THE THOMAS-FERMI EQUATION:

COMPARISON OF SOLUTIONS BY VARIOUS METHODS

by

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Dedicated to my Parents
Siblings, Friends
and my Late
Grand Father.

Abstract

In this dissertation, several techniques have been used to determine solutions of the Thomas-Fermi equation. This is an important nonlinear ordinary differential equation which models the effective nuclear charge in heavy atoms. This model is also used to determine charge density, which is helpful to study the electrons in an atom. First Adomian Decomposition Method is used to find a series solution of the equation. Accuracy is enhanced when this solution is expressed in terms of Padé approximants. Secondly we find an analytical solution based on the Majorana transformation. Finally we solve the problem by using the Spectral Method. These solutions are compared with each other and also with Liao's solution found with the Homotopy Analysis Method.

Javeria Ayub.

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Those scientists who have deep knowledge fear Allah better, Verily; Allah is All-Mighty, Oft-Forgiving. (Quran 35:28)

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Contents

Chapter 1

Introduction

There are many problems in science and engineering associated with physical phenomena, which are modeled by researchers by differential equations with imposed initial or boundary conditions or both. Engineering, mechanics, economics, seismology and climate science are few examples which make use of mathematical models to solve important problems in their respective fields.

1.1 Thomas-Fermi Equation

The simplest atomic system is the hydrogen atom for which a complete solution exists. It is modeled as a two body problem, including one proton and one electron. Problems become complex when we deal with multi-electron atoms because electrons interact not only with the attractive central electrostatic field of the nucleus, but also undergo mutual repulsion whose strength depends on the mutual distance between the electrons. Various methods of approximation described to model this interaction are present in the literature [15]. Here we describe the theory developed independently by Thomas and Fermi suitable for heavy atoms containing many electrons [13].

The statistical model of an atom was first introduced by Thomas and Fermi in 1927 and was named after them. It was originally introduced to study a multi-electron atom. After that it has found major applications in molecular theory, solid state theory and also in defining the contribution from the electrons to the equation of state of matter at high pressures. The Thomas-Fermi Model is applied to determine the charge densities and potentials in an atom of numerous electrons with atomic number Z.

Now we derive the Thomas-Fermi equation. The electron density which is the number of electrons per unit volume $n(r)$ is defined below, where r is the distance from the nucleus

$$n(r) = \frac{1}{\pi^2 h^3} \int_0^{p_m} p^2 dp = \frac{p_m^3}{3\pi^2 h^3}, \tag{1.1}$$

where

$$\frac{p_m^2}{2m} = \mu - E(r). \tag{1.2}$$

Here m is the mass of an atom, h^3 is the volume, μ is the chemical potential, p is the electron momentum, p_m is the maximum electron momentum and $E(r)$ potential energy function. From Eq.(1.2) we write

$$p_m^3 = (2m[\mu - E(r)])^{3/2},$$

which leads to,

$$n(r) = \frac{(2m[\mu - E(r)])^{3/2}}{3\pi^2 h^3}. \tag{1.3}$$

The function $\psi(r)$ is the electrostatic potential, which is related to potential energy function through $E(r) = -e\psi(r)$, where e is the magnitude of the electronic charge. We can write an expression which shows the relation between the electron density and the electrostatic potential

$$n(r) = \frac{(2m[\mu + e\psi(r)])^{3/2}}{3\pi^2 h^3}. \tag{1.4}$$

Eq.(1.4) represents the Thomas-Fermi relation between $n(r)$ and $\psi(r)$. We can rewrite Eq.(1.4) as

$$n(r) = \frac{(2me[\psi - \psi_0])^{3/2}}{3\pi^2 h^3}, \tag{1.5}$$

where $\psi_0 = -\mu/e$. The Poisson equation relates the potential and the charge density through:

$$\nabla^2 \psi = 4\pi e n(r). \tag{1.6}$$

With substitution of $n(r)$ in Eq. (1.6) we get

$$\nabla^2(\psi - \psi_0) = \frac{4e}{3\pi h^3}(2me[\psi - \psi_0])^{3/2}. \tag{1.7}$$

Assuming nucleus at the origin of the coordinate system such that the potential is spherically symmetric. Therefore, we write the Laplacian for $(\psi - \psi_0)$ as:

$$\nabla^2(\psi - \psi_0) = \frac{1}{r}\frac{d}{dr}\big[r^2 \frac{d}{dr}(\psi - \psi_0)\big]. \tag{1.8}$$

When distance from the nucleus $r \to 0$ it means that it is approching to nucleus. We assume a dimensionless function $y(r)$:

$$(\psi - \psi_0) = \frac{Ze}{r} y(r). \tag{1.9}$$

When $r \to 0$, we have $(\psi - \psi_0) \to \frac{Ze}{r}$. From this we have a condition $y(0) = 1$. First compare Eq.(1.7) and Eq.(1.8) then put Eq.(1.9) in them and after doing some calculation we arrive at:

$$\frac{d^2 y}{dr^2} = \Big[\frac{4Z^{1/2}}{3\pi h^3}(2me^2)^{3/2}\Big]\frac{y^{3/2}}{r^{1/2}}. \tag{1.10}$$

We introduce here a dimensionless variable x, to make Eq.(1.10) take a simpler form:

$$r = \beta x. \tag{1.11}$$

Use Eq.(1.11) in Eq.(1.10). We can write it as

$$\frac{d^2y}{dx^2} = \beta^{3/2}\Big[\frac{4Z^{1/2}}{3\pi h^3}(2me^2)^{3/2}\Big]\frac{y^{3/2}}{x^{1/2}}. \tag{1.12}$$

Now we chose β such that the term in the bracket becomes unity

$$\beta = \frac{1}{2}\Big(\frac{3\pi}{4}\Big)^{3/2}\frac{h^3}{me^2}\frac{1}{Z^{1/3}} \approx \frac{0.88534b_0}{Z^{1/3}}, \tag{1.13}$$

where

$$b_0 = \frac{h^3}{me^2} \approx 0.529 \times 10^{-8}cm. \tag{1.14}$$

Thus b_0 represents the Bohr radius. Putting the value of β in Eq.(1.12), we obtain the dimensionless Thomas-Fermi differential equation which is valid for all Z

$$y'' = \frac{y^{\frac{3}{2}}}{x^{\frac{1}{2}}}, \tag{1.15}$$

$$y(0) = 1 \quad , \quad y(\infty) = 0. \tag{1.16}$$

By using an appropriate substitution, we can transform it into well-known differential equations. Let us assume $y = x^{-3}\psi(z)$ and $z = \ln x$, the Thomas-Fermi equation is transformed into the following:

$$\psi^{''} - 7\psi^{'} + 12\psi – \psi^{\frac{3}{2}} = 0, \tag{1.17}$$

where $\psi^{'}$ and $\psi^{''}$ are the first and second derivatives of ψ with respect to z. Also, using $y = x^{-3}z$ and $x = exp[\int dz\psi(z)]$, one can transform it into the Abel equation of the first type

$$\psi^{'} + 7\psi^2 + (z^{\frac{1}{2}} - 12)z\psi^3 = 0. \tag{1.18}$$

Here, we can find a way to predict the potential curve $y(x)$ as a function of the distance between the nuclei. We can easily find electron density $n(x)$.

$$n(x) = \frac{32}{9\pi^3}\frac{Z^2}{b_0^3}\left[\frac{y(x)}{x}\right]. \tag{1.19}$$

From this, we are able to know all the structural properties of the molecule. Molecular electrostatic potential also demonstrate facts about the charge distribution of a molecule. Electrostatic potential gives knowledge about the charge distribution of a molecule because of the properties of the nucleus and nature of electrostatic potential energy. Thus a high electrostatic potential displays the comparative absence of electrons and a low electrostatic potential indicates large number of electrons.

Liao [11] used Homotopy analysis method to determine an approximate solution and further used Padé approximate method for finding slope. Salvatore Esposito used old Majorana transformation to convert the Thmas-Fermi equation in a first order differential equation and found an analytical solution [10]. Both of them are vary accurate results. However the Thomas-Fermi equation has been applied as a testing ground for a broad assortment. For example Wazwaz [4] has used the Modified decomposition method, V. Rudrapatna [7] has used Analytical approximation method and Noor [8] has used Homotopy perturbation analysis. Further Padé approximants [4, 8, 11], Spectral Methods with different basis functions in [6, 9] and a technique from old notes of Ettore Majorana [10] have also been applied for this problem.

Reference	Methods
$RV.Ramnath$[7]	New analytical approximation
$A-M.Wazwaz$[4]	Modified decomposition method
$S.Esposito$[10]	Majorana transformation
$Liao$[11]	Homotopy analysis solution
$M.A.Noor$[8]	Homotopy Perturbation Method
$F.Bayatbabolghani, K.Parand$[6]	Use Hermite function to approximate solution
$R.Jovanovicetal.$[9]	Uses Exponential functions

Table 1.1: Thomas-Fermi bibliography

The problem consists of a nonlinear ordinary differential equation on a semi infinite interval. There are very few methods of solving nonlinear differential equations with exact results. When we cannot obtain the exact solution we use approximate methods. Some of the popular approximate methods are Spectral Methods, Adomian decomposition method, Homotopy methods, etc. Success of the method is measured by its accuracy, efficiency and by its convergence rate.

We use several techniques for solving the nonlinear ordinary differential equation i.e. the Thomas-Fermi equation. In Chapter 2, we have presented Wazwaz solution by the Adomian decomposition method [4]. In Chapter 3, we describe in detail, an analytical solution of the problem. This solution was found by Majorana but it remained unpublish and S. Esposito worked out the details and published it in 2002 [10]. In chapter 4, we solve the problem by Chebyshev Spectral method. These solutions are compared with each other in chapter 5.

Chapter 2

Adomian Decomposition Method

In this chapter, we have presented the solution of the problem by Wazwaz [4]. He used the Adomian decomposition method to solve the Thomas-Fermi problem. A slight change in Adomian decomposition method gives a solution in which an unknown coefficient appears. To estimate this unknown coefficient we further apply Padè approximants method.

2.1 Adomain Decomposition Method (ADM)

Adomain decomposition method is a simple process, it is easily utilized and is a convenient tool for the direct application to the problem. It was first presented by George Adomian [14] and was developed between 1970's to the 1990's. Adomain decomposition method is widely applicable to different types of problems in different fields and produces accurate results. It can be applied to all types of ordinary or partial differential equations whether these are linear or nonlinear.

We consider a general non-linear differential equation

$$Wy = w, \tag{2.1}$$

where W is the nonlinear operator, y and w are the functions of x. Now, we can spilt W into three parts like:

$$Xy + Yy + Zy = w. \tag{2.2}$$

Where Xy represents the linear portion and Yy represents the remainder of the linear portion of Wy in Eq.(2.1). Finally Zy represents the nonlinear portion of Wy. Now we apply the inverse operator of X on both sides of the Eq. (2.2):

$$\begin{aligned} X^{-1}Xy + X^{-1}Yy + X^{-1}Zy &= X^{-1}w, \\ X^{-1}Xy &= X^{-1}w - X^{-1}Yy - X^{-1}Zy, \\ y(x) &= g(x) - X^{-1}Yy - X^{-1}Zy. \end{aligned} \tag{2.3}$$

As X is a linear operator, so we have got an equation for $y(x)$. By taking integration of Eq.(2.2) and using initial condition, we got $X^{-1}w = g(x)$. Now we will take $y(x)$ as an approximate solution by taking the sum of infinite components and write as:

$$y(x) = \sum_{i=0}^{\infty} y_i(x). \tag{2.4}$$

To find the nonlinear term Zy, it can be approximated into infinite series of polynomial

$$Zy = \sum_{i=0}^{\infty} A_i. \tag{2.5}$$

In the above equation A_i represents the Adomain polynomials which has its general form

$$A_i = \frac{1}{i!}\Big[\frac{d^i}{d\lambda^i}Zy(\lambda)\Big]_{\lambda=0}. \tag{2.6}$$

By putting $Eq.(2.4),(2.5)$ into $Eq.(2.2)$ we get

$$\sum_{i=0}^{\infty} y_i = y_0 - X^{-1}\sum_{i=0}^{\infty} Yy_i - X^{-1}\sum_{i=0}^{\infty} A_i, \tag{2.7}$$

If we take

$$\begin{aligned} y_0 &= g(x),\\ &\vdots\\ y_{i+1} &= X^{-1}Yy_i + X^{-1}A_i. \end{aligned}$$

From the above relation, we can find $y_1, y_2, \cdots$ in a recursive manner. The sum of $y_{i's}$ give us the approximate solution $y(x)$. Now many researchers use Modified decomposition method by doing some slight change in the ADM according to their problem. This change in ADM improves the accuracy level.

2.1.1 Example

Consider a first order nonlinear ordinary differential equation with the initial value problem

$$\frac{dy}{dx} = y^2, \tag{2.8}$$

$$y(0) = 1. \tag{2.9}$$

Its exact solution is $y(x) = \frac{1}{1-x}$. Let X be a linear operator, say

$$X = \frac{d}{dx}, \tag{2.10}$$

and inverse operator is given as

$$X^{-1} = \int_0^x ()dx. \tag{2.11}$$

Let M be a nonlinear operator, then Eq.(2.8) becomes

$$Xy = My, \tag{2.12}$$

$$My = y^2. \tag{2.13}$$

Apply X^{-1} on the above equation we have

$$X^{-1}Xy = y(x) - y(0). \tag{2.14}$$

By using initial condition we have

$$X^{-1}Xy = y(x) - 1. \tag{2.15}$$

By putting Eq.(2.15) in Eq.(2.12), we have

$$y(x) = 1 + X^{-1}My. \tag{2.16}$$

By Adomian Decomposition Method we can take the infinite series $y(x) = \sum_{i=0}^{\infty} y_n(x)$. And nonlinear term My as the infinite series of Adomian polynomials $My = \sum_{i=0}^{\infty} A_i$. The above equation becomes

$$\sum_{i=0}^{\infty} y_i(t) = 1 + X^{-1} \sum_{i=0}^{\infty} A_i. \tag{2.17}$$

By definition Adomian polynomials are

$$A_i = \frac{1}{i!} \frac{d^i}{d\lambda^i} \big(My(\lambda) \big) \mid_{\lambda=0}, \tag{2.18}$$

$$y(\lambda) = \sum_{i=0}^{\infty} \lambda_i y_i, \tag{2.19}$$

where λ_i are scalars. Adomian polynomials found for this example are given below.

$$A_0 = y_0^2,$$
$$A_1 = 2y_0y_1,$$
$$A_2 = 2y_0y_2 + y_1^2,$$
$$A_3 = 2y_0y_3 + 2y_1y_2,$$
$$\vdots$$

By Adomian Decomposition Method we can write Eq.(2.17) as

$$y_0 = 1, \tag{2.20}$$
$$y_{i+1} = X^{-1}A_i. \tag{2.21}$$

We get from above

$$y_0 = 1,$$
$$y_1 = x,$$
$$y_2 = x^2,$$
$$y_3 = x^3,$$
$$\vdots$$

These series solution is formed from $\sum_{i=0}^{\infty} x^i$ so

$$y(x) = \sum_{i=0}^{\infty} x^i. \tag{2.22}$$

It is recognized as the Taylor series of $\frac{1}{1-x}$,

$$y(x) = \frac{1}{1-x}. \tag{2.23}$$

2.2 Modified Decomposition Method

For a slight change or modification in Eq.(2.5), here we split $g(x)$ into two components as given below:

$$g(x) = g_0(x) + g_1(x), \tag{2.24}$$

The next step is to take y_0 equal to the first component g_0.The second component g_1 is added to the rest of the series of y_i. The rest of the term remains the same for $y_{i's}$ with $i \geq 2$. The new recursive relationship is written below.

$$\begin{aligned} y_0 &= g_0, \\ y_1 &= g_1 - X^{-1}Yy_0 - X^{-1}A_0, \\ &\vdots \\ y_{i+2} &= -X^{-1}Yy_{i+1} - X^{-1}A_{i+1}, i \geq 0. \end{aligned}$$

Making some small changes in the ADM, first it increases the convergence of the solution and second it reduces the calculation. By properly choosing g_0 and g_1, the exact solution $y(x)$ can be found by using very few components and sometimes by only two components. The level of success in modification depends on the best choice of g_0 and g_1. If $g(x)$ has only one component, then the standard Adomian decomposition method is applied in this situation.

2.3 Application

The Thomas-Fermi Equation is a nonlinear ordinary differential equation with $[0, \infty)$. It is used to find potentials and charge densities of multi electron atoms. It also determines the effective nuclear charge in heavy atoms.

$$\frac{d^2y}{dx^2} = \frac{y^{\frac{3}{2}}}{x^{\frac{1}{2}}},$$
$$y(0) = 1 \quad , \quad y(\infty) = 0. \tag{2.25}$$

We apply Modified decomposition method (MDM) on equation (2.25). First step is to write above problem in operator form.

$$Xy = \frac{y^{\frac{3}{2}}}{x^{\frac{1}{2}}}. \tag{2.26}$$

Here X is the second order linear differential operator. Apply X^{-1} on both sides of (2.26) to find the solution $y(x)$

$$X^{-1}Xy = X^{-1}\big(y^{\frac{3}{2}}x^{\frac{-1}{2}}\big) + Dx + E \quad , \quad y(0) = 1,$$
$$y(x) = 1 + Dx + X^{-1}\big(y^{\frac{3}{2}}x^{\frac{-1}{2}}\big). \tag{2.27}$$

Take derivative of (2.27) with respect to x then we have $y'(0) = D$. According to Modified decomposition method we can write approximate solution of problem (2.25) as given below.

$$y(x) = \sum_{i=0}^{\infty} y_i(x). \tag{2.28}$$

Here the nonlinear term $y^{\frac{3}{2}}$ can be written as approximated infinite series of polynomial by ADM,

$$y^{\frac{3}{2}}(x) = \sum_{i=0}^{\infty} A_i(x). \tag{2.29}$$

where A_i are the Adomain polynomials. By substituting Eq.(2.28) and (2.29) in Eq.(2.27)

$$\sum_{i=0}^{\infty} y_i(x) = 1 + Dx + X^{-1}\Big(x^{\frac{-1}{2}} \sum_{i=0}^{\infty} A_i(x)\Big). \tag{2.30}$$

It is easy to recognize the first component y_0, zeroth component is given below:

$$y_0(x) = 1 + Dx = g(x), \tag{2.31}$$

$$y_{i+1}(x) = X^{-1}\Big(x^{\frac{-1}{2}} A_i(x)\Big), \quad i{\geq}0. \tag{2.32}$$

Here we apply Modified decomposition method so that we can split $g(x)$ into two components g_0 and g_1.

$$g_0(x) = 1, \qquad g_1(x) = Dx. \tag{2.33}$$

Here we have

$$y_0 = g_0 = 1, \tag{2.34}$$

$$y_1 = g_1 + X^{-1}\Big(x^{\frac{-1}{2}} A_0(x)\Big) = Dx + X^{-1}\Big(x^{\frac{-1}{2}} A_0(x)\Big), \tag{2.35}$$

$$\vdots$$

$$y_{i+2} = X^{-1}\Big(x^{\frac{-1}{2}} A_{i+1}(x)\Big) \quad , \quad i{\geq}0. \tag{2.36}$$

Taking $y_0 = 1$, instead of $y_0 = 1 + Dx$, it leads to more simplification in calculation. By using this modification we make a remarkable improvement in the state of convergence of the series solution. Here is the list of Adomain polynomials A_i.

$$\begin{aligned}
A_0 &= 1,\\
A_1 &= \frac{3}{2}y_1,\\
A_2 &= \frac{3}{8}y_1^2 + \frac{3}{2}y_2,\\
A_3 &= \frac{-1}{16}y_1^3 + \frac{3}{4}y_1y_2 + \frac{3}{2}y_3,\\
A_4 &= \frac{3}{128}y_1^4 - \frac{3}{16}y_1^2y_2 + \frac{3}{8}(y_2^2 + 2y_1y_3) + \frac{3}{2}y_4,
\end{aligned}$$

$$A_5 = \frac{3}{32}y_1^3y_2 + \frac{1}{16}(- 3y_1y_2^2 - 3y_1^2y_3) + \frac{3}{8}(2y_2y_3 + 2y_1y_4) + \frac{3}{2}y_5 + \frac{-3}{256}y_1^5,$$

$$A_6 = \frac{7}{1024}y_1^6 - \frac{15}{256}y_1^4y_2 + \frac{3}{8}(y_3^2 + 2y_2y_4 + 2y_1y_5) + \frac{1}{16}(- y_2^3 - 6y_1y_2y_3 - 3y_1^2y_4) + \frac{3}{128}(6y_1^2y_2^2 + 4y_1^3y_3) + \frac{3}{2}y_6,$$

$$A_7 = \frac{-9}{2048}y_1^7 + \frac{21}{512}y_1^5y_2 - \frac{3}{256}(10y_1^3y_2^2 + 5y_1^4y_3) + \frac{3}{128}(4y_1y_2^3 + 12y_1^2y_2y_3 + 4y_1^3y_4) + \frac{1}{16}(- 3y_2^2y_3 - 3y_1y_3^2 - 6y_1y_2y_4 - 3y_1^2y_5) + \frac{3}{8}(2y_3y_4 + 2y_2y_5 + 2y_1y_6) + \frac{3}{2}y_7,$$

$$A_8 = \frac{99}{32768}y_1^8 - \frac{63}{2048}y_1^6y_2 + \frac{7}{1024}(15y_1^4y_2^2 + 6y_1^5y_3) - \frac{3}{256}(10y_1^2y_2^3 + 20y_1^3y_2y_3 + 5y_1^4y_4) + \frac{3}{128}(y_2^4 + 12y_1y_2^2y_3 + 6y_1^2y_3^2 + 12y_1^2y_2y_4 + 4y_1^3y_5) + \frac{1}{16}(- 3y_2y_3^2 - 3(y_2^2 + 2y_1y_3)y_4 - 6y_1y_2y_5 - 3y_1^2y_6) + \frac{3}{8}(y_4^2 + 2y_3y_5 + 2y_2y_6 + 2y_1y_7) + \frac{3}{2}y_8,$$

$$\begin{aligned}
A_9 = &\frac{-143}{65536}y_1^9 + \frac{99}{4096}y_1^7 y_2 - \frac{9}{2048}(21y_1^5 y_2^2 \\
&+ 7y_1^6 y_3) + \frac{7}{1024}(20y_1^3 y_2^3 + 30y_1^4 y_2 y_3 \\
&+ 6y_1^5 y_4) - \frac{3}{256}(5y_1 y_2^4 + 30y_1^2 y_2^2 y_3 \\
&+ 10y_1^3 y_3^2 + 20y_1^3 y_2 y_4 + 5y_1^4 y_5) \\
&+ \frac{3}{128}(4y_2^3 y_3 + 12y_1 y_2 y_3^2 + 4(3y_1 y_2^2 \\
&+ 3y_1^2 y_3)y_4 + 12y_1^2 y_2 y_5 + 4y_1^3 y_6) \\
&+ \frac{1}{16}(- y_3^3 - 6y_2 y_3 y_4 - 3y_1 y_4^2 \\
&- 3(y_2^2 + 2y_1 y_3)y_5 - 6y_1 y_2 y_6 - 3y_1^2 y_7) \\
&+ \frac{3}{8}(2y_4 y_5 + 2y_3 y_6 + 2y_2 y_7 + 2y_1 y_8) + \frac{3}{2}y_9,
\end{aligned}$$

By using $y_0 = 1$ from Eq.(2.34) , the remaining components can be found.

$$\begin{aligned}
y_0 &= 1, \\
y_1 &= Dx + \frac{4x^{\frac{3}{2}}}{3}, \\
y_2 &= \frac{2}{5}Dx^{\frac{5}{2}} + \frac{x^3}{3}, \\
y_3 &= \frac{3}{70}D^2 x^{\frac{7}{2}} + \frac{2Dx^4}{15} + \frac{2x^{\frac{9}{2}}}{27}, \\
y_4 &= \frac{-1}{252}D^3 x^{\frac{9}{2}} + \frac{D^2 x^5}{175} + \frac{31Dx^{\frac{11}{2}}}{1485} + \frac{4x^6}{405}, \\
y_5 &= \frac{x^{\frac{11}{2}}61425D^4 + 164736D^3 x^{\frac{1}{2}} + 360936D^2 x + 374400Dx^{\frac{3}{2}} + 124432x^2}{64864800}, \\
y_6 &= \frac{-3D^5 x^{\frac{13}{2}}}{9152} - \frac{29D^4 x^7}{24255} - \frac{623D^3 x^{\frac{15}{2}}}{351000} - \frac{46D^2 x^8}{45045} - \frac{113Dx^{\frac{17}{2}}}{1178100} + \frac{23x^9}{473850},
\end{aligned}$$

$$y_7 = \frac{7D^6x^{\frac{15}{2}}}{49920} + \frac{68D^5x^8}{105105} + \frac{153173D^4x^{\frac{17}{2}}}{116424000} + \frac{1046D^3x^9}{675675} + \frac{799399D^2x^{\frac{19}{2}}}{698377680} + \frac{51356Dx^{10}}{103378275} + \frac{35953x^{\frac{21}{2}}}{378132300},$$

$$y_8 = \frac{-x^{\frac{17}{2}}}{8905153473216000}\Big(613866278025D^7 + 3426706483200D^6x^{\frac{1}{2}} + 8590664370420D^5x + 12533963464704D^4x^{\frac{3}{2}} + 11434694685040D^3x^2 + 6492922168320D^2x^{\frac{5}{2}} + 2132373014464Dx^3 + 317159180800x^{\frac{7}{2}}\Big),$$

$$y_9 = \frac{99D^8x^{\frac{19}{2}}}{2646016} + \frac{256D^7x^{10}}{1044225} + \frac{705965027D^6x^{\frac{21}{2}}}{966226060800} + \frac{43468D^5x^{11}}{33622875} + \frac{1861464749D^4x^{\frac{23}{2}}}{1253187936000} + \frac{27134428D^3x^{12}}{23880381525} + \frac{17319117797D^2x^{\frac{25}{2}}}{30580884180000} + \frac{494880923Dx^{13}}{2936459901375} + \frac{172159489x^{\frac{27}{2}}}{7487019540000},$$

and so on. By taking $t = x^{\frac{1}{2}}$, the approximation $y(t)$ becomes

$$\begin{aligned} y(t) = {} & 1 + Dt^2 + \frac{4}{3}t^3 + \frac{2}{5}Dt^5 + \frac{1}{3}t^6 + \frac{3}{70}D^2t^7 + \frac{2}{15}Dt^8 + \Big(\frac{2}{27} - \frac{1}{252}D^3\Big)t^9 \\ & + \frac{1}{175}D^2t^{10} + \Big(\frac{31}{1485}D + \frac{61425}{64864800}D^4\Big)t^{11} + \Big(\frac{164736}{64864800}D^3 + \frac{4}{405}\Big)t^{12} \\ & - \Big(\frac{3}{9152}D^5 + \frac{360936}{64864800}D^2\Big)t^{13} + \Big(\frac{374400}{64864800}D - \frac{29}{24255}D^4\Big)t^{14} \\ & - \Big(\frac{623}{351000}D^3 + \frac{124432}{64864800} + \frac{7}{49920}D^6\Big)t^{15} - \Big(\frac{46}{45045}D^2 + \frac{68}{105105}D^5\Big)t^{16} \\ & + \Big(\frac{153173}{116424000}D^4 - \frac{613866278025}{8905153473216000}D^7 - \frac{113}{1178100}D\Big)t^{17} \\ & + \Big(\frac{23}{473850} + \frac{1046}{675675}D^3 - \frac{3426706483200}{8905153473216000}D^6\Big)t^{18} \\ & + \Big(\frac{799399}{698377680}D^2 + \frac{99}{2646016}D^8 - \frac{8590664370420}{8905153473216000}D^5\Big)t^{19} \\ & + \Big(\frac{51356}{103378275}D - \frac{12533963464704}{8905153473216000}D^4 + \frac{256}{1044225}D^7\Big)t^{20} \\ & + O(t^{21}). \end{aligned}$$

2.4 Padé Approximants

Padé approximants converge on the whole real axis for any function $y(x)$ if it has no singularity on the real axis. The advantage of Padé approximants is to get more information of the function $y(x)$ by converting polynomial approximation into a rational function. For function $y(x)$ and two integers $m \geq 0$ and $n \geq 1$, the Padé approximant of order $[m/n]$ is the rational function.

$$R(x) = \frac{\sum_{j=0}^{m} a_j x^j}{1 + \sum_{k=1}^{n} b_k x^k}. \tag{2.37}$$

Above rational functions satisfy following property

$$\begin{aligned}
y(0) &= R(0), \\
y'(0) &= R'(0), \\
y''(0) &= R''(0), \\
&\vdots \\
y^{m+n}(0) &= R^{m+n}(0).
\end{aligned}$$

The Padé approximant is unique for every m and n and all the coefficients can easily be found. Here we use Padé approximant to estimate the value of $y'(0) = D$. In the Thomas-Fermi Equation we use the diagonal approximant $[m/m]$ only, because they are efficient and stable. All the diagonal approximants $[m/m]$ will vanish by using the boundary condition $y(\infty) = 0$. To satisfy the condition, take the coefficient of the highest power of t in the numerator equal to zero and calculate the roots of polynomials of D through Mathematica or Maple. An important fact that the Thomas-Fermi equation has a solution which is decreasing so $y'(0) < 0$. Using this fact, complex roots and positive roots can be ignored automatically. We used Kobayashi [2] and Anderson [3] results as a reference. Kobayashi found a highly accurate numerical solution of the Thomas-Fermi equation, and a slope $y'(0) = -1.588071$. Anderson calculated the upper and lower bound of $y'(0)$ by using principles of complementary variation method $-1.589 < y'(0) < -1.563$.

Padé approximation	Initial slope $y'(0)$	Comparison with [2]
[2/2]	-1.21413729	23.71
[4/4]	-1.550525919	2.36
[7/7]	-1.586021037	12.9×10^{-2}
[8/8]	-1.588076820	3.66×10^{-4}

Table 2.1: Padé approximation and initial slopes $y'(0)$

In above Table 2.1 diagonal approximants [2/2] and [4/4] initial slope $y'(0)$ does not lie between the limits of Anderson. By increasing the degree of the Padé approximants the initial slope $y'(0)$ improves rapidly. The initial slope for [7/7] and [8/8] lies between the limit of Anderson and also approaches the initial slope of Kobayashi.

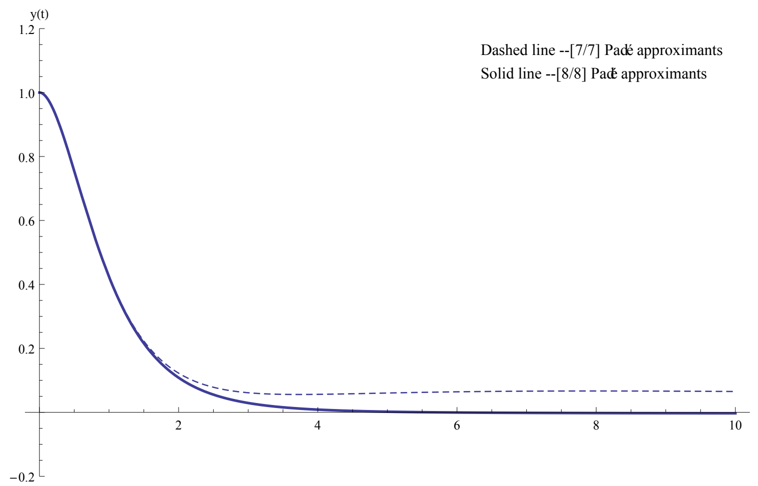


Figure 2.1: Padé approximants [7/7] and [8/8] of the approximations of the potential $y(t)$.

From figure 2.1, we can see that both the approximants have fast convergence initially but comparatively [7/7] Pade approximant is a better option. It slowly converges to zero but it has a dip near $t = 4$. On the other hand [8/8] is efficient but becomes negative after $t = 5.75$. Both these features are bad marks as far as the accuracy is concerned. More precise view of [7/7] and [8/8] Padé approximant is following:

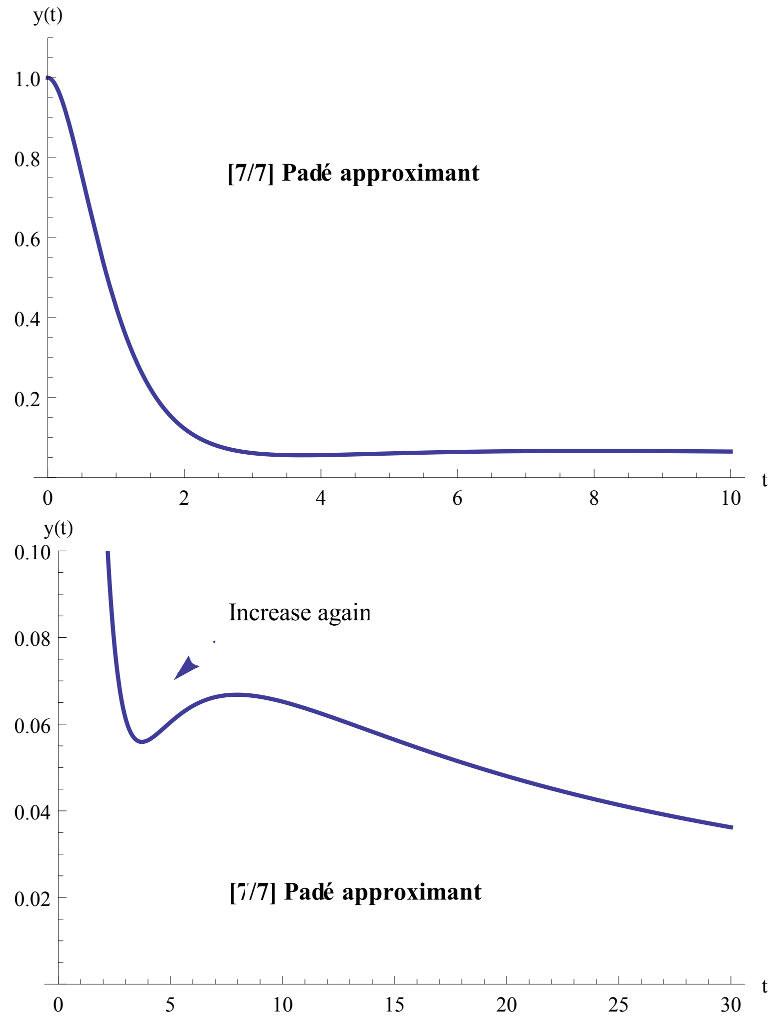


Figure 2.2: More precise view of Padé approximant [7/7].

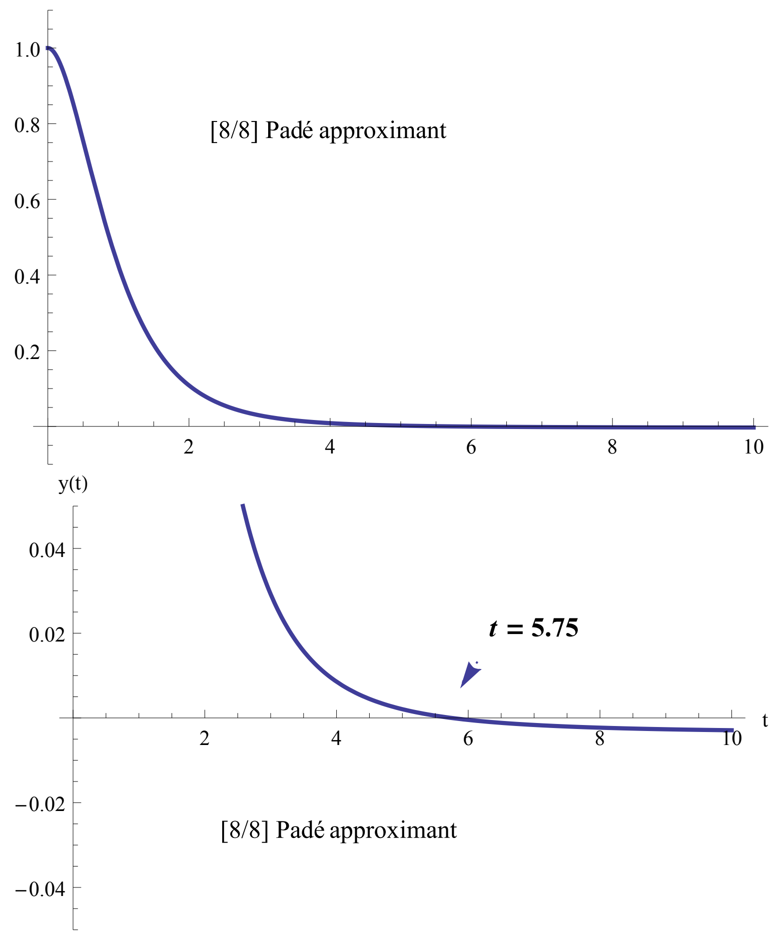


Figure 2.3: More precise view of Padé approximant [8/8].

From figure 2.2 and 2.3 we can well differentiate between Padé approximants [7/7] and [8/8]. Numerical values of Padé approximants [7/7] and [8/8] are given in the table below:

t	[7/7] Padé approximants	[8/8] Padé approximants
00.50	0.7557383	0.7552
01.00	0.426623	0.424
01.50	0.222946	0.215866
02.00	0.12256	0.108321
02.50	0.0784775	0.0554392
03.00	0.0613384	0.0292216
04.00	0.0563062	0.0085627
05.00	0.0604499	0.00205949
05.50	0.0625399	0.000535552
05.75	0.0634375	-0.0000160073
06.00	0.0642223	-0.000469363
10.00	0.0652132	-0.00290523
20.00	0.0480175	-0.00296214
30.00	0.036208	-0.00244271

Table 2.2: Comparrison between Padé approximants.

These Padé approximants give us good initial slope $y'(0)$ but the assuracy deteriorate for values of t near 5. The [8/8] approximant becomes negative beyond 5.75 which is, of course, absurd. Also the [7/7] approximant appears to slowly converge to zero but it has a dip in value near $t = 4$.

Chapter 3

Majorana Solution of the Thomas-Fermi Equation

In this chapter, we use Majorana method to obtain the solution of the Thomas-Fermi equation. We use Majorana transformations to convert the Thomas-Fermi equation in a first order differential equation and solve it to get a series solution. It is an analytical method of finding solution of the Thomas-Fermi equation. It was discovered by Majorana but remained unpublish until S. Esposito improved it and published it in 2002 [10].

3.1 Majorana Transformation

The Thomas-Fermi Model is applied to estimate the electron density and this electron density is used to compute the electrostatic potential due to the nucleus and the cloud of electrons.

$$y'' = \frac{y^{\frac{3}{2}}}{x^{\frac{1}{2}}}, \tag{3.1}$$

$$y(0) = 1, \tag{3.2a}$$

$$y(\infty) = 0. \tag{3.2b}$$

Eq.(3.1) is the Thomas-Fermi equation with boundary conditions (3.2a) and (3.2b). Unfortunately, there exists no sufficiently good approximate analtical solution which satisfies the boundary condition (3.2a) and (3.2b) of Eq (3.1). Sommerfeld [12] discovered an exact particular solution of the Thomas-Fermi equation which satisfy condition (3.2b) but his solution had a divergent first derivative at $x = 0$ (doesnot satisfy condition (3.2a)),

$$y = \frac{144}{x^3}. \tag{3.3}$$

In 1928 Majorana discovered a semi-analytical series solution of the Thomas-Fermi equation with appropriate boundary conditions but unfortunately it remained unpublished. The Majorana solution can be viewed as a modification of (3.3).

Let us take a parameter t:

$$x = x(t), \tag{3.4a}$$

$$y = y(t). \tag{3.4b}$$

These equations are called a parametric representation of the solution of the Thomas-Fermi equation. Here is a scheme adopted by Majorana i.e to use double change of variables. If $x \to t$ then $y(x) \to z(t)$. Now the new unknown function is $z(t)$. This relation is taken as invertible and connecting the two sets of variables which has differential nature.

$$t = t(x, y), \tag{3.5a}$$

$$z = z(y, y'). \tag{3.5b}$$

The above equations are in their general form. By using these we can transform second-order differential equation (3.1) for y into a first-order differential equation in z. In addition, these equations are also implicit equations for t and z, because x and y depend on them. For the Thomas-Fermi equation, Majorana presented the following transformation shift:

$$t = 144^{-\frac{1}{6}} x^{\frac{1}{2}} y^{\frac{1}{6}}, \tag{3.6}$$

$$z = -\left(\frac{16}{3}\right)^{\frac{1}{3}} y^{-\frac{4}{3}} y'. \tag{3.7}$$

We can see that (3.6) is similar to the Sommerfeld solution (3.3), because it can be written to the given pattern:

$$y = \frac{144}{x^3} t^6. \tag{3.8}$$

For determining the differential equation for $z(t)$, we take derivative of (3.7) with respect to t and obtain the following:

$$\frac{dz}{dt} = -\left(\frac{16}{3}\right)^{\frac{1}{3}} \dot{x} y^{-\frac{4}{3}} \left[-\frac{4}{3}\frac{y'^2}{y} + y'' \right], \tag{3.9}$$

by inserting (3.1) in above equation we have:

$$\frac{dz}{dt} = -\left(\frac{16}{3}\right)^{\frac{1}{3}} \dot{x} y^{-\frac{4}{3}} \left[-\frac{4}{3}\frac{y'^2}{y} + \frac{y^{\frac{3}{2}}}{x^{\frac{1}{2}}} \right]. \tag{3.10}$$

By using (3.6) and (3.7) to eliminate $x^{1/2}$ and y'^2 respectively, we have:

$$\frac{dz}{dt} = \left(\frac{16}{3}\right)^{\frac{1}{3}} \left(\frac{4}{3}\right) \dot{x} y^{-7/3} \left[\left(\frac{3}{16}\right)^{\frac{2}{3}} y^{8/3} z^2 \right] - \left(\frac{16}{3}\right)^{\frac{1}{3}} \frac{\dot{x} y^{1/6}}{[t y^{-1/6} 144^{1/6}]},$$

$$\frac{dz}{dt} = \left(\frac{2}{3}\right)^{\frac{2}{3}} \dot{x}y^{1/3}z^2 - \left(\frac{2}{3}\right)^{\frac{2}{3}} \frac{\dot{x}y^{1/3}}{t},$$

by substitution the values of $x^{1/2}$ and y'^2 we have:

$$\frac{dz}{dt} = \left(\frac{4}{9}\right)^{\frac{1}{3}} \left[\frac{tz^2 - 1}{t}\right] \dot{x}y^{1/3}. \tag{3.11}$$

In the above equation, we have only $\dot{x}y^{1/3}$ to express into a function of z and t. We use here (3.6):

$$x = 144^{1/3}t^2y^{-1/3}. \tag{3.12}$$

Differentiate with respect to t both sides of (3.12) explicitly, we have,

$$\dot{x} = 144^{1/3}\Big[2ty^{-1/3} + t^2\dot{x}(-\frac{1}{3}y^{-4/3}y')\Big], \tag{3.13}$$

$$\dot{x}y^{1/3} + \frac{144^{1/3}}{3}t^2y^{-4/3}y'\dot{x}y^{1/3} = 144^{1/3}2t,$$

$$\dot{x}y^{1/3} = 144^{1/3}\frac{2t}{1 + \frac{144^{1/3}}{3}t^2y^{-4/3}y'},$$

and after calculation we reach to the following results

$$\dot{x}y^{1/3} = 144^{1/3}\frac{2t}{1 - zt^2}. \tag{3.14}$$

Put (3.14) in (3.11), we finally obtain the differential equation for $z(t)$

$$\frac{dz}{dt} = 8\frac{tz^2 - 1}{1 - t^2z}. \tag{3.15}$$

In Eq.(3.6) for condition (3.2a), we have $t = 0$ for $x = 0$. And also from (3.7) we have:

$$z(0) = \left(\frac{16}{3}\right)^{\frac{1}{3}} y'_0. \tag{3.16}$$

Where $y'_0 = y'(x = 0)$. The unique solution $z(t)$ of (3.15) obtained with boundary condition(3.2b) must satisfy the initial condition of (3.16). By using Sommerfeld expression (3.3) in (3.6) and (3.7). This means that at $x \to \infty$, we have $t = 1$, and

$$z(1) = 1. \tag{3.17}$$

Thus we find t varies between $t = 0$ and $t = 1$. In this interval we look for the solution of (3.15) by using a series of expansion in powers of the variable $\nu = 1 - t$:

$$z = a_0 + a_1\nu + a_2\nu^2 + a_3\nu^3 + \cdots \tag{3.18}$$

From (3.17) we have:

$$a_0 = 1. \tag{3.19}$$

Using $\nu = 1 - t$, we convert (3.15) into following:

$$\frac{dz}{d\nu} = -8\frac{(1-\nu)z^2 - 1}{1 - (1-\nu)^2 z}. \tag{3.20}$$

$$\frac{1}{8}[(1-\nu)^2 z - 1]\frac{dz}{d\nu} = 8[(1-\nu)z^2 - 1],$$

We use (3.18) series of expansion in above, then we compare the coefficients of ν^i. For ν^0, we have

$$\frac{1}{8}[a_0 - 1] = [a_0^2 - 1]. \tag{3.21}$$

Eq. (3.21) is satisfied for $a_0 = 1$, and for ν^1, we have

$$\frac{1}{8}[a_1^2 - 2a_0a_1 - 2a_2 + 2a_2a_0] = [-a_0^2 + 2a_0a_1], \tag{3.22}$$

$$\frac{1}{8}[a_1^2 - 2a_1 - 2a_2 + 2a_2] = [2a_1 - 1], \quad \text{with} \quad a_0 = 1,$$

we solve (3.22) for a_1 and get

$$a_1 = 0.455996. \tag{3.23}$$

Let $z = \sum_{p=0}^{\infty} a_p \nu^p$ in (3.20), we have:

$$\frac{1}{8}\Big[\sum_{k=0}^{n-1}\sum_{n=1}^{\infty}(k+1)a_{n-k}a_{k+1}\nu^n - 2\sum_{k=0}^{n-1}\sum_{n=1}^{\infty}(k+1)a_{n-k-1}a_{k+1}\nu^n + \sum_{k=0}^{n-2}\sum_{n=2}^{\infty}(k+1)a_{n-k-2}a_{k+1}\nu^n\Big] - \sum_{k=0}^{n}\sum_{n=0}^{\infty}a_{n-k}a_k\nu^n + \sum_{k=0}^{n-1}\sum_{n=1}^{\infty}a_{n-k-1}a_k\nu^n = 0. \tag{3.24}$$

For $n = 2$ we can obtain an equation for a_2, which is

$$\frac{1}{8}[a_1a_2 + 2a_2a_1 - 2a_1^2 - 4a_2 + a_0a_1] = [a_0a_2 + a_1^2 + a_0a_2 - a_0a_1 - a_0a_1], \tag{3.25}$$

$[3a_1a_2 - 2a_1^2 - 4a_2 + a_1] = 8[a_1^2 + 2a_2 - 2a_1]$, with $a_0 = 1$, $a_1 = 0.455996$,

put value of a_1 from (3.23) in above then we have

$$a_2 = 0.304455. \tag{3.26}$$

Rewriting (3.24), we obtain the following recurrence relation by setting coefficients of ν^n in (3.24) to zero:

$$\sum_{k=0}^{n-1}\sum_{n=1}^{\infty}(k+1)a_{n-k}a_{k+1} - 2\sum_{k=0}^{n-1}\sum_{n=1}^{\infty}(k+1)a_{n-k-1}a_{k+1} + \sum_{k=0}^{n-2}\sum_{n=2}^{\infty}(k+1)a_{n-k-2}a_{k+1} - 8\sum_{k=0}^{n}\sum_{n=0}^{\infty}a_{n-k}a_k + 8\sum_{k=0}^{n-1}\sum_{n=1}^{\infty}a_{n-k-1}a_k = 0, \tag{3.27}$$

$$
\begin{aligned}
a_n[a_1 + na_1 - 2n - 2] = 2\sum_{k=0}^{n-2}(k+1)a_{n-k-1}a_{k+1} - \sum_{k=1}^{n-2}(k+1)a_{n-k}a_{k+1} \\
- \sum_{k=0}^{n-2}(k+1)a_{n-k-2}a_{k+1} + 8\sum_{k=1}^{n-1} a_k a_{n-k} \\
- 8\sum_{k=0}^{n-1} a_k a_{n-k-1},
\end{aligned}
$$

from above steps we can easily get an expression for a_n where $n \geq 3$,

$$
a_n = \frac{A(n)}{2 - \frac{1}{8}[(n+1)a_1 - 2n]}, \tag{3.28}
$$

where

$$
\begin{aligned}
A(n) = \sum_{k=1}^{n-2}(k+1)a_{n-k}a_{k+1} - 2\sum_{k=0}^{n-2}(k+1)a_{n-k-1}a_{k+1} \\
+ \sum_{k=0}^{n-2}(k+1)a_{n-k-2}a_{k+1} - 8\sum_{k=1}^{n-1} a_k a_{n-k} \\
+ 8\sum_{k=0}^{n-1} a_k a_{n-k-1}.
\end{aligned}
$$

We can figure out that the sum on the right-hand side involves coefficient a_j with $j \leq n-1$. In order to have the relation in which (3.28) gives explicitly the value of a_n where all the previous ones $n-1$ coefficients are known. By letting $\nu = 1$, we have $t = 0$, when we place it in (3.18), certainly we have $z(0) = \sum_{n=0}^{\infty} a_n$. Assign this value of z at $t = 0$ in (3.16), here we get the value of initial slope.

$$
-y_0' = (\frac{3}{16})^{1/3} \sum_{n=0}^{\infty} a_n. \tag{3.29}
$$

The above equation shows that for the finite sum of series in (3.16) we also have finite value of y_0'. As the slope at initial point y_0' of the Thomas-Fermi equation is approximately $y_0' \simeq -1.588071$. For some fixed value of n we can easily approach this value. Notice that the $a_{i'}s$ are positive definite and that the series in (3.29) shows geometric convergence with $a_n/a_{n-1} \sim 4/5$ for $n \to \infty$.

n	$\sum_{n=0}^{\infty} a_n$	a_n/a_{n-1}	y_0'
20	2.75597	0.806429	-1.5774
40	2.77432	0.814719	-1.5879
60	2.77458	0.818761	-1.58807

Table 3.1: Initial slope for various values of n.

By using the above expression for a_n, we can find $z(t)$ for different n.

Here we take $n = 60$:

$$\begin{aligned} z(t) \; = \; & 2.77461 - 7.99965t + 30.7825t^2 - 125.537t^3 + 524.566t^4 - 2212.5t^5 + 9296.78t^6 \\ & -38389.8t^7 + 153707.t^8 - 589657.t^9 + 2.14688 \times 10^6 t^{10} - 7.36728 \times 10^6 t^{11} \\ & +2.37173 \times 10^7 t^{12} - 7.14212 \times 10^7 t^{13} + 2.00866 \times 10^8 t^{14} - 5.27245 \times 10^8 t^{15} \\ & +1.29155 \times 10^9 t^{16} - 2.9535 \times 10^9 t^{17} + 6.30844 \times 10^9 t^{18} - 1.25936 \times 10^{10} t^{19} \\ & +2.3514 \times 10^{10} t^{20} - 4.10914 \times 10^{10} t^{21} + 6.72531 \times 10^{10} t^{22} - 1.03151 \times 10^{11} t^{23} \\ & +1.48341 \times 10^{11} t^{24} - 2.00114 \times 10^{11} t^{25} + 2.53321 \times 10^{11} t^{26} - 3.00996 \times 10^{11} t^{27} \\ & +3.3575 \times 10^{11} t^{28} - 3.51614 \times 10^{11} t^{29} + 3.45694 \times 10^{11} t^{30} - 3.19027 \times 10^{11} t^{31} \\ & +2.76286 \times 10^{11} t^{32} - 2.24449 \times 10^{11} t^{33} + 1.70956 \times 10^{11} t^{34} - 1.22005 \times 10^{11} t^{35} \\ & +8.15195 \times 10^{10} t^{36} - 5.09478 \times 10^{10} t^{37} + 2.97503 \times 10^{10} t^{38} - 1.62107 \times 10^{10} t^{39} \\ & +8.23012 \times 10^9 t^{40} - 3.88654 \times 10^9 t^{41} + 1.70378 \times 10^9 t^{42} - 6.91789 \times 10^8 t^{43} \\ & +2.59485 \times 10^8 t^{44} - 8.96454 \times 10^7 t^{45} + 2.84259 \times 10^7 t^{46} - 8.23993 \times 10^6 t^{47} \\ & +2.17327 \times 10^6 t^{48} - 518660.t^{49} + 111267.t^{50} - 21287.6t^{51} + 3597.06t^{52} \\ & -530.378t^{53} + 67.1962t^{54} - 7.16818t^{55} + 0.626149t^{56} - 0.0430083t^{57} \\ & +0.00217836t^{58} - 0.0000723397t^{59} + 1.18161 \times 10^{-6} t^{60}. \end{aligned}$$

Now we look for the parametric result ($x = x(t)$) and ($y = y(t)$). First, we make an assumption which also satisfies initial condition $y(0) = 1$.

$$y(t) = e^{\int_0^t w(t)dt}, \tag{3.30}$$

where $w(t)$ is to be resolved in terms of $z(t)$. By substituting (3.30) in (3.7) and using (3.14) we find that:

$$z = -\left(\frac{16}{3}\right)^{1/3} \frac{w}{\dot{x} y^{1/3}},$$

$$w = -\frac{6zt}{1 - t^2 z}. \tag{3.31}$$

Briefly, the parametric solution of the Thomas-Fermi equation (3.1) with boundary condition in (3.2) is:

$$x(t) = \sqrt[3]{144}\, t^2 e^{2\eta(t)}, \tag{3.32a}$$

$$y(t) = e^{-6\eta(t)}, \tag{3.32b}$$

where

$$\eta(t) = \int_0^t \frac{zt}{1 - t^2 z} dt. \tag{3.33}$$

Expression for $z(t)$ is derived above and by using (3.32) the Majorana solution of the Thomas-Fermi equation we can figure out the solution.

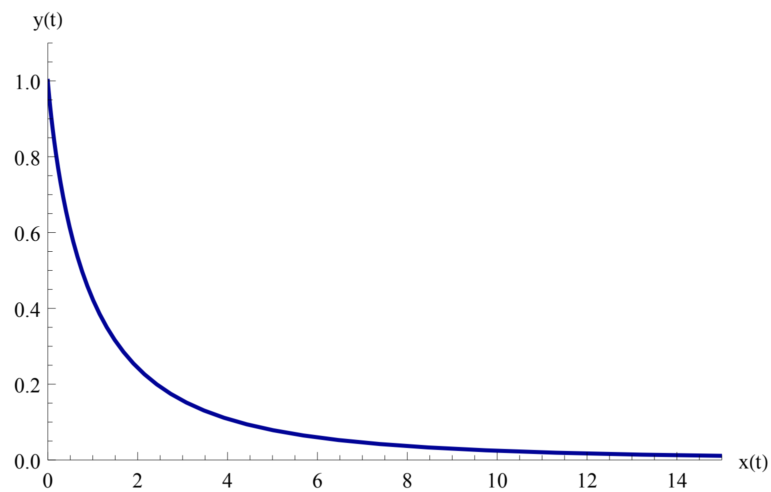


Figure 3.1: Majorana solution of the Thomas-Fermi equation.

t	x(t)	y(t)
0.00	0.00	1
0.06	0.0190407	0.973236
0.12	0.0780538	0.904205
0.18	0.182384	0.807301
0.24	0.340928	0.694452
0.30	0.567102	0.575581
0.36	0.880773	0.458759
0.42	1.31167	0.350256
0.48	1.90544	0.254581
0.54	2.73493	0.174536
0.60	3.9225	0.111322
0.66	5.688	0.0646767
0.72	8.46396	0.0330854
0.78	13.2173	0.0140444
0.84	22.5707	0.00439949
0.90	46.4753	0.000762342
0.96	169.244	0.0000232514

Table 3.2: Numerical result of Majorana solution of the Thomas-Fermi equation.

Figure 3.1 and Table 3.2 depict this solution which is a highly accurate solution of the Thomas-Fermi equation.

Chapter 4

Chebyshev Spectral Method

4.1 Introduction

The origin of the term, "spectral" is not known but probably arises from the original use of Fourier sines and cosines as basis functions, especially in the fundamental frequencies of a process, namely the "spectrum". Spectral methods are generally based on the representation of a real and continuous function $g(x)$, on some interval not necessarily bounded. In spectral methods, basis functions are global smooth functions.

If we have an equation for any arbitrary function $z(x)$ where $x \in \mathrm{J} \subseteq \mathbb{R}^n$

$$Lz = g, \tag{4.1}$$

$$Bz = 0 \ , \ x \in dJ, \tag{4.2}$$

then this function $z(x)$ can be approximated on the interval J as:

$$z(x) \approx z_N(x) = \sum_{i=0}^{N} c_i^{(n)} \psi_i(x). \tag{4.3}$$

where J denotes a bounded domain $\mathbb{R}^a$ with $a = 1, 2$, or 3 and ψ_i are the basis functions with constant coefficients c_i which are to be determined. Put $z_N(x)$ in Eq. (4.1) then the residual R can be calculated as

$$R_N(x) = Lz_N(x) - g(x) \neq 0, \quad x \in J. \tag{4.4}$$

We have to force the residual R to zero, it requires

$$(R_N, \phi_i) := \int_J R_N(x)\phi_i(x)w(x) = 0, \quad 0 \leq i \leq N, \tag{4.5}$$

where ϕ_i are members of an orthogonal set of functions

$$< R_N, \phi_i >_{N,w} := \sum_{j=0}^{N} R_N(x_j)\phi_i(x_j)w_j = 0, \quad 0 \leq i \leq N, \tag{4.6}$$

where x_j with $j = 0, 1, ...N$ are a set of collocation points and w_j are the weights. As z is an approximate solution so the residual R is about to vanish for all $x \in J$. For high accuracy, the residual function R is minimized. Later we have to find c_i the unknown coefficients, so that the choice of the function approximates the exact solution in the best way.

4.1.1 Properties of Orthogonal Polynomials

Some properties are mentioned here which are very useful in spectral methods to find unknown coefficients. We state some of them. Proof may be found in [5].

Theorem 4.1.1. *The polynomials of an orthogonal set stisfy a recurrence relation of the form*

$$x\psi_i(x) = E_i\psi_{i+1}(x) + F_i\psi_i(x) + G_i\psi_{i-1}(x), \quad i \geq 1.$$

where E_i, F_i and G_i are constants that may depend on i.

Theorem 4.1.2. *The jth degree polynomial ψ_j of an orthogonal set has j real distinct zeros, all of which lie in the interval (a, b).*

In the particular case where $w(x) = 1$ for $a \leq x \leq b$, g_1 and g_2 are said to be *simply orthogonal*. Simply, set of functions $\{\phi_i(x)\}_{i=0}^{\infty}$ is called an *orthogonal set of functions* if the functions are pairwise orthogonal $< \phi_i(x), \phi_j(x) >= 0$ for $i \neq j$.

A spectral method of solution of differential equations is based on the expansion of the solution in a basis set of linearly independent functions. The choice of basis functions based on the problem. The most commonly used basis functions are trigonometric functions and orthogonal polynomials which include following:

1. Fourier Spectral Method
2. Laguerre Spectral Method
3. Chebyshev Spectral Method
4. Legendre Spectral Method
5. Hermite Spectral Method

Here is a list of several classical polynomials orthogonal with respect to weight function $w(x)$ on the specified interval $[a, b]$.

Name	Symbol	w(x)	[a,b]
$Legendre$	$P_n(x)$	1	$[-1,1]$
$Chebyshev$	$T_n(x)$	$\frac{1}{\sqrt{1-x^2}}$	$[-1,1]$
$Sine$	$\sin(n\pi x)$	1	$[-1,1]$
$Cosine$	$\cos(n\pi x)$	1	$[-1,1]$
$Hermite$	$H_n(x)$	e^{-x^2}	$[-\infty,\infty]$
$Hermite$	$h_n(x)=e^{-\frac{x^2}{2}}H_n(x)$	1	$[-\infty,\infty]$
$AssociatedLaguerre$	$L_n^{(\alpha)}(x)$	$x^\alpha e^{-x}$	$[0,\infty]$

Table 4.1: List of basis functions.

Let an example to see how to apply Spectral Methods on a problem.

4.1.2 Example

Let us solve a first order nonlinear ordinary differential equation,

$$Rz = z' + q(x) + \frac{1}{p(x)}z^2 = 0. \tag{4.7}$$

is called the Riccati differential equation. Where $p(x)$ and $q(x)$ are continuous on $\mathbb{R}$ and $p(x) > 0$ on $\mathbb{R}$. For $p(x) = q(x) = 1$, we have

$$Rz = z' + 1 + z^2 = 0 \quad , \quad z(0) = 0. \tag{4.8}$$

Let the approximate solution of above equation by using Chebyshev spectral method be given as

$$z(x) = \sum_{i=0}^{N} c_i T_i(x). \tag{4.9}$$

As exact solution of (4.8) is $z(x) = -\tan(x)$ defined on an interval $(-\frac{\pi}{2}, \frac{\pi}{2})$. So, first step is to transform by using

$$\mathbb{T}_i(x) = T_i\Big(\frac{\pi}{2}x\Big). \tag{4.10}$$

```
In[2]:= Array[T, 100, 0];

In[3]:= Array[L, 100, 0];

In[4]:= T[n_][x_] := Sum[((n)! x^(n-2k) (x^2 - 1)^k)/((2 k)! (n - 2 k)!), {k, 0, n/2}]

In[5]:= For[n = 0, n < 100, L[n][x_] = T[n][π/2 x]; n++]

In[6]:= ff := f'[x] + 1 + f[x]^2

In[7]:= ff

Out[7]= 1 + f[x]^2 + f'[x]
```

Then (4.9) becomes

$$z(x) = \sum_{i=0}^{N} c_i \mathbb{T}_i(x). \tag{4.11}$$

For $N = 3$, unknown coefficients c_i can easily be computed by using roots $x_{i'}s$ of Chebyshev polynomial from Theorem 4.1.2 and these are as well called the Gauss-Radau nodes.

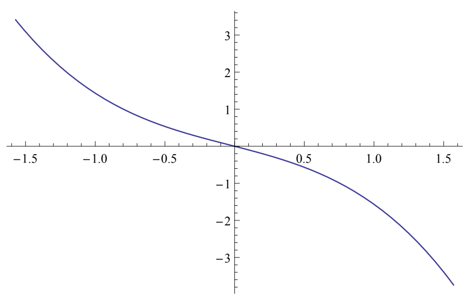
```
In[10]:= "h[i]=ith root of L[n]+L[n+1]"
         n = 3
         f[x_] = Sum[j[i] L[i][x], {i, 0, n}];
         TT = NSolve[L[n + 1][x] + L[n][x] == 0, Reals]
         For[i = 1, i < n + 2, pp[i] = x /. TT[[i]]; i++]
         For[i = 1, i < n + 2, h[i] = pp[i]; i++]
         Print["h[1]=", h[1], "      ", "h[", n + 1, "]=", h[n + 1]]

Out[10]= h[i]=ith root of L[n]+L[n+1]

Out[11]= 3

Out[13]= {{x → -0.63662}, {x → -0.396926}, {x → 0.141661}, {x → 0.573575}}

         h[1]=-0.63662      h[4]=0.573575

In[17]:= g[x_] = ff;
```

By using these N nodes in (4.8), we have N number of unknowns and N number of equations. By solving these systems of equations (4.12) we approach the solution.

$$Rz(x_i) = z'(x_i) + 1 + z^2(x_i) = 0. \tag{4.12}$$

```
In[18]:= LP[3] = FindRoot[{f[0] == 0, g[h[1]] == 0, g[h[2]] == 0, g[h[3]] == 0}
           , {{j[0], 1}, {j[1], 0.4}, {j[2], 0.5}, {j[3], -.5}}]

Out[18]= {j[0] → -0.0136434, j[1] → -0.7192, j[2] → -0.0136434, j[3] → -0.0341808}

In[19]:= fg[3][x_] = Simplify[f[x] /. LP[3]]

Out[19]= 0. - 0.968644 x - 0.0673276 x^2 - 0.52991 x^3

In[21]:= ga3 = Plot[fg[3][x], {x, -π/2, π/2}, PlotRange → All]
```

Out[21]=



By using Mathematica, we can find good accuracy by taking $N = 50$.

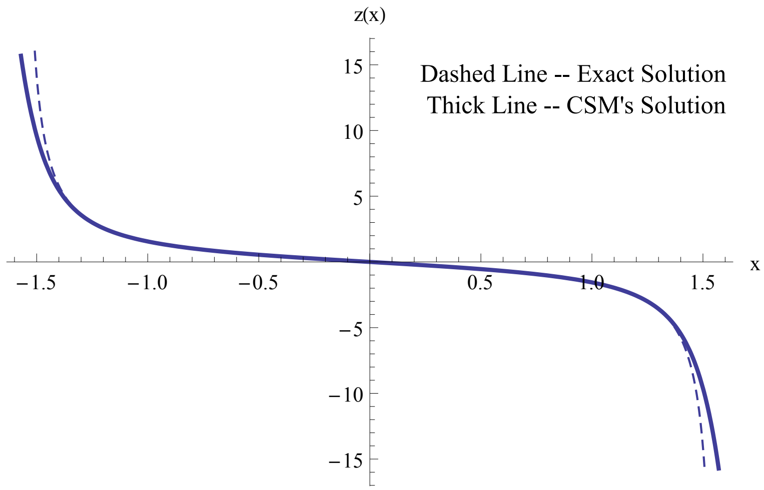


Figure 4.1: Comparison of Chebyshev Spectral method with exact solution of Riccati equation.

For $N = 50$, we can easily find the best solution of Riccati equation using Mathematica. Also, we can compare it with the exact solution of Riccati equation. In figure 4.1, approximated solution calculated by using Chebyshev spectral method is a good accurate numerical solution of Riccati equation.

4.2 Solution of the Thomas-Fermi Equation by using Chebyshev Spectral Method

In this section, we have utilized one of the spectral methods on the Thomas-Fermi Equation which is a nonlinear second order ordinary differential equation. We have used Chebyshev polynomials as the basis set of orthogonal polynomials. As interval of Chebyshev polynomial is $[-1, 1]$, so first we transform its interval according to our problem. Then use roots of these polynomials to find unknown coefficients.

4.2.1 Application

As we saw in section-4.1 that Spectral methods are suitable for nonlinear problems with complicated coefficients. The Thomas-Fermi equation is defined on the semi infinite interval and we can't solve it exactly. So we use Spectral methods on Thomas-Fermi equation. Here we are using its standard form.

$$xy''^2 - y^3 = 0, \tag{4.13}$$

$$y(0) = 1 \quad , \quad y(\infty) = 0. \tag{4.14}$$

First, we write y in its approximated form. Let $\{\phi_i(x)\}_0^\infty$ be a set of basis functions and c_i are unknown coefficients then we can write it as:

$$y_N(x) = \sum_{i=0}^{N} c_i \phi_i(x) \tag{4.15}$$

It is an approximate solution of the Thomas-Fermi equation. From Eq.(4.13), (4.14) the residual function $R_n(x)$ can be written as

$$R_N(x) = x(y_N''(x))^2 - (y_N(x))^3. \tag{4.16}$$

In order to find $n + 1$ unknown coefficients in Eq.(4.15), we need to solve $n + 1$ systems of equations. By applying boundary conditions on Eq.(4.15) we find following equations

$$\sum_{i=0}^{n} c_i^n \phi_i(0) = 1, \tag{4.17}$$

$$\sum_{i=0}^{n} c_i^n \phi_i(\infty) = 0. \tag{4.18}$$

For rest of n equations we set residual to zero at N from $n+1$ nodes $x_i, i = 1, 2, ..., n+1$. For finding these nodes x_i we use a approach what are called Gauss-Radau nodes. In this method we use zeros of $\phi_n(x) + \phi_{n+1}(x)$ as x_i in Eq.(4.16).

$$R_n(x_i) = 0\ ,\ \ i = 1, 2, ..., n. \tag{4.19}$$

4.2.2 Chebyshev Spectral Methods

For finding a solution of the Thomas-Fermi equation by spectral methods, we use $\phi_i(x)$ as Chebyshev polynomials in Eq.(4.15). Chebyshev polynomials of the first kind $T_n(x)$, are solutions of the Chebyshev differential equation

$$(1-x^2)T_n''(x) - xT_n'(x) + n^2 T_n(x) = 0, \tag{4.20}$$

which is written in summation form as given below

$$T_n(x) = \sum_{k=0}^{\frac{n}{2}} \frac{n! x^{n-2k}(x^2-1)^k}{(2k)!(n-2k)!}, n \geq 0.$$

Our problem is defined over the interval $[0, \infty)$ and Chebyshev polynomials are defined on $[-1, 1]$. First step is to transform its interval from $[-1, 1]$ to $[0, \infty)$. We use small program on Mthematica for the transformation of the interval

$$\mathbb{T}_n(x) = T_n(\frac{x-1}{x+1}). \tag{4.21}$$

```
In[1]:= Array[T, 100, 0];

In[2]:= Array[L, 100, 0];
```

In[3]:= $T[n\_][x\_] := \sum_{k=0}^{n/2} \frac{(n)!\, x^{n-2k} (x^2-1)^k}{(2k)!\,(n-2k)!}$

In[4]:= $\text{For}\left[n = 0,\ n < 61,\ L[n][x\_] = T[n]\left[\frac{x-1}{x+1}\right];\ n{+}{+}\right]$

```
In[5]:= ff := x f''[x]^2 - f[x]^3

In[6]:= ff
```

Out[6]= $-f[x]^3 + x\, f''[x]^2$

Now, the second step is to use transformed Chebyshev polynomial $\mathbb{T}_i(x)$ as basis function in Eq.(4.15). We have

$$y_N(x) = \sum_{i=0}^{N} c_i \mathbb{T}_i(x). \tag{4.22}$$

By increasing number of terms N the residual function $R_N(x)$ minimized easily

$$R_N(x) = x(y_N''(x))^2 - (y_N(x))^3. \tag{4.23}$$

Then, the next step is to find unknown coefficient c_i. From Theorem **??** in section-4.1 we know that if set of polynomials $\{\phi_i(x)\}_0^\infty$ is orthogonal then there exist n zeros of ϕ_n. So Chebyshev polynomial $\mathbb{T}_i(x)$ have N zeros. We can also use zeros of $\mathbb{T}_i(x)$ or $\mathbb{T}_i(x) + \mathbb{T}_{i+1}(x)$, the second one is also called Gauss-Radau nodes. we use Mathematica to find these nodes.

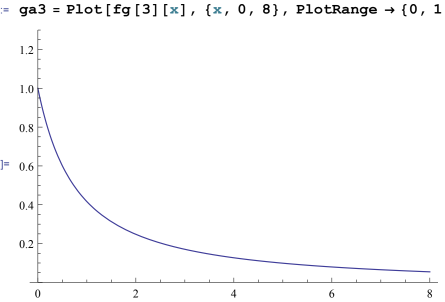
```
In[7]:= "h[i]=ith root of L[n]+L[n+1]"
        n = 3
        f[x_] = Sum[j[i] L[i][x], {i, 0, n}];
        TT = NSolve[L[n + 1][x] + L[n][x] == 0, Reals]
        For[i = 1, i < n + 2, pp[i] = x /. TT[[i]]; i ++]
        For[i = 1, i < n + 2, h[i] = pp[i]; i ++]
        Print["h[1]=", h[1], "      ", "h[", n + 1, "]=", h[n + 1]]

Out[7]= h[i]=ith root of L[n]+L[n+1]

Out[8]= 3

Out[10]= {{x → 0.}, {x → 0.231914}, {x → 1.57242}, {x → 19.1957}}

        h[1]=0.     h[4]=19.1957
```

The above program is for $N = 3$, we can easily improve the solution by increasing N. We use these nodes x_i in Eq.(4.22) and use these $y(x_i)$ in Eq.(4.23). In this manner we have N equations to find N unknown coefficients c_i

$$R_N(x_i) = x_i(y''_N(x_i))^2 - (y_N(x_i))^3 = 0. \tag{4.24}$$

```
In[14]:= g[x_] = ff;

In[15]:= LP[3] = FindRoot[{f[0] == 1, g[h[2]] == 0, g[h[3]] == 0, g[h[4]] == 0}
           , {{j[0], 1}, {j[1], 0.4}, {j[2], 0.5}, {j[3], -.5}}]

Out[15]= {j[0] → 0.451652, j[1] → -0.517543, j[2] → 0.0354849, j[3] → 0.00468068}

In[16]:= fg[3][x_] = Simplify[f[x] /. LP[3]]

Out[16]= (1. + 1.76529 x + 0.589779 x^2 - 0.0257255 x^3) / (1. + x)^3

In[17]:= ga3 = Plot[fg[3][x], {x, 0, 8}, PlotRange → {0, 1.3}]
```

Out[17]=



By using Chebyshev Spectral Method, here are some solutions of The Thomas-Fermi equation $y_N(x)$ for $N = 10, 15$ and 20.

$$y_{10}(x) = \frac{1}{(1.+x)^{10}}\Big(1. + 8.52548x + 34.8683x^2 + 72.6484x^3 + 121.032x^4 + 99.6885x^5 + 67.2864x^6 + 25.4258x^7 + 3.78336x^8 - 0.0799839x^9 + 0.000338145x^{10}\Big),$$

$$y_{15}(x) = \frac{1}{(1.+x)^{15}}\Big(1. + 13.4888x + 89.1748x^2 + 316.538x^3 + 1103.05x^4 + 1129.41x^5 + 4320.5x^6 + 524.37x^7 + 4785.99x^8 + 188.725x^9 + 1262.04x^{10} + 91.3591x^{11} + 67.0276x^{12} + 1.34155x^{13} - 0.013637x^{14} + 0.0000259715x^{15}\Big),$$

$$y_{20}(x) = \frac{1}{(1.+x)^{20}}\Big(1. + 18.4701x + 168.444x^2 + 845.934x^3 + 4686.6x^4 + 2313.17x^5 + 69388.1x^6 - 106352.x^7 + 413903.x^8 - 453600.x^9 + 635853.x^{10} - 330078.x^{11} + 221883.x^{12} - 33677.3x^{13} + 16952.6x^{14} + 1828.59x^{15} + 393.202x^{16} + 83.4827x^{17} + 0.744736x^{18} - 0.0047709x^{19} + 5.30493 * 10^{-6}x^{20}\Big).$$

We can see that for different values of N, solutions are displayed in a very simple and short form. Here is the graphical view for different values of N.

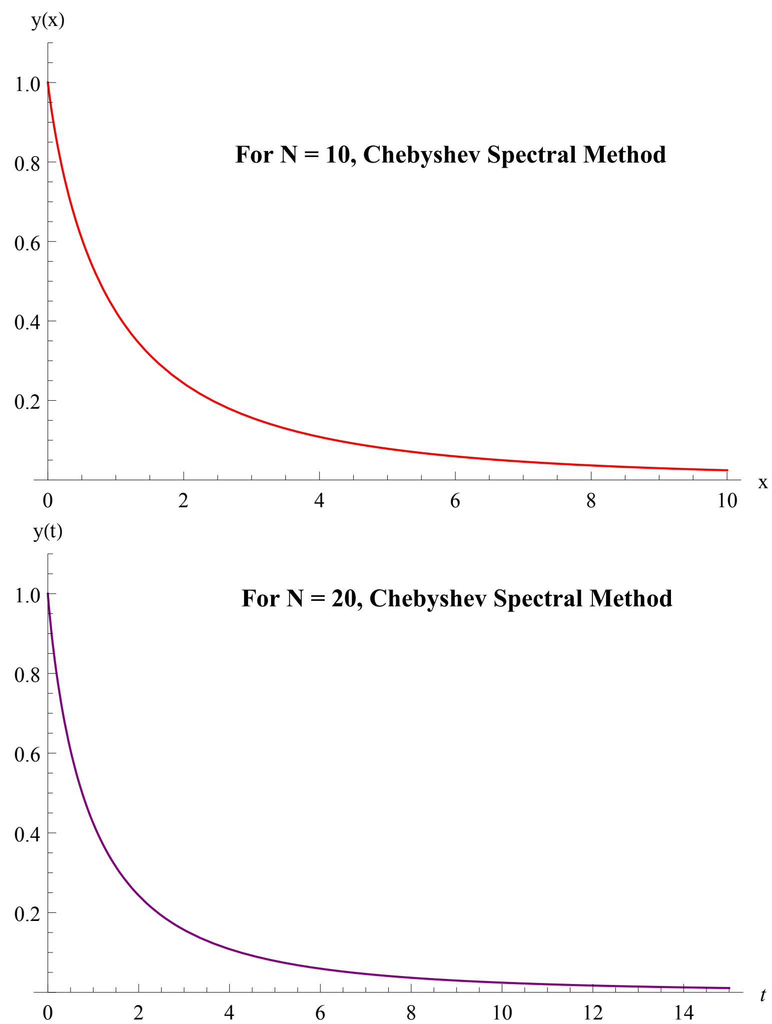


Figure 4.2: Plot For N = 10, 20 using Chabyshev Spectral Method.

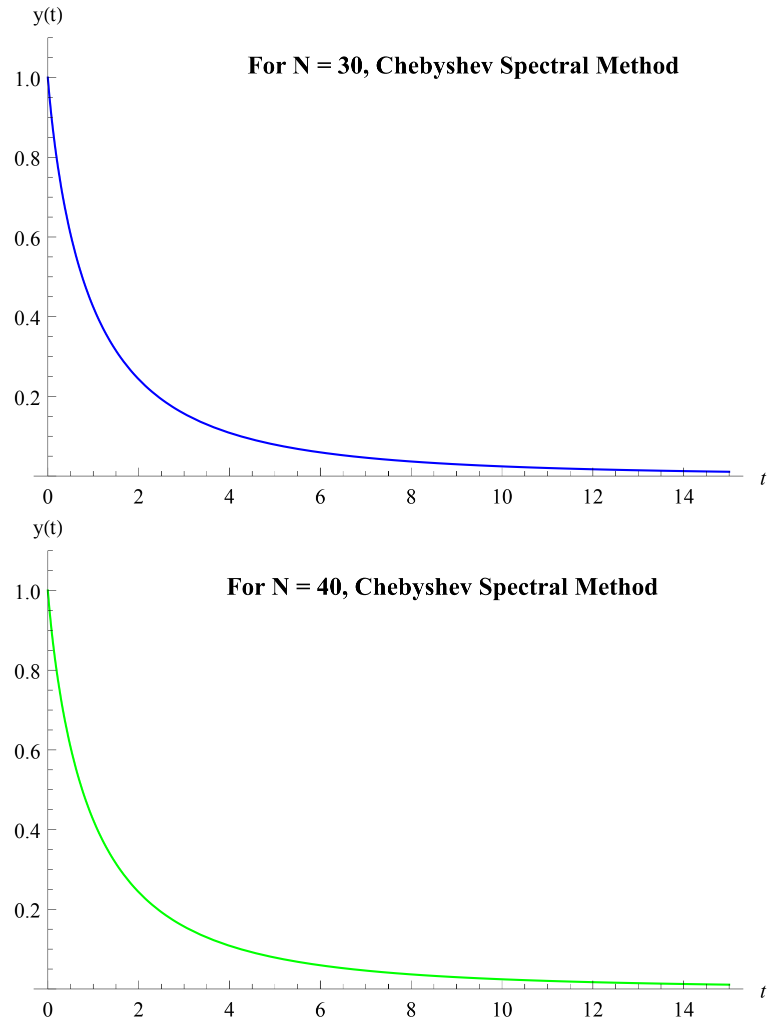


Figure 4.3: Plot For N = 30, 40 using Chabyshev Spectral Method.

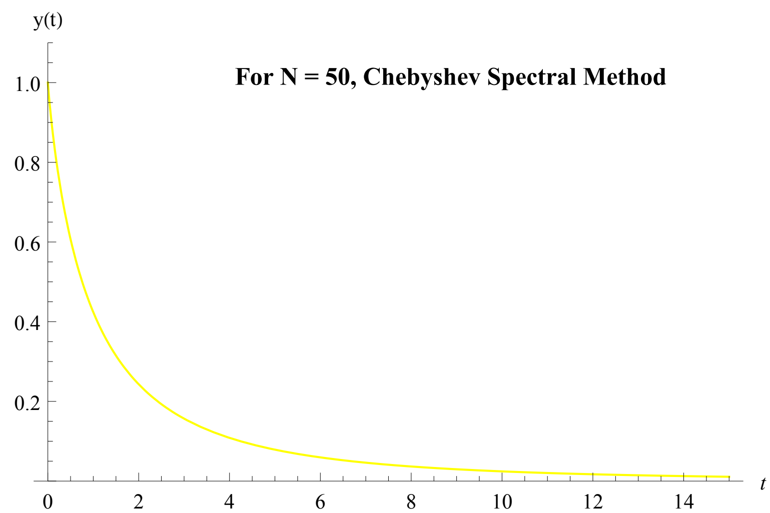


Figure 4.4: Plot For N = 50 using Chabyshev Spectral Method.

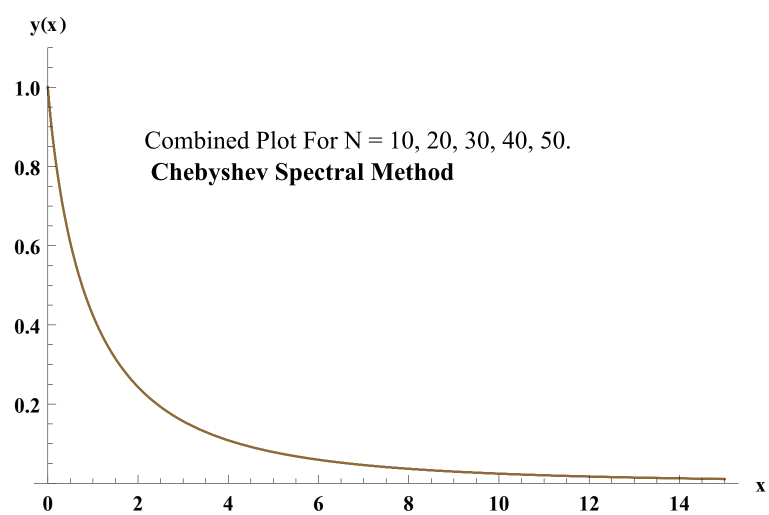


Figure 4.5: Combined Plot For N = 10, 20, 30, 40, 50 using Chabyshev Spectral Method.

From figure 4.2, 4.3, 4.6 and 4.5 we can easily observe that by increasing N, solution of the problem approximately remains the same.

x	$N = 10$	$N = 20$	$N = 30$	$N = 40$	$N = 50$
0.5	0.607045	0.606993	0.606988	0.606987	0.606987
1.0	0.424003	0.424014	0.424009	0.424009	0.424008
2.0	0.243087	0.243014	0.24301	0.243009	0.243009
3.0	0.156647	0.156631	0.156633	0.156633	0.156633
4.0	0.108321	0.108408	0.108404	0.108404	0.108404
5.0	0.0787195	0.0788086	0.0788083	0.0788077	0.0788078
10.0	0.024464	0.0243177	0.0243148	0.0243144	0.0243144
20.0	0.00578872	0.00578131	0.00578519	0.00578495	0.00578489
30.0	0.00209271	0.00225696	0.00225594	0.00225587	0.00225589
40.0	0.000880967	0.00111761	0.0011132	0.00111338	0.00111359
50.0	0.000382537	0.000636264	0.000631891	0.000632181	0.000632242

Table 4.2: Approximate solution varies by increasing N.

In the above table we can see that by increasing number of terms N the solution also rapidly converges.

From Kobayashi and Anderson [2, 3] we can compare how much our solution is precise at the starting points. Kobayashi calculated highly accurate numerical solution of the Thomas-Fermi equation and found $y'(0) = -1.588071$. Anderson calculated the upper and lower bound of $y'(0)$ by using complementary variation method principles

$$-1.589 < y'(0) < -1.563. \tag{4.25}$$

By using Chebyshev Spectral Method our slop is $y'(0) = -1.56801$, which is a much better result as compared with Liao [11].

Order N	$y\prime(0)$ SM	% Comparison with [2]	$y\prime(0)$ Liao [11]	% Comparison with [2]
10	-1.47452	7.15	-1.28590	19.03
20	-1.52987	3.66	-1.40932	11.26
30	-1.54894	2.50	-1.46306	7.87
40	-1.5586	1.85	-1.49236	6.03
50	-1.56443	1.49	-1.51063	4.88
60	-1.56801	1.26	-1.52309	4.09

Table 4.3: Comparison of initial slope $y\prime(0)$ with Liao[11], and compared with Kobayashi's numerical result $y'(0) = -1.58801$.

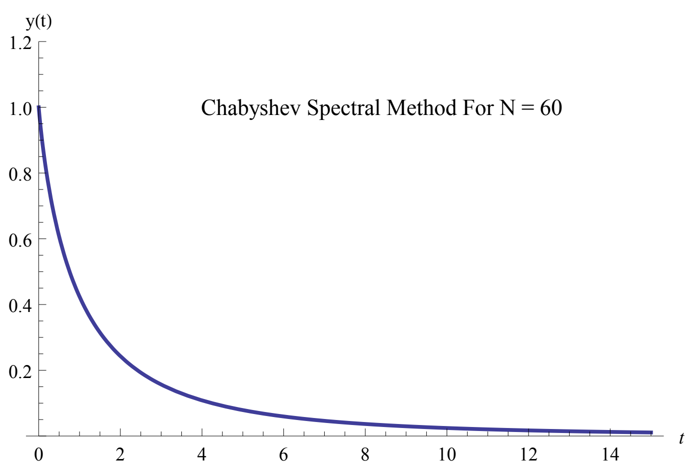


Figure 4.6: Approximate Solution by Using Chabyshev Spectral Method for N=60.

4.2.3 Results and Discusion

We know that $y(x)$ tends to zero algebraically as $x \to \infty$. Under this condition we have obtained the convergent results of the original Thomas-Fermi equation in the whole region $0 \leq x < \infty$.

x	Expo	RC-SK	RC-TK	Hermite	CSM
0.5	0.606986951	0.605270502	0.602998554	0.606658908	0.606987
1.0	0.424010148	0.420343948	0.416399658	0.423811203	0.424008
1.5	0.314780118	0.318737461	0.314761643	—	0.363202
2.0	0.243010373	0.256010764	0.252344355	0.242918233	0.243009
2.5	0.192984580	0.213705386	0.210384924	0.192917948	0.192984
3.0	0.156631657	0.183318729	0.180313058	0.156573773	0.156633
3.5	0.129367328	0.160461449	0.157728304	0.129316613	0.12937
4.0	0.108401057	0.142653971	0.140154047	0.108360441	0.108404
5.0	0.078803669	0.116720187	0.114592127	—	0.0788078
15	0.010808302	0.041370727	0.040533524	0.010803774	0.0108054
20	0.005789307	0.031271686	0.030630632	0.005792831	0.00578493
30	0.002260351	—	—	0.002252634	0.00225587
50	0.000632255	0.012687078	0.012420906	—	0.000632268
75	0.000219970	0.008484835	0.008305908	—	0.0002182
100	0.000101341	0.006373709	0.006238954	—	0.000100214

Table 4.4: Comparrison of the Thomas-Fermi equation solution by using (CSM) with other spectral methods using different basis functions.

In the above table, solution are given by using Exponential function as a basis function (Expo)[9], Rational Chebyshev second kind(RC-SK), Rational Chebyshev third kind(RC-TK), Hermite function as basis function (Hermite)[6] and our Chebyshev Spectral method (CSM).

x	PA [7/7]	PA [8/8]	Majorana	Liao [11]	CSM
00.50	0.755738	0.7552	0.606982	0.606987	0.606987
01.00	0.426623	0.424	0.424007	0.424008	0.424008
02.00	0.12256	0.108321	0.243009	0.243009	0.243009
03.00	0.0613384	0.0292216	0.156633	0.156633	0.156633
04.00	0.0563062	0.0085627	0.108404	0.108404	0.108404
05.00	0.0604499	0.00205949	0.0788078	0.0788078	0.0788078
10.00	0.0652132	-0.00290523	0.0243142	0.0243143	0.0243143
15.00	0.056417	-0.00316081	0.0108054	0.0108054	0.0108054
20.00	0.0480175	-0.00296214	0.00578493	0.00578494	0.00578493
25.00	0.0413783	-0.00269538	0.00347375	0.00347375	0.00347375
50.00	0.0239109	-0.00172492	0.000632257	0.000632255	0.000632268
75.00	0.0167075	-0.00124431	0.000218206	0.000218210	0.0002182
100.0	0.0128253	-0.000970104	0.000100243	0.000100243	0.000100214
1000	0.00136446	-0.00010745	—	1.3513×10^{-7}	2.25317×10^{-7}

Table 4.5: Comparrison between Chebyshev Spectral Method $T_n(x)$ and Analytic results of Liao [11].

Spectral methods has been a new approach for solving the Thomas-Fermi equation. We have demonstrated by using Chebyshev polynomials as basis function, a very high level of accuracy of the approximate solution can be attained when we compare it with more accurate results of Liao[11] and

Majorana[10].

Chapter 5

Conclusion

We have presented the solution of Wazwaz [4] by using the Adomian decomposition method to solve the Thomas-Fermi problem. A slight change in Adomian decomposition method gives a solution in which an unknown coefficient appears which is equal to initial slope. Then we use Padé approximants, which give us good value for initial slope $y'(0)$. But these results have bad marks as far as the accuracy is concerned. After that we describe an analytical solution of the problem. This solution was founded by famous Italian physicist Majorana but it remained unpublished and S. Esposito [10] worked out the details and published it in 2002. We observe that the Majorana solution of the Thomas-Fermi equation is a highly accurate solution of the Thomas-Fermi equation. Then we utilized one of the spectral methods on the Thomas-Fermi Equation. We have used Chebyshev polynomials as the basis set of orthogonal polynomials. As the interval of Chebyshev polynomial is $[-1, 1]$ we transform its interval according to our problem. We use roots of these polynomials to find unknown coefficients. We have demonstrated by using Chebyshev polynomials as basis function, a very high level of accuracy and compare it with accurate result of Majorana [10]. Also, we find that both the Spectral solution and the Majorana solution can be made as accurate as desired by increasing the number of terms.

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