Theoretical Considerations

2.1 Many electron system

All atoms except Hydrogen atom and certain ions of the light elements, contain several electrons, this will lead to arise a difficulty, that is the impossibility of describing the motion of each individual electron because of, in addition to considering the electrical interaction of each electron with the nucleus, there is a mutual interaction among the electrons with each other, so that, Hamiltonian operator in the Schrödinger equation have an added cross term as [22]

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m} \nabla_i^2 - \sum_{i=2}^{N} \frac{Ze^2}{r_1} + \sum_{j>i}^{N} \sum_{i=1}^{N} \frac{e^2}{r_{ij}} \qquad (2.1)$$

The first term in (2.1) represents the kinetic energy operators for the N-electrons, the second is the potential energy for the attractions between the electrons and the nucleus of charge Z and the last is the potential energy of the inter electronic repulsions[23]. The restrictions j > i avoids counting the same inter electronic repulsions twice, and avoids terms like $\frac{e^2}{r_{ii}}$.

The Schrödinger equation for the atom is not separable because of the inter electronic repulsion terms $\frac{e^2}{r_{ij}}$

This equation is not exactly soluble because of two problems:

1-The spin-orbital magnetic interaction phenomenon

2-the repulsive interaction between each pair of electrons that called cross-term (i.e. $\frac{e^2}{r_{ij}}$)that avoid equation (2-1) to be separable equation(i.e. set of equations involving coordinates of only one electron ,which can be solved exactly).

The first problem are tackled by the neglecting for the spin-orbital magnetic interaction, so that, the total wavefunction will be product of the special part of the wavefunction with the spin part

$$\psi(r,\theta,\phi,s) \Rightarrow \psi(r,\theta,\phi) \times \delta(s)$$

Where $\psi(r,\theta,\phi)$ is the radial & angular part of the wavefunction

$\delta(s)$ is the spin part of the wavefunction

The second problem will be tackled by using method called "**central field model**" [24]

2. 2 Central Field Model

This method assumed that the electron to be subjected to a potential V that represent the combined effect to a potential of the nucleus and all the other electrons .if further one takes a spherical averaged over the latter ,so that ,V is a function of r only and not of the angle (i.e. V(r))..

One arrives at the central field model .so that, the radial part to be separable from the angular part.

The angular part will be assumed to have same solution of the hydrogen atom as a spherical harmonics $Y_l^m = (const.)e^{im\varphi} p_l^m(\cos\theta)$, where $p_l^m(\cos\theta)$ are the associated Legender Polynomials ($m = 0. \pm 1, \pm 2, l \geq |m|$), so that the spatial wavefunction will write as:

$$\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$$

Radial part will be different from the hydrogen atom because of V(r) no longer have simple coulombs form.

The problem of calculating potential $V_i(r)$ for electron of order i is tackled by using computational technique called "**self-consistent field**" [25].

2.3 Self-consistent field

Self consistent field (SCF) method of calculating atomic wavefunction for atomic structure was originated by Hartree, improved by Fock, and used by most every one.

The basses of the method is to guess the wavefunction for all the electrons in the system .then one electron is selected and the potential in which it more is calculated by freezing the distribution of all the other electrons treating them as the source of the potential. The Schrödinger equation for the electron is solved for this potential and so a new wavefunction for the electron is obtained. This procedure is repeated for the electron is obtained. This procedure is repeated for all electrons in the system, using the electrons in the frozen orbital as the source of potential, when the cycle is completed as shown in Fig. (2-1) on possesses asset of orbital for all the electron of the system, and general these will differ from the original, guessed set. Now the cycle is repeated but improved wavefunction generated by the first cycle are used as the initial guess, complete cycle generates a new set of improved function .This sequence is continued until passing asset of orbital through the cycle leads to no change the orbital are then self consistent.

But because of the electrons are indistinguishable particle and the electrons under rule of Pauli Exclusion Principle that states "No more than one electron may occupy particular state".

This means that sign of wavefunction will be changed under changing the labels of electrons and it will be called symmetric wavefunction.

$$\psi(1,2) = -\psi(2,1) \Rightarrow \psi_a(1)\psi_b(2) = -\psi_a(2)\psi_b(1)$$

so that wavefunction for fermions (electrons) will written as:

$$\psi(1,2) = \frac{1}{2}[\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)]$$

Where ½ is the normalization constant [26].

For many electron systems "**Slater determinant**" are used to include "Pauli Exclusion Principle".

start here

Guess $R_1, R_2, \ldots, R_N$

Solve Schrödinger equation for R'_1 in field of electrons in $R_2, R_3, \ldots R_N$

Obtain $R'_1, R_2, \ldots, R_N$

Compare: repeat cycle until not significantly different

Repeat prosses field $R'_1, R'_2, R'_3 \ldots, R'_N$

Obtain $R'_1, R'_2, R'_3 \ldots, R'_N$

Solve Schrödinger equation for R'_2 in field of electrons in $R_1, R_3, \ldots R_N$
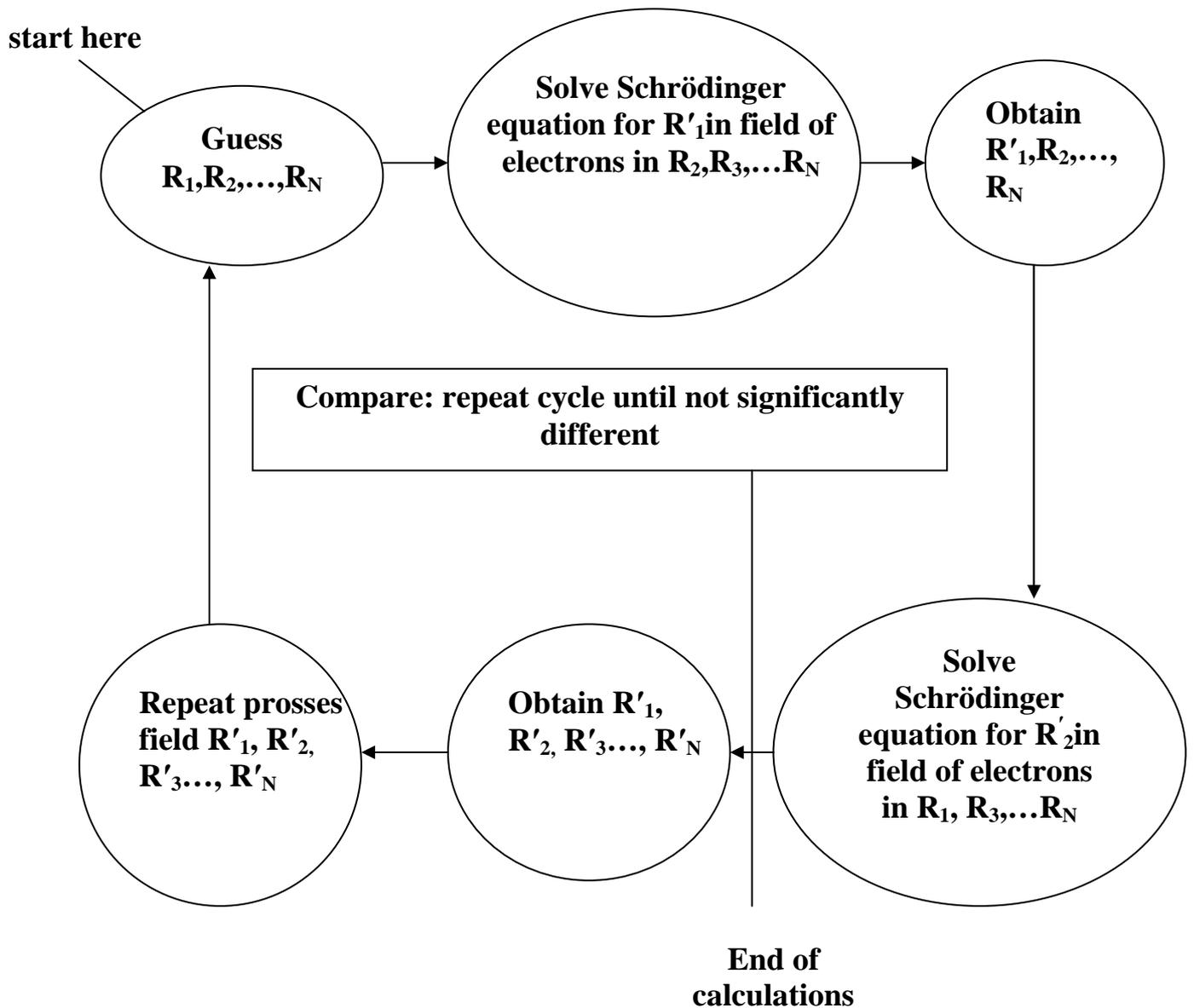
End of calculations

Fig.(2-1) Self consistent cycle [25]

2.4 Slater determinant

According to Pauli principle the wavefunction for system of electrons must change sign where the coordinates of any two electrons are interchanged , so that, from mathematical point of view, determinate will solve this problem, as Slater Pointed out in the 1920s, so that, many body wavefunctions wrote be of the form:

$$\Psi (1,2,.... N) = \frac{1}{\sqrt{(N!)}} \begin{vmatrix} \phi_1(1)\phi_2(1)........ & \phi_N(1) \\ \phi1(2)\phi_2(2)...... & \phi_N(2) \\ . \\ . \\ . \\ \phi_1(N)\phi_2(N).... & \phi_N(N) \end{vmatrix} \qquad (2.2)$$

where:

$\frac{1}{\sqrt{N!}}$ is the normalization constant and the component of one particle function

$\phi_i(i)$ is referred to as Spin-orbital . Any spin-orbital may be written as the product of a space function φ_i and a spin function α or β.

The numbers in the parentheses denote the particle, and the subscripts 1,2...N denote the eigenstate. The interchange of any two particles causes the sign of ψ to change, since it involves the interchange of corresponding two columns, and also when two electrons occupy the same spin orbital, i.e. two columns of the determinate are identical, the wavefunction is equal to zero. [26]

$$\phi_i(i) = \varphi(r,\theta,\phi)\delta(s) \qquad (2.3)$$

and $\varphi(i)$ is the spatial part

$\delta(s)$ The spin part

$$\varphi(r,\theta,\phi) = R(r)Y(\theta,\phi) \qquad (2.4)$$

$R_p(r)$:r is the radial part of special part of the total wavefunction

$Y(\theta,\phi)$:is the angular part of the special part of the total wavefunction [26]

The last wavefunction called "**Roothan-Hartree-Fock (RHF) wavefunction**" [27], [28].

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2.5 Roothaan-Hartree-Fock (RHF) Wavefunction

Analytical self consistent field atomic wavefunction in the radial atomic orbital are expanded as a linear combination of a complete set of known function ,called basis function

$$R(r) = \sum_{p}^{M} c_p \chi_p(r)$$

M: is the Number of states

c_p :is an expanded coefficient [29]

2.6 Slater Type Orbital (STO)

Atomic orbital in many-electron atoms have completed dependence on position which can be represented accurately by listing there amplitude numerically for many purposes its desirable to have an analytical function rather a table of numbers, and the Slater atomic orbital are analytical function based on the numerical results, but defined to reproduce them with moderate accuracy, each orbital have radial, dependence given by:

$$\chi_p(r) = N \times r^{(n_p - 1)} e^{-\zeta r} \qquad (2.6)$$

Where

N is the normalization constant and is equale to:

$$N = \sqrt{\frac{(2\zeta_p)^{n+1}}{(2n_p)!}}$$

then $\qquad \varphi(r,\theta,\phi) = [\sum_{p}^{M} c_p N \times r^{(n_p - 1)} e^{-\zeta r}] Y(\theta,\varphi) \qquad (2.7)$

And n_p, ζ_p are constants [29].

But wavefunction $\psi(1,2,3,...,N)$ itself, however, has no direct physical significant, But there is an interpretation made by Max Born [30]in 1926 used the probability density $|\psi(1,2,....N)|^2$,that reflects the possibility of body presence, this lead to:

$$|\psi(1,2,....N)|^2 = \psi(1.2.....N)^* \times \psi(1.2.....N) \tag{2-8}$$

$$|\psi(1,2,....N)|^2 = \frac{1}{N!} \begin{vmatrix} \phi_1(1)\phi_2(1)........ & \phi_N(1) \\ \phi_1(2)\phi_2(2)...... & \phi_N(2) \\ . \\ . \\ . \\ \phi_1(N)\phi_2(N).... & \phi_N(N) \end{vmatrix} \times \begin{vmatrix} \phi_1(1)\phi_2(1)........ & \phi_N(1) \\ \phi_1(2)\phi_2(2)...... & \phi_N(2) \\ . \\ . \\ . \\ \phi_1(N)\phi_2(N).... & \phi_N(N) \end{vmatrix} \tag{2-9}$$

For many electron systems this treatment will be more complicated, so that, there is a quantum mechanical technique to reduce this calculation to easing states called "**Second order reduced density matrix** $\Gamma_{HF}(x_m,x_n)$"

2.7 Second Order Reduced Density Matrix $\Gamma_{HF}(\chi_m,\chi_n)$

Lödin in its researches has shown that for given wavefunction $\psi(1,2,3,...,N)$ there exist a unique orbital basis, so that, called natural spin orbital (NSO) of that $\psi(1,2,3,...,N)$ and has shown that the reduced density matrix provide available tool to analyzing the properties of the wav function, the 2nd order density matrix $\Gamma_{HF}(x_m,x_n)$ is expressed in term of normalized wavefunction [31].

$$\Gamma_{ij}(x_m,x_n) = \frac{1}{2}\sum_{i\prec j}^{N} A_{ij}^{mn}\left(A_{ij}^{mn}\right)^* \tag{2.9}$$

$$\therefore \Gamma(x_m,x_n) = \sum_{i\prec j}\Gamma_{ij}(x_m,x_n) \tag{2.10}$$

where,

$$A_{ij}^{mn} = \left[\phi_i(m)\phi_j(n) - \phi_i(n)\phi_j(m)\right] \tag{2.11}$$

i and j represents spin orbital labels and m , n refer to electron labels, the density $\Gamma_{HF}(\chi_m, \chi_n)$ for each pair (i, j) is normalized for unity.

Atomic Properties

3.1 Overview

This chapter is designed to show calculation of nuclear magnetic shielding constant σ for $1s^2, 1s^2 2s$ and $1s^2 2s^2$ configurations .

These calculations must go through calculating, $\Gamma'(x_m, x_n), D(r)$ and $< r_1^n >$ before calculating the aimed property (i.e. σ).

Another properties are calculated for checking the calculations and for discuss the results such as $\rho(0)$ and Δr_1 .

The steps of calculating the aimed property is shown in Fig.(3.1)

$$\boxed{\Gamma(x_m, x_n)}$$

$$\downarrow$$

$$\boxed{\Gamma'(x_m, x_n)}$$

$$\downarrow$$

$$\boxed{D(r_1)} \longrightarrow \boxed{\rho(0)}$$

$$\downarrow$$

$$\boxed{\Delta r_1} \longleftarrow \boxed{< r_1^n >}$$
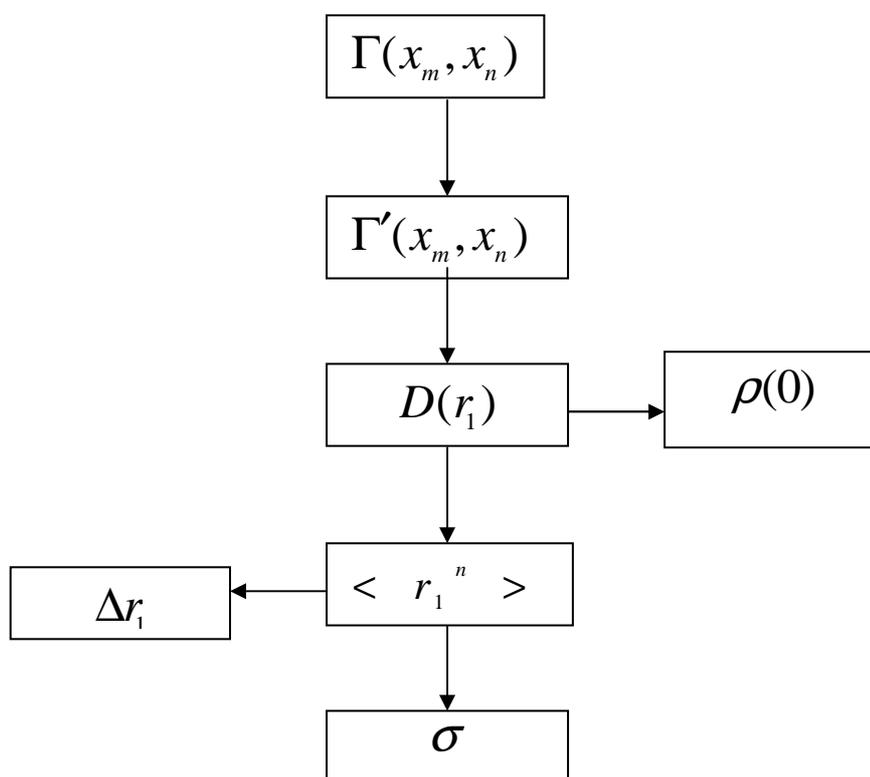
$$\downarrow$$

$$\boxed{\sigma}$$

Fig.(3.1) Steps of calculating the nuclear magnetic shielding constant

3.1 Second Order Reduced Density Matrix

For any N-electron atomic system, the two particle density can be written as: [32, 33 and 34,]

$$\Gamma_{HF}(x_m, x_n) = \begin{bmatrix} N \\ 2 \end{bmatrix} \int \Psi^*(x_1, x_2, ..., x_N) \Psi(x_1, x_2, x_3, ... x_N) dx_1 ... dx_N \qquad (3.1)$$

As usual, x_N represents combined space and spin coordinates of electron N and $(dx_1...dx_N)$ indicates integration summation over all N electrons except m and n.

The factor $\begin{bmatrix} N \\ 2 \end{bmatrix}$ is the 2nd ordered density matrix normalized to the number of electron pairs within the system:

$$\int \Gamma_{HF}(x_m, x_n) dx_m dx_n = \begin{bmatrix} N \\ 2 \end{bmatrix} = \frac{N}{[2!(N-2)!]} \qquad (3.2)$$

For that there is $\begin{bmatrix} N \\ 2 \end{bmatrix}$ number of state for atomic system of N electrons, this

lead to $\begin{bmatrix} N \\ 2 \end{bmatrix}$ number of $\Gamma_{ij}(x_m, x_n)$, with $i < j$.

$$\Gamma_{ij}(x_m, x_n) = \frac{1}{2} \sum_{i<j}^{N} A_{ij}^{mn} (A_{ij}^{mn})^* \qquad (3.3)$$

where

$$A_{ij}^{mn} = [\phi_i(m)\phi_j(n) - \phi_j(m)\phi_i(n)] \qquad (3.4)$$

where $\phi_i(m)$ =(spatial part)$\times$ (spin part)

$\Gamma_{ij}(x_m, x_n)$ Normalized to unity for each pair (i, j) .

- **1s^2 configuration:**

This configuration have one shell is K shell that contain 2-electrons, so that

$$\begin{bmatrix} N \\ 2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \end{bmatrix} = 1 \text{ pair}$$

$$\Gamma_{12}(K_\alpha, K_\beta) = \frac{1}{2}[\phi_i(1)\phi_j(2) - \phi_j(1)\phi_i(2)]^2 \qquad (3.5)$$

$$\Gamma_{12}(K_\alpha, K_\beta) = \frac{1}{2}[1s(1)\alpha(1)1s(2)\beta(2) - 1s(2)\beta(1)1s(1)\alpha(2)]^2 \qquad (3.6)$$

$$\Gamma_{12}(K_\alpha, K_\beta) = \frac{1}{2}1s(1)^2 \, 1s(2)^2 \, [\alpha(1)\beta(2) - \beta(1)\alpha(2)]^2 \qquad (3.7)$$

- **$1s^2$ 2s configuration:**

This configuration have has two shells   intra-shell(K-shell) and inter-shell(KL-shell), this configuration have 3- electrons, so that,

$$\begin{bmatrix} N \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \end{bmatrix} = \frac{3!}{2!(3-2)!} = 3 \text{ pairs} \qquad (3.8)$$

$$\therefore \Gamma(x_m, x_n) = \sum_{i \prec j} \Gamma_{ij}(x_m, x_n) = \Gamma_{12}(K_\alpha, K_\beta) + \Gamma_{13}(K_\alpha, L_\alpha) + \Gamma_{23}(K_\beta, L_\alpha) \qquad (3.9)$$

$$\Gamma_{12}(K_\alpha, K_\beta) = \frac{1}{2}[1s(1)\alpha(1)1s(2)\beta(2) - 1s(2)\beta(1)1s(1)\alpha(2)]^2 \qquad (3.10)$$

$$= \frac{1}{2}1s(1)^2 \, 1s(2)^2 \, [\alpha(1)\beta(2) - \beta(1)\alpha(2)]^2 \qquad (3.11)$$

$$\Gamma_{13}(K_\alpha, L_\alpha) = \frac{1}{2}[1s(1)\alpha(1)2s(2)\alpha(2) - 1s(2)\alpha(2)2s(1)\alpha(1)]^2 \qquad (3.12)$$

$$= \left[\frac{1s(1)2s(2) - 1s(2)2s(1)}{\sqrt{2}}\right]^2 \alpha(1)^2 \, \alpha(2)^2 \qquad (3.13)$$

$$\Gamma_{23}(K_\beta, L_\alpha) = \frac{1}{2}[1s(1)\beta(1)2s(2)\alpha(2) - 1s(2)\beta(2)2s(1)\alpha(1)]^2 \qquad (3.14)$$

- **$1s^2 2s^2$ configuration:**

This configuration of 4- electron has 6-pairs of electrons divided to intra and inter shells with 4-electrons, so that:

$$\begin{bmatrix} N \\ 2 \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix} = \frac{4!}{2!(4-2)!} = 6 \text{ pairs of electrons}$$

$$\therefore \Gamma(x_m, x_n) = \sum_{i \prec j} \Gamma_{ij}(x_m, x_n) = \Gamma_{12}(K_\alpha, K_\beta) + \Gamma_{13}(K_\alpha, L_\alpha) + \Gamma_{14}(K_\alpha, L_\beta)$$
$$+ \Gamma_{23}(K_\beta, L_\alpha) + \Gamma_{24}(K_\beta, L_\beta) + \Gamma_{34}(L_\alpha, L_\beta) \qquad (3.15)$$

$$\Gamma_{12}(K_\alpha, K_\beta) = \frac{1}{2}[\phi_i(1)\phi_j(2) - \phi_j(1)\phi_i(2)]^2 \tag{3.16}$$

$$= \frac{1}{2}[1s(1)\alpha(1)1s(2)\beta(2) - 1s(2)\alpha(2)1s(1)\beta(1)]^2 \tag{3.17}$$

$$= \frac{1}{2}1s(1)^2 1s(2)^2 [\alpha(1)\beta(2) - \alpha(2)\beta(1)]^2 \tag{3.18}$$

$$\Gamma_{13}(K_\alpha, L_\alpha) = \frac{1}{2}[1s(1)\alpha(1)2s(2)\alpha(2) - 1s(2)\alpha(2)2s(1)\alpha(1)]^2 \tag{3.19}$$

$$= \left[\frac{1s(1)2s(2) - 1s(2)2s(1)}{\sqrt{2}}\right]^2 \alpha(1)^2 \alpha(2)^2 \tag{3.20}$$

$$\Gamma_{23}(K_\beta, L_\alpha) = [\frac{1s(1)2s(2) + 1s(2)2s(1)}{\sqrt{2}}]^2 [\frac{\alpha(1)\beta(2) - \alpha(1)\beta(2)}{\sqrt{2}}]^2 \tag{3.21}$$

$$\Gamma_{24}(K_\beta, L_\beta) = \frac{1}{2}[1s(1)\beta(1)2s(2)\beta(2) - 1s(2)\beta(2)s(1)\beta(1)]^2 \tag{3.22}$$

$$= \frac{1}{2}[1s(1)2s(2) - 2s(2)1s(1)]^2 \beta(1)^2 \beta(2)^2 \tag{3.23}$$

$$\Gamma_{14}(K_\alpha, L_\beta) = [\frac{1s(1)2s(2) - 1s(2)2s(1)}{\sqrt{2}}]^2 [\frac{\alpha(1)\beta(2) + \alpha(1)\beta(2)}{\sqrt{2}}]^2 \tag{3.24}$$

$$\Gamma_{34}(L_\alpha, L_\beta) = \frac{1}{2}[2s(1)\alpha(1)2s(2)\beta(2) - 2s(1)\beta(1)2s(2)\alpha(2)]^2$$

$$= \frac{1}{2}2S(1)^2 2S(2)^2[\alpha(1)\beta(2) - \alpha(2)\beta(1)]^2 \tag{3.25}$$

The total value

$$\Gamma_{total} = \frac{1}{6}\left[\Gamma_{k(1s)} + \Gamma_{L(1s)} + \Gamma_{KL(1s)} + 3\Gamma_{KL(3s)}\right] \tag{3.26}$$

From calculating $\Gamma(x_n, x_m)$ for each shell for each configuration, equation of k-shell is same for all studied configurations this will be repeated for $\Gamma(x_n, x_m)$ to other shells.

3.2 Spin-less two-particle density $\Gamma'(x_m x_n)$

Because of these calculations are neglecting the spin-orbit interaction the equation $\Gamma(x_m x_n)$ can be simplified to $\Gamma'(x_m x_n)$ as:

$$\Gamma'(x_1, x_2) = \int \Gamma(x_1, x_2) d\delta_1 d\delta_2 \qquad (3.27)$$

- $1s^2$ configuration:

For ground state, K-shell can be described by Substituting equation (3-7) in (3-27)

$$\Gamma'(x_1, x_2) = \int \Gamma(x_1, x_2) d\delta_1 d\delta_2 \qquad (3.27)$$

$$\Gamma'_{12}(K_\alpha, K_\beta) = \iint \frac{1}{2} 1s(1)^2 1s(2)^2 [\alpha(1)\beta(2) - \alpha(2)\beta(1)]^2 \, d\delta_1 d\delta_2 \qquad (3.28)$$

$$= \frac{1}{2} 1s(1)^2 1s(2)^2 [1 - 2\times 0 + 1] \qquad (3.29)$$

$$= 1s(1)^2 1s(2)^2 \qquad (3.30)$$

Since: $\int \alpha^2(1) d\delta_1 = 1, \int \beta^2(2) d\delta_2 = 1$

Because of the normalized condition

$$\int \alpha(1)\beta(2) d\delta = \int \alpha(2)\beta(1) d\delta = 0$$

Because of the orthogonally condition

- **$1s^2 1s$-condition:**

$\Gamma'_{12}(K_\alpha, K_\beta)$ for this configuration is equal to that of equation (3-30)

For KL-shell Substitute equation (3-13) in (3-27) gives:

$$\Gamma'_{13}(K_\alpha, L_\alpha) = \iint \left\{ \frac{1}{2} [1s(1)\ 2s(2) - 2s(1)1s(2)]^2 \alpha(1)^2 \alpha(2)^2 \right\} d\delta_1 d\delta_2 \qquad (3.31)$$

$$= \frac{1}{2} [1s(1)2s(2) - 2s(1)1s(2)]^2 \qquad (3.32)$$

For KL-shell Substitute equation (3-14) in (3-27) gives:

$$\Gamma'_{23}(K_\beta, L_\alpha) = \iint \frac{1}{2} [1s(1)\beta(1)2s(2)\alpha(2) - 1s(2)\beta(2)2s(1)\alpha(1)]^2 d\delta_1 d\delta_2 \qquad (3.33)$$

$$= \frac{1}{2} 1s(1)^2 2s(2)^2 + \frac{1}{2} 1s(2)^2 2s(1)^2 \qquad (3.34)$$

- **$1s^2 2s^2$ configuration:**

$\Gamma'_{12}(K_\alpha, K_\beta), \Gamma'_{23}(K_\beta, L_\alpha) \& \Gamma'_{13}(K_\alpha, L_\alpha)$ for this configuration is equal to that of equation (3-30),(3-32),(3-34).

To calculate $\Gamma'_{14}(K_\alpha, L_\beta)$ substitute equation (3.24) in equation (3.27)

$$\Gamma'_{14}(K_\alpha, L_\beta) = \iint [\frac{1s(1)2s(2) - 1s(2)2s(1)}{\sqrt{2}}]^2 [\frac{\alpha(1)\beta(2) + \alpha(1)\beta(2)}{\sqrt{2}}]^2 d\delta_1 d\delta_2 \qquad (3.35)$$

$$= \frac{1}{2} 1s(1)^2 2s(2)^2 + \frac{1}{2} 1s(2)^2 2s(1)^2 \qquad (3.36)$$

To calculate $\Gamma'_{24}(K_\alpha, L_\beta)$ substitute equation (3-23) in equation (3-27)

$$\Gamma'_{24}(K_\alpha, L_\beta) = \iint \frac{1}{2} [1s(1)2s(2) - 2s(2)1s(1)]^2 \beta(1)^2 \beta(2)^2 d\delta_1 d\delta_2 \qquad (3.37)$$

$$= \frac{1}{2} [1s(1)2s(2) - 2s(2)1s(1)]^2 \qquad (3.38)$$

To calculate $\Gamma'_{34}(L_\alpha, L_\beta)$ substitute equation (3-24) in equation (3-27)

$$\Gamma'_{34}(L_\alpha, L_\beta) = \iint \frac{1}{2} 2s(1)^2 2s(2)^2 [\alpha(1)\beta(2) - \beta(1)\alpha(2)]^2 d\delta_1 d\delta_2 \qquad (3.39)$$

$$= 2s(1)^2 2s(2)^2 \qquad (3.40)$$

3.3 One particle Electron Density $D(r)$

This property is very important $D(r)$ to study the electron in atom, which means the probability of finding electrons in each shell and it represents the density distribution of one electron in each shell an is defined as [35, 36 and 37]

$$D(r) = \int_0^\infty \Gamma'_{12}(x_m, x_n) r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \qquad (3.41)$$

$$d\Omega = \sin(\theta) d\theta d\phi$$

- **1s²-configuration:**

To calculate $D_K(r_1)$ substitute equation (3-30) in equation (3-41)

$$D_K(r_1) = \int_0^\infty \Gamma_{12}'(K_\alpha, K_\beta) r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \tag{3.42}$$

$$= \int_0^\infty 1s(1)^2 1s(2)^2 r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \tag{3.43}$$

$$= R_{1s}^2(r_1) r_1^2 \iint y_{1s}^2(\theta_1, \phi_1) y_{1s}^2(\theta_2, \phi_2) d\Omega_1 d\Omega_2 \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2 \tag{3.44}$$

$$= R_{1s}^2(r_1) r_1^2 \tag{3.45}$$

Since: $\int_0^{2\pi}\int_0^\pi y_{1s}^2(\theta_1, \phi_1)\sin\theta_1 d\theta_1 d\phi_1 = \int_0^{2\pi}\int_0^\pi y_{2s}^2(\theta_2, \phi_2)\sin\theta_2 d\theta_2 d\phi_2 = 1$

Because of normalization condition

$$\int_0^\infty R_{2s}^2(r_2)^2 r_2^2 dr_2 = 1$$

Because of normalization condition

Substitute (2-6) in (3-45)

$$D_K(r_1) = \sum_i C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} e^{-(2\xi_i)r_1} r_1^{2n_i} \tag{3.46}$$

Where

C_i, are the variation determined expansion coefficients (1s)

N_i are the normalization constant and is given by:

ξ_i: is the orbital components

- ## $1s^2 1s$-configuration:

$D_{kk}(r_1)$ is equal to that in the $1s^2$-configuration in equation

Substitute equation (3-32) in (3-41)

$$D_{KL3}(r_1) = \int_0^\infty \Gamma'_{13}(K_\alpha, L_\alpha) r_1^2 r_2^2 \, dr_2 d\Omega_2 \tag{3.47}$$

$$= \int \frac{1}{2} [1s(1)2s(2) - 1s(2)2s(1)]^2 \, r_1^2 r_2^2 \, dr_1 d\Omega_1 d\Omega_2 \tag{3.48}$$

$$= \frac{1}{2} R_{1s}(r_1)^2 r_1^2 \int y^2{}_{1s}(\Omega_1) d\Omega_1 \int y^2{}_{2s}(\Omega_2) d\Omega_2 \int_0^\infty R_{2s}^2(r_2) r_2^2 \, dr_2$$

$$- \frac{1}{2} \cdot 2 \int y_{1s}(\Omega_1) y_{2s}(\Omega_2) y_{2s}(\Omega_1) y_{1s}(\Omega_2) d\Omega_1 d\Omega_2 \int_0^\infty R_{1s}(r_1) R_{2s}(r_2) R_{1s}(r_2) R_{2s}(r_1) r_1^2 r_2^2 \, dr_2 \tag{3.49}$$

$$+ \frac{1}{2} \int_0^\infty R_{1s}^2(r_2) r_2^2 \, dr_2 \int y^2{}_{2s}(\Omega_1) d\Omega_1 \int y^2{}_{1s}(\Omega_2) d\Omega_2 R_{2s}^2(r_1) r_1^2$$

$$= \frac{1}{2} R_{1s}(r_1)^2 r_1^2 + \frac{1}{2} R_{2s}^2(r_1) r_1^2 \tag{3.50}$$

Substitute (2-6) in (3-50)

$$D_{KL3}(r_1) = \frac{1}{2} \sum_i C_i^2 \frac{(2.\xi_i)^{n+1}}{[(2.n_i)!]^{\frac{1}{2}}{}_i} e^{-(2\xi_i)r_1} r_1^{2n_i} + \frac{1}{2} \sum_j C_j^2 \frac{(2.\xi_j)^{n+1}}{[(2.n_j)!]^{\frac{1}{2}}{}_i} e^{-(2\xi_j)r_1} r_1^{2n_i} \tag{3.51}$$

Since:

$$\int y^2{}_{1s}(\Omega_1) d\Omega_1 = \int y^2{}_{2s}(\Omega_2) d\Omega_2 = 1$$

$$\int y^2{}_{2s}(\Omega_1) d\Omega_1 = \int y^2{}_{1s}(\Omega_2) d\Omega_2 = 1$$

$$\int y_{1s}(\Omega_1) y_{2s} d\Omega_1 = \int y_{2s}(\Omega_2) y_{1s}(\Omega_2) d\Omega_2 = 1$$

$$\int y_{1s}(\Omega_2) y_{2s}(\Omega_2) d\Omega_2 = 1$$

Because of the quantum number are equal in the two subshells (i.e. $y_{1s} \to l, m_l = 0, \ y_{2s} \to l, m_l = 0$)

$$\int R_{1s}(r_2)^2 r_2^2 \, dr_2 = \int R_{2s}^2(r_2) r_2^2 \, dr_2 = 1$$

Because of normalization condition

$$\int\limits_0^\infty R_{2s}(r_2)R_{1s}(r_2)r_2^2 dr_2 = 0$$

Because of the principle quantum number for 1s-subshell (i.e. n=1) not equal to that of 2s-subshell (i.e. n=2) this lead to the apply the orthogonal condition.

Substitution equation (3-34) in (3-41)

$$D_{KL3}(r_1) = \int\limits_0^\infty \Gamma_{23}'(K_\beta, L_\alpha)r_2^2 dr_1 dr_2 d\Omega_1 d\Omega_2 \qquad (3.52)$$

$$= \int\limits_0^\infty [\frac{1}{2}1s(1)^2 2s(2)^2 + \frac{1}{2}1s(2)^2 2s(1)^2]r_2^2 dr_1 dr_2 d\Omega_1 d\Omega_2 \qquad (3.53)$$

$$= \frac{1}{2}R_{1s}(r_1)^2 r_1^2 \int\limits_0^\infty R_{2s}(r_2)^2 r_2^2 dr_2 + \frac{1}{2}R_{2s}(r_1)^2 r_1^2 \int\limits_0^\infty R_{1s}(r_2)^2 r_2^2 dr_2 \qquad (3.54)$$

$$= \frac{1}{2}R_{1s}(r_1)^2 r_1^2 + \frac{1}{2}R_{2s}(r_1)^2 r_1^2 \qquad (3.55)$$

Note that the later equation (3-55) is equal to that of (3-50)

$$D_{KL1}(r_1) = D_{KL3}(r_1)$$

- **$1s^2 2s^2$ configuration:**

The one particle radial density distribution for k-shell is equal to that for k-shell for $1s^2$ configuration as in equation (3-41).

Substitute equation (3-40) in (3-41)

$$D_{LL}(r_1) = \int \Gamma_{34}'(L_\alpha, L_\beta)r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \qquad (3.56)$$

$$D_{LL}(r_1) = \int 2s(r_1)^2 \cdot 2s(r_2)^2 r_1^2 r_2^2 dr_1 dr_2 d\Omega_1 d\Omega_2$$

$$R_{2s}^2(r_1)r_1^2 \int y_{1s}(\Omega_1)^2 \cdot d\Omega_1 \int y_{1s}(\Omega_2)^2 d\Omega_2 \cdot \int R_{2s}^2(r_2)r_2^2 dr_2$$

$$= R_{2s}^2(r_1)r_1^2 \qquad (3.57)$$

One-particle radial density for KL-shell has 4-states in these shells will represent a probable states for D(r):

$$D_{KL}(r) = \int \Gamma'_{13}(K_\alpha, L_\alpha) r_1^2 r_2^2 dr_1 d\Omega_1 d\Omega_2 \tag{3-58}$$

The result of this integral is equal to the result of equation (3-47).

The 2nd probable state gives for the interaction of x_1 & x_4

$$\therefore D_{KL}(r_1) = \int \Gamma'_{14}(K_\alpha, L_\beta) r_1^2 r_2^2 dr_2 \tag{3.59}$$

Substitute equation (3-36) in (3-41)

$$\int_0^\infty R_{2s}^2(r_2) r_2^2 dr_2 = \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2 = 1$$

$$\left.\begin{array}{l} D_{KL}(r_1) = \int \left[\dfrac{1}{2} 1s(1)^2 2s(2)^2 + \dfrac{1}{2} 1s(2)^2 2s(1)^2 \right] r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \\[3mm] = = \dfrac{1}{2} R_{1s}(r_1)^2 r_1^2 \int y_{1s}(\Omega_1)^2 d\Omega_1 \int y_{2s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{2s}^2(r_2) r_2^2 dr_2 \\[3mm] + \dfrac{1}{2} R_{2s}(r_1)^2 r_1^2 \int y_{2s}(\Omega_1)^2 d\Omega_1 y_{1s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2 \end{array}\right\} \tag{3.60}$$

$$D_{KL}(r_1) = \frac{1}{2} R_{2s}(r_1)^2 r_1^2 + \frac{1}{2} R_{2s}(r_1)^2 r_1^2 \tag{3.61}$$

The third probable state for x_2, x_3 coupling

$$D_{KL}(r_1) = \int \Gamma'_{23}(K_\beta, L_\alpha) r_2^2 r_3^2 dr \tag{3.62}$$

Substitute equation (3-34) in (3-41)

$$
\left.\begin{aligned}
D_{KL}(r_1) &= \int \left[\frac{1}{2} 1s(1)^2 2s(2)^2 + \frac{1}{2} 1s(2)^2 2s(1)^2 \right] r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \\
&= \frac{1}{2} R_{1s}(r_1)^2 r_1^2 \int y_{1s}(\Omega_1)^2 d\Omega_1 \int y_{2s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{2s}^2(r_2) r_2^2 dr_2 \\
&\quad + \frac{1}{2} R_{2s}(r_1)^2 r_1^2 \int y_{2s}(\Omega_1)^2 d\Omega_1 y_{1s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2
\end{aligned}\right\} \quad (3.63)
$$

$$
= \frac{1}{2} R_{2s}(r_1)^2 r_1^2 + \frac{1}{2} R_{2s}(r_1)^2 r_1^2 \qquad (3.64)
$$

Since:

$$
\int y_{1s}^2(\Omega_1) d\Omega_1 = \int y_{2s}(\Omega_2) d\Omega_2 = 1 : \int_0^\infty R_{2s}^2(r_2) r_2^2 dr_2 = \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2 = 1
$$

The 4-th probable state for D(r) is

$$
D_{KL}(r) = \int \Gamma_{14}'(K_\alpha, L_\beta) r_1^2 r_2^2 dr_2 d\Omega_2 d\Omega_1 \qquad (3.65)
$$

Substitute equation (3-36) in (3-55)

$$
\left.\begin{aligned}
D_{KL}(r_1) &= \int \left[\frac{1}{2} 1s(1)^2 2s(2)^2 + \frac{1}{2} 1s(2)^2 2s(1)^2 \right] r_1^2 r_2^2 dr_2 d\Omega_1 d\Omega_2 \\
&= \frac{1}{2} R_{1s}(r_1)^2 r_1^2 \int y_{1s}(\Omega_1)^2 d\Omega_1 \int y_{2s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{2s}^2(r_2) r_2^2 dr_2 \\
&\quad + \frac{1}{2} R_{2s}(r_1)^2 r_1^2 \int y_{2s}(\Omega_1)^2 d\Omega_1 y_{1s}(\Omega_2)^2 d\Omega_2 \int_0^\infty R_{1s}^2(r_2) r_2^2 dr_2
\end{aligned}\right\} \quad (3.64)
$$

$$
= \frac{1}{2} R_{2s}(r_1)^2 r_1^2 + \frac{1}{2} R_{2s}(r_1)^2 r_1^2
$$

$$
\int y_{1s}(\Omega_2) y_{2s}(\Omega_2) d\Omega_2 = 1
$$

Because of $y_{1s} \rightarrow l, m_l = 0, \ y_{2s} \rightarrow l, m_l = 0$

  The one-particle radial density D(r) for KL-shell has 4-probable states and all states are equals as in equations:

(3-50), (3-54), 3-57), and (3-61).

Final forms of one particle radial density distribution for studied configurations will be given by applying STO-wavefunction, as follow:

$$R(r) = \sum_{i=1}^{N} C_i N_i r^{n_i-1} e^{-(\xi_i)r_i} \tag{3.67}$$

- for K-shell for N-electron system

Substitute (3-62) in (3-42)

$$D_{KK}(r_1) = \sum_{i=1}^{N} C_i^2 N_i^2 r^{2n_i} e^{-2\xi_i r_i} \tag{3.68}$$

- for KL-shell for N-electron system

Substitute equation(3-62) in any one of equations(3-51), (3-54), 3-57), and (3-61).

$$D_{KL}(r_1) = \frac{1}{2} \sum_{i=1}^{N} C_i^2 N_i^2 r^{2n_i} e^{-2\xi_i r_i} + \frac{1}{2} \sum_{j=1}^{N} C_j^2 N_j^2 r^{2n_j} e^{-2\xi_j r_j} \tag{3.69}$$

- for L-shell N-electron system

Substitute (3-62) in (3-50)

$$D_{LL}(r_1) = \sum_{j=1}^{N} C_j^2 N_j^2 r^{2n_j} e^{-2\xi_j r_j} \tag{3.70}$$

3.4 One particle Expectation Values $<r_1^n>$

The one particle expectation values $<r_1^n>$ is defined by equations [46, 42, 44, 47, 48]

$$<r_1^n> = \int_0^\infty D(r_1) r_1^n dr_1 \tag{3.71}$$

When n is the power of $<r_1>$ and equal to (-2.-1.0.1.2)

But for n=0, then ,$<r_1^n> = 1$,because of normalization condition :

Since

$$\int_0^\infty D(r)r_1^0 dr_1 = \int_0^\infty D(r_1)dr_1 = 1$$

The one particle expectation value depends directly with $D(r_1)$ for N-electron system have the same form as in K-shell for $1s^2$, $2s^2 1s$ and $1s^2\ 2s^2$ configurations and same thing in KL and LL shells for $1s^2$, $1s^2 2s^2$ configuration, so that, states of $<r^n>$ for K, LL, and KL will have same formula for any in any 4-electron systems that satisfy Hartree-Fock condition.

- For k-shell

Substitute (3-45) in (3-71)

By using integral Gamma-fuction

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$\therefore <r^n>_{KK} = \sum_{i=1}^N C_i^2 N_i^2 \cdot \frac{[2n_i + n]!}{[2\zeta_i]^{2n_i+n+1}} \tag{3.73}$$

- For KL-shell for any N-electron system

Substitute (3-50) in (3-71)

$$<r^n>_{KL} = \frac{1}{2}\sum_{i=1}^N C_i^2 N_i^2 \int_0^\infty r^{2n_i+n} e^{-2\zeta_i r_1} dr_1 + \frac{1}{2}\sum_{j=1}^N C_j^2 N_j^2 \int_0^\infty r^{2n_j+n} e^{-2\zeta_j r_j} dr \tag{3.74}$$

$$\therefore <r_1^n>_{KL} = \frac{1}{2}\sum_{i=1}^N C_i^2 N_i^2 \frac{[2n_i + n]!}{(2\zeta_i)^{2n_i+n+1}} + \frac{1}{2}\sum_{j=1}^N C_j^2 N_j^2 \frac{[2n_j + n]!}{(2\zeta_j)^{2n_j+n+1}} \tag{3.75}$$

- For LL-shell for any N-electron system

Substitute (3-57) in (3-71)

$$< r^n > = \sum_{j=1}^{N} C_j^2 N_j^2 \int_0^\infty r_j^{2n_j+n} e^{-2\zeta_j r_j} dr \tag{3.76}$$

$$= \sum_{j=1}^{N} C_j^2 N_j^2 \cdot \frac{\lfloor 2n_j + n \rfloor!}{\lfloor 2\zeta_j \rfloor^{2n_j+n+1}} \tag{3.77}$$

3.5 Electronic Density at Nucleus $\rho(0)$:

The electron density at the nucleus can be evaluated using [39, 40,and41]

$$\rho(o) = \left[\frac{D(r)}{4\pi r^2} \right]_{r \to 0} \tag{3.78}$$

- For K-shell

Substitute(3-46) in (3-78)

$$\rho_{KK}(o) = \left[\frac{1}{4\pi} \sum_i^N C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} r_i^{2n_i-2} e^{-2\zeta_i r_i} \right]_{r \to 0} \tag{3.79}$$

For KL-shell substitute (3-57) in (3-78)

$$\rho_{KL}(o) = \left[\frac{1}{8\pi} \sum_{i=1}^N C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} r_i^{2n_i-2} e^{-2\zeta_i r_i} + \frac{1}{8\pi} \sum_{j=1}^N C_j^2 \frac{(2.\xi_j)^{n_j+1}}{(2.n_j)!} r_j^{2n_j-2} e^{-2\zeta_j r_j} \right. \tag{3.80}$$

For L-shell

$$\rho_{LL}(o) = \left[\frac{1}{4\pi} \sum_{i=1}^N C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} r_i^{2n_i-2} e^{-2\zeta_i r_i} \right]_{r \to 0} \tag{3.81}$$

3.6 Standard deviation of Δr_1

The Standard deviation of Δr_1 is defined as [42 and 43]

$$\Delta r_1 = \sqrt{<r_1^2> - <r_1>^2}$$ (3.82)

For K-shell, substitute (3-73) into (3-82)with n=2, n=1

$$\Delta r_{1K-shell} = \left[\sum_{i=1}^{N} C_i^2 N_i^2 \cdot \frac{[2n_i + 2]!}{[2\zeta_i]^{2n_i+3}} - \sum_{i=1}^{N} C_i^4 N_i^4 \cdot \frac{[(2n_i + 1)!]^2}{[2\zeta_i]^{4n_i+4}} \right.$$ (3.83)

For KL-shell, substitute (3-75) in (3-82)

$$\Delta r_{1KL-shell} = \left[\frac{1}{2} \sum_{i=1}^{N} C_i^2 N_i^2 \cdot \frac{[2n_i + 2]!}{[2\zeta_i]^{2n_i+3}} + \frac{1}{2} \sum_{j=1}^{N} C_j^2 N_j^2 \cdot \frac{[2n_j + 2]!}{[2\zeta_j]^{2nj+3}} \right.$$ (3.84)

$$\left. - \frac{1}{4} \sum_{i=1}^{N} C_i^4 N_i^4 \cdot \frac{[(2n_i + 1)!]^2}{[2\zeta_i]^{4n_i+4}} + \frac{1}{4} \sum_{j=1}^{N} C_j^4 N_j^4 \cdot \frac{[(2n_j + 1)!]^2}{[2\zeta_j]^{4n_j+4}} \right]^{1/2}$$

For LL-shell, substitute (3-77) in (3-82)

$$\Delta r_{1LL} = \left[\sum_{j=1}^{N} C_j^2 N_j^2 \cdot \frac{[2n_j + 2]!}{[2\zeta_j]^{2nj+3}} - \sum_{j=1}^{N} C_j^4 N_j^4 \cdot \frac{[(2n_j + 1)!]^2}{[2\zeta_j]^{4nj+4}} \right]^{\frac{1}{2}}$$ (3.85)

3.7 Nuclear Magnetic Shielding Constant σ :

The Nuclear magnetic shielding constant, is determined from formula [3,4,5 and 44]

$$\sigma = \frac{1}{3}\alpha^2 \sum_{i=1}^{N} <r_i^{-1}>$$ (3.86)

Where α: is the fine structure constant, whose value is taken [81]

$\alpha = e^2 / 4\pi t_o \hbar c = 7.29735308*10^{-3}$

Final mathematical formula of nuclear magnetic shielding constant for studied configuration .

- For k-shell, substitute (3-73)in (3-87)

$$\sigma_{KK-shell} = \frac{1}{3}\alpha^2 \sum_{i=1}^{N} C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} \frac{[2n_i-1]!}{(2\zeta)^{2n_i}} \qquad (3.87)$$

- For KL-shell, substitute (3-75) in (3-87)

$$\sigma_{KL-shell} = \frac{1}{6}\alpha^2 \sum_{i=1}^{N} C_i^2 \frac{(2.\xi_i)^{n_i+1}}{(2.n_i)!} \frac{[2n_i-1]!}{(2\zeta)^{2n_i}} + \sum_{j=1}^{N} C_j^2 \frac{(2.\xi_j)^{n_j+1}}{(2.n_j)!} \frac{[2n_j-1]!}{(2\zeta)^{2n_j}}$$

For $1s^2 2s$ configuration KL will have two states only KL(^{1}S), KL(^{3}S) but with $1s^2 2s^2$ 4-states one fo(KL^{1}S)& three fort (KL^{3}S)

For L-shell , substitute (3-77) in (3-82)

$$\sigma_{LL-shell} = \frac{1}{3}\alpha^2 \sum_{j=1}^{N} C_j^2 \frac{(2.\xi_j)^{n_j+1}}{(2.n_j)!} \frac{[2n_j-1]!}{(2\zeta)^{2n_j}} \qquad (3.88)$$

Results, Discussion and Conclusions

4-1 Introduction

This work has been designed to investigate the physical phenomena that reflected from tables and figures ,that contain the results which produced for main atomic properties such as, one-particle electronic density D(r1),one particle expectation value $\langle r_1^n \rangle$,when n=-2to2, one particle standard deviation Δr_1,nuclear magnetic shielding constant σ and electronic density at the nucleus $\rho(0)$ by using Data in appendix(C), for (He-isoelectronic series , Li-isoelectronicseries,Li^{-1}, Be).

These results are arranged in two categories to direct the discussion for the results in the direction of the mean aim of this work (i.e. studying nuclear magnetic shielding constant σ for Z=2 to10).

First category discuss all properties of the work except the nuclear magnetic shielding constant σ for (He-isoelectronicseries, Li-isoelectronic series, Li^{-1} ion, Be atom).

Second category rearranged the atomic systems in a new 5samples to investigate physical ideas behind results in tables and figures nuclear magnetic shielding constant σ, and these samples are:

Sample 1: He-isoelectronic series.

Sample2: Li-ioelectric series.

Sample3: Li^{+1}, Li and Li^{-1}.

Sample5: He, Li and Be.

Sample4: individual K(^{1}S),KL(^{1}S),KL(^{3}S) and L(^{1}S) shells with in Be atom.

Results of these calculations are checked by using three specific procedures

1- Calculating total energy for all studied atomic systems, as in appendices (A and B.

2- Checking normalization condition (i.e. checking $\langle r^0 \rangle$ =1).

3- Comparing results with other published works.

Part A

4. A.1 One-particle expectation value $<r_1^n>$

4. A.1.1 He-isoelectronic series:

After analysis from Table (4.1) and figure (4.1and 4.2), one may be found many important behaviors such as:

1-The largest value for one particle expectation value $<r_1^n>$ with power n=1, in is for He-atom and equal to 0.91911, because of this atom has the smallest atomic number (Z=2) with respect to other ions in this series, this lead to smallest coulombs attraction between the nucleus and the electron in the K-shell for this ground state elements (Z goes from 2 to 10).

2- When Z increase the one particle expectation value $<r_1^n>$ increase when n equal to -1 ,-2 because of the increasing in Z will increase the attraction force between the electrons and the nucleus (i.e. total energy proportional directly with $Z<r_1^{-1}>$will decrease when n goes from 1 to 2 due to the weakly attraction force between the nucleus in outer shells.

3-For each Z, $<r_1^n>$ increase when n goes from -1 to -2, and decrease when n goes from 1 to 2.

4-When n go to zero, the expectation value $<r1^0>$ go to unity because of the normalization condition has been applied, this will certificate results in table (4.1).

5-The $<r_1^{-1}>$ increase with increasing of the atomic number, the fast of increasing approximately constant and equal [1.006, 1.0000, and 0.09999] per each element in the series this will be expressed in this equation:

$<r1^{-1}>_{i+1}-<r1^{-1}>_i=\Delta_{i,i+1}$

$\Delta_{i,i+1}=(1.006,1.0000,0.09999)\times10^{-5}$

Where $\Delta_{i,i+1}$ represent the absolute value of difference between two adjacent values of one particle expectation value .

Where i represent the order of the element in the series

4. A.1.2 Li-isoelectronic series:

After analysis for tables (4.2, 4.3and 4.4) and figures (4.3, 4.4, 4.5, and 4.6), many important behaviors can describe:

1-The largest value for one particle expectation value $<r_1^n>_{KK}$ with power n=1in this series is for Li atom and equal to 0.57312 (i.e. $<r_1>$ for Be^{+1}=0.41500 and for B^{+2}=0.32522) this happened because of this atom has the smallest atomic number (Z=3) with respect to other ions in this series. This leads to smallest coulomb, attraction between the nucleus and the electron in the K-shell for these ground state elements.

2-For each Z, the one particle expectation value $<r_1^n>$for k-shell are increasing when n goes from -1to -2 n and decrease when n goes from 1 to 2.

3-Where n goes from -1 to -2 the one particle expectation value$<r_1^n>$ increase with the increasing of the atomic number Z along the series.

4-For n go from 1, 2 the one particle expectation value $<r1^n>$ decrease by increasing the atomic number Z, due to the weakly attraction force between the nucleus and the electrons in outer shells as mentioned before.

5-The values of the one particle expectation value for $<r1^n>_{KL1}=<r1^n>_{KL3}$ equal to that of $KL(^3S)$-shells for all n for all selected ions since there is no difference between them.

5-The expectation value for $KL(^1S)$ and $KL(^3S)$ shells increase when n goes from -1 to -2 and 1 to 2 for all Z.

7-The total values of one particle expectation value for selected ions, represent the average value for different in atom and given by:

$$< r^n >= \frac{1}{3}[< r^n >_K +2 < r^n >_{KL}]$$

4. A.1.3 Four Electron Atoms (Li^{-1}, Be):

Table (4.5, 4.6) and figure (4.7, 4.8, 4.9 and 4.10), show many important behaviors such as:

1-The one particle expectation value $<r_1^n>$ for k-shell is decreases, when n goes from +1 to +2 and increase when n goes from -1 to -2.

2- One particle expectation value $<r_1^{-1}>$ for K-shell greater than that for KL(^{1}S), KL(^{3}S) and the latest greater than that for L-shells in Li^{-1} ion and Be atom ,this behavior will lead to give energy in K-shell greater than that for energy of KL-shell as in Appendix A and B.

3-One particle expectation value $<r_1^n>$ for KL(^{1}S) equal that for KL(^{3}S) for Li^{-1} ion and Be atoms.

4-For n=0 expectation value go to unity ($<r^0>=1$).

5-Total expectation value of one particle expectation value, represent the average value for different shells in atom and given by:

$$< r^n >= \frac{1}{6}[< r^n >_K + < r^n >_{KL(1S)} +3 < r^n >_{KL(3S)} + < r^n >_L]$$

4. A.2 Electronic Density at Nucleus $\rho(0)$:

4. A.2.1 He-isoelectronic series:

The results that shown in table (4.7) and figure (4.11 and 4.12), shows that: Electronic density at nucleus $\rho(0)$ increases with the increasing of atomic number Z because of the coulomb attraction force between the nucleus and the electrons.

4. A.2.2 Li-sioelectric series:

From the analysis of table (4.11), many important notes can be captured:

1-Electronic density at nucleus $\rho(0)$ increase with increasing of the atomic number Z, this happened for all shells, in each atom in the sequence.

2-Electronic density at nucleus $\rho(0)$ for K-shell greater than that for KL(^{1}s), KL (^{3}s) shells because of increasing of the distance between the electrons and the nucleus when the location of electrons changed from K-shell to KL-shell (in the two state singlet and triplet states).

3-Electronic density at nucleus for (Li atom, Be^{+1}ion&B^{+2} ion) of the Li-isoelectronic series have the same value at the KL(^{1}S) and KL(^{3}S) ,because of D$_{KL1}$ is equal to that of D$_{KL3}$as in figure(4.5).

4-Total electron density at the nucleus for each Z represents the average value for different shells at the atom in this series given by:

$$\rho_{total}(0) = \frac{1}{3}[\rho_{KK}(0) + 2\rho_{KL}(0)]$$

4. A.2.3 Four Electron atoms (Li^{-1}, Be)

After analysis for table (4.8, 4.9) and figure (4.13), many important behaviors can be captured:

1-Electronic density at nucleus $\rho(0)$ for K-shell for Be atom is greater than that for Li^{-1}, because of the atomic number for Be atom is greater than that for Li^{-1} atom as shown in figure (4.7).

2- Electronic density at nucleus $\rho(0)$ for K-shell is greater than that for KL (singlet, triplet states) for both atoms (Be, Li^{-1}) because of the increasing in the distance between the nucleus and the electrons.

3- Electronic density at nucleus ρ(0) for KL(^{1}s)(singlet)is equal to that for KL(^{3}s)for both atoms.

4- Electronic density at nucleus $\rho(0)$ for L-shell for both atoms (Be, Li^{-1}) approaches to each other at outer shell as shows in figure(4.6) because of the L-shell represents the farer shell than the nuclease ,so that ,the electronic cloud

will be focused farer the nucleus ,this can be expressed   one-particle radial density $D(r_1)$ as in the figure(4.9).

5-Total value of electronic density at the nucleus $\rho(0)$ represents the average value for different shells in atom and given by:

$$\rho_{total}(0) = \frac{1}{6}[\rho_{KK}(0) + \rho_{KL(^1S)}(0) + 3\rho_{KL(^3S)}(0) + \rho_{LL}(0)]$$

4. A.3 Standard Deviation Δr_1

4. A.3.1 He-isoelectronic series:

Table (4.1) shows many important behaviors ,such as standard deviation Δr_1 decrease with increasing of the atomic number and start from (0.56986) for He-atom to (0.09087)forNe^{+8} ion.

Mathematically decreasing behavior appears as a result of direct proportionality with respect to one particle expectation value, this from mathematical point of view, but from physical point of view ,increases in the atomic number increases coulombs attraction force, this will lead to decrease one particle expectation value ,this means that moving region for electrons will be smaller and smaller with increasing of atomic number Z ,and the uncertainty (i.e. $\Delta x \Delta p \geq \hbar/2$) of finding the electronic position will decreases and the certainty of finding r_1 will be increased .

4. A.3.2 Li-isoelectronic series:

From tables (4.2, 4.3 and 4.4) one may found some results.

1-As mentioned for He-isoelectronic series standard deviation Δr_1 decrease with increasing of atomic Number for all shells in series.

2- Standard deviation Δr_1 for K-shell is smaller than that for KL-shells (singlet, triplet states), physically when the region of freedom for electrons in their shells increases the probability of finding the exact position of this moving electron will be more harder, so that, the uncertainty of measuring the position of

electron will be increased, so, when electron move from K-shell to KL (singlet or triplet) Δr_1 will be increase.

4. A.3.3 Four Electron Atoms (Li^{-1}, Be).

After analysis for tables (4.5 and 4.6), many important behaviors can be captured:

1- Standard deviation Δr_1 for Be is smaller than for negative ions (Li^{-1}) for all shells.

2- Standard deviation Δr_1 for Be atom and Li $^{-1}$ ion for both singlet and Triplet states are equal.

3- Standard deviation Δr_1 for K-shell is smaller than that for L-shell and the latest is smaller than that for KL-shell (singlet, triplet) (i.e. $\Delta r_{1KK} < \Delta r_{1LL} < \Delta r_{1KL}$).

Part B

4. B. Nuclear Magnetic Shielding Constant σ:

4B.1.(sample1): He-isoelectronic series:

He-isoelectronic series is a group of atoms have 2-electrons in K-shell in ground state, and the atomic number expanded from 2 to10 with $1s^2$ electronic configuration.

After analysis for table (4.10) and figures (4.14,4.15 and 4.16), many important phenomena can be detected:

1- Nuclear magnetic shielding constant increase with increasing of the atomic number Z (2 to 10), physically this happened because of increasing with in $D(r_1)$ figure(4.3), in the same time peak $D(r_1)$ is shifted toward nucleus with

because of the increasing in the D(r1) ,this will lead to magnetic shielding for nucleus. .

2-The fast of the increasing in the series approximately constant and is fluctuated between $(3.550 \times 10^{-5}, 3.549 \times 10^{-5})$ per each order of increasing, so that, after checking values of σ He-isoelectronic series ,there is a relationship between any two adjacent values ,this behavior can be restricted by this relation :

$$\sigma_{i+1} - \sigma_i = \Delta_{i,i+1}$$

$$\Delta_{i,i+1} = 3.550 \times 10^{-5}, 3.549 \times 10^{-5}$$

This increasing have constant increasing for values of σ along series this behavior can be expressed mathematically by :

$\dfrac{\sigma_{i+1} - \sigma_i}{\sigma_{i+2} - \sigma_{i+1}}$ These values approximately go to unity

 (i.e. the fast of increasing is approximately constant).

4- Indirectly when nuclear magnetic shielding constant σ increase the electronic density at the nucleus $\rho(0)$ increase in the density.

5- Nuclear magnetic shielding constant increasing with the decreases of the energy.

6-Nuclear magnetic shielding constant increases with decreases of the volume of electronic cloud that surround nucleus.

4. B.2.(sample2): Li-isoelectronic series

Li-isoelectronic series is a group of atoms have same number of charges (i.e.3-electrons) with atomic number Z=3 to 5, these atoms in ground state with electronic configuration $1s^2 2s^1$ (i.e. Z changes from 3to5, number of electrons constant)

After analysis for table (4.11) and figure(4.17,4.18,4.19 and 4.20), many important phenomena can be detected:

1- Nuclear magnetic shielding constant σ increase with increase of the number of electrons 3 to 5, because of magnetic field proportional directly with No. of electrons.

2- Fast of increasing is approximately constant and fluctuated between $(4.0058 \times 10^5), (3.9982 \times 10^5)$ per each order of increasing as mentioned for He-isoelectronic series in the previous discussion, the increasing of σ can be described mathematically as:

$$\sigma_{i+1} - \sigma_i = \Delta_{i,i+1}$$

$$\Delta_{i,i+1} = 4.0058 \times 10^5 \text{ or } 3.9982 \times 10^5$$

And

$\dfrac{\sigma_{i+1} - \sigma_i}{\sigma_{i+2} - \sigma_{i+1}}$ This value approximately goes to unity (i.e. the fast of increasing is approximately constant)

4-From Figures (4.18, 4.19 and 4.20), we can see that shielding constant in Li-isoelectronic series shared between K-shell and KL (singlet, triplet) shells.

5-Nuclear magnetic shielding constant σ for KL(^{1}S)-shell equal to that of KL(^{3}S)-shell because of, $D(r_1)_{KL1}$ equale to that of $D(r1)_{KL3}$, $<r_1^n>_{KL1}$ equal to that of $<r_1^n>_{KL3}$

6-The nuclear magnetic shielding constant for KK(^{1}S) is smaller than that for KL(^{1}S),KL(^{3}S).

7-Total values of nuclear magnetic shielding constant for (Li,Be^{+1} ,and B^{+2}) Will shared between K-shell and both KL(singlet and triplet) shells with percentage of sharing as:

Li: K-shell=46.978%, Total KL=53.022% .

Be^{+1}: K-shell=46.19127%, Total KL-shell=53.8088%.

B^{+2}: K-shell=45.776%, Total KL-shell=54.219% .

Where KL-shells=KL(^{1}S)+KL(^{3}S),since KL(^{1}S)= KL(^{3}S).

This means that a percentage of magnetic shielding will be transferred from K-shell to KL-shells (singlet and triplet), but this transformation is little.

8-As mentioned for He-isoelectronic series, nuclear magnetic shielding constant σ increase with decreasing of total energy, because of both total energy and σ have a direct proportionality with $\langle r_1^{-1} \rangle$.

9- Nuclear magnetic shielding constant σ increases with decreasing of volume of electronic cloud of the atom, because of the volume of the electronic cloud decreases with the increasing of Z.

10- The increasing of the K-shell in (sample1) He-isoelectronic series is faster than that for Li-isoelectronic series (i.e. $\Delta_{i,i+1}$ for K-shell=0.177 for Li but for He-isoelectronic series to 3.550) because of sharing by KL(^{1}S)& KL(^{3}S) state in Li-isoelectronic seriese .

4. B.3.(sample3): Positively and Negatively Ionization for Li Atom (Li^{+1}ion and Li^{-1}ion):

This sample have two ions with same atomic number (Z=3), with different number of electrons ,the analysis produced shows that :

1- Total value of nuclear magnetic shielding constant for Li from table (4.11) is 10.145×10^{-5} shared between two shells K-shell and KL(^{1}S), KL(^{3}S) shells.

2-When Li positively ionized (i.e. Li^{+1}) (i.e. Z =3 and Number of electrons=2), the all shielding will done by 2-elelctron in K-shell with shielding constant of value 9.5411×10^{-5} .

3-The 3-rd electron, that located in the KL ($\sigma_{KL} = \sigma_{KL1} + \sigma_{KL3}$) in Li^{-1} ion will add 0.60392×10^{-5}, to the total value of nuclear magnetic shielding constant, for K-shell (since $\sigma_{Li} > \sigma_{Li+1}$) and ($\sigma_{Li-1} - \sigma_{Li} = 060392 \times 10^{-5}$).

4-From table (4.9) and (4.11) the 4-th electron that located in the L-shell in the

Li^{-1} ion will add 0.27452×10^{-5} (since $\sigma_{Li-1} > \sigma_{Li}$) to total value of the shielding

for K-shell and KL-shell ($\sigma_{KL} = \sigma_{KL1} + \sigma_{KL3}$) and $\sigma_{Li-1} - \sigma_{Li} = 0.27452 \times 10^{-5}$

5-The increasing from Li^{+1} to Li^{-1} is not constant.

6-In Li-atom$<r_1>_{KL1}=<r_1>_{KL3}=2.2232$, but when Li is ionized negatively the 3-rd

electron affected with the addition of new electron, and Li^{-1} $<r1>_{KL1}=<r1>_{Kl3}$ and

equal to 3.16016, so that, the addition of new electron will make the single

electron in KL (triplet and singlet states) distant from nuclease, and σ will

decrease in KL (singlet, triplet states).

4. B.2. (Sample4) Individual shells with in Be Atom:

   This sample atomic number Z= 4, number of electrons=4, and after analysis

for table (4.8) and figure (4.22,4.23), many important phenomena can be

detected such as:

1- Nuclear magnetic shielding constant is shared among four shells, K-shell, KL

(singlet, triplet) and L-shell in the atom, so that, the percentage of sharing for

each individual shell is   :

For K-shell=43.786%.

For L-shell=6.214 %.

For KL-shells=KL(^{1}S)+KL(^{3}S)=50 %(Because of KL(^{1}S)= KL(^{3}S))

Since: $[\frac{\sigma_{shell}}{\sigma_{total}}] \times 100$

2- Nuclear magnetic shielding constant will decreases when go from K-shell to

L-shell through KL(singlet and triplet states) ,this decreasing had been restricted

be same relation that restrict the increasing for the total value of σ for He-

isoelectronic series and Li-isoelectronic series as mentioned in previous

discussions.

4. B.2. (Sample5): Parallel Increasing of Atomic Number and Number of Charges for He, Li and Be Atoms:

Atomic number in this sample Z=2, 3, 4, number of charges=2, 3 and 4 From figure (4.17) nuclear magnetic shielding constant for this sample linearly increases with increase of Z and number of electrons.

4-2 Conclusions:

After analysis for results that introduced in this work, many ideas are detected and they can be summarized as follow:

1- Nuclear magnetic shielding constant σ have a restricted increasing with increasing of Z, along series as in [He-isoelectronic series, Li-isoelectronic series] for fixed number of charges

2- Nuclear magnetic shielding constant σ have a restricted increasing with increasing of number of electrons for [He-isoelectronic series, Li-isoelectronic series] for fixed atomic number Z in each atom.

3- Nuclear magnetic shielding constant σ have unrestricted increasing with increasing of both Z and number of charges for He, Be and Li.

4- There is a relation, restricts the values of σ for ions and atoms in He-isoelectronicserise, Li-isoelectronic serise , can be described as:

$$\sigma_{i+1} - \sigma_i = \Delta_{i,i+1}.$$

5-The same relation, that restricts He-isoelectronicserise, Li-isoelectronic serise will restricts the decreasing for values of σ with in the individual shells of Be atom.

6-There restricted behavior restricts the increasing of values of $<r_1^{-1}>$ along He-isoelectronic series and this behavior can be described mathematically with a relation have same form of the relation that restricts values of σ as:

$$<r_1^{-1}>_{i+1}-<r_1^{-1}>_i=\Delta_{i,i+1}$$

7-There is a small change in total value of σ when the Li atom is positively and negatively ionized (Li^{-1}, Li^{+1}), but there is larger change in the total value of the σ when the atomic number (Z) is changed with constant number of electrons as in (Li, Be^{+1}&B^{+2}).

8-Shielding effect usually shared between shells, within many electron atoms.

9-when Z increases in each sequence the uncertainty decreasing (i.e. Δr_1 decrease).

Suggestions for future work

We suggest some studies as flows:

1-Astudy for the nuclear magnetic shielding constant by using correlated wave function and finding the difference with the results of using the uncorrelated wave function.

2- Using the graphical integration to find the nuclear magnetic shielding constant from practical data of x-ray forming factor.

3-Study for the nuclear magnetic shielding constant for Be-isoelectronic series, Z=4 to 10.

1. INTRODUCTION

1.1 Extra Nucleus Magnetic Generators within Atomic Structure

The building of the atom naturally contains charged units are "electrons and protons" that are negatively and positively charged respectively.

These charged particles do not have a static state but they are moving particle and obeying the Heisenberg uncertainty principle $(\Delta x \Delta p \geq \hbar/2)$.

This will produce a magnetic phenomena affect the behavior of these charged particles with each other and affects the nearest atoms if the atom is a unit of building for bigger structure such as molecules or solids.

1.2 The Nuclear Magnetic Shielding Phenomenon

High precision measurement of nuclear magnetic moments for light nuclei such as H and He by the Rabi resonance method [1] have proved its necessarily to take in account the faint shielding of their magnetic field in the nuclear region by the Larmor precession of outer electronic shells.

Dr. H.L. Anderson was the first to turn the attention of physicists of the world to importance of this problem [2].

Theoretically an applied electronic or magnetic multipole field induces an electric and magnetic multipole moments in closed shell atom or ion this induced moment is proportional to the applied field.

The induced electric or magnetic moments give rise to secondary field which has the special symmetry of the applied field., so that, for one- electron atom, the diminution of homogeneous external magnetic field

$$\vec{H} = \nabla \times \vec{A} \tag{1.1}$$

$$\vec{A} = \frac{1}{2}[\vec{H} \times \vec{r}] \tag{1.2}$$

Where:

$\vec{A}$ is magnetic vector potential

$\vec{H}$ is the vector quantity of the external applied field

$\vec{r}$ is distance between nucleus and electron inside atomic system

At the center of the atom can be obtained from the Biot-Savart law

$$\Delta\vec{H} = (e/c)\frac{(\vec{r} \times \vec{V})}{r^3} \tag{1.3}$$

Expressing e by $\vec{V}$ by the aid of the equation

$$m\vec{V} = \vec{P} + (e/c)\vec{A} \tag{1.4}$$

And averaging over a stationary state of atom, usually the ground state.

If the angular momentum $\vec{r} \wedge \vec{P}$ is Zero, there remains from (1.3)

$$-\Delta\vec{H} = (e^2/mc^2)\frac{(\vec{r} \times \vec{A})}{r^3} \tag{1.5}$$

$$= e^2/2mc^2)[\frac{\vec{r} \times (\vec{H} \times \vec{r})}{r^3}] \tag{1.6}$$

On averaging over spherically symmetric state, the result is

$$(-\frac{\Delta H}{H}) = \frac{1}{3}\alpha^2 < \frac{a_H}{r} >_{Av.} \tag{1.7}$$

Where a_H is the Bohr radius and α the fine structure constant.

For many electron system with spherically symmetric state

$$\sigma = (\frac{-\Delta H}{H}) = \frac{1}{3}\alpha^2\sum_{i=1}^{N} < \frac{a_H}{r_i} >_{Av.} \tag{1.8}$$

σ is the nuclear magnetic shielding constant where r_i is the distance between

the nucleus and electron with label "i"

N is number of electrons inside atom [3, 4, 5]

$$< \frac{a_H}{r_i} >_{Av.} = \int \psi^* (\frac{a_H}{r_i}) \psi d\tau \tag{1.9}$$

Then $$\sigma = (\frac{\alpha^2}{3}) \int \psi^* [\sum_{i=1}^{N} (1/r_i)] \psi d\tau \tag{1.10}$$

Since:

$< \dfrac{a_H}{r_i} >_{Av.}$ Average value of $(a_H r_i^{-1})$

$r_i = r_i / a_H$

1.3 The Importance of Studying the Nuclear Magnetic Shielding Constant

The studying of the nuclear magnetic shielding constant may be used many applications but the most famous applications are:

1- Finite Nuclear Size:

Interest in atomic shielding factor results from there effect for reducing the apparent coupling of the nuclear multipoles with external applied fields.

The magnetic dipole is of particular interest in this regard since measurements of nuclear magnetic moment are sufficiently precise to warrant inclusion of shielding correction. Experiments to measure nuclear magnetic moments involve the interaction energy of the applied field with the nuclear magnetic moment. For a nucleus described by a state function in $\Psi(\vec{r}_1, ..., \vec{r}_A)$ magnetic field B(r_i),the interaction energy is:

$$E_I = -\mu_N \int d^3 r_1 .... d^3 r_A \Psi^* (\vec{r}_1, ..., \vec{r}_A) \times \sum_{i=1}^{A} [g_l(i)\vec{I}_i + g_s(i)\vec{S}_i \times \vec{B}(r_i) \Psi(\vec{r}_1, ..., \vec{r}_A)]$$

$$\tag{1.11}$$

Where $\mu_N = \dfrac{e\hbar}{2Mc}$ is the nuclear Bohr magneton, $g_s(i)$ is the gyro magnetic ratio of the nucleon, and $g_l(i)$ is one for proton and Zero for neutron; $\vec{I}_i$ is the orbital angular momentum, and $\vec{S}_i$ is the spin.

After many simplifications, the interaction energy given as:

$$E_I = -\vec{\mu} \cdot \vec{B}(1 - \sigma - \delta\sigma) \tag{1.11}$$

where σ is the dipole shielding factor

$\delta\sigma$: Additional contribution correction to the nuclear magnetic shielding factor [5]

2- Checking the Experimental and Theoretical Data of the x-ray form Factor

The experimental data of the formula that results relating x-ray forming factor with nuclear magnetic shielding constant that produced by the "Yukio Obata"

$$\int_0^\infty f(k)dk = 3/2(\pi/\alpha^2)\sigma \tag{1.12}$$

Where $f(k)$:is the form factor

$K = (2\pi/\lambda)(\vec{S} - \vec{S}_0), \vec{S} \ \& \ \vec{S}_0$ are unite vectors along the direction of the diffraction and incident beam, λ is the wave length of radiation.

By making the graphical integration, for the experimental results of x-ray scattering. the integration will solved easily ,and compared with other side of the formula [6].

1.4 Historical Development

1941 ‖ W. E. Lamb ,JR [2]

From 40s of the 20th century to the middle of the first decade of 21st century, many researchers (physists and chemists) were trying to calculate the nuclear magnetic shielding constant by using different Quantum mechanical methods that represent the form of the wave function, different published Data for wave functions, different mathematical tools and different computers.

So that, the historical growth of development for calculations are detected as follows:

-*Main work:*

1-An equation has been derived to describe the induced magnetic shielding constant at nuclease that put under influence of an external magnetic field in term of $\vec{H}$ & Z (where $\vec{H}$ is the external magnetic field).

2-the correction on g-factor calculations

-*Method that used:*

The Fermi-Thomas atom models are used.

1950	E. Hylleraas and S. Skavlem [1]

-*Main work:*

1-The nuclear magnetic shielding constant are calculated for He atom

2-The nuclear magnetic shielding constant for the atom H_2

-*Method that used::*

Wave function that used in this calculations for He atom are:

1)1st order Approximation

2)2nd order approximation

3)3rd order approximation

4) $\Psi = \Psi(r_{1a}, r_{1b}, r_{2a}, r_{2b}, r_{12}, r_{ab})$

1958	F. T.Ormand and F.A. Matsen [3]

-Main work:

The nuclear magnetic shielding constant for:

1)Two-electron system (He,H^{-1},Li^{+1},Be^{+2})

2)Three electron system (Li,Be^{+1})

3)4-electron system(Be)

- Method that used:

 wave function that used are:

1-open configuration wave function

2-closed configuration wave function

1959	T.P.Das and R.Bersohn [7]

-Main work:

nuclear magnetic field was found for the H_2-molcule

- Method that used:

The Variation method are used in these calculations

1961	G.G.Hall [8]

-Main work:

For isoelectronic sequence

1) σ determined theoretically

2) σ determined experimentally

-Method that used:

The energy was the start point in this calculation and in two categories:

1) Non-relativistic energy for theoretical calculations

2) Relativistic energy for experimental calculations

1962	J. N. Silverman and Y.Obata [6]

-Main work:

He found sum rule relating coherent X-ray scattering Data to the diamagnetic nuclear shielding constant & σ was computed for Br atom

-Method that used:

Graphical integration of the experimentally determined X-ray scattering factor curve for Br

-Computers that used:

Assembly program for one-electron operators developed for the IBM360/75 computer

1963	M.L.Rustgi and P.Tiwari [4]

-Main work:

The nuclear magnetic shielding constant for two ,three & four electron system :

1) He-isoelectric series(He,Li^{+1},Be^{+2})

2)Li-isoelectric series (Li,Be^{+1})

3)Be-atom

-Method that used:

1) The best SCF wave function of Roothan,sachs & Weiss are used, and the method of E.Q.Hyllaraas and Skav.lem are used

2) The method of Silverman and Obata for calculating the nuclear magnetic shielding constant by using X-ray form factor.

-Computers that used:

The university of southern California Honey well 800 electronic computer

| **1964** | M. R. Baker,C. H. Anderson and N. Ramsey[9] |

-Main work:

Diamagnetic shielding constant for atom is specific molecules are calculated such as:

(1)F in HF   (2)F in F$_2$ (3)N in N$_2$

1969	F.D.Feiock and W.R.Johnson [5]

-Main work:

The nuclear magnetic shielding constant for

1) Atoms of atomic No. (Z=1to92)

2)All shells of natural Hg-atom

3)For some atoms of He-isoelectronic series

4)Comparison are made with non-relativistic coupled HF calculated

-Method that used :

the closed-shell atomic system based on relativistic Hartree-Fock salater (RHFS) electron theory

-Computer that used:

 UNIVAC-1107 COMPUTER AT Notre Dame

1972	R. Benesch [10]

-Main work:

 He did work on the convergence of the Z^{-1} expansion of the nuclear magnetic shielding constant σ for 2,3 &4-electronic system ,for these atoms &ions:

1)He-isoelectronic series ,Z=2 to10

2)Li-isoelectronic ,Z=3to10

3)Be-isoelectronic series Z=4 to10

-Method that used:

The Z^{-1} series expansion of Hartree-Fock equations are used.

-Computer that used:

1) IBM360/75 computer at the University of Water100

2) IBM 360/50 computer at Queen University.

1976	M.L. Sachdeva and S.P.Puri[11]

-Main work:

The nuclear magnetic shielding constant are evaluated for Cs^{+1},Cs

-Method that used:

1)Self consistent field Hartree-Fock wave function by Roothan expansion

2)Virial theorm are used in these computations

1977	C. F.Bunge [12]

-Main work:

The nuclear magnetic shielding constant are determined for Be ground state atom with uncertainty 2%

 -Method that used:

An external configuration interaction (CI) wave function one used

1982	E.Klempt, R.Schuze and H.Walf [13]

-Main work:

The nuclear magnetic shielding constant are determined of protons

for(HBr and H_2O)

-*Method that used:*

THE High resolution NMR are used for these determinations

| **1988** | F. W.king [14] |

-*Main work*:

High accurate calculations are made for nuclear magnetic shielding constant σ for Be^{+1} and the accuracy make them useful bench mark for more approximate computational schemes.

-*Method that used:*

Extensive variational calculations on the ^{2}S ground state of Be^{+1},using four term expansion of Hyleraas-type functions

-*Computer that used:*

Supper computer time by Cray research, Inc. at the computer center of university Wisconsin-Ean.

| **1989** | F. W. King [15] |

-*Main work*: the nuclear magnetic shielding constant σ for same members of the Li-isoelectronic series ^{2}S ground state for these atoms: (Li,B^{+1},N,O,F&Ne)

-*Method that used*:

Extensive Variation calculations using Hyleraas-type functions are used

-Computer that used:

The computerized calculation was made at :

1)University of Wisconsin-Ean clair computer center

2)National center for supper computer application.

| **1990** | F. W.King [16] |

-Main work:

The nuclear magnetic shielding constant σ determined for some low-lying exited state ^{2}S states of Li-isoelectronic series   for $3 \leq Z \leq 10$,the 3^2S,4^2S &5^2S state are studied for Li and Be and 3^2S & 4^2S state for the other ions

-Method that used:

Hyllaraas basis set are used.

-Computer that used:

The calculations was made at:

1)Claire computer center at Wisconsin-Eau University

2)National center for supper computer application at the university of Illinois at Urbana Champaign

| **1991** | F. W.King [17] |

-Main work:

The nuclear magnetic shielding constant σ are calculated for some low-lying exited ^{2}S state of Li-isoelectronic series

-Method that used:

The Hylleraas-type wave functions are used *-Computer that used:* Super computer of the National center for supper computer application at the university of Illinois at Urbana champing.	

1995	J. Komasa ,W. Cenek and J. Rychlewski [18]

-Main work:

Nuclear magnetic shielding constant for ^{1}S ground state Be atom.

-Method that used:

-Corrected Gaussian wave function are used with 1200 term

-Variational theorm.

1997	F. W. King [18]

-Main work:

The nuclear magnetic shielding constant σ calculated for Li ground state atom.

-Method that used:

Hyllaraas wave function with 602 & 760 term.

2002	B. K. Abass [19]

-Main work:

The nuclear magnetic shielding constant σ is calculated for Li^{-1} ground state atom.

-Method that used:

Clementi and Roetti wave function are used uncorrelated wave function

-Computer that used:

PC computer

2004	M. A. AlKaabi [20]

-Main work:

The nuclear magnetic shielding constant σ is calculated for Li ground state atom.

-Method that used:

1) Correlated wave function arte used by using configuration interaction method where Weiss (1961) with correlated 2-particle density of AL-Bayati(1984)

2) Uncorrelated Hartree-Fock (HF) wave function

Computer that used:

PC computer(pentume3)

Aim of work

The aim of this work is to evaluate the total and individual values of nuclear magnetic shielding constant for five atomic samples in the way to finding a relation relates values of nuclear magnetic shielding constant through 2, 3-electron like ions , and a relation relates values of nuclear magnetic shielding constant for individual shells inside 4-electron structure.

Appendix(C)
Data of wave functions

1-*Data that used is for He-isoelectronic series published by* ***Clementi*** *and* ***Roetti****[45]*

- Li^{+1} ion:

n	ζ	C
1	2.45055	0.89066
1	4.57259	0.12328
1	6.67032	0.00088

- **Be^{+2} ion:**

n	ζ	C
1	3.43071	0.89855
1	5.63150	0.09068
1	7.35143	0.02158

- **B^{+3} ion:**

n	ζ	C
1	4.44422	0.93036
1	7.90274	0.77860
1	11.31380	0.00013

- C^{+4} **ion:**

n	ζ	C
1	5.44726	0.94428
1	9.80425	0.06382
1	14.61460	-0.00125

- N^{+5} ion:

n	ζ	C
1	6.45215	0.95445
1	11.6988	0.05228
1	19.74440	-0.00096

- **O^{+6} ion :**

n	ζ	C
1	7.45601	0.96175
1	13.66210	0.04445
1	22.59050	-0.00121

- **F^{+7} ion:**

n	ζ	C
1	8.44950	0.96398
1	15.20300	0.04150
1	24.63050	-0.00103

- **Ne^{+8} ion:**

n	ζ	C
1	9.45544	0.96961
1	17.36970	0.03573
1	27.77710	-0.00138

2-*Data that used for three ions of Li-isoelectronic series published by* **Weiss** *for(Li atom,Be^{+1}ion &B^{+3}ion) [46]*

- Li atom:

n	l	ζ	C1	C2
1	0	3.0	0.89116	-0.13923
3	0	9.6	-0.00089	0.00039
3	0	3.38	0.10842	-0.01706
3	0	2.25	0.05032	0.01642
3	0	1.24	-0.00087	0.39542
3	0	0.757	0.00075	0.65346

- **Be^{+1} ion:**

n	l	ζ	C1	C2
1	0	4.0	0.91711	-0.19922
3	0	10.81	-0.00129	0.00045
3	0	4.68	0.07960	-0.01081
3	0	3.40	0.04314	0.00728
3	0	1.97	-0.00331	0.42943
3	0	1.31	0.00178	0.61599

- **B^{+2} ion:**

n	l	ζ	C1	C2
1	0	5.0	0.93299	-0.23270
3	0	12.0	-0.00151	0.00050
3	0	5.97	0.06390	-0.00787
3	0	4.28	0.03661	0.00451
3	0	2.70	-0.00409	0.42344
3	0	1.863	0.00192	0.62350

3- *Data that used for ground state Be and He atoms published by CARLOS.F. Bungee [29]*

- **He atom**

n	C	ζ
1	1.4595	1.347900
3	5.3244	-0.001613
2	2.6298	-0.100506
2	1.7504	-0.270779

- **Be atom:**

n	ζ	*C1*	*C2*
1	5.7531	0.285107	-0.16378
1	3.7156	0.474813	-0.155066
3	9.9670	-0.001620	0.000426
3	3.7128	0.052852	-0.059234
2	4.4661	0.243499	-0.031925
2	1.2919	0.000106	0.387968
2	0.8555	-0.000032	0.685674

*Data that used for ground state Li^{-1} ion published by **Clementi** [45]*

n	ζ	C1	C2
1	2.47472	0.89760	-0.10034
1	4.69209	0.11212	-0.01100
2	0.26763	-0.00003	0.39768
2	0.53399	0.00016	0.56089
2	1.01192	-0.00108	0.20478
2	1.66285	0.00750	-0.07906

Appendix (A)
Ground State Energy calculations

In theoretical atomic calculations the energy results used as a tool to certificate the results and the programs that used.

So that, the energy are calculated in this work and the results are tabulated to certificate our results and the accuracy of the programs that used in these calculations.

For any N-electron atomic wave function that satisfies the Viral theorem the energy expectation value is related to the potential energy by:

<E>=1/2<V>................. (A.1)

Where <E> the total expectation value of the energy ,<V>the total expectation value of the potential energy that simplified the sum of the electron –nuclear attraction energy &the inter electronic repulsion energy [46],which given as:

$$< V >= -Z\sum_{i}^{N} < r_i^{-1} > + \sum_{i<j}^{N} < r_{ij}^{-1} > \ \ldots\ldots. (A.2)$$

Where Z is the atomic no. of atom, N is the no. of electrons in atom $< r_i^{-1} >$ is the one particle expectation value and $< r_{ij}^{-1} >$ is the inter particle expectation value with power n=-1.

Table (A-1) Kinetic, Potential and Total Energy for Li

Shell	Present work Vee	Present work Ven	Present work V	Present work T	Present work E_{total}	Published work[46] E_{total}
KK	1.649877	-8.05503	-6.40515	3.202577	-3.202577	-----
KL(^{1}S)	0.322679	-4.5456	-4.22292	2.111461	-2.111461	-----
KL(^{3}S)	0.308384	-4.5456	-4.23722	2.11861	-2.11861	-----
Total	2.28094	-17.1462	-14.8653	7.43265	-7.43265	-7.43272

Table (A-2) Kinetic, Potential and Total Energy for B^{+2}

Shell	Present work Vee	Present work Ven	Present work V	Present work T	Present work E_{total}	Published work[46] E_{total}
KK	2.91448	-23.4034	-20.4889	10.24446	-10.24446	-----
KL(^{1}S)	0.76923	-13.8597	-13.0905	6.54523	-6.54523	-----
KL(^{3}S)	0.71165	-13.8597	-13.1481	6.57402	-6.57402	-----
Total	4.39536	-51.1228	-46.7274	23.36372	-23.36372	-23.37599

Table (A-3) Kinetic, Potential and Total Energy for Be^{+1}

Shell	Present work Vee	Present work Ven	Present work V	Present work T	Present work E_{total}	Published work[46] E_{total}
KK	2.27324	-14.7297	-12.4565	6.22824	-6.22824	-----
KL(^{1}S)	0.51275	-8.57944	-8.06669	4.03334	-4.03334	-----
KL(^{3}S)	0.54832	-8.57944	-8.03112	4.01556	-4.01556	-----
Total	3.33431	-31.8886	-28.5543	14.27715	-14.27715	-14.27739

Table (A-4) Kinetic, Potential and Total Energy for Li[-1]

Shell	Present work Vee	Present work Ven	Present work V	Present work T	Present work E_{total}	Published work[20] E_{total}
KK	1.650308	-8.05649	-6.40619	3.203093	-3.203093	-----
KL(^{1}S)	0.238628	-4.40255	-3.92529	1.962645	-1.962645	-----
KL(^{3}S)	0.231686	-4.40255	-3.93917	1.969587	-1.969587	-----
LL	0.162769	-1.675	-1.51223	0.756114	-0.756114	-----
Total	2.753704	-18.5366	-15.7829	7.891438	-7.42822	-7.42822

Table (A-5) Kinetic, Potential and Total Energy for Be

Shell	Present work Vee	Present work Ven	Present work V	Present work T	Present work E_{total}	Published work[45] E_{total}
KK	2.272987	-14.7275	-12.4545	6.227257	-6.227257	-----
KL(^{1}S)	0.480908	-8.4088	-7.92789	3.963944	-3.963944	-----
KL(^{3}S)	0.455559	-8.4088	-7.95324	3.976619	-3.976619	-----
LL	0.343229	-2.09009	-1.74686	0.873432	-0.873432	-----
Total	-33.6352	4.48915	-29.146	14.57302	-14.57302	-14.57301

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Appendix (B)
Inter particle expectation value$<r_{12}{}^{n}>$

To calculate the coulomb energy that restrict electron-electron interaction, the antiparticle expectation value $<r_{12}{}^{n}>$ must be calculated

$$< r_{12}{}^{n} >= \int\limits_{0}^{\infty} r^{n}{}_{12} f(r_{12}) dr_{12}$$

Where n=1, 2, 0,-1 and-2

By using the method of coulson and A.H.Neilson 1961

$$f(r_{12}) = \frac{1}{2}\left\{ \int\limits_{0}^{r_{12}} \int\limits_{r_{12}-r_1}^{r_{12}+r_1} \Gamma'(r_1,r_2) r_1 r_2 dr_1 dr_2 + \int\limits_{r_{12}}^{\infty} \int\limits_{r_1-r_{12}}^{r_{12}+r_{12}} \Gamma'(r_1,r_2) r_1 r_2 dr_1 dr_2 \right\} r_{12}$$

This function is normalized to unity [47]

$$\int\limits_{0}^{\infty} f(r_{12}) dr_{12} = 1$$

Table (B-1) One-particle expectation value $< r_{12}^n >$ and standard

deviation $\Delta \mathbf{r_{12}}$ for He-isoelectric series

Z	symbol	-2	-1	0	1	2	$\Delta \mathbf{r_{12}}$
2	He	1.84205	1.02577	1.00000	1.36213	2.36965	0.71712
3	Li^{+1}	4.72704	1.65174	1.00000	0.83659	0.88504	0.43029
4	Be^{+2}	8.94387	2.27706	1.00000	0.60583	0.46369	0.3109
5	B^{+3}	14.49501	2.9023	1.00000	0.47431	0.28372	0.24238
6	C^{+4}	21.37925	3.52744	1.00000	0.38978	0.1914	0.19866
7	N^{+5}	29.5256	4.15256	1.00000	0.3308	0.13775	0.16829
8	O^{+6}	39.14896	4.77773	1.00002	0.28734	0.10387	0.14597
9	F^{+7}	50.03141	5.40264	1.00003	0.25399	0.08113	0.12892
10	Ne^{+8}	62.24807	6.02762	1.00000	0.22756	0.0651	0.11541

Table (B-2) One-particle expectation value $<r_{12}{}^{n}>$ and standard deviation Δr_{12} for Li atom

Shell	-2	-1	0	1	2	Δr_{12}
KK	4.71716	1.64988	1.00000	0.8395	0.89361	0.43456
KL(^{1}S)	0.11995	0.30838	1.00000	3.92703	18.17525	1.67186
KL(^{3}S)	0.19511	0.32268	1.00000	3.92175	18.17525	1.65943

Table (B-3) particle expectation value $<r_{12}{}^{n}>$ and standard deviation Δr_{12} for B^{+2} ion

Shell	-2	-1	0	1	2	Δr_{12}
KK	14.9319	2.91448	1.00000	0.4838	0.29328	0.24335
KL(^{1}S)	0.62346	0.71165	1.00000	1.68878	3.29057	0.67809
KL(^{3}S)	1.17342	0.76923	1.00000	1.68313	3.29275	0.66226

Table (B-4) particle expectation value $\langle r_{12}{}^n \rangle$ and standard deviation $\Delta \mathbf{r_{12}}$ for Be^{+1} ion

Shell	-2	-1	0	1	2	$\Delta \mathbf{r_{12}}$
KK	8.1721	2.27324	1.00000	0.60717	0.46608	0.31213
KL(^{1}S)	0.327	0.51275	1.00000	2.33131	6.33399	0.96391
KL(^{3}S)	0.59024	0.54832	1.00000	2.32483	6.33399	0.94814

Table (B-5) One-particle expectation value $\langle r_{12}{}^n \rangle$ and standard deviation $\Delta \mathbf{r_{12}}$ for Li^{-1}

Shell	-2	-1	0	1	2	$\Delta \mathbf{r_{12}}$
KK	4.71906	1.65031	1.00000	0.83922	0.89275	0.43413
KL(^{1}S)	0.11016	0.23863	1.00000	5.78402	43.95767	3.2408
KL(^{3}S)	0.07382	0.23169	1.00000	5.78661	43.95768	3.23617
LL	0.04423	0.16277	1.00000	8.31543	87.00189	4.22558

Table (B-6) One-particle expectation value $<r_1^n>$ and standard deviation $\Delta \mathbf{r_{12}}$

Shell	-2	-1	0	1	2	$\Delta \mathbf{r_{12}}$
KK	8.91469	2.27299	1.00000	0.60714	0.46591	0.31192
KL(^{1}S)	0.45121	0.48091	1.00000	2.68717	8.65907	1.19925
KL(^{3}S)	0.26454	0.45556	1.00000	2.69184	8.65906	1.18872
LL	0.19042	0.34323	1.00000	3.75524	16.85231	1.65846

Table (A-6) Kinetic, Potential and Total Energy for He-isoelectronic series

Z	symbol	Vee	Ven	Present work V	Published work[46] V	Present work[46] T	Published work[46] T	Present work[46] E	Published work[46] E
2	He	1.01609	-6.72244	-5.706	-5.723	2.85317	2.86166	-2.85317	-2.86167
3	Li^{+1}	1.65174	-16.1255	-14.474	-14.473	7.2369	7.2372	-7.2369	-7.2364
4	Be^{+2}	2.27706	-29.4996	-27.223	-27.2225	13.61127	13.61121	-13.61127	-13.61129
5	B^{+3}	2.9023	-46.8748	-43.973	43.9730	21.98625	21.98682	-21.98625	-21.98623
6	C^{+4}	3.52744	-68.2501	-64.723	-64.7222	32.36134	32.36119	-32.36134	-32.36119
7	N^{+5}	4.15256	-93.6258	-89.473	-89.472	44.73664	44.73656	-44.73664	-44.73616
8	O^{+6}	4.77773	-123.002	-118.224	-11.8223	59.11233	59.11196	-59.11233	59.11114
9	F^{+7}	5.40264	-156.375	-150.972	-150.970	75.48627	75.48405	-75.48627	-75.48612
10	Ne^{+8}	6.02762	-193.749	-187.7216	-187.7198	93.86079	93.85872	-93.8608]	-93.8611

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A Study for Nuclear Magnetic Shielding Constant for Z = 2 to 10

A thesis

Submitted to College of Science at Nahrain University in Partial Fulfillments of the Requirements for the Degree of Master of Science in Physics

By

Wissam Ahmed Al-Meshhedany
(B.Sc. 2003)

Supervised By

Prof. Dr. Khalil H. Al-Bayati

2006 A.D.   **1427 A.H.**

Abstract

The nuclear magnetic shielding constant σ has calculated for He-isoelectronic series (Z=2to10), Li-isoelectronic series (Z=3to5), Be and Li^{-1} by using RHF method and Data published by Andrew W. Weiss 1963) , Cleminty and Roetti (1974) .

The calculations of σ must go through calculating many properties, so that, Electron radial density distribution $D(r_1)$ and one particle

expectation value $< r_1^n >$ are calculated, with power equal to -2, -1,

0,1and 2.

For checking the results the energy are calculated for all studied atoms and ions and all results are restricted with normalization conditions.

Electronic density at the nucleus $\rho(0)$ and Stander deviation Δr_1 are

calculated.

All introduced results physically analyzed to find the idea behind these data.

These calculations are mad by using mathcad program version 11

By using PC (Pentium 4) and all results are in atomic unite (a.u.).

v

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I would like to express my deepest appreciation and gratitude to my supervisor Prof .Dr. Kahlil H. AL-Bayati for his continuous   help and stimulated discussion during the work.

I would like to express my thanks to my friends.

Finally, I am very grateful to my family to there continuous support through this work.

Wissam Ahmed. Al-Meshhedany

CERTIFICATION

We certify that this thesis was prepared under my supervision at the College of science, Nahrain University as a partial fulfillment of the requirement for the degree of Master of Science in physics.

Signature:

Name: Dr. Khalil H. Al-Bayati
Title: Professor.
Date: /   /2006

In view of the available recommendations, I forward this thesis for debate by the examination committee.

Signature:

Name: Dr. A.K. Ahmad
Title: Assistant Professor.
Address: Head of Physics Department
Date: /   /2006

Contents

List of Appendices

Examination Committee Certification

We certify that this thesis entitled ***"A Study for Nuclear Magnetic Shielding Constant"***, is submitted by the student **Wissam Ahmed Al-Meshhedany**, and as Examination Committee, examined the student in its contents and that in our opinion, it meets the standard of a thesis for the degree of Master of Science in physics.

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Approved by University Committee of Postgraduate Studies

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Name: Dr. LAITH ABDUL AZIZ AL-AN
Title: Assistant Professor
Dean of the College of Science
Date:

List of Symbols

Symbol	Meaning
$\vec{H}$	Applied magnetic field
$\vec{A}$	Magnetic vector potential
$\vec{r}$	vector of distance between electron and nucleus
e	Electron charge
$\Delta\vec{H}$	Induced magnetic field at nucleus
m	Mass of electron
α	Fine structure
a_H	Bohr radius
ψ	Wave function
E_I	Interaction Energy for protons
μ_N	Bohr magneton
$g_s(i)$	Gyromagnetic ratio
I_i	Orbital angular momentum quantum number
$\vec{B}$	Magnetic field density
$\delta\sigma$	Additional contribution correction for nuclear magnetic shielding constant
σ	Nuclear magnetic shielding constant
$f(k)$	X-ray forming factor
λ	Wave length
$\vec{S}, \vec{S}_0$	Unit vector
Z	Atomic number
r_{12}	Distance between any tow electron for atomic structure
$\rho(0)$	Electronic density at nucleus
Δr_1	Standard deviation
E_{total}	Total energy
$\hat{H}$	Hamiltonian operator
$\delta(s)$	Spin wavefunction
$R(r)$	Radial part of wavefunction
$Y(\theta,\phi)$	Angular part of wavefunction
ϕ_i	Spin orbital wavefunction
$\varphi_i(r,\theta,\phi)$	Spatial part of wavefunction

HF	Hartree-Fock
STO	Slater Type Orbital
RHF	Roothaan Hartree Fock
χ_p	Slater Type Orbital wavefunction
p_l^m	associated Legender Polynomials
SFC	Self-Consistent field
C_p	Expansion coefficient
ζ_p	Orbital exponents
n_p	Expansion coefficient
N	Normalization costant
M	Number of States
$\Gamma(x_m, x_n)$	*Second Order Reduced Density Matrix*
$\Gamma'(x_m, x_n)$	*Spin-less two-particle density*
$D(r_1)$	*One particle Electron Density*
α	Spin up
β	Spin down
$KL(^1S)$	Singlet state
$KL(^3S)$	Triplet state
$\Delta_{i,i+1}$	Absolute value of the different between $\sigma_{i+1} \& \sigma_i$
V_{ee}	Electron -electron potential energy
V_{en}	Electron -nucleus potential energy
V	Total potential energy
T	Kinetic energy
Δr_{12}	Standard deviation for r_{12}
C_1, C_2	Expansion coefficient

دراسة ثابت الحجب النووي المغناطيسي للعدد الذري من ٢ الى ١٠
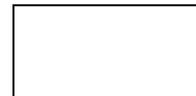
من قبل
وسام احمد امين المشهداني
(بكلوريوس،جامعة النهرين2003)

باشراف
الأستاذ د.خليل هادي البياتي

الخلاصة

تم حساب ثابت الحجب النووي لسلسلة الذرات الشبيهة بالهيليوم للعدد الذري من ٢ الى ١٠والذرات الشبيهة بالليثيوم ذات العدد الذري من ٣ الى ٥ بالاضافة الى ذرتي البريليوم والايون السالب لليثيوم باستخدام طريقة (RHF)و باستخدام البيانات المنشورة من قبل Weiss (١٩٦٣) و (Cleminityو Roetti) (١٩٧٤) .

لذلك تم حساب دالة توزيع الكثافة الشعاعية لجسيم واحد ،القيم المتوقعة لجسيم واحد للأس ٢ ،١ ،٠، ١-، ٢-، لغرض التأكد من الحسابات تم حساب الطاقة لكل الذرات والأيونات المدروسة وتم التأكد من الشرط العياري لكل الذرات المدروسة.

تم حساب الكثافة الألكترونية عند النواة والأنحراف المعياري.

كل النتائج التي تم الحصول عليها تم تحليلها فيزيائيا ويجاد التفسير الفيزيائي خلف هذه الأرقام.

هذه الحسابات تم عملها بأستخدام برنامج الماثكاد الأصدار١١باستخدام الحاسب الشخصي(بنتيوم٤) .