Study the atomic properties of 2s shell for some atoms

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Abstract

Ground state energies and other properties of 2S shell for some atoms as Be(Z=4), B(Z=5), C(Z=6) and N(Z=7) were calculated by using Hartree-Fock wave function. We found the values of potential energies in hartree unit (3.8369, 6.78565, 10.18852 and 14.41089) respectively and the other proprieties like expectation values of the position $< r_1^m >$ were in agreement with the published results. All the studied atomic properties were normalized.

Key words
Atomic Hartree-Fock, atomic properties.

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دراسة الخواص الذرية للقشرة 2S لبعض الذرات

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الخلاصة

طاقات الحالة الأرضية والخواص الأخرى لغلاف 2S لبعض الذرات مثل البريليوم (Z=4)، البورون(Z=5)، الكربون (Z=6) والنتروجين(Z=7) قد حسبت باستخدام دالة هارتري – فوك. لقد تم ايجاد قيم الطاقات الكامنة بوحدات الهارتري (3.8369، 6.78565، 10.18852 و 14.41089) على التوالي، والخواص الأخرى مثل القيمة المتوقعة للموقع $< r_1^m >$ وكانت متوافقة مع النتائج المنشورة عالميا. كل الخواص الذرية المدروسة كانت عياريه.

Introduction

Any system can be described by a wave function; it is a mathematical expression which used to describe the system properties such as the position, momentum and energy etc. The exact calculation of wave functions for many electron atoms becomes difficult because of the many electron-electron repulsions that should be ignored for simplicity. There are two main kinds of the wave functions that have been used in the approximation methods, the first one is the uncorrelated wave function Hartree-Fock (HF) which used in the present research, and the second one is the correlated wave function such as Configuration Interaction (CI) [1].

The uncorrelated wave function

According to Pauli principle the wave function for system of electrons must change sign when the coordinates of any two electrons are interchanged, so that, from mathematical point of view, the many body wave function is written as Slater determinant [2]:

$$\psi_{HF}(123...N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\Phi_1(1) & \cdots & \Phi_1(N)\\ \vdots & \ddots & \vdots\\ \Phi_N(1) & \cdots & \Phi_N(N)\end{vmatrix} \qquad (1)$$

where $\frac{1}{\sqrt{N!}}$ the multiplying factor introduced to ensure that the wave function is normalized after integrating over all the space and spin coordinates such that.[3]

$$\int \Psi^*\Psi d\tau = 1 \qquad (2)$$

where ψ^* represents the complex conjugate of the wave function and the component of one particle function is referred to as spin-orbital. Any spin-orbital may be written as the product of a space function and a spin function, where α- spin up and β-spin down.The spin wave functions are orthonormal, where:

$$\int \alpha^*(1)\alpha(1)d\sigma_1 = 1 \qquad (3a)$$

$$\int \beta^*(1)\beta(1)d\sigma_1 = 1 \qquad (3b)$$

$$\int \alpha^*(1)\beta(1)d\sigma_1 = 0 \qquad (3c)$$

The wave function for N-electron system is constructed from a basis set containing several orbital; this wave function can be written as [3].

$$\Psi_{HF}(123\cdots N)=\frac{1}{\sqrt{N!}}\left|\phi_1(1)\cdots\Phi_N(N)\right| \qquad (4)$$

$$\Phi_i(i)=\Phi(r,\theta,\Phi)\sigma(s) \qquad (5)$$

$$\Phi_{nl}=\sum_{i=1}^{j}c_n^i\chi_{nlm} \qquad (6)$$

where Φ is the spatial part, $\sigma(s)$ the spin part and the numbers in the parentheses denote the particle, and the subscripts 1, 2... N denotes the eigen state. The special function is defined by [1].

$$\chi_{nlm}(r,\theta,\Phi)=R_{NL}(r)Y_{lm}(\theta,\Phi) \qquad (7)$$

the radial part of special part of the total wave function is given by:

$$R_{nl}(r)=N_{nlm}S_{nl}(r) \qquad (8)$$

where N_{nlm} is the normalization constant, and given by

$$N_{nlm}=\sqrt{\frac{(2\xi)^{2n+1}}{(2n)!}} \qquad (9)$$

and $S_{nl}(r)=r^{n-1}e^{-\xi r}$ (10)

where $S_{nl}(r)$ is called the Slater-Type-Orbitals (STO) and ξ represents the orbital exponent.

Results and discussion

In this research we using the atomic data for Hartree-Fock wave function of Clementi and Roetti [4].

Table1: Atomic data for Hartree-Fock functions for studied atoms[4].

Be(Z=4)			*B(Z=5)*			*C(Z=6)*			*N (Z=7)*		
n	ξ	C_{2s}	*n*	ξ	C_{2s}	*n*	ξ	C_{2s}	*n*	ξ	C_{2s}
1	*3.47116*	*-0.17092*	*1*	*4.44561*	*-0.19484*	*1*	*5.43599*	*-0.20814*	*1*	*6.45739*	*-0.21677*
1	*6.36861*	*-0.01455*	*1*	*7.91796*	*-0.01254*	*1*	*9.48256*	*-0.01071*	*1*	*11.17200*	*-0.00846*
2	*0.77820*	*0.21186*	*2*	*0.86709*	*0.06941*	*2*	*1.05749*	*0.08099*	*2*	*1.36405*	*0.17991*
2	*0.94067*	*0.62499*	*2*	*1.21924*	*0.75234*	*2*	*1.52427*	*0. 75045*	*2*	*1.89734*	*0.67416*
2	*1.48725*	*0.26662*	*2*	*2.07264*	*0.31856*	*2*	*2.68435*	*0.33549*	*2*	*3.25291*	*0.31297*
2	*2.71830*	*-0.09919*	*2*	*3.44332*	*-0.12642*	*2*	*4.20096*	*-0.14765*	*2*	*5.08238*	*-0.14497*

One- particle radial density distribution function D(r1)

We calculated one-electron radial density distribution function $D(r_1)$ (the probability of finding the electron in a spherical shell of distance r_1 from the nucleus) using the following equation [5] :

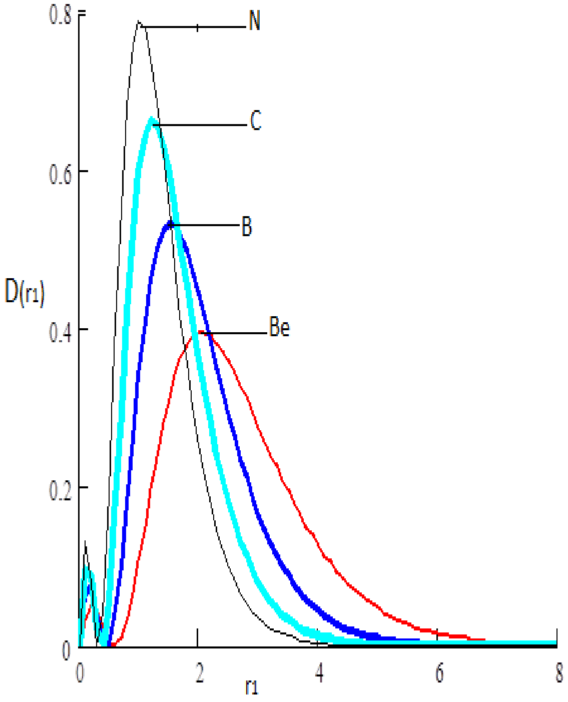
$$D(r_1)_{2s} = R^2{}_{2s}(r_1) r_1{}^2 \qquad (11)$$

where $R_{2S}(r_1)$ represented the radial part of the wave function.

In Table 2 we listed the results of maximum values of $D(r_1)$ with the corresponding position r_1, Fig. 1 represents relation between $D(r_1)$ with the position for 2S shell of studied atoms. We noted from Table 2 that the maximum values for $D(r_1)$ increase when the atomic number increases, that means the probability of finding an electron increase, and the locations of these peaks are contracted toward the nucleus due to effect of nuclear charge increases.

Table 2: The values of positions and maximum values of the $D(r_1)$ for studied system for 2S shell.

Atom	2S-shell			
	Peak 1		Peak 2	
	R_1	$D_{max}(r_1)$	R_1	$D_{max}(r_1)$
Be	0.21	0.053	2.10	0.396
B	0.18	0.082	1.55	0.533
C	0.15	0.111	1.20	0.663
N	0.12	0.139	1.00	0.791



Figure(1):Relation between the one-particle radial density distribution function D(r1)and the position (r1)

One-particle expectation value $\langle r^m{}_1 \rangle$

The one-particle expectation value and the standard deviation Δr_1 were calculated by using the following equations [5]:

$$\langle r_1{}^m \rangle = \int_0^\infty D(r_1) r_1{}^m dr_1 \qquad (12)$$

$$\Delta r_1 = \left[\langle r_1{}^2 \rangle - \langle r_1 \rangle^2 \right]^{1/2} \qquad (13)$$

Consecutively for different values for m where m is integer number and takes the values $-2 \leq m \leq 2$, the results of the radial expectation values of $< r_1{}^m >$ and the standard deviation for 2S shell of studied atoms are tabulated in Table 3.

Table 3:The values of one-particle expectation values and standard deviation for 2S shell of studies atoms.

Atom		$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^{0} \rangle$	$\langle r_1^{1} \rangle$	$\langle r_1^{2} \rangle$	Δr_1
Be	Present work	1.056119	0.522515	0.9999993	2.649405	8.426407	1.18619
	Ref.[6]	1.055647	0.522522	_-__	2.649414	8.426431	-
B	Present work	2.04951	0.71887	1.0000011	1.977096	4.709244	0.89461
	Ref.[6]	2.024533	0.712882	-	1.977064	4.709135	-
C	Present work	3.255826	0.896783	1.000008	1.589342	3.05171	0.72504
	Ref.[6]	3.255510	0.896798	-	1.589344	3.052064	-
N	Present work	4.754181	1.078189	1.000011	1.332295	2.149463	0.61193
	Ref.[6]	4.753636	1.078176	-	1.332277	2.149438	-

From Table 3 we noted :

The one-particle expectation value < r_1^m > increase as the atomic number (Z) increases for negative value of m, The $\langle r_1^{-1} \rangle$ represents to the attraction energy expectation value and $\langle r_1^{-2} \rangle$ indicates how the density distribution in near regions of the nucleus.

For positive value of m the one particle expectation value decreases as Z increases.

The standard deviation for all studied systems Δr_1 decreases with increasing atomic number, because the distance between electron-nucleus becomes small.

Inter-particle radial density distribution function $f(r_{12})$

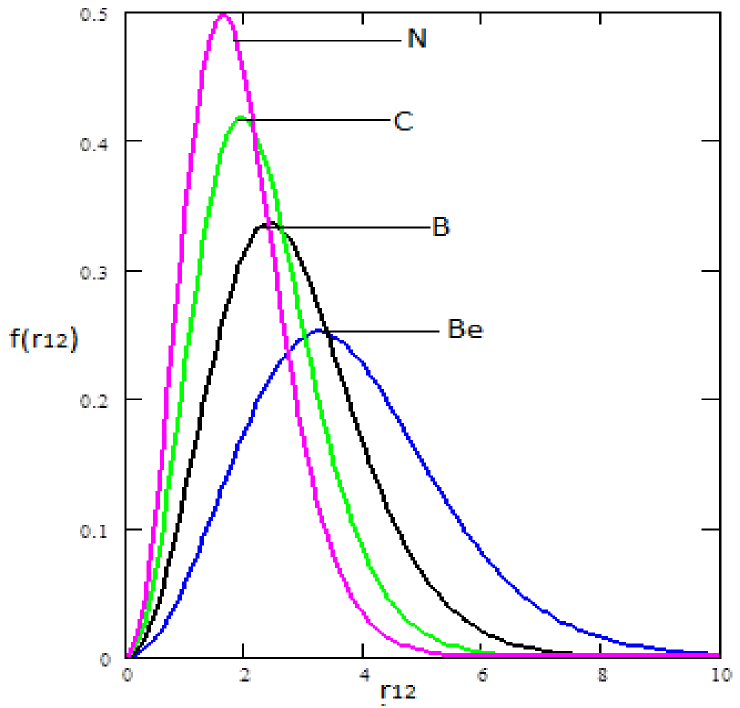
The inter-particle radial density distribution function $f(r_{12})$ was evaluated using the following equation below [7]:

$$f(r_{12})_{(2S)} = 0.5 r_{12} \left[\begin{array}{l} \int_{r_{12}}^{\infty} r_1 \int_{r_1 - r_{12}}^{r_1 + r_{12}} R_{2S}{}^2(r_1) R_{2S}{}^2(r_2) r_2 dr_2 dr_1 + \\ \int_{0}^{r_{12}} r_1 \int_{r_{12} - r_1}^{r_{12} + r_1} R_{2S}{}^2(r_1) R_{2S}{}^2(r_2) r_2 dr_2 dr_1 \end{array} \right] \quad (14)$$

where $f(r_{12})$ represented the Coulomb repulsion between a pair of electron in L-shell. The results for all systems as tabled in Table 4, and Fig. 2 indicates the relation between $f(r_{12})$ and inters electronic distance r_{12}.

Table4:The location and maximum values of $f(r_{12})$ for studied systems.

Atom	r_{12}	$f(r_{12})$
Be	3.33	0.251
B	2.5	0.336
C	2	0.417
N	1.67	0.497



Figure(2):Relation between inter-particle radial density distribution function and the distance (r12).

From Table 4 and Fig. 2 we notes:

As atomic number increase, the distance r_{12} between two electron decrease, this behavior from the fact that, each shell shrinkage toward the nucleus because the Coulomb attraction force will be greater than the Coulomb repulsion force between unlike spin in 2S shell.

The maximum value $f(r_{12})$ increases as Z increases because of increasing the atomic number which lead to increases the attraction force between the nucleus and the electrons.

Inter-particle expectation value $\langle r_{12}^{m} \rangle$

The inter-particle expectation value $\langle r_{12}^{m} \rangle$ and standard deviation Δr_{12} can be defined as [8]:

$$< r_{12}{}^{m} >= \int_{0}^{\infty} f(r_{12}) r_{12}{}^{m} dr_{12} \qquad (15)$$

$$\Delta r_{12} = \sqrt{< r_{12}{}^{2} > - < r_{12} >^{2}} \qquad (16)$$

The results are presented in Table 5.

Table 5: expectation values $\langle r_{12}^{m} \rangle$ where -2≤m≤2 and standard deviation.

Atom		$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^{0} \rangle$	$\langle r_{12}^{1} \rangle$	$\langle r_{12}^{2} \rangle$	Δr_{12} Standard deviation
Be	Present work	0.19041	0.34322	0.9999	3.75523	16.8527	1.65859
	Ref.. [9]	0.1904 1	0.34322	1.00000	3.73524	16.85233	1.65846
B		0.34456	0.46027	1.00002	2.80513	9.41859	1.24492
C		0.53609	0.57288	1.00002	2.25673	6.10347	1.00531
N		0.76614	0.68376	1.0002	1.89291	4.29894	0.84606

from analyzing the results in Table 5 we noted :

The inter-particle expectation value $\langle r_{12}^{m} \rangle$ increase as Z increases for -ve values of m, where as these values decreases for positive of m. The standard deviation decrease when Z increase for all systems. The standard deviation contains much information concerning the shape of the two-particle radial density distribution function $f(r_{12})$, the Δr_{12} shape results indicate $f(r_{12})$ become less diffuse.

The expectation values of potential energy $\langle V \rangle$

The total energy and the potential energy in atomic unit can be written as [8].

$$\langle V \rangle = -Z\left\langle \frac{1}{r_1} \right\rangle + \left\langle \frac{1}{r_{12}} \right\rangle \tag{17}$$

$$\langle T \rangle = \frac{\langle V \rangle}{2} \tag{18}$$

and the results are listed in Table 6.

Table 6: The expectation values for attraction, repulsion and kinetic energies of the 2s shell for studied atoms.

Atom		$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$
Be	present work	4.18012	0.34322	3.8369	1.91845
	Ref.[9]	4.18018	0.34322	3.83696	1.91848
B		7.12887	0.34322	6.78565	3.392825
C		10.7614	0.57288	10.18852	5.094258
N		15.09465	0.68376	14.41089	7.205443

From the Table 6, The results of the expectation values for attraction potential $\langle V_{en} \rangle$ and the repulsion potential $\langle V_{ee} \rangle$ nucleus-electron, and the results the expectation values of the total energy or Hartree-Fock energy are consistent with published results. Both $\langle V_{en} \rangle$ and $\langle V_{ee} \rangle$ increase when atomic number increases. This result can be understood from the fact that all shell shrink toward the nucleus due to the attraction force between the protons and the electrons increase because the distance between nucleus-electron and electron-electron decrease, this result leads to increase in repulsion potential energy and attraction potential energy, the expectation values for total potential energy $\langle V \rangle$ increase in each system because the increase of $\langle V_{en} \rangle$ are larger than that of $\langle V_{ee} \rangle$. we noted that the increase the energy of attraction is greater that the increase in the energy of repulsion when Z increase in order to maintain the entity of v the atom. The expectation energy for kinetic energy $\langle T \rangle$ increase when Z increases.

Conclusions

The kinetic and potential energies of selected atoms (Be, B,C AND N) have been investigated theoretically. It was found that these energies increased with respect to atomic numbers Z. Anther atomic properties such as one-particle radial density distribution function $D(r_1)$ and inter-particle radial distribution function $f(r_{12})$ were studied. the results showed $D(r_1)$ and $f(r_{12})$ were increased with atomic number. Moreover, the expectation values of position $\langle r^{m}{}_{1} \rangle$ was in perfect agreement with published results for various values of m(-2,-1,1and2).

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