CHAPTER I

INTRODUCTION

Rationale for the Study

When we explore an atom, where electrons travel around the nucleus of an atom, Electron's position cannot be exactly identified according to the Heisenberg uncertainty principle. However, electrons are likely to be in specific regions of an atom. This is the most modern and accepted form of the atom called "The electron cloud model". The density of electrons cloud is the probability density of the electrons, named "electron distribution".

The simplest atomic system is the hydrogen atom. It can be viewed as static electricitybetween proton in nucleus and electron. Electron distribution model can be explained via quantum mechanics. However, for a heavy atom (e.g. Mercury; Hg) many electrons exist. There are not only the interactions between protons and electrons but also the electron-electron interaction. Hence, the calculation of electron distribution is likely to be complicated. For the ground state of a complex atom, electron distribution can somehow be proposed by Thomas-Fermi model.

Thomas-Fermi model can be written in the form of dimensionless ordinary differential equations (ODE); $y'' = \frac{y^{3/2}}{x^{1/2}}$ which has been called "Thomas-Fermi equation". This equation is in the form of nonlinear ODE, which is not easy to solve. Several methods have been used to find the solution, one of them is mathematical technique called "Modified Adomian Decomposition Method (MADM), incorporating Padé approximants". The solution of this method has the form of polynomials, and infinite series after being operated by Padé approximants.

Motivated by Thomas-Fermi model, we would like to study it and build mathematical technique to describe electron distribution of a heavy atom. We compare Thomas-Fermi solution with Thomas-Fermi equation solution by the Differential Analyzer [1]. Mercury atom is chosen because its data are available for comparison [1, 3].

Review methods for Thomas-Fermi model

There are several methods for solving the Thomas-Fermi model. Some of them [1,11,12,13,14] require a huge size of computational work. Chan and Hon [15] used the monotone method and Green's function for calculating the solution of Thomas-Fermi equation, but using another set of boundary conditions. However, Hon [16] improves the calculations of Chan and Hon [15] by using the modification of Adomian decomposition method made by Cherruault [17] combined with Green's function, but Green's function is not always easy to find. The work of Venkatarangan [18] provided improvements over other methods; a transformation formula was used to encounter the difficulty caused by the nonlinearly of the radical power. In the work of Venkatarangan [18], the accuracy level in the initial slope was not enhanced, compared to other methods because only few terms of the approximation were derived [5]. In Pathria [2], the solution of Thomas-Fermi equation is in asymptotic form. So, electron distribution given by this solution was similar to electron distribution solution from Differential Analyzer [1, 3] in asymptotic condition.

Thus, in this work, we use the "Modified Adomian Decomposition Method (MADM) incorporated with Padé approximants" for solving Thomas-Fermi equation (see Chapter III).

Review methods for Adomian Polynomials

The Modified Adomian Decomposition Method (MADM) can be computed in a recursive way for a linear function. However, a nonlinear term can be expressed by infinite series of the so-called "Adomian Polynomials; $A_n = A_n(y_0, y_1, \cdots, y_n)$". The original methods proposed by Adomian [19] can generate Adomian Polynomials of form

$$A_0 = f(y_0)$$

$$A_1 = y_1 \frac{df(y_0)}{dy_0}$$

$$A_2 = y_2 \frac{df(y_0)}{dy_0} + \frac{y_1^2}{2!} \frac{d^2 f(y_0)}{dy_0^2}$$

$$A_3 = y_3 \frac{df(y_0)}{dy_0} + y_1 y_2 \frac{d^2 f(y_0)}{dy_0^2} + \frac{y_1^3}{3!}\frac{d^3 f(y_0)}{dy_0^3}$$

$$\vdots$$

$$A_n = \sum_{\nu=1}^{n} c(\nu,n) f^{(\nu)}(y_0); n \geq 1.$$

For example, if $f(y) = y^2$, we will have $A_0 = y_0^2$, $A_1 = 2y_0 y_1$, $A_2 = y_1^2 + 2y_0 y_2$, $A_3 = 2y_1 y_2 + 2y_0 y_3, \cdots$. Note that in this scheme, the sum of the subscripts in each term of the A_n is equal to n. The $c(\nu,n)$ are products (or the sum of products) of ν component of y whose subscripts sum to n, divided by the factorial of the number of repeat subscripts. Therefore, $c(1,3) = y_3$, $c(2,3) = y_1 y_2$, and $c(3,3) = (1/3!) y_1^3$. In some works [4, 20, 21, 22,23,24], the authors used algorithm for generated A_n by

$$A_n = \frac{1}{n!}\frac{d^n}{d\lambda^n}\left[F\left(\sum_{i=0}^{n} y_i \lambda^i\right)\right]_{\lambda=0}, n = 0,1,2,\cdots.$$

While, Zhu [25] used another algorithm for calculating A_n in the form

$$\left.\frac{\partial^n F\left(\sum_{k=0}^{n} y_k \lambda^k\right)}{\partial \lambda^n}\right|_{\lambda=0} = \left.\frac{\partial^n F\left(\sum_{k=0}^{n} A_k \lambda^k\right)}{\partial \lambda^n}\right|_{\lambda=0}.$$

Both algorithms [4,20,21,22,23,24,25] provided improvement on the Adomian [19]. They used the extraction parameter λ to make program simple by computational calculation. However, the methods presented by those works [4, 20, 21, 22, 23, 24, 25] are difficult to investigate due to human error. For examples, Adomian polynomials order A_5, A_6 and A_9 for nonlinear function e^u are incorrect [24].

Thus, we propose a new algorithm for generating Adomian Polynomials; A_n called "Order-By-Order Extraction Technique (OBOET)" (see Chapter IV).

Purpose of the Study

Applying Modified Adomian decomposition method (MADM) to calculate electron distribution for Mercury atom by Thomas-Fermi equation $y'' = \frac{y^{3/2}}{x^{1/2}}$.

Building new mathematical technique for calculation "Adomian polynomials" called "Order-By-Order Extraction Technique".

Applying Padé approximants to be combined with power series for work calculation, because the solution of Thomas-Fermi equation in practice has truncated series, it has an effect on rapidly divergent solution.

Applying Padé approximants to calculate initial slope of the Thomas-Fermi potential.

Significance of the Study

We may use electron distribution to calculate binding energy of heavier atoms.

We may apply Modified Adomian Decomposition Method (MADM) to solvenonlinear ODEs in other physics problem.

We may use manipulation languages such as Mathematica or other languages in computational physics works.

Scope of the Study

Scope of this work is calculation of electron distribution excluding binding energy. In this work we calculate electron distribution for heavy atoms by applying Thomas-Fermi model. This model is based on quantum statistical mechanics which is applicableto many-electron atoms.