



An efficient numerical method for solving nonlinear Thomas-Fermi equation

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Abstract. In this paper, the nonlinear Thomas-Fermi equation for neutral atoms by using the fractional order of rational Chebyshev functions of the second kind (FRC2), $FU_n^\alpha(t, L)$, on an unbounded domain is solved, where L is an arbitrary parameter. Boyd (*Chebyshev and Fourier Spectral Methods, 2ed, 2000*) has presented a method for calculating the optimal approximate amount of L and we have used the same method for calculating the amount of L . With the aid of quasilinearization and FRC2 collocation methods, the equation is converted to a sequence of linear algebraic equations. An excellent approximation solution of $y(t)$, $y'(t)$, and $y'(0)$ is obtained.

1 Introduction

In this section, the introduction of numerical methods used for solving equations in unbounded domains is expressed. Furthermore, the mathematical model of Thomas-Fermi equation is introduced.

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1.1 The problems on unbounded domains

There are several numerical methods for solving differential equations on unbounded domains, such as:

1. *Finite difference method (FDM)*: One of the oldest and the simplest methods for solving differential equations is using the FDM approximations for derivatives. The FDMs are in a class of the discretization methods [2].
2. *Finite element method (FEM)*: One of the important methods used for solving the boundary value problems for partial differential equations is the finite element method [2].
3. *Meshfree methods*: Meshfree methods are those that do not require a connection between nodes of the simulation domain, i.e. a mesh, but are rather based on the interaction of each node with all its neighbors [3]. The use of Radial Basis Functions (RBFs) in meshless methods is very common in solving differential equations [4, 5]. This approach has recently received a great deal of attention from researchers [6, 7].
4. *Spectral methods*: Several approaches in Spectral methods have been proposed for solving the problems on unbounded domains:
 - (a) Using functions such as Hermite, Sinc, Laguerre, and Bessel functions that are defined on the unbounded domains. This approach investigated by Parand et al. [8, 9], Funaro & Kavian [10], and Guo & Shen [11].
 - (b) Mapping an unbounded equation to a bounded equation. Authors of [12, 13] have applied this approach in their works.
 - (c) Replacing unbounded domains with $[-B, B]$ or $[0, B]$ by choosing B sufficiently large. This method is named domain truncation [14, 15].
 - (d) Mapping the bounded basic functions to the unbounded basic functions. In this approach, the basic functions on a bounded domain convert to the functions on an unbounded domain. For example, Boyd [16] introduced a new spectral basis, called rational Chebyshev functions, on the unbounded domain by mapping on the Chebyshev polynomials, and also in Refs. [17, 18, 19]. There are three important mappings for this approach:

- (A) Algebraic mapping: basic functions on a bounded domain $t \in [a, b]$ by using the transformation of $t = \frac{bx+al}{x+L}$ convert to functions on an unbounded domain $x \in [0, \infty)$, where L is an arbitrary parameter [21].
- (B) Exponential mapping: basic functions on a bounded domain $t \in [a, b]$ by using the transformation of $t = b + (a - b)e^{-\frac{x}{L}}$ convert to functions on an unbounded domain $x \in [0, \infty)$ [20].
- (C) Logarithmic mapping: basic functions on a bounded domain $t \in [a, b]$ by using the transformation of $t = a + (b - a) \tanh(2\frac{x}{L})$ convert to functions on an unbounded domain $x \in [0, \infty)$.

In this paper, a Spectral method is introduced to solve unbounded problems by using the fractional order of rational Chebyshev orthogonal functions of the second kind.

1.2 The Thomas-Fermi equation

The Thomas-Fermi equation is an important nonlinear singular differential equation which is defined on semi-infinite domain [22, 23]:

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

The nonlinear Thomas-Fermi equation appears in the problem of determining the effective nuclear charge in heavy atoms, therefore, many great scholars were considered it, such as Fermi [24], Feynman (physics) [25], and Slater (chemistry) [26].

The initial slope $y'(0)$ is difficult for computing by any means and plays an important role in determining many properties of the physical of Thomas-Fermi atom [27]. It determines the energy of a neutral atom in Thomas-Fermi approximation:

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

where Z is the nuclear charge.

For these reasons, the problem has been studied by many researchers and has been solved by different techniques where a number of them are listed in Table 1, in this table, the calculated value of $y'(0)$ by researchers is shown.

The rest of the paper is constructed as follows: the FRC2s and their properties are expressed in section 2. The methodology is explained in section 3. In section 4, results and discussions of the method are shown. Finally, a conclusion is provided.

2 Fractional order of rational Chebyshev functions of the second kind

In this section, the definition of the fractional order of rational Chebyshev functions of the second kind (FRC2s) and some theorems for them is provided.

2.1 The FRC2s definition

Using some transformations, some researchers have generalized the Chebyshev polynomials to semi-infinite or infinite domains, for example the rational Chebyshev functions on the semi-infinite domain [28], the rational Chebyshev functions on an infinite domain [1], and the generalized fractional order of the Chebyshev functions (GFCF) on finite interval $[0, \eta]$ [29, 30, 31] are introduced by using transformations $x = \frac{t-L}{t+L}$, $x = \frac{t}{\sqrt{t^2+L}}$, and $x = 1 - 2(\frac{t}{\eta})^\alpha$, respectively.

In the proposed work, by new transformation $x = \frac{t^\alpha - L}{t^\alpha + L}$, $L > 0$ on the Chebyshev polynomials of the second kind, the fractional order of rational Chebyshev functions of the second kind on domain $[0, \infty)$ is introduced, which is denoted by $FU_n^\alpha(t, L) = U_n(\frac{t^\alpha - L}{t^\alpha + L})$ where L is a numerical parameter.

The $FU_n^\alpha(t, L)$ can be calculated by using the following relation:

$$\begin{aligned} FU_0^\alpha(t, L) &= 1, & FU_1^\alpha(t, L) &= 2 \frac{t^\alpha - L}{t^\alpha + L}, \\ FU_{n+1}^\alpha(t, L) &= 2 \frac{t^\alpha - L}{t^\alpha + L} FU_n^\alpha(t, L) - FU_{n-1}^\alpha(t, L), & n &= 1, 2, \dots, \end{aligned} \quad (3)$$

and we can also calculate:

$$FU_n^\alpha(t, L) = \sum_{k=0}^n \beta_{n,k} (t^\alpha + L)^{-k}, \quad (4)$$

where

$$\beta_{n,k} = (-4L)^k \frac{(n+k+1)!}{(n-k)!(2k+1)!} \quad \text{and} \quad \beta_{0,k} = 1.$$

2.2 Approximation of functions

Any function of continuous and differentiable $y(t)$, $t \in [0, \infty)$, can be expanded as follows:

$$y(t) = \sum_{n=0}^{\infty} a_n \text{FU}_n^\alpha(t, L),$$

where the coefficients a_n can be obtained by:

$$a_n = \frac{8\alpha L^{\frac{3}{2}}}{\pi} \int_0^\infty \text{FU}_n^\alpha(t, L) y(t) w(t) dt, \quad n = 0, 1, 2, \dots.$$

In the numerical methods, we have to use first $(m + 1)$ -terms FRC2s and approximate $y(t)$:

$$y(t) \approx y_m(t) = \sum_{n=0}^m a_n \text{FU}_n^\alpha(t, L). \quad (5)$$

Theorem 1 *The FRC2, $\text{FU}_n^\alpha(t, L)$, has precisely n real simple zeros on the interval $(0, \infty)$ in the form*

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

Proof. Chebyshev polynomial of the second kind $U_n(x)$ has n real simple zeros [1]:

$$x_k = \cos\left(\frac{k\pi}{n+1}\right), \quad k = 1, 2, \dots, n.$$

Therefore $U_n(x)$ can be written as

$$U_n(x) = (x - x_1)(x - x_2)\dots(x - x_n).$$

Using transformation $x = \frac{t^\alpha - L}{t^\alpha + L}$ yields to

$$\text{FU}_n^\alpha(t, L) = \left(\left(\frac{t^\alpha - L}{t^\alpha + L} \right) - x_1 \right) \left(\left(\frac{t^\alpha - L}{t^\alpha + L} \right) - x_2 \right) \dots \left(\left(\frac{t^\alpha - L}{t^\alpha + L} \right) - x_n \right),$$

so, the real zeros of $\text{FU}_n^\alpha(t, L)$ are $t_k = \left(L \frac{1+x_k}{1-x_k} \right)^{\frac{1}{\alpha}}$. □

Theorem 2 *The FRC2s are orthogonal on domain $[0, \infty)$ for all $L > 0$ with positive weight function $w(t) = \frac{t^{\frac{3}{2}\alpha-1}}{(t^\alpha+L)^3}$ as follows:*

$$\int_0^\infty F U_n^\alpha(t, L) F U_m^\alpha(t, L) w(t) dt = \frac{\pi}{8\alpha L^{\frac{3}{2}}} \delta_{mn}, \quad (6)$$

where δ_{mn} is the Kronecker delta.

Proof. The Chebyshev polynomials of the second kind $U_n(x)$ are orthogonal as [1]:

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

Now, by using transformation $x = \frac{t^\alpha-1}{t^\alpha+L}$, $L > 0$ on the integral, the theorem can be proved. \square

3 The methodology

The quasi-linearization method (QLM) based on the Newton-Raphson method has introduced by Bellman and Kalaba [32, 33]. Some researchers have used this method in their works [34, 35, 36, 37].

Occasionally the linear ordinary differential equation that gets from the QLM at each iteration does not solve analytically. Hence we can use the Spectral methods to approximate the solution.

The QLM for Thomas-Fermi equation (1) is as follows:

$$\frac{d^2 y_{n+1}}{dt^2} - \frac{3}{2\sqrt{t}} (y_n(t))^{1/2} y_{n+1}(t) = -\frac{1}{2\sqrt{t}} (y_n(t))^{3/2}, \quad (7)$$

$$y_{n+1}(0) = 1, \quad y_{n+1}(\infty) = 0, \quad (8)$$

where $n = 0, 1, 2, 3, \dots$.

The QLM iteration requires an initialization or "initial guess" $y_0(t)$. We assume that $y_0(t) \equiv 1$, i.e. the initial guess satisfies in the boundary condition at zero. Mandelzweig and Tabakin in Ref. [38] have shown that if the initial function is true in one of the conditions of (8) then the QLM is convergent.

Baker has shown that the solution of Eq. (1) is generated by the powers of $t^{\frac{1}{2}}$ as follows [39]:

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

for this reason, in Eq. (3), we assume that $\alpha = \frac{1}{2}$.

We apply the FRC2s collocation method to solve the linear ordinary differential equations at each iteration Eq. (7) with boundary conditions (8).

Approximation of functions $y_{n+1}(t)$ by using Eq. (5) is shown by $y_{m,n+1}(t)$. Now, for applying the collocation method, we construct the residual function for the Thomas-Fermi equation by substituting $y_{m,n+1}(t)$ for $y(t)$ in Eq. (1):

$$\text{RES}_n^m(t) = \frac{d^2}{dt^2} (y_{m,n+1}(t)) - \frac{1}{\sqrt{t}} (y_{m,n+1}(t))^{\frac{3}{2}}. \quad (10)$$

In this study, the roots of the FRC2s in the semi-infinite domain $[0, \infty)$ (Theorem 1) have been used as collocation points. Also, consider that all of the computations have been done by Maple 2015.

Boyd in Ref. [1] has provided the method of the experimental trial-and-error for calculating the approximation of the optimal value of L :

“The experimental trial-and-error method (Optimizing infinite Interval Map Parameter) (Page 377 in Ref. [1]):

Plot the coefficients a_i versus degree on a log-linear plot. If the graph abruptly flattens at some m , then this implies that L is TOO SMALL for the given m , and one should increase L until the flattening is postponed to $i = m$.”

It must be noted that the optimal value of L is dependent on m .

Fig. 1 presents the graph of the coefficients of $\log(|a_i|)$ for different values of L , $m = 200$ and $n = 50$, according to the above experimental trial-and-error method, the approximation optimal amount of L is about 21.

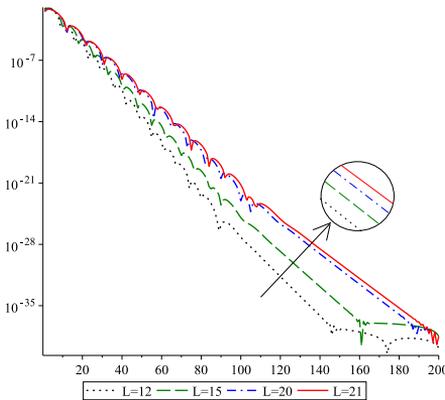


Figure 1: Graph of logarithm of coefficients $|a_i|$ with $m = 200$, $n = 50$, and different values of L , for calculating an approximation optimal value of L

Bellman & Kalaba [32] and Mandelzweig & Tabakin [38] proved the convergence of the QLM. Let $\delta \mathbf{y}_{n+1}(\mathbf{t}) \equiv \mathbf{y}_{n+1}(\mathbf{t}) - \mathbf{y}_n(\mathbf{t})$, then it can show that $\|\delta \mathbf{y}_{n+1}\| \leq k \|\delta \mathbf{y}_n\|^2$ where k is a positive real constant [38]. Therefore, the convergence rate is of the order of 2, i.e. $O(h^2)$. We can also obtain for $(n + 1)$ -th iteration:

$$\|\delta \mathbf{y}_{n+1}\| \leq (k \|\delta \mathbf{y}_1\|)^{2^n} / k. \quad (11)$$

Furthermore, it can be hoped that even if the initial guess is not appropriate, then after a while the solution converges [32].

4 Results and discussion

Calculating the amount of $\mathbf{y}'(0)$ of Thomas-Fermi potential is very important for determining many physical properties of Thomas-Fermi atom.

Comparison of methods: Zaitsev et al. [40] showed that the Adams-Bashforth and Runge-Kutta methods to solve this equation on unbounded domains are ill-conditioned, hence, researchers have used the methods of numerical and semi-analytical for solving the equation, and some researchers can calculate very good solutions. For example, authors of [55, 57, 58, 59, 60, 61, 64, 68, 70] used the analytical methods for solving the equation and Amore et al. [68] were able to calculate the best solution using Pade-Hankel method, correct to 26 decimal places. Authors of [54, 56, 62, 63, 65, 66, 67] used the numerical methods for solving the equation and Parand & Delkhosh [73] were able to calculate the best solution using the combination of the quasilinearization method and the fractional order of rational Chebyshev collocation method, correct to 37 decimal places. In numerical methods, there is usually a numerical arbitrary parameter which selected by authors. Such as, in [54] the parameter is chosen 0.258497 to accuracy 10^{-6} , in [56] is chosen 0.93799968 to accuracy 10^{-8} , in [63] is chosen 0.62969503 to accuracy 10^{-6} , in [65] is chosen 0.0958885 to accuracy 10^{-7} , and in [67] is chosen 1.588071 to accuracy 10^{-7} . Here we choose $L = 21$ to accuracy 10^{-37} .

Table 1 presents some of the calculated values of $\mathbf{y}'(0)$ of Thomas-Fermi potential by some researchers. It is clear that some researchers were able to calculate good solution and accuracy. The last three rows present the best solution obtained by the present method for different values of m .

Table 1: Comparison of the obtained values of $y'(0)$ by researchers, inaccurate digits are **bold**.

Author/Authors	Obtained value of $y'(0)$
Fermi (1928) [24]	-1.58
Baker (1930) [39]	-1.588 558
Bush and Caldwell (1931) [41]	-1.589
Miranda (1934) [42]	-1.5880 464
Slater and Krutter (1935) [26]	-1.58808
Feynman et al. (1949) [25]	-1.588 75
Kobayashi et al. (1955) [43]	-1.58807 0972
Mason (1964) [44]	-1.5880710
Laurenzi (1990) [45]	-1.588 588
MacLeod (1992) [46]	-1.5880710226
Wazwaz (1999) [47]	-1.58807 6779
Epele et al. (1999) [48]	-1.588 102
Esposito (2002) [49]	-1.588
Liao (2003) [50]	-1.58 712
Khan and Xu (2007) [51]	-1.58 6494973
El-Nahhas (2008) [52]	-1.5 5167
Yao (2008) [53]	-1.5880 04950
Parand and Shahini (2009) [54]	-1.58807 02966
Marinca and Herianu (2011) [55]	-1.5880 659888
Oulne (2011) [56]	-1.5880710 34
Abbasbandy and Bervillier (2011) [57]	-1.5880710226113753127189
Fernandez (2011) [58]	-1.588071022611375313
Zhu et al. (2012) [59]	-1.58807 411
Turkylmazoglu (2012) [60]	-1.58801
Zhao et al. (2012) [61]	-1.5880710226
Boyd (2013) [62]	-1.5880710226113753127186845
Parand et al. (2013) [63]	-1.58807 0339
Marinca and Ene (2014) [64]	-1.588071 9992
Kilicman et al. (2014) [65]	-1.588071 347
Jovanovic et al. (2014) [66]	-1.588071022 811
Bayatbabolghani & Parand(2014)[67]	-1.588071
Amore et al. (2014) [68]	-1.588071022611375312718684508
Fatoorehchi & Abolghasemi(2014)[69]	-1.58807 6818
Liu and Zhu (2015) [70]	-1.5880 72
Parand et al. (2016) [71]	-1.588071022611375312718684509
Parand et al. (2016) [72]	-1.588071022611375312718684509423
Parand and Delkhosh (2017) [73]	-1.5880710226113753127186845094239501095
Parand and Delkhosh (2017) [74]	-1.588071022611375312718684509
This paper [m=200]	-1.5880710226113753127186845094239501093
” ” [m=100]	-1.5880710226113753127186845094239
” ” [m=50]	-1.588071022611375312728

Table 2 presents the absolute errors in the calculation of $y'(0)$ for different values of m and the obtained results are compared with the best solution calculated in Ref. [73].

Table 2: Absolute errors of $y'(0)$ for different values of m and iterations

m	L_{opt}	10th Iter.	20th Iter.	30th Iter.	40th Iter.	50th Iter.
25	0.5	3.970e-08	3.939e-08	3.939e-08	3.939e-08	3.939e-08
75	5	6.667e-13	3.926e-18	5.878e-24	4.065e-30	4.646e-30
100	7	6.524e-13	5.656e-20	4.026e-24	8.314e-31	1.976e-33
175	19	6.524e-13	1.065e-25	1.349e-27	4.240e-31	1.908e-34
200	21	6.524e-13	3.477e-25	6.072e-29	9.237e-32	1.974e-37

Table 3: Obtained values of $y(t)$ by the present method for different values t

t	$y(t)$	t	$y(t)$	t	$y(t)$
0.25	0.7552014653133312	5	7.880777925136990e-2	125	5.423519678389911e-5
0.50	0.6069863833559799	6	5.942294925042258e-2	150	3.263396444625690e-5
0.75	0.5023468464123686	7	4.609781860449858e-2	175	2.115958647941346e-5
1.00	0.4240080520807056	8	3.658725526467680e-2	200	1.450180349694576e-5
1.25	0.3632014144595141	9	2.959093527054687e-2	300	4.548571953616680e-5
1.50	0.3147774637004581	10	2.431429298868086e-2	400	1.979732628112504e-5
1.75	0.2754513279960917	15	1.080535875582389e-2	500	1.034077168199939e-5
2.00	0.2430085071611195	20	5.784941191566940e-3	1000	1.351274773541057e-7
2.25	0.2158946265761301	25	3.473754416765632e-3	2000	1.733984751613821e-8
2.50	0.1929841234580007	50	6.322547829849047e-4	3000	5.189408334513832e-9
3.00	0.1566326732164958	75	2.182104320497469e-4	5000	1.130926706343084e-9
4.00	0.1084042569189077	100	1.002425681394073e-4	10000	1.42450045099559e-10

Tables 3 and 4 present the obtained results of $y(t)$ and $y'(t)$ by the present method for different values of t .

Table 4: Obtained values of $y'(t)$ by the present method for different values t

t	$y'(t)$	t	$y'(t)$	t	$y'(t)$
0.25	-0.7223069849102349	5	-2.356007495470051e-2	125	-1.202665391336449e-6
0.50	-0.4894116125745380	6	-1.586754953340707e-2	150	-6.091399478608917e-7
0.75	-0.3583068801675136	7	-1.114253181486708e-2	175	-3.410947673774533e-7
1.00	-0.2739890515933062	8	-8.088602969645474e-3	200	-2.057532316475268e-7
1.25	-0.2157941303007336	9	-6.033074714457392e-3	300	-4.365949618530290e-8
1.50	-0.1737387990139451	10	-4.602881871269254e-3	400	-1.436682305996181e-8
1.75	-0.1423209371968936	15	-1.515323082023606e-3	500	-6.034363442475256e-9
2.00	-0.1182431916254876	20	-6.472543327776920e-4	1000	-3.98801070822799e-10
2.25	-0.0994093212014470	25	-3.240429977697511e-4	2000	-2.57608536992070e-11
2.50	-0.0844261867988090	50	-3.249890204825881e-5	3000	-5.15300117644723e-12
3.00	-0.0624571308541209	75	-7.777974714283007e-6	5000	-6.75339712163883e-13
4.00	-0.0369437578241234	100	-2.739351068678330e-6	10000	-4.26161647550093e-14

Fig. 2 presents the graphs of the residual errors of RES_n^m of Eq. (10) with $m = 50, 75, 100, 150, 200$ and $n = 50$, and the logarithm of coefficients $|a_i|$ with $m = 200$ and $n = 50$, for showing the convergence of the method. It can see that the residual errors are very small value, about 10^{-39} .

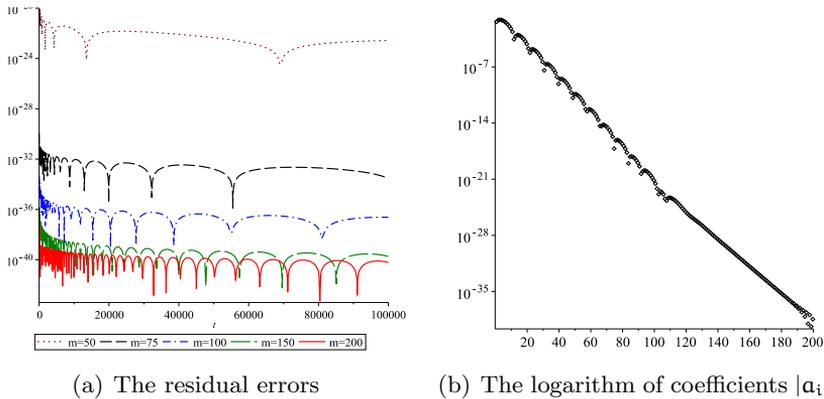


Figure 2: Graphs of the residual errors for different values of m and the logarithm of coefficients $|a_i|$, for showing the convergence of the method.

5 Conclusion

In this paper, the combination of the methods of the quasilinearization and the FRC2s collocation is used for constructing an approximation of the solution of the nonlinear singular Thomas-Fermi equation on unbounded domain. The present method has several advantages. For example, for the first time, the fractional order of rational Chebyshev functions of the second kind (FRC2s) has been introduced as a new basic for Spectral methods. The fractional basis were used to solve an ordinary differential equation and this provides an insight into an important issue. The roots of the FRC2s are used on unbounded domain $[0, \infty)$ as collocation points for solving Thomas-Fermi equation and the problem does not convert to a bounded domain. Some researchers solved the equation by changing the variables in this equation [58, 62] or domain truncation [38] but we solved the problem without any changing on variables or domain in this equation. An approximate optimal value of L is calculated. The convergence of the obtained results is shown. The accurate solutions for $y(t)$, $y'(t)$ and $y'(0)$ by 200 collocation points are obtained. This article provided a good history of solving Thomas-Fermi equation by other researchers

and the numerical methods to solve equations in unbounded domains.

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