CHAPTER V

RESULTS AND DISCUSSION

In this chapter, we propose the results of the methodology from Chapter III. All of these could be computed by manipulation program (see Appendix C).

Adomian Polynomials for the nonlinear term of Thomas-Fermi equation via OBOET

According to (3.1.6), Adomian polynomials, A_n are generated via Order-By-Order Extraction Technique (OBOET).

From the previous chapter where $F(y)=y^{3/2};y=\sum_{k=0}^{p}y_k\lambda^k$,we can rewrite $F(y)$ in the form

$$F(y)\equiv F(y(\lambda))=y_0^{3/2}\left(1+\frac{3w}{2}+\frac{3w^2}{8}-\frac{w^3}{16}+\cdots\right);w\equiv\frac{1}{y_0}\sum_{k=1}^{p}y_k\lambda^k.$$

Next, consider equation (4.2)

$$\sum_{n=0}^{\infty}A_n\lambda^n\equiv F[y(\lambda)]=F\left(\sum_{n=0}^{\infty}y_n\lambda^n\right).$$

The algorithm for calculating canbe seen in Chapter IV.Theypertain to the Thomas-Fermi equation, which are calculated from A_0 to A_{10} as follows:

$$A_0=1,$$

$$A_1=\frac{3y_1}{2},$$

$$A_2=\frac{3y_1^2}{8}+\frac{3y_2}{2},$$

$$A_3=-\frac{y_1^3}{16}+\frac{3y_1y_2}{4}+\frac{3y_3}{2},$$

$$A_4=\frac{3y_1^4}{128}-\frac{3}{16}y_1^2y_2+\frac{3y_2^2}{8}+\frac{3y_1y_3}{4}+\frac{3y_4}{2},$$

$$A_5=-\frac{3y_1^5}{256}+\frac{3}{32}y_1^3y_2-\frac{3}{16}y_1y_2^2-\frac{3}{16}y_1^2y_3+\frac{3y_2y_3}{4}+\frac{3y_1y_4}{4}+\frac{3y_5}{2},$$

$$A_6=\frac{7y_1^6}{1024}-\frac{15}{256}y_1^4y_2+\frac{9}{64}y_1^2y_2^2-\frac{y_2^3}{16}+\frac{3}{32}y_1^3y_3-\frac{3}{8}y_1y_2y_3+\frac{3y_3^2}{8}-\frac{3}{16}y_1^2y_4+\frac{3y_2y_4}{4}$$
$$+\frac{3y_1y_5}{4}+\frac{3y_6}{2},$$

$$A_7=-\frac{9y_1^7}{2048}+\frac{21}{512}y_1^5y_2-\frac{15}{128}y_1^3y_2^2+\frac{3}{32}y_1y_2^3-\frac{15}{256}y_1^4y_3+\frac{9}{32}y_1^2y_2y_3-\frac{3}{16}y_2^2y_3$$
$$-\frac{3}{16}y_1y_3^2+\frac{3}{32}y_1^3y_4-\frac{3}{8}y_1y_2y_4+\frac{3y_3y_4}{4}-\frac{3}{16}y_1^2y_5+\frac{3y_2y_5}{4}+\frac{3y_1y_6}{4}+\frac{3y_7}{2},$$

$$A_8=\frac{99y_1^8}{32768}-\frac{63y_1^6y_2}{2048}+\frac{105y_1^4y_2^2}{1024}-\frac{15}{128}y_1^2y_2^3+\frac{3y_2^4}{128}+\frac{21}{512}y_1^5y_3-\frac{15}{64}y_1^3y_2y_3+\frac{9}{32}y_1y_2^2y_3$$
$$+\frac{9}{64}y_1^2y_3^2-\frac{3}{16}y_2y_3^2-\frac{15}{256}y_1^4y_4+\frac{9}{32}y_1^2y_2y_4-\frac{3}{16}y_2^2y_4-\frac{3}{8}y_1y_3y_4+\frac{3y_4^2}{8}+\frac{3}{32}y_1^3y_5$$
$$-\frac{3}{8}y_1y_2y_5+\frac{3y_3y_5}{4}-\frac{3}{16}y_1^2y_6+\frac{3y_2y_6}{4}+\frac{3y_1y_7}{4}+\frac{3y_8}{2},$$

$$A_9=-\frac{143y_1^9}{65536}+\frac{99y_1^7y_2}{4096}-\frac{189y_1^5y_2^2}{2048}+\frac{35}{256}y_1^3y_2^3-\frac{15}{256}y_1y_2^4-\frac{63y_1^6y_3}{2048}+\frac{105}{512}y_1^4y_2y_3$$
$$-\frac{45}{128}y_1^2y_2^2y_3+\frac{3}{32}y_2^3y_3-\frac{15}{128}y_1^3y_3^2+\frac{9}{32}y_1y_2y_3^2-\frac{y_3^3}{16}+\frac{21}{512}y_1^5y_4-\frac{15}{64}y_1^3y_2y_4+\frac{9}{32}y_1y_2^2y_4$$
$$+\frac{9}{32}y_1^2y_3y_4-\frac{3}{8}y_2y_3y_4-\frac{3}{16}y_1y_4^2-\frac{15}{256}y_1^4y_5+\frac{9}{32}y_1^2y_2y_5-\frac{3}{16}y_2^2y_5-\frac{3}{8}y_1y_3y_5+\frac{3y_4y_5}{4}$$
$$+\frac{3}{32}y_1^3y_6-\frac{3}{8}y_1y_2y_6+\frac{3y_3y_6}{4}-\frac{3}{16}y_1^2y_7+\frac{3y_2y_7}{4}+\frac{3y_1y_8}{4}+\frac{3y_9}{2},$$

$$A_{10}=\frac{429y_1^{10}}{262144}-\frac{1287y_1^8y_2}{65536}+\frac{693y_1^6y_2^2}{8192}-\frac{315y_1^4y_2^3}{2048}+\frac{105y_1^2y_2^4}{1024}-\frac{3y_2^5}{256}+\frac{99y_1^7y_3}{4096}$$
$$-\frac{189y_1^5y_2y_3}{1024}+\frac{105}{256}y_1^3y_2^2y_3-\frac{15}{64}y_1y_2^3y_3+\frac{105y_1^4y_3^2}{1024}-\frac{45}{128}y_1^2y_2y_3^2+\frac{9}{64}y_2^2y_3^2+\frac{3}{32}y_1y_3^3$$
$$-\frac{63y_1^6y_4}{2048}+\frac{105}{512}y_1^4y_2y_4-\frac{45}{128}y_1^2y_2^2y_4+\frac{3}{32}y_2^3y_4-\frac{15}{64}y_1^3y_3y_4+\frac{9}{16}y_1y_2y_3y_4-\frac{3}{16}y_3^2y_4$$
$$+\frac{9}{64}y_1^2y_4^2-\frac{3}{16}y_2y_4^2+\frac{21}{512}y_1^5y_5-\frac{15}{64}y_1^3y_2y_5+\frac{9}{32}y_1y_2^2y_5+\frac{9}{32}y_1^2y_3y_5-\frac{3}{8}y_2y_3y_5$$
$$-\frac{3}{8}y_1y_4y_5+\frac{3y_5^2}{8}-\frac{15}{256}y_1^4y_6+\frac{9}{32}y_1^2y_2y_6-\frac{3}{16}y_2^2y_6-\frac{3}{8}y_1y_3y_6+\frac{3y_4y_6}{4}+\frac{3}{32}y_1^3y_7$$
$$-\frac{3}{8}y_1y_2y_7+\frac{3y_3y_7}{4}-\frac{3}{16}y_1^2y_8+\frac{3y_2y_8}{4}+\frac{3y_1y_9}{4}+\frac{3y_{10}}{2}.$$

Thomas-Fermi equation solved by MADM via OBOET

After obtaining A_0 to A_{10} from the previous section, we show the detailed derivation of equations (3.1.8-10). The modified recursive relations for components $y_0(x)$ to $y_{11}(x)$ in equation (3.1.8) have the form

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

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

$$y_0(x) = 1,$$
$$y_1(x) = Bx + \frac{4x^{3/2}}{3},$$
$$y_2(x) = \frac{2}{5}Bx^{5/2} + \frac{x^3}{3},$$
$$y_3(x) = \frac{3}{70}B^2x^{7/2} + \frac{2Bx^4}{15} + \frac{2x^{9/2}}{27},$$
$$y_4(x) = -\frac{1}{252}B^3x^{9/2} + \frac{B^2x^5}{175} + \frac{31Bx^{11/2}}{1485} + \frac{4x^6}{405},$$
$$y_5(x) = \frac{B^4x^{11/2}}{1056} + \frac{4B^3x^6}{1575} + \frac{557B^2x^{13/2}}{100100} + \frac{4Bx^7}{693} + \frac{101x^{15/2}}{52650},$$
$$y_6(x) = -\frac{3B^5x^{13/2}}{9152} - \frac{29B^4x^7}{24255} - \frac{623B^3x^{15/2}}{351000} - \frac{46B^2x^8}{45045} - \frac{113Bx^{17/2}}{1178100} + \frac{23x^9}{473850},$$
$$y_7(x) = \frac{7B^6x^{15/2}}{49920} + \frac{68B^5x^8}{105105} + \frac{153173B^4x^{17/2}}{116424000} + \frac{1046B^3x^9}{675675} + \frac{799399B^2x^{19/2}}{698377680}$$
$$+ \frac{51356Bx^{10}}{103378275} + \frac{35953x^{21/2}}{378132300},$$
$$y_8(x) = -\frac{3B^7x^{17/2}}{43520} - \frac{4B^6x^9}{10395} - \frac{1232941B^5x^{19/2}}{1278076800} - \frac{99856B^4x^{10}}{70945875} - \frac{33232663B^3x^{21/2}}{25881055200}$$
$$- \frac{250054B^2x^{11}}{342953325} - \frac{22773977Bx^{23/2}}{95108013000} - \frac{823x^{12}}{23108085},$$
$$y_9(x) = \frac{99B^8x^{19/2}}{2646016} + \frac{256B^7x^{10}}{1044225} + \frac{705965027B^6x^{21/2}}{966226060800} + \frac{43468B^5x^{11}}{33622875} + \frac{1861464749B^4x^{23/2}}{1253187936000}$$
$$+ \frac{27134428B^3x^{12}}{23880381525} + \frac{17319117797B^2x^{25/2}}{30580884180000} + \frac{494880923Bx^{13}}{2936459901375} + \frac{172159489x^{27/2}}{7487019540000},$$

$$y_{10}(x) = -\frac{143B^9x^{21/2}}{6537216} - \frac{6272B^8x^{11}}{38105925} - \frac{4524629159B^7x^{23/2}}{7953566100480} - \frac{14756758B^6x^{12}}{12455257815}$$
$$-\frac{2383837819589B^5x^{25/2}}{1455090436800000} - \frac{96201013897B^4x^{13}}{61665657928875} - \frac{308663609101B^3x^{27/2}}{301554110088000}$$
$$-\frac{303011686294B^2x^{14}}{678322237217625} - \frac{1487118494129Bx^{29/2}}{12613018163803200} - \frac{50500903x^{15}}{3509540409375},$$
$$y_{11}(x) = \frac{143B^{10}x^{23/2}}{10551296} + \frac{2048B^9x^{12}}{17782765} + \frac{144926432597B^8x^{25/2}}{319825938432000} + \frac{3474669398B^7x^{13}}{3197478559275}$$
$$+\frac{50468746588277B^6x^{27/2}}{28696914005760000} + \frac{8824737028748B^5x^{14}}{4396533019003125} + \frac{605561615787857B^4x^{29/2}}{369981866138227200}$$
$$+\frac{3016967993986B^3x^{15}}{3201870700153125} + \frac{31823185257584653B^2x^{31/2}}{86728773867896160000} + \frac{15076074226306Bx^{16}}{172443607708246875}$$
$$+\frac{3220476338281x^{33/2}}{331899576208200000}.$$

After that, we sum the previous components to obtain equation (3.1.9)

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

Then, we have the solution of Thomas-Fermi equation solved by MADM via OBOET in term of $y(x)$;

$$y(x) = 1 + Bx + \frac{4x^{3/2}}{3} + \frac{2}{5}Bx^{5/2} + \frac{x^3}{3} + \frac{3}{70}B^2x^{7/2} + \frac{2Bx^4}{15} + \frac{2x^{9/2}}{27} - \frac{1}{252}B^3x^{9/2} + \frac{B^2x^5}{175}$$
$$+\frac{31Bx^{11/2}}{1485} + \frac{B^4x^{11/2}}{1056} + \frac{4x^6}{405} + \frac{4B^3x^6}{1575} + \frac{557B^2x^{13/2}}{100100} - \frac{3B^5x^{13/2}}{9152} + \frac{4Bx^7}{693} - \frac{29B^4x^7}{24255}$$
$$+\frac{101x^{15/2}}{52650} - \frac{623B^3x^{15/2}}{351000} + \frac{7B^6x^{15/2}}{49920} - \frac{46B^2x^8}{45045} + \frac{68B^5x^8}{105105} - \frac{113Bx^{17/2}}{1178100} + \frac{153173B^4x^{17/2}}{116424000}$$
$$-\frac{3B^7x^{17/2}}{43520} + \frac{23x^9}{473850} + \frac{1046B^3x^9}{675675} - \frac{4B^6x^9}{10395} + \frac{799399B^2x^{19/2}}{698377680} - \frac{1232941B^5x^{19/2}}{1278076800}$$
$$+\frac{99B^8x^{19/2}}{2646016} + \frac{51356Bx^{10}}{103378275} - \frac{99856B^4x^{10}}{70945875} + \frac{256B^7x^{10}}{1044225} + \frac{35953x^{21/2}}{378132300} - \frac{33232663B^3x^{21/2}}{25881055200}$$
$$+\frac{705965027B^6x^{21/2}}{966226060800} - \frac{143B^9x^{21/2}}{6537216} - \frac{250054B^2x^{11}}{342953325} + \frac{43468B^5x^{11}}{33622875} - \frac{6272B^8x^{11}}{38105925}$$
$$-\frac{22773977Bx^{23/2}}{95108013000} + \frac{1861464749B^4x^{23/2}}{1253187936000} - \frac{4524629159B^7x^{23/2}}{7953566100480} + \frac{143B^{10}x^{23/2}}{10551296}$$

$$-\frac{823x^{12}}{23108085}+\frac{27134428B^{3}x^{12}}{23880381525}-\frac{14756758B^{6}x^{12}}{12455257815}+\frac{2048B^{9}x^{12}}{17782765}+\frac{17319117797B^{2}x^{25/2}}{30580884180000}$$
$$-\frac{2383837819589B^{5}x^{25/2}}{1455090436800000}+\frac{144926432597B^{8}x^{25/2}}{319825938432000}+\frac{494880923Bx^{13}}{2936459901375}$$
$$-\frac{96201013897B^{4}x^{13}}{61665657928875}+\frac{3474669398B^{7}x^{13}}{3197478559275}+\frac{172159489x^{27/2}}{7487019540000}-\frac{308663609101B^{3}x^{27/2}}{301554110088000}$$
$$+\frac{50468746588277B^{6}x^{27/2}}{28696914005760000}-\frac{303011686294B^{2}x^{14}}{678322237217625}+\frac{8824737028748B^{5}x^{14}}{4396533019003125}$$
$$-\frac{1487118494129Bx^{29/2}}{12613018163803200}+\frac{605561615787857B^{4}x^{29/2}}{369981866138227200}-\frac{50500903x^{15}}{3509540409375}$$
$$+\frac{3016967993986B^{3}x^{15}}{3201870700153125}+\frac{31823185257584653B^{2}x^{31/2}}{86728773867896160000}+\frac{15076074226306Bx^{16}}{172443607708246875}$$
$$+\frac{3220476338281x^{33/2}}{331899576208200000}.$$

The initial slope for each Padé approximants order [n/n]

After considering the solution $y(x)$ from the previous section, we find it diverges rapidly when x is not small. Thus, we will use Padé approximants to solve this problem. However, the previous solution $y(x)$ is in an inappropriate form. Hence, we will set $x^{1/2}=t$ and transform the solutions of (3.1.9) into the appropriate form (3.1.10) of

$$y(t)=\sum_{n=0}^{11}y_n(t),$$

Thus, we have the solution of Thomas-Fermi equation solved by MADM via OBOET in term of $y(t)$;

$$
\begin{aligned}
y(t) &= 1 + Bt^2 + \frac{4t^3}{3} + \frac{2Bt^5}{5} + \frac{t^6}{3} + \frac{3B^2t^7}{70} + \frac{2Bt^8}{15} + (\frac{2}{27} - \frac{B^3}{252})t^9 + \frac{B^2t^{10}}{175} \\
&+(\frac{31B}{1485} + \frac{B^4}{1056})t^{11} + (\frac{4}{405} + \frac{4B^3}{1575})t^{12} + (\frac{557B^2}{100100} - \frac{3B^5}{9152})t^{13} + (\frac{4B}{693} - \frac{29B^4}{24255})t^{14} \\
&+(\frac{101}{52650} - \frac{623B^3}{351000} + \frac{7B^6}{49920})t^{15} + (-\frac{46B^2}{45045} + \frac{68B^5}{105105})t^{16} \\
&+(-\frac{113B}{1178100} + \frac{153173B^4}{116424000} - \frac{3B^7}{43520})t^{17} + (\frac{23}{473850} + \frac{1046B^3}{675675} - \frac{4B^6}{10395})t^{18} \\
&+(\frac{799399B^2}{698377680} - \frac{1232941B^5}{1278076800} + \frac{99B^8}{2646016})t^{19} + (\frac{51356B}{103378275} - \frac{99856B^4}{70945875} + \frac{256B^7}{1044225})t^{20} \\
&+(\frac{35953}{378132300} - \frac{33232663B^3}{25881055200} + \frac{705965027B^6}{966226060800} - \frac{143B^9}{6537216})t^{21} \\
&+(-\frac{250054B^2}{342953325} + \frac{43468B^5}{33622875} - \frac{6272B^8}{38105925})t^{22} \\
&+(-\frac{22773977B}{95108013000} + \frac{1861464749B^4}{1253187936000} - \frac{4524629159B^7}{7953566100480} + \frac{143B^{10}}{10551296})t^{23} \\
&+(-\frac{823}{23108085} + \frac{27134428B^3}{23880381525} - \frac{14756758B^6}{12455257815} + \frac{2048B^9}{17782765})t^{24} \\
&+(\frac{17319117797B^2}{30580884180000} - \frac{2383837819589B^5}{1455090436800000} + \frac{144926432597B^8}{319825938432000})t^{25} \\
&+(\frac{494880923B}{2936459901375} - \frac{96201013897B^4}{61665657928875} + \frac{3474669398B^7}{3197478559275})t^{26} \\
&+(\frac{172159489}{7487019540000} - \frac{308663609101B^3}{301554110088000} + \frac{50468746588277B^6}{28696914005760000})t^{27} \\
&+(-\frac{303011686294B^2}{678322237217625} + \frac{8824737028748B^5}{4396533019003125})t^{28} \\
&+(-\frac{1487118494129B}{12613018163803200} + \frac{605561615787857B^4}{369981866138227200})t^{29} \\
&+(-\frac{50500903}{3509540409375} + \frac{3016967993986B^3}{3201870700153125})t^{30} + \frac{31823185257584653B^2t^{31}}{86728773867896160000} \\
&+\frac{15076074226306Bt^{32}}{172443607708246875} + \frac{3220476338281t^{33}}{331899576208200000}.
\end{aligned}
$$

These solutions $y(t)$ can be taken into Padé approximants for converging the solution to generate the initial slope $B = y'(0)$. Several values of the initial slope for each Padé approximants order are shown in Table 1.

Table 1 Several values of initial slope $B = y'(0)$ calculated by Padé approximants

Padé approximants	$B = y'(0)$	Error(%) of $y'(0)$, (compare Kobayashi)
[2/2]	-1.211413729	23.7179
[4/4]	-1.550525919	2.36419
[7/7]	-1.586021035	0.129085
[8/8]	-1.588076820	0.00036651
[10/10]	-1.588069657	0.0000845376

From Table 1, we can see that the initial slope of high order [10/10] is the nearest result compared with Kobayashi's initial slope [7]. Then, the initial slope is used to converge the solution of Thomas-Fermi equation. The solutions for each order [n/n] will be shown in the next section.

The solutions of Thomas-Fermi equation for each order [n/n]

The solutions of Thomas-Fermi equation due to MADM via OBOET, MADM via OBOET incorporated Padé approximants orders [4/4], [7/7], and [10/10] are compared with the solution of Thomas-Fermi equation obtained by the Differential Analyzer [1] as shown in Figure 5.

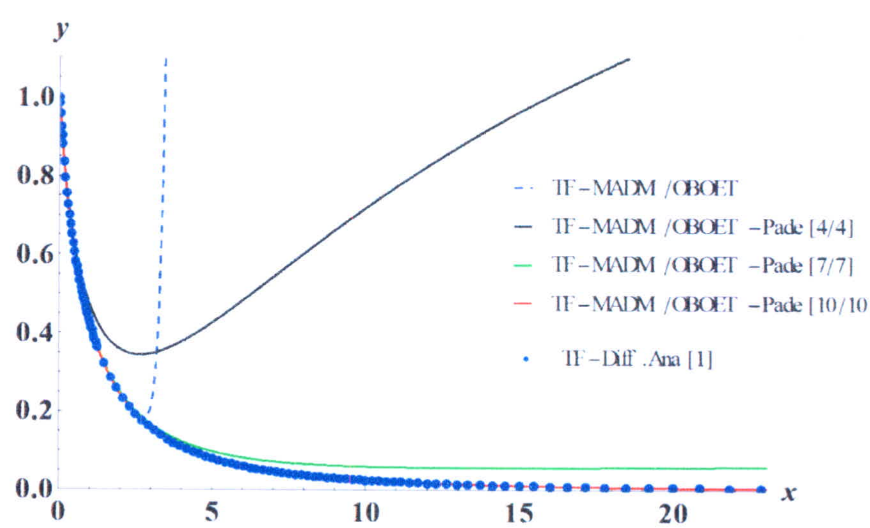

Figure 5 Comparison of solutions of Thomas-Fermi equation obtained by the Differential Analyzer [1], MADM via OBOET, MADM via OBOET incorporated Padé approximants orders [4/4], [7/7], and [10/10]

From Figure 5, the solution of MADM via OBOET is consistent with the solution of Differential Analyzer when x is small ($x \leq 2.7$) because for a small value of x, the high order term in equation 3.1.9 can be neglected. On the other hand, for a high value of x, the high order term in equation 3.1.9 are dominant. For this reason, the graph of MADM via OBOET diverges rapidly when x is large. So the solution of MADM via OBOET can be improved by increasing number of terms in the summation of equation 3.1.9.

The solution of Padé approximants orders [4/4] is consistent with the solution of Differential Analyzer when x is small (x<1) and then diverges from the solution of Differential Analyzer when x is sufficiently large. However, the solution of MADM via OBOET diverges more rapidly than solution of Padé approximants orders [4/4].

The solution of Padé approximants orders [7/7] is better than the solution of Padé approximants orders [4/4] because the former solution contains number of terms more than the latter solution. Moreover, initial slope of the former solution is more accurate than the latter solution, compared with the result of Kobayashi [7]. However, the former solution does not converge to zero when $x \to \infty$, while the standard solution [1] converge to zero when $x \to \infty$.

The solution of Padé approximants orders [10/10] is the best; it is consistent with for the standard solution [1] for all values of x and converges to zero when $x \to \infty$. The disadvantage of Padé approximants orders [10/10] is that we cannot calculate the solution with package programs because it contains too many numbers of terms to be calculated. (Our computer specification is Intel(R) (64 bit) Core i5-3570 CPU @ 3.40 GHz and 16.0 GB of RAM). Hence, we write the program specifically for computing the solution of Padé approximants [10/10] (see Appendix C).

The results of electron distribution for Mercury atom

In this section, we plot electron distribution for Mercury atom. Figure 6 shows electron distributions for MADM via OBOET, MADM via OBOET incorporated Padé approximants orders [4/4], [7/7], and [10/10].They are compared with the solution of electron distribution obtained by the Differential Analyzer [1, 3]

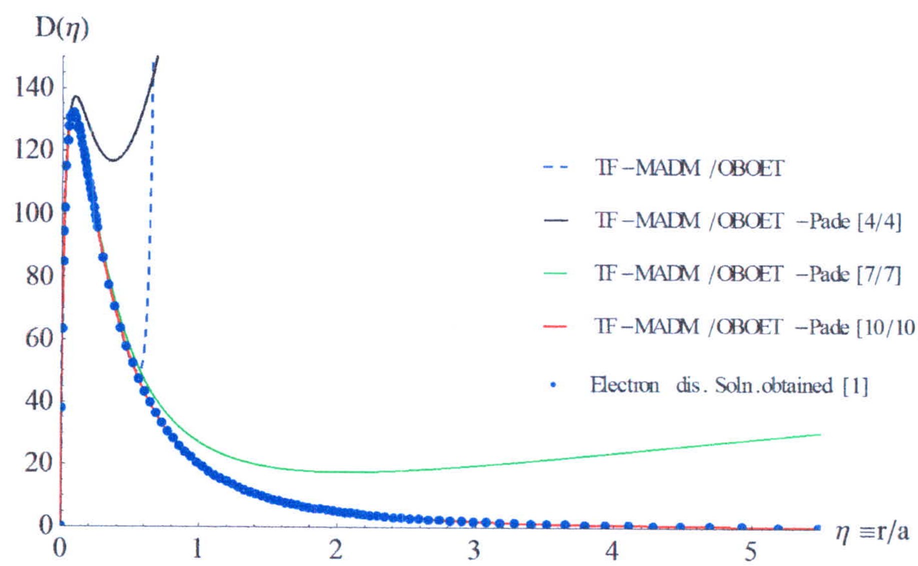

Figure 6 Electron distributions obtained by the Differential Analyzer [1, 3], MADM via OBOET, MADM via OBOET incorporated Padé approximants orders [4/4], [7/7], and [10/10]

Similar to Figure 5, electron distributions due to MADM via OBOET, MADM via OBOET incorporated Padé approximants orders [4/4], and [7/7] in Figure 6 are consistent with the distribution due to Differential Analyzer [1,3] when x is sufficiently small. While, the distribution due to Padé approximants orders [10/10] is likely to agree with the standard solution [1, 3] everywhere.

After considering electron distribution of Padé approximants orders [10/10] which is the electron distribution in the ground state, we find that electrons distribute densely at the length $r \approx 0.08a_B$ (a_B is the Bohr radius), which is very close to the nucleus. This is because electrons are influenced by the nucleus of the heavy atom.

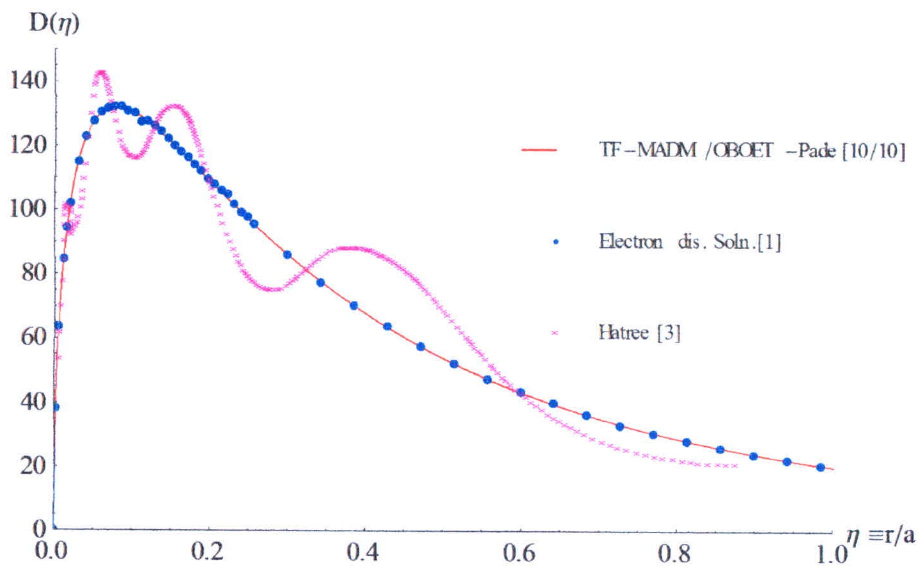

Figure 7 Comparison of the electron distributions of an atom of mercury; using MADM via OBOET incorporated Padé approximants orders [10/10], the Differential Analyzer [1], and Hatree [3]

Figure 7 shows electron distributions for an atom of mercury, using MADM via OBOET incorporated Padé approximants orders [10/10], the Differential Analyzer [1], and Hatree [3]. We can see that the result of MADM via OBOET incorporated Padé approximants orders [10/10] and that due to the Differential Analyzer [1] have the same tendency as the result due to Hatree [3]. Hence, those two results are likely to be the average electron distribution of Hatree [3].