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Approximate Variational Solutions of the Thomas-Fermi Equation Using Exponential Functions

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ABSTRACT. The variational method is used to obtain an approximate solution to the Thomas-Fermi equation. Group of exponential functions are used in attempt to improve the desired results. This method eliminates the shortcomings of the exact solution, such as the behaviour of the electronic density far away and close to the nucleus. Also it enables us to use the Thomas-Fermi equation to treat the negative ions. The method has been tested by calculating the diamagnetic susceptibilities of the neutral atoms and the ions and comparing them with the experimental values and the Thomas-Fermi results.

The Thomas-Fermi model (Thomas 1926 and Fermi 1928) for atoms is a crude approximation to the N-electron Schrodinger equation. It is useful for obtaining effective potentials which can be used as initial potential in the self-consistent field method. This model is described by a nonlinear second order differential equation. However, this model has two major defects: First, the electron density, and therefore the kinetic energy, becomes infinite at the nucleus. Second, at large distances the electron density vanishes as $1/r^6$ instead of the exponential decay of the exact density. These shortcomings can be eliminated if the Thomas-Fermi equation is replaced by an equivalent variational treatment (Csavinszky 1968 and 1973). In the original (TF) theory the density of positive ions abruptly drops to zero after a finite radius. The use of the variational method eliminates this discontinuity. So, the negative ions can be treated as well as the neutral atoms and the positive ions. This method has been implemented by Csavinszky 1976 and 1979 and by Csavinszky and Morrow (1981) and leads to significant corrections to the results which obtained from the (TF) theory.

In this work we selected a group of trial functions as approximate solutions to the (TF) equation. These functions satisfy the exponential behavior of the density at large distances and satisfy the boundary conditions of the (TF) equation. Our results are in better agreement with experimental results compared to those of (TF). Three different trial functions have been used and the results show the importance of choosing the trial function. In section II the variational principle is used to obtain an approximate solution to the (TF) equation with three different exponential functions. In this section, neutral atoms, positive ions, and negative ions are examined.

Study Area

1. Neutral atoms

For neutral atom the (TF) equation has the form

$$\frac{d^2\phi(x)}{dx^2} = \frac{\phi(x)^{3/2}}{x^{\frac{1}{2}}} \tag{1}$$

The electron density n(r) within the atom is related to $\phi(x)$ by

$$n(r) = \frac{Z}{4\pi b^3}\left[\frac{\phi(x)}{x}\right]^{3/2} \tag{2}$$

The dimensionless measure x of the distance r from the nucleus is defined by

$$r = bx = \frac{1}{4}\left[\frac{9\pi^2}{2Z}\right]^{1/3} x = (0.88534/Z^{1/3}) \cdot x(a.u) \tag{3}$$

and the solution $\phi(x)$ is satisfying the boundary conditions

$$\phi(0) = 1,\ \phi(\infty) = 0, \text{ and } \phi'(\infty) = 0 \tag{4}$$

with the usual normalization condition

$$\int n(r)dv = N \tag{5}$$

where N is the number of electrons.

Since the exact solution of Eqn. (1) gives, at large distances from the nucleus, an electron density with the radial dependence $1/r^6$, while its behavior must be exponential, we have used a trial function yielding an approximate solution to equation (1) and insuring the exponential behavior. The form of this function is

$$\phi(x) = [a.e^{-\beta x} + b.e^{-\gamma x} + \cdots]^m, \quad m=1,2,.. \tag{6}$$

where, a, b, β, and γ are parameters to be determined such that $\phi(x)$ satisfies equation (1) under the boundary conditions, (4), and the normalization condition, (5). To determine the parameters we make use of the variational principle (Goldstein 1965)

$$J(\phi) = \int F(\phi,\phi', x)dx \tag{7}$$

where

$$F = \frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 + \frac{2}{5}\left(\frac{\phi^{2/5}}{x^{\frac{1}{2}}}\right) \tag{8}$$

Equation (7) is equivalent to Eqn. (1) when we substitute Eqn. (8) in Euler-Lagrange equation

$$\frac{\delta F}{\delta \phi} - \frac{d}{dx}\left(\frac{\delta F}{\delta \phi'}\right) = 0 \tag{9}$$

with the condition

$$a + b + \cdots = 1 \tag{10}$$

and the normalization condition. Equation (7) should be minimized with respect to the parameters a, b, β, and γ.

In this work we have used $\phi(x)$ of equation (6) with three values for the power m. The reason for this is to find out how important is the choice of the function. The difficulties in the calculations have restricted us to small values of m. We have used three values m=1,2,4. Using $\phi(x)$ given in equation (6), we have calculated $F(\phi,\phi',x)$ and then evaluated the integral in equation (7). Using the notations

$$J(\phi) = J(a,n) = J_1(a,n) + J_2(a,n)$$

where

$$J_1(a,n) = \frac{1}{2} \int (\phi'_m)^2 dx \tag{11}$$

and

$$J_2(a,n) = \frac{2}{5} \int \phi_m^{2/5} / x^{1/2} dx \tag{12}$$

where

$$n = \beta/\gamma \tag{13}$$

Furthermore, the extremalization should be carried out subject to the normalization condition (5).

For m=1 we have obtained

$$J_1(a,n) = \frac{1}{2} \beta \left[a^2 + n(1-a)^2 + \frac{na(1-a)}{1+n}\right], \tag{14}$$

$$J_2(a,n) = \frac{\sqrt{\pi}}{\sqrt{\beta}} \left[0.1012a^{5/2} + \frac{5a^{3/2}b}{2(1.5+n)^{\frac{1}{2}}} + \frac{15a^{\frac{1}{2}}b^2}{8(\frac{1}{2}+2n)^{\frac{1}{2}}} + \right.$$

$$\left. \frac{15a^{-\frac{1}{2}}b^3}{48(3n-\frac{1}{2})^{\frac{1}{2}}}\right] \tag{15}$$

The normalization condition gives

$$\beta = 0.922635 \left\{\frac{Z}{N}\left[\left(\frac{2}{3}a\right)^{3/2} + \frac{3a^{\frac{1}{2}}b}{2(\frac{1}{2}+n)^{3/2}} + \frac{3a^{-\frac{1}{2}}b^2}{8(2n-\frac{1}{2})^{3/2}}\right]\right\}^{2/3} \tag{16}$$

For m = 2:

$$J_1(a,n) = \beta\left[\frac{1}{2}a^4 + 4a^3(1-a)\left(\frac{1+n}{3+n}\right) + a^2(1-a)^2\left(\frac{1+4n+n^2}{1+n}\right) + 4a(1-a)^3\right.$$

$$\left.\left(\frac{n+n^2}{1+3n}\right) + \frac{1}{2}(1-a)^4 n\right] \tag{17}$$

and

$$J_2\ (a,n) = \frac{2\sqrt{\pi}}{\sqrt{\beta}}\left\{\frac{a^5}{5^{3/2}} + \frac{a^4(1-a)}{(4+n)^{\frac{1}{2}}} + \frac{2a^3(1-a)^2}{(3+2n)^{\frac{1}{2}}} + \right.$$

$$\left.\frac{2a^2(1-a)^3}{(2+3n)^{\frac{1}{2}}} + \frac{a(1-a)^4}{(1+4n)^{\frac{1}{2}}} + \frac{(1-a)^5}{5(5n)^{\frac{1}{2}}}\right\} \tag{18}$$

and the normalization condition gives

$$\beta = .922635\left\{\frac{Z}{N}\left\{\frac{a^3}{3^{3/2}} + \frac{3a^2(1-a)}{(2+n)^{3/2}} + \frac{3a(1-a)^2}{(1+2n)^{3/2}} + \frac{(1-a)^2}{(3n)^{3/2}}\right\}\right\}^{2/3} \tag{19}$$

For m = 4:

$$J_1\ (a,n) = \beta\left\{a^8 + \frac{16a^7(1-a)(3+n)}{7+n} + \frac{4a^6(1-a)^2(15+12n+n^2)}{3+n} + \right.$$

$$\frac{16a^5(1-a)^3(10+15n+3n^2)}{5+3n} + \frac{10a^4(1-a)^4(3+8n+3n^2)}{1+n} +$$

$$\frac{16a^3(1-a)^5(3+15n+10n^2)}{3+5n} + \frac{4a^2(1-a)^6(1+12n+15n^2)}{1+3n} +$$

$$\left.\frac{16a(1-a)^7(1+3n)}{1+7n} + n(1-a)^8\right\} \tag{20}$$

and

$$J_2\ (a,n) = \frac{4\sqrt{\pi}}{\sqrt{\beta}}\left\{\frac{a^{10}}{10^{\frac{1}{2}}} + \frac{10a^9(1-a)}{(9+n)^{\frac{1}{2}}} + \frac{45a^8(1-a)^2}{(8+2n)^{\frac{1}{2}}} + \right.$$

$$\frac{120a^7(1-a)^3}{(7+3n)^{\frac{1}{2}}} + \frac{210a^6(1-a)^4}{(6+4n)^{\frac{1}{2}}} + \frac{252a^5(1-a)^5}{(5+5n)^{\frac{1}{2}}} + \frac{210a^4(1-a)^6}{(4+6n)^{\frac{1}{2}}} +$$

$$\left.\frac{120a^3(1-a)^7}{(3+7n)^{\frac{1}{2}}} + \frac{45a^2(1-a)^8}{(2+8n)^{\frac{1}{2}}} + \frac{10a(1-a)^9}{(1+9n)^{\frac{1}{2}}} + \frac{(1-a)^{10}}{(10n)^{\frac{1}{2}}}\right\} \tag{21}$$

and the normalization condition gives

$$\beta = 0.922635 \left\{ \frac{a^6}{6^{1.5}} + \frac{6a^5(1-a)}{(5+n)^{1.5}} + \frac{15a^4(1-a)^2}{(4+2n)^{1.5}} + \frac{20a^3(1-a)^3}{(3+3n)^{1.5}} + \right.$$

$$\left. \frac{15a^2(1-a)^4}{(2+4n)^{1.5}} + \frac{6a(1-a)^5}{(1+5n)^{1.5}} + \frac{(1-a)^6}{(6n)^{1.5}} \right\}^{2/3} \tag{22}$$

In equations 16,19 and 22 we see that β is a function of the parameters a and n. We also have N/Z=1 for a neutral atoms. The substitution for β in equation (6) leaves $J(\phi)$ with only two parameters, a and n. Now J(a,n) can be minimized with respect to the parameters a and n. The minimum of J(a,n) is reached when the parameters have the values listed in Table 1, where we used Eqns. (10) and (13) to obtain b and γ.

To test our approximated function, $\phi(x)$, with the different values of the parameters some of the properties of the neutral atom such as the total energy needed for complete ionization of an atom and its diamagnetic susceptibility, have been considered. The total energy is given by the relation (March 1975):

$$E = .4840748Z^{7/3} \left[\phi'(0) + \left(1 - \frac{N}{Z}\right)^2 / x_o\right] \tag{23}$$

where, for neutral atoms the second term in parenthesis vanishes.

Since the expectation value of the squared distance provides a sensitive test of the density at large r (Englert and Schwinger 1984), we have calculated the expectation values for some atoms and use the results to calculate the diamagnetic susceptibility by

$$\langle r^2 \rangle = 4\pi \int r^4 n(r) dr \tag{24}$$

and

$$X_m = -[1/137]^2 N_A a_o^3 I = 4.752 \times 10^{-6} I, \tag{25}$$

where, the constants are in atomic units, and

$$I = \frac{\langle r^2 \rangle}{6} \tag{26}$$

Table (2) contains the results for the total ionization energy obtained from Eqn. (23) together with (TF) and the experimental results for a group of species hanging in mass from very light to very heavy atoms. The Table shows that the present approximations give ionization energies much better than those obtained from the original (TF) equation. One can say that up to medium weight atoms m=2 gives very good agreement with experimental results. However, for very heavy atoms (Hg and U) m=1 seems to do a better job.

From Table 3 it is clear that as the atomic weight gets progressively larger, a choice of higher value of m gives better agreement with experiment. This can be physically understood since a higher value of m leads to a slower change of the density for heavy atoms.

The variation in our predictions for values of m used is within 15%, where its very little for energies but larger for the other properties, this can be seen from Tables 1 and 3.

2. Positive Ions

For positive ions we have used the same procedures employed for neutral atoms except that the nuclear charges are not equal to the number of electrons. So, for each ion we have different parameters. When 1-N/Z becomes close to zero the parameters will have values close to that of neutral atoms, (Eqns. (11)-(13)). The values of the parameters for various positive ions are listed in Tables 5 and 6. These were used to obtain $<r^2>$ and the diamagnetic susceptibility, X_m. These results are listed in Tables 7 and 8.

3. Negative ions

According to Fermi-Amaldi (FA) correction (Gombas 1949) we have for a singly negative ion

$$n(r) = \frac{Z}{4\pi b^{*3}} \cdot \frac{N}{(N-1)} \left(\frac{\phi(x)}{x}\right)^{3/2} \tag{27}$$

where x is defined by

$$x = r/b^* \tag{28}$$

r stands for the distance from the nucleus and b^* is a constant defined by

$$b^* = \frac{N}{N-1} \cdot b^{2/3} = \left(\frac{N}{N-1}\right) \cdot (.92202)/Z^{2/9} \tag{29}$$

The normalization condition is

$$\int n(r)r^2dr = N \tag{30}$$

from Eqns. (19) and (22) we get

$$\int \left(\frac{\phi}{x}\right)^{3/2} \cdot x^2dx = \frac{(N-1)}{Z} = 1 \tag{31}$$

for singly charged negative ions.

To compare our variational method with the (FA) approximation we followed the same procedure employed for neutral atoms except we have different parameters for each ion. These parameters are listed in Table 9, keeping in mind the fact that since ϕ is exponentially varying, then n(r) is not zero for $r > r_0$. These parameters were used in equations (24) and (25) to predict $<r^2>$ and X_m which are shown in Table 10. Our results for X_m are better than those of (FA) approximation.

Table 1. The values of the parameters of equation (6) for neutral atoms with three different values of the power m

m	a	b	β	γ
1	0.96202	0.03798	0.59199	22.12869368
2	0.721834	0.2781663	0.1782559	1.759339
4	0.8416	0.1584	0.086951	1.4967917

Table 2. Comparison of total ionization energies (in atomic units) of this investigation, TF, and experiment

	m=1	m=2	m=4	TF	Experiment
H	.6825	.5984	.6009	.769	.5
He	3.43968	3.01565	3.0285	3.875	2.904
Be	17.3344	15.1984	15.2623	19.53	14.68
C	44.6482	39.1441	39.3108	50.3	37.86
Ne	147.0452	128.918	129.4671	165.7	129.5
Kr	2920.7211	2560.6639	2571.57	3291	2704
Hg	18821.788	16501.499	16571.7873	21210	18680
U	26078.895	22863.972	22961.3623	29380	25520

Table 3. Predictions of $\langle r^2 \rangle$ by the present investigation compared with TF and the experimental results for neutral atoms

Z	m=1	m=2	m=4	TF	Experiment
Ne 10	8.0484	19.0611	19.7097	84.596	8.5101
Ar 18	9.7904	23.1867	23.9756	102.2727	24.7475
Kr 36	12.3351	29.2135	30.20732	128.7879	36.3636
Xe 54	14.1202	33.4411	34.5788	147.7273	55.4293
Rn 86	16.4895	39.0524	40.3811	172.6	

Table 4. Diamagnetic susceptibilities per gram atom (in units of 1×10^{-6} cm^3) of atoms as listed by experiment, TF, and the present investigation

Z	m=1	m=2	m=4	TF	Experiment
Ne 10	− 6.3743	−15.0964	−15.6101	− 67.0	− 6.74
Ar 18	− 7.754	−18.364	−18.9887	− 81.0	−19.9
Kr 36	− 9.7694	−23.1371	−23.9242	−102.0	−28.8
Xe 54	−11.1832	−26.4854	−27.3864	−117.8	−43.9
Rn 86	−13.0597	−30.9295	−31.9818	−136.0	−

Table 5. Values of the parameters a, b, β, and γ for various positive ions using equation (6) where the power m=2 is used

N	Z	a	b	β	γ
	10	.769986	.230014	.21283	2.030143
9	11	.81	.190	.2464357	2.3360138
	12	.8437	.1563	.2789749	2.69216386
	18	.74865	.25135	.1967869	1.9016933
17	19	.7727	.2273	.2149545	2.048495
	20	.7955	.2045	.2331893	2.2195195
	36	.7333	.2667	.1866592	1.811042
35	37	.7473	.2527	.1960273	1.893017
	38	.7591	.2409	.2048064	1.960878
	54	.7305	.2695	.1841882	1.80075
53	55	.7389	.2611	.1900242	1.8462411
	56	.7476	.2524	.1960653	1.8952068

Table 6. Values of the parameters a, b, β, and γ for various positive ions using equation (6) where the power m=4 is used

N	Z	a	b	β	γ
	10	.8729	.1271	.1050074	1.772734
9	11	.8979	.1021	.1224892	2.090756
	12	.9160992	.08391	.1384998	2.40569
	18	.859	.141	.0965563	1.6374394
17	19	.87429	.12571	.1059858	1.7847
	20	.888	.112	.11528	1.94752
	36	.8506	.1494	.09173039	1.565462
35	37	.8587	.1413	.09632938	1.6361738
	38	.867	.133	.1011448	1.7130895
	54	.8484	.1516	.0903216	1.553351
53	55	.8541	.1458	.09346809	1.597407
	56	.859	.141	.096381	1.64040173

Table 7. Predictions of $<r^2>$ and X_m of some positive ions by the present work using the parameters of table 5

N	Z	$<r^2>$	X_m
	10	12.42126	− 9.8364
9	11	8.920126	− 7.06474
	12	6.7116283	− 5.31561
	18	18.2848	−14.48156
17	19	15.01489	−11.89179
	20	12.52024	− 9.91603
	36	26.06456	−20.64313
35	37	23.44039	−18.56479
	38	21.25604	−16.83478
	54	30.90217	−24.47452
53	55	28.84	−22.84232
	56	26.92594	−21.32534

Table 8. Predictions of $<r^2>$ and X_m of some positive ions by the present work using the parameters of table 6

N	Z	$<r^2>$	X_m
	10	12.65193	−
9	11	9.00292	− 7.13513
	12	6.80847	− 5.39231
	18	18.77062	−14.866331
17	19	15.31427	−12.1289
	20	12.72657	−10.07944
	36	26.69451	−21.14205
35	37	24.013	−19.01829
	38	21.62301	−17.12543
	54	31.76018	−25.15406
53	55	29.49731	−23.36187
	56	27.57393	−21.83855

Table 9. Predictions of the diamagnetic susceptibilities of some singly charged negative ions using the FA approximation

(Z,N)	m=1	m=2	m=4	Experiment
(9,10)	− 7.8696	−18.6375	−19.27171	−11
(17,18)	− 8.69310	−20.5879	−21.2883	−26
(35,36)	−10.33563	−24.4781	−25.311	−36

Table 10. The parameters a, b, β, and γ for singly charged negative ions using equation (6) with m=4

(Z,N)	a	b	β	γ
(9,10)	.8078	.1922	.0707100	1.288216
(17,18)	.8237	.1763	.0779184	1.3802689
(35,36)	.833	.167	.0824699	1.43863
(53,54)	.83583	.1642	.0839393	1.4571444
(92,93)	.838	.162	.0851077	1.47155589

Table 11. Predictions of $<r^2>$ and X_m of some negative ions by the present work using the parameters of table 9

(Z,N)	$<r^2>$	X_-	X_m(exp)
(9,10)	30.63506	−24.262966	−11
(17,18)	30.33775	−24.0275	−26
(35,36)	33.83173	−26.79473	−36
(53,54)	37.2684	−29.51656	−52
(92,93)	43.33985	−34.3252	−−

Table 12. The parameters a, b, β, and γ for singly charged negative ions using equation (6) with m=2

(Z,N)	a	b	β	γ
(9,10)	.6692	.3308	.146198	1.534492
(17,18)	.6935	.3065	.1604401	1.631034
(35,36)	.708	.292	.1694133	1.692269
(53,54)	.713	.287	.172469	1.717412
(92,93)	.7167	.2833	.1749019	1.7342926

Table 13. Predictions of $<r^2>$ and X_m of some negative ions by the present work using the parameters of table 11

(Z,N)	$< r^2>$	X_m	X_m(exp)
(9,10)	29.333	−23.2317	−11
(17,18)	29.1814	−23.112	−26
(35,36)	32.6427	−25.853	−36
(53,54)	35.95662	−28.47764	−52
(92,93)	41.787	−33.0953	−−

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حلول تقريبية ذات متغير لمعادلة توماس ـ فيرمي باستخدام بعض الدّوال الأسية

عويش حربي مبارك

قسم الفيزياء ـ كلية العلوم ـ جامعة الملك عبدالعزيز
ص. ب: ٩٠٢٨ ـ جدة ٢١٤١٣ ـ المملكة العربية السعودية

يعد حل تـوماس ـ فـيرمي التقريبي لمعـادلة شرودنجـر حلاً غـير دقيق ولكنه مفيد للحصول عـلى جهود تقـريبية تمثـل الجهد الأولي المستخـدم في طريقـة الحل الذاتي المتساوي للمجال (Self - Consistent Field Mothed) .

وهذا التمثيل عبارة عن حل لمعادلة من الدرجة الثانية ولهـا عيبين رئيسيـين، أولهما أن للكثافة قيمة غير معروفة عند مركز الذرة وثانيهما أنه عند مسافـات بعيدة عن النـواة تنتهي الكثافـة على الشكـل $1/r^6$ بدلاً من التخـامد الأسي الـذي يصف الكثافة الفعلية .

هذه العيوب يمكن تفاديها إذا استعيض عن معادلة تـوماس ـ فـيرمي بمعادلـة مكافئة تعتمد على تغير الثوابت .

ومن العيوب الظاهرة لنظريـة تومـاس ـ فيرمي الأصليـة أن كثافـة الأيونـات المـوجبة تؤول إلى الصفـر عند مسـافة محـددة، كذلـك لا يمكن استخدامهـا عنـد التعـامل مـع الأيونـات السالبـة وباستخـدام الطريقـة المكافئـة فإن هـذه العيوب تختفي . وبإجراء الحسـابات العـادية نجـد كذلـك تحسن واضح في النتـائج عنـد المقارنة بين هذه الطريقة والطريقة الأصلية .

وفي هـذا البحث قمنا بـاختيار مجمـوعـة دوال تحـوي متغـيرات تحـدد قيمهـا باستخدام قاعدة المتغيرات والتي تحدد على أساس الحصول على أقـل قيمة للطاقـة (Ground State Energy) .

واشترطنا في هذه الدوال تحقيق شرطين أساسيين أولهما تحقيق الشرط الأسي للكثافة عند مسافات كبيرة، وثانيهما تحقيق الشروط الحدية لمعادلة توماس ـ فيرمي الأصلية. وقد اخترنا ثلاث دوال أسية تحقق الشرطين السابقين وتحقّق سهولة الحسابات. ولاحظنا أن النتائج جميعها أفضل من النتائج المستخرجة من النظرية الأصلية. ولكن الفرق بين النتائج المستخرجة من هذه الدوّال ليس كبيراً والفرق في حدود ١٥ ٪ عند دراسة خصائص العناصر المختلفة. أما الطاقة فإن الاختلاف صغيرٌ جداً.

في الفصل الثاني استخدمنا نظرية المتغير (Variation Principle) للحصول على الحل التقريبي لنظرية توماس ـ فيرمي.

وقمنا بتحديد الثوابت التي تعطي أقل قيمة للطاقة، هذه الثوابت رصدت في الجدول ١ للذرات المتعادلة وفي الجدولين ٥ و ٦ للأيونات الموجبة وفي الجدول ٩ للأيونات السالبة. وباستخدام هذه الثوابت استنتجنا الطاقة الكلية لمجموعة من العناصر المتعادلة (جدول ٢). كذلك درسنا متوسط مربع نصف القطر (r^2) لمجموعة الذرات والأيونات (الجداول ٣ و ٧ و ١١) التي منها استنتجنا خاصية التأثر لثنائي القطب المغناطيسي. وفي كل الأحوال تمت المقارنة بين نتائج هذا العمل ونتائج التجربة والنظرية الأصلية.

كذلك لاحظنا أن هناك ثوابت وحيدة لكافة الذرات المتعادلة. أما الأيونات فإن لكل أيون ثوابته الخاصة وكل هذه الثوابت لها جداولها الخاصة.