Analysis of Thomas-Fermi Energy Functional Under Two Potentials

C.O. Ogabi
Department of Physics, Lagos State University, Ojo, Lagos, Nigeria
PMB 0001, LASU Post Office, Ojo, Lagos State, Nigeria
Phone Number: 234-08035754124

ABSTRACT— ***In this paper, by constructing Free-energy Functionals, the Thomas-Fermi theory has been extended to include the non-zero temperature effects in many-particle systems. Using the Sobolev-Lieb and the Hőlder inequalities, the constructed Free-energy Functionals were put into a form from which an extended Thomas-Fermi equation was derived. Hitherto, in this work, the two states $\Psi_0(r)$ and $\Psi_1(r)$, corresponding respectively to the square root of two densities $\rho_0(r)$ and $\rho_1(r)$, had been used to construct the new free-energy Functionals $F[\rho_0(r)]$ and $F[\rho_1(r)]$. The states $\Psi_0(r)$ and $\Psi_1(r)$ were required to be mutually orthogonal, and the functional $F[\rho_0(r)]$ was considered as the ground state functional while $F[\rho_1(r)]$ was the excited state functional with temperature ≥ 0. From the functionals, the electron density matrix was derived and finally the total energy was computed for many-electrons system under the influence of the Coulomb and Yukawa Potentials. Various results were obtained and discussed.***

Keywords— Thomas-Fermi theory, Sobolev-Lieb inequality, Density functional method, Free-Energy functional, Functional derivative, Density matrix.

1. INTRODUCTION

1.1 The Thomas-Fermi theory

The theory of Thomas and Fermi, now known as Thomas-Fermi theory provides a functional form for the kinetic energy of a non interacting electron gas in some known external potential $V(r)$(usually due to impurities) as a function of the density. It is a local density functional (LDF) and is based on a semi classical approximation. The formulation becomes exact for a uniform electron gas.

In a uniform system of Fermions of spin $S = 1/2$ in 3 dimensional physical spaces, the Fermi momentum k_F is related to the density $n(r)$ via the following relation:

$$\frac{4\pi}{3}k_F^3/\frac{(2\pi)^3}{\Omega} = \frac{N}{2} \Rightarrow 3\pi^2 n = k_F^3$$

The kinetic energy of the uniform system is given by

$$T = \sum_{k<k_F}\sum_{\sigma}\frac{\hbar^2k^2}{2m} = 2\frac{\Omega}{(2\pi)^3}\int_0^{k_F}4\pi k^2\,dk\,\frac{\hbar^2k^2}{2m} = \frac{\Omega}{\pi^2}\frac{\hbar^2}{10m}k_F^5 \quad (1)$$

The total electron number can be obtained in a similar fashion:

$$N = \sum_{k<k_F}\sum_{\sigma}1 = 2\frac{\Omega}{(2\pi)^3}\int_0^{k_F}4\pi k^2\,dk = \frac{\Omega}{3\pi^2}k_F^3 \quad (2)$$

One can thus calculate the kinetic energy per unit volume or per particle using $3\pi^2 n = k_F^3$ in equation (1) to give:

$$T = \Omega\frac{3}{5}\frac{\hbar^2k_F^2}{2m}n = N\frac{3}{5}\frac{\hbar^2k_F^2}{2m} \quad (3)$$

In a non-uniform system where the density is a function of the position $n(r)$one assumes the same functional form (the semi classical approximation) and thus the Fermi momentum becomes position-dependent:

$$n(r) = \frac{k_F^2(r)}{3\pi^2} \quad (4)$$

and the kinetic energy within TF becomes;

$$T[n] = \int d^3r\,\frac{3}{5}\frac{\pi^2k_F^2(r)}{2m}n(r) \quad (5)$$

The relationship between the external potential and the density is obtained by minimizing the total (here the kinetic plus external) energy with respect to the density with the constraint of constant electron number: subject to the normalization condition $\int n(r)dr = N$;

$$\frac{\delta}{\delta n}\left(T + \int n(r)V(r)d^3r - \mu\int n(r)d^3r\right) = 0$$

In the semi classical approximation, the local Fermi momentum is obtained by solving the above minimization equation:

$$\mu = \frac{\hbar^2 k_F^2(r)}{2m} + V(r) \quad (6)$$

Where the Lagrange multiplier, $\mu = \partial E_{tot}/\partial N$ is identified as the equilibrium chemical potential of the system. This semi classical approximation is valid if the variations in the external potential are weak in the scale of the Fermi wavelength: $|\nabla V(r)|/V(r)| \ll k_F(r)$. See reference, [1, 2]

1.2.Definition:

A function *f* is said to be in L^a if $[\int |f(x)|^a dx]^{1/a} \equiv ||f||_a$ is finite, $1 \le a \le \infty$.
$||f||_\infty \equiv ess\ \sup |f(x)|$. If $f \in L^a \cap L^b$ with $a < b$
then $f \in L^t$ for all $a \le t \le b$. $||f||_t \le ||f||_a^{\lambda} ||f||_b^{1-\lambda}$,
where $\lambda a^{-1} + (1-\lambda)b^{-1} = t^{-1}$.
By Sobolev Inequality, we have:

$$T_\psi \equiv \int |\nabla\psi|^2 dV \ge S\left(\int \rho_\psi^3\, dV\right)^{1/3} \quad (7)$$

where, $\rho_\psi = |\psi|^2$, and *S*, some numerical constant.
[1, 2] using Holder's Inequality,

$$\left(\int |f|^p\right)^{1/p} * \left(\int g^q\right)^{1/q} \ge \int |fg|, \quad \frac{1}{p} + \frac{1}{q} = 1\ and\ p, q > 1 \quad (8)$$

And letting $f = |\psi|^2 = \rho, g = |\psi|^{4/3} = \rho^{2/3}, p = 3, q = 3/2.$ the Sobolev inequality is refined to give a weaker but more useful inequality:

$S(\int \rho^3)^{1/3} * \left(\int \rho^{\left(\frac{2}{3}\right)\left(\frac{3}{2}\right)}\right)^{2/3} \ge \int \rho\rho^{3/2}$ But, $\int \rho = 1$ therefore equation (7) can be written as:

$T_\psi \equiv \int |\nabla\psi|^2 dV \ge S\left(\int \rho_\psi^3\, dV\right)^{1/3} \ge K \int \rho^{5/3} d\,V$, where $K \cong 2.8712$

Using the above inequalities, the kinetic energy density is seen to be proportional $\int \rho^{5/3}\, d^3r$ so that kinetic energy per particle is: see reference [5]

$T_\psi \equiv K \int \rho^{5/3} d^3 r$

For an interacting system, if the form of the interaction potential is known as a function of the ground state density, such as in the density functional theory, one can also add this contribution to the external potential $V(r)$, and solve the non-linear equations again, now with an effective potential $V_{eff} = V + V_H + V_{xc}$;

$$\rho(r) = \frac{1}{3\pi^2\hbar^3}\{2m\left[\mu - V(r) - e^2 \int d^3r' \frac{\rho(r')}{|r-r'|} - V_{xc}[\rho(r)]\right]\}^{3/2} \quad (9)$$

Here, the newly added terms are respectively the Coulomb interaction (Hartree potential) and the exchange-correlation potential seen by an electron. The latter has a simple expression in the local density approximation (LDA) of the density functional theory. Within the Hartree-Fock theory, the exchange energy of the Jellium model was derived as the function of the density. From this functional, it is possible to deduce an exchange-only potential which is obtained by differentiating the exchange energy with respect to ρ. Using this potential in the TF equation above yields the Thomas-Fermi-Dirac equation in a suitable unit:

$$\mu = V(r) + e^2 \int d^3r' \frac{\rho(r')}{|r-r'|} - \alpha\rho(r)^{1/3} + \frac{\hbar^2 k_F^2(r)}{2m} \quad (10)$$

That is, for a given μ and a given external potential, the solution needs to be found iteratively as the equation has become an integral equation.
One can transform the Thomas-Fermi equation into the integral form (10) into a differential form. The function to search for will be the electrostatic potential generated by $\rho(r)$. We introduce this potential as:

$$U(r) = e \int d^3r' \frac{\rho(r')}{|r-r'|}$$

It must satisfy the Poisson equation:

$$\Delta U(r) = -4\pi e\rho(r). \quad (11)$$

From Eq. (9) one extracts the electron density:

$$\rho(r) = -\frac{32\pi^2 e}{3h^3}(2m)^{\frac{3}{2}}[\mu - eV_{ext.}(r) - eU(r)]^{\frac{3}{2}}. \quad (12)$$

This is the Thomas-Fermi equation in differential form.
In summary, we can write the energy functional of Thomas-Fermi as:

$$\mathrm{E}[\rho] = K\int \rho(r)^{5/3} d^3 r - \int V(r)\rho(r) d^3 r + \frac{1}{2}\iint \frac{\rho(r)\rho(r')d^3 r d^3 r'}{|r-r'|} + \mho \qquad (13)$$

In suitable units$(e^2 = 1)$, where: $(r) = \sum_{i=1}^{j} Z_i |r - R_i|^{-1}, \mho = \sum_{1\le s<i\le j} Z_s Z_i |R_s - R_i|^{-1}$

And $K \cong 2.8712$ numerically, the constraint on $\rho(r)$ is $\rho(r) \geq 0$ & $\int \rho(r) d^3 r = 1$ the functional $\rho \to E[\rho]$ is convex.

The justification for this TF functional is this:

- The first term in equation (13) is roughly the minimum quantum-mechanical kinetic energy of *N* electrons needed to produce an electron density$\rho(r)$. The fact that electrons are fermions is crucial here. This minimum energy is, in fact, the semi classical energy and is known to be exact in the limit where the shape of $\rho(r)$ is fixed and *N* goes to ∞ The first term is also conjectured by [3] to be a lower bound to the electronic kinetic energy when the density is $\rho(r)$.
- The second term is the attractive interaction of the *N* electrons with the *K* nuclei, via the Coulomb potential *V*.
- The third term is approximately the electron-electron repulsive energy.
- $\mho$ is the nuclear-nuclear repulsion. While it is a constant, it is an important constant because it determines whether or not binding can occur, i.e., whether or not the energy can be lowered by moving the nuclei far apart from each other.
- The minimum energy is gotten by first taking the functional derivative of equation (13) multiplying the result by $\rho(r)$ and integrate and finally subtracting the output from the same which yields:

$$\mathrm{E}_{min} = -\frac{2K}{3}\int \rho^{5/3} d^3 r - \frac{1}{2}\int U(r)\rho(r) d^3 r \qquad (14)$$

1.3 *The Free Energy Functional*

Consider the foregoing results when the temperature of the system is low, but non-zero.

A thermodynamic system can also be described in terms of *Helmholtz free energy*, *F(T,V,N)*, the energy available for work at temperature θ. It is given by

$$F = U - \theta S, \qquad (15)$$

Where S is the entropy. Like internal energy U, F is a state function, and takes its minimum value under every given constraint..

The minimization of Helmholtz free energy is a very useful principle. *Many features such as phase transitions and formation of complex patterns in equilibrium systems can be analyzed using this principle.* For our purpose, we construct the entropy ***S*** ≡ - ***σ*** and thereby construct the free energy functional; Let $\rho(r, r')/N$ be the density matrix of a system, then the ***entropy*** is defined by (see reference, [4, 6])

$$\sigma = NTr\left(\rho(r,r')\right) In\left(\rho(r,r')\right) \qquad (16)$$

Where

$$Tr\rho(r,r') = \int \rho(r,r) dr = 1$$

Under the approximation

$\rho(r,r') \approx \rho(r,r) \equiv \rho(r)$ We have the entropy functional;

$$\sigma[\rho] = N\int \left(\rho(r,r')\right) In\left(\rho(r,r')\right) dr = -S = N\int \rho(r) In\rho(r) dr \qquad (17)$$

$$S \approx -N\int \rho(r) In\rho(r) dr (\geq 0) \qquad (18)$$

Now at some finite temperature, Let $\rho_o(r)$ be the ground state density and $\rho_1(r)$ the excited density, i.e $\rho(r) = \alpha\rho_o(r) + (1-\alpha)\rho_1(r),\ \alpha \in [0,1]$ the energy functional per particle is

$$\varepsilon[\rho] = k\int \rho(r)^{5/3} dr + \int V(r)\rho(r) dr + \frac{g}{2}\iint \rho(r)\rho(r')V(r-r') d^3 r' d^3 r \qquad (19)$$

Hence the Helmholtz free energy functional per particle is:

$$F[\rho] = \varepsilon[\rho] + \theta\sigma[\rho]\ \ (\equiv U - \theta S) \qquad (20)$$

where *g is the strength of interaction*, and *θ is a measure of temperature*. With the constraint $\int \rho(r) dr = N \leq Z$, we have, to minimize: [7]

$$F[\rho]=k\int\rho(r)^{5/3}dr+\int V(r)\rho(r)dr+\frac{g}{2}\iint\rho(r)\rho(y)V(r-r')d^3r'd^3r+\theta\int\rho(r)In\rho(r)d^3r \quad (21)$$
$$-\theta\int\rho(r)In\rho d^3r+\lambda\left(\int\rho(r)d^3r-1\right)$$

where $\rho(r)=\alpha\rho_o(r)+(1-\alpha)\rho_1(r),\ \alpha\in[0,1]$ and λ is the Lagrange multiplier. This *F[ρ]* is strictly convex and therefore has a unique minimum That is,

$$\frac{\delta F[\rho(r)]}{\delta\rho(r)}=\frac{5k}{3}\rho(r)^{2/3}+V(r)+g\int\rho(r')V(r-r')d^3r'+\theta(In\,\rho(r)+1-In(N))+\lambda=0 \quad (22)$$

Clearly equation (22) has a unique solution; it shall be solved under Coulomb and Yukawa potentials respectively: $V(r)=-Z/|r-r'|$, $V(r)=-Z\exp(-b|r-r'|)/|r-r'|$

2. RESULTS

Equations (11), (12) and (13) were computed together with *Coulomb potential* under the influence of electron-electron repulsive energy (*interaction*) and the following results depicted in figures 1 & 2 were obtained for a very small and very large neutral atom

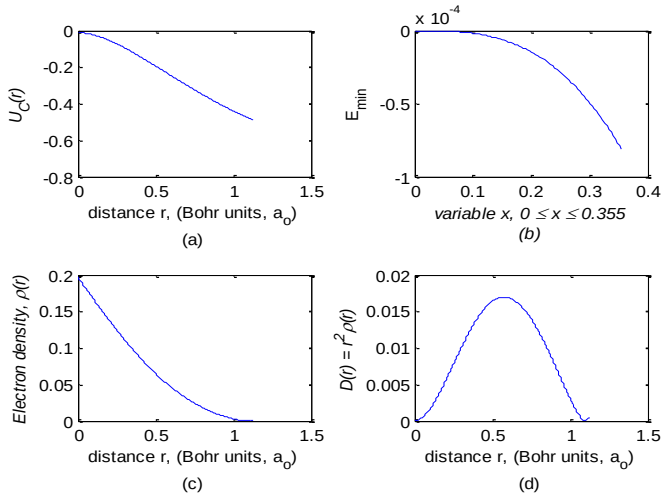

Figure 1, Z=1 Coulomb

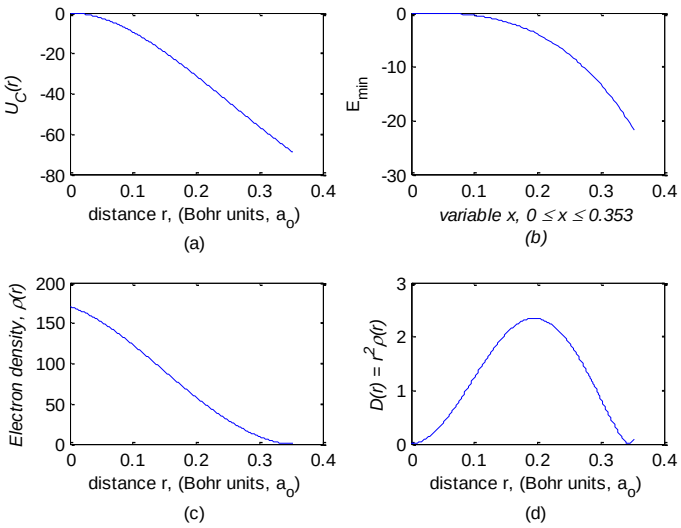

Figure 2 Z = 90 (Th) Coulomb

Figures 1&2: (a) the plot of Coulomb internal potential $U(r) = \int dr' \frac{\rho(r')}{|r-r'|}$ versus radial distance r, (in Bohr units). (b) The plot of minimum energy, $E_{min} \cong \int \rho(r)^{5/3} d^3r + \int U(r)\rho(r) d^3r$ versus parameter/variable x. (c) The plot of electron density, $\rho(r) \cong \{\mu - V_{ext}(r) - U(r)\}^{3/2}$versus radial distance r. (d) the plot of electron distribution $D(r) = r^2\rho(r)$ versus radial distance. Plots 1, (a) to (d) are results of computations under Coulomb potential,$V_{ext}(r) = -Z/r$ with $Z = 1, Hydrogen, (H)$ and Plots 2, (a) to (d) are results for Z = 90, Thorium (Th) likewise.

Similarly, equations (11), (12) and (13) were computed together with *Yukawa potential* under the influence of electron-electron repulsive energy (*interaction*) and the following results depicted in figures 3 & 4 were obtained for a very small and very large neutral atom

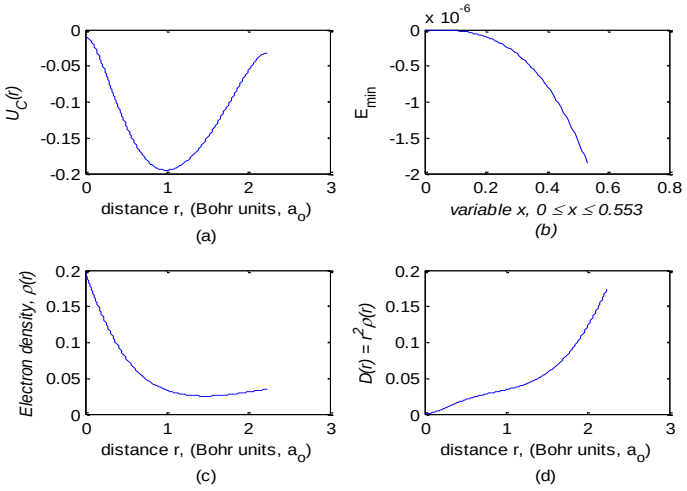

Figure 3 Z = 1, Hydrogen (H) , Yukawa potential

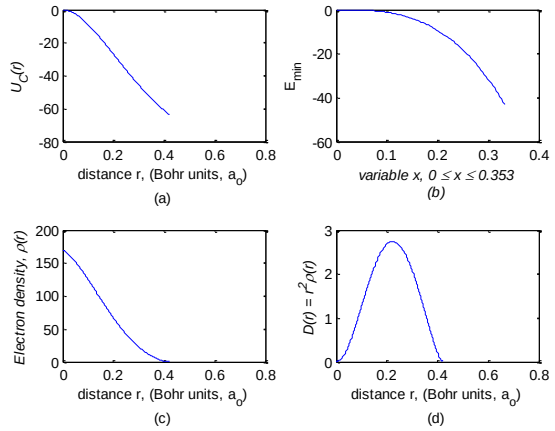

Figure 4 Z = 90, (Th) Yukawa potential

Figures 3&4: (a) the plot of Yukawa internal potential $U(r) = \int dr' \frac{\rho(r')e^{-br}}{|r-r'|}$ versus radial distance r, (in Bohr units). (b) The plot of minimum energy, $E_{min} \cong \int \rho(r)^{5/3} d^3r + \int U(r)\rho(r) d^3r$ versus parameter/variable x. (c) The plot of electron density, $\rho(r) \cong \{\mu - V_{ext}(r) - U(r)\}^{3/2}$versus radial distance r. (d) the plot of electron distribution $D(r) = r^2\rho(r)$ versus radial distance. Plots of figure 3, (a) to (d) are results of computations under Yukawa potential,$V_{ext}(r) = -Ze^{-br}/r$ with $Z = 1, Hydrogen, (H)$ and Plots of figure 4, (a) to (d) are results for Z = 90, Thorium (Th) likewise.

2.1. ***Perturbed Under Coulomb Potential:***

In this case, the potential $V(r)$ is written $-Z/|r-r'|$, so that one solves

$$\frac{5k}{3}\rho(r)^{2/3} - \frac{Z}{r} + g\int \frac{\rho(r')d^3r'}{|r-r'|} + \theta\, In\,\rho(r) - \theta\, In\,\tau(r) + \lambda = 0 \qquad (23)$$

Under the condition that g = 1, θ = 1, λ – θ → λ we have

$$\frac{5k}{3}\rho(r)^{2/3} - \frac{Z}{r} + \int \frac{\rho(r')d^3r'}{|r-r'|} + In\,\rho(r) - In\tau(r) + \lambda = 0 \tag{24}$$

Let η be a perturbation in ρ such that it is possible to write the latter as:

$$\rho \to \tau + \eta \tag{25}$$

where τ is the unperturbed electron density and the solution of

$$\frac{5k}{3}\rho(r)^{2/3} - \frac{Z}{r} + g\int \frac{\rho(r')d^3r'}{|r-r'|} + \lambda = 0 \tag{26}$$

Hence using (24), equation (23) can be written as

$$\frac{5k}{3}\left(\tau(r)+\eta(r)\right)^{2/3} - \frac{Z}{r} + g\int\left(\tau(r')+\eta(r')\right)V(r-r')d^3r' + \theta\,In(\tau(r)+\eta(r)) - \theta\,In\tau(r) + \lambda = 0 \tag{27}$$

Applying binomial theorem to the first and the fourth terms in equation (26) we can write the following expressions

$$\frac{5k}{3}\tau(r)^{2/3} + \frac{10k}{9}\eta(r)\tau(r)^{(-1/3)} - \frac{Z}{r} + g\int \tau(r')\frac{d^3r'}{|r-r'|} + g\int \frac{\eta(r')d^3r'}{|r-r'|} + \theta\,In(\tau(r)) \tag{28}$$

$$-\theta\,In\,\tau(r) + \theta\frac{\eta(r)}{\tau(r)} + \lambda = 0$$

But, $$\frac{5k}{3}\tau(r)^{2/3} - \frac{Z}{r} + g\int \tau(r')\frac{d^3r'}{|r-r'|} + \lambda = 0 \tag{29}$$

Hence $$\frac{10k}{9}\eta(r)\tau(r)^{(-1/3)} + g\int \frac{\eta(r')d^3r'}{|r-r'|} + \theta\frac{\eta(r)}{\tau(r)} = 0 \tag{30}$$

Immediately, the potential of perturbation, $\varphi_\eta(r)$, attached to the internal core is identified as

$$\varphi_\eta(r) = \int \frac{\eta(r')d^3r'}{|r-r'|}, \tag{31}$$

and using the concept of Dirac distribution on (30) we have;

$$\nabla^2\varphi_\eta(r) = -4\pi\eta(r) \tag{32}$$

So that equation (29) can be written as;

$$\eta(r) = -\frac{g\tau(r)\varphi_\eta(r)}{\frac{10k}{9}\tau(r)^{2/3} + \theta} \tag{33}$$

Equations (32), (31), (17) and (24) were computed together and the following results depicted in figures 5 & 6 were obtained for a very small and very large neutral atoms.

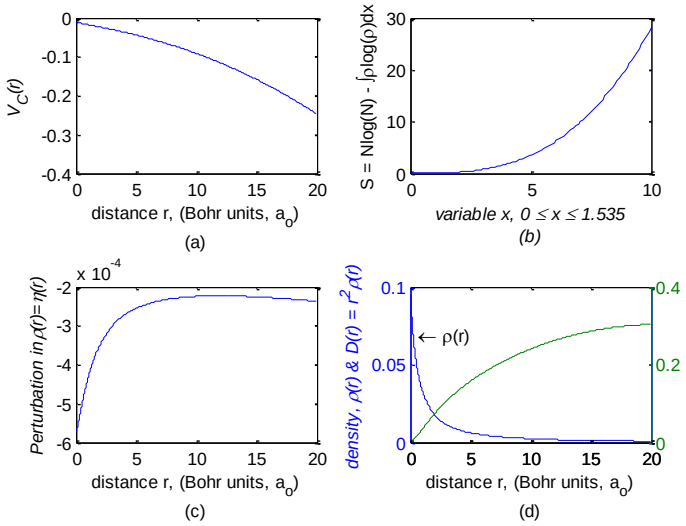

Figure 5 Z = 1, (H) perturbed Coulomb

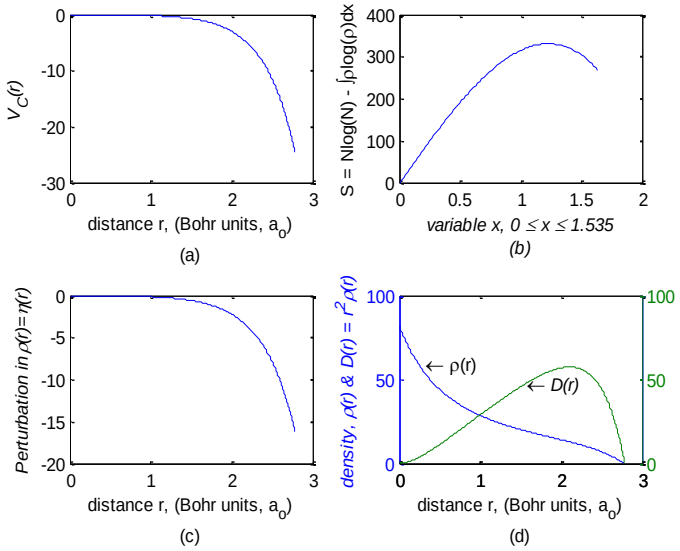

Figure 6, Z = 90, (Th) ,Perturbed Coulomb

Figures 5&6: (a) the plot of perturbed Coulomb internal potential $\varphi_\eta(r) = \int dr' \frac{\rho(r')}{|r-r'|}$ versus radial distance$r$, (in Bohr units). (b) The plot of entropy $S \cong Nlog(N) - \int \rho\log(\rho) d^3r$ versus some parameter x. (c) The plot of perturbation of electron density, $\eta(r) \cong \frac{\tau(r)\varphi_\eta(r)}{\frac{10k}{9}\tau(r)^{2/3}+\theta}$ with $\theta = 1$versus radial distance r. (d) the plot of perturbed electron density, $\rho(r) = \tau(r) + \lambda\eta(r), where\ \lambda = 1$ and perturbed electron radial distribution $D(r) = r^2\rho(r)$ versus radial distance. Plots of figure 5, (a) to (d) are results of computations under Coulomb potential,$V_{ext}(r) = -Z/r$ with $Z = 1, Hydrogen, (H)$.and Plots of figure 6, (a) to (d) are results with Z = 90, Thorium (Th) likewise.

2.2 ***Perturbed Under Yukawa Potential***

In this case, the potential V(r) is written $-Ze^{-br}/r$, so that one solves;

$$\frac{5k}{3}\rho(r)^{2/3} - \frac{Ze^{-b|r-r'|}}{r} + g\int \rho(r')V(r-r')d^3r' + \theta\, In\,\rho(r) - \theta\, In\,\tau(r) + \lambda = 0 \qquad (34)$$

Under the condition that g = 1, θ = 1, λ – θ → λ we have

$$\frac{5k}{3}\rho(r)^{2/3} - \frac{Ze^{-bx}}{r} + \int \rho(r')V(r-r')d^3r' + In\,\rho(r) - In\tau(r) + \lambda = 0 \qquad (35)$$

Following the same procedure as in section 3.1 above, we have the following equations

$$\nabla^2\varphi_\eta(r) = 4\pi\eta(r) - b^2\varphi_\eta(r) - 2b\nabla\varphi_\eta(r) \qquad (36)$$

$$\eta(r) = -\frac{\tau(r)\varphi_\eta(r)}{\frac{10k}{9}\tau(r)^{2/3}+1} \qquad (37)$$

Equation (34), (35), 24 and (17) were computed together and the following results depicted in figures 7 & 8 obtained for a very small and very large neutral atoms.

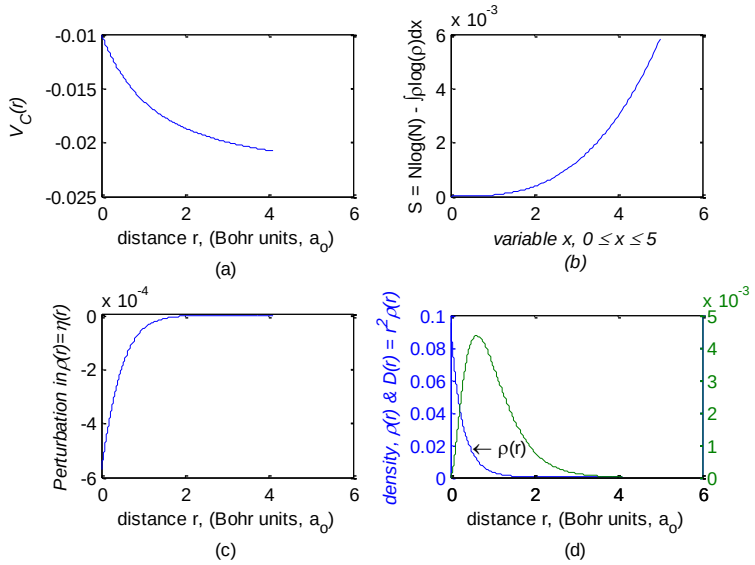

Figure 7 Z = 1 (H) Perturbed, Yukawa.

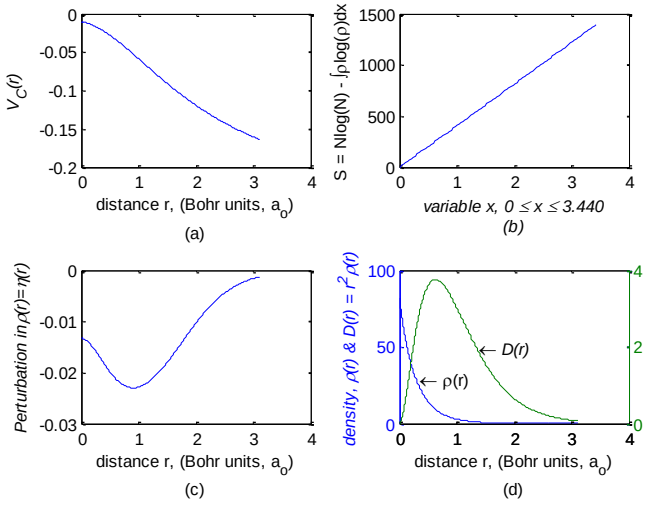

Figure 8 Z = 90 (Th) Perturbed, Yukawa.

Figures 7&8: (a) the plot of perturbed Yukawa internal potential $\varphi_\eta(r) = \int dr' \frac{\rho(r')}{|r-r'|}$ versus radial distance$r$, (in Bohr units). (b) The plot of entropy $S \cong Nlog(N) - \int \rho \log(\rho) d^3r$ versus some parameter x. (c) The plot of perturbation of electron density, $\eta(r) \cong \frac{\tau(r)\varphi_\eta(r)}{\frac{10k}{9}\tau(r)^{2/3}+\theta}$ with $\theta = 1$versus radial distance r. (d) the plot of perturbed electron density, $\rho(r) = \tau(r) + \lambda\eta(r), where\ \lambda = 1$ and perturbed electron radial distribution $D(r) = r^2\rho(r)$ versus radial distance. Plots of figure 7, (a) to (d) are results of computations under Yukawa potential,$V_{ext}(r) = -Z/r$ with $Z = 1, Hydrogen, (H)$.and Plots of figure 8, (a) to (d) are results with Z = 90, Thorium (Th) likewise.

4. DISCUSSION

Figures 1&2 and 3&4 are plots of the atom under constraints which is equivalent to the excited state of the atom. The imposed constraints can be interpreted as the chemical potential of the electrons. It is also observed that atoms under Coulomb potential are more negative, that is more bound and stable than the Yukawa because Coulomb potential is long ranged while Yukawa potentials is short ranged.

The plots revealed that negativity increases with nuclear charge, *Z*, making larger atoms more stable. This is one of the outstanding features of TF theory

3.1 *Comparisons*

The various plots in sections 3.1 and 3.2 clearly reveal the differences between electron density graphs and their corresponding electron radial distributions. Under Coulomb potential, when temperature parameter, θ is non zero, there is an increase in the *radial spread* of the electron density and their corresponding electron radial distributions, whereas when θ is zero, there is a decrease in the *radial spread* of the electron density and their corresponding electron radial distributions. In particular, figure 6d, the *radial spread* of electron radial distribution is 2.795 for θ = 1 while figure 2d, the *radial spread* electron radial distribution is 0.351 for $\theta = 0$. Similar effects are noticed under Yukawa potential.

3.2 *Suggestions for Further Studies*

This work has been charted towards stability (at zero temperature) and weak excitation of atoms and molecules at non zero but low temperature. These have been observed under two potentials, (The Coulomb and the Yukawa).

All the obtained results should be treated under Dirac correction (i.e. correlation taken into account) and also under Scott correction. The relevant equations are likely to be harder to solve and the computational work more intricate.

4. REFERENCES

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