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AN INTERMEDIATE SOLUTION BETWEEN CSAVINSZKY'S AND KESARWANI-VARSHNI'S TRIAL DENSITY FUNCTIONS

Mario D. Glossman, María C. Donnamaría* and Eduardo A. Castro

INIFTA, División Química Teórica
Suc.4, C.C.16, 1900 La Plata/ ARGENTINA

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*To whom any correspondence should be addressed

ABSTRACT : An approximate variational solution of the Thomas-Fermi equation for atoms is proposed in order to obtain some atomic properties like total ionization energy of atoms and diamagnetic susceptibilities. The results obtained by the suggested function describe the behaviour of medium atomic number elements, while those ones from Csavinzky's and Kesarwani- Varshni's are better for light and heavy atoms respectively.

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I. INTRODUCTION

The statistical theory of the atom /1,2/ is very useful in dealing with a lot of physical problems where a more fundamental quantum mechanical approach is not feasible. Historically, the density functional formalism initiated with the idea that locally the behaviour of a collection of particles, the electron cloud , could be represented and approximated by that of a free electron gas of the same density at that point. The Thomas-Fermi (TF) model /3,4/ was in many aspects very successful and showed the basic stepts to obtain the density functional for the total energy,that is to say by using standard quantum mechanics based on wave functions it is easy to find out,from a well- defined model, a direct relationship between the total energy and the electronic density. The TF theory ,providing a differential equation for the self-consistent determination of the charge density,stands as an appropriate procedure for the study of a system instead of using the associated wave function /5/ to carry it.out. Recently, there has been renewed interest in the approximate analytical solution of the TF equation. One of these solutions has been obtained by making use of an equivalent variational principle /6/, on the other hand, it has been rigurously justified /7/.

Csavinszky /8/ has proposed the trial function :

$$\phi_1 = (a_o e^{-\alpha_o x} + b_o e^{-\beta_o x})^2 \tag{1}$$

where

$a_o = 0.7218337$, $\alpha_o = 0.1782559$

$b_o = 0.2781663$, $\beta_o = 1.759339$

while Kesarwani and Varshni /9/ have suggested :

$$\phi_2 = (a\, e^{-\alpha x} + b e^{-\beta x} + c e^{-\gamma x})^2 \tag{2}$$

where

$a = 0.52495$, $\alpha = 0.12062$

$b = 0.43505$, $\beta = 0.84795$

$c = 0.04$, $\gamma = 6.7469$

When they are used to calculate some atomic properties, the function of Csavinszky is more suitable for light elements, while that one of Kesarwani and Varshni's is more adecuate for high atomic number elements .

It is the aim of the present paper to present an intermediate variational solution of the TF equation which gives better results for properties of medium-atomic-number atoms. A comparison among the three trial density functions is then made.

II. THEORY

II.1. It is a shortcoming of the TF theory of the atom that it leads to a radial electron density which decreases in the same way as the inverse fourth power of the distance from the nucleus does, whereas the Hartree approximation , its quantum mechanical equivalent, gives an exponential decrease. The drawback mentioned above can be eliminated by making use of the flexibility in imposing boundary conditions when the TF equation is replaced by an equivalent variational principle.

The TF differential equation for a neutral atom is

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

x being a dimensionless variable defined by :

$$x = 4(2Z/ 9\pi^2)^{1/3}(r/a_B) \qquad (4)$$

r is the distance from the nucleus, in units of the Bohr radius a_B, and Z is the atomic number . Equation (3) has to be solved subjected to the boundary conditions

$$\phi(0) = 1, \ \phi(\infty) = 0 \ , \ \phi'(\infty) = 0 \qquad (5)$$

and the subsidiary normalization condition

$$\int \rho \, dv = N \qquad (6)$$

N is the electron number, dv is the volume element , and ρ is the electron density, which is related to the screening function ϕ by

$$\rho = Z(\phi/x)^{3/2}/4\mu^3 \tag{7}$$

with

$$\mu = (9\pi^2/2Z)^{1/3} a_B/4$$

Choosing

$$F(\phi,\phi';x) = (d\phi/dx)^2/2 + (2/5)\,\phi^{5/2}\,x^{-1/2} \tag{8}$$

in conjuntion with the variational principle

$$L(\phi) = \int_0^{\infty} F\,dx \tag{9}$$

is the equivalent of equation (3) since substitution of equation (9) for the Euler Lagrange equation (10)

$$\frac{d}{dx}\left(\frac{\partial F}{\partial \phi'}\right) - \frac{\partial F}{\partial \phi} = 0 \tag{10}$$

results in the TF equation .

We must now select a trial density function ϕ_3 which satisfies the boundary conditions in equation (5). So, we are going to choose a form which allows computational simplicity in connection with the integral in equation (9). The proposed trial is as follows

$$\phi_3 = \left(ae^{-\alpha x} + be^{-\beta x} + ce^{-\gamma x} \left(1 - e^{-\delta x}\right) \right)^2 \qquad (11)$$

$a, b, c, \alpha, \beta, \gamma$ and δ are unspecified variational parameters . In order to satisfy equation (5), it is neccessary to fulfil the relationship :

$$a + b = 1 \qquad (12)$$

with equation (11) it is possible to calculate F in equation (8) and then to evaluate the integral in equation (9). The resulting expression is then extremalized as regards those parameters subjected to the subsidiary condition that the electron density must be normalized. It is important that the electron density be normalized when one calculates specific physical quantities for a neutral atom on the basis of approximate solutions of the TF equation .

It is convenient to write L as :

$$L = L_1 + L_2 \qquad (13)$$

with

$$L_1 = \int_0^\infty \frac{1}{2} \left(\frac{d\phi}{dx}\right)^2 dx \qquad (14)$$

and

$$L_2 = \int_0^\infty \frac{2}{5} \phi^{5/2} x^{-1/2} dx \qquad (15)$$

All integrals involved in equations (6), (14) and (15) can be evaluated analytically. Details of calculations are given in the Appendix. The results can be summarized as follows :

$$a = 0.70110 \qquad \alpha = 0.17029321$$
$$b = 0.29890 \qquad \beta = 1.6041808$$
$$c = -0.00243 \qquad \delta = 31.67791$$
$$\gamma = 1.3180541$$

II. 2. To test the validity of the approximate TF function of equation (11) some atomic properties are calculated, such as the ionization energy of several neutral atoms and the diamagnetic susceptibility of noble gas atoms. The energy neccessary to remove all electrons of an atom is calculated within the TF formalism by the expression /1/ :

$$E = (12/7)(2/9\pi^2)^{1/3}\ \phi'(0)\ Z^{7/3}(e^2/a_B) \tag{16}$$

The susceptibility is given as follows /1/:

$$\chi = -L\ (\ e_0{}^2/6m_0c^2)\ \langle r_0{}^2\rangle \tag{17}$$

where L is the Avogadro's number, m_0 is the electron mass and c is the speed of light, while for a spherically symmetric electron distribution

$$\langle r_0{}^2\rangle = \pi\, 4\int_0^{\infty}\rho\, r^4 dr \tag{18}$$

Using equation (11) we find :

$$\langle r_o^2\rangle = (15/8)\,\pi^{1/2}\mu^2 Z\Big[a^3(3\alpha)^{-7/2} + 3a^2b\,(2\alpha+\beta)^{-7/2} + 3ab^2(\alpha+2\beta)^{-7/2} + b^3(3\beta)^{-7/2} + 3a^2c\big[(2\alpha+\gamma)^{-7/2} - (2\alpha+\gamma+\delta)^{-7/2}\big] + 6abc\big[(\alpha+\beta+\gamma)^{-7/2} - (\alpha+\beta+\gamma+\delta)^{-7/2}\big] + 3b^2c\big[(2\beta+\gamma)^{-7/2} - (2\beta+\gamma+\delta)^{-7/2}\big] + 3ac^2\big[(\alpha+2\gamma)^{-7/2} - 2(\alpha+2\gamma+\delta)^{-7/2} + (\alpha+2\gamma+2\delta)^{-7/2}\big] + 3bc^2\big[(\beta+2\gamma)^{-7/2} - 2(\beta+2\gamma+\delta)^{-7/2} + (\beta+2\gamma+2\delta)^{-7/2}\big] + c^3\big[(3\gamma)^{-7/2} - 3(3\gamma+\delta)^{-7/2} + 3(3\gamma+2\delta)^{-7/2} - (3\gamma+3\delta)^{-7/2}\big]\Big] \qquad (19)$$

III. DISCUSSION

In order to compare the approximate solution of the TF equation with the exact solution, the ratio of these quantities as a function of x is listed in Table I. Due to the fact that the proposed trial function has an exponential behaviour, the largest deviation occurs only at large x values.

The ionization energy ,from equation (16), for several atoms is listed in Table II. For the sake of comparison, the same property calculated through equation (1) and equation (2) are shown together with the standard values obtained from an experimental way or from Hartree-Fock theoretical data /11/. It is evident that for light elements Csavinszky's approximation is convenient, for medium Z elements our formalism is better than the other approaches, while for high Z elements Kesarwani-Varshni's results are the best as regards Hartree-Fock calculations.

The diamagnetic susceptibilities for the noble gas atoms, Ne, Ar, Kr, Xe and Rn have been calculated from equations (17)-(19). In Table III the results are compared with those ones obtained by numerical TF approach /1/, by Kesarwani-Varshni's and Csavinszky's trial density functions and by experimental form /12/. The present procedure represents a significant improvement over the original TF theory, since the latter greatly overestimates the magnitude of diamagnetic susceptibilities. This is attributed to the fact that the radial TF electron density goes to zero in the same way as the inverse fourth power of the distance from the nucleus does. This behaviour is seen through the integral in equation (18) over $\langle r_o^2 \rangle$ and hence χ comes out to be too large. In spite of this wrong situation, the present solution gives good results for medium Z element diamagnetic susceptibilities.

To conclude with, we have found that for medium Z elements, the suggested trial density function ,equation (11), gives a more satisfactory approximation to the exact solution ϕ than those from Csavinszky's and Kesarwani-Varshni's.

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IV. APPENDIX

Substituting equation (8) into equation (9) and then introducing the notation

$$L = L_1 + L_2 \tag{A 1}$$

$$L_1 = \frac{1}{2}\left(\frac{d\phi}{dx}\right)^2 dx \tag{A 2}$$

$$L_2 = \frac{2}{5}\,\phi^{5/2}\,x^{-1/2}dx \tag{A 3}$$

and using

$$\theta = \gamma + \delta \tag{A 4}$$

a straightforward evaluation of the integrals leads to :

$$L_1 = 0.5\Bigg[a^4\frac{\alpha}{2} + b^4\frac{\beta}{2} + (ab)^2(\alpha+\beta) + (ac)^2(\alpha+\gamma) + (ac)^2(\alpha+\theta)$$

$$+(bc)^2(\beta+\gamma) + (bc)^2(\beta+\theta) + c^4\frac{\gamma}{2} + c^2(\theta+\gamma) + c^4\frac{\theta}{2}$$

$$+\frac{4a^3b\,\alpha(\alpha+\beta)}{3\alpha+\beta} + 4a^3c\left[\alpha\frac{(\alpha+\gamma)}{3\alpha+\gamma} - \frac{(\alpha+\theta)}{3\alpha+\theta}\right] + \frac{2(ab)^2\alpha\beta}{\alpha+\beta}$$

$$+4a^2bc\left[\frac{\beta+\gamma}{2\alpha+\beta+\gamma} - \frac{\beta+\theta}{2\alpha+\beta+\theta}\right]\alpha + 2(ac)^2\frac{\alpha\gamma}{(\alpha+\gamma)}$$

$$-4(ac)^2\left[\frac{\alpha(\theta+\gamma)}{(2\alpha+\theta+\gamma)}\right] + 2(ac)^2\frac{\alpha\theta}{\alpha+\theta} + 4a^2bc\frac{(\alpha+\beta)(\alpha+\gamma)}{2\alpha+\beta+\gamma}$$

$$- \frac{4a^2bc(\alpha+\beta)(\alpha+\theta)}{2\alpha+\beta+\theta} + \frac{4ab^3\beta(\alpha+\beta)}{\alpha+3\beta} + \frac{4ab^2c(\alpha+\beta)(\beta+\gamma)}{\alpha+2\beta+\gamma}$$

$$- \frac{4ab^2c(\alpha+\beta)(\beta+\theta)}{\alpha+2\beta+\theta} + \frac{4abc^2\gamma(\alpha+\beta)}{\alpha+\beta+2\gamma} - \frac{4abc^2(\alpha+\beta)(\theta+\gamma)}{\alpha+\beta+\gamma+\theta}$$

$$+ \frac{4abc^2\theta(\alpha+\beta)}{\alpha+\beta+2\theta} - \frac{4(ac)^2(\alpha+\gamma)(\alpha+\theta)}{2\alpha+\gamma+\theta} + \frac{4ab^2c\beta(\alpha+\gamma)}{\alpha+2\beta+\gamma}$$

$$+ \frac{4abc^2(\alpha+\gamma)(\beta+\gamma)}{\alpha+\beta+2\gamma} - \frac{4abc^2(\alpha+\gamma)(\beta+\theta)}{\alpha+\beta+\gamma+\theta} + \frac{4ac^3\gamma(\alpha+\gamma)}{\alpha+3\gamma}$$

$$- \frac{4ac^3(\alpha+\gamma)(\theta+\gamma)}{\alpha+\gamma+2\theta} + \frac{4ac^3\theta(\alpha+\theta)}{\alpha+3\theta} - \frac{4ab^2c\beta(\alpha+\theta)}{\alpha+2\beta+\theta}$$

$$- \frac{4abc^2(\beta+\gamma)(\alpha+\theta)}{\alpha+\beta+\gamma+\theta} + \frac{4abc^2(\alpha+\theta)(\beta+\theta)}{\alpha+\beta+2\theta} - \frac{4ac^3\gamma(\alpha+\theta)}{\alpha+\theta+2\gamma}$$

$$+ \frac{4ac^3(\alpha+\theta)(\gamma+\theta)}{\alpha+\gamma+2\theta} - \frac{4ac^3\theta(\alpha+\theta)}{\alpha+3\theta} + \frac{4b^3c\beta(\beta+\gamma)}{3\beta+\gamma}$$

$$- \frac{4b^3c\beta(\beta+\theta)}{3\beta+\theta} + \frac{2(bc)^2\beta\gamma}{\beta+\gamma} - \frac{4(bc)^2\beta(\theta+\gamma)}{2\beta+\theta+\gamma} + \frac{2(bc)^2\beta\theta}{\beta+\theta}$$

$$- \frac{4(bc)^2(\beta+\gamma)(\beta+\theta)}{2\beta+\gamma+\theta} + \frac{4bc^3\gamma(\beta+\gamma)}{2\beta+\theta+\gamma} - \frac{4bc^3(\beta+\gamma)(\theta+\gamma)}{\beta+\theta+2\gamma}$$

$$+ \frac{4bc^3\theta(\beta+\gamma)}{\beta+\gamma+2\theta} - \frac{4bc^3\gamma(\beta+\theta)}{\beta+\theta+2\gamma} + \frac{4bc^3(\beta+\theta)(\theta+\gamma)}{\beta+\gamma+2\theta} - \frac{4bc^3\theta(\beta+\theta)}{\beta+3\theta}$$

$$- \frac{4c^4\gamma(\theta+\gamma)}{\theta+3\gamma} + \frac{2c^4\theta\gamma}{\theta+\gamma} - \frac{4c^4\theta(\theta+\gamma)}{3\theta+\gamma}\Bigg] \qquad (A\ 5)$$

and

$$L_2 = \frac{2\sqrt{\pi}}{5}\left[\frac{a^5}{(5\alpha)^{1/2}} + \frac{5a^4b}{(4\alpha+\beta)^{1/2}} + \frac{10a^3b^2}{(3\alpha+2\beta)^{1/2}} + \frac{10a^2b^3}{(2\alpha+3\beta)^{1/2}}\right.$$

$$+ \frac{5ab^4}{(\alpha+4\beta)^{1/2}} + \frac{b^5}{(5\beta)^{1/2}} + \frac{5a^4c}{(4\alpha+\gamma)^{1/2}} + \frac{20a^3bc}{(3\alpha+\beta+\gamma)^{1/2}}$$

$$+ \frac{30a^2b^2c}{(2\alpha+2\beta+\gamma)^{1/2}} + \frac{20ab^3c}{(\alpha+3\beta+\gamma)^{1/2}} + \frac{5b^4c}{(4\beta+\gamma)^{1/2}} - \frac{5a^4c}{(4\alpha+\theta)^{1/2}}$$

$$- \frac{20a^3bc}{(3\alpha+\beta+\theta)^{1/2}} - \frac{30a^2b^2c}{(2\alpha+2\beta+\theta)^{1/2}} - \frac{20ab^3c}{(\alpha+3\beta+\theta)^{1/2}}$$

$$- \frac{5b^4c}{(4\beta+\theta)^{1/2}} + \frac{10a^3c^2}{(3\alpha+2\gamma)^{1/2}} + \frac{30a^2bc^2}{(2\alpha+\beta+2\gamma)^{1/2}}$$

$$+ \frac{30ab^2c^2}{(\alpha+2\beta+2\gamma)^{1/2}} + \frac{10b^3c^2}{(3\beta+2\gamma)^{1/2}} - \frac{20a^3c^2}{(3\alpha+\gamma+\theta)^{1/2}}$$

$$- \frac{60a^2bc^2}{(2\alpha+\beta+\gamma+\theta)^{1/2}} - \frac{60ab^2c^2}{(\alpha+2\beta+\gamma+\theta)^{1/2}} - \frac{20b^3c^2}{(3\beta+\gamma+\theta)^{1/2}}$$

$$+ \frac{10a^3c^2}{(3\alpha + 2\theta)^{1/2}} + \frac{30a^2bc^2}{(2\alpha+\beta+2\theta)^{1/2}} + \frac{30ab^2c^2}{(\alpha+2\beta+2\theta)^{1/2}}$$

$$+ \frac{10b^3c^2}{(3\beta+2\theta)^{1/2}} + \frac{10a^2c^3}{(2\alpha+3\gamma)^{1/2}} + \frac{20abc^3}{(\alpha+\beta+3\gamma)^{1/2}} + \frac{10b^2c^3}{(2\beta+3\gamma)^{1/2}}$$

$$- \frac{30a^2c^3}{(2\alpha+2\gamma+\theta)^{1/2}} - \frac{60abc^3}{(\alpha+\beta+2\gamma+\theta)^{1/2}} - \frac{30b^2c^3}{(2\beta+2\gamma+\theta)^{1/2}}$$

$$+ \frac{30a^2c^3}{(2\alpha+\gamma+2\theta)^{1/2}} + \frac{60abc^3}{(\alpha+\beta+\gamma+2\theta)^{1/2}} + \frac{30b^2c^3}{(2\beta+\gamma+2\theta)^{1/2}} - \frac{10a^2c^3}{(2\alpha+3\theta)^{1/2}}$$

$$- \frac{20abc^3}{(\alpha+\beta+3\theta)^{1/2}} - \frac{10b^2c^3}{(2\beta+3\theta)^{1/2}} + \frac{5ac^4}{(\alpha+4\gamma)^{1/2}} + \frac{5bc^4}{(\beta+4\gamma)^{1/2}}$$

$$- \frac{20ac^4}{(\alpha+3\gamma+\theta)^{1/2}} - \frac{20bc^4}{(\beta+3\gamma+\theta)^{1/2}} + \frac{30ac^4}{(\alpha+2\gamma+2\theta)^{1/2}} + \frac{30bc^4}{(\beta+2\gamma+2\theta)^{1/2}}$$

$$- \frac{20ac^4}{(\alpha+\gamma+3\theta)^{1/2}} - \frac{20bc^4}{(\beta+\gamma+3\theta)^{1/2}} + \frac{5ac^4}{(\alpha+4\theta)^{1/2}} + \frac{5bc^4}{(\beta+4\theta)^{1/2}}$$

$$+ \frac{c^5}{(5\gamma)^{1/2}} - \frac{5c^5}{(4\gamma+\theta)^{1/2}} + \frac{10c^5}{(3\gamma+2\theta)^{1/2}} - \frac{10c^5}{(2\gamma+3\theta)^{1/2}}$$

$$+ \frac{5c^5}{(\gamma+4\theta)^{1/2}} - \frac{c^5}{(5\theta)^{1/2}} \Bigg] \qquad (16)$$

In order to evaluate the integral of the subsidiary condition, equation (6), equations (11) and (7) are used , then the following expression is obtained

$$\left[\frac{a^3}{(3\alpha)^{3/2}}+\frac{3a^2b}{(2\alpha+\beta)^{3/2}}+\frac{3ab^2}{(\alpha+2\beta)^{3/2}}+\frac{b^3}{(6\beta)^{3/2}}+\frac{3a^2c}{(2\alpha+\gamma)^{3/2}}\right.$$

$$+\frac{6abc}{(\alpha+\beta+\gamma)^{3/2}}+\frac{3b^2c}{(2\beta+\gamma)^{3/2}}-\frac{3a^2c}{(2\alpha+\theta)^{3/2}}-\frac{6abc}{(\alpha+\beta+\theta)^{3/2}}$$

$$-\frac{3b^2c}{(2\beta+\theta)^{3/2}}+\frac{3ac^2}{(\alpha+2\gamma)^{3/2}}-\frac{6ac^2}{(\alpha+\gamma+\theta)^{3/2}}+\frac{3ac^2}{(\alpha+2\theta)^{3/2}}+\frac{3bc^2}{(\beta+2\gamma)^{3/2}}$$

$$-\frac{6bc^2}{(\beta+\gamma+\theta)^{3/2}}+\frac{3bc^2}{(\beta+2\theta)^{3/2}}+\frac{c^3}{(3\gamma)^{3/2}}+\frac{3c^3}{(2\gamma+\theta)^{3/2}}+\frac{3c^3}{(\gamma+2\theta)^{3/2}}$$

$$\left.+\frac{c^3}{(3\theta)^{3/2}}\right]=\frac{2}{\sqrt{\pi}}\frac{N}{Z} \qquad \text{(A 7)}$$

For neutral atoms $(N/Z) = 1$ and, for this reason, the solution of the TF equation remains universal.

To extremalize L in equation (A1) subjected to the subsidiary conditions in equation (A 7), the following procedure is carried out. Some values for α , β , γ and δ are picked at random. Then a value for c is held and modified in order that for each value of c a particular a satisfies equation (A 4). Using the fixed $(\alpha, \beta, \gamma, \delta)$ and the different c and a values, L is calculated. When that value of c is found which makes L a minimum, then it is kept constant and α is varied. This method lowers the magnitude of the minimum. This cycling is repeated with the other parameters β, γ and δ and continued until the minimum of L as a function of a, c, α, β, γ and δ is found. The numerical values are displayed in the text.

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TABLE I

x	ϕ / ϕ_{TF}
0.00	1.000
0.05	1.004
0.10	1.006
0.50	0.994
1.00	0.999
1.20	1.000
1.40	1.023
1.60	1.039
1.80	1.056
2.00	1.073
3.00	1.142
4.00	1.164
5.00	1.137
5.50	1.108
6.00	1.072
6.50	1.018
7.00	0.983
7.50	0.924
8.00	0.881
8.50	0.821
9.00	0.775
9.50	0.717
10.00	0.671
15.00	0.271
20.00	0.094
50.00	0.008

TABLE II

Atom	Z	Eq.(1)	Error %	Eq.(2)	Error %	Eq.(11)	Error %	Standard
He	2	3.016	3.8	3.426	17.9	3.298	13.5	2.905
C	6	39.14	7.3	44.47	17.4	42.80	12.9	37.88
Ne	10	128.9	-0.2	146.4	13.4	140.97	9.2	129.1
Ar	18	508.1	-4.0	577.2	9.0	555.60	4.9	529.4
Ni	28	1424	-6.2	1618	6.5	1557.8	2.6	1519
Kr	36	2861	-8.1	2909	4.4	2800.1	0.5	2786
Pd	46	4537	-9.9	5154	2.3	49610	-1.5	5036
Xe	54	6595	-11.2	7491	0.9	7211.9	-2.9	7427
Hf	72	12905	-13.8	14659	-2.1	14111.5	-5.8	14977
Hg	80	16501	-15.1	18745	-3.5	18044.4	-7.1	19431
Rn	86	19535	-16.0	22191	-4.6	21361.3	-8.1	23253
U	92	22864	-16.9	25972	-5.6	25001.7	-9.1	27506
Fm	100	27774	-18.1	31550	-6.9	30371.4	-10.4	33896

TABLE III

Atom	Z	$\chi_{expt.}$	χ_{TF}	$\chi_{present}$	$\chi_{Csav.}$ #	χ_{K-V} #
Ne	10	-6.74	-67.0	-16.3	-15.1	-24.2
Ar	18	-19.6	-81.0	-19.8	-18.4	-29.4
Kr	36	-28.8	-102.0	-24.9	-23.1	-37.1
Xe	54	-43.9	-117.0	-28.5	-26.5	-42.5
Rn	86	---	-136.7	-33.3	-30.9	-49.6

Csav. : Csavinszky ; K-V : Kesarwani-Varshni

CAPTIONS FOR TABLES

TABLE I RATIO BETWEEN THE PRESENT ϕ AND THAT FROM THE THOMAS -FERMI EXACT SOLUTION

TABLE II COMPARISON OF TOTAL IONIZATION ENERGIES (UNITS OF e^2/a_B)

TABLE III DIAMAGNETIC SUSCEPTIBILITIES PER GRAM ATOM (UNITS OF $10^{-6}cm^3$)