Calculation of the atomic properties of excited states for B-atom using Hartree – Fock approximation

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Abstract

In this paper were studied some atomic properties for Boron atom and like ions such as (C^{+1} and N^{+2}) for different excited states($1S^2 2S^2\, nS^1$)where nequal (3,4,5). This system consists of five –electron : two electron each in(1S,2S-Level) with same quantum number except spin component ,where the first electron with spin up (α)and the other –down(β) and the Fifth electron puts in(n S-Level)with spin up(α).using Hartree –Fock approximation in position spaceand electron density at the nucleus ρ(0) have been calculated for these states of the same atom .

Key words: Boron excited state ,Hartree- Fock approximation , Electron density at the nucleus ,Atomic properties, ($1S^2 2S^2\, nS^1$).

Introduction

The Schrödinger equation for atoms (ions) with more than one electron has not been solved analytically. Approximate methods must be applied in order to obtain the wave functions or another physical attributes from quantum mechanical calculation[1].

The Hartree-Fock(HF) equations were first proposed by Fock in 1930.since then, the Hartree- Fock method has taken a central role in studies of atomic and molecular electronic structure the development of effective computational methods for Hartree-Fock equations there are two computation methods for Hartree-Fock equations numerical and algebraic [2]. Numerical computational methods for atomic HF equations have been developed by Froese Fischer [3,4].

The Hartree-Fock method(HF) is known to be successful in calculating properties of electron systems, in particular , the ground state properties of atoms. Based on a variational principle ,the HF method estimate the ground state energy E of the electron system ,from above,i.e$E_{HF} \geq E$,where E_{HF} is the ground state energy calculated within the HF method if the ground state wave function of N- electrons is approximated by a single N-electron Slater determinant, the HF solution delivers minimum value E_{HF} on the set of all such determinants. Agreement, or otherwise, with the HF result is often used to estimate the success of other approximate computational schemes[5]

1.Two-particle density distribution function $\Gamma_{HF}(x_m, x_n)$

The Two-particle density $\Gamma_{HF}\ (xi, xj)$ for N electron system is given by[6]

$$\Gamma_{HF}(X_i, X_j) = \binom{N}{2} \int \phi_i\left(x_1, x_2, \ldots\ldots, x_n\right) - \phi_j\left(x_1, x_2, \ldots\ldots, x_n\right) dx_p \ldots\ldots dx_N \tag{1}$$

Where $\binom{N}{2}$ is the Binomial factor defined as [6].

$$\binom{N}{2} = \left[\frac{N!}{(2!(N-2)!)}\right] \tag{2}$$

Where N is the number of electrons within system and $dx_P \ldots . dx_N$ indicates that the integration is over N electrons except i and j .Since the partitioning technique enable correlation to be examined in depth for various intra and inter shells electron pairs thus we had employed this technique to pair-wise components (p,q) [7].

$$\Gamma_{HF}(X_i, X_j) = \sum_{p<q}^{N} \Gamma_{pq}(X_i, X_j) \tag{3}$$

Hence

$$\Gamma_{pq}(X_i, X_j) = \frac{1}{2} \sum_{p>q}^{N} \left[\psi_p(x_i)\psi_q(x_j) - \psi_q(x_i)\psi_p(x_j)\right]^2 \tag{4}$$

Where Ψ is the occupied normalized Hartree –Fock spin orbital, the

symbol (p,q) represent the spin orbital labels and (x_i, x_j) indicates the electron labels[7].

2.one particle radial density distribution $D_{pq}(r_1)$ and expectation values $\langle r_1^k \rangle$

The radial correlation contained within a correlated wave function may be investigated by evaluating the two-particle radial density distribution $D_{ij}^{\cdot}(r_1, r_2)$, which defined as[8]:

$$D_{pq}^{\cdot}(r_1, r_2) = \iint \Gamma_{pq}'^{\cdot}\, r_1^2 r_2^2 d\Omega_1 d\Omega_2 \qquad (5)$$

Where $d\Omega$ refer to solid angles, r is the distance between electrons and nucleus. $\Gamma_{pq}'^{\cdot}$ defined as:

$$\Gamma_{pq}'^{\cdot} = \iint \Gamma_{pq}^{\cdot} d\sigma_1 d\sigma_2 \qquad (6)$$

Here $d\sigma$ denotes spin-part (α spin up, β spin down).

The determination of expectation value $\langle r_1^k \rangle$ requires evaluation of one particle radial density distribution $D_{pq}^{\cdot}(r_1)$ which is defined as[9]

$$D_{pq}^{\cdot}(r_1) = \int_0^\infty D_{pq}^{\cdot}(r_1, r_2) dr_2 \qquad (7)$$

Then the expectation value $\langle r_1^k \rangle$, where $-2 \le k \le 2$, is determined from the expression[8]

$$\langle r_1^m \rangle = \int_0^\infty D_{pq}^{\cdot}(r_1) r^k dr_1 \qquad (8)$$

3.standard deviation Δr_1

The standard deviation of distance of the test electron from the nucleus is defined as[10][11].

$$\Delta r_1 = \sqrt{< r_1^{\ 2} > - < r_1 >^2} \qquad (9)$$

While the standard deviation of the inter electronic distance of the two electrons, is defined

as .

$$\Delta r_{12} = \sqrt{< r_{12}^{\ 2} > - < r_{12} >^2} \qquad (10)$$

4.Inter-particle distribution function $f_{pq}^{\cdot}(r_{12})$ and the expectation value of $\langle r_{12}^k \rangle$

Coulson and Neilson proposed a distribution function for inter-electronic separation of $f_{pq}(r_{12})$ of s-states associated with spin - orbital pair (p,q) [11] .

$$f_{pq}(r_{12}) = \int \Gamma_{pq}(r_1, r_2)\ dr_1 dr_2 \qquad (11)$$

Where the function $f_{pq}(r_{12})$is the probability distribution distance between electron 1 and electron 2; this function of great importance in both Fermi and Coulomb holes and $r_{12}$is the distance between the two electrons, this function satisfies the normalization condition [12][13].

$$\int f_{pq}(r_{12})\ dr_{12} = 1 \qquad (12)$$

Then $f_{pq}(r_{12})$ can be as follows

$$f_{pq}(r_{12}) = 8\pi^2 r_{12}\{J_1 + J_2\} \qquad (13)$$

Where :

$$\left.\begin{aligned} J_1 &= \int_0^{r_{12}} r_1 \int_{|r_{12}-r_1|}^{|r_{12}+r_1|} \Gamma\,(r_1, r_2)\, r_2\, dr_2 dr_1 \\ J_2 &= \int_{r_{12}}^{\infty} r_1 \int_{|r_1-r_{12}|}^{|r_1+r_{12}|} \Gamma\,(r_1, r_2)\, r_2\, dr_2 dr_1 \end{aligned}\right\} \qquad (14)$$

$$\langle r_{12}^{k}\rangle = \int_{0}^{\infty} f_{pq}(r_{12})\, r_{12}^{k} dr_{12} \qquad (15)$$

5.Electron density at the nucleus ρ(0)

The electron density at the nucleus can be evaluated using the following form [14] .

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

Results and discussion

The results obtained in the present of one-particle expectation values for different powers (k =-2 to 2)in addition to calculate the standard deviation for different excited states $(1S^2 2S^2\, 3S^1), (1S^2 2S^2\, 4S^1)\ and\ (1S^2 2S^2\, 5S^1)$of B- like ions up to Z=7 are listed in tables(1,2,3).From this tables we noted effect the increase in atomic number with fixed the number of electrons, where observed when (k) takes negative values the expectation values of $\langle r_1^k\rangle$ increase with increasing the atomic number while when(k) takes positive values the expectation values of $\langle r_1^k\rangle$ are decreases because the distance between the electron and the nucleus become smallest as nuclear charge increases .Normalization condition has been applied for all wave functions.The values of standard deviation are decreases as atomic number increase because it depend on the values of $\langle r_1^1\rangle$ and$\langle r_1^2\rangle$.

Tables: (4,5,6) contain The results of inter-particle expectation value$\langle r_{12}^k\rangle$,we noted when(k) takes negative values the expectation values$\langle r_{12}^k\rangle$ increase as atomic number increases for all studied system ,while when n takes positive values the $\langle r_{12}^k\rangle$ decreases. also standard deviation decreases for all intra and inter shells.

Table (6) represents the electron density at the nucleus calculated from equation (). we could see the for (1s)-shell is larger than that for other shells because (1s) shell closer to the nucleus than other shells. We could see from those tables The effect of the atomic number upon the electron density, where the density increases by increasing the atomic number Z is due to the Coulomb attraction forces.

Figure (1,2,3) show that the relation between the one–electron radial density distribution function(r1) with the position for 1s, 2s,3s,4s and 5s shells respectively ,where noted for each shell the maximum values of D(r1) increase when atomic number increase and location of these peaks contracted to ward of the nucleus ,also observed the value of D(r1) vanishes when the distance equal zero or infinity, in the figure(1,2,3) (B) noted two peaks ,the first represent the probability of finding the electron in small distance from the nucleus and the second represent the probability of finding the electron in 2sshell. Also noted in figure (1,2,3) (C) three peaks in (3s) shells, four peaks in (4s) shells and five peaks in (5s) shells

Table (1): The one- particle expectation values and the standard deviation of the excited state in position space for B - like ions($1S^2 2S^2\, 3S\alpha$) .

Shell	z	$\langle r_1^{-2}\rangle$	$\langle r_1^{-1}\rangle$	$\langle r_1^{0}\rangle$	$\langle r_1^{1}\rangle$	$\langle r_1^{2}\rangle$	$\Delta r1$
$1S\alpha\ 1S\beta$	5	44.60126	4.67893	1.00000	0.32529	0.14271	0.19208
	6	65.44193	5.67664	1.00000	0.26745	0.09628	0.15733
	7	90.27919	6.67487	1.00000	0.22705	0.06930	0.13321
$2S\alpha\ 2S\beta$	5	2.40547	0.77866	1.00000	1.80277	3.85005	0.77464
	6	4.2590	1.03096	1.00000	1.37731	2.2359	0.58217
	7	6.61598	1.28226	1.00000	1.11668	1.46569	0.46768
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	23.50337	2.72879	1.00000	1.06403	1.99638	0.92963
	6	34.85047	3.35380	1.00000	0.82238	1.16609	0.69985
	7	48.44759	3.97857	1.00000	0.67186	0.76749	0.56222
$1S\alpha\ 3S\alpha \equiv 1S\beta\ 3S\alpha$	5	22.38548	2.43413	1.00000	3.52814	25.77519	3.65067
	6	32.98532	2.99435	1.00000	2.26379	10.29523	2.27387
	7	45.66370	3.55205	1.00000	1.70172	5.73020	1.68356
$2S\alpha\ 3S\alpha \equiv 2S\beta\ 3S\alpha$	5	1.2875	0.48399	1.00000	4.26688	27.62886	3.06962
	6	2.39386	0.67151	1.00000	2.81872	11.36504	1.84929
	7	3.83210	0.85574	1.00000	2.14653	6.42839	1.34937

Table (2): The one- particle expectation values and the standard deviation of the excited state in position space for B – like ions $(1S^2 2S^2\ 4S\alpha)$.

Shell	z	$\langle r_1^{-2}\rangle$	$\langle r_1^{-1}\rangle$	$\langle r_1^{0}\rangle$	$\langle r_1^{1}\rangle$	$\langle r_1^{2}\rangle$	$\Delta r1$
$1S\alpha\ 1S\beta$	5	44.60391	4.67910	1.00000	0.32528	0.14269	0.19206
	6	65.44926	5.67702	1.00000	0.26742	0.09626	0.15731
	7	90.29208	6.67544	1.00000	0.22702	0.06928	0.13318
$2S\alpha\ 2S\beta$	5	2.41156	0.77976	1.00000	1.79934	3.83141	0.77057
	6	4.27564	1.03326	1.00000	1.37334	2.21985	0.57774
	7	6.64400	1.28538	1.00000	1.11326	1.45467	0.46403
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	23.50773	2.72943	1.00000	1.06231	1.98705	0.92658
	6	34.86245	3.35514	1.00000	0.82038	1.15806	0.69644
	7	48.46804	3.98041	1.00000	0.67014	0.76197	0.55936
$1S\alpha\ 4S\alpha \equiv 1S\beta\ 4S\alpha$	5	22.32817	2.38522	1.00000	7.46261	120.0161	8.02032
	6	32.81513	2.91812	1.00000	4.43054	41.50322	4.67691
	7	45.33455	3.44993	1.00000	3.21493	21.62508	3.35995
$2S\alpha\ 4S\alpha \equiv 2S\beta\ 4S\alpha$	5	1.23192	0.43555	1.00000	8.19965	121.86045	7.39096
	6	2.22829	0.59624	1.00000	4.98350	42.56501	4.21067
	7	3.51053	0.75490	1.00000	3.65805	22.31778	2.98939

Table (3): The one- particle expectation values and the standard deviation of the excited state in position space for B - like ions$(1S^2 2S^2\ 5S\alpha)$.

Shell	z	$\langle r_1^{-2}\rangle$	$\langle r_1^{-1}\rangle$	$\langle r_1^{0}\rangle$	$\langle r_1^{1}\rangle$	$\langle r_1^{2}\rangle$	$\Delta r1$
$1S\alpha\ 1S\beta$	5	44.60459	4.67914	1.00000	0.32527	0.14269	0.19206
	6	65.45132	5.67712	1.00000	0.26742	0.09625	0.1573
	7	90.29589	6.67561	1.00000	0.22701	0.06927	0.13318
$2S\alpha\ 2S\beta$	5	2.41281	0.77998	1.00000	1.79870	3.82809	0.76992
	6	4.27916	1.03374	1.00000	1.37257	2.21694	0.57704
	7	6.65004	1.28604	1.00000	1.11258	1.45262	0.46345
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	23.50870	2.72956	1.00000	1.06199	1.98539	0.92605
	6	34.86524	3.35543	1.00000	0.81999	1.15659	0.69585
	7	48.47297	3.98083	1.00000	0.66980	0.76095	0.55885
$1S\alpha\ 5S\alpha \equiv 5S\beta\ 5S\alpha$	5	22.31319	2.36648	1.0000	12.89314	363.21120	14.03489
	6	32.76946	2.88694	1.00000	7.34403	116.38455	7.90252
	7	45.23451	3.40693	1.00000	5.22610	58.51737	5.58616
$2S\alpha\ 5S\alpha \equiv 2S\beta\ 5S\alpha$	5	1.21778	0.41691	1.0000	13.62986	365.05390	13.38958
	6	2.18122	0.56525	1.00000	7.89660	117.44489	7.42216
	7	3.41410	0.71214	1.00000	5.66888	59.20904	5.20315

Table (4): The Two - particle expectation values and the standard deviation of the excited state in position space for B - like ions($1S^2 2S^2\ 3S\alpha$) .

Shell	z	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}^{0}\rangle$	$\langle r_{12}^{1}\rangle$	$\langle r_{12}^{2}\rangle$	$\Delta r12$
$1S\alpha\ 1S\beta$	5	14.43771	2.89601	1.00000	0.47559	0.28542	0.24338
	6	21.29082	3.51944	1.00000	0.39085	0.19256	0.1995
	7	29.47570	4.14322	1.00000	0.33171	0.13859	0.169
$2S\alpha\ 2S\beta$	5	0.40984	0.50269	1.00000	2.54764	7.70010	1.09983
	6	0.70356	0.65708	1.00000	1.94449	4.47180	0.83112
	7	1.07218	0.80957	1.00000	1.57558	2.93107	0.6698
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$	5	0.53912	0.65540	1.00000	1.84168	3.99276	0.77523
	6	0.89871	0.84902	1.00000	1.41210	2.33218	0.5815
	7	1.34385	1.04019	1.00000	1.14777	1.53495	0.46644
$1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	0.97559	0.70138	1.00000	1.83664	3.99276	0.78708
	6	1.68007	0.91625	1.00000	1.40723	2.33218	0.59319
	7	2.56034	1.12863	1.00000	1.14324	1.53498	0.47748
$1S\alpha\ 3S\alpha$	5	0.05363	0.18175	1.00000	6.73988	51.54826	2.47431
	6	0.13996	0.29134	1.00000	4.27028	20.59041	1.53464
	7	0.25512	0.39352	1.00000	3.18644	11.46034	1.14323
$1S\beta\ 3S\alpha$	5	0.08036	0.18453	1.00000	6.73959	51.54826	2.4751
	6	0.22860	0.29881	1.00000	4.26977	20.59040	1.53605
	7	0.43448	0.40623	1.00000	3.18583	11.46034	1.14491
$2S\alpha\ 3S\alpha$	5	0.03329	0.16622	1.00000	6.97971	55.25821	2.5577
	6	0.07869	0.25623	1.00000	4.49501	22.73009	1.58902
	7	0.13792	0.33942	1.00000	3.38501	12.85553	1.18205
$2S\beta\ 3S\alpha$	5	0.04622	0.17354	1.00000	6.95894	55.25822	2.6137
	6	0.11767	0.27229	1.00000	4.47053	22.73007	1.65663
	7	0.21305	0.36377	1.00000	3.36171	12.85557	1.24679

Table (5): The Two - particle expectation values and the standard deviation of the excited state in position space for B - like ions($1S^2 2S^2\ 4S\alpha$) .

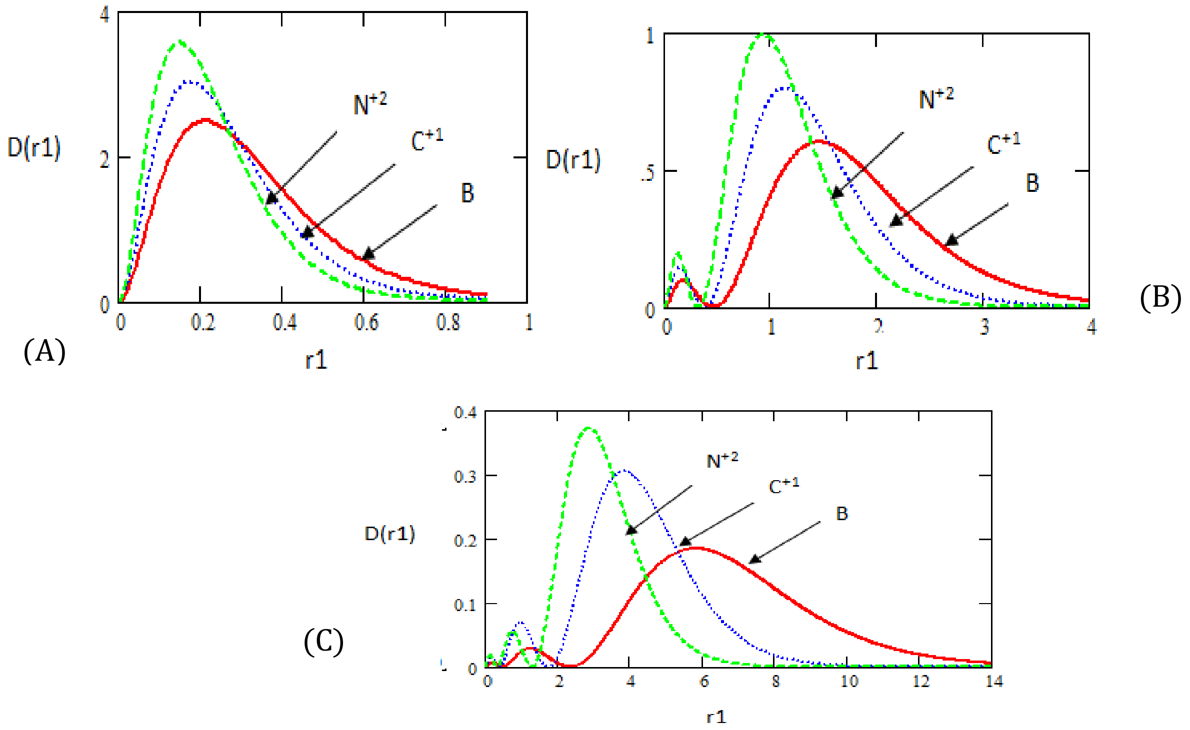
Shell	z	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}^{0}\rangle$	$\langle r_{12}^{1}\rangle$	$\langle r_{12}^{2}\rangle$	$\Delta r12$
$1S\alpha\ 1S\beta$	5	14.43882	2.89614	1.00000	0.47556	0.28538	0.24336
	6	21.29393	3.51973	1.00000	0.39081	0.19252	0.19947
	7	29.48119	4.14365	1.00000	0.33167	0.13855	0.16897
$2S\alpha\ 2S\beta$	5	0.41107	0.50351	1.00000	2.54230	7.66281	1.09522
	6	0.70685	0.65874	1.00000	1.93835	4.43971	0.82614
	7	1.07837	0.81202	1.00000	1.57055	2.90934	0.66536
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$	5	0.54020	0.65618	1.00000	1.83830	3.97410	0.7712
	6	0.90150	0.85059	1.00000	1.40821	2.31611	0.57712
	7	1.34895	1.04249	1.00000	1.14448	1.52395	0.46272
$1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	0.97782	0.70228	1.00000	1.83326	3.97410	0.78312
	6	1.68602	0.91808	1.00000	1.40332	2.31611	0.5889
	7	2.57516	1.13164	1.00000	1.13990	1.52395	0.4739
$1S\alpha\ 3S\alpha$	5	0.01688	0.08902	1.00000	14.59559	239.8512	5.1788
	6	0.04907	0.15221	1.00000	8.59800	82.99420	3.01141
	7	0.09409	0.21173	1.00000	6.20798	43.24884	2.17021
$1S\beta\ 3S\alpha$	5	0.02503	0.08986	1.00000	14.59550	239.85118	5.17905
	6	0.07902	0.15472	1.00000	8.59783	82.99420	3.01189
	7	0.15773	0.21621	1.00000	6.20777	43.24884	2.17081
$2S\alpha\ 3S\alpha$	5	0.01079	0.08452	1.00000	14.71681	243.70977	5.2082
	6	0.02903	0.14116	1.00000	8.71023	85.12915	3.0432
	7	0.05410	0.19407	1.00000	6.30909	44.63536	2.1979
$2S\beta\ 3S\alpha$	5	0.01454	0.08657	1.00000	14.71155	243.70942	5.22301
	6	0.04124	0.14590	1.00000	8.70402	85.12913	3.06092
	7	0.07850	0.20141	1.00000	6.30322	44.63536	2.21467

Table (6): The Two - particle expectation values and the standard deviation of the excited state in position space for B - like ions($1S^2 2S^2\ 5S\alpha$) .

Shell	z	$\langle r_{12}^{-2}\rangle$	$\langle r_{12}^{-1}\rangle$	$\langle r_{12}^{0}\rangle$	$\langle r_{12}^{1}\rangle$	$\langle r_{12}^{2}\rangle$	$\Delta r12$
$1S\alpha\ 1S\beta$	5	14.43910	2.89617	1.00000	0.47556	0.28538	0.24335
	6	21.29480	3.51981	1.00000	0.39080	0.19251	0.19946
	7	29.48281	4.14377	1.00000	0.33166	0.13854	0.16896
$2S\alpha\ 2S\beta$	5	0.41131	0.50367	1.00000	2.54131	7.65618	1.09449
	6	0.70753	0.65907	1.00000	1.93719	4.43387	0.82534
	7	1.07953	0.81247	1.00000	1.56953	2.90524	0.66469
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$	5	0.54042	0.65634	1.00000	1.83767	3.97078	0.77056
	6	0.90209	0.85092	1.00000	1.40745	2.31319	0.57642
	7	1.34994	1.04293	1.00000	1.14382	1.52189	0.46214
$1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	0.97828	0.70246	1.00000	1.83262	3.97078	0.78249
	6	1.68728	0.91846	1.00000	1.40256	2.31319	0.58822
	7	2.57730	1.13216	1.00000	1.13923	1.52189	0.47333
$1S\alpha\ 3S\alpha$	5	0.00738	0.05280	1.00000	25.47241	727.33114	8.85932
	6	0.02274	0.09352	1.00000	14.41401	232.57906	4.98149
	7	0.04481	0.13226	1.00000	10.22583	116.99390	3.52508
$1S\beta\ 3S\alpha$	5	0.01092	0.05316	1.00000	25.47237	727.33114	8.85943
	6	0.03647	0.09467	1.00000	14.41394	232.57906	4.98171
	7	0.07474	0.13437	1.00000	10.22574	116.9939	3.52537
$2S\alpha\ 3S\alpha$	5	0.004757	0.05089	1.00000	25.52694	730.03298	8.85484
	6	0.01365	0.08860	1.00000	14.48997	234.86289	4.99037
	7	0.02625	0.12420	1.00000	10.29027	118.41232	3.53873
$2S\beta\ 3S\alpha$	5	0.006358	0.05176	1.00000	25.52480	730.03294	8.86102
	6	0.01910	0.09067	1.00000	14.48739	234.86282	4.99783
	7	0.03735	0.12745	1.00000	10.28784	118.41229	3.5458

Table (7): the electron density at the nucleus ρ(0) for all shell in the different excited states ($1S^2 2S^2\ 3S\alpha$), ($1S^2 2S^2\ 4S\alpha$) ,($1S^2 2S^2\ 5S\alpha$) of B - like ions.

($1S^2 2S^2\ 3S\alpha$)			($1S^2 2S^2\ 4S\alpha$)			($1S^2 2S^2\ 5S\alpha$)		
Shell	**z**	$\rho(0)$	**Shell**	**z**	$\rho(0)$	**Shell**	**z**	$\rho(0)$
$1S\alpha\ 1S\beta$	5	34.605	$1S\alpha\ 1S\beta$	5	34.607	$1S\alpha\ 1S\beta$	5	34.608
	6	61.174		6	61.182		6	61.185
	7	98.744		7	98.762		7	98.767
$2S\alpha\ 2S\beta$	5	1.6997	$2S\alpha\ 2S\beta$	5	1.704	$2S\alpha\ 2S\beta$	5	1.705
	6	3.706		6	3.721		6	3.725
	7	6.826		7	6.857		7	6.864
$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2S\beta$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2S\alpha$	5	18.152	$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2$	5	18.156	$1S\alpha\ 2S\alpha \equiv 1S\beta\ 2$ $1S\alpha\ 2S\beta \equiv 1S\beta\ 2$	5	18.157
	6	32.44		6	32.452		6	32.455
	7	52.785		7	52.81		7	52.815
$1S\alpha\ 3S\alpha \equiv 1S\beta\ 3S\alpha$	5	17.355	$1S\alpha\ 4S\alpha \equiv 1S\beta\ 4$	5	17.32	$1S\alpha\ 5S\alpha \equiv 1S\beta\ 5$	5	17.311
	6	30.803		6	30.664		6	30.626
	7	49.89		7	49.566		7	49.471
$2S\alpha\ 3S\alpha \equiv 2S\beta\ 3S\alpha$	5	0.903	$2S\alpha\ 4S\alpha \equiv 2S\beta\ 4$	5	0.868	$2S\alpha\ 5S\alpha \equiv 2S\beta\ 5$	5	0.86
	6	2.069		6	1.934		6	1.896
	7	3.931		7	3.614		7	3.519



(A)

(B)

(C)

Figure 1: The relation between one-electron radial density distribution function with the position for - like ions. ($1S^2 2S^2\ 3S\alpha$) A (1S),B(2S)and C(3S) .

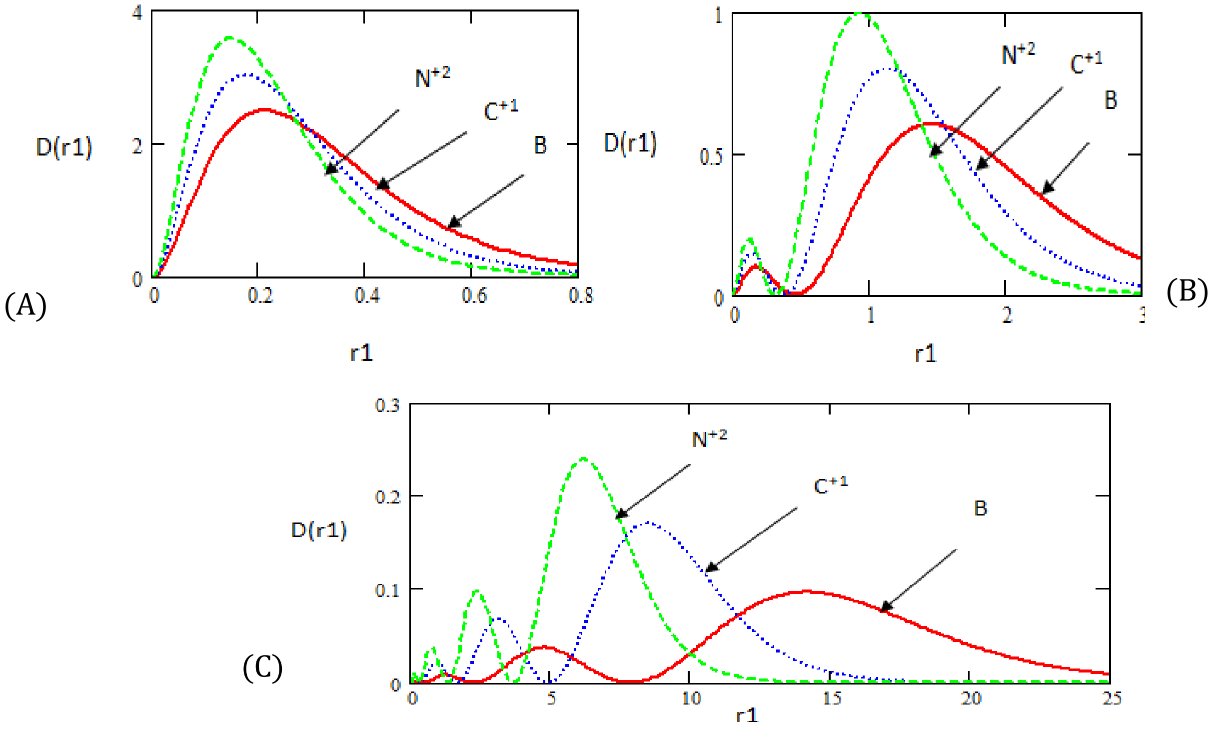


Figure 2 : The relation between one-electron radial density distribution function with the position forB - like ions. $(1S^2 2S^2\, 4S\alpha)$ A (1S),B(2S)and C(4S) .

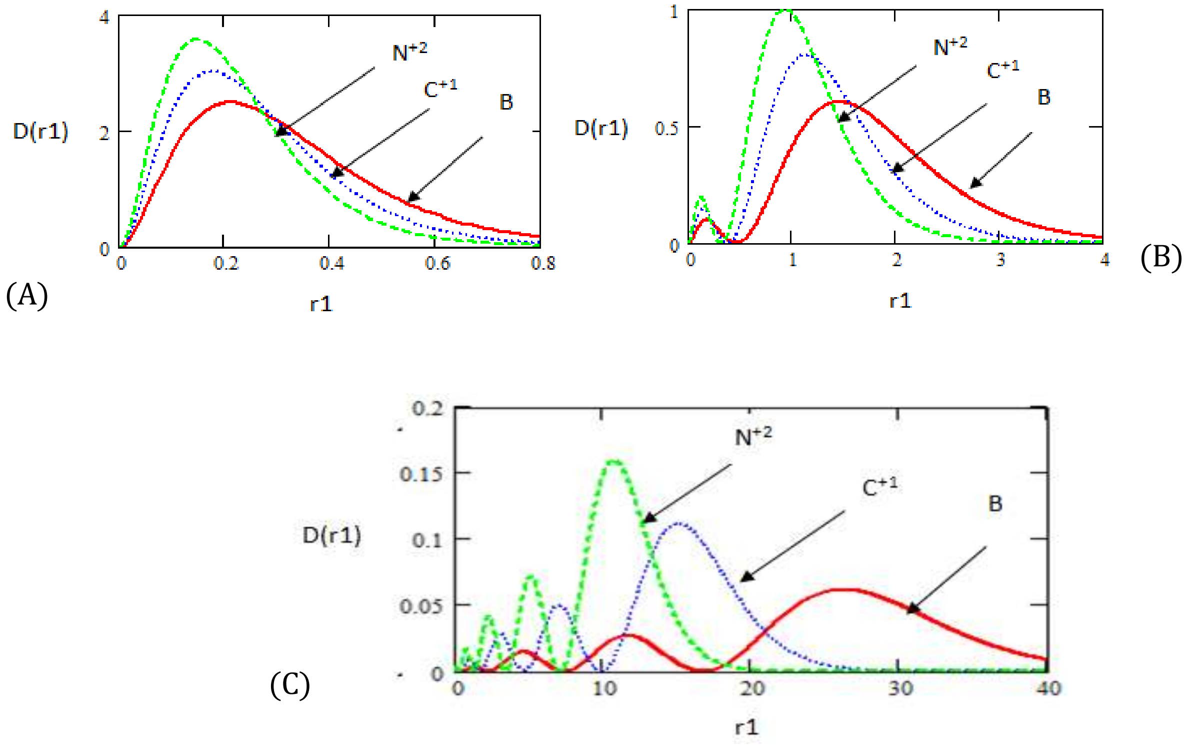


Figure 3 :The relation between one-electron radial density distribution function with the position for - like ions. $(1S^2 2S^2\, 5S\alpha)$ A (1S),B(2S)and C(5S) .

Conclusions

From these results can be conclude the followings:

expectation values of $\langle r_1^n \rangle$ and $\langle r_{12}^n \rangle$ increase when (n) takes negative values and the inverse for positive values as atomic number increase .As the atomic number Z increases , for both approximations the one particle radial density distribution function $D(r_1)$,the electron density at the nucleus $\rho(0)$. The Hartree-Fock method also allows one to study how the electron density at the nucleus behaves for all shells in different configurations .

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