AIMS Mathematics

http://www.aimspress.com/journal/Math

AIMS Mathematics, 8(5): 10529–10546.
DOI: 10.3934/math.2023534
Received: 08 December 2022
Revised: 14 February 2023
Accepted: 15 February 2023
Published: 02 March 2023

Research article

Generalized Thomas-Fermi equation: existence, uniqueness, and analytic approximation solutions

Lazhar Bougoffa[1,*], **Smail Bougouffa**[2] **and Ammar Khanfer**[3]

[1] Department of Mathematics, Faculty of Science, Imam Mohammad Ibn Saud Islamic University, Riyadh 11623, Saudi Arabia

[2] Department of Physics, Faculty of Science, Imam Mohammad Ibn Saud Islamic University, Riyadh 11623, Saudi Arabia

[3] Department of Mathematics and Sciences, Prince Sultan University, Riyadh, Saudi Arabia

* **Correspondence:** Email: bougoffa@hotmail.com.

Abstract: The existence and uniqueness theorem for the generalized boundary value problem of the Thomas-Fermi equation:

$$\begin{cases} y'' + f(x,y) = 0, \ 0 < x < \infty, \\ y(0) = 1, \ y(\infty) = 0, \end{cases}$$

where

$$f(x,y) = -y\left(\frac{y}{x}\right)^{\frac{p}{p+1}}, \ p > 0, \ 0 < x < \infty,$$

is proved. Also, highly accurate approximate solutions are obtained explicitly for this new boundary value problem which arises in particular studies of many-electron systems (atoms, ions, molecules, metals, crystals). To the best of our knowledge, the results obtained here are new and provide the lower and upper bounds approximate solutions for the generalized Thomas-Fermi problem.

Keywords: Thomas-Fermi equation; existence and uniqueness theorem; approximate solution; lower and upper bounds; Adomian decomposition method; Adomian polynomials
Mathematics Subject Classification: 34B16, 34B40, 65N35

1. Introduction

The classical Thomas-Fermi problem for the neutral atom is a second-order non-linear ordinary differential equation, named after Llewellyn Thomas and Enrico Fermi [1–5] which can be derived by applying the Thomas-Fermi model to atoms. The Thomas-Fermi model assumes that all electrons are subject to the same conditions and energy conservation law, and has potential energy $e\Phi$ [6] so when assuming that the potential is spherically symmetric, then the charge density ρ and the potential energy are related through the Poisson's equation

$$\frac{1}{r}\frac{d^2}{dr^2}\left(r\Phi(r)\right) + 4\pi\rho(r) = 0, \tag{1.1}$$

where $\hbar$ is the Planck's constant, r is the distance from the nucleus, and ρ is given by

$$\rho = \frac{-1}{3\pi^2\hbar^3}(2m)^{3/2}[e\Phi(r)]^{3/2}, \tag{1.2}$$

where e is the electronic charge and m is the mass. Substituting in the above equation yields

$$\frac{1}{r}\frac{d^2}{dr^2}\left(r\Phi(r)\right) - \frac{4e}{3\pi}\left(\frac{2m}{\hbar}\right)^{3/2}[e\Phi(r)]^{3/2} = 0, \tag{1.3}$$

with the corresponding boundary conditions:

$$\lim_{r\to 0} r\Phi(r) = eZ, \tag{1.4}$$

where Z is the atomic number, and

$$\lim_{r\to\infty} \Phi(r) = 0. \tag{1.5}$$

By introducing the following transformation $r = \mu x$ for some appropriate parameter μ and $y = \dfrac{r\Phi(r)}{eZ}$, we arrive at the so-called differential equation of the Thomas-Fermi equation

$$y'' = x^{-\frac{1}{2}}y^{\frac{3}{2}},\ 0 < x < \infty, \tag{1.6}$$

$$y(0) = 1,\ y(\infty) = 0. \tag{1.7}$$

This equation models the charge distribution of a neutral atom as a function of the radius x. It should be noted here that the basic Thomas-Fermi (TF) model for ions is subject to the boundary conditions $y(0) = 1$ and $y(x_0) = 0$, where $x_0 > 0$ is the dimensionless ion size which measures the boundary radius and satisfies the relation $-x_0 y'(x_0) = q$ for some ionization factor q. When the nuclear charge equals the number of (bound) electrons, then $q = 0$ which occurs when $x_0 \longrightarrow \infty$, and the the problem, in this case, describes the neutral atom model case [7]. The TF equation (1.6) has connections to other important partial differential equations, for example, it is considered a special case of the well-known Poisson equation, and can also be viewed as an Euler-Lagrange equation associated with the Fermi energy [8]. The Thomas-Fermi model has deep connections to the quantum gravity theory where it is reformulated at the Planck scale [9–11].

The equation has a particular solution $y_p(x)$, which satisfies the boundary condition $y \to 0$ as $x \to \infty$, but not the initial condition $y(0) = 1$. This particular solution is $y_p(x) = \frac{144}{x^3}$.

Arnold Sommerfeld used this particular solution and provided an approximate solution that can satisfy the other boundary condition [4]:

$$y_s(x) = y_p(x)\left(1 + y_p(x)^{\lambda_1/3}\right)^{\lambda_2/2}, \tag{1.8}$$

where $\lambda_1 = 0.772$ and $\lambda_2 = -7.772$. This solution predicts the correct solution accurately for large x but still fails near the origin. A considerable amount of literature is devoted to the numerical solutions for the classical version of this problem [12–16]. In [12], numerical solution was obtained using the variational principle. J. Boyd [13] obtained a numerical solution using rational Chebyshev functions. The authors in [14, 15] obtained numerical solutions using a spectral method based on the fractional order of rational Bessel functions. Pikulin [16] used a semi-analytical numerical method to compute the solution. Furthermore, different methods such as homotopy analysis and iterative methods are used to investigate the approximate solutions to this problem, see, e.g., [17–21].

However, a free boundary value issue is also implemented to approach the initial Thomas-Fermi equation. As a result, the free boundary value issue is changed into a nonlinear boundary value problem that is defined on a closed interval. An adaptive approach is used to tackle the issue utilizing the moving mesh finite element method [22].

The present paper investigates the generalized boundary value problem of the Thomas-Fermi equation

$$\begin{cases} y'' + f(x,y) = 0, \ 0 < x < \infty, \\ y(0) = 1, \ y(\infty) = 0, \end{cases} \tag{1.9}$$

where

$$f(x,y) = -y\left(\frac{y}{x}\right)^{\frac{p}{p+1}}, \ p > 0, \ 0 < x < \infty, \tag{1.10}$$

and we assume that $0 \leq y(x) \leq 1$.

The Thomas-Fermi equation is a special case of this equation when $p = 1$. As pointed out in [23], this generalized TF equation is related to non-integrable Abel equations, and therefore no closed solutions are possible for any case of this type of equation.

In this paper, we aim to provide an analytic approximate solution in explicit form for problem (1.9) with (1.10). In Section 2, we establish a theorem that provides the lower and upper bounds of the solution y and guarantees the existence of the solution to this problem as well as a theorem on the uniqueness of the solution. In Section 3, we present analytic approximate solutions in different explicit forms to this problem. Also, an interesting variation of the Adomian decomposition method (ADM) [24–33] is presented, which allows the determination of the solution in an easily-computed series. In Section 4, we carry out an analysis of the solution and compare it with other numerical solutions.

2. An existence and uniqueness theorem

2.1. Existence theorem

We first prove a result on the double inequalities for the lower and upper bounds of the solution y, which is an important tool in the proof of the existence of the solution to problem (1.9) with (1.10).

Theorem 2.1. *The generalized boundary value problem of TF equation (1.9) with (1.10) has at least one solution $y \in \mathbb{C}^2[0,\infty)$ such that*

$$y_1 \leq y \leq y_2 \ \text{on} \ [0,\infty), \tag{2.1}$$

where $y_1(x) = \frac{1}{(x+1)^{\frac{1+\sqrt{5}}{2}}}$, $y_2(x) = -x\Big((K(0,x) - K(1,x))\Big)$*, and* K *is the modified Bessel function of the second kind.*

Proof. Using the following inequality:

$$\left(\frac{1}{x}\right)^r < \left(1+\frac{1}{x}\right)^r,\ r = \frac{p}{p+1} < 1,\ x > 0, \tag{2.2}$$

we obtain

$$\left(\frac{1}{x}\right)^r < 1+\frac{1}{x},\ r = \frac{p}{p+1} < 1,\ x > 0, \tag{2.3}$$

which will be helpful later.

In view of $0 \le y(x) \le 1$, it follows that

$$\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \le \left(1+\frac{1}{x}\right)y^{\frac{p}{p+1}},\ \text{for } 0 \le y \le 1, \tag{2.4}$$

and with $y^{\frac{p}{p+1}} \le 1$, we have

$$\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \le 1+\frac{1}{x},\ \text{for } 0 \le y \le 1. \tag{2.5}$$

Consequently,

$$y\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \le \left(1+\frac{1}{x}\right)y,\ \text{for } 0 \le y \le 1. \tag{2.6}$$

Hence,

$$f(x,y) = -y\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \ge -\left(1+\frac{1}{x}\right)y,\ \text{for } 0 \le y \le 1. \tag{2.7}$$

On the other hand, in view of the solution y remains in the interval $[0, 1]$ and since $\frac{p}{p+1} < 1$, we have

$$y^{\frac{p}{p+1}} \ge y. \tag{2.8}$$

Using now $x < x+1$ to obtain $\frac{1}{x} > \frac{1}{x+1}$. Hence, $\left(\frac{1}{x}\right)^{\frac{p}{p+1}} > \frac{1}{(x+1)^{\frac{p}{p+1}}}$. Thus,

$$\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \ge \frac{1}{(x+1)^{\frac{p}{p+1}}} \tag{2.9}$$

or

$$\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \ge \frac{y}{x+1}. \tag{2.10}$$

It can be checked easily that

$$y\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \ge \frac{y}{(x+1)^2},\ \text{for } 0 \le y \le 1. \tag{2.11}$$

Hence,

$$f(x,y) = -y\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \le -\frac{y}{(x+1)^2},\ \ \text{for } 0 \le y \le 1. \tag{2.12}$$

Thus, from (2.7) and (2.12), we obtain

$$G_2(x,y) \leq f(x,y) = -y\left(\frac{y}{x}\right)^{\frac{p}{p+1}} \leq G_1(x,y),\ \text{for } 0 \leq y \leq 1, \tag{2.13}$$

where

$$G_1(x,y) = -\frac{1}{(x+1)^2}y \text{ and } G_2(x,y) = -\left(1+\frac{1}{x}\right)y,\ \text{for } 0 \leq y \leq 1. \tag{2.14}$$

For comparison purposes, we have the following linear boundary value problems:

$$\begin{cases} y_1'' + G_1(x,y_1) \leq 0,\ 0 < x < \infty, \\ y_1(0) = 1,\ y_1(\infty) = 0, \end{cases} \tag{2.15}$$

and

$$\begin{cases} y_2'' + G_2(x,y_2) \geq 0,\ 0 < x < \infty, \\ y_2(0) = 1,\ y_2(\infty) = 0. \end{cases} \tag{2.16}$$

Then, suitable comparison problems are

$$\begin{cases} y_1'' - \dfrac{1}{(1+x)^2}y_1 = 0,\ 0 < x < \infty, \\ y_1(0) = 1,\ y_1(\infty) = 0, \end{cases} \tag{2.17}$$

and

$$\begin{cases} y_2'' - \left(1+\dfrac{1}{x}\right)y_2 = 0,\ 0 < x < \infty, \\ y_2(0) = 1,\ y_2(\infty) = 0. \end{cases} \tag{2.18}$$

To find the solution y_1 of problem (2.17), we write

$$(1+x)^2\, y_1'' - y_1 = 0. \tag{2.19}$$

Let $\xi = x + 1$. Thus this equation becomes

$$\xi^2 y_1''(\xi) - y_1(\xi) = 0. \tag{2.20}$$

The substitution $\xi = e^{-t}$ leads to a constant coefficient linear equation

$$y_1''(t) - y_1'(t) - y_1(t) = 0. \tag{2.21}$$

Thus,

$$y_1(x) = \frac{C_1}{(x+1)^{\frac{1+\sqrt{5}}{2}}} + \frac{C_2}{(x+1)^{\frac{1-\sqrt{5}}{2}}}, \tag{2.22}$$

where C_1 and C_2 are two constants. Using the boundary conditions $y_1(0) = 1,\ y_1(\infty) = 0$ to find $C_1 = 1$ and $C_2 = 0$. This gives

$$y_1(x) = \frac{1}{(x+1)^{\frac{1+\sqrt{5}}{2}}}. \tag{2.23}$$

To find the solution y_2 of problem (2.18), we bring back the form of the confluent hypergeometric equation with parameters a and b [34–36]:

$$xy'' + (b - x)y' - ay = 0, \tag{2.24}$$

which has a regular singularity at 0 and an irregular one at infinity; and whose solution is ${}_1F_1(a; c; x)$.

The equation of problem (2.18) can be simply written as

$$y_2'' - \left(1 + \frac{2}{2x}\right) y_2 = 0. \tag{2.25}$$

We introduce the change of variables $\xi = 2x$ and $y_2(x) = v(\xi)$. Then

$$4\xi v''(\xi) - (\xi + 2)\, v(\xi) = 0. \tag{2.26}$$

The transformation $v(\xi) = \xi e^{-\frac{\xi}{2}} w(\xi)$ leads to

$$\xi w''(\xi) + (2 - \xi)\, w'(\xi) - \frac{3}{2} w(\xi) = 0, \tag{2.27}$$

which is the confluent hypergeometric equation with parameters $a = 3/2$ and $b = 2$.

Thus the general solution of problem (2.18) is given in terms of the modified Bessel functions as

$$y_2(x) = x\Big(c_1(I(0, x) + I(1, x)) + c_2(K(0, x) - K(1, x))\Big), \tag{2.28}$$

where I and K are the modified Bessel functions of the first and second kind, respectively. c_1 and c_2 are arbitrary constants, which can be determined from the boundary conditions. Indeed, to satisfy these conditions $y_2(0) = 1$ and $y_2(\infty) = 0$, we get $c_1 = 0$ and $c_2 = -1$, and so the required solution is given by

$$y_2(x) = -x\Big((K(0, x) - K(1, x))\Big). \tag{2.29}$$

For small x, we have

$$y_2(x) \approx 1 + x(\ln(\frac{x}{2}) + \gamma) + O(x^2) \text{ as } x \to 0^+. \tag{2.30}$$

Hence, the condition $y_2(0) = 1$ is satisfied.

We are now able to apply the method of upper and lower solutions. For more details about this technique, we refer the reader to (Chapter 7, [37]), which is applicable when $f(x, y)$ has a singularity at $x = 0$ and the Lipschitz constants $L_1(x) = -\frac{1}{(x+1)^2}$ and $L_2(x) = -\left(1 + \frac{1}{x}\right)$ are functions of the independent variable x and continuous everywhere except for $L_2(x)$ at $x = 0$.

It should be noted here that y_1 and y_2 are both twice continuously differentiable and satisfy the above differential inequalities functions (2.15) and (2.16) on $(0, \infty)$ with $y_1 < y_2$. Furthermore, the function $f(x, y)$ is continuous and bounded in

$$\mathbb{S} = \{(x, y) :\ 0 \le x < \infty,\ y_1 \le y \le y_2\}. \tag{2.31}$$

This completes the proof. □

To show the variation of these two extremum functions, we present in Figure 1 the variation of the upper and lower functions in terms of the independent variable x. In addition, the extremum functions are independent of the parameters p, which makes them the optimum functions for all kinds of Thomas-Fermi equations.

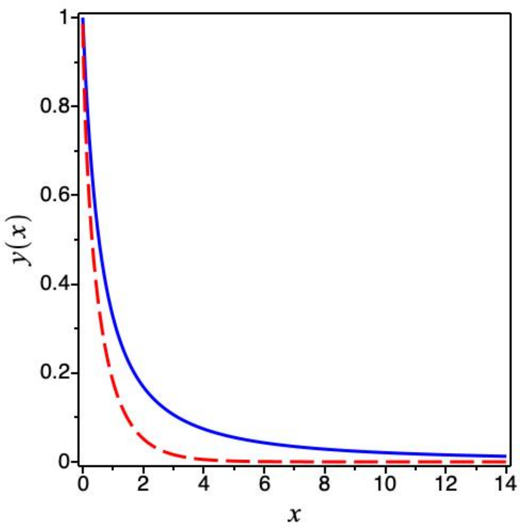

Figure 1. The variation of the extremum functions $y_1(x)$ and $y_2(x)$ versus the independent variable x. Lower function: red dashed line; Upper function: blue solid line.

2.2. Uniqueness theorem

Theorem 2.2. *The generalized boundary value problem of TF equation (1.9) with (1.10) has at most one solution* $y \in \mathbb{C}^2[0,\infty)$.

Proof. To obtain an important result on the uniqueness, we assume that $\bar{y}_1$ and $\bar{y}_2$ are two different solutions to problem (1.9) with (1.10). Then,

$$\begin{cases} \bar{y}_1'' = g(x, \bar{y}_1), \ 0 < x < \infty, \\ \bar{y}_1(0) = 1, \ \bar{y}_1(\infty) = 0, \end{cases} \tag{2.32}$$

and

$$\begin{cases} \bar{y}_2'' = g(x, \bar{y}_2), \ 0 < x < \infty, \\ \bar{y}_2(0) = 1, \ \bar{y}_2(\infty) = 0, \end{cases} \tag{2.33}$$

where $g(x, y) = y\left(\frac{y}{x}\right)^{\frac{p}{p+1}}$.

Consider the positive function $h(x) = \frac{1}{2}(\bar{y}_1 - \bar{y}_2)^2$. Thus h vanishes at zero and infinity. Therefore, if is not identically zero it must have a positive maximum at a point $\bar{x}$, where $\bar{x} > 0$. Thus, its graph is concave down at $\bar{x} > 0$, and we have

$$h''(\bar{x}) = \left[\frac{1}{2}(\bar{y}_1 - \bar{y}_2)^2\right]'' |_{x=\bar{x}} \leq 0. \tag{2.34}$$

Since

$$\left[\frac{1}{2}(\bar{y}_1-\bar{y}_2)^2\right]''|_{x=\bar{x}}=(\bar{y}_1''(\bar{x})-\bar{y}_2''(\bar{x}))(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x}))+(\bar{y}_1'(\bar{x})-\bar{y}_2'(\bar{x}))^2, \tag{2.35}$$

or

$$\left[\frac{1}{2}(\bar{y}_1-\bar{y}_2)^2\right]''|_{x=\bar{x}}=(\bar{y}_1''(\bar{x})-\bar{y}_2''(\bar{x}))(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x})). \tag{2.36}$$

Hence,

$$(\bar{y}_1''(\bar{x})-\bar{y}_2''(\bar{x}))(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x}))\le 0. \tag{2.37}$$

From (2.32) and (2.33), we have

$$\bar{y}_1''(x)-\bar{y}_2''(x)=g(x,\bar{y}_1)-g(x,\bar{y}_2). \tag{2.38}$$

Applying the mean value theorem to the function g with respect to $\bar{y}$, we obtain

$$\bar{y}_1''(x)-\bar{y}_2''(x)=\frac{\partial g}{\partial y}(x,\bar{y}^*)(\bar{y}_1(x)-\bar{y}_2(x)), \tag{2.39}$$

where $0\le\bar{y}_1<\bar{y}^*<\bar{y}_2\le 1$.

On the other hand, differentiating the function $g(x,y)$ with respect to y, we obtain

$$\frac{\partial g}{\partial y}(x,y)=\left(\frac{2p+1}{p+1}\right)\left(\frac{y}{x}\right)^{\frac{p}{p+1}}. \tag{2.40}$$

Hence,

$$\frac{\partial g}{\partial y}(\bar{x},\bar{y}^*)=\left(\frac{2p+1}{p+1}\right)\left(\frac{\bar{y}^*(\bar{x})}{\bar{x}}\right)^{\frac{p}{p+1}},\ \bar{x}>0. \tag{2.41}$$

Consequently,

$$\bar{y}_1''(\bar{x})-\bar{y}_2''(\bar{x})=\left(\frac{2p+1}{p+1}\right)\left(\frac{\bar{y}^*(\bar{x})}{\bar{x}}\right)^{\frac{p}{p+1}}(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x})). \tag{2.42}$$

Substituting this into (2.37), we obtain

$$\left(\frac{2p+1}{p+1}\right)\left(\frac{\bar{y}^*(\bar{x})}{\bar{x}}\right)^{\frac{p}{p+1}}(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x}))^2\le 0, \tag{2.43}$$

which contradicts the assumption that $\frac{2p+1}{p+1}>0$, $\frac{\bar{y}^*(\bar{x})}{\bar{x}}>0$, $\bar{x}>0$ and $(\bar{y}_1(\bar{x})-\bar{y}_2(\bar{x}))^2>0$. So $h(x)=\frac{1}{2}(\bar{y}_1-\bar{y}_2)^2\equiv 0$. This shows the uniqueness of the solution and completes the proof of the theorem. □

3. Explicit approximate solutions

We conclude here based on Theorem 2.1, which may offer advantages in finding out lower and upper solutions of our problem (1.9) with (1.10) in explicit forms such that $y_1\le y\le y_2$ on $[0,\infty)$, and consequently we should expect y to take similar explicit forms in the whole region with the corresponding boundary conditions.

3.1. The first approximation

To obtain an approximate solution y to problem (1.9) with (1.10), we first make the following approximation.

A possible linear approximation of a function $f(x)$ at $x = x_0$ may be obtained using the equation of the tangent line

$$f(x) \approx f(x_0) + f'(x_0)(x - x_0). \tag{3.1}$$

If we choose $f(x) = \sqrt{\beta x}$, $\beta > 0$ and $x_0 = \frac{1}{\beta}$, then

$$\sqrt{\beta x} \approx \frac{1 + \beta x}{2}, \tag{3.2}$$

when x is close enough to $x_0 = \frac{1}{\beta}$. Hence,

$$\beta x \approx \frac{(1 + \beta x)^2}{4}. \tag{3.3}$$

Substituting (3.3) into the nonlinear term of the ODE of problem (1.9), we obtain

$$y'' - \frac{2^{\frac{2p}{p+1}} \beta^{\frac{p}{p+1}}}{(1 + \beta x)^{\frac{2p}{p+1}}} y^{\frac{p}{p+1}+1} = 0. \tag{3.4}$$

For the solution y of the approximate equation (3.4), by Theorem 2.1, we expect that the solution y can be obtained in the form

$$y = (1 + \beta x)^m, \tag{3.5}$$

where $\beta > 0$ and $m < 0$ are two parameters to be determined. Inserting the ansatz given by (3.5) into Eq (3.4), we obtain

$$m(m - 1)\beta^2 (1 + \beta x)^{m-2} = 2^{\frac{2p}{p+1}} \beta^{\frac{p}{p+1}} (1 + \beta x)^{\frac{mp}{p+1}+m-\frac{2p}{p+1}}. \tag{3.6}$$

If we assume that $m - 2 = \frac{mp}{p+1} + m - \frac{2p}{p+1}$, that is $m = -\frac{2}{p}$, then, we derive the following relation between the parameters

$$\frac{2}{p} \frac{p + 2}{p} = 2^{\frac{2p}{p+1}} \beta^{-\frac{p+2}{p+1}}, \tag{3.7}$$

that is

$$\beta = \frac{2^{\frac{2p}{p+2}}}{\left(\frac{2}{p} \frac{p+2}{p}\right)^{\frac{p+1}{p+2}}}. \tag{3.8}$$

Thus the first analytic approximate solution to the generalized TF equation is given by

$$y_1(x; p) = \frac{1}{(1 + \beta x)^{\frac{2}{p}}}, \text{ where } \beta = \frac{2^{\frac{2p}{p+2}}}{\left(\frac{2}{p} \frac{p+2}{p}\right)^{\frac{p+1}{p+2}}}. \tag{3.9}$$

3.2. The second approximation

The term $(\beta x)^{\frac{p}{p+1}}$ can be approximated by $(1+\beta x)^{\frac{p}{p+1}}$ for sufficiently large values of βx; that is,

$$(\beta x)^{\frac{p}{p+1}} \approx (1+\beta x)^{\frac{p}{p+1}} . \tag{3.10}$$

Substituting (3.10) into the nonlinear term of the ODE of problem (1.9), we obtain

$$(m^2+m)\beta^2 (1+\beta x)^{-2} = \beta^{\frac{p}{p+1}} (1+\beta x)^{-\frac{(m+1)p}{p+1}} . \tag{3.11}$$

It follows that $m = 1+\frac{2}{p}$ and $\beta = \left[\left(\frac{p+2}{p}\right)^2 + \frac{p+2}{p}\right]^{-\frac{p+1}{p+2}}$.

Thus, the second analytic approximate solution to the generalized TF equation for x large is given as

$$y_2(x;p) = \frac{1}{(1+\beta x)^{1+\frac{2}{p}}}, \text{ where } \beta = \left[\left(\frac{p+2}{p}\right)^2 + \frac{p+2}{p}\right]^{-\frac{p+1}{p+2}} . \tag{3.12}$$

3.3. The third approximation

For x near 1, we can substitute $x \approx 1$ in the denominator of the nonlinear term of the ODE of problem (1.9) to find

$$(m^2+m)\beta^2 (1+\beta x)^{-2} = (1+\beta x)^{-\frac{(m+1)p}{p+1}} . \tag{3.13}$$

It follows that $m = 2+\frac{2}{p}$ and $\beta = \left[\left(\frac{2p+2}{p}\right)^2 + \frac{2p+2}{p}\right]^{-\frac{1}{2}}$.

Thus, the third analytic approximate solution to the generalized TF equation for x near 1 is given as

$$y_3(x;p) = \frac{1}{(1+\beta x)^{2+\frac{2}{p}}}, \text{ where } \beta = \left[\left(\frac{2p+2}{p}\right)^2 + \frac{2p+2}{p}\right]^{-\frac{1}{2}} . \tag{3.14}$$

Thus, our approximate solutions can be obtained by direct approaches.

3.4. The fourth approximation using ADM

In this section, we consider an interesting variation of the modified Adomian decomposition method (ADM) [24–34], which permits the determination of the solution of nonlinear initial-boundary value problem (1.9) with (1.10).

Rewrite the ODE of problem (1.9) with (1.10) in Adomian's operator-theoretic form

$$Ly = x^{-\frac{p}{p+1}} N(y), \ 0 < x < \infty, \tag{3.15}$$

where $L = \frac{d^2}{dx^2}$ and $N(y) = y^{\frac{2p+1}{p+1}}$.

Applying L^{-1} to both sides of Eq (3.15) and using the initial condition $y(0) = 1$, we obtain

$$y = 1 + Bx + \int_0^x \int_0^x \left[x^{-\frac{p}{p+1}} N(y)\right] dxdx, \tag{3.16}$$

where $B = y'(0)$ is an unknown constant to be determined by using the boundary condition $y(\infty) = 0$.

According to the Adomian decomposition method [24–33], assuming the decomposition

$$y = \sum_{n=0}^{\infty} y_n \text{ and } N(y) = y^{\frac{2p+1}{p+1}} = \sum_{n=0}^{\infty} A_n, \tag{3.17}$$

where A_n are the Adomian polynomials [24, 25, 33]. Thus, Eq (3.16) becomes

$$\sum_{n=0}^{\infty} y_n = 1 + Bx + \int_0^x \int_0^x \left[x^{-\frac{p}{p+1}} \sum_{n=0}^{\infty} A_n \right] dxdx. \tag{3.18}$$

We identify

$$y_0 = 1,\ y_1 = Bx \text{ and } \sum_{n=2}^{\infty} y_n = \int_0^x \int_0^x \left[x^{-\frac{p}{p+1}} \sum_{n=0}^{\infty} A_n \right] dxdx. \tag{3.19}$$

Hence, a new recurrence relation for $y_n,\ n \geq 0$, is established as

$$\begin{cases} y_0 &= 1, \\ y_1 &= Bx, \\ y_{n+2} &= \int_0^x \int_0^x \left[x^{-\frac{p}{p+1}} A_n \right] dxdx, \end{cases} \tag{3.20}$$

where the Adomian polynomials A_n [24, 25, 33] for the $N(y) = y^{\frac{2p+1}{p+1}}$ term are

$$\begin{cases} A_0(y_0) &= y_0^{\frac{2p+1}{p+1}}, \\ A_1(y_0, y_1) &= \frac{2p+1}{p+1} y_1 y_0^{\frac{p}{p+1}}, \\ A_2(y_0, y_1, y_2) &= \frac{2p+1}{p+1} y_2 y_0^{\frac{p}{p+1}} + \frac{1}{2!} \frac{2p+1}{p+1} \frac{p}{p+1} y_1^2 y_0^{-\frac{p+2}{p+1}}, \\ &\cdots \end{cases} \tag{3.21}$$

The first few components of the solution $y_n,\ n \geq 0$ are given by

$$\begin{cases} y_0 &= 1, \\ y_1 &= Bx, \\ y_2 &= \frac{(p+1)^2}{p+2} x^{\frac{p+2}{p+1}}, \\ y_3 &= B \frac{(p+1)(2p+1)}{(p+2)(2p+3)} x^{\frac{2p+3}{p+1}}, \\ y_4 &= \frac{(p+1)^3(2p+1)}{2(p+2)^2(p+3)} x^{\frac{2p+4}{p+1}} + B^2 \frac{p(2p+1)}{2(3p+4)(2p+3)} x^{\frac{3p+4}{p+1}}, \\ &\cdots \end{cases} \tag{3.22}$$

Hence,

$$y = 1 + Bx + \frac{(p+1)^2}{p+2} x^{\frac{p+2}{p+1}} + B \frac{(p+1)(2p+1)}{(p+2)(2p+3)} x^{\frac{2p+3}{p+1}} + ... \tag{3.23}$$

3.4.1. Computation of B

It remains now to apply the second boundary condition $y \to 0$ as $x \to \infty$ to the function $y(x)$. This boundary condition cannot be applied directly to the series (3.23). Recall that it is customary to combine the series solutions obtained by the decomposition method with the Padé approximants to provide an effective tool to treat boundary value problems on an infinite or semi-infinite interval [33]. To illustrate this, we choose $p = 1$. For convenience, we list below, by using (3.21), few terms of the Adomian polynomials A_n

$$\begin{cases} A_0(y_0) = 1, \\ A_1(y_0, y_1) = \frac{3}{2}y_1, \\ A_2(y_0, y_1, y_2) = \frac{3}{2}y_2 + \frac{3}{8}y_1^2, \\ A_3(y_0, y_1, y_2) = \frac{3}{2}y_3 + \frac{3}{4}y_1y_2 - \frac{1}{16}y_1^2, \\ \qquad ... \end{cases} \tag{3.24}$$

The first few components of the solution $y_n,\ n \geq 0$, are given by

$$\begin{cases} y_0 = 1, \\ y_1 = Bx, \\ y_2 = \frac{4}{3}x^{\frac{3}{2}}, \\ y_3 = \frac{2}{5}Bx^{\frac{5}{2}}, \\ y_4 = \frac{1}{3}x^3 + \frac{3}{70}B^2x^{\frac{7}{2}}, \\ \quad ... \end{cases} \tag{3.25}$$

Hence,

$$y = 1 + Bx + \frac{4}{3}x^{\frac{3}{2}} + \frac{2}{5}Bx^{\frac{5}{2}} + \frac{1}{3}x^3 + \frac{3}{70}B^2x^{\frac{7}{2}} + \frac{2}{15}Bx^4 + ... \tag{3.26}$$

Setting $x^{\frac{1}{2}} = \xi$ into (3.26), we obtain

$$y = 1 + B\xi^2 + \frac{4}{3}\xi^3 + \frac{2}{5}B\xi^5 + \frac{1}{3}\xi^6 + \frac{3}{70}B^2\xi^7 + \frac{2}{15}B\xi^8 + ..., \tag{3.27}$$

which is indeed the same approximation of y that obtained by Baker in 1930 [5] and Wazwaz [33]. In applying the boundary condition $y(\infty) = 0$ to the diagonal Padé approximants $P_{10,10} = [10/10]$, we obtain the approximation for the initial slope $B = y'(0) = -1.588077$, which is a very good approximation to accuracy 10^{-5} comparing to the value obtained by Parand et al. as -1.588071 [14]. These values are also in good agreement with the obtained numerical value $y_n'(0) = -1.564036$ for $p = 1$.

4. Analysis of solutions

We are now in the position to explore some mathematical results and investigate the numerical treatment of the boundary value problem (1.9) with (1.10). In Figure 2, we present the different solutions of problem (1.9) with (1.10) with the particular case $p = 1$. The first approximation (solid blue line) is in good agreement with the numerical solution and Sommerfeld's approximation. On the other hand, the third approximation (black dash-dotted line) is in good agreement with the numerical solution for small values of the independent variable x. While the second approximation diverges slightly from the other solutions for small and intermediate values of the independent variable x. All solutions coincide together for large values of x. Due to the potential limits of the numerical volume [38–40], we chose the maximum value of the independent variable as $x = 14$. The numerical solution is obtained, using the Maple software, and the available mid-rich sub-method, which is a midpoint method with the same enhancement schemes. So, the midpoint sub-methods are capable of handling harmless end-point singularities that the trapezoid sub-methods cannot. For the enhancement schemes, Richardson extrapolation is generally faster, but deferred corrections use less memory on difficult problems [41,42].

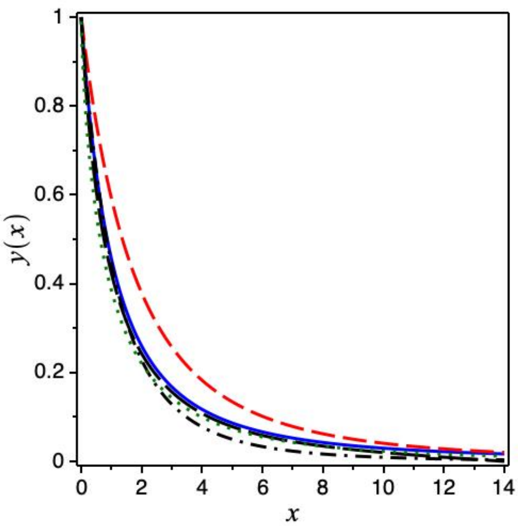

Figure 2. The variation of the different solutions $y(x)$ of (1.9) with (1.10) versus the independent variable x. Numerical solution: black long dashed line; Sommerfeld's solution: green dotted line; first approximation: blue solid line; second approximation: red dashed line; third approximation: black dash-dotted line. All solutions are obtained for $p = 1$.

In addition, we present in Tables 1 and 2 a comparison between the numerical solution and different proposed approximations for the case $p = 1$, for small and large values of the independent variables x. These numerical values show clearly that the first and third approximations agree very well with the numerical solution in all ranges of the independent value x.

Now, we can explore other interesting cases with $p \neq 1$, to show the efficiency of the suggested approximations and their validity ranges. In Figure 3, we present the different solutions of (1.9) with (1.10) with the particular cases $p = 2, 3$. The first and third approximations (solid blue line, black dash-dotted line) are in good agreement with the numerical solution for small values of the independent variable x. On the other hand, the third approximation remains in good agreement with the numerical solutions, while the first approximation diverges from the numerical solution by increasing the parameter p. The second approximation is still larger than all approximations over the small and intermediate domains of x.

Table 1. Comparison between different approximations and numerical solutions of problem (1.9) with (1.10) for the case $p = 1$, and small values of the independent variable x. y_n = Numerical solution, y_s = Sommerfeld's approximation, $y_{1;1}$ = First solution, $y_{2;1}$ = Second approximation and $y_{3;1}$ = Third approximation.

x	y_n	y_s	$y_{1;1}$	$y_{2;1}$	$y_{3;1}$
.100000	.890589	.836423	.910357	.944876	.915349
.200000	.800549	.740601	.832265	.893735	.839461
.300000	.725548	.666917	.763802	.846210	.771278
.400000	.662283	.606766	.703443	.802028	.709884
.500000	.608242	.556122	.649967	.760838	.654476
.600000	.561517	.512617	.602373	.722429	.604368
.700000	.520665	.474709	.559820	.686559	.558968
.800000	.484586	.441319	.521616	.653027	.517735
.900000	.452445	.411651	.487194	.621639	.480250
1.00000	.423598	.385104	.456075	.592235	.446096

Table 2. Comparison between different approximations and numerical solutions of (1.9) with (1.10) for the case $p = 1$, and large values of the independent variable x. y_n = Numerical solution, y_s = Sommerfeld's approximation, $y_{1;1}$ = First solution, $y_{2;1}$ = Second approximation and $y_{3;1}$ = Third approximation.

x	y_n	y_s	$y_{1;1}$	$y_{2;1}$	$y_{3;1}$
1.	.423598	.385104	.456075	.592235	.446096
2.	.242734	.220660	.259910	.379212	.227968
3.	.156335	.142841	.167656	.257243	.128316
4.	.107979	.0993388	.117042	.182448	.0776398
5.	.781469e-1	.725516e-1	.863148e-1	.134052	.496894e-1
6.	.584026e-1	.549358e-1	.662721e-1	.101365	.332598e-1
7.	.445657e-1	.427789e-1	.524786e-1	.784985e-1	.230930e-1
8.	.343581e-1	.340689e-1	.425827e-1	.620228e-1	.165308e-1
9.	.264419e-1	.276399e-1	.352432e-1	.498537e-1	.121427e-1
10.	.199817e-1	.227745e-1	.296497e-1	.406706e-1	.911860e-2
11.	.144286e-1	.190161e-1	.252895e-1	.336111e-1	.698002e-2
12.	.940720e-2	.160612e-1	.218248e-1	.280956e-1	.543328e-2
13.	.465612e-2	.137020e-1	.190263e-1	.237236e-1	.429216e-2
14.	0.	.117932e-1	.167334e-1	.202137e-1	.343549e-2

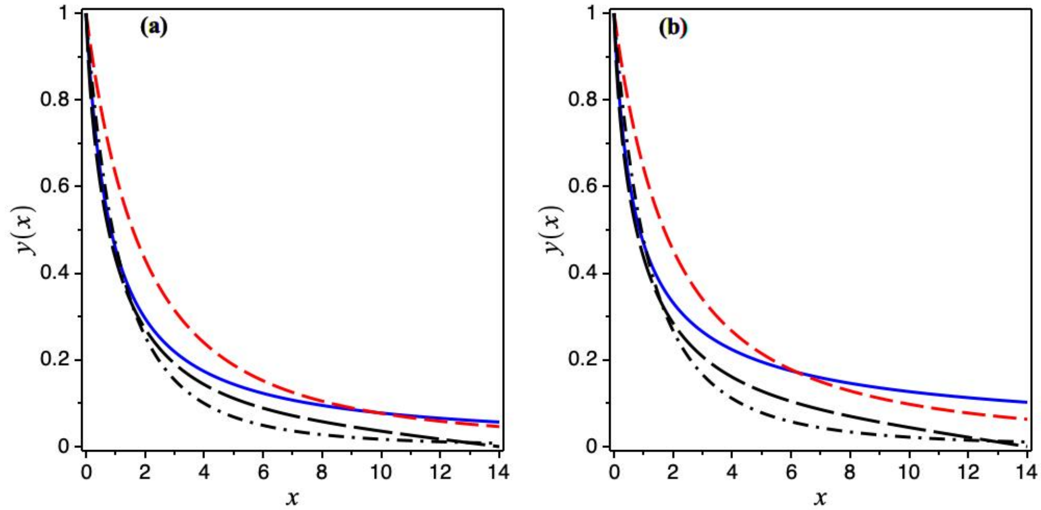

Figure 3. The variation of the different solutions $y(x)$ of (1.9) with (1.10) versus the independent variable x. Numerical solution: black long dashed line; first approximation: blue solid line; second approximation: red dashed line; third approximation: black dash-dotted line. (a) for $p = 2$ and (b) for $p = 3$.

Our overall findings demonstrate that it is possible to acquire a good approximation to the generalized TF equation. The charge distribution of a neutral atom as a function of radius x is also well-known to be described by this equation if and only if $y(x)$ approaches zero as x grows in size. Solutions with $y(x) = 0$ at a finite x are used to mimic positive ions. For solutions where $y(x)$ becomes significant and positive as x increases significantly, it can be viewed as a model of a compressed atom, where the charge is squeezed into a smaller region. These broad comments are adequately supported by our plots. The proposed investigation might be useful in dense media where quantum gravity's effects could be felt strongly.

5. Conclusions

The goal of this study is to solve the generalized TF equation which governs several physical issues, such as quantum systems, that naturally differ significantly from Fermi or Bose statistics, as well as some astrophysical or cosmological contexts where quantum electrostatics may exhibit more intertwined screening effects. The TF equation is modeled in this investigation as a singular boundary value problem with an upper and lower solution theory. The existence-construction of the aforementioned upper-lower solutions is also explored. Excellent approximations are proposed and the obtained results are in good agreement with those obtained numerically. We anticipate that the approximation solutions we have presented will be useful in assisting with the investigation of the TF model-governed physics issues.

Acknowledgements

The authors extend their appreciation to the Deanship of Scientific Research at Imam Mohammad Ibn Saud Islamic University for funding this work through Research Group no. RG-21-09-14.

Conflict of interest

The authors declare that they have no competing interests.

References

1. L. H. Thomas, The calculation of atomic fields, *Math. Proc. Cambridge Philos. Soc.*, **23** (1927), 542–548. https://doi.org/10.1017/S0305004100011683
2. E. Fermi, Eine statistiche methode zur bestimmung einiger eigenschaften des atoms und ihre anwendung auf die theorie des periodischen systems der elemente, *Z. Phys.*, **48** (1928), 73–79. https://doi.org/10.1007/BF01351576
3. S. L. Shapiro, S. A. Teukolsky, *Black holes, white dwarfs and neutron stars: the physics of compact objects*, New York: Wiley, 1983. https://doi.org/10.1002/9783527617661
4. A. Sommerfeld, Integrazione asintotica dell'equazione differenziale di Thomas-Fermi, *Rend. R. Accad. Lincei*, **15** (1932), 293–308.
5. E. B. Baker, The application of the Fermi-Thomas statistical model to the calculation of potential distribution in positive ions, *Phys. Rev.*, **36** (1930), 630–647. https://doi.org/10.1103/PhysRev.36.630
6. V. Marinca, R. D. Ene, Analytical approximate solutions to the Thomas-Fermi equation, *Cent. Eur. J. Phys.*, **12** (2014), 503–510. https://doi.org/10.2478/s11534-014-0472-9
7. A. A. Mavrin, A. V. Demura, Approximate solution of the Thomas-Fermi equation for free positive ions, *Atoms*, **9** (2021), 1–11. https://doi.org/10.3390/atoms9040087
8. A. Hasan-Zadeh, Examination of minimizer of Fermi energy in notions of Sobolev spaces, *Res. J. Appl. Sci. Eng. Technol.*, **15** (2018), 356–361. http://dx.doi.org/10.19026/rjaset.15.5926
9. H. Shababi, On the Thomas-Fermi model at the noncommutative framework, *Eur. Phys. J. Plus*, **137** (2022), 376. https://doi.org/10.1140/epjp/s13360-022-02596-9
10. H. Shababi, K. Ourabah, On the Thomas-Fermi model at the Planck scale, *Phys. Lett. A*, **383** (2019), 1105–1109. https://doi.org/10.1016/j.physleta.2019.01.019
11. H. Shababi, K. Ourabah, Thomas-Fermi theory at the Planck scale: a relativistic approach, *Ann. Phys.*, **413** (2020), 168051. https://doi.org/10.1016/j.aop.2019.168051
12. M. Oulne, Variation and series approach to the Thomas-Fermi equation, *Appl. Math. Comput.*, **218** (2011), 303–307. https://doi.org/10.1016/j.amc.2011.05.064
13. J. P. Boyd, Rational Chebyshev series for the Thomas-Fermi function: endpoint singularities and spectral methods, *J. Comput. Appl. Math.*, **244** (2013), 90–101. https://doi.org/10.1016/j.cam.2012.11.015
14. K. Parand, A. Ghaderi, M. Delkhosh, H. Yousefi, A new approach for solving nonlinear Thomas-Fermi equation based on fractional order of rational Bessel functions, *Electron. J. Differ. Equ.*, **331** (2016), 1–18. https://doi.org/10.48550/arXiv.1606.07615

15. K. Parand, K. Rabiei, M. Delkhosh, An efficient numerical method for solving nonlinear Thomas-Fermi equation, *Acta Univ. Sapientiae Math.*, **10** (2018), 134–151. https://doi.org/10.2478/ausm-2018-0012
16. S. V. Pikulin, Analytical-numerical method for calculating the Thomas-Fermi potential, *Russ. J. Math. Phys.*, **26** (2019), 544–552. https://doi.org/10.1134/S1061920819040113
17. L. Bougoffa, R. C. Rach, Approximate analytical solutions of the Thomas-Fermi equation by a direct method, *Rom. Journ. Phys.*, **60** (2015), 1032–1039.
18. H. Fatoorehchi, H. Abolghasemi, An explicit analytic solution to the Thomas-Fermi Equation by the improved differential transform method, *Acta Phys. Pol. A*, **125** (2014), 1083–1087. https://doi.org/10.12693/APHYSPOLA.125.1083
19. H. Fatoorehchi, M. Alidadi, The extended Laplace transform method for mathematical analysis of the Thomas-Fermi equation, *Chin. J. Phys.*, **55** (2017), 2548–2558. https://doi.org/10.1016/j.cjph.2017.10.001
20. S. J. Liao, An explicit analytic solution to the Thomas-Fermi equation, *Appl. Math. Comput.*, **144** (2003), 495–506. https://doi.org/10.1016/S0096-3003(02)00423-X
21. C. X. Liu, S. F. Zhu, Laguerre pseudospectral approximation to the Thomas-Fermi equation, *J. Comput. Appl. Math.*, **282** (2015), 251–261. https://doi.org/10.1016/j.cam.2015.01.004
22. S. F. Zhu, H. C. Zhu, Q. B. Wu, Y. Khan, An adaptive algorithm for the Thomas-Fermi equation, *Numer. Algorithms*, **59** (2012), 359-–372. https://doi.org/10.1007/s11075-011-9494-1
23. H. C. Rosu, S. C. Mancas, Generalized Thomas-Fermi equations as the Lampariello class of Emden-Fowler equations, *Phys. A*, **471** (2017), 212–218. https://doi.org/10.1016/j.physa.2016.12.007
24. G. Adomian, *Solving frontier problems of physics: the decomposition method*, Dordrecht: Springer, 1994. https://doi.org/10.1007/978-94-015-8289-6
25. R. Rach, G. Adomian, Multiple decompositions for computational convenience, *Appl. Math. Lett.*, **3** (1990), 97–99. https://doi.org/10.1016/0893-9659(90)90147-4
26. R. Rach, G. Adomian, R. E. Meyers, A modified decomposition, *Comput. Math. Appl.*, **23** (1992), 17–23. https://doi.org/10.1016/0898-1221(92)90076-T
27. G. Adomian, R. Rach, Transformations of series, *Appl. Math. Lett.*, **4** (1991), 69–71. https://doi.org/10.1016/0893-9659(91)90058-4
28. J. S. Duan, R. Rach, A. M. Wazwaz, A new modified Adomian decomposition method for higher-order nonlinear dynamical systems, *CMES*, **94** (2013), 77–118. https://doi.org/10.3970/cmes.2013.094.077
29. L. Bougoffa, J. S. Duan, R. Rach, Exact and approximate analytic solutions of the thin film flow of fourth-grade fluids by the modified Adomian decomposition method, *Int. J. Numer. Methods Heat Fluid Flow*, **26** (2016), 2432–2440. https://doi.org/10.1108/HFF-07-2015-0278
30. L. Bougoffa, S. Bougouffa, Adomian method for solving some coupled systems of two equations, *Appl. Math. Comput.*, **177** (2006), 553–560. https://doi.org/10.1016/j.amc.2005.07.070
31. L. Bougoffa, S. Bougouffa, Solutions of the two-wave interactions in quadratic nonlinear media, *Mathematics*, **8** (2020), 1–10. https://doi.org/10.3390/math8111867

32. L. Bougoffa, A. Mennouni, R. C. Rach, Solving Cauchy integral equations of the first kind by the Adomian decomposition method, *Appl. Math. Comput.*, **219** (2013), 4423–4433. https://doi.org/10.1016/j.amc.2012.10.046

33. A. M. Wazwaz, *Partial differential equations and solitary waves theory*, Berlin, Heidelberg: Springer, 2009. https://doi.org/10.1007/978-3-642-00251-9

34. M. van Hoeij, V. J. Kunwar, Classifying (almost)-Belyi maps with five exceptional points, *Indagat. Math.*, **30** (2019), 136–156. https://doi.org/10.1016/j.indag.2018.09.003

35. V. J. Kunwar, M. van Hoeij, Second order differential equations with hypergeometric solutions of degree three, In: *Proceedings of the 38th International Symposium on Symbolic and Algebraic Computation*, 2013, 235–242. https://doi.org/10.1145/2465506.2465953

36. E. Imamoglu, M. van Hoeij, Computing hypergeometric solutions of second order linear differential equations using quotients of formal solutions and integral bases, *J. Symb. Comput.*, **83** (2017), 254–271. https://doi.org/10.1016/j.jsc.2016.11.014

37. P. B. Bailey, L. F. Shampine, P. E. Waltman, *Nonlinear two point boundary value problems*, Academic Press, 1968.

38. W. M. Seiler, M. Seiss, On the numerical integration of singular initial and boundary value problems for generalized Lane-Emden and Thomas-Fermi equations, 2023, arXiv: 2301.01041v1.

39. C. Y. Chan, Y. C. Hon, Computational methods for generalized Thomas-Fermi models of neutral atoms, *Q. Appl. Math.*, **46** (1988), 711–726.

40. J. Shahni, R. Singh, A fast numerical algorithm based on Chebyshev-wavelet technique for solving Thomas-Fermi type equation, *Eng. Comput.*, **38** (2022), 3409–3422. https://doi.org/10.1007/s00366-021-01476-7

41. U. M. Ascher, R. M. M. Mattheij, R. D. Russell, *Numerical solution of boundary value problems for ordinary differential equations*, SIAM, 1995. https://doi.org/10.1137/1.9781611971231

42. U. M. Ascher, L. R. Petzold, *Computer methods for ordinary differential equations and differential-algebraic equations*, SIAM, 1998.