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A NEW APPROACH FOR SOLVING NONLINEAR THOMAS-FERMI EQUATION BASED ON FRACTIONAL ORDER OF RATIONAL BESSEL FUNCTIONS

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Abstract. In this article, we introduce a fractional order of rational Bessel functions collocation method (FRBC) for solving the Thomas-Fermi equation. The problem is defined in the semi-infinite domain and has a singularity at $x = 0$ and its boundary condition occurs at infinity. We solve the problem on the semi-infinite domain without any domain truncation or transformation of the domain of the problem to a finite domain. This approach at first, obtains a sequence of linear differential equations by using the quasilinearization method (QLM), then at each iteration the equation is solves by FRBC method. To illustrate the reliability of this work, we compare the numerical results of the present method with some well-known results, to show that the new method is accurate, efficient and applicable.

1. Introduction

Many problems in mathematics, fluid dynamics, quantum mechanics, astrophysics, physics, and engineering are arisen on the infinite or semi-infinite domains. In this section, we have expressed some of the approaches for solving problems which are defined in unbounded domains and a brief history of Thomas-Fermi equation that is defined on the semi-infinite domain.

1.1. **Solving problems over unbounded domains.** Recently, various approaches have been successfully proposed for solving problems which are arisen on unbounded domains. Such as numerical, analytical and semi-analytical methods.

Different numerical methods have been introduced to the problems which is defined in the semi-infinite domain, such as the Finite difference method (FDM) [56, 14], Finite element method (FEM) [14, 17], Meshfree methods [73, 62, 74], and Spectral methods [66, 58].

The study of analytical and semi-analytical solutions of differential equations (DEs) plays an important role in mathematical physics, engineering, and the other sciences. In the past several decades, various methods for obtaining solutions of DEs have been presented, such as the Adomian decomposition method [35, 82], Homotopy perturbation method [36, 78], Variational iteration method [80], Exp-function method [37] and so on.

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The spectral approximations for DEs on finite domains have achieved great success and popularity in recent years, but spectral approximations for DEs on infinite domains have only received limited attention. Several spectral methods for treating infinite/semi-infinite domain problems have been utilized by different researchers: (1) There is an effective approach to solve these problems by applying the basis of Sinc, Hermite and rational Christov functions that are orthogonal on the interval $(-\infty, \infty)$ [32, 68] and the basis of Laguerre polynomials that are orthogonal on the interval $[0, \infty)$ [64, 20]. (2) Another approach for solving such problems which is based on rational approximations. This method transfers polynomials on interval $[\alpha, \beta]$ to functions on interval $[0, \infty)$ by using the algebraic mapping $x \to \frac{\beta x+\alpha L}{x+L}$ that $L > 0$ is a scaling/stretching factor [75]. The Jacobi polynomials are a class of classical orthogonal polynomials, also the Gegenbauer polynomials, the Legendre and Chebyshev polynomials, are special cases of these polynomials which have been used in several literatures for solving some problems. In some papers have been provided the collocation method for natural convection heat transfer equations embedded in porous medium, nonlinear differential equation and nonlinear integro-differential equation based on rational Gegenbauer, Legendre, Chebyshev functions [58, 64, 65, 72]. Doha et al have presented Jacobi rational-Gauss collocation method based on Jacobi rational functions and Gauss quadrature integration to solve nonlinear Lane-Emden equation [25]. Isik et al have used Bernstein polynomials to solve high order initial and boundary value problems. Their approximate solution has a better convergence rate than the one found by using the collocation method [40]. (3) Guo [33, 34] has applied a method that proceeds by mapping the original problem in an unbounded domain to a problem in a bounded domain, and then using suitable Jacobi polynomials such as the Gegenbauer polynomials to approximate the resulting problems. (4) A further approach consists of replacing the infinite domain with $[-K, K]$ and the semi-infinite domain with $[0, K]$ by choosing K sufficiently large. This method is named domain truncation [12, 39].

In this investigation, we attempt to introduce a Spectral method based on the fractional order of rational Bessel functions (FRB) to solve Thomas-Fermi on the semi-infinite domain.

1.2. **Thomas-Fermi equation.** One of the most important nonlinear ordinary differential equations that occurs in semi-infinite interval is Thomas-Fermi equation as follows [83, 22, 16]:

$$\frac{d^2y(x)}{dx^2} - \frac{1}{\sqrt{x}}y^{3/2}(x) = 0, \quad x \in [0, \infty), \tag{1.1}$$

where the boundary conditions for this equation are as follows:

$$y(0) = 1, \quad \lim_{x\to\infty} y(x) = 0. \tag{1.2}$$

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) [81] and Richard Feynman (physics) [31] and of course Enrico Fermi [29].

One measure of the rapidity of the convergence of the procedure is provided by the calculation of the value of the initial slope $y'(0)$ of the Thomas-Fermi potential [47]. The problem is useful for calculating form-factors and for obtaining effective potentials which can be used as initial trial potentials in self-consistent field calculations. The initial slope $y'(0)$ is difficult to compute by any means and plays an important role in determining many physical properties of the Thomas-Fermi atom. It determines the energy of a neutral atom in the Thomas-Fermi approximation:

$$E = \frac{6}{7}\Big(\frac{4\pi}{3}\Big)^{2/3} Z^{7/3} y'(0), \tag{1.3}$$

where Z is the nuclear charge.

For these reasons, the problem has been studied by many researchers and by the different techniques have been solved, that a number of them are as follows: Baker in 1930 [7] studied the singularity of this equation and calculated an analytical solution as follows:

$$y(x) = 1 - Bx + \frac{4}{3}x^{3/2} - \frac{2}{5}Bx^{5/2} + \frac{1}{3}x^3 + \frac{3}{70}B^2x^{7/2} - \frac{2}{15}Bx^4 + \dots,$$

where $-B$ is the value of the first derivative at the origin that has calculated $y'(0) = -B = -1.588558$.

Esposito in 2002 [28] reported an original method, due to Majorana, that leads to a semi-analytical series solution of the Thomas-Fermi equation with appropriate boundary conditions in terms of only one quadrature, and proved that the series expansion is uniformly convergent in the interval $[0, 1]$, and has calculated $y'(0) = -1.588$.

Liao in 2003 [49] employed the Homotopy analysis method and gave an explicit analytic solution of the Thomas-Fermi equation and the related recurrence formula of constant coefficients. The corresponding mth-order approximation is

$$y(x) = \sum_{k=0}^{m} \sum_{n=1}^{4k+1} \alpha_{k,n}(1 + x)^{-n},$$

where $\alpha_{k,n}$ is defined in [49, Eq. 26]. He calculated $y'(0) = -1.58712$.

Kobayashi et al in 1955 [46] examined the asymptotic solution of obtained by Coulson and March [21], and improved their solution:

$$y(x) = \frac{144}{x^3}\big(1 - z + 0.6256974977z^2 - 0.3133861150z^3 + 0.1373912767z^4 - \dots\big),$$

where $z = \frac{F}{x^c}$, and $F = 13.27097391$ and $c = 0.7720018726$, and calculated $y'(0) = -1.588070972$.

Adomian in 1998 [3] introduced a standard decomposition method for solving Thomas-Fermi equation. As briefly as follows:

$$y(x) = c_1 + c_2x + L^{-1}x^{-1/2}\sum_{n=0}^{\infty} A_n \tag{1.4}$$

where L^{-1} denotes a two-fold integration, A_n denotes the Adomian polynomials generated for $y^{3/2}$, and c_1, c_2 are constants of integration. The Adomian decomposition method employs the recursive relation.

Marinca and Herianu in 2011 [52] used a new method to find an analytical approximate solution to Thomas-Fermi equation and called it the Optimal Parametric Iteration Method (OPIM) that this new iteration approach provides us with a convenient way to optimally control the convergence of the approximate solution. This new iteration approach containing a new iteration scheme involves the presence of a finite number of initially unknown parameters, which are optimally determined. In this way, the approximate initial slope is $y'(0) = -1.5880659888022421$.

Zhu et al in 2012 [93] approximated the original Thomas-Fermi equation by a nonlinear free boundary value problem (FBVP) and applied an iterative method to solve the FBVP. They transformed the FBVP to a nonlinear singular BVP defined on $[0, 1]$ by a change of variables and also employed an adaptive finite element method based on moving mesh to obtain the best approximate solution at each iteration. Best approximation obtained by this method is $y'(0) = -1.58794357$.

A simple and more precise solution to the Thomas-Fermi equation is obtained by making use of the famous Ritz Variational method. Oulne in 2011 [57] used a new simple Variational solution of the Thomas-Fermi equation which reproduces the numerical solution accurately in a wide range with a correct asymptotic behavior at long distances from the origin and which allows us to calculate with exactness the initial slope. The proposed solution will be developed in power series which have the same form as series solutions that have been obtained previously by Baker [7]. In this method, the approximate initial slope is $y'(0) = -1.588071034$.

Abbasbandy and Bervillier in 2011 [1] compared three methods based respectively on Taylor (Maclaurin) series, Padé approximates and conformal mappings. $y'(0) = -1.588071022611375312718 9 \pm 7 * 10^{-22}$ was obtained by using the Padé-Hankel method.

Boyd in 2013 [13] applied collocation method based on the rational Chebyshev functions on semi-infinite intervals $TL_n(y; L)$ which L is a user-choosable numerical. Boyd employed Newton-Kantorovich iteration to reduce the nonlinear differential equation to a sequence of linear differential equations, and he has calculated

$$y'(0) = -1.588071022611375312718 6845$$

with $L = 64$ and 600 collocation points.

MacLeod in 1992 [50] used two differing approximations on Chebyshev polynomial according to behavior Thomas-Fermi function, one for small $x < 40$, one for large x. In this method, the approximate initial slope is $y'(0) = -1.5880710226$.

Parand et al [59, 71, 8, 63] proposed collocation method on rational Chebyshev, Hermite polynomials and Sinc functions to solve Thomas-Fermi on semi-infinite interval without truncating it to a finite domain. These methods reduce the solution of this problem to the solution of a system of algebraic equations.

Jovanovic et al in 2014 [41] solved the Thomas-Fermi equation by applying a spectral method using an exponential basis set in a semi-infinite domain. The goal of the spectral method approach is to find the values of coefficients a_i that best satisfy the equation

$$y(x) = \sum_{i=1}^{N} a_i R_i, \quad R_i = e^{-\beta_i x}, \tag{1.5}$$

where values of R_i are selected in an intuitive way to cover all the possible decay rates. They have reported detailed about the convergence rate of the initial slope $y'(0)$ for an exponential basis set.

Liu and Zhu in 2015 [48] proposed an iterative method based on the Laguerre pseudospectral approximation which the solution of the Thomas-Fermi equation as the sum of two parts due to its singularity at the origin. One "singular" part is a power series expansion. The other "smooth" part satisfies a nonlinear two-point boundary value problem. In this method, the approximate initial slope is $y'(0) = -1.588072$.

Yao in 2008 [88] solved the Thomas-Fermi equation with a kind of analytic technique, named Homotopy analysis method and his answer is $y'(0) = -1.588004950$.

Amore et al in 2014 [5] obtained highly accurate solutions to the Thomas-Fermi equations for atoms and atoms in very strong magnetic fields. And they apply the Padé-Hankel method, numerical integration, power series with Padé and Hermite-Padé approximates and Chebyshev polynomials. They solved Thomas-Fermi for different x and obtain answers for $y(x)$ and $y'(x)$. Their best answer is $y'(0) = -1.588071022611375312718684509$.

Fernandez in 2011 [30] showed that a simple and straightforward rational approximation to the Thomas-Fermi equation provides the slope at the origin with unprecedented accuracy and that Padé approximates of relatively low order are far more accurate than more elaborate approaches proposed recently by other authors. He calculated $y(x)$ for different values of x and compare their method with Chebyshev and numerical method, and calculated $y'(0) = -1.588071022611375313$.

Epele et al in 1999 [27] used Padé approximate approach to solving Thomas-Fermi equation. They have calculated $y'(0) = -1.5881$.

Khan and Xu in 2007 [44] used an analytic technique, namely the Homotopy analysis method (HAM). Their best answer for $y'(0)$ was -1.586494973 when they selected [30,30] for Homotopy-Padé approximations.

The rest of this paper is arranged as follows: Section 2 introduces a novel the fractional order of rational Bessel functions (FRB). Section 3 describes a brief formulation of quasilinearization method (QLM) introduced in [51]. In section 4 at first, by utilizing QLM over Thomas-Fermi equation a sequence of linear differential equations is obtained and then at each iteration the fractional order of rational Bessel functions collocation method (FRBC) is used for solving the linear differential equations. We in section 5 compared our solutions with some well-known results, comparisons show that the present solutions are highly accurate, we also describe our results via tables and figures. Finally, we give a brief conclusion in section 6.

2. Fractional order of rational Bessel functions (FRB)

The Bessel functions arise in many problems in physics possessing cylindrical symmetry, such as the vibrations of circular drumheads and the radial modes in optical fibers. Bessel functions are usually defined as a particular solution of a linear differential equation of the second order which known as Bessel's equation. Bessel functions first defined by the Daniel Bernoulli on heavy chains (1738) and then generalized by Friedrich Bessel. More general Bessel functions were studied by Leonhard Euler in (1781) and in his study of the vibrating membrane in (1764) [18, 38].

2.1. **Definition of Bessel polynomials.**

The Bessel differential equation of order $n \in \mathbb{R}$ is

$$x^2 \frac{d^2y(x)}{dx^2} + x\frac{dy(x)}{dx} + (x^2 - n^2)y(x) = 0, \quad x \in (-\infty, \infty). \tag{2.1}$$

One of the solutions of equation (2.1) by applying the method of Frobenius as follows [9]:

$$J_n(x) = \sum_{r=0}^{\infty} \frac{(-1)^r}{r!(n+r)!} (\frac{x}{2})^{2r+n}, \tag{2.2}$$

where series (2.2) is convergent for all $x \in (-\infty, \infty)$.

Bessel functions and polynomials are used to solve a number of problems in physics, engineering, mathematics, and etc., such as Blasius equation, Lane-Emden equations, integro-differential equations of the fractional order, unsteady gas equation, systems of linear Volterra integral equations, high-order linear complex differential equations in circular domains, systems of high-order linear Fredholm integro-differential equations, etc. [70, 60, 69, 23, 79, 90, 89, 84].

Bessel polynomials have been introduced as follows [91]:

$$B_n(x) = \sum_{r=0}^{[\frac{N-n}{2}]} \frac{(-1)^r}{r!(n+r)!} (\frac{x}{2})^{2r+n}, \quad x \in [0, 1]. \tag{2.3}$$

where $n \in \mathbb{N}$, and N is the number of the basis of Bessel polynomials.

Let $\Gamma = \{x : 0 \le x \le 1\}$ and $L^2_w(\Gamma) = \{v : \Gamma \to \mathbb{R} | v$ is measurable and $\|v\|_w < \infty\}$, where

$$\|v\|_w = \Big(\int_0^1 |v(x)|^2 w(x) dx \Big)^{1/2},$$

with $w(x) = 1$, is the norm induced by the inner product of the space $L^2_w(\Gamma)$ as follows:

$$\langle v(x), u(x) \rangle_w = \int_0^1 v(x) u(x) w(x) dx.$$

Now, suppose that

$$\mathfrak{B} = \operatorname{span}\{B_0(x), B_1(x), \dots, B_N(x)\},$$

where $\mathfrak{B}$ is a finite-dimensional subspace of $L^2_w(\Gamma)$, $\dim \mathfrak{B} = N+1$, so $\mathfrak{B}$ is a closed subspace of $L^2(\Gamma)$. Therefore, $\mathfrak{B}$ is a complete subspace of $L^2(\Gamma)$. Assume that $f(x)$ is an arbitrary element in $L^2(\Gamma)$. Thus f has a unique best approximation in $\mathfrak{B}$ subspace, say $\hat{b}(x) \in \mathfrak{B}$; that is,

$$\exists\ \hat{b}(x) \in \mathfrak{B}, \quad \forall b(x) \in \mathfrak{B}, \quad \|f(x) - \hat{b}(x)\| \le \|f(x) - b(x)\|. \tag{2.4}$$

Notice that we can write $b(x)$ vector as a combination of the basis vectors of $\mathfrak{B}$ subspace.

We know function of $f(x)$ can be expanded by $N+1$ terms of Bessel polynomials as:

$$f(x) = f_N(x) + R(x);$$

that is,

$$f_N(x) = \sum_{n=0}^{N} a_n B_n(x) = A^T B(x), \tag{2.5}$$

where $B(x) = [B_0(x), B_1(x), \dots, B_N(x)]^T$ and $R(x) \in \mathfrak{B}^\perp$ that $\mathfrak{B}^\perp$ is the orthogonal complement. So $(f(x) - f_N(x)) \in \mathfrak{B}^\perp$ and $b(x) \in \mathfrak{B}$ are orthogonal which we denote it by

$$(f(x) - f_N(x)) \perp b,$$

thus $f(x) - f_N(x)$ vector is orthogonal over all of basis vectors of $\mathfrak{B}$ subspace as:

$$\langle f(x) - f_N(x), B_i(x)\rangle_w = \langle f(x) - A^T B(x), B_i(x)\rangle_w = 0, \quad i = 0, 1, \dots, N,$$

hence

$$\langle f(x) - A^T B(x), B^T(x)\rangle_w = 0,$$

therefore A can be obtained by

$$\langle f(x), B^T(x)\rangle_w = \langle A^T B(x), B^T(x)\rangle_w,$$
$$A^T = \langle f(x), B^T(x)\rangle_w \langle B(x), B^T(x)\rangle_w^{-1}, \quad n = 0, 1, \dots, N.$$

2.2. **Definition of FRB.** Some researchers have proposed the series expansions $\sum_{i=0}^{N} c_i x^{i\alpha}$, $(\alpha > 0)$ to solve the fractional differential equations, for instance, Bhrawy et al constructed shifted fractional-order Jacobi orthogonal functions to solve the nonlinear initial value problem of fractional order α and a class of time-fractional partial differential equations with variable coefficient [11]. Authors [42, 2] have proposed fractional-order Legendre functions to solve fractional-order differential equations and the time-fractional convection-diffusion equation. Alshbool et al. have utilized operational matrices of new fractional Bernstein functions for approximating solutions to fractional differential equations [4]. Parand and Delkhosh have introduced the fractional order of the Chebyshev functions for solving Volterra's population growth model of arbitrary order [67].

Baker [7] proved that the answer to Thomas-Fermi equation is as fractional forms, for this reason, we have applied new FRB to solve the Thomas-Fermi equation in the semi-infinite interval, $\{FB_n\}$:

$$FB_n^{\alpha}(x, L) = B_n\Big(\frac{x^{\alpha}}{x^{\alpha} + L}\Big), \quad n = 0, 1, \dots, N$$

or

$$FB_n^{\alpha}(x, L) = \sum_{r=0}^{[\frac{N-n}{2}]} \frac{(-1)^r}{r!(n+r)!}\Big(\frac{x^{\alpha}}{2(x^{\alpha} + L)}\Big)^{2r+n}, \quad n = 0, 1, \dots, N \tag{2.6}$$

where $\alpha > 0$, $x \in [0, \infty)$, $B_n(x)$ is Bessel polynomials of order n, and the constant parameter $L > 0$ is a scaling/stretching factor.

Let $\Lambda = \{x : 0 \le x < \infty\}$ and $L_w^2(\Lambda) = \{z : \Lambda \to \mathbb{R} | z$ is measurable and $\|z\|_w < \infty\}$, where

$$\|z\|_w = \Big(\int_0^{\infty} |z(x)|^2 w(x, L) dx\Big)^{1/2},$$

with $w(x, L) = \frac{\alpha x^{\alpha-1} L}{(x^{\alpha}+L)^2}$, is the norm induced by the inner product of the space $L_w^2(\Lambda)$ as follows:

$$\langle z, g\rangle_w = \int_0^{\infty} z(x) g(x) w(x, L) dx.$$

Now, suppose that

$$\mathfrak{FB} = \operatorname{span}\{FB_0^{\alpha}(x, L), FB_1^{\alpha}(x, L), \dots, FB_N^{\alpha}(x, L)\},$$

Let $y(x) \in L^2(\Gamma)$ be a function defined over interval $[0, \infty)$ can be expanded by $N + 1$ terms of FRB as:

$$y_N(x) = \sum_{n=0}^{N} a_n FB_n^{\alpha}(x, L) = A^T FB(x, L), \tag{2.7}$$

where $FB(x,L) = [FB_0^\alpha(x,L), FB_1^\alpha(x,L), \dots, FB_N^\alpha(x,L)]^T$. Hence

$$\langle y(x) - A^T FB(x,L), FB^T(x,L)\rangle_w = 0, \tag{2.8}$$

therefore A can be obtained by

$$\langle y(x), FB^T(x,L)\rangle_w = \langle A^T FB(x,L), FB^T(x,L)\rangle_w,$$
$$A^T = \langle y(x), FB^T(x,L)\rangle_w \langle FB(x,L), FB^T(x,L)\rangle_w^{-1}, \ n = 0,1,\dots,N.$$

3. Quasilinearization method (QLM)

The QLM is a generalization of the Newton-Raphson method [19, 77] to solve the nonlinear differential equation as a limit of approximating the nonlinear terms by an iterative sequence of linear expressions. Bellman and Kalaba have introduced the QLM method about fifty years ago [43, 10]. The QLM techniques are based on the linearization of the high order ordinary/partial differential equation and require the solution of a linear ordinary differential equation at each iteration. Mandelzweig and Tabakin [51] have determined general conditions for the quadratic, monotonic and uniform convergence of the QLM method to solve both initial and boundary value problems in nonlinear ordinary n-th order differential equations in N-dimensional space. Recently, the QLM method has been successfully applied by researchers to solve the various types of fractional differential equations and some ordinary nonlinear equation [76, 61, 87, 24].

We have considered second-order nonlinear ordinary differential equations in one variable on the interval $[0,\infty)$ as follows:

$$\frac{d^2u}{dx^2} = F(u'(x), u(x), x), \tag{3.1}$$

with the boundary conditions: $u(0) = A$, $u(\infty) = B$, where A and B are real constants and F is nonlinear functions.

By using the QLM for solving (2.8) determines the $(r+1)$-th iterative approximation $u_{r+1}(t)$ as a solution of the linear differential equation:

$$\frac{d^2u_{r+1}}{dx^2} = F(u'_r, u_r, x) + (u_{r+1} - u_r)F_u(u'_r, u_r, x) + (u'_{r+1} - u'_r)F_{u'}(u'_r, u_r, x), \tag{3.2}$$

with the boundary conditions

$$u_{r+1}(0) = A, \quad u_{r+1}(\infty) = B, \tag{3.3}$$

where $r = 0,1,2,\dots$ and the functions $F_u = \partial F/\partial u$ and $F_{u'} = \partial F/\partial u'$ are functional derivatives of functional $F(u'_r, u_r, x)$.

4. Solution of Thomas-Fermi equation by FRBC-QLM

By utilizing QLM technique on (1.1), we have

$$\frac{d^2y_{r+1}(x)}{dx^2} - \frac{3}{2\sqrt{x}}(y_r(x))^{1/2} y_{r+1}(x) = -\frac{1}{2\sqrt{x}}(y_r(x))^{3/2}, \tag{4.1}$$

with the boundary conditions:

$$y_{r+1}(0) = 1, \quad y_{r+1}(\infty) = 0, \tag{4.2}$$

where $r = 0,1,2,\dots$.

For rapid convergence is actually sufficient that the initial guess be sufficiently best to ensure the smallness of just one of the quantity $q_r = k||y_{r+1} - y_r||$, where k

is a constant independent of r. Usually, it is advantageous that $y_0(t)$ would satisfy at least one of the boundary conditions (4.2) [76], thus set $y_0(x) = 1$ for the initial guess of Thomas-Fermi equation. In this paper have been considered two terms $\frac{1}{x^2+1}$ and $\frac{x}{x^2+1}$ to satisfy boundary conditions (4.2). Thus we can approximate $y_{r+1}(x)$ by $N + 1$ basis of FRB as:

$$y_{r+1}(x) \approx y_{N,r+1}(x) = \frac{1}{x^2+1} + \frac{x}{x^2+1} \sum_{n=0}^{N} \hat{c}_i FB_n^{\alpha}(x, L). \tag{4.3}$$

where $\alpha > 0$ and $r = 0, 1, 2, \dots$. In all of the spectral methods, the purpose is to find $\hat{c}_i$ coefficients.

To apply the collocation method, we constructed the residual function for $(r+1)$-th iteration in QLM method by substituting $y_{r+1}(x)$ by $y_{N,r+1}(x)$ into (4.1) as follows:

$$Res_{r+1}(x) = \frac{d^2 y_{N,r+1}}{dx^2} - \frac{3}{2\sqrt{x}}(y_r(x))^{1/2} y_{N,r+1}(x) + \frac{1}{2\sqrt{x}}(y_r(x))^{3/2}. \tag{4.4}$$

A method for forcing the residual function (4.4) to zero can be defined as collocation algorithm. There is no limitation to choose the point in the collocation method. The $N + 1$ collocation points which are roots of rational Chebyshev functions on interval $[0, \infty)$ (i.e. $x_i = (1 - cos(\frac{(2i-1)\Pi}{2N+2}))/(1 + cos(\frac{(2i-1)\Pi}{2N+2})), i = 1, 2, \dots, N + 1$ [71]) have been substituted $Res_{r+1}(x)$, therefore:

$$\mathrm{Res}_{r+1}(x_i) = 0, \quad i = 0, 1, \dots, N + 1. \tag{4.5}$$

A linear system of equations has been obtained, all of these equations can be solved by Newton method for the unknown coefficients. We have also done all of the computations by Maple 2015 on PC with CPU Core i5, Windows 7 64bit, and 8GB of RAM.

Now we can employ the FRBC-QLM iterative algorithm to solve Thomas-Fermi equation as follows:

BEGIN

Input variable of I that is the number of iterations of QLM method.
Input variable of N that is the number of basic of the FRB.
Set $y_{N,0}(x) = 1$.

For $r = 0$ to I do

Construct the series (4.3) for approximating $y_{r+1}(x)$ as $y_{N,r+1}(x)$.
Construct the linear differential equation (4.4) by using QLM method on (1.1).
Substitute $y_{N,r+1}(x)$ into the equation (4.4) and create residual function $Res_{r+1}(x)$.
Now we have $N+1$ unknown $\{\hat{c}_i\}_0^N$. To obtain these unknown coefficients, we need $N + 1$ equations.
Choose the roots of order $N + 1$ of Rational Chebyshev functions as $N + 1$ collocation points: $\{x_i\}_0^N$.
Substitute collocation points $\{x_i\}_0^N$ into the $Res_{r+1}(x)$ and create the $N+1$ equations.
Solve the $N + 1$ linear equations with $N + 1$ unknown coefficients, for calculating $y_{N,r+1}(x)$.

End For
END

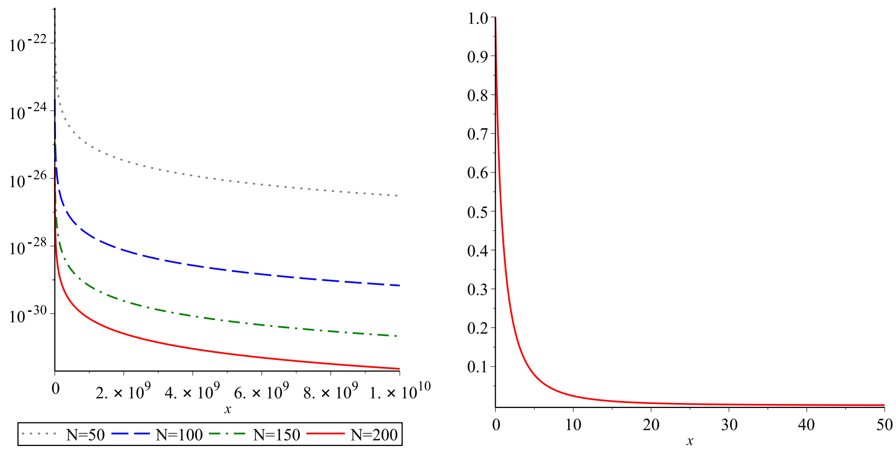
5. Numerical Results

The initial slope $y'(0)$ is difficult to compute by any means and plays an important role in determining many physical properties of the Thomas-Fermi atom. It determines the energy of a neutral atom in the Thomas-Fermi approximation. Zaitsev et al [92] have shown that the methods of Runge-Kutta and Adams-Bashforth can apply to solve the Thomas-Fermi equation in the semi-infinite interval, although their methods are ill-condition and have not high accuracy for more scheme. Exact solution for Thomas-Fermi differential equation, which is defined on the semi-infinite interval and has a singularity at $x = 0$ and its boundary condition occurs at infinity, is not available, so approximating this solution is very important.

Table 1 shows a list of the number of calculations $y'(0)$ of the Thomas-Fermi potential. As can be seen, some researchers have achieved good results and accuracy. The last three rows show best approximations of $y'(0)$ for various value of N and a fixed value of $L = 1$ by the present method which shows that the present solution is highly accurate. Tables 2 and 3 show values obtained of $y(x)$ and $y'(x)$ by the present method respectively, for different values of N and the 45-th iteration. Obviously, Table 4 and 5 present some numerical example to illustrate the accuracy and convergence of our suggested method by increasing the number of points and iterations. It should be mentioned that all calculations are done by software Maple for various values N and iterations. Figure 1 shows the resulting graph of Thomas-Fermi equation obtained by the present method for $N = 200$ and iteration 45 which tends to zero as x increases by boundary condition $y(\infty) = 0$, and graphs of residual error of the problem with $N = 50,\ 100,\ 150,\ 200$, and the 45-th iteration, note that the residual error decreases with the increase of the collocation points. Comparing the computed results by this method with the others shows that this method provides more accurate and numerically stable solutions than those obtained by other methods.

6. Conclusion

The fundamental goal of this paper has been to construct an approximation to the solution of nonlinear Thomas-Fermi equation in a semi-infinite interval which has a singularity at $x = 0$ and its boundary condition occurred in infinity. In the above discussion, we applied a new method to solve the Thomas-Fermi equation that is nonlinear ordinary differential equation on a semi-infinite interval. By using an analytical method for solving Thomas-Fermi equation has proved that the answer to this problem is as fractional forms [7]. So for the first time, we solved the problem based on the new fractional order of rational Bessel functions without any domain truncation or transformation of the domain of the problem to a finite domain. In this work, first, by utilizing QLM over Thomas-Fermi equation a sequence of linear differential equations is obtained. Second, at each iteration the linear differential equation is solved by novel FRBC method. We obtained accurately to 30 decimal places for initial slope, $y'(0) = -1.588071022611375312718684509423$, only by using 200 collocation points and successfully have been applied to find the most accurate values of $y(x)$ and $y'(x)$. A known open problem in spectral methods is finding the optimal value for L [12], but in this paper, for simplicity, we set $L = 1$. The



Graphs of residual error Graph of $y(x)$

FIGURE 1. Graphs of residual error with $N = 50, 100, 150, 200$, and iteration 45, and Thomas-Fermi graph obtained by present method.

numerical results of solving this problem show that this method is higher accurate than obtained results of other famous methods. Finally, the comparison results have shown that the present method is an acceptable approach and good candidate to solve this type of problems that occur in the semi-infinite interval and the nonlinear singular two point boundary value problems effectively.

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

Author/Authors	Obtained value of $y'(0)$
Fermi (1928) [29]	-1.58
Baker (1930) [7]	-1.588**558**
Bush and Caldwell (1931) [15]	-1.58**9**
Miranda (1934) [55]	-1.5880**464**
Slater and Krutter (1935) [81]	-1.5880**8**
Feynman et al (1949) [31]	-1.588**75**
Kobayashi et al. (1955) [46]	-1.58807**0972**
Mason (1964) [54]	-1.5880710
Laurenzi (1990) [47]	-1.588**588**
MacLeod (1992) [50]	-1.5880710226
Wazwaz (1999) [86]	-1.58807**6779**
Epele et al (1999) [27]	-1.588**1**
Esposito (2002) [28]	-1.588
Liao (2003) [49]	-1.58**712**
Khan and Xu (2007) [44]	-1.58**6494973**
El-Nahhas (2008) [26]	-1.5**5167**
Yao (2008) [88]	-1.5880**04950**
Fernandez (2008) [30]	-1.588071022611375313
Parand and Shahini (2009) [71]	-1.58807**02966**
Marinca and Herianu (2011) [52]	-1.5880**659888**
Oulne (2011) [57]	-1.588071**034**
Abbasbandy and Bervillier (2011) [1]	-1.58807102261137531271**8**9
Zhu et al. (2012) [93]	-1.58**794357**
Turkylmazoglu (2012) [85]	-1.5880**1**
Zhao et al (2012) [94]	-1.5880710226
Parand et al (2013) [63]	-1.58807**0339**
Boyd (2013) (with m=600) [13]	-1.5880710226113753127186845
Amore et al (2014) [5]	-1.588071022611375312718684508
Marinca and Ene (2014) [53]	-1.588071**9992**
Bayatbabolghani and Parand(2014)[8]	-1.588071
Kilicman et al (2014) [45]	-1.588071**347**
Liu and Zhu (2015) [48]	-1.58807**2**
This article [N=100]	-1.5880710226113753127
This article [N=150]	-1.5880710226113753127186845
This article [N=200]	-1.588071022611375312718684509423

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TABLE 2. Values of $y(x)$ for various values of x with iteration 45 and N=200

x	$y(x)$	x	$y(x)$
0.25	0.755201465313331276073659062048	30	2.255836616202855884224e-3
0.50	0.606986383355979909494446070174	40	1.113635638833368812571e-3
0.75	0.502346846412368627446521794036	50	6.322547829849047267797e-4
1.00	0.424008052080705600224612007418	60	3.939113666854170020266e-4
1.25	0.363201414459514114681451617277	70	2.622652998120112937417e-4
1.50	0.314777463700458172973580939810	80	1.835457597407102401554e-4
1.75	0.275451327996091785680113852782	90	1.335458289537346235905e-4
2.00	0.243008507161119555299806749733	100	1.002425681394073316855e-4
2.25	0.215894626576130144431137496637	200	1.450180349694576468040e-5
2.50	0.192984123458000701287136925252	300	4.548571953616680184257e-6
2.75	0.173441292490063451179594691770	400	1.979732628112504742575e-6
3.00	0.156632673216495841339813440477	500	1.034077168199939706035e-6
3.25	0.142069642692650781317847467819	600	6.068687696675251337105e-7
3.5	0.129369596993799111381550504704	700	3.861765157037986162218e-7
3.75	0.118229001616846686506107664622	800	2.608137304998336353315e-7
4.00	0.108404256918907711089847680321	900	1.843724151350651789179e-7
4.25	0.099697845864740046922595440377	1000	1.351274773541058315394e-7
4.50	0.091948133826563845114632113892	2000	1.733984751613850910820e-8
4.75	0.085021743728059499429131697623	3000	5.189408334543857341875e-9
5.00	0.078807779251369904256091892542	4000	2.201209082423027362721e-9
6.00	0.059422949250422580797949567059	5000	1.130926706419984771574e-9
7.00	0.046097818604498589876456260102	6000	6.56056637887703224451e-10
8.00	0.036587255264676802392315804375	7000	4.13886522087042381058e-10
9.00	0.029590935270546873724362041806	8000	2.77658195353364145555e-10
10.00	0.024314292988680864190110388176	9000	1.95225879692802747067e-10
20.00	0.005784941191566940442010571504	10000	1.42450044462688615523e-10

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TABLE 3. Values of $y'(x)$ for various values of x with iteration 45 and $N = 200$

x	$y'(x)$	x	$y'(x)$
0.25	- 0.722306984910234919519668083864	30	-1.806700064769926350e-4
0.50	-0.489411612574538088647005847557	40	-6.966802854032586631e-5
0.75	-0.358306880167513621987250767311	50	-3.249890204825881462e-5
1.00	-0.273989051593306251989464686519	60	-1.719770008309986259e-5
1.25	-0.215794130300733601274300529492	70	-9.956533393052361268e-6
1.50	-0.173738799013945185681936465228	80	-6.166195528764075475e-6
1.75	-0.142320937196893658885960452965	90	-4.024473703766734693e-6
2.00	-0.118243191625487620571255867534	100	-2.739351068678330086e-6
2.25	-0.099409321201447030009355248089	200	-2.057532316475268926e-7
2.50	-0.084426186798809043812545918214	300	-4.365949618530290454e-8
2.75	-0.072335044846097235621822505698	400	-1.436682305996181021e-9
3.00	-0.062457130854120976228704899999	500	-6.034363442475256759e-9
3.25	-0.054300422911798016711579461695	600	-2.961822515102276227e-9
3.5	-0.047501046582295208950097689053	700	-1.619832187577198029e-9
3.75	-0.041785207716826396797995883443	800	-9.59243855994648160e-10
4.00	-0.036943757824123486354813738987	900	-6.03766177055436240e-10
4.25	-0.032814785443993540385309640573	1000	-3.98801070822799359e-10
4.50	-0.029271448448803843379269452384	2000	-2.57608536991971054e-11
4.75	-0.026213311168397937715703460851	3000	-5.15300117640232003e-12
5.00	-0.023560074954700512881180449080	4000	-1.64161860704260568e-12
6.00	-0.015867549533407079812737615662	5000	-6.75339712187831946e-13
7.00	-0.011142531814867088405578460800	6000	-3.26676807336313998e-13
8.00	-0.008088602969645474322126751847	7000	-1.76730816571737264e-13
9.00	-0.006033074714457392439143608348	8000	-1.03777992089730866e-13
10.00	-0.004602881871269254502543511851	9000	-6.48790244833915206e-14
20.00	-0.000647254332777692033047085589	10000	-4.26161649603483992e-14

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Table 4. Numerical solution $y(x)$ with various values of x, N and iterations.

N	x	15th iteration	45th iteration
50	10	0.024314292988800	0.024314292988680865622793862360
	100	0.000100242576939	0.000100242568139361977721849610
	200	0.000014501554262	0.000014501803498894699818187404
	300	0.000004548556111	0.000004548571957423423877537837
	400	0.000001982372128	0.000001979732627197689616236145
	500	0.000001042194934	0.000001034077156421974180242224
100	10	0.024314292988681	0.024314292988680864190110392609
	100	0.000100242573102	0.000100242568139407331736524506
	200	0.000014501912109	0.000014501803496945768054100507
	300	0.000004549264630	0.000004548571953616663090340995
	400	0.000001982297142	0.000001979732628112377070251772
	500	0.000001040782592	0.000001034077168200025910092884
150	10	0.024314292988682	0.024314292988680864190110388161
	100	0.000100242577603	0.000100242568139407331685518495
	200	0.000014502011929	0.000014501803496945764680397208
	300	0.000004549891945	0.000004548571953616680172305663
	400	0.000001984616067	0.000001979732628112504797936584
	500	0.000001046957055	0.000001034077168199940285585132
200	10	0.024314292988682	0.024314292988680864190110388176
	100	0.000100242578682	0.000100242568139407331685585932
	200	0.000014502034840	0.000014501803496945764680403612
	300	0.000004550038335	0.000004548571953616680184257373
	400	0.000001985153638	0.000001979732628112504742575794
	500	0.000001048360910	0.000001034077168199939706035334

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Table 5. Numerical solution $y'(x)$ with various values of x, N and iterations.

N	x	15th iteration	45th iteration
50	0	-1.58798412034597	-1.588071022461220318498896590154
	10	-0.00460288187129	-0.004602881871269254843810395419
	100	-0.00000273935089	-0.000002739351068678834237868374
	200	-0.00000020575729	-0.000000205753231612157754759952
	300	-0.00000004364704	-0.000000043659496195672746505803
	400	-0.00000001432569	-0.000000014366823142132220490812
	500	-0.00000000596694	-0.000000006034363572464639504768
100	0	-1.58806849943926	-1.588071022611375312724621425500
	10	-0.00460288187126	-0.004602881871269254502543510545
	100	-0.00000273935085	-0.000002739351068678330084039598
	200	-0.00000020575078	-0.000000205753231647526755494256
	300	-0.00000004364886	-0.000000043659496185303784906289
	400	-0.00000001433829	-0.000000014366823059962315807005
	500	-0.00000000597884	-0.000000006034363442469561014542
150	0	-1.58807102261138	-1.588071022611375312718684517975
	10	-0.00460288187126	-0.004602881871269254502543511856
	100	-0.00000273935065	-0.000002739351068678330086729788
	200	-0.00000020574848	-0.000000205753231647526892514803
	300	-0.00000004365807	-0.000000043659496185302905165385
	400	-0.00000001431185	-0.000000014366823059961806903847
	500	-0.00000000592789	-0.000000006034363442475252124155
200	0	-1.58807102261137	-1.588071022611375312718684509423
	10	-0.00460288187126	-0.004602881871269254502543511851
	100	-0.00000273935060	-0.000002739351068678330086744132
	200	-0.00000020574799	-0.000000205753231647526892605535
	300	-0.00000004363715	-0.000000043659496185302904545958
	400	-0.00000001430608	-0.000000014366823059961810213641
	500	-0.00000000591587	-0.000000006034363442475256759610

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