New Numerical Solution For Solving Nonlinear Singular Thomas-Fermi Differential Equation

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Abstract

In this paper, the nonlinear singular Thomas-Fermi differential equation on a semi-infinite domain for neutral atoms is solved by using the generalized fractional order of the Chebyshev orthogonal functions (GFCFs) of the first kind. First, this collocation method reduces the solution of this problem to the solution of a system of nonlinear algebraic equations. Second, using solve a system of nonlinear equations, the initial value for the unknown parameter *L* is calculated, and finally, the value of *L* to increase the accuracy of the initial slope is improved and the value of y'(0) =-1.588071022611375312718684509 is calculated. The comparison with some numerical solutions shows that the present solution is highly accurate.

1 Introduction

In this section, the used methods for solving the equations on unbounded domains are expressed. Also, it is tried that a history for Thomas-Fermi equation is provided.

1.1 Differential equations on unbounded domains

Many of the problems that are formulated in fluid dynamics, astrophysics, quantum mechanics, and other sciences are defined on unbounded domains. The dif-

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ferent methods are introduced for solving this class of equations, such as semianalytical and numerical methods.

1. **Numerical methods:** Various numerical methods are provided to solve New Numerical Solution For Solving Nonlinear Singular Thomas-Fermiproblems on unbounded domains, such as the finite difference method [1], the finite element method [2], the Spectral methods [3, 4], and the Meshfree methods [5, 6].

The Spectral approximations for ordinary differential equations (ODEs) on finite domains have achieved great success and popularity in recent years, but Spectral approximations for solving ODEs on infinite or semi-infinite domains have only received limited attention. Several Spectral methods for treating infinite or semi-infinite domain problems have been proposed by different researchers:

- (a) Direct approaches, by using functions such as Laguerre, Bessel, Hermite, and Sinc functions that are orthogonal over the unbounded domains, were used by Parand et al. [7, 8], Guo & Shen [9], and Funaro & Kavian [10], and etc.
- (b) Mapping an unbounded problem to a bounded problem, for example Guo [11] has introduced a method that coverts the original problem in an infinite domain to a problem in [−1, 1], and then using the Jacobi polynomials to approximate the resulting problems. Rad et al. [12, 13] have converted an infinite domain to interval [0, 1] and then were approximate the solutions of the problems.
- (c) Another class of Spectral methods is based on rational approximations. In this approach, the basic functions on a bounded domain convert to the functions on an unbounded domain. For example, Christov [14] and Boyd [15] have developed some Spectral methods on infinite domains by using mutually orthogonal systems of rational functions. Authors of [16, 17] have applied this approach for solving many of differential equations.
- (d) A further approach consists of replacing the infinite domain with [-A, A] and the semi-infinite domain with [0, A] by choosing A sufficiently large. This method is named domain truncation. [18]
- 2. **Analytical methods:** The study of analytical and semi-analytical solutions of differential equations (DEs) play an important role in engineering, mathematical physics, and the other applied sciences. In the past several decades, various methods for obtaining solutions of DEs are presented, such as Adomian decomposition method [19], Homotopy perturbation method [20], Variational iteration method [21], Exp-function method [22, 23], and so on.

In this paper, it is attempted to introduce a Spectral method based on the generalized fractional order of the Chebyshev functions for solving Thomas-Fermi equation.

1.2 The Thomas-Fermi equation

The nonlinear singular Thomas-Fermi equation is defined as [24, 25, 26]:

$$\frac{d^2 y(t)}{dt^2} - \frac{1}{\sqrt{t}} y^{\frac{3}{2}}(t) = 0, \quad t \in [0, \infty),$$
(1)

with the boundary conditions:

$$y(0) = 1, \quad \lim_{t \to \infty} y(t) = 0.$$
 (2)

The Thomas-Fermi equation appears in the problem of determining the effective nuclear charge in heavy atoms, and because of its importance to theoretical physics, computing its solutions has attracted the attention of the Nobel laureates John Slater (chemistry) [33] and Richard Feynman (physics) [34] and of course Enrico Fermi [27].

One measure of the rapidity of convergence of the procedure is provided by the calculation of the value of the initial slope y'(0) of Thomas-Fermi potential [28]. The initial slope y'(0) is difficult to compute by any means, and plays an important role in determining many physical properties of Thomas-Fermi atom. It determines the energy of a neutral atom in Thomas-Fermi approximation:

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

where *Z* is the nuclear charge. For these reasons, the problem has been studied by many researchers and has been solved by the different techniques, that some of them are listed in Table 1.

The paper is constructed as follows: in section 2, the GFCFs and their properties are introduced. In Section 3, the method is expressed. In Section 4, results and discussions of the method are shown. Finally, a conclusion is provided.

2 Generalized Fractional order of the Chebyshev functions

In this section, the generalized fractional order of the Chebyshev functions (GFCF) are introduced.

2.1 The GFCF definition

The Chebyshev polynomials are frequently used in the polynomial approximation, Gauss-quadrature integration, integral and differential equations and Spectral methods, and also have many properties, such as orthogonal, recursive, simple real roots, complete in the space of polynomials. For these reasons, many researchers have used these polynomials in their researches [89, 90].

Author/Authors	Year	A/N	Technique
Fermi [27]	1928	А	Statistical method
Baker [29]	1930	А	Monotone and Taylor's series
Bush and Caldwell [30]	1931	Ν	Differential analyzer
Sommerfeld [31]	1932	Α	Asymptotic behavior
Feynman et al. [34]	1949	А	Taylor's series
Coulson and March [35]	1949	А	Asymptotic series
Kobayashi et al. [36]	1955	А	Asymptotic series
Mason [37]	1964	А	Rational functions
Hille [38]	1970	А	Asymptotic behavior and Taylor's series
More [39]	1976	А	Local density approximation
Graef et al. [40]	1976	Α	Asymptotic behavior
Laurenzi [41]	1990	А	Perturbative procedure
MacLeod [42]	1992	Ν	Chebyshev collocation method
Al-Zanaidi, Grossmann [43]	1996	N	Monotone discretization principle
Adomian [44]	1998	A	Adomian decomposition method(ADM)
Wazwaz [45]	1999	A	Pade - ADM
Epele et al. [46]	1999	A	Pade approximant
Mandelzweig, Tabakin [47]	2001	N	Quasilinearization iteration method
Esposito [48]	2001	A	Majorana method
Kiessling [49]	2002	A	Asymptotic behavior
Liao [50]	2002	A	Homotopy analysis method
He [51]	2003	A	Hybrid of semi-inverse and Ritz methods
Ramos [52]	2003	N	Piecewise quasilinearization technique
Zaitsev et al. [53]	2004	N	Iterative and sweep methods
	2004	A	Direct variational method
Desaix et al. [54]			
Khan and Xu [55]	2007	A	Homotopy analysis method
El-Nahhas [56]	2008	A	Homotopy analysis method
Iacono [57]	2008	A	By exploiting integral properties
Yao [58]	2008	A	Homotopy analysis method
Parand and Shahini [59]	2009	N	Rational Chebyshev collocation method
Ebaid [60]	2011	A	Improved Adomian decomposition method
Marinca and Herianu [61]	2011	Α	Optimal parametric iteration method
Oulne [62]	2011	N	Variational method
Abbasbandy, Bervillier [63]	2011	A	Pade-Hankel method
Dong [64]	2011	А	Density matrix
Caetano and Reis [65]	2011	Ν	Neural networks
Fernandez [66]	2011	A	Pade-rational approximation
Fewster-Young, Tisdell [67]	2012	A	Existence of solutions for BVP
Kusano et al. [68]	2012	Α	Existence solution and asymptotics behavior
Kusano and Manojlovic[69]	2012	Α	Solutions of Fourth Order T-F equation
Zhu et al. [70]	2012	А	Iterative and finite element methods
Turkylmazoglu [71]	2012	А	Homotopy analysis method
Zhao et al. [72]	2012	А	Improved homotopy analysis method
Ourabah and Tribeche[73]	2013	А	Revisited the T-F model with thermal effects
Boyd [74]	2013	Ν	Rational 1-kind Chebyshev collocation method
Parand et al. [75]	2013	Ν	Sinc-collocation method
Marinca and Ene [76]	2014	А	Optimal homotopy asymptotic method
Jaros and Kusano [77]	2014	А	Asymptotic behavior
Kusano et al. [78]	2014	А	Asymptotic analysis
Kilicman et al. [79]	2014	Ν	Rational 2-kind Chebyshev collocation method
Jovanovic et al. [80]	2014	Ν	Spectral method on exponential basis set
Bayat and Parand [81]	2014	Ν	Collocation method on Hermite polynomials
Amore et al. [82]	2014	А	Pade-Hankel method
Feng et al. [83]	2015	A	Existence of solutions for fractional BVP
Dahmani and Anber [84]	2015	A	ADM and VIM for fractional T-F model
Liu and Zhu [85]	2015	A	Iterative method on Laguerre pseudoSpectral
Parand et al. [86]	2015	N	Iterative method on Eagleric pseudospectral Iterative method based on the fractional order of rational Euler functions
Parand et al. [87]	2016	Ν	Quasilinearization-Fractional-Rational Bessel collocation method
Parand and Delkhosh[88]	2017	Ν	Quasilinearization-Fractional-Rational Chebyshev collocation method

Table 1: A summary of the methods used to solve the Thomas-Fermi equation, marked with Analytical or Numerical methods (A/N)

Using some transformations, a number of researchers extended Chebyshev polynomials to various domains, for example by using the transformation of $x = \frac{t-L}{t+L}$, L > 0 the rational Chebyshev functions on semi-infinite domain [91, 92], and by using transformation of $x = \frac{t}{\sqrt{t^2+L}}$, L > 0 the rational Chebyshev functions on an infinite domain [93] are introduced.

In the proposed work, by transformation $z = 1 - 2(\frac{t}{\eta})^{\alpha}$, $\alpha, \eta > 0$ on classical Chebyshev polynomials of the first kind, the GFCFs in interval $[0, \eta]$ are defined, that be denoted by ${}_{\eta}FT_{n}^{\alpha}(t) = T_{n}(1 - 2(\frac{t}{\eta})^{\alpha})$.

Fig. 1 shows graphs of GFCFs for various values of *n* and α and η = 5.

The $_{\eta}FT_{n}^{\alpha}(t)$ can be obtained using the recursive relation as follows:

$${}_{\eta}FT_{0}^{\alpha}(t) = 1 \quad , \quad {}_{\eta}FT_{1}^{\alpha}(t) = 1 - 2(\frac{t}{\eta})^{\alpha},$$

$${}_{\eta}FT_{n+1}^{\alpha}(t) = (2 - 4(\frac{t}{\eta})^{\alpha}) \; {}_{\eta}FT_{n}^{\alpha}(t) - {}_{\eta}FT_{n-1}^{\alpha}(t), \quad n = 1, 2, \cdots.$$

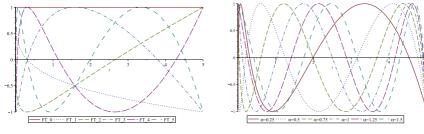
The analytical form of ${}_{\eta}FT_n^{\alpha}(t)$ of degree $n\alpha$ is given by

$${}_{\eta}FT_{n}^{\alpha}(t) = \sum_{k=0}^{n} \beta_{n,k,\eta,\alpha} t^{\alpha k}, \quad t \in [0,\eta],$$
(4)

where

$$\beta_{n,k,\eta,\alpha} = (-1)^k \frac{n2^{2k}(n+k-1)!}{(n-k)!(2k)!\eta^{\alpha k}}$$
 and $\beta_{0,k,\eta,\alpha} = 1.$

Note that $_{\eta}FT_{n}^{\alpha}(0) = 1$ and $_{\eta}FT_{n}^{\alpha}(\eta) = (-1)^{n}$, for all n, η , and $\alpha > 0$.



(a) Graphs of GFCFs with $\alpha = 0.25$ (b) Graphs of GFCFs with n = 5 and and various values of n various values of α

Figure 1: Graphs of GFCFs for various values of *n* and α .

Theorem 1. The GFCFs are orthogonal in the interval $[0, \eta]$ with weight function $w(t) = \frac{t^{\frac{\alpha}{2}-1}}{\sqrt{\eta^{\alpha}-t^{\alpha}}}$ as follows:

$$\int_0^\eta {}_{\eta} FT_n^{\alpha}(t) {}_{\eta} FT_m^{\alpha}(t) w(t) dt = \frac{\pi}{2\alpha} c_n \delta_{mn}, \tag{5}$$

where δ_{mn} is Kronecker delta, $c_0 = 2$, and $c_n = 1$ for $n \ge 1$.

Proof: The Chebyshev polynomials are orthogonal as follows [94]:

$$\int_{-1}^{1} T_n(x) T_m(x) \frac{1}{\sqrt{1-x^2}} dx = \frac{\pi}{2} c_n \delta_{mn}.$$

Now, by transformation $x = 1 - 2(\frac{t}{\eta})^{\alpha}$, $\alpha, \eta > 0$ on the above integral, the theorem can be proved.

Theorem 2. The singular Sturm-Liouville differential equation for the GFCFs with weight function $w(t) = \frac{t^{\frac{\alpha}{2}-1}}{\sqrt{\eta^{\alpha}-t^{\alpha}}}$ is as follows:

$$\frac{d}{dt}\left(\frac{1}{w(t)}\frac{d}{dt}_{\eta}FT_{n}^{\alpha}(t)\right)+\lambda_{n}w(t)_{\eta}FT_{n}^{\alpha}(t)=0,$$

where $\lambda_n = n^2 \alpha^2$ and $t \in [0, \eta]$.

Proof: The singular Sturm-Liouville differential equation for Chebyshev polynomials is as follows [94]:

$$\frac{d}{dx}\left(\sqrt{1-x^2}\frac{d}{dx}T_n(x)\right) + \frac{n^2}{\sqrt{1-x^2}}T_n(x) = 0.$$

Now, by transformation $x = 1 - 2(\frac{t}{\eta})^{\alpha}$, $\alpha, \eta > 0$ on the above equation, calculating $\frac{dy}{dx} = \frac{\eta^{\alpha}}{-2\alpha t^{\alpha-1}} \frac{dy}{dt}$, and $\sqrt{1 - x^2} = \frac{2t^{\alpha-1}}{\eta^{\alpha}} w(t)$, the theorem can be proved.

2.2 Approximation of functions

We consider $\Gamma = \{t \mid 0 \le t \le \eta\}$ and $L^2_w(\Gamma) = \{\mu : \Gamma \longrightarrow \mathbb{R} \mid \mu \text{ is measurable and } \|\mu\|_w < \infty\}$, where

$$\|\mu\|_{w}^{2} = \int_{0}^{\eta} |\mu(t)|^{2} w(t) dt, \quad w(t) = \frac{t^{\frac{\alpha}{2}-1}}{\sqrt{\eta^{\alpha} - t^{\alpha}}},$$
(6)

is the norm produced by the inner product on the space $L^2_w(\Gamma)$:

$$\langle \nu, \mu \rangle_w = \int_0^\eta \nu(t) \ \mu(t) \ w(t) \ dt.$$
⁽⁷⁾

Now, we assume

$$\mathcal{GFCF}_m = span\{ \ _{\eta}FT_0^{\alpha}(t), \ _{\eta}FT_1^{\alpha}(t), \cdots, \ _{\eta}FT_{m-1}^{\alpha}(t) \},$$

is finite dimensional subspace, therefore \mathcal{GFCF}_m is a complete subspace of $L^2_w(\Gamma)$ [93, 94]. The interpolating function of a smooth function y(t) on a finite interval is denoted by $y_m(t)$. It is an element of \mathcal{GFCF}_m and

$$y(t) \approx y_m(t) = \sum_{n=0}^{m-1} a_n \,_{\eta} F T_n^{\alpha}(t) = A^T \Phi(t),$$
 (8)

with

$$A = [a_0, a_1, \cdots, a_{m-1}]^T, (9)$$

$$\Phi(t) = [{}_{\eta}FT_0^{\alpha}(t), {}_{\eta}FT_1^{\alpha}(t), \cdots, {}_{\eta}FT_{m-1}^{\alpha}(t)]^T.$$
(10)

If $y_m(t)$ is the best projection of y(t) upon \mathcal{GFCF}_m with respect to the inner product Eq. (7) and the norm Eq. (6). Then, we have

$$\langle y_m(t) - y(t), \eta FT_n^{\alpha}(t) \rangle = 0 \quad \forall \eta FT_n^{\alpha}(t) \in \mathcal{GFCF}_m.$$

The coefficients a_n are obtained by using the orthogonality property of the GFCFs (Theorem 1) as follows:

$$a_n = \frac{2\alpha}{\pi c_n} \int_0^{\eta} {}_{\eta} FT_n^{\alpha}(t) y(t) w(t) dt, \quad n = 0, 1, 2, \cdots.$$

2.3 Convergence analysis

The following theorem shows that by increasing *m*, the approximation solution $f_m(t)$ is convergent to f(t) exponentially.

Theorem 3. Suppose that $D^{k\alpha}f(t) \in C[0,\eta]$ for k = 0, 1, ..., m, and F_m^{α} is the subspace generated by $\{ {}_{\eta}FT_0^{\alpha}(t), {}_{\eta}FT_1^{\alpha}(t), ..., {}_{\eta}FT_{m-1}^{\alpha}(t) \}$. If $f_m = A^T \Phi$ (in Eq. (8)) is the best approximation to f(t) from F_m^{α} , then the error bound is presented as follows

$$\|f(t) - f_m(t)\|_w \leq \frac{\eta^{m\alpha} M_\alpha}{2^m \Gamma(m\alpha + 1)} \sqrt{\frac{\pi}{\alpha m!}},$$

where $M_{\alpha} \ge |D^{m\alpha}f(t)|$, $t \in [0, \eta]$.

Proof. See Ref. [95].

Theorem 3 shows that if $m \to \infty$ then $|| f(t) - f_m(t) ||_w \to 0$.

Theorem 4. The GFCF, $_{\eta}FT_{n}^{\alpha}(t)$, has precisely *n* real zeros on interval $(0, \eta)$ in the form

$$t_k = \eta \left(\frac{1 - \cos(\frac{(2k-1)\pi}{2n})}{2} \right)^{\frac{1}{\alpha}}, \quad k = 1, 2, ..., n$$

Moreover, $\frac{d}{dt} {}_{\eta} FT_n^{\alpha}(t)$ has precisely n - 1 real zeros on interval $(0, \eta)$ in the following points:

$$t'_{k} = \eta \left(\frac{1 - \cos(\frac{k\pi}{n})}{2}\right)^{\frac{1}{\alpha}}, \qquad k = 1, 2, ..., n - 1.$$

Proof. See Ref. [95].

3 Application of the method

The efficient methods have been used by many researchers to solve the differential equations (DEs) is based on series expansion of the form $\sum_{i=0}^{n} c_i t^i$, such as Adomian's decomposition method [96] and Homotopy perturbation method [97]. But the exact solution of some DEs can't be estimated by polynomial basis, therefore, a new basis for Spectral methods to solve them has been defined as follows:

$$\Phi_n(t) = \sum_{i=0}^n c_i t^{i\alpha}.$$

In this section, the GFCFs collocation method is applied to solve Thomas-Fermi equation.

For satisfying the boundary conditions, we satisfy conditions Eq. (2) by multiplying the function $y_m(t)$ (in Eq. (8)) in $t e^{-2(t+2)}$ and adding it to $\frac{L}{t+L}$ as follows:

$$\widehat{y_m}(t,L) = \frac{L}{t+L} + t \ e^{-2(t+2)} \ y_m(t), \tag{11}$$

where $y_m(t)$ is defined in Eq. (8) and L > 0 is an arbitrary numerical parameter. Now, $\widehat{y_m}(t, L) = 1$ when t tends to zero, and $\widehat{y_m}(t, L) = 0$ when t tends to ∞ for all L > 0. The term $e^{-2(t+2)}$ is selected for accelerating convergence to zero. So the function $\widehat{y_m}(t, L)$ is satisfied in the conditions of Eq. (2) and is defined on semi-infinite domain.

The method of satisfying the boundary conditions is used in some papers, for examples see Ref. [98, 99]. Furthermore, in fact, the basic functions used in the paper can be considered as $e^{-2t} \,_{\eta} F T_n^{\alpha}(t)$. It is clear that the growth of the exponential function e^{-2t} in the interval of $[0, \infty]$ is much faster than the GFCFs. For this reason, the basic functions considered in the paper can be considered convergent.

To apply the collocation method, the residual function is constructed by substituting $\widehat{y_m}(t, L)$ in Eq. (11) for y(t) in the Eq. (1):

$$Res(t; a_0, \cdots, a_{m-1}, L) = \frac{d^2}{dt^2} \widehat{y_m}(t, L) - \frac{1}{\sqrt{t}} \left(\widehat{y_m}(t, L) \right)^{\frac{3}{2}}.$$
 (12)

One of the problems that exists in all the papers is to calculate the initial value and the optimal value for the parameter *L*. We have done two stages working to fix this problem in this paper:

Stage 1: The equations for obtaining the initial value for the parameter *L* arise from equalizing Res(t) to zero on (m + 1) collocation points:

$$Res(t_i; a_0, \cdots, a_{m-1}, L) = 0, \quad i = 1, 2, ..., m + 1.$$
 (13)

i.e. we have added the parameter of *L* as an unknown to the unknowns and have solved the system of equations generated by m + 1 equations and m + 1 unknowns. At this stage, the initial value for the parameter *L* is calculated with accuracy 10^{-8} for y'(0) compared with Parand et al. [86]. Tables 2 and 3 show that the approximation solution for this stage is calculated with a good accuracy. In this study, we used the roots of $_{\eta}FT_{m+1}^{\alpha}(t)$ in the interval $[0, \eta]$ (Theorem 4), as collocation points.

Stage 2: In this stage, with trial and error method, accurate value for the parameter *L* is computed (see Table 3).

The equations for obtaining the coefficient $\{a_i\}_{i=0}^{m-1}$ with the accurate value of *L* arise from equalizing Res(t) to zero on *m* collocation points (the roots of $_{\eta}FT_m^{\alpha}(t)$ in the interval $[0, \eta]$ (Theorem 4)):

$$Res(t_i; a_0, \cdots, a_{m-1}, L) = 0, \quad i = 1, 2, ..., m.$$
 (14)

By solving the obtained set of equations, we have the approximating function $\widehat{y_m}(t)$ in the Eq. (11).

Baker in 1930 [29] has calculated an analytical solution as follows:

$$y(t) = 1 + Bt + \frac{4}{3}t^{\frac{3}{2}} + \frac{2}{5}Bt^{\frac{5}{2}} + \frac{1}{3}t^{3} + \frac{3}{70}B^{2}t^{\frac{7}{2}} + \frac{2}{15}Bt^{4} + \frac{4}{63}(\frac{2}{3} - \frac{1}{16}B^{3})t^{\frac{9}{2}} + \cdots,$$
(15)

where *B* is the value of the first derivative at the origin. The solution in Eq. (15) has been generated by the powers of $t^{\frac{1}{2}}$, i.e. we can generate this solution using the basic set $\{1, t^{\frac{1}{2}}, t, t^{\frac{3}{2}}, t^2, \cdots\}$. For this reason, we solve Thomas-Fermi equation by using new basic of the GFCFs in the Eq. (4) with $\alpha = \frac{1}{2}$ where have been generated by the powers of $t^{\frac{1}{2}}$. Also consider that all of the computations have been done by Maple 2015.

4 Results and discussion

Calculation of the value of the initial slope y'(0) of Thomas-Fermi potential has always been of great interest and plays an important role in determining many physical properties of Thomas-Fermi atom.

Comparison with previous works: Zaitsev et al. [53] have shown that the methods of the Runge-Kutta and Adams-Bashforth for solving Thomas-Fermi equation are ill-conditioned on semi-infinite domains. For this reason, many researchers have used numerical and semi-analytical methods to solve this equation, and some of them have calculated very good results. For examples, recently, authors of [61, 63, 66, 70, 71, 72, 76, 82, 85] have used analytical methods to solve this equation, and the best solution for y'(0) was calculated by Amore et al. [82] by using Pade-Hankel method, correct to 26 decimal places. Authors of [59, 62, 74, 75, 79, 80, 81] have used numerical methods to solve this equation, and the best solution for y'(0) was calculated by Parand et al. [86] by using an iterative method based on the fractional order of rational Euler functions, correct to 27 decimal places. In these numerical methods, there is a numerical parameter that is selected by the authors. For examples, in [59] is selected 0.258497 to accuracy 10^{-6} , in [62] is selected 0.93799968 to accuracy 10^{-8} , in [75] is selected 0.62969503 to accuracy 10^{-6} , in [79] is selected 0.0958885 to accuracy 10^{-7} , and in [81] is selected 1.588071 to accuracy 10^{-7} . Table 2 shows a list of the number of calculations y'(0) of Thomas-Fermi equation by many researchers. We can see that some researchers have achieved good results and accuracy. The last two rows show the best approximation obtained by the present method in two stages. The solutions in both stages are more accurate than many previous results.

Table 3 shows the obtained values of y'(0) for various values of L and m = 45, and the absolute error with Parand et al. [86]. Table 4 shows comparison of the obtained values of y(t) between the present method, Parand and Shahini [59], Jovanovic [80], and Liao [100] for various values of t. Table 5 shows the obtained values of y'(t) by the present method for various values of t.

Fig. 2 shows the graphs of residual error Res(t) of the Eq. (12) with m = 45, and logarithmic of coefficients $|a_i|$ to show the convergence of the present method. Fig. 3 shows the resulting graphs of Thomas-Fermi equation for y(t) and y'(t) with m = 45.

5 Conclusion

The fundamental goal of the paper has been to construct an approximation to the solution of nonlinear Thomas-Fermi equation in a semi-infinite domain which has a singularity at t = 0 and its boundary condition occurred in infinity. To achieve this goal, the generalized fractional order of the Chebyshev orthogonal functions (GFCFs) of the first kind are used. The present method has several advantages, such as:

- 1. The generalized fractional order of the Chebyshev functions (GFCFs) of the first kind have been introduced as a new basis for Spectral methods and this basis can be used to develop a framework or theory in Spectral methods.
- 2. The fractional basis was used for solving an ordinary differential equation (nonlinear singular Thomas-Fermi differential equation) and it provided insight into an important issue.
- 3. We know that calculate the initial value and the optimal value for the parameter *L* is one of the problems in many papers, but in this method we calculated the initial value for *L* by solving a system of (m + 1) equations and unknowns, i.e. we calculated the initial value *L* with no attempt.
- 4. The differential equation is solved without any change of variable in it.
- 5. The comparison of the obtained values with the others shows that the present method provides good numerical solution.
- 6. A good accuracy to 27 decimal places for y(t), y'(t), and y'(0) are achieved.
- This article tells a good history as follows: (a) A history of the methods to solve this equation by other researchers. (b) A history of the numerical methods to solve the equations in unbounded domains.

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Author/Authors	Obtained value of $y'(0)$
Fermi (1928) [27]	-1.58
Baker (1930) [29]	-1.588 558
Bush and Caldwell (1931) [30]	-1.58 9
Miranda (1934) [32]	-1.5880 464
Slater and Krutter (1935) [33]	-1.5880 8
Feynman et al. (1949) [34]	-1.588 75
Kobayashi et al. (1955) [36]	-1.58807 0972
Mason (1964) [37]	-1.5880710
Laurenzi (1990) [41]	-1.588 588
MacLeod (1992) [42]	-1.5880710226
Wazwaz (1999) [45]	-1.58807 6779
Epele et al. (1999) [46]	-1.588 102
Esposito (2002) [48]	-1.588
Liao (2003) [50]	-1.58 712
Khan and Xu (2007) [55]	-1.58 6494973
El-Nahhas (2008) [56]	-1.5 5167
Yao (2008) [58]	-1.5880 04950
Parand and Shahini (2009) [59]	-1.58807 02966
Marinca and Herianu (2011) [61]	-1.5880 659888
Oulne (2011) [62]	-1.5880710 34
Abbasbandy and Bervillier (2011) [63]	-1.588071022611375312718 9
Fernandez (2011) [66]	-1.588071022611375313
Zhu et al. (2012) [70]	-1.58807 411
Turkylmazoglu (2012) [71]	-1.5880 1
Zhao et al. (2012) [72]	-1.5880710226
Boyd (2013) [74]	-1.5880710226113753127186845
Parand et al. (2013) [75]	-1.58807 0339
Marinca and Ene (2014) [76]	-1.588071 9992
Kilicman et al. (2014) [79]	-1.588071 347
Jovanovic et al. (2014) [80]	-1.588071022 811
Bayatbabolghani & Parand(2014)[81]	-1.588071
Amore et al. (2014) [82]	$-1.58807102261137531271868450{\color{black}{8}}$
Liu and Zhu (2015) [85]	-1.58807 2
Parand et al. (2016) [86]	-1.588071022611375312718684509
This article (Stage 1)	-1.58807094
This article (Stage 2)	-1.588071022611375312718684509

Table 2: Comparison of the obtained values of y'(0) by researchers, inaccurate digits are **bold**.

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Stage	L	Obtained value	Abs. Err.
1	0.108	-1.58807094	7.297e-08
2	0.107	-1.58807105	2.738e-08
2	0.1072822	-1.588071022613	1.624e-12
2	0.10728222052	-1.588071022611375190	1.227e-16
2	0.107282220518793	-1.58807102261137531270	1.868e-20
2	0.107282220518792882	-1.58807102261137531271866	2.450e-23
2	0.10728222051879288180562	-1.588071022611375312718684509	3.989e-28
	Parand et al. (2016) [86]	-1.588071022611375312718684509	

Table 3: Obtained values of y'(0) for various values of *L* and the absolute errors with Ref. [86]

Table 4: The comparison of the obtained values of y(t) by the present method and other methods

t	Present method	Jovanovic[80]	Liao [100]	Parand [59]
0.25	0.75520146	0.755202096	0.75520200	0.75588075
0.50	0.60698638	0.606986951	0.60698700	0.60670000
0.75	0.50234684	0.502348140	0.50234700	0.50296404
1.00	0.42400805	0.424010148	0.42400800	0.42433317
1.25	0.36320141	0.363203991	0.36320200	0.36322793
1.50	0.31477746	0.314780118	0.31477800	0.31466064
1.75	0.27545132	0.275453712	0.27545100	0.27523384
2.00	0.24300850	0.243010373	0.24300900	0.24267858
2.25	0.21589462	0.215895823	0.21589500	0.21543933
2.50	0.19298412	0.192984580	0.19298400	0.19240632
2.75	0.19298412	0.173440997	0.17344100	0.17275869
3.00	0.15663267	0.156631657	0.15663300	0.15587186
3.25	0.14207167	0.142067963	0.14207000	0.14126050
3.50	0.12937199	0.129367328	0.12937000	0.12854138
3.75	0.11823180	0.118226225	0.11822900	0.11740805
4.00	0.10840425	0.108401057	0.10840400	0.10761295
4.25	0.09970158	0.099694306	0.09969790	0.09895432
4.50	0.09195242	0.091944333	0.09194820	0.09126645
4.75	0.08502664	0.085017755	0.08502180	0.08441228
5.00	0.07881335	0.078803669	0.07880780	0.07827775
6.00	0.05943190	0.059418888	0.05942300	0.05923642
7.00	0.04611150	0.046094375	0.04609780	0.04623102
8.00	0.03660733	0.036584707	0.03658730	0.03698065
9.00	0.02961945	0.029589375	0.02959090	0.03018090
10.0	0.02435370	0.024313708	0.02431430	0.02504474
15.0	0.01095404	0.010808302	0.01080540	0.01173122
20.0	0.00619613	0.005789307	0.00578494	0.00658563
25.0	0.00435986	0.003478434	0.00347375	0.00410440

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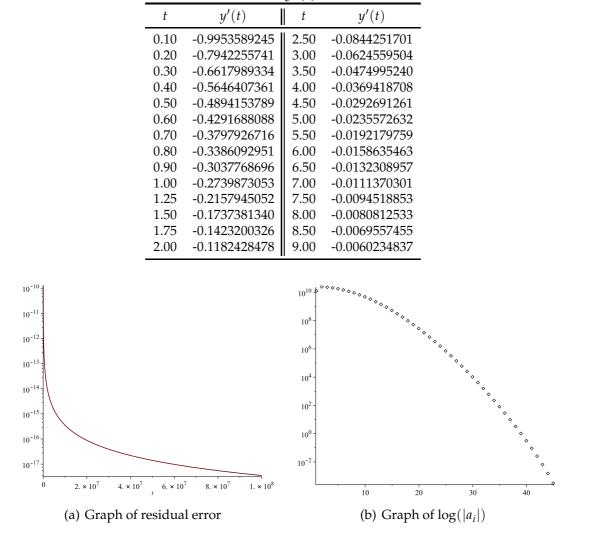
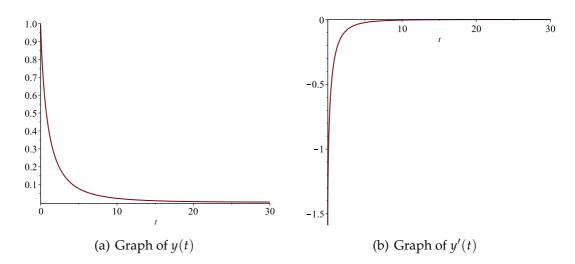
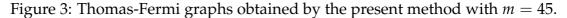


Table 5: Obtained values of y'(t) for various values of *t*

Figure 2: Graphs of residual error with m = 45, and logarithmic of coefficients $|a_i|$ to show the convergence of the method.

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