CHAPTER III

RESEARCH METHODOLOGY

Modified Adomian Decomposition Method

In this section, Thomas-Fermi equation's solution will be extracted by Modified Adomian Decomposition Method (MADM) (see Appendix A). This work is aims to obtain an approximate solution to the Thomas-Fermi equation (2.3.10), $y''(x)=\frac{y^{3/2}(x)}{x^{1/2}}$.We shall focus our attention here to the boundary conditions

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

For a detailed discussion of MADM, we first rewrite (2.3.10) in an operator form

$$\hat{L}(y)=\frac{y^{3/2}}{x^{1/2}}, \tag{3.1.1}$$

where $\hat{L}$ is a second order differential operator, and hence $\hat{L}^{-1}$ is a two-fold integration operator defined by

$$\hat{L}^{-1}(.)=\int_0^x\int_0^x(.)\,dx\,dx. \tag{3.1.2}$$

Operating with $\hat{L}^{-1}$ on both sides of equation (3.1.1) and using the boundary condition $y(0)=1$, we obtain

$$y(x)=1+Bx+\hat{L}^{-1}\left(x^{-1/2}y^{3/2}\right), \tag{3.1.3}$$

where

$$B\equiv y'(0). \tag{3.1.4}$$

B in equation (3.1.4) actually is **the initial slope of Thomas-Fermi potential.**

The standard Adomian decomposition method defines the solution $y(x)$ by the series

$$y(x)=\sum_{n=0}^{\infty}y_n(x), \tag{3.1.5}$$

where the components $y_n(x), n\geq 0$ will be determined recursively. Substituting (3.1.5) into both sides of (3.1.3) gives

$$\sum_{n=0}^{\infty} y_n(x) = 1 + Bx + \hat{L}^{-1}\left(x^{-1/2}\sum_{n=0}^{\infty} A_n\right), \tag{3.1.6}$$

where A_n are the **Adomian polynomials** .They may be calculated via **Order-by-order extraction technique (OBOET)** that is shownin detail in Chapter IV. Some results of A_n are also shown in the following Chapter V. Recall that the Adomian decomposition method defines the zeroth component $y_0(x)$ by all terms that are not included under the inverse operator $\hat{L}^{-1}$. In other words, the Adomian decomposition method employs the recursive relation

$$\begin{aligned} y_0(x) &= f(x) = 1 + Bx, \\ y_{k+1}(x) &= \hat{L}^{-1}\left(x^{-1/2}A_k\right), k \geq 0. \end{aligned} \tag{3.1.7}$$

However, the modified decomposition method suggests that the function $f(x)$ be divided into two parts, one is assigned to the component $y_0(x)$, and the other part is added to the definition of the component $y_1(x)$. Under this assumption, we set the modified recursive relation [5].

$$\begin{aligned} y_0(x) &= 1, \\ y_1(x) &= Bx + \hat{L}^{-1}\left(x^{-1/2}A_0\right), \\ y_{k+2}(x) &= \hat{L}^{-1}\left(x^{-1/2}A_{k+1}\right), k \geq 0. \end{aligned} \tag{3.1.8}$$

Thus, we will have $y_0(x)$ to $y_{11}(x)$.

Hence, solution of Thomas-Fermi equation by MADM, has the approximate form;

$$y(x) = \sum_{n=0}^{11} y_n(x), \tag{3.1.9}$$

However, we getunknown $B = y'(0)$. Although, if we substitute $B = y'(0) = -1.588071$, (Kobayashi [7]) into equation (3.1.9), itwill further accelerate the divergence of the Thomas-Fermi equation solution by the Differential Analyzer [1], because we cannot obtainthe solution in exact infinite series. Thus, we will incorporate Padé approximants [4].This method enablesfurther solution to converge. One benefit of Padé approximants is that we may calculate the initial slope $B = y'(0)$. First, we set

$x^{1/2} = t$ .So, the approximated solution of (3.1.9) can be transformed to $y(t)$, readily found to be

$$y(t) = \sum_{n=0}^{11} y_n(t). \tag{3.1.10}$$

For more details associated with equations (3.1.8) to (3.1.10), please see inthe following Chapter V. After that, we take $y(t)$ from (3.1.10) into Padé approximants.

The Padé approximants

Padé approximants for extends the truncated series solution

Padé approximants [4] represents a function by the ratio of two polynomials. The coefficients of the polynomials in the numerator and in the denominator are determined by using the coefficients in the Taylor expansion of the function. To explore the need of Padé approximants, we consider the example function

$$f(x) = \sqrt{\frac{1+3x}{1+x}}. \tag{3.2.1}$$

The Taylor series of $f(x)$ in equation (3.2.1) is given by

$$f(x) = 1 + x - \frac{3}{2}x^2 + \frac{5}{2}x^3 - \frac{37}{8}x^4 + \frac{75}{8}x^5 - \frac{327}{16}x^6 + \frac{753}{16}x^7 + O(x^8). \tag{3.2.2}$$

The Taylor series from equation (3.2.2) is often used to approximate $f(x)$ for values of $x$within the radius of convergence. However, if the polynomial obtained from using a finite number of the Taylor series from equation (3.2.2) is to be evaluated for very large positive values of x, the series or any truncated number of terms of equation (3.2.2) will definitely fail to provide a converging expression. Padé introduced a powerful tool that should be combined with power series for calculations.

Padé approximants, symbolized by $[m/n]$, is a rational function defined by

$$[m/n] = \frac{a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m}{1 + b_1 x + b_2 x^2 + \cdots + b_n x^n}, \tag{3.2.3}$$

where we have considered $b_0=1$, the numerator and denominator have no common factors. If we select $m=n$, then the approximants $[m/n]$ are called diagonal approximants.

In the following we shall introduce the simple and straightforward method to construct Padé approximants. Suppose that $f(x)$ is written in Taylor series form given by

$$f(x)=\sum_{k=0}^{\infty} c_k x^k. \tag{3.2.4}$$

Assuming that $f(x)$ can be manipulated by the diagonal Padé approximant defined in (3.2.3), where $m=n$. This admits the use of

$$\frac{a_0+a_1x+a_2x^2+\cdots+a_nx^n}{1+b_1x+b_2x^2+\cdots+b_nx^n}=c_0+c_1x+c_2x^2+\cdots+c_{2n}x^{2n}. \tag{3.2.5}$$

By using cross multiplication in (3.2.5) we find

$$a_0+a_1x+a_2x^2+\cdots+a_nx^n=c_0+(c_1+b_1c_0)x+(c_2+b_1c_1+b_2c_0)x^2+\cdots. \tag{3.2.6}$$

Equating powers of x leads to

coefficient of x^0 : $a_0=c_0$,

coefficient of x^1 : $a_1=c_1+b_1c_0$,

coefficient of x^2 : $a_2=c_2+b_1c_1+b_2c_0$,

coefficient of x^3 : $a_3=c_3+b_1c_2+b_2c_1+b_3c_0$,

$\vdots$

coefficient of x^n : $a_n=c_n+\sum_{k=1}^{n} b_k c_{n-k}$.

Notice that coefficients of $x^{n+1}, x^{n+2}, \ldots, x^{2n}$ must be equated to zero. This completes the determination of the constants of the polynomials both in the numerator and denominator [4].

Padé approximants and Boundary Value Problems

In this section, the boundary value problems on infinite or semi-infinite intervals will be investigated. In what follows, we outline the basic steps to be followed for handling the boundary value problems on an unbounded domain of validity. In the first step, we use the decomposition method or the modified decomposition method to derive a series solution. In the second step, we form the diagonal Padé approximants $[n/n]$, because it is the most accurate and efficient approximation. Recall that

$$[n/n]=\frac{a_0+a_1x+a_2x^2+\cdots+a_nx^n}{1+b_1x+b_2x^2+\cdots+b_nx^n}. \qquad (3.2.7)$$

In the last step, the most effective use of the diagonal approximant is that it can be evaluated in the limit $x\to\infty$. In this case

$$\lim_{x\to\infty}[n/n]=\frac{a_n}{b_n}. \qquad (3.2.8)$$

However, if the boundary condition at $x=\infty$ is given by

$$y(\infty)=0, \qquad (3.2.9)$$

it follows immediately that

$$a_n=0. \qquad (3.2.10)$$

Notice here that a_n is an expression that contains values from the prescribed boundary conditions. Consequently, equation (3.2.10) can be solved to find the unknown parameters of the given boundary condition [4].

For Thomas-Fermi model, we apply Padé approximants. In this work, we use manipulation language such as Maple or Mathematica to calculate Padé approximants of (3.1.10), obtaining

$$[2/2]=\frac{9B^2-12Bt+\left(9B^3+16\right)t^2}{9B^2-12Bt+16t^2},$$

$$[4/4]=\frac{G(t)}{H(t)},$$

where

$$G(t)=27B^4+97B+\left(\frac{140}{9}+\frac{33}{10}B^3\right)t+\left(\frac{675}{28}+\frac{437}{5}B^2\right)t^2$$
$$+\left(\frac{453}{14}B^4+\frac{1070}{9}B\right)t^3+\left(-\frac{81}{28}B^6-\frac{1096}{175}B^3+\frac{455}{27}\right)t^4,$$

and

$$H(t)=27B^4+97B+\left(\frac{140}{9}+\frac{33}{10}B^3\right)t+\left(\frac{81}{28}+\frac{48}{5}B^2\right)t^2$$
$$-\left(\frac{243}{35}B^4+26B\right)t^3-\left(\frac{186}{175}B^3+\frac{35}{9}\right)t^4.$$

Other Padé approximants order can also computed.

To determine the initial slope $B=y'(0)$, in this case

$$\lim_{t\to\infty}[n/n]=\frac{a_n}{b_n}, \tag{3.2.11}$$

we use the boundary condition $t\to\infty$ given by

$$\lim_{t\to\infty}[n/n]\equiv\lim_{t\to\infty}y(t)=0, \tag{3.2.12}$$

it followsfrom (3.2.11) and (3.2.12) immediately that $a_n=0$,

For example, consider Padé approximants of order [2/2]

$$[2/2]=\frac{9B^2-12Bt+\left(9B^3+16\right)t^2}{9B^2-12Bt+16t^2},$$

$$\lim_{t\to\infty}[2/2]=\frac{\left(9B^3+16\right)}{16},\ ;a_n=9B^3+16,\text{and } b_n=16.$$

We use the boundary condition $t \to \infty$ given by

$$\lim_{t\to\infty}[2/2] \equiv \lim_{t\to\infty} y(t) = 0,$$

$$9B^3 + 16 = 0.$$

Finally, we get initial slope $B = y'(0)$, for Padé approximants of order [2/2]

$$B = -1.211413729.$$

Previous methods can be programmed to calculate initial slope. For other orders of Padé approximants the initial slope can also be computedusing the same process. The error of initial slope has been calculated by using the highly accurate numerical solution of the Thomas- Fermi equation provided by Kobayashi [7] as

$$y'(0) = -1.588071. \qquad (3.2.13)$$

The resulting value of the initial slope $B = y'(0)$, are tabulated in Table 5.1have been shown in the following Chapter V.

When obtaining the initial slope $B = y'(0)$, we make a change of variable $t^2 = x$, and replace initial slope of each Padé approximants.

For example, consider Padé approximants of order [2/2],

$$[2/2] = \frac{9B^2 - 12Bt + (9B^3 + 16)t^2}{9B^2 - 12Bt + 16t^2},$$

we make a change of variable $t^2 = x$, and replace initial slope of each Padé approximants $B = -1.211413729$, we get the approximant solution

$$[2/2] \equiv y(x) = \frac{1}{1 + 1.100642416298209\sqrt{x} + 1.21141372855476x}$$
$$+ \frac{1.100642416298209\sqrt{x}}{1 + 1.100642416298209\sqrt{x} + 1.21141372855476x}$$
$$+ \frac{2.689878827577008 \times 10^{-16} x}{1 + 1.100642416298209\sqrt{x} + 1.21141372855476x}.$$

Previous methods can be programmed to calculate the solution. For other Padé orders the solution can also be computed via the same process. We plot MADM, [4/4], [7/7], [10/10] and compare them with Thomas-Fermi equation solution by the Differential

Analyzer [1] as shown in the following Chapter V. Data for Thomas-Fermi equation solution by the Differential Analyzer show in Appendix B.

Electron distribution for Mercury atom

Let us consider the electron distribution function, $D(r) = 4\pi r^2 \cdot n(r)$.

From equation (2.3.11), we have

$$D(r) = 4\pi r^2 \cdot \frac{(2me)^{3/2}}{3\pi^2\hbar^3}\left\{\frac{Ze}{r}y(x)\right\}^{3/2}, \tag{3.3.1}$$

Bohr radius $a = \dfrac{\hbar^2}{me^2}$, and setting $\eta \equiv \dfrac{r}{a} = \dfrac{0.88534}{Z^{1/3}}x$, we can reform equation(3.3.1) to the form of $D(\eta)$,

$$D(\eta) = \frac{2^{7/2}}{3\pi}\cdot\left(\frac{Z}{a}\right)^{3/2}(\eta a)^{1/2}\left\{y\left[\frac{Z^{1/3}}{0.88534}\eta\right]\right\}^{3/2}. \tag{3.3.2}$$

For the atomic unit of length, we can setting $a = 1$. So, we have;

$$D(\eta) = \frac{2^{7/2}}{3\pi}\cdot Z^{3/2}\eta^{1/2}\cdot\left\{y\left[\frac{Z^{1/3}}{0.88534}\eta\right]\right\}^{3/2}. \tag{3.3.3}$$

For mercury atom, $Z = 80$. The distance is expressed in terms of the atomic unit of length $\eta \equiv \dfrac{r}{a}$. The results of electron distribution have been showninthe following Chapter V.