Linear Increasing in Radial Electronic Density Distribution for K and L Shells throughout Some Be-Like Ions

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Abstract:

Maximum values of one particle radial electronic density distribution has been calculated by using Hartree-Fock (HF)wave function with data published by[A. Sarsa et al. Atomic Data and Nuclear Data Tables 88 (2004) 163–202] for K and L shells for some Be-like ions. The Results confirm that there is a linear behavior restricted the increasing of maximum points of one particle radial electronic density distribution for K and L shells throughout some Be-like ions. This linear behavior can be described by using the nth term formula of arithmetic sequence, that can be used to calculate the maximum radial electronic density distribution for any ion within Be like ions for Z<20.

Key words: Hartree-Fock, Radial electronic density distribution, Be like ions.

Introduction:

From the beginning of quantum theory, the atomic electronic structure of ground state Be atom was one of the most interesting problems because of its relative simplicity with respect to other structure problems that occur in nuclear, molecular or solid state physics. The atomic spectrum was one of the first accurately interpreted spectrums using quantum mechanics. A large deal of the advances of quantum theory is attributed to its successful application to atomic structure theory [1]. Four electron atoms or ions represent an excellent testing ground for checking new calculation approaches and for studying photoelectron and other atomic processes. However, the Schrodinger equation for atoms/ions with more than one electron cannot be solved analytically. Approximate methods must be applied in order to solve the problem. A large variety of techniques were developed to obtain the nonrelativistic properties for the mentioned system[2]. It's well-known that the radial electronic density would be considered as a probe to determine the quality of the wave function over whole configuration space. Most of theoretical calculations for the electronic density so far have been restricted to two-electron systems[3]. Some works used mainly ***Hyllaraas*** approach, for example ***Coulson and Nilson***, which obtained the electron-electron distribution function[4]. Using 20 terms Hyllaraas-type wavefunction, ***Benesch*** calculated the radial electron-nucleus distribution function for He-like ions[5]. ***To our knowledge this study seems to be the first time which has been done in the scientific literature .***

Theoretical background:

The one particle radial electronic density[6]:

$$D(r) = r^2 p(r) \quad (1)$$

where,

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$$p(r) = N\int_0^{\pi}\int_0^{2\pi} d\Omega_1 \int \Psi^*(x_1,x_2,\dots,x_N)\times\Psi(x_1,x_2,\dots,x_N)ds_1dx_2\dots ds_Ndx_N \quad (2)$$

$d\Omega = \sin\theta_1 d\theta_1 d\Phi_1$ and $x_i = (r_i,s_i)$ are combined the spatial and spin coordinates for i-th electrons, and$\Psi(x_1,x_2,\dots,x_N)$ is normalized position-space representation of the wavefunction, the number of electron (N)=2, for each individual shells. Throughout this work the origin of coordinates is taken to be the nucleus. you can see for example [3],[5]. The (HF) wavefunction$\psi_{HF}$are used to perform calculations in this research. The HF wavefunction for individual K and L shells given as follow:

$$\psi_{HF}(1,2) = \frac{1}{\sqrt{2}}[\Phi_1(1)\Phi_2(2) - \Phi_1(2)\Phi_2(1)] \quad (3)$$

where,
$\Phi_j(r,\theta,\phi) = R(r)Y(\theta,\phi)$.
$R(r)$is one particle radial wavefunction and $Y(\theta,\phi)$ is the one particle angular wavefunction of the total wavefunction$\psi_{HF}(1,2)$.In terms of (HF) radial wavefunction the one particle radial density distribution can be written as follow:

$$D(r) = [r\,R(r)]^2 \quad (4)$$

The Slater-type orbital (STO's) is used as a radial wavefucntion, $R(r)$, and substituted within HF wavefunction, as you can see for example Ref.[1],

$$R(r) = \sum_{k=1}^{M} C_k N_k r^{n_i-1}\, e^{-(\xi_k)r_k} \quad (5)$$

where M is the number of basis sets, $n_i$is the principle quantum number, ξ_i is the orbital exponent, C_i is the expansion coefficient, and N_i is the normalization constant agiven by: $N_i = \sqrt{\frac{(2\xi_i)^{2n_i+1}}{(2n_i)!}}$.

In terms of STO's parameters one particle radial electronic density distribution given by:

$$D(r) = \sum_{i=j=1}^{M} C_i^{\,2} N_i^{\,2} r^{2n_i} e^{-2r\xi_i} + 2[\textstyle\sum_{i<j}^{M} C_iC_jN_iN_j r^{n_i+n_j}\, e^{-(\xi_i+\xi_j)r}] \quad (6)$$

There is one maximum point for $D(r)$ for K-shell and two for L-shell for any atom $\frac{d}{dr}D(r) = 0$ (7)

within the series under studying, as shown in Figures (1and2). To find maximum value $D(r)$the derivative must be taken and equalized to zero as below:

But the derivative for $D(r)$given by:

$$\frac{d}{dr}D(r) = \sum_{i=j=1}^{M} C_i^{\,2} N_i^{\,2}[2n_i r^{2n_i-1} e^{-2r\xi_i} + r^{2n_i}\, 2\xi_i e^{-\xi_i r}] + 2[\sum_{i<j}^{M} C_iC_jN_iN_j\,(-r^{n_i+n_j}\,(\xi_i+\xi_j)\,e^{-(\xi_i+\xi_j)r} + (n_i+n_j)\,e^{-(\xi_i+\xi_j)r} r^{n_i+n_j-1})]. \quad (8)$$

After substituting equation (8) in equation (7) and solving the final equation numerically this lead to find the location r_0.$D(r_0)_{max}$for K and L shellscan be found by substituting the value of r_0 within equation (1).

Results and Conclusions:

Maximum values of radial electronic density distribution $D(r_0)_{max}$ was calculated numerically for Z=4-10 by using HFwavefunction with data published by A. Sarsa,[7] and all results are tabulated within tables (1,2and 3). For checking, a two graphs between$\frac{d}{dr}D(r)$via distance between nucleus and each individual electron r are plotted for K and L shells, as shown in Figures (3 and 4). These two figures can be used to measure $D(r_1)_{max}$ by finding the intercepts of derivative with *r*-axis. The Maximum values of K-shell for $B^{+1}$is greater than that of Be atom, and values for $C^{+2}$is greater than that for B^{+1} and so on, this is so clear in third column of the Table(1). The same thing happened for the first and second maximum values for L-shell, as shown in third column of Table (2 and 3). This means that the values of $D(r_1)_{max}$increase linearly through K-shells and L-shell sthroughout Be-like ions. So, there is a common difference between any two adjacent values of $D(r_1)_{max}$ within Be-like ions for K and L shells, as shown in fourth column of the Tables (1,2and 3) this means that there is a fixed amount of charge shifting toward nucleus with the increasing of the atomic number Z throughout Be- like ions.

The common difference is used to develop a simple arithmetic sequence in which the n^th^ term is given by$D(Z,D_0,d)$which depends only on a three parameters, first one is atomic number Z, second one isD_0 which is the initial maximum value in the series (i.e.$D(r_0)_{max}$of Be atom) and the third one is$d$ which is the common difference as mentioned before.This n^th^term formula represents $D(r_0)_{max}$ for any atom throughout Be like ions. After simple mathematical manipulations$D(Z,D_0,d)$can be given as follow:

Table(1): The Maximum values of radial electronic density distribution for B-like ions for electrons in K-shell.

Atom	Z	$D(r)_{max}$ a	d	$D(r)_{max}$ b
Be	4	1.9416		1.9416
B^{+1}	5	2.4788	0.5372	2.4749
C^{+2}	6	3.0152	0.5364	3.0082
N^{+3}	7	3.5495	0.5343	3.5415
O^{+4}	8	4.0797	0.5302	4.0748
F^{+5}	9	4.6153	0.5356	4.6081
Ne^{+6}	10	5.1419	0.5266	5.1414
Average of d			0.5333	

a:present work by using HF wavefunction
b:present work by using eq.(9).

In this work, Equation (9) used to calculate$D(r_0)_{max}$ for Z=4-10 as shown in fifth column of the Tables (1,2and 3). There is a little difference between the results given by using HF wavefunction and the results given by using equation (9), so that this arithmetic sequence can be used as a fast method to calculate $D(r_0)_{max}$ for Be- like ions for Z<20because the relativistic effect that may affect the results.

$$D(r_0)_{max} = D(Z,D_0,d) = D_0 + (Z-4)\, d\, ; Z \geq 4 \qquad (9)$$

Table(2): The Maximum values of radial electronic density distribution for B-like ions for first maximum for electrons in L-shell.

Atom	Z	$D(r)_{max}{}^a$	$d$for 1^st^ max. value	$D(r)_{max}{}^b$
Be	4	0.05670		0.05670
B^{+1}	5	0.08610	0.02940	0.08504
C^{+2}	6	0.11350	0.02740	0.11338
N^{+3}	7	0.13910	0.02560	0.14172
O^{+4}	8	0.17126	0.03216	0.17006
F^{+5}	9	0.19702	0.02576	0.19840
Ne^{+6}	10	0.22675	0.02973	0.22674
Average of d			0.02834	

a:present work by using HF wavefunction.
b:present work by using eq.(9).

Table(3): The Maximum values of radial electronic density distribution for B-like ions for second maximum for electrons in L-shell.

Atom	Z	$D(r)_{max}$	d for 2nd max. value	$D(r)_{max}{}^{b}$
Be	4	0.39620		0.39620
B^{+1}	5	0.53620	0.14000	0.52735
C^{+2}	6	0.66730	0.13110	0.65850
N^{+3}	7	0.79610	0.12880	0.78965
O^{+4}	8	0.93101	0.13491	0.92080
F^{+5}	9	1.05250	0.12149	1.05195
Ne^{+6}	10	1.18310	0.13060	1.18310
Average of d			0.13115	

a:present work by using HF wavefunction
b:present work by using eq.(9).

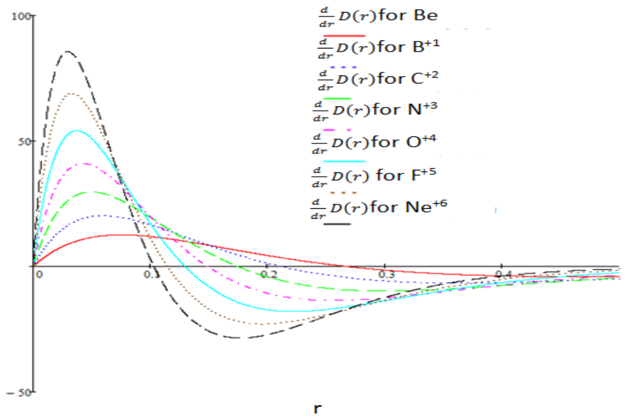

Fig.(1): $\frac{d}{dr}D(r)$ via r for K-shell , all results in atomic units (a.u.).

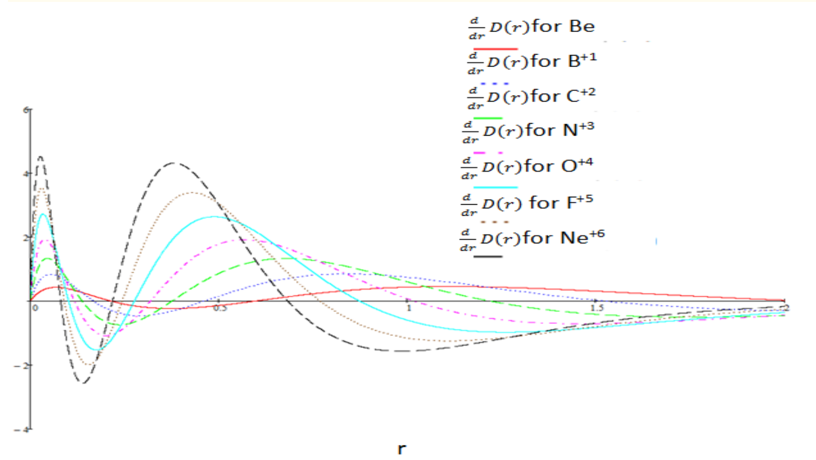

Fig. (2): $\frac{d}{dr}D(r)$ via r for L-shell , all results in atomic units (a.u.).

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الزيادة الخطية في دالة التوزيع القطرية الالكترونية لجسم واحد لذرة البريليوم والذرات الشبيهة بها للقشرة K وL

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الخلاصة:

تم حساب القيم العظمى لدالة التوزيع القطرية الالكترونية لذرة البريليوم والذرات الشبيهة بها باستخدام دالة هارتريفوكباستخدام البيانات المنشورة من قبل [A. Sarsa et al. Atomic Data and Nuclear Data Tables 88 (2004) 163–202]، للقشرة K وللقشرة L. اظهرت النتائج ان هنالك زيادة خطية في قيم دالة التوزيع لكلا الغلافين في ذرة البريليوم والذرات الشبيهة بها. وقد تم تطوير صيغة نونية لمتوالية عددية لحساب القيمة العظمى لدالة التوزيع لأي ايون شبيه بالبريليوم للإعداد الذريةz<20.