Studying the x- ray atomic Scattering form Factor and Nuclear Magnetic Shielding Constant for Be atom in its Excited state ($1s^2$ 2s 3s) and the Be - like ions

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Abstract:

The division partitioning technique has been used to analyze the four electron systems into six-pairs electronic wave functions for ($K\alpha K\beta, K\alpha L\alpha, K\beta L\alpha, K\alpha M\alpha, K\beta M\alpha L\alpha M\alpha$) $shell$ for the Beryllium atom in its excited state ($1s^2$ 2s 3s) and like ions (B^{+1},C^{+2}) using Hartree-Fock wave functions . The aim of this work is to study atomic scattering form factor *f(s)* for and nuclear magnetic shielding constant. The results are obtained numerically by using the computer software (Mathcad).

Key words: Hartree-Fock(HF), two electron density function, atomic scattering form factor

Introduction:

This study deals with the first excited state (**$1s^2$ 2s 3s**) of beryllium atom. This system consists of four –electrons : two in K-shell with same quantum number except spin component ,where the first electron with spin up (α)and the other –down(β), the third electron puts in L-shell with spin-up (α) and the fourth electron puts in M-shell with spin up(α) .This is a general distribution of electrons in orbitals for excited state of the present system. For Partitioning technique we deal with pair of electron only therefore, intra and inter shells will arise. The intra shells is represented by K-shell and the inter shells are represented by ($K\alpha L\alpha, K\beta L\alpha, K\alpha M\alpha, K\beta M\alpha L\alpha M\alpha$) shells, each shell has two electrons with parallel or anti –parallel spin.

Theory:

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

The function $\Gamma(1,2)$ represents the probability of finding two electrons simultaneously at position 1 and 2. For any N-electron atomic system, the two-particle density $\Gamma_{HF}(x_m,x_n)$ can be written as [1, 2,3]

$$\Gamma_{HF}(x_m,x_n)=\frac{N(N-1)}{2}\iint\left|\psi(x_1,x_2,..x_q)\right|^2 dx_p...dx_q$$ …(1)

Where x_n represents the combined space and spin coordinates of electron n, and $dx_p..dx_q$ indicates integration summation over all N-electrons except m and n. $\frac{N(N-1)}{2}$ represents the number of electron pairs which can be obtained by integrating the second-order reduced density matrix, so $\Gamma_{HF}(x_m,x_n)$ is normalized to the number of independent electron pairs within the system as : [4,5]

$$\int\int\Gamma_{HF}(x_m,x_n)dx_m dx_n=\frac{N(N-1)}{2}$$ ….(2)

Where:

$\frac{N(N-1)}{2}=6$ for the Be-like ions.

And

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$$\Gamma_{HF}(x_m, x_n) = \sum_{i<j}^{N} \Gamma(x_m, x_n) \ldots(3)$$

For Be-like ions

$$\Gamma_{HF} Total = \Gamma_{12} + \Gamma_{13} + \Gamma_{14} + \Gamma_{23} + \Gamma_{24} + \Gamma_{34} \quad \ldots (4)$$

2- Two-particle radial distribution function $D(r_1, r_2)$:

Two-particle density distribution function $D(r_1, r_2)$ is defined as [6,7]

$$D(r_1, r_2) = \int\int \Gamma(r_1, r_2) r_1^2 r_2^2 \, d\Omega_1 d\Omega_2 d\sigma_1 d\sigma_2 \quad ..(5)$$

Where $d\Omega_i$ denotes that the integration is over all angular coordinates of the position vector and it is simply defined as:

$$\int d\Omega_k = \int_0^{2\pi} \int_0^{\pi} \sin\theta_k \; d\theta_k d\phi_k \quad \ldots.(6)$$

Where k =1 or 2 and the normalization condition for two-particle radial density distribution function $D(r_1, r_2)$ can define as

$$\int\int D(r_1, r_2) \, d\, r_1 dr_2 = 1 \quad \ldots (7)$$

This means the two-particle density distribution $D(r_1,r_2)dr_1dr_2$ is a measure of probability of finding the two-electron simultaneously and their radial coordinates are in the range r_1 and $r_1 + dr_1$,and r_2 to $r_2 + dr_2$ [7]

3- One-particle Radial distribution function $D(r_1)$:

The radial density distribution function $D(r_1)$ is of extreme importance in the study of atom and ions because it measure the probability of finding an electron in each shell, and it is define as [6,8,9]

$$D(r_1) = \int_0^{\infty} D(r_1, r_2) \, dr_2 \quad \ldots (8)$$

4- The atomic form factor f(S) :

The quantity f(s) is used to describe the "efficiency" of scattering of a given atom in a given direction, and it is defined as a ratio of amplitude: [10,11]

$$f(s) = \frac{\text{Amplitude of the wave scattered by an atom}}{\text{Amplitude of the wave scattered by one free elctron}} \quad \ldots..(9)$$

Mathematically, the relation of X-ray form factor $f(s)$ to the electron distribution function $D(r)$ in the atom is expressed by the formula [12,13].

$$f(s) = \int_0^{\infty} D(r) \frac{\sin 4\pi sr}{4\pi sr} dr \quad \ldots.(10)$$

Where: $4\pi S$ is called the momentum transfer, $\frac{\sin sr}{sr}$ is the spherical Bessel function of zero order [14,15] and $s = \sin\theta/\lambda$

5- Nuclear Magnetic Shielding Constant σ_d

The Nuclear Magnetic Shielding Constant is determined from the formula [2,15,16]:

$$\sigma_d = \frac{1}{3}\alpha^2 \left\langle \Psi \left| \sum_{i=1}^{n} (r_i)^{-1} \right| \Psi \right\rangle \quad \ldots..(11)$$

where α is the fine structure constant and it is equal to(7.297353*10^{-3} au(atomic unit) and r_i represented the distance from the nucleus to the electron (i)

Results and Discussion:

1.The atomic form factor f(s):

It results from Table (1) and fig (1),(2),(3),(4),(5) show the behavior of atomic form factor starts from the maximum value, (at zero angle) which equal to the number of electrons for each shell, and gradually decline with increasing the scattering angle until reach to the minimum value. These maximum and minimum values are different from an element to another. Physically the maximum value of atomic form factor means that the full scattering of x-rays is occurred since all scattering rays in forward direction (θ=0) from the electrons of different locations are in the same phase because of their equal light pathways, so that, amplitude of scattering beam equals to

the amplitude of scattering waves resulting from one electron multiplied by the atomic number Z.
According to this, increasing of the scattering the angle lead to increase of the light differences pathways between the scattered waves from the different electrons. This leads to partial distractive interference and decreasing in the total amplitude of the scattered wave associated with increasing the scattering angle and the minimum value means that the lowest scattering of x-rays is occurred also, where the path differences between the scattered waves by different location electrons are very large which results in more probability for occurrence of distractive interference which produces final resultant amplitude of small value.

2. Nuclear Magnetic Shielding σ_d

Table (2) shows that the nuclear magnetic shielding constant increases as Z increases, this is due to the attraction force between the electrons and protons .

Table(1) : The variation of atomic form factors for individual electronic shells and the total values of Be and like ions (B^{+1} ,C^{+2}) with scattering angel.

shell	Atom or Ion	$f(s)$ ($1s^2$ 2s 3s) $s=\frac{\sin\theta}{\lambda}$					
		0.0	0.2	0.4	0.6	0.8	1.0
Kα Kβ	Be	2 2	1.58957 1.590Ref.[17]	0.91606 0.916Ref.[17]	0.47486 0.475Ref.[17]	0.24857 0.249Ref.[17]	0.13648 0.136Ref.[17]
	B^{+1}	2 2	1.7311 1.731Ref.[17]	1.1906 1.191 Ref.[17]	0.7280 0.728 Ref.[17]	0.4312 0.431 Ref.[17]	0.2584 0.258 Ref.[17]
	C^{+2}	2 2	1.8120 1.812Ref.[17]	1.3868 1.387 Ref.[17]	0.9537 0.953 Ref.[17]	0.6245 0.624 Ref.[17]	0.4048 0.404 Ref.[17]
KαLα ≡ KβLα	Be	2	0.7711	0.4764	0.2499	0.1309	0.0719
	B^{+1}	2	0.8755	0.6073	0.3862	0.2305	0.1384
	C^{+2}	2	1.0237	0.6851	0.5017	0.3359	0.2189
KαMα ≡ KβMα	Be	2	0.7929	0.4595	0.2385	0.1248	0.0686
	B^{+1}	2	0.8778	0.5961	0.3668	0.2176	0.1309
	C^{+2}	2	0.9464	0.6905	0.4804	0.3162	0.2055
LαMα	Be	2	-0.0255	0.0196	0.0133	$6.9796^{*}10^{-3}$	$5.7888^{*}10^{-3}$
	B^{+1}	2	0.0222	0.0128	0.0251	0.0169	0.0107
	C^{+2}	2	0.1581	-0.0112	0.0284	0.0275	0.0193
Total	Be	4	1.564	0.9359	0.4885	0.2558	0.1424
	B^{+1}	4	1.7533	1.2034	0.7531	0.4481	0.2691
	C^{+2}	4	1.9701	1.3756	0.9820	0.6520	0.4240

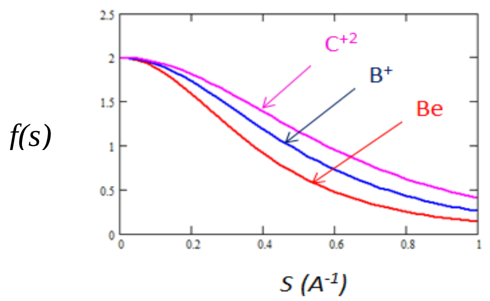

Fig. (1) Atomic scattering factor $f(s)$ relationship with the unit vector s for the K-shell of Be and like ions (B^{+1}, C^{+2}).

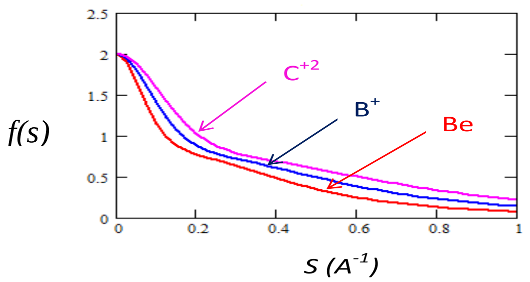

Fig. (2) Atomic scattering factor $f(s)$ relationship with the unit vector s for the KL-shell of Be and like ions (B^{+1}, C^{+2}).

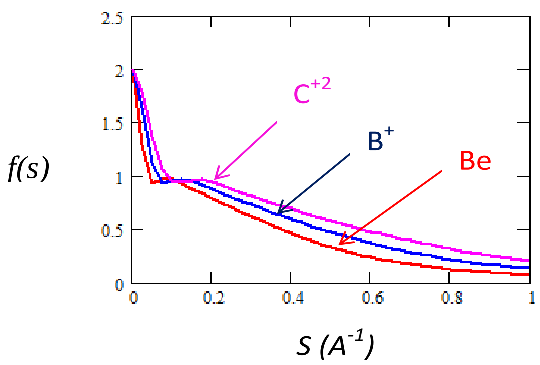

Fig. (3) Atomic scattering factor $f(s)$ relationship with the unit vector s for the KM-shell of Be and like ions (B^{+1}, C^{+2}).

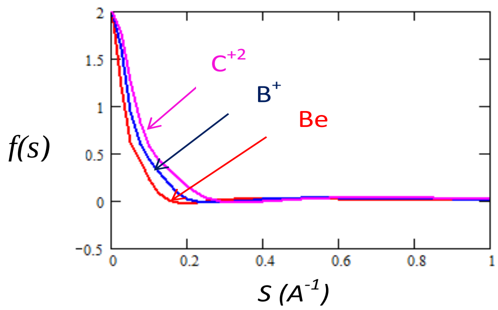

Fig. (4) Atomic scattering factor $f(s)$ relationship with the unit vector s for the LM-shell of Be and like ions (B^{+1}, C^{+2}).

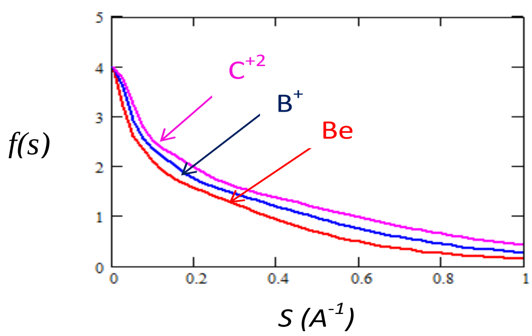

Fig. (5) Atomic scattering factor $f(s)$ relationship with the unit vector s for the total of Be and like ions (B^{+1}, C^{+2}).

Table(2) : Values of the Nuclear Magnetic Shielding Constant for individual electronic shells and the total values of Be and like ions (B^{+1} ,C^{+2}) .

Z	$\sigma_d * 10^{-5}$				
	Kα Kβ	KαLα ≡ KβLα	KαMα ≡ KβMα	LαMα	Total
4	6.536	3.809	3.414	0.6872	3.611
5	8.306	4.923	4.402	1.018	4.662
6	20.16	12.07	10.78	2.689	5.711

Conclusions:

1.The largest relative effects on x-ray scattering factor for the shell of smallest effective nuclear charge and greatest radius in an atom.

2.The maximum value of the form factor is obtained when the scattering angles is maximum (i.e. θ=0) which mean that the full scattering of x-rays is occurred.

3. The nuclear magnetic shielding constant increases by increasing the atomic number (Z) .

4. The values of Nuclear Magnetic Shielding Constant σ_d for K- shell larger than for KL, KM, and LM because K-shell is nearest for nucleus .

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دراسة عامل الاستطاره الذري للاشعه السينيه وثابت الحجب النووي المغناطيسي لذرة البريليوم في الحالة المتهيجه $(1s^2\ 2s\ 3s)$ والايونات المشابهه لها

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الخلاصه :
استخدمت تقنية التجزئة لتحليل أنظمة تحتوي على اربعة الكترونات الى ستة ازواج من الدوال الموجية الالكترونية $K\beta M\alpha, L\alpha M\alpha)(K\alpha K\beta, K\alpha L\alpha, K\beta L\alpha, K\alpha M\alpha,$ لذرة البيريلوم و بعض الايونات المشابهة لذرة البيريليوم في الحاله المتهيجه $(1s^2\ 2s\ 3s)$ وهي (B^+, C^{+2}) باستخدام دالة الموجة لهارتري فوك (Hartree-Fock) .هدف البحث هو دراسة عامل الاستطارة الذري وثابت الحجب النووي المغناطيسي،والنتائج المستحصلة تم حسابها عددياً باستخدام البرامج الحاسوبيه (MATHCAD).