\alpha(x)$ and $\beta(x)$ are not unique. We can consider other expressions for $y_0$, $\alpha(x)$ and $\beta(x)$, such as:

$$\begin{aligned} y_0(x) =& C'_1 e^{-\lambda x} + C'_2 e^{-2\lambda x}, \\ \alpha(x) =& C'_3 e^{-\lambda x} + C'_4 e^{-2\lambda x} + C'_5 e^{-3\lambda x}, \\ \beta(x) =& C'_6 e^{-\lambda x} + C'_7 e^{-2\lambda x} + C'_8 e^{-3\lambda x} + C'_9 e^{-4\lambda x} \end{aligned} \tag{25}$$

and so on, with the constants $\lambda$ and $C'_1, C'_2, \ldots, C'_9$, which can be determined in the same way from Eqs. (24).

***Remark 2.3.***
Eq. (1) can be written as

$$y'' - \frac{2}{(\lambda x+1)^2} y = f(x, y, y''), \tag{26}$$

where

$$f(x, y, y'') = x y''^2 + y'' - \frac{2}{(\lambda x+1)^2} y - y^3.$$

In this case, the initial approximation and the functions $\alpha(x)$ and $\beta(x)$ can be chosen in the form

$$y_0 = \frac{C_1}{\lambda x+1}, \quad y_0'' = \frac{2\lambda^2 C_1}{(\lambda x+1)^3}, \tag{27}$$

$$\alpha(x) = \frac{C_2}{\lambda x+1} + \frac{C_3}{(\lambda x+1)^2}, \tag{28}$$

$$\beta(x) = \frac{C_4}{\lambda x+1} + \frac{C_5}{(\lambda x+1)^2} + \dots. \tag{29}$$

We underline that the basic ideas of the proposed procedure are the construction of the new iteration scheme (12) and the involvement of the constants $C_1, C_2, \dots$, which are optimally determined, providing a rigorous way to control the convergence of the solution.

## 3. Numerical examples

In order to demonstrate the effectiveness of the proposed method, we follow the procedure described in the previous section and use the solution analytically obtained in (21) and Eq. (24) to find numerical results

$$\begin{aligned} \lambda &= 0.8142096804743827, \\ C_1 &= -0.1463669113967, \\ C_2 &= -417.8208014694533, \\ C_3 &= -855.9241157162435, \\ C_4 &= -281.4804345074634, \\ C_5 &= -735.7393406374861, \\ C_6 &= 95.01941123786105. \end{aligned} \tag{30}$$

From Eqs. (30) and (22), the coefficients $A, B, C, D, E, F, G$ and $H$ are determined as follows:

$$\begin{aligned} A &= 2.7581329751336514, \\ B &= -11.451371899334289, \\ C &= 27.47101530791185, \\ D &= -39.64505180499373, \\ E &= 26.92197372053835, \\ F &= 47.77913460422296, \\ G &= -1.8543596994158142, \\ H &= 4.317289100105105. \end{aligned} \tag{31}$$

In this way, the first-order approximate solution (21) of Thomas-Fermi equation is well determined.
From Eq. (21) we obtain

$$y_0' = A + C + E + G - \lambda(B + 2D + 3F + 4H). \tag{32}$$

From Eqs. (31) and (32), the approximate initial slope $y_1'(0)$ becomes

$$y_1'(0) = -1.5880659888022421 \tag{33}$$

and therefore the energy neutral atom given by Eq. (3) is well determined.
Kobayashi [1] gave the numerical result for the same problem as $y_1'(0) = -1.588071$. A comparison between different approximations of the initial slop $y_1'(0)$ is presented in Table 1. It is clear that the present result for the initial slope is better than those given by Liao's method [9, 10].

| Order of approximation | Liao [10] | Liao [9] | Present work (first-order approximation) | Kobayashi [1] |
|---|---|---|---|---|
| 10 | -1.28590 | -1.50014 | -1.5880659888 | -1.588071 |
| 20 | -1.40932 | -1.54093 | | |
| 30 | -1.46306 | -1.55595 | | |
| 40 | -1.49236 | -1.56373 | | |
| 50 | -1.51063 | -1.56848 | | |
| 60 | -1.52309 | -1.57168 | | |
| 70 | -1.53211 | -1.57399 | | |
| 80 | -1.53895 | -1.57572 | | |
| 90 | -1.54430 | -1.57708 | | |
| 100 | -1.54860 | -1.57816 | | |

**Table 1.** Comparison between different approximations of the initial slope $y_1'(0)$.

Figure 1 presents a comparison between our first-order approximate solution (21) and Liao's results [9]. The first-order analytic approximate solution $y(x)$ for $x \in [0, \infty)$

given by Eq. (21) is compared with the 60th-order approximation obtained by Liao [9]. From Fig. 1 it can be seen that the solution obtained through the proposed procedure (after only one iteration) is nearly identical with the 60th-order approximation of the series solution obtained by means of the homotopy analysis method for the same problem.

To the best of our knowledge, it is the first time then such an explicit analytic approximate solution to the Thomas-Fermi equation is given. Some series solutions were reported [9–12], without providing an explicit analytical solution in the traditional meaning of the word "analytical".

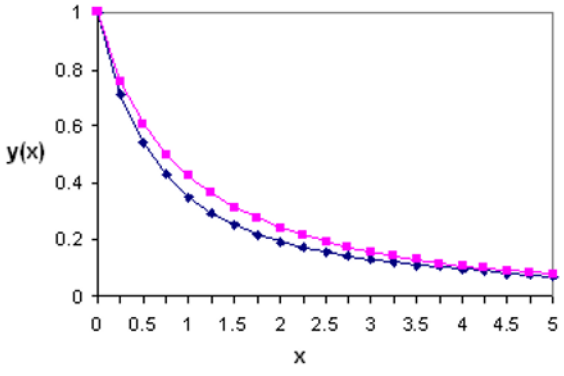


**Figure 1.** Comparison between the first-order approximate solution (21) and Liao's 60th-order approximation [9]; ♦ - present results (21), ■ - Liao's results [9].

## 4. Conclusions

In this paper a new iteration procedure, namely the Optimal Parametric Iteration Method (OPIM), is employed to propose a new analytic approximate solution for the Thomas-Fermi equation. The proposed procedure is valid even if the nonlinear equation does not contain small or large parameters. This method provides us with a simple and rigorous way to control the convergence of the solution by means of the constants $\lambda, C_1, C_2, \ldots$, which are optimally determined. Very good approximations are obtained in only a few terms. The proposed procedure provides a very good solution after only one iteration, unlike Liao's solutions [9, 10] which converge upwards after 60th-order of approximation. The proposed solution and Kobayashi's solution [1] are both higher that Liao's [9, 10] in terms of the initial slope. Besides, the present solution is an explicit analytic approximate solution and to the best of our knowledge this is the first explicit analytic approximate solution reported in the literature to the Thomas-Fermi equation.

This new iterative approach proves to be very rapid, effective and accurate and this is proved by comparing the solution obtained through the proposed method after only one iteration with the solutions obtained by means of the homotopy analysis method. For more complicated problems, if the results obtained through OPIM after the first iteration are not satisfactory, the iteration process can continue to get better results. This is not the case in this paper since after only one iteration we get an error less than $10^{-5}$ for the initial slope, which is excellent.

The technique presented in this work can be easily applied to handle other strongly nonlinear problems, including systems with damping. This paper shows one step in the attempt to develop a new nonlinear analytical technique in the absence of small or large parameters.

## References

[1] S. Kobayashi et al., J. Phys. Soc. Jpn. 10, 759 (1955)
[2] B.L. Burrows, P.W. Core, Q. Appl. Math. 42, 73 (1984)
[3] M.S. Wu, Phys. Rev. A 6, 57 (1982)
[4] J.H. He, H.M. Liu, Nonlinear Anal. Theory Methods Appl. 63, 919 (2005)
[5] H. Krutter, J. Comput. Phys. 47, 308 (1982)
[6] C. Grossmann, J. Comput. Phys. 98, 26 (1992)
[7] A. Cedillo, J. Math. Phys. 34, 2713 (1993)
[8] A.M. Wazwaz, Math. Comput. 105, 11 (1999)
[9] S.J. Liao, Appl. Math. Comput. 144, 495 (2003)
[10] S.J. Liao, Beyond perturbation: introduction to the homotopy analysis method (Chapmann & Hall/CRC Press, Boca Raton, 2003)
[11] H. Khan, H. Xu, Phys. Lett. A 365, 111 (2009)
[12] B. Yao, Appl. Math. Comput. 203, 396 (2008)
[13] C.Y. Chan, Y.C. Han, Q. Appl. Math. 45, 591 (1989)
[14] J.I. Ramos, Comput. Phys. Commun. 158, 14 (2004)
[15] J.H. He, G.C. Wu, F. Austin, Nonlinear Science Letters A, 1, 1 (2010)
[16] N. Herişanu, V. Marinca, Nonlinear Science Letters A, 1, 183 (2010)
[17] R.E. Mickens, J. Sound Vib. 16, 185 (1987)
[18] C.W. Lim, B.S. Wu, J. Sound Vib. 257, 202 (2002)
[19] V. Marinca, N. Herişanu, Acta Mech. 184, 231 (2006)
[20] N. Herişanu, V. Marinca, Int. J. Nonlin. Sci. Num. 10, 353 (2009)