Evaluation the Atomic Properties in Momentum Space for Three-electronSystems (Z=10-14) using Hartree-Fock Method

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Abstract

In This paper we study the atomic properties for three-electron systems Ne^{+7}, Na^{+8}, $Mg^{+9,}$ Al^{+10} and Si^{+11} in momentum space Like ,one-electron radial density function $D(p_1)$,inter –electron distribution function $f(p_{12})$,Fermi hole $\Delta f_{kl}(p_{12})$ one- particle expectation value $\langle p_1^n \rangle$,inter- particle expectation value $\langle p_{12}^n \rangle$, for n= -*2* to *2* . All properties calculated using atomic units .

Keywords: Hartree-Fock, momentum space, atomic properties.

الخلاصة

درس في هذا البحث الخواص الذرية لأنظمة ثلاثية الالكترونات Si+11 و Ne+7, Na+8, Mg+9, Al+10 في فضاء الزخم مثل دالة الكثافة القطرية لجسيم واحد ، دالة التوزيع البينية، فجوة فيرمي، القيمة المتوقعة لجسيم واحد، القيمة المتوقعة لجسيمين n= −2 to 2. كل الخواص الذرية حسبت باستخدام الوحدات الذرية.

الكلمات المفتاحية : هارتري–فوك ، فضاء الزخم، الخواص الذرية .

Introduction

Quantum mechanics play a fundamental role in the description and understanding of physical and chemical phenomena [Schweizer, 2002]. It is the set of laws governing the behavior of very small particles including electrons and atomic nuclei. At this small scale the usual laws of classical mechanics fail to provide an accurate description of the behavior of matter[Hill, 2010]. In 1926 Erwin Schrodinger developed an equation, called a wave equation, to describe the behavior of matter wave. By using Schrodinger's equations scientists can find the wave function which solves a particular problem in quantum mechanics. Unfortunately, it is usually impossible to find an exact solution to the equation, so certain assumptions are used in order to obtain an approximate answer for the particular problem[Iqbal, 2012]. The Hartree–Fock method (HF) is widely employed for calculations of various properties of multi electron systems because of its internal logical rigidity and relative simplicity. It is noteworthy that the HF method enables calculation not only of the ground state but also excited states of atoms and ions, the symmetry of which differs from that of the ground state. Thus, many excited configurations giving excited states can be examined for any system [Malykhanov *et al.*, 2008].

Theory

The Hartree-Fock approach is a method for obtaining approximate total wave functions for many-electron systems. It has been applied successfully to many areas of quantum mechanics including atomic, molecular, and solid-state systems nuclear, elementary particle fields.The method is based on both the central field approximation and the variation principle. In the central field approximation electrons are assumed to move independently of each other in an average field due to the nucleus; the other electrons are with additional assumption that the average potential is spherically symmetric [Al-Hayani 2006] . The wave function $\Psi(r_1, \ldots, r_N)$ representing the whole

electron gas is expressed as a product of N wave functions representing each electron [Sée *et al.*, 2002].

$$\Psi(r_1,\dots,r_N)=\psi(r_1)\times\cdots\times\psi_N(r_N) \quad \text{.....(1)}$$

The basis function as a standard normalized Slater –type orbital (STO's), which is given without spin in momentum space by [E.M.Al-Robayi 2006].

$$\chi_{nlm}(\vec{p})=R_{nl}(\vec{p})Y_{lm_l}(p) \quad \text{.....(2)}$$

Where $\chi_{nlm}(\vec{p})$ is the basis function and $R_{nl}(\vec{p})$ is the radial factor which describes how the wave function Ψ of the electron varies with distance from the nucleus, and the angular factor $Y_{lm_l}(p)$.

Where N_{nlm_l} is a normalized constant given by [E.M.Al-Robayi 2006].

$$N_{nlm_l}=\frac{(2\xi_{nl})^{n+0.5}}{\sqrt{[(2n)!]}} \quad \text{.....(3)}$$

The normalized factor N_{nlm_l} and the radial part of the various STO's used in this work [E.M.Al-Robayi 2006].

a- for 1s orbital the normalized factor $N_{nlm_l}=\sqrt{(4\xi^3)}$ and radial part of the various STO's= $2\xi\sqrt{(^2/_\pi)}\ A^{-2}$

b- for 2s orbital the normalized factor $N_{nlm_l}=\sqrt{\left(^{4\xi^3}/_3\right)}$ and radial part of the various

$$\mathbf{STO's}=\sqrt{(^8/_\pi)}\,(3\xi^2-b^-)A^{-2}$$

Where $A=\xi^2+p^2$

where ξ is orbital exponent.

Atomic properties

a- One-particle radial density distribution function $D(p_1)$:

The one – particle radial density function is very important for study the electrons in an atom , which means the probability of finding electrons in each shell [Al-Hayhani 2002].The one – particle radial density function for each shell is [Al-Robayi 2006] :

$$D(p_1)_{K(^1S)}=R_{1s}^2(p_1)p_1^2 \quad \text{.....(4)}$$

$$D(p_1)_{KL(^1S)}=D(p_1)_{KL(^3S)}=\frac{1}{2}.p_1^2[R_{1s}^2(p_1)+R_{2s}^2(p_2)] \quad \text{.....(5)}$$

b- Inter –electron distribution function f(p_{12}) and Fermi hole $\Delta f_{kl}(p_{12})$:

Inter –electron distribution function can be defined as the measure of the probability distance between two electrons *i* and *j* respectively[H.S.abdul baqi 2010]. Inter–electron distribution function $f(p_{12})$ is given by[F. W. King et al 1991]:

$$f(p_{12}) = 0.5 * p_{12}\left[\int_0^{p_{12}} p_1\,dp_1 \int_{|p_1-p_2|}^{|p_1+p_{12}|} \Gamma(\mathbf{p_1},\mathbf{p_2})\,p_2\,dp_2 + \int_{p_{12}}^{\infty} p_1\,dp_1 \int_{|p_{12}-p_1|}^{|p_{12}+p_1|} \Gamma(\mathbf{p_1},\mathbf{p_2})\,p_2\,dp_2\right] \quad \text{.....(6)}$$

Where $\Gamma(\mathbf{p_1},\mathbf{p_2})$ is The electron pair density function that deserves much study because the concept of electron pairs is fundamental to chemistry[Ajit.J.Thakkar 2003].

A Fermi hole refers to the probability of finding two electrons together with the same spin, can be studied as a difference between the triplet state KL(^{3}S) and singlet state KL(^{1}S) for the inter-particle distribution function [Al-Robayi 2007; Al-Bayati *et al.*, 2005].

$$\Delta f_{KL}(p_{12}) = f_{KL}(^3\mathrm{S})\,(p_{12}) - f_{KL}(^1\mathrm{S})\,(p_{12}) \quad \text{.....(7)}$$

c- One – particle expectation value $\langle p_1^n \rangle$ and Inter – particle expectation value $\langle p_{12}^n \rangle$:

The one-particle expectation value is defined by [Esquivelt *et al.*, 1992] :

$$\langle p_1^n \rangle = \int_0^{\infty} D(p_1) p_1^n dp_1 \quad \text{.....(8)}$$

The inter – particle expectation value $\langle p_{12}^n \rangle$ is given by [King, 1991]:

$$\langle p_{12}^n \rangle = \int_0^{\infty} f(p_{12}) p_{12}^n dp_{12} \quad \text{.....(9)}$$

Results and discussion

Table (1) shows the values of maximum one – particle density function $D_{max}(p_1)$ in momentum space corresponding of momentum values for individual shells (*K*, *KαLα, KβLα*), from these results we noted as atomic no. increases the values of $D_{max}(p_1)$ decreases for each shell, while the values of momentum increase because that increase the attraction force which leads to decreases in the distance between the nucleus and the electrons, in order to overcome to it's the momentum will be increased.

Fig. (1) and Fig. (2) represented the values of p_1 scaled plots of the $D(p_1)$ for *K*-shell and *(KαLα≡KβLα*) respectively. It is to be noted these as Z increases note only dose $D(p_1)$ becomes more diffuse but also decrease in magnitude.

Table (2), shows the values of maximum of inter –particle density function $f(p_{12})$ corresponding of the inter particle momentum values p_{12}, fig.(3), fig.(4) and fig.(5)

represented the p_{12} scaled plots of $f(p_{12})$ for *K*- shell , *KαLα*-shell and *KβLα* –shell , respectively . The behavior of function $f(p_{12})$ is the same of $D(p_1)$ but noted at small p_{12} ,the *KαLα*-shell curves give a flat region due to the presence of the Fermi effect .

Table (3), indicates the radius of Fermi hole $\Delta f_{KL}(p_{12})$ for studied systems, fig.(6) shows the relation between $\Delta f_{KL}(p_{12})$ and p_{12}, by investigated these results we noted that the values of radius of Fermi hole increase as Z increases .

Table (4), which represented the relation between one- particle expectation values of momentum for different values of n with atomic number for each shell and the average, while the table (5) represented the relation between inter- particle expectation values of momentum for the same values of n with atomic number for each shell and the average of the system.

From tables (4) and (5) we noted when n negative is (n=-2, -1), the values of $\langle p_1^n \rangle$ **and** $\langle p_{12}^n \rangle$ decreases for each shell and average of each system as atomic no. increases, while these increases are when they take positive values (n= 1, 2).

The interpretation of these is results due to as Z increase the distance between the nucleus and the electron also the distance between two electrons decrease which lead to increases the velocity and the momentum for overcome to the attraction energy.

Table(1): Values of momentum p_1 corresponding to maximum values $D(p_1)$ for studied systems.

Ion	*K-shell*		*KαLα-Shell ≡KβLα-Shell*			
	p_1	$D_{max}(p_1)$	*First peak*		*Second peak*	
			P_1	$D_{max}(p_1)$	p_2	$D_{max}(p_2)$
Ne^{+7}	5.48	0.12001	1.657	0.26472	5.20	0.05766
Na^{+8}	5.99	0.11088	1.86	0.23904	6.39	0.05327
Mg^{+9}	6.62	0.10147	2.05	0.21810	7.84	0.04759
Al^{+10}	7.18	0.09464	2.25	0.20051	8.74	0.04352
Si^{+11}	7.76	0.09069	2.45	0.18569	8.97	0.04177

Table(2): Values of momentum p_{12} corresponding to maximum values $f(p_{12})$ for studied systems.

	K-shell	*KαLα-Shell*	*KβLα-Shell*

ion	p_{12}	$f_{max}(p_{12})$	p_{12}	$f_{max}(p_{12})$	p_{12}	$f_{max}(p_{12})$
Ne^{+7}	8.77	0.08214	6.73	0.11815	5.81	0.11619
Na^{+8}	9.67	0.07592	7.47	0.10809	6.44	0.10696
Mg^{+9}	10.59	0.06949	8.21	0.09886	7.06	0.09845
Al^{+10}	11.49	0.06482	8.95	0.091627	7.67	0.09168
Si^{+11}	12.39	0.06212	9.69	0.08632	8.28	0.08676

Table (3) : The radius of Fermi hole $\Delta f_{KL}(p_{12})$ using Hartree-Fock approximation for studied systems .

Ion	$p_{12}(radius)$
Ne^{+7}	6.20
Na^{+8}	6.97
Mg^{+9}	7.76
Al^{+10}	8.51
Si^{+11}	9.28

Table(4): Expectation values of p_1 for each individual shell and the average for studied systems.

Ion	Shell	$\langle p_1^{-2}\rangle$	$\langle p_1^{-1}\rangle$	$\langle p_1^{1}\rangle$	$\langle p_1^{2}\rangle$
Ne^{+7}	K	0.05929	0.19106	8.76519	100.10868
	$K\alpha L\alpha \equiv K\beta L\alpha$	0.41226	0.44356	5.25772	51.11789
	Average	0.29460	0.35939	6.42670	67.44815
Na^{+8}	K	0.0496	0.17646	9.85348	124.02786
	$K\alpha L\alpha \equiv K\beta L\alpha$	0.33321	0.40096	5.86328	62.78656
	Average	0.23867	0.32612	7.19334	83.20032
Mg^{+9}	K	0.04147	0.16142	10.78288	148.34009
	$K\alpha L\alpha \equiv K\beta L\alpha$	0.27486	0.36556	6.43240	75.14225
	Average	0.19706	0.29751	7.88256	99.54153
Al^{+10}	K	0.03560	0.15072	11.84657	176.78362
	$K\alpha L\alpha \equiv K\beta L\alpha$	0.23076	0.33625	7.03265	89.06428
	Average	0.16570	0.27440	8.63729	118.30406
Si^{+11}	K	0.03161	0.14417	13.18496	211.95680
	$K\alpha L\alpha \equiv K\beta L\alpha$	0.19662	0.31205	7.69469	105.08239
	Average	0.141616	0.25609	9.52478	140.70719

Table(5) : Expectation values of p_{12} for each individual shell and the average studied systems.

Ion	Shell	$\langle p_{12}^{-2}\rangle$	$\langle p_{12}^{-1}\rangle$	$\langle p_{12}^{1}\rangle$	$\langle p_{12}^{2}\rangle$
	K	0.02446	0.12490	12.80160	200.21761
	$K\alpha L\alpha$	0.02475	0.13868	9.20510	109.68493

Ne^{+7}	***Kβ'Lα***	0.05300	0.18176	9.08788	105.95943
	Average	0.03407	0.14844	10.36486	138.62065
Na^{+8}	***K***	0.02048	0.11539	14.38925	248.05540
	KαLα	0.02035	0.12655	10.30659	135.66918
	Kβ'Lα	0.04410	0.16716	10.18831	130.97448
	Average	0.02831	0.13636	11.62805	171.56635
Mg^{+9}	***K***	0.01713	0.10558	15.74494	296.67830
	KαLα	0.01690	0.11552	11.33318	163.40882
	Kβ'Lα	0.03704	0.15377	11.22272	157.71715
	Average	0.02369	0.12495	12.76694	205.9347
Al^{+10}	***K***	0.01471	0.09846	17.29670	353.56675
	KαLα	0.01434	0.10688	12.42644	194.70068
	Kβ'Lα	0.03172	0.14310	12.31911	187.84979
	Average	0.02025	0.116146	14.01408	245.37240
Si^{+11}	***K***	0.01307	0.00433	19.24935	423.91604
	KαLα	0.01247	0.10054	13.65502	230.85851
	Kβ'Lα	0.02780	0.13534	13.55179	222.67048
	Average	0.01778	0.08007	15.48538	292.48167

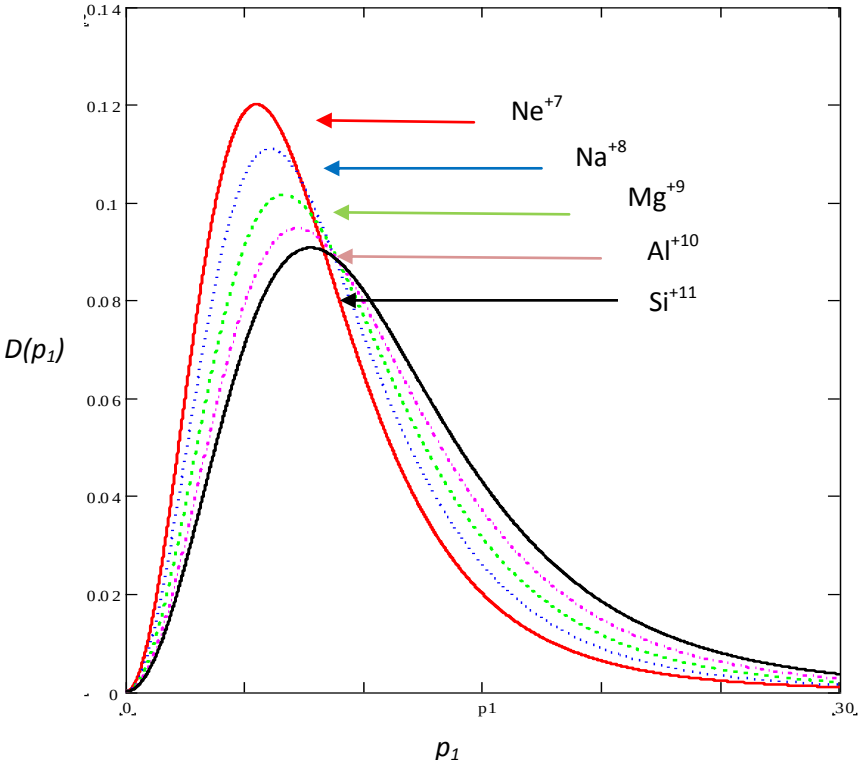

Fig.(1) : The relation between one -particle radial density function $D(p_1)$ and p_1 for K-shell in momentum space.

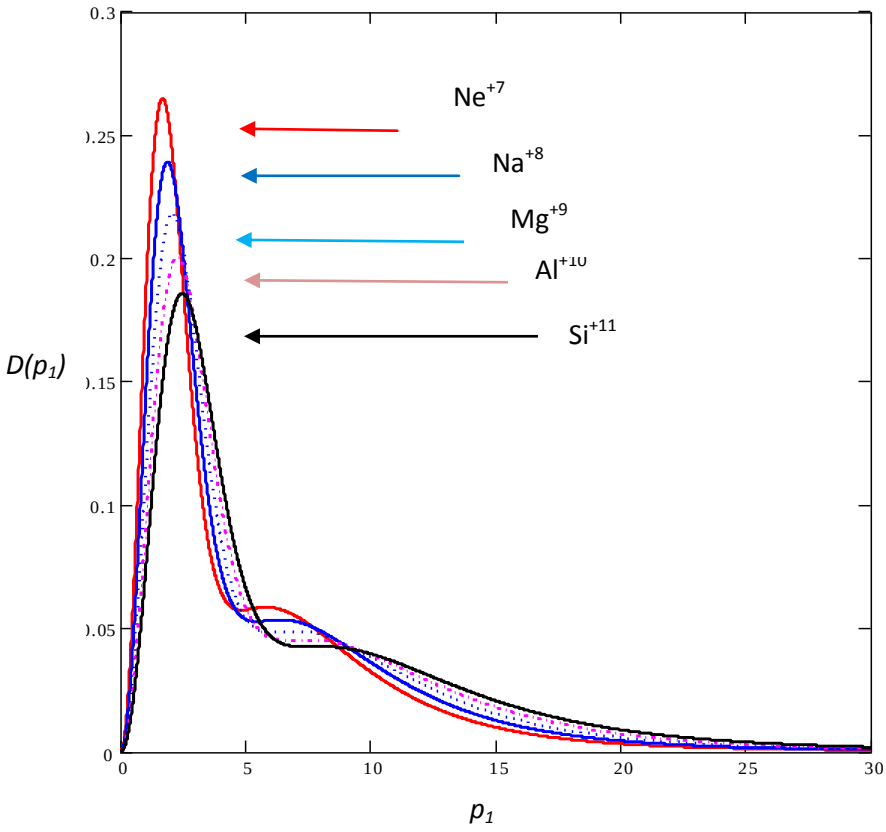

Fig.(2): The relation between one -particle radial density function $D(p_1)$ and p_1 for (KαLα≡KβLα-shell) in momentum space

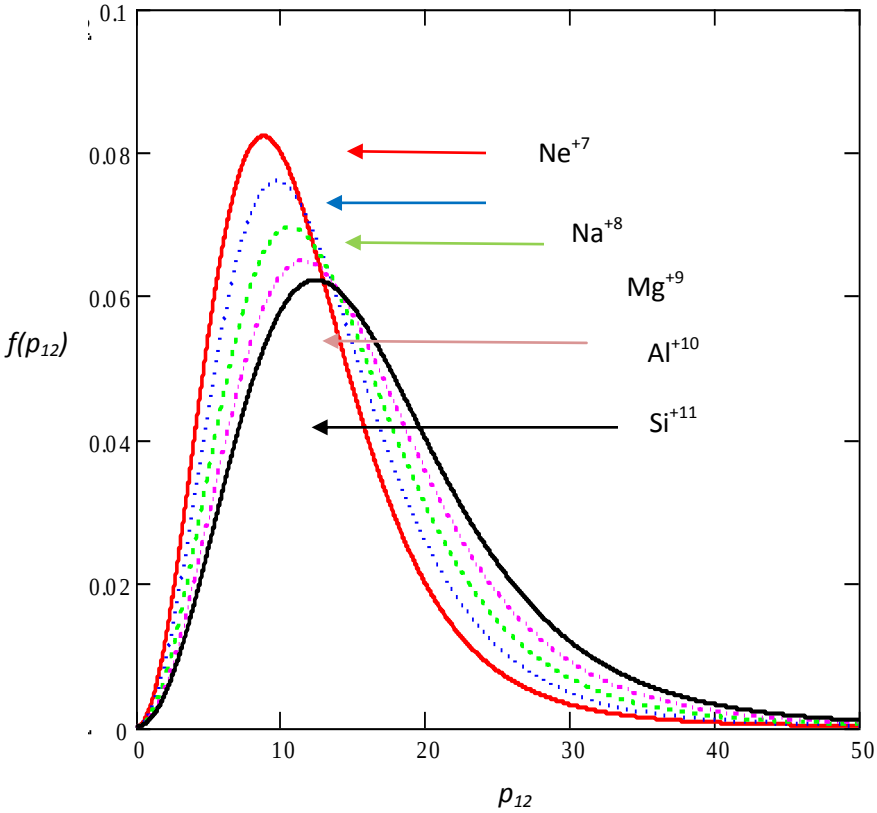

Fig.(3): The relation between inter-particle distribution function $f(p_{12})$ and p_{12} for (K-shell) in momentum

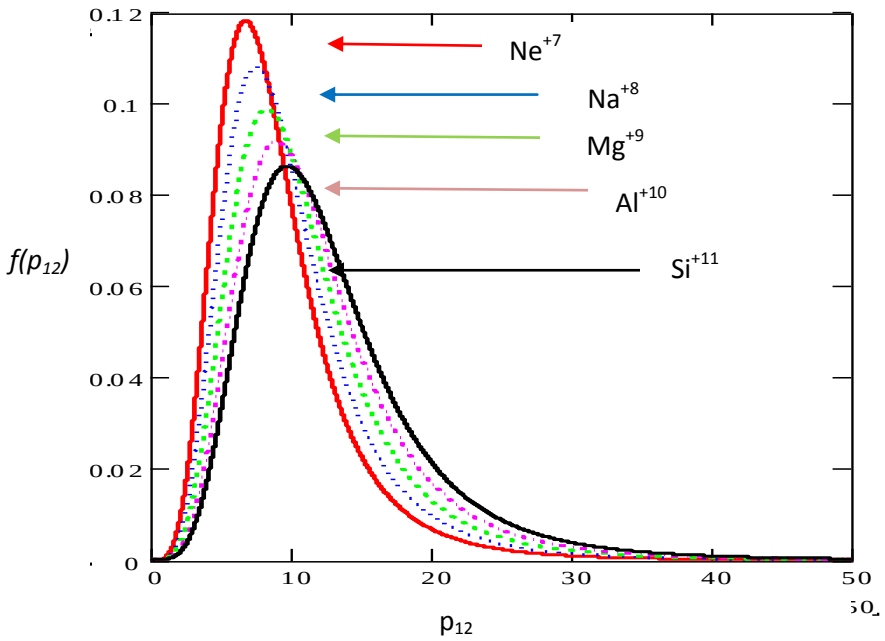

Fig.(4): The relation between inter -particle distribution function $f(p_{12})$ and p_{12} for (KαLα -shell) in momentum space .

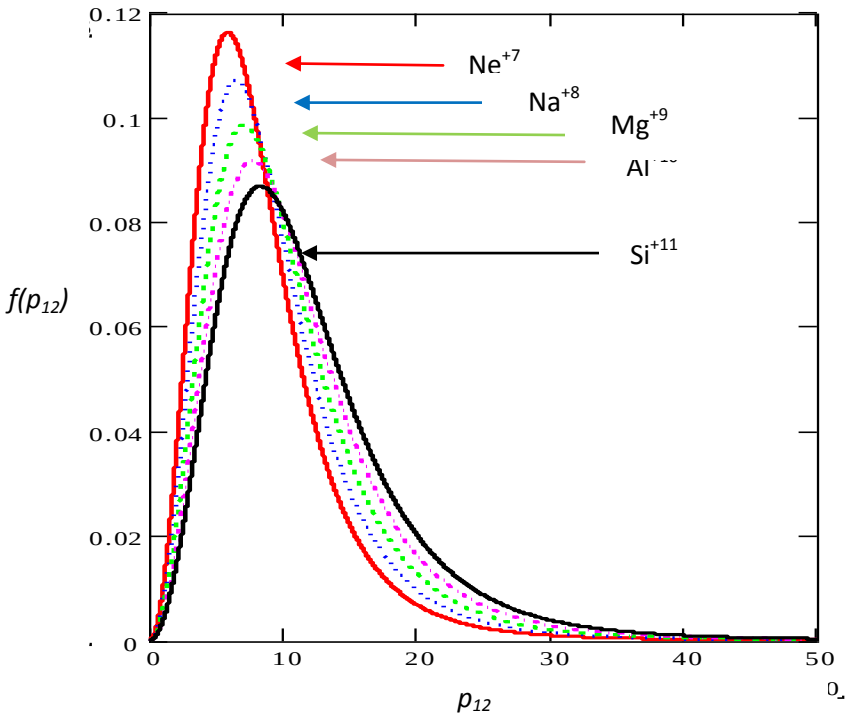

Fig.(5): The relation between inter -particle distribution function $f(p_{12})$ and p_{12} for (KβLα -shell) in momentum space .

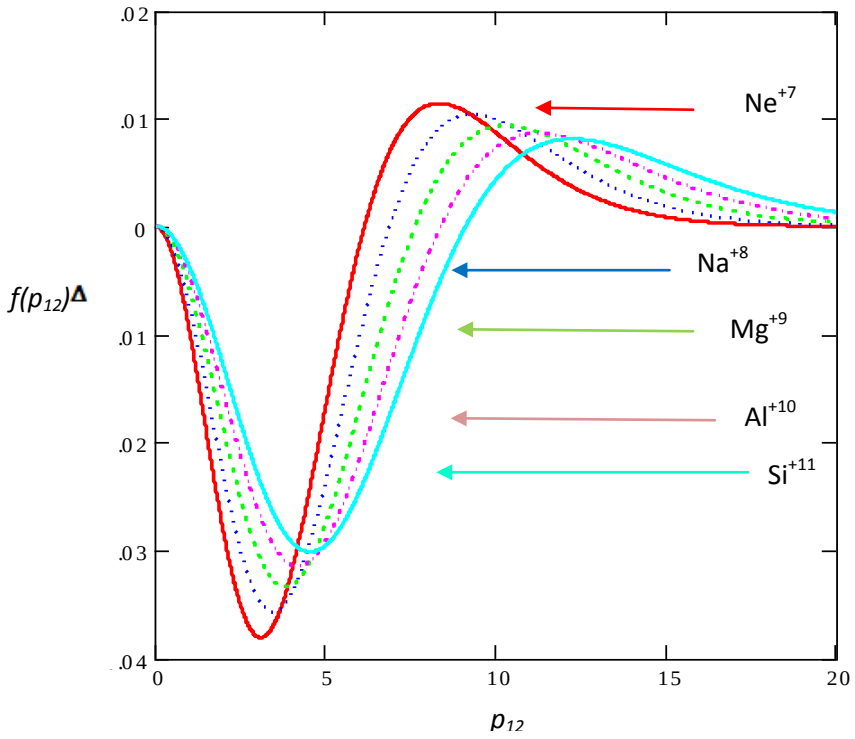

Fig.(6):Fermi hole as a difference between the inter – particle distribution function $f(p_{12})$ of KαLα - shell and KβLα- shell in momentum space .

Conclusions

1- The maximum value of $D(p_1)$ decreases as the atomic number (Z) increases and the location of these maximum increases.
2- The maximum probability of pair distribution function $f(p_{12})$ decreases as atomic number increases ,while the locations of their maxima increases.
3- The radius of Fermi hole increases and the depth of them decreases as Z increases.
4- For each shell as Z increases the one particle radial expectation values decreases when *n* takes negative values -1 and -2 ,and increases when *n* take positive values 1 and 2.
5- For n=1,2 the inter-particle expectation values $\langle p_{12}^n \rangle$ increase by increasing the atomic number and decrease when n takes the values -1,-2.

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