

Radial expectation values and electron density at the nucleus of four electron systems

القيم المتوقعة القطرية والكثافة النووية عند النواة للأنظمة الرباعية الإلكترون

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Abstract:

In this paper it is formulated the Hartree-Fock equations for multi-electron systems in terms of two electron density function $\Gamma(r_1, r_2)$ in order to solve Hartree-Fock equations in the algebraic approximation which called Hartree-Fock-Roothaan (H-F-R) method using slater type atomic orbitals published by ref. [31] for Be atom and ref. [32] for B^{+1} ion . The radial expectation values of one particle $\langle r_1^n \rangle$, two particles $\langle r_1^n \cdot r_2^n \rangle$ and inter particles $\langle r_{12}^n \rangle$ where (n=-1,-2, 1,2) of Be atom and B^{+1} ion in its ground state are calculated using Hartree-Fock wave function with analysis the one electron radial density function $D(r_1)$ and inter electron density function $f(r_{12})$ for each shell. Electron density at the nucleus $\rho(o)$ also evaluated for each shell and for total systems , using partitioning technique ,were in these systems there are six shells : $K\alpha K\beta(K(1S))$, $K\alpha L\alpha (KL(3S))$, $K\beta L\alpha (KL(1S))$, $K\alpha L\beta (KL(3S))$, $K\beta L\beta (KL(3S))$, $L\alpha L\beta (L(1S))$

Keywords: Hartree-Fock-Roothaan method, slater type orbitals, two electron density function, radial expectation values, electron density at the nucleus

الخلاصة :

في هذا البحث تم صياغة معادلات هارترى - فوك للأنظمة متعددة الإلكترونات في صيغة دالة كثافة الزوج الإلكتروني $\Gamma(r_1, r_2)$ لغرض حل معادلات هارترى - فوك في التقريب الجبري التي تسمى طريقة هارترى-فوك-روثنان باستخدام اوربتالات نوع سليتر المنشورة بواسطة مصدر [31] لذرة البريليوم Be ومصدر [32] لايون البورون B^{+1} . القيم المتوقعة القطرية لجسيم واحد $\langle r_1^n \rangle$, ولجسيمين $\langle r_1^n \cdot r_2^n \rangle$, وللمسافة بين جسيمين $\langle r_{12}^n \rangle$ حيث (n=-1,-2,1,2) لذرة البريليوم Be وايون البورون B^{+1} في الحالة الأرضية قد تم حسابها باستخدام الدالة الموجية لهارترى فوك مع تحليل دالة الكثافة القطرية للإلكترون واحد ودالة المسافة البينية $f(r_{12})$. الكثافة الإلكترونية عند النواة أيضا تم حسابها للأنظمة المدروسة باستخدام تقنية التجزئة حيث تحتوي هذه الأنظمة على ست قشرات هي :

$K\alpha K\beta(K(1S))$, $K\alpha L\alpha (KL(3S))$, $K\beta L\alpha (KL(1S))$, $K\alpha L\beta (KL(3S))$, $K\beta L\beta (KL(3S))$, $L\alpha L\beta (L(1S))$

الكلمات المفتاحية: طريقة هارترى فوك روثان, اوربتالات نوع سليتر, دالة كثافة الزوج, القيم المتوقعة القطرية, الكثافة عند النواة

1-Introduction

Hartree-Fock theory is one of the simplest approximate theories for solving the many-body problem. [1]. Atomic Hartree–Fock equations are solved usually by two methods, that is, a numerical method and an analytic method. A numerical Hartree–Fock (NHF) method has been formulated by Froese Fischer , and it can give very accurate results. On the other hand, an analytic Hartree–Fock method has been developed by Roothaan using the Rayleigh–Ritz variational procedure, and is often called the Hartree–Fock–Roothaan (HFR) method. The HFR method can be applied to polyatomic molecules because wave functions are represented as basis set expansions. As the basis set, Slater-type functions (STFs) or Gaussian-type functions (GTFs) are usually employed. [2]. This method is based on the mean-field approximation. This approximation implies that interelectron coulomb repulsion is accounted for by means of an average integration of the repulsion term, i.e. the interaction of one electron with the others are accounted for as the interaction of this electron with an average field induced by other electrons. The electron correlation (interaction between electrons) for the electrons of opposite spin is completely neglected . A certain amount of electron correlation is already considered within the HF approximation, found in the electron exchange term describing the correlation between electrons with parallel spin[3]

2-Theory and wave function

In the Hartree-Fock approximation, the many body wave function $\psi(x_1, x_2 \dots x_N)$ is approximated by a single Slater determinant . We can write wave function as [4,5,6],

$$\Psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) \cdots & \phi_1(x_N) \\ \phi_2(x_1) & \phi_2(x_2) \cdots & \phi_2(x_N) \\ \vdots & \vdots & \vdots \\ \phi_3(x_1) & \phi_3(x_2) \cdots & \phi_3(x_N) \end{vmatrix} \dots(1)$$

The factor $\frac{1}{\sqrt{N!}}$ ensures the normalization condition on the wave function . Here the variables x_i include the coordinates of spin and space , $\phi_i(x_j)$ terms are called spin orbitals and these spin orbitals are orthonormal functions, which are spatial orbitals times a spin functions. The wave function Ψ_{HF} in equation (1) is clearly antisymmetric because interchanging any pair of particles is equivalent to interchanging two columns and hence changes the sign of the determinant. Moreover, if any pair of particles are in the same single-particle state, then two rows of the Slater determinant are identical and the determinant vanishes, in agreement with the Pauli exclusion principle.

The one-electron orbitals used to construct the ϕ_i each consist of a radial function $R_{nl}(r)$, a spherical harmonic $Y_{lm}(\theta, \phi)$ and a spin function $\sigma_{m_s}(s)$ as [7,8,9],

$$\phi = R_{nl}(r)Y_{lm_1}(\theta, \phi)\sigma_{m_s}(s) \dots(2)$$

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The spatial part of one-electron spin orbital may be expressed as linear combination of Slater type orbital called basis functions,

$$\Phi_{nlm}(r, \theta, \phi) = \sum_i c_i \mathcal{X}_i \quad \dots(3)$$

Where c_i the expansion coefficient determined by minimizing the energy using one of several procedures and this process is continued until \hat{H}_{HF} and Ψ_{HF} converge, at which point a self-consistent field (SCF) has been achieved. This usually yields the lowest-energy single determinant within the basis. \mathcal{X}_i is a Slater type orbital.

The most frequently used basis functions for atomic calculations are Slater type orbitals (STO) defined as [10,11,12],

$$\chi_{nlm_1}(\xi, r) = R_{nl}(\xi, r) Y_{lm_1}(\theta, \phi) \quad \dots(4)$$

The radial part is:

$$R_{nl}(\xi, r) = (2\xi)^{n+\frac{1}{2}} [(2n)!]^{-\frac{1}{2}} r^{n-1} \exp(-\xi r) \quad \dots(5)$$

Here, $\xi_i > 0$ is the orbital exponent. The quantity n occurring in eq. (5) is a positive principal quantum number of (STO). The determination of nonlinear parameters n and ξ is very important for describing the atomic orbitals.

3-Expectation values

3-1 Expectation value for one-electron

Expectation value for one-electron $\langle r_1^n \rangle$ is determined by the following expression [13,14,15],

$$\langle r_1^n \rangle = \int_0^\infty D(r_1) r_1^n dr_1 \quad \dots(6)$$

Where n integer number ($-2 \leq n \leq 2$), $D(r_1)$ is The one-electron radial density function which represents the probability density function of finding an electron at a distance between r_1 and $r_1 + dr_1$ from the coordinate origin (i.e nucleus) . Though $D(r_1)$ is a one-dimensional condensation of the wave function $\psi(x_1, x_2, \dots, x_N)$, radial physical properties which depend solely on the radial variable r are completely determined by the knowledge of $D(r_1)$. The single-electron radial density $D(r_1)$ is obtained from integration over two–electron radial density function $D(r_1, r_2)$ and defined as[16,17],

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \quad \dots(7)$$

Where the two-electron radial density function $D(r_1, r_2)$ is given by [18],

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$$D(r_1, r_2) = \frac{N(N-1)}{2} r_1^2 r_2^2 \int |\psi(x_1, x_2, \dots, x_N)|^2 dx_3, \dots, dx_N ds_1 ds_2 d\Omega_1 d\Omega_2 \quad \dots(8)$$

$$d\Omega_i = \sin \theta_i d\theta_i d\phi_i \quad \dots(9)$$

Where Ω_i is the solid angle .The two-electrons radial density represents the probability density that one electron is located at a radius r_1 and the other electron at a radius r_2 simultaneously. The function $D(r_1, r_2)$ is meaningful only when $r_1 > 0$ and $r_2 > 0$, and for such values of r_1 and $D(r_1, r_2) > 0$.

The two-electron radial density $D(r_1, r_2)$ can be written as [19].

$$D(r_1, r_2) = \iint \Gamma(r_1, r_2) r_1^2 r_2^2 ds_1 ds_2 d\Omega_1 d\Omega_2 \quad ..(10)$$

Where $\Gamma(r_1, r_2)$ is the two electron density function and contains all of the information necessary to calculate the energy and many properties of the atom. It is obtained by integrating the spin and spatial coordinates of all electrons except two electrons (m, n) from the N-particle density matrix [20], so the two-electron reduced density matrix $\Gamma(x_1, x_2)$ is then given by [21],

$$\Gamma(x_1, x_2) = \frac{N(N-1)}{2} \int \dots \int |\psi(x_1, x_2, \dots, x_N)|^2 dx_3 \dots dx_N \quad \dots(11)$$

Where $x_i = (r_i, s_i)$ combined space and spin variable with $s = \alpha$ (spin up) or β (spin down) [22]. Two electron density function gives the probability that one electron will be found at x_1 and another at x_2 of N electrons [23]. $\frac{N(N-1)}{2}$ represents the number of electron pairs which can be obtained by integrating the second-order reduced density matrix, so $\Gamma(x_1, x_2)$ is normalized to the number of independent electron pairs within the system as [24,25].

$$\int \int \Gamma(x_1, x_2) dx_1 dx_2 = \frac{N(N-1)}{2} \quad \dots(12)$$

3-2 Two particle expectation value

Two particle expectation value $\langle r_1^n r_2^n \rangle$ is defined as [26].

$$\langle r_1^n r_2^n \rangle = \int_0^\infty \int_0^\infty D(r_1, r_2) r_1^n r_2^n dr_1 dr_2 \quad \dots(13)$$

3-3 Inter particle expectation value

Inter particle expectation value $\langle r_{12}^n \rangle$ is given by the relation [27].

$$\langle r_{12}^n \rangle = \int_0^\infty f(r_{12}) r_{12}^n dr_{12} \quad \dots(14)$$

where r_{12} represents the distance between two-electrons. $f(r_{12})$ is radial electron-electron distribution function $f(r_{12})$, which describes the probability of locating two electrons separated by distance r_{12} from each other, was first introduced by Coulson and Neilson in their study of electron correlation for

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He(1S) in the ground state. The electron-electron distribution function $f(r_{12})$ plays a central role in the discussion of correlation holes in many electron systems .[27,28].Pair distribution function can be written as [29].

$$f(r_{12}) = 8\pi^2 r_{12} \left[\int_0^{r_{12}} r_1 dr_1 \int_{r_1-r_{12}}^{r_1+r_{12}} \Gamma(r_1, r_2) r_2 dr_2 + \int_{r_{12}}^{\infty} r_1 dr_1 \int_{r_{12}-r_1}^{r_{12}+r_1} \Gamma(r_1, r_2) r_2 dr_2 \right] \dots (15)$$

4-Electron density at the nucleus $\rho(o)$

The electron density at the nucleus can be evaluated using the following form[30].

$$\rho(o) = \left[\frac{D_0(r)}{4\pi r^2} \right]_{r \rightarrow 0} \dots (16)$$

..

5.Result and discussion

Using Mathcad 2001i program , we have calculated the expectation values of one electron $\langle r_1^n \rangle$, expectation values for two-electron $\langle r_1^n r_2^n \rangle$ and expectation values for inter-electron $\langle r_{12}^n \rangle$, also analysis one electron radial density function $D(r_1)$ and radial electron-electron distribution function. $f(r_{12})$ for Be atom ($Z=4$) and B^{+1} ion ($Z=5$) in their ground states. On the other hand it should be mentioned that all numerical calculations have been performed in the Hartree-Fock frame work using Ref. [31] for atomic data of Be atom and Ref. [32] for atomic data of B^{+1} ion where in these systems there are six shells: $K\alpha K\beta$ (K(1S)), $K\alpha L\alpha$ (KL (3S)), $K\beta L\alpha$ (KL (1S)), $K\alpha L\beta$ (KL (3S)), $K\beta L\beta$ (KL(3S)), $L\alpha L\beta$ (L(1S)) .Table (1) shows the calculated one electron expectation values and standard deviation for studied systems. Table (2) represents expectation values for two electrons and table (3) represents expectation values for inter electrons and standard deviation of four electron systems. we noticed for each electronic individual shell and for total system, the expectation values for one electron and two electrons and inter electrons when n takes negative values increases as atomic number Z increases and vice-versa when n takes positive values, also it is noticed the expectation values for K (1S)-shell is larger than those for L(¹S)-shell when n is negative and vice-versa when n is positive , $\langle r_{12}^n \rangle$ and $\langle r_1^n . r_2^n \rangle$ for KL(¹S) when n negative values is larger than those for KL(³S)-shell and vice-versa when n positive values. Standard deviation Δr_1 and Δr_{12} decrease as Z increases .

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Table(1) one particle expectation value $\langle r_1^n \rangle$ and standard deviation Δr_1 for Be atom and B+ve for each individual electronic shell and for total system .

Z	shell	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$	Δr_1
4	K(1S)	27.68783	3.67641	0.41622	0.23507	0.24865
	L(1S)	1.12016	0.52805	2.64728	8.42233	1.18610
	KL(1S) \equiv KL(3S)	14.40400	2.10223	1.53175	4.32870	1.40799
	total	14.40400	2.10223	1.53175	4.32870	1.17778
5	K(1S)	44.60768	4.67920	0.32527	0.14268	0.19204
	L(1S)	2.41502	0.78015	1.79819	3.82590	0.76968
	KL(1S) \equiv KL(3S)	23.51136	2.72967	1.06173	1.98429	0.92575
	total	23.51131	2.72967	1.06173	1.98429	0.77746

*the total system for $\langle r_1^n \rangle$ is given by $1/6 [K(^1S) + L(^1S) + KL(^1S) + 3 KL(^3S)]$

Table(2) two particles expectation values $\langle r_1^n \cdot r_2^n \rangle$ for Be atom and B+ve for each individual electronic shell and for total system .

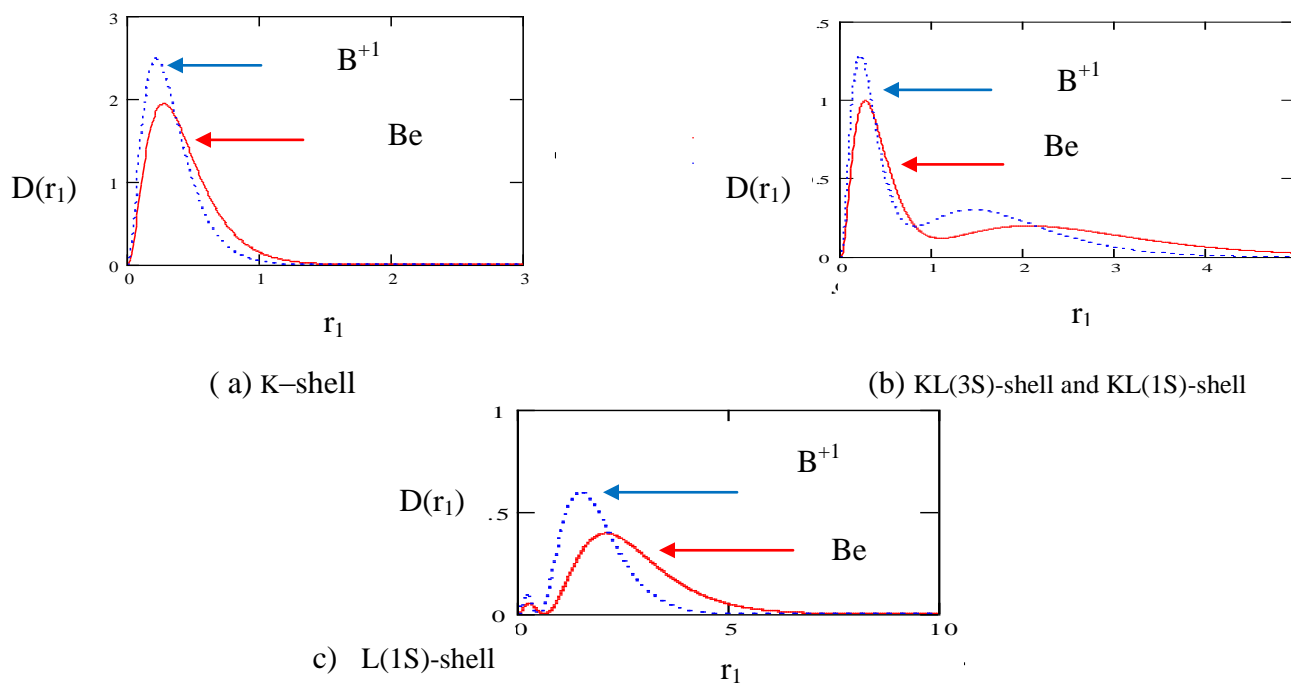
Z	shell	$\langle r_1^{-2} \cdot r_2^{-2} \rangle$	$\langle r_1^{-1} \cdot r_2^{-1} \rangle$	$\langle r_1^1 \cdot r_2^1 \rangle$	$\langle r_1^2 \cdot r_2^2 \rangle$
4	K(1S)	766.61605	13.51602	0.17324	0.05526
	L(1S)	1.25476	0.27884	7.00808	70.93572
	KL(1S)	54.01511	2.14174	1.11438	2.02234
	KL(3S)	8.01447	1.74094	1.08933	1.93729
	total	140.98822	3.52657	1.92728	13.13753
5	K(1S)	1989.83611	21.89478	0.10580	0.02036
	L(1S)	5.83229	0.60863	3.23349	14.63752
	KL(1S)	188.61705	4.07736	0.59311	0.55883
	KL(3S)	26.838847	3.223551	0.576686	0.532924
	total	377.46700	6.04190	0.94374	0.94374

Table(3) inter particle expectation values $\langle r_{12}^n \rangle$ and standard deviation Δr_{12} for Be atom and B⁺ ion for each individual electronic shell and for total system .

Z	shell	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^1 \rangle$	$\langle r_{12}^2 \rangle$	Δr_{12}
4	K(1S)	8.88564	2.26837	0.60917	0.47013	0.31472
	L(1S)	0.19125	0.34354	3.75336	16.84467	1.66042
	KL(1S)	0.66604	0.51074	2.68025	8.65740	1.21394
	KL(3S)	0.26476	0.45572	2.69093	8.65740	1.19007
	total	1.61101	0.66040	2.59929	8.90193	1.12655
5	K(1S)	14.43951	2.89621	0.47555	0.28536	0.24171
	L(1S)	0.41150	0.50381	2.54054	7.65181	1.09429
	KL(1S)	1.41656	0.74873	1.82707	3.96859	0.79397
	KL(3S)	0.54058	0.65646	1.83717	3.96859	0.77032
	total	2.98155	1.01969	1.72578	3.96859	0.74016

Figure (1) exemplify the one-electron radial density function $D(r_1)$ as a function of r_1 for Be atom and B⁺ ion for each individual electronic shell ,we find in this figure the $D(r_1)$ increase as Z increases and decrease their positions towards the nucleus when Z increases where in curve (a) presented in this figure it is found one peak in the K(1S)-shell which represents the probability of finding the electron in the K-shell , while in curve (b) we can see two peaks for KL(1S)-shell and KL(3S)-shell(where $D(r_1)_{KL(1S)} \equiv D(r_1)_{KL(3S)}$), the first peak represents the probability of finding the electron in the K-shell , the second peak represents the probability of finding the electron in the L-shell and it is clearly from this curve the probability of finding the electron in the K-shell is larger than that for L-shell because K-shell closer to the nucleus than L-shell. In curve (c) it is found two peaks the first peak represents the probability of finding the electron in the K-shell as a results of penetration effect and the second peak represents the most probability of finding the electron in the L-shell.

Figure(1) one- particle radial density function for three shells of Be atom and B⁺ ion . Atomic unit are used.



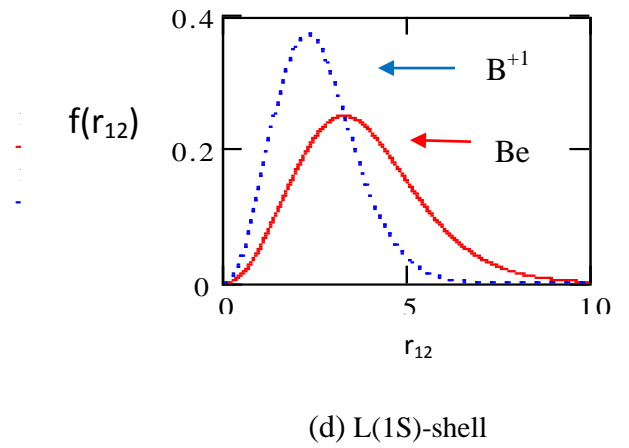
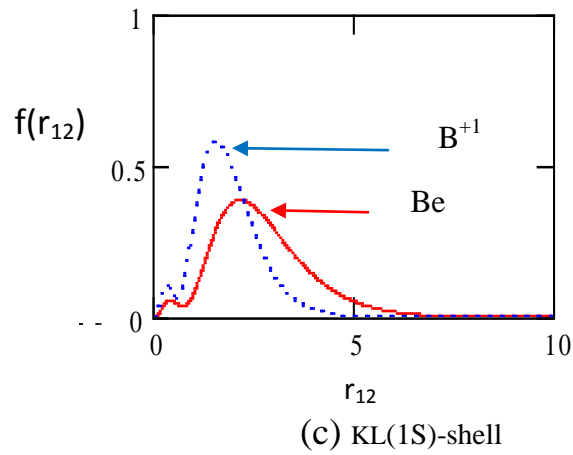
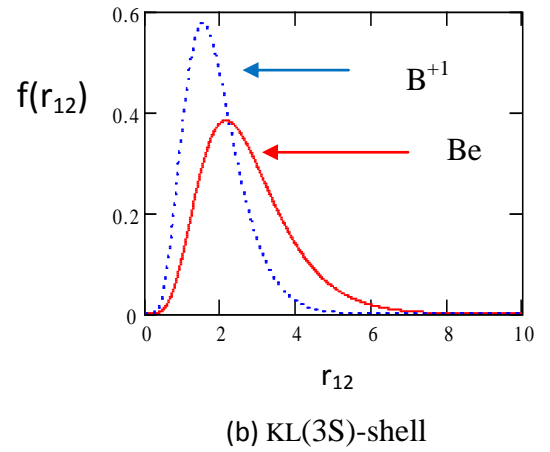
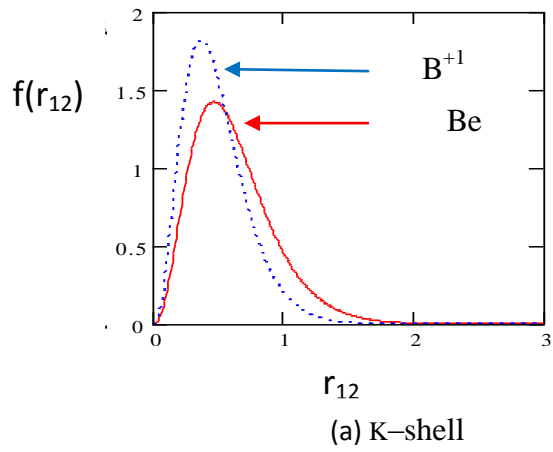


Figure (2) radial electron-electron distribution function $f(r_{12})$ for Be atom and B^{+1} ion. Atomic unit are used.

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Figure (2) illustrates the inter particle distribution function $f(r_{12})$ which represents the probability of finding two electrons separated by distance r_{12} between them. It is clear from all curves (a, b, c and d) the values of pair distribution function $f(r_{12})$ increase as Z increases and the inter distance between two electrons r_{12} decreases for all shells because of the influence of increasing the attraction nuclear force, we can also see the maximum values of $f(r_{12})$ for K-shell is larger than that for L-shell because k-shell closer to the nucleus than L-shell . In curves (b and c) it is found one peak for KL(3S)-shell and two peaks in KL(1S)-shell the first peak represents the probability of finding two electrons separated by small distance between them and it is the small probability as a results of neglecting the correlation between the electrons by Hartree-Fock approximation , the second peak represents the probability of finding two electrons separated by larger distance (r_{12}) between them and it is the most probability. Table (4) shows the maximum values of $D(r_1)$ and the position r_1 . It is noticeable when Z increases the maximum values of $D(r_1)$ increase too and the position of maximum values r_1 decrease this results agreement with coulomb law because increasing in Z leads to increasing in attraction force between the nucleus and the electrons which leads to increasing in the probability of finding the electron $D(r_1)$ and decreasing in the position towards the nucleus .Table (5) represents the maximum values of $f(r_{12})$ and the inter distance between two electrons r_{12} , it is found the maximum probability of pair distribution function $f(r_{12})$ increases as Z increases because the influence of increasing in attraction nuclear force and r_{12} decrease.

Table (4) maximum values of $D(r_1)$ and their position r_1 for Be atom and B^{+1} ion for all shells.

Z	K(1S)-shell		KL(3S)-shell \equiv KL(1S)-shell				L(1S)-shell			
	r_1	$D(r_1)$	Peak1		Peak 2		Peak1		Peak 2	
			r_1	$D(r_1)$	r_1	$D(r_1)$	r_1	$D(r_1)$	r_1	$D(r_1)$
4	0.27	1.941	0.26	0.997	2.05	0.198	2.06	0.396	0.21	0.0567
5	0.21	2.485	0.21	1.289	1.44	0.302	1.45	0.62	0.17	0.0996

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Table (5) maximum values of $f(r_{12})$ and their position r_{12} for Be atom and B^{+1} ion for each shells.

Z	K(1S)-shell		KL(3S)-shell		KL(1S)-shell				L(1S)-shell	
	r_{12}	$f(r_{12})$	r_{12}	$f(r_{12})$	Peak1		Peak 2		r_{12}	$f(r_{12})$
					r_{12}	$f(r_{12})$	r_{12}	$f(r_{12})$		
4	0.45	1.421	2.12	0.384	0.37	0.0623	2.14	0.388	3.25	0.252
5	0.36	1.822	1.50	0.576	0.29	0.1047	1.52	0.582	2.25	0.3741

Table (6) the electron density at the nucleus for all shell and total systems for Be atom and B^{+1} ion

Z	shell	$\rho(o)$
4	K(1S)	17.0789
	L(1S)	0.6201
	KL(1S)	8.8495
	KL(3S)	8.8495
	total	8.8495
5	K(1S)	34.6276
	L(1S)	1.7129
	KL(1S)	18.1702
	KL(3S)	18.1702
	total	18.1702

In table (6) the electron density at the nucleus $\rho(0)$ calculated from equation (16). we could see the $\rho(0)$ for K(1S)-shell is larger than that for other shells because K-shell closer to the nucleus than other shells and we could see also the values of $\rho(0)$ increases when Z increase.

Conclusion:

It has been shown how the radial expectation values act when atomic Z increases ,numerical results have been discussed for Be like systems ($Z= 3 , 4$) in the Hartree-Fock framework . The Hartree-Fock method also allows one to study how the electron density at the nucleus $\rho(0)$ increases when Z increases for all shells and for total systems . In the present study ,the one electron radial density function $D(r_1)$ and pair distribution function $f(r_{12})$ introduced as a function of r_1 and r_{12} respectively .

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